2012 CASL Round Table Virtual Meeting

June 11-14, 2012

Consortium for Advanced Simulation of LWRs

MULTIPHYSICS and MULTISCALE

--- VOCC AGENDA ---

From	To	Monday, June 11	Tuesday, June 12	Wednesday, June 13
All times are EDT			**SESSION 3** Chair: Ken Yueh	**SESSION 6** Chair: H. Zhang
10:30	11:00		SLT – 10 Year Strategic Planning – D. Kothe & SLT	AMA – Challenge Problem Integration – Z. Karoutas
11:00	11:30		VRI/MPO – GTRF Challenge Problem Integration – R. Summers / S. Sham	VUQ – Verification Tools – K. Copps
11:30	12:00		THM – GTRF Turbulence Modeling – J. Bakosi	AMA –Requirements Update – S. Hess
12:00	1:00		**--- BREAK ---**	
All times are EDT		**SESSION 1** Chair: R. Szilard	**SESSION 4** Chair: B. Kochunas	**SESSION 7** Chair: C. Webster
1:00	1:30	MPO – Fuel Performance Upscaling – C. Stanek	RTM – Pin Resolved 3D Transport Full Core Capability – J. Wagner	Safety Challenge Problems – J. Gaertner
1:30	2:00	THM – Multiphase flow Analysis – M. Christon	RTM – Denovo Framework – T. Evans	MPO – Accident Tolerant Fuels – B. Wirth
2:00	2:30	DOE Overview – Alex Larzelere	RTM – CFD and MPACT coupling – T. Downar	VOCC – Validation Data Center – N. Dinh / H. Lee
2:30	3:30	**--- BREAK** ---		
All times are EDT		**SESSION 2** Chair: Ben Collins	**SESSION 5** Chair: Rose Montgomery	**SESSION 8** Chair: S. Pannala
3:30	4:00	AMA/MPO – CRUD Challenge Problem Integration – J. Secker / A. Manera	VRI – VERA Strategy & RSICC Release – J. Turner	THM – Intrusive UQ for Thermal Hydraulics – J. Shadid
4:00	4:30	AMA/VRI – Core Simulator – S. Palmtag	VRI/RTM – Cross Sections – B. Rearden	THM – RELAP7 – R. Martineau
4:30	5:00	VRI – Input and Analysis Capability – A. Godfrey	VOCC Update & Strategic Plan – A. Lewis	VUQ – UQ Hybrid Framework – H. Abdel-Khalik

From	To	Thursday, June 14
All times are EDT		**SESSION 9** Chair: M. Pernice
10:30	11:00	AMA – Industry Achievements – J. Yan/J. Gehin
11:00	11:30	VUQ – V&V Workflow – W. Rider
11:30	12:00	VRI – SIERRA – R. Bond
12:00	1:00	**BREAK**
All times are EDT		**SESSION 10** **AWARD CEREMONY**
1:00	1:45	

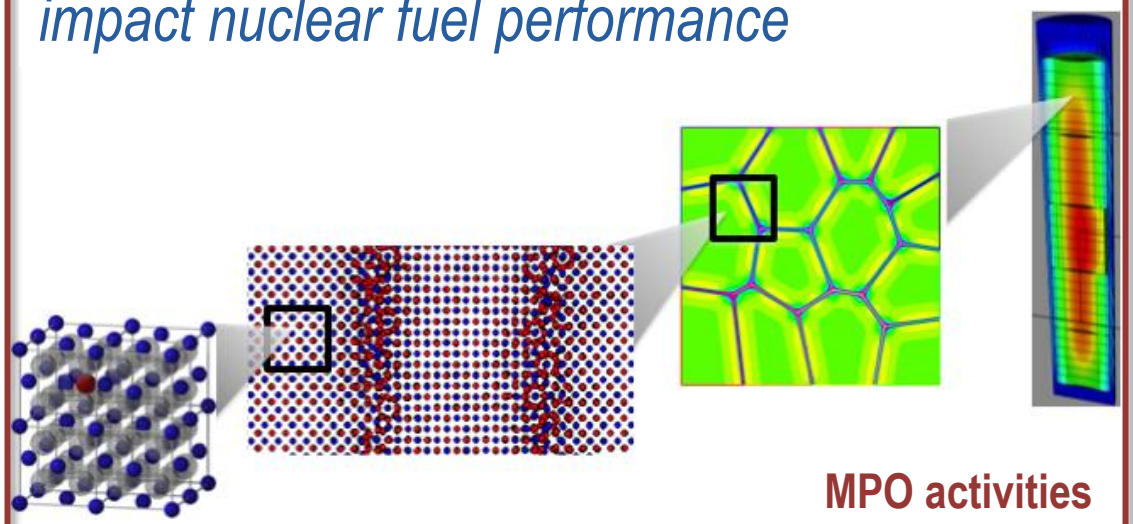
Fuel Upscaling

Chris Stanek, LANL

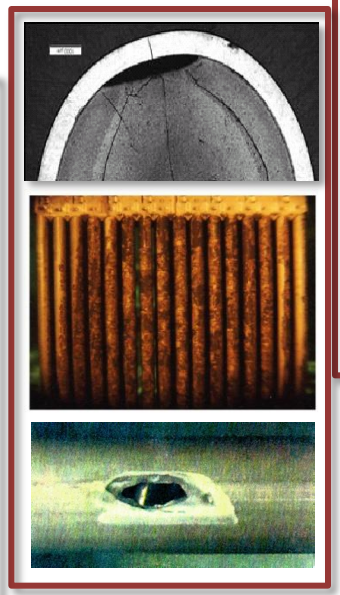
Materials Performance Optimization (MPO)

Enabling Improved Fuel Performance through Predictive Simulation

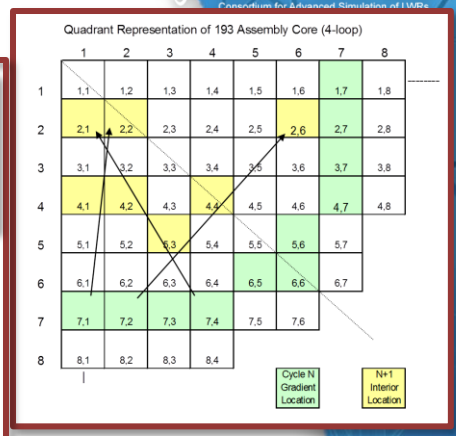
Challenging, multiscale processes impact nuclear fuel performance



MPO activities



CASL Challenge Problems



VERA CS

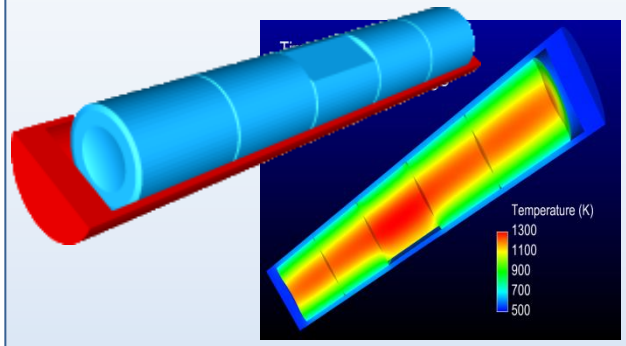
- Provide physics-based materials models of fuel/clad/internals property evolution to enable predictive modeling of CRUD, GTRF and PCI within 3D, multi-physics, virtual reactor simulator
- Improved physics and chemistry insight delivered via constitutive relations

- VERA CS will be used to highlight assemblies of interest, and provide conditions of specific fuel rods.
- Improved understanding of fuel conditioning will facilitate improved fuel utilization.

MPO delivers materials physics-based constitutive models to the virtual reactor for CASL challenge problems

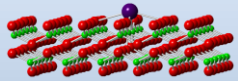
For CRUD, GTRF and PCI, identify 3-D, high resolution coupled physics simulation capability for interface with virtual reactor;

PCI

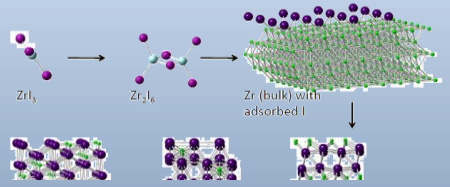


Peregrine

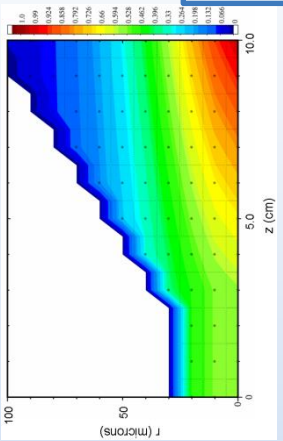
(Fuel Performance)

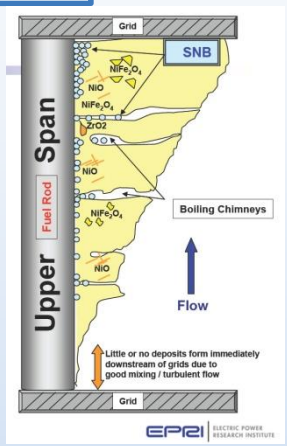


ZrO_2 / I_2 Interaction



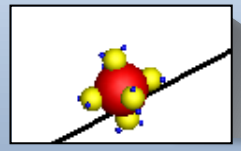
CRUD



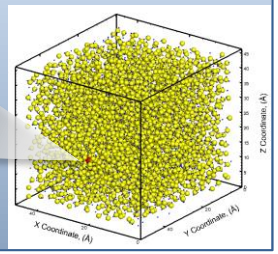


MAMBA

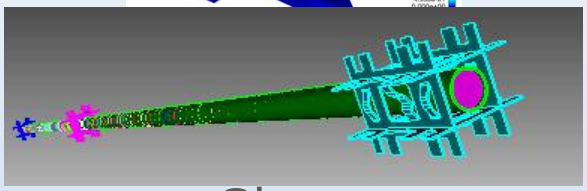
(MPO Advanced Model for Boron Analysis)



ΔH_{MD}

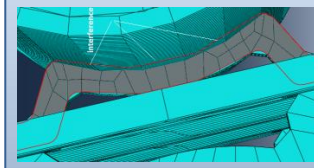


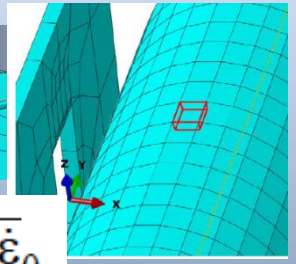
GTRF



Sierra

(Structural Mechanics)





$$\dot{\bar{\varepsilon}} = \bar{\bar{M}} : \bar{\bar{\sigma}} + \dot{\bar{\varepsilon}}_0$$

Initiate a series of microscale activities to provide mechanistic/physical insight into complex degradation phenomena

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Complexities of PCI Failure Process

- State of pellet and cladding interaction is a complex function of the prior irradiation history
  - Role of Pellet
    - Densification => opens gap; Relocation/pellet cracking, Thermal expansion, Swelling => closes gap
  - Role of Cladding
    - Thermal/irradiation creep => closes gap or induces plastic strain
  - Role of fission products
    - Production/release/decay => availability of reactive species for SCC
- Leads to processes of <u>conditioning</u> (able to withstand power change with minimal change in stress) or <u>deconditioning</u> (power change will induce large increase in stress)
  - Defined by residual (or cold) pellet-cladding gap (larger -> conditioned, smaller-> deconditioned)

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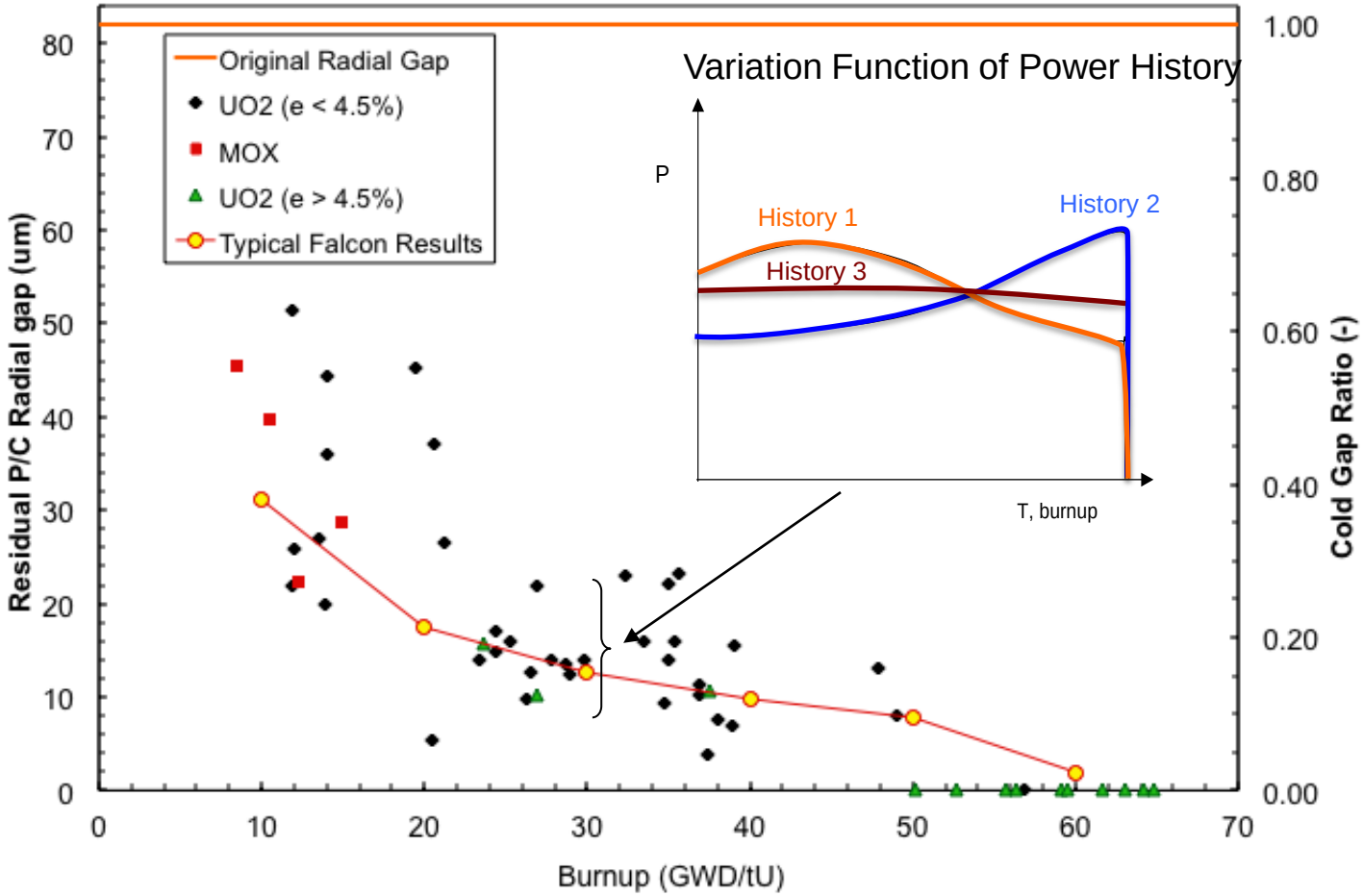
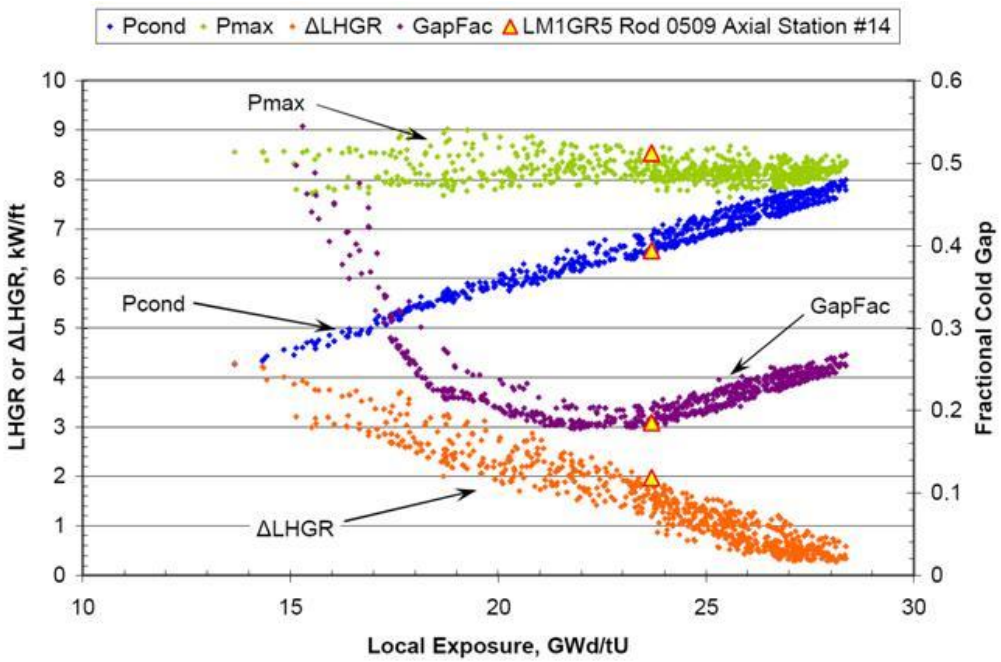
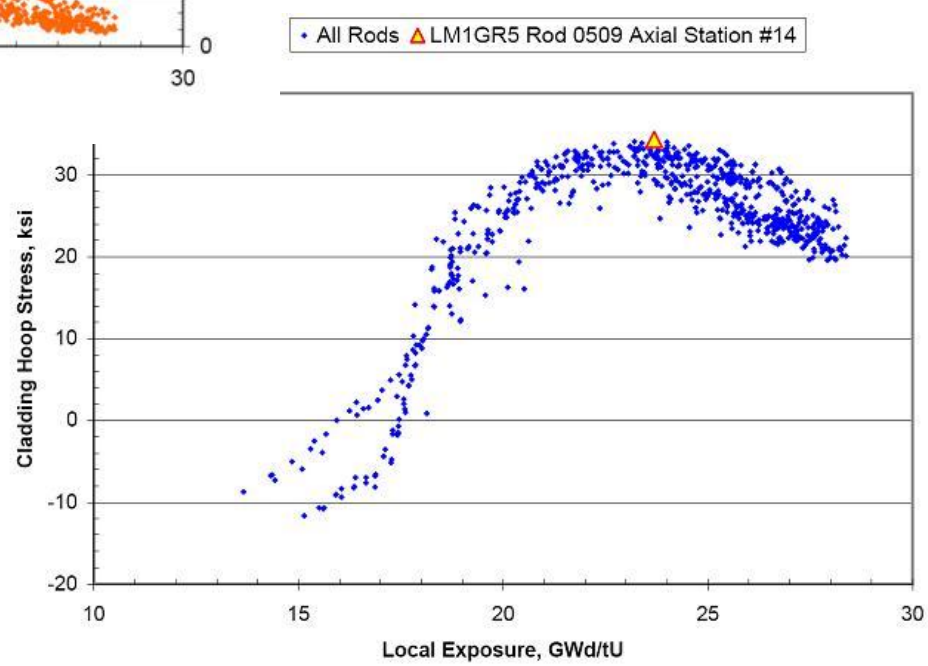
Data on Conditioned State in PWR Fuel:
Not All Burnups are Created Equal



PCI Failure Vulnerable Rod Assessment

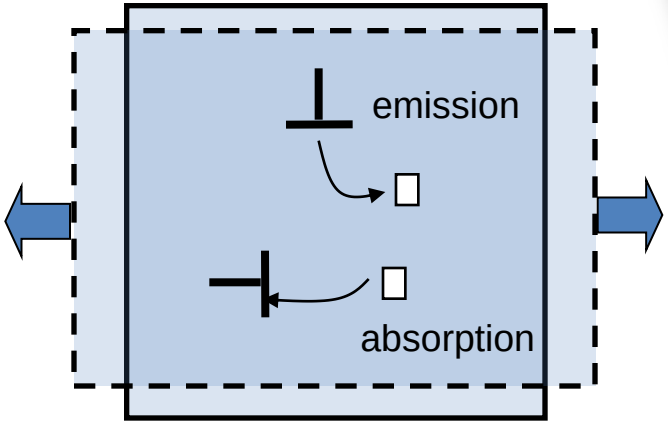


- Local Power and Gap Characteristics – 792 rods (~230,000 pellets)
- One data set per rod corresponding to peak stress node

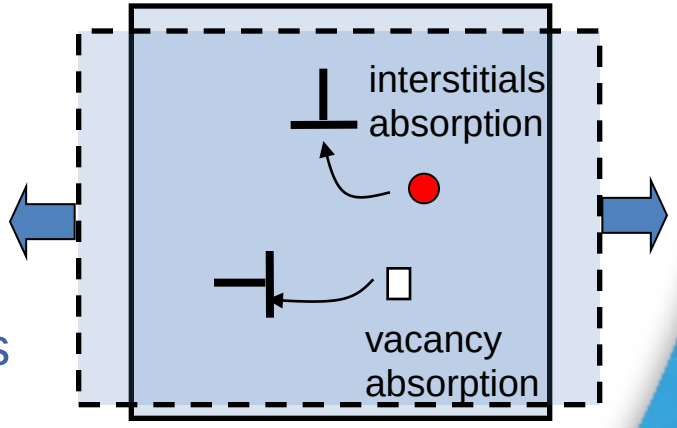


Mechanisms of Thermal and Irradiation Creep

Thermal creep: thermally activated vacancy diffusion
→ climb-controlled glide of dislocations
→ need to balance sources and sinks
→ relevant at high temperature or for close-to-yield stresses



Irradiation creep: driven by super-saturation of vacancies and interstitials
→ climb of dislocation loops
→ climb and glide of edge dislocations
→ relevant at all irradiation temperatures



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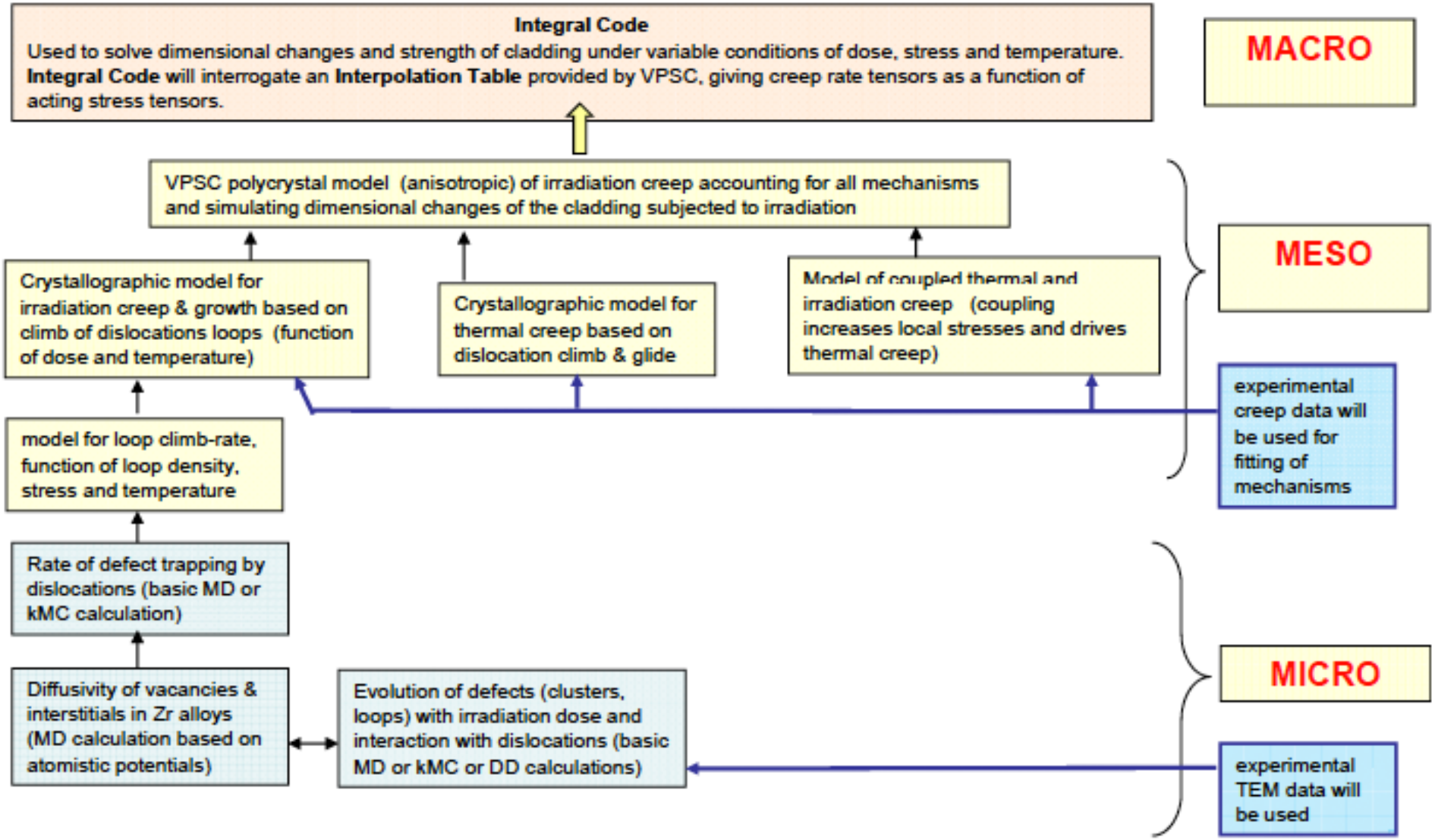
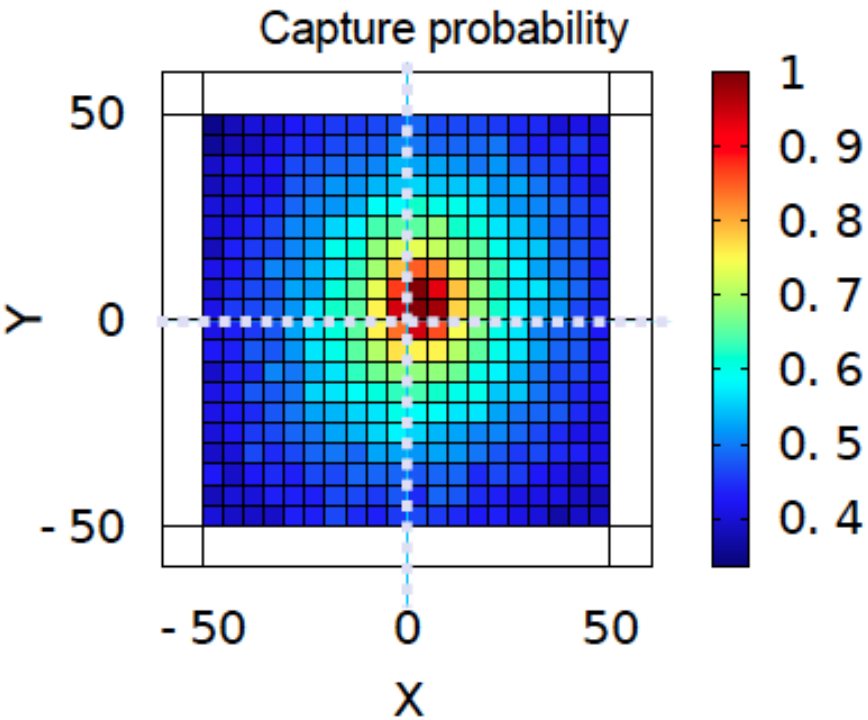
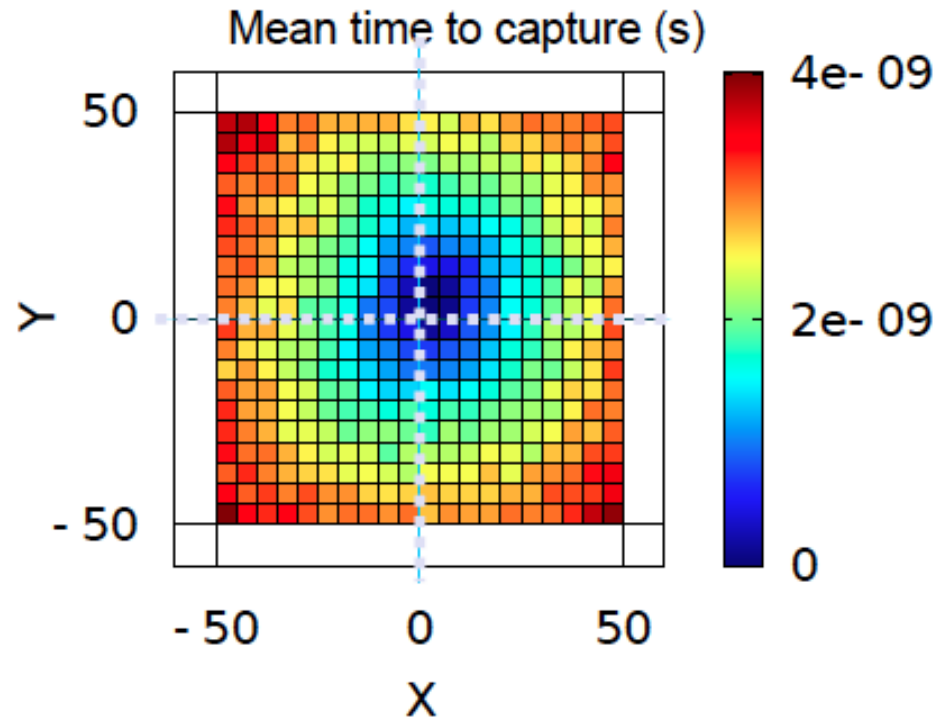
Multiscale Modeling of Thermal and Irradiation Creep in Zr



Absorption rate of point defects by a population of sinks from atomistics





- Edge dislocation with b = 1/3 < 1 1 -2 0 > at origin. Defect = single interstitial
- **Total number of runs = 8.6 x 10^5**
- Anisotropy of strain field reflected in capture probability & time
- Simulations can be carried out for sinks (e.g. dislocations, loops, etc) of arbitrary size and orientation

NEAMS Interface: *Fission Gas Behavior*

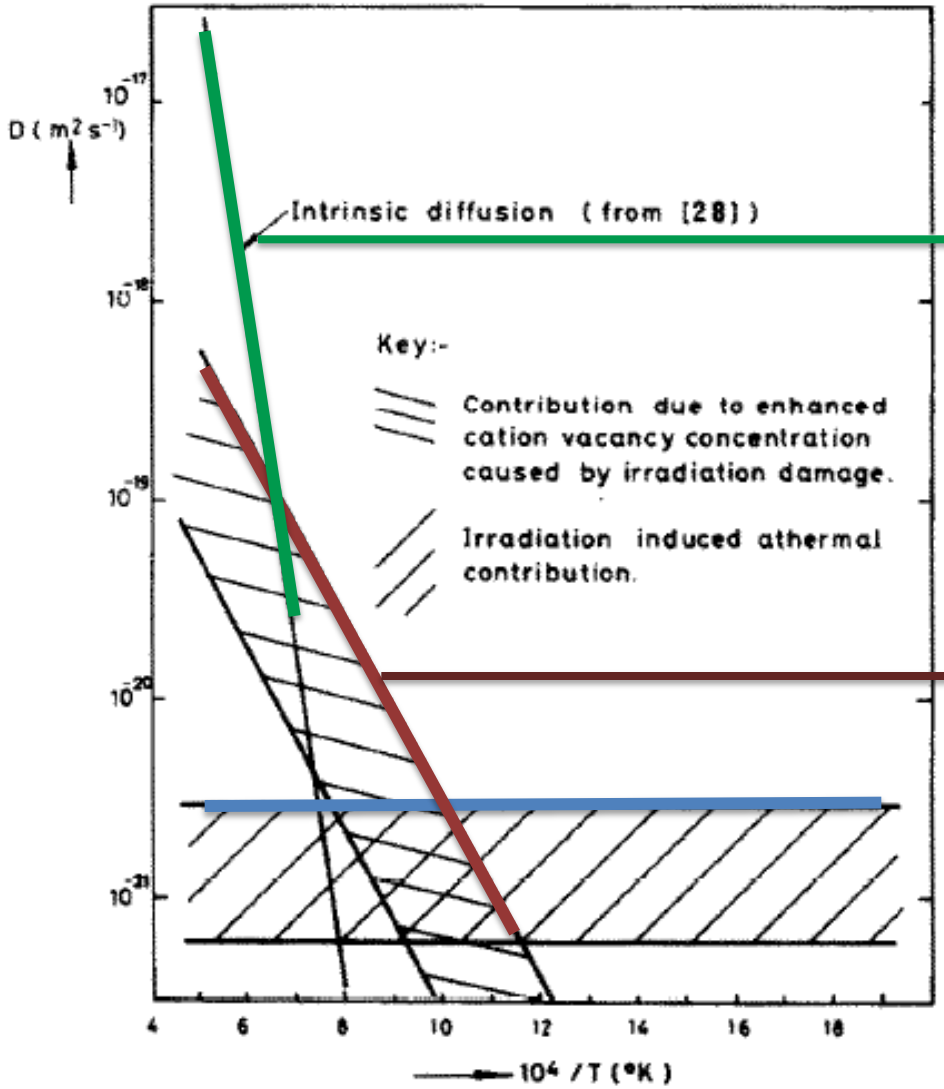


Fig. 10. Possible components of the in-pile rare gas diffusion coefficient.

Thermal diffusion: $D = 7.6 \times 10^{-10} \exp\left(-\frac{3.04}{k_B T}\right)$

Calculations for the same conditions yield 3.94 eV, in good agreement with more recent measurements of intrinsic diffusion (3.9 eV).

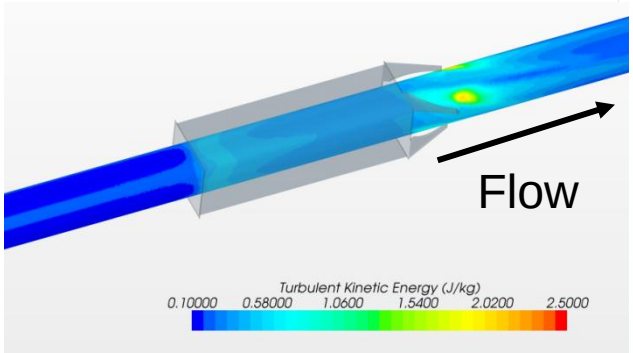
Enhanced diffusion: $D = C' \sqrt{\dot{F}} \exp\left(-\frac{1.20}{k_B T}\right)$

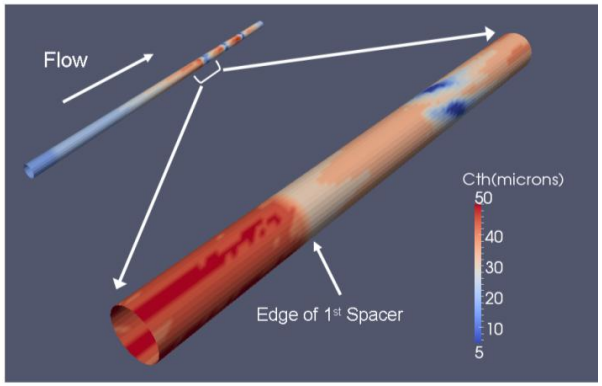
Enhanced vacancy concentration due to irradiation. Improved data for unit processes yields 3.17 eV. Better agreement with FG bubble transport controlled by surface diffusion (1.00-1.25 eV).

Turnbull et al., J. Nucl. Mater. 107, 168 (1982).

MAMBA: *Destination for CRUD Physics Models*

A matrixed CASL team from LANL, MIT, University of Michigan, EPRI, and ORNL has developed an advanced, pin scale, coupled, multi-physics, 3D approach for simulating crud deposition and assessing the crud-induced power shift (CIPS) risk for a single fuel rod with three spacers and integral mixing vanes





New CASL CRUD capability known as "MAMBA" calculates cladding surface heat flux, crud surface temperature, and is coupled DeCART (neutronics) / STAR-CCM+ (thermal-hydraulics) calculation

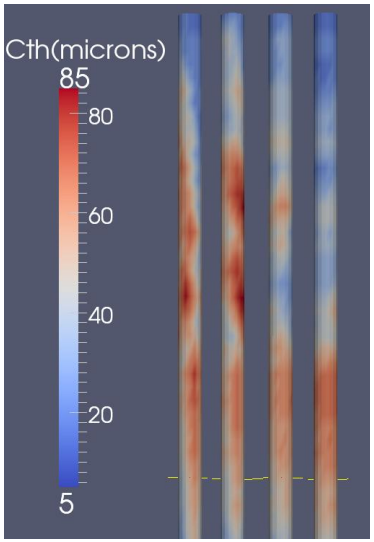
The simulation produced findings useful to PWRs :

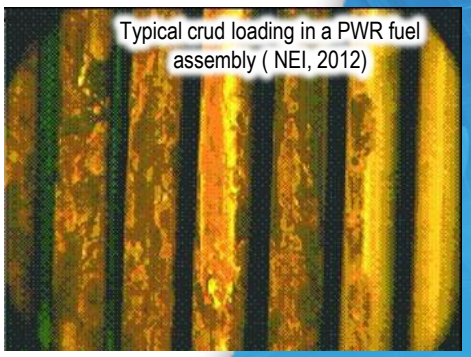
** Significant azimuthal temperature variations on the cladding surface (see right)*

** Varying crud deposition and erosion rates resulting in streak deposits (observed in operating PWRs, see right)*

** Cladding "hot spots" were observed for thicker crud*

This new coupled simulation capability is still under development and hence has only been qualitatively validated. Comparisons with Westinghouse out-of-pile data (in their WALT facility) currently underway





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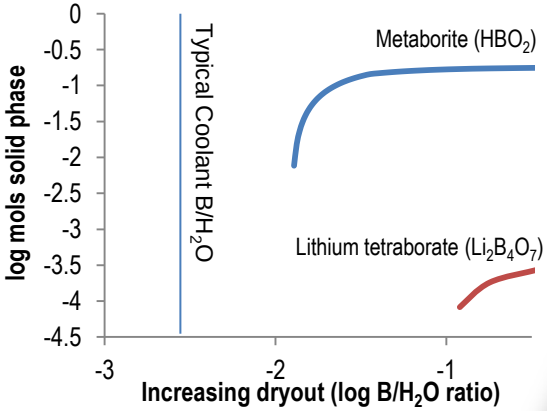
Improved Thermodynamic Models for CRUD

- Current industry code (BOA) only includes two borate compounds: lithium metaborate ($LiBO_2$) or lithium tetraborate ($Li_2B_4O_7$)
- Analysis under MPO found metaborite (HBO_2) can form as well as the lithium borates
- That prediction has been recently supported by the discovery of a sizable metaborite "rock“ in the residual heat removal cooling system of a PWR
- Calculations illustrated in the plot indicate metaborite formation as a function of increasing dryout of the coolant (i.e., evaporation of cooling water)

Where and how will CRUD form and how can we anticipate and mitigate it?

Thermochemical models of CRUD informed by DFT

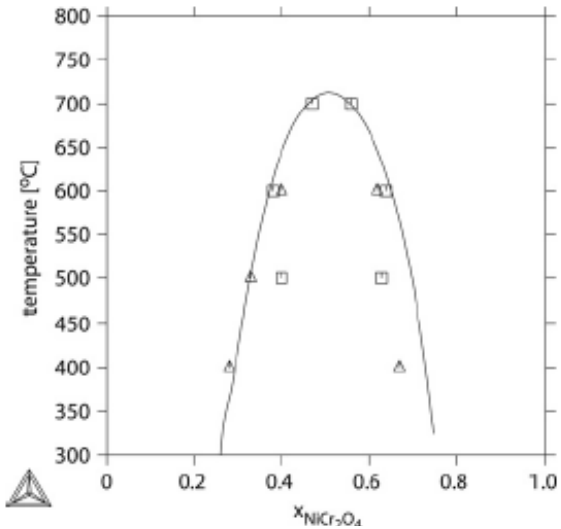
A largely metaborite 7.5 cm “rock” found in a reactor residual heat removal system

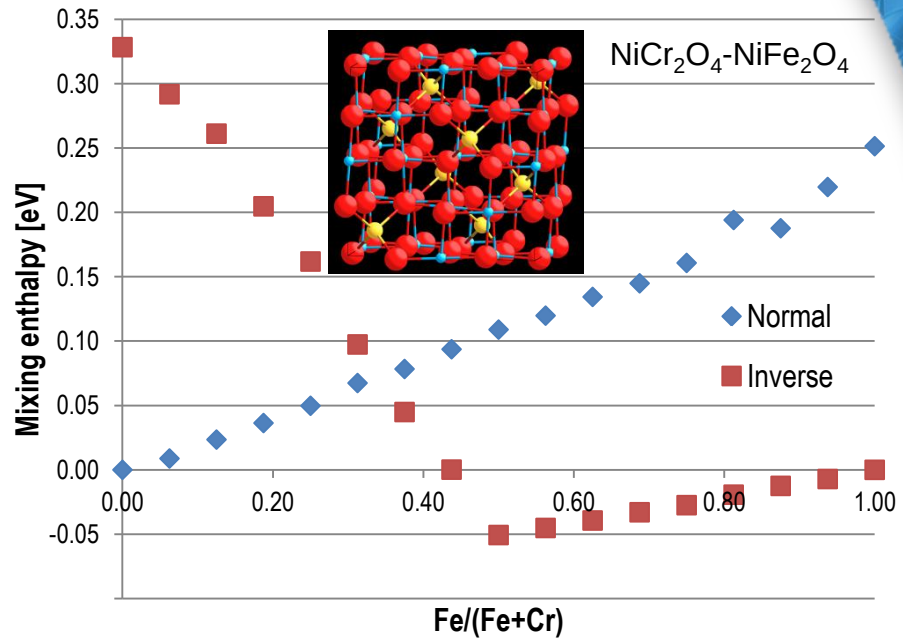


Plot of increasing dryout resulting in predicted metaborite formation.

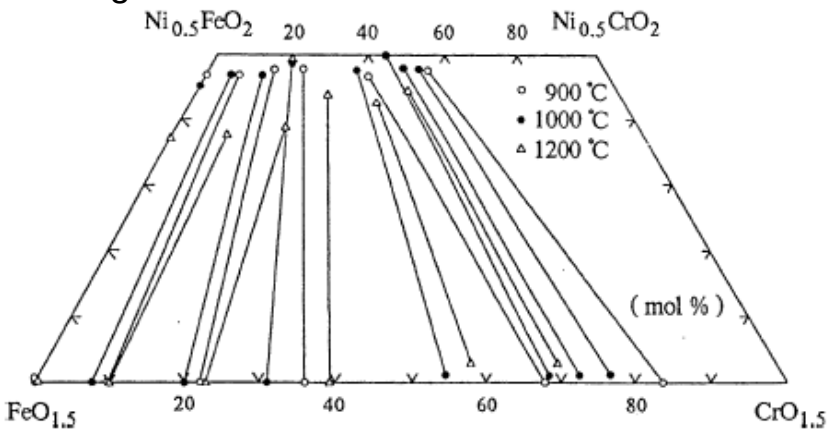
$NiCr_2O_4$-$NiFe_2O_4$ mixing enthalpies from DFT

Phase diagram due to S. E. Ziemniak et al.[1]





Phase diagram due to B.-H. Park et al.[2]



- DFT modeling supports Park et al., but disagrees with Ziemniak et al (current thermodynamic models).

- $NiCr_2O_4$ is a normal spinel.
- The Cr ions are anti-ferromagnetically ordered on the octahedral sites.
- $NiCr_2O_4$ has negative solution energy in $NiFe_2O_4$ up to $NiFe_1Cr_1O_4$, i.e. when the Cr ions have filled all available B (octahedral) sites and starts filling A (tetrahedral) sites.

[1]S. Ziemniak, and A. Gaddipati, P. Sander, J. Phys. Chem. Solids **66**, 1112 (2005).
[2]B.-H. Park, and D.–S. Kim, Bull. Korean Chem. Soc. **20**, 939 (1999).

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DFT lattice stabilities used in CALPHAD assessment

Spinel compound	Formation energy, normal spinel	Formatioin energy, inverse spinel	Experiment (298 K)
$FeZn_2O_4$	-10.420526	-11.129450	
$FeNi_2O_4$	-9.283824	-9.092449	
$CrNi_2O_4$	-10.796869	-10.941382	
$CrZn_2O_4$	-12.575370	-13.164124	
$ZnCr_2O_4$	-15.788417	-13.981118	
$ZnNi_2O_4$	-7.562001	-8.222975	
$NiZn_2O_4$	-8.517137	-9.796126	
$CrFe_2O_4$	-4.863822	-13.259188	
$NiFe_2O_4$	-9.908768	-11.237851	-11.239970
$ZnFe_2O_4$	-12.071988	-11.976264	-12.215662
$FeCr_2O_4$	-15.110068	-13.640414	-14.584208
$NiCr_2O_4$	-14.212902	-13.277367	-14.241458
Fe_3O_4	-11.591219	-11.591219	
Ni_3O_4	-7.647856		
Zn_3O_4	-9.414027		
Cr_3O_4	-15.344572		

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Challenges & Future Plans

Agility & Expectation of Multiscale: Evolution of MPO team to reflect engineering scale priority & appropriate multiscale balance requires proper identification of materials phenomena conducive to multiscale simulation. Need interaction & leveraging across external programs of mutual interest (e.g., NEAMS, EFRCs, exascale, LWR-S, etc.)

Multiphysics Coupling: Improved coordination across FAs is required for future success, as fuel performance/structural engineering frameworks are informed by higher fidelity, physics-based materials performance models

Validation of Materials Models: A wide range of data is required, from full integrated data to specialized separate effects. Possible sources: NE-KAMS, FCRD, EFRCs, etc.

Flexibility & Innovation: Responsiveness to NE community needs (e.g., accident tolerant fuels, additional challenge problems) & ability to evaluate innovative advanced fuel concepts

Multiphase Flow Analysis in Hydra-TH

J. Bakosi, M. A. Christon, M. M Francois, R.B. Lowrie
Los Alamos National Laboratory

R. Nourgaliev
Idaho National Laboratory

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June 11 – 14, 2012

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OVERVIEW

- Requirements & Design Principles
- Survey of Codes & Solution Algorithms
- Hydra-TH Model Formulation
- Candidate Hydra-TH Solution Algorithms
- Hydra-TH Status
- Summary & Future Directions

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HYDRA-TH: requirements & design principles

- Multi-(*N*)-fluid (user-specified) formulation
- (Discrete) mass, momentum, and energy conservation
- Ability to cover all-speeds (from nearly-incompressible to fully-compressible)
- Ability to deal with numerically stiff fluid (water) equation of state
- Robust treatment of phase appearance and disappearance
- Ability to deal with boiling/condensation (tight coupling with energy equation)
- For [1-fluid, ρ=*const*, operator-splitting] option, should reduce to the original HYDRA algorithm (proven to be robust/accurate/efficient)
- Solvability: hyperbolicity/well-posedness
- Efficient for large-scale unstructured-mesh HPC applications (scalable)
- Can be tightly coupled with Next-Generation System Analysis codes

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Survey of Codes & Solution Algorithms

- Codes Surveyed: NPHASE, NEPTUNE, CATHARE, StarCD & CCM+, Fluent, CFX, MFIX, CFDLib, TRAC, TRACE, RELAP5, RETRAN, …
  - Documented in "Effective-Field Modeling for Multi-Fluid Flows" working notes
- Basic formulations are similar in terms of ensemble averaged conservation equations, degrees-of-freedom, and closures
  - Volume fractions, multiple velocities, multiple energy eq.'s, etc.
  - Virtually all are using a single-pressure approximation
- Approaches to hyperbolize equations
  - Bulk pressure difference, interface dynamic pressure, added mass
  - 7 equation-model of Saurel, Berry, et al. preserves hyperbolicity -- invisicid
- Solution algorithms
  - Virtually all are pressure-based
  - Many are based on SIMPLE (aka Uzawa iteration)
    - Expect slow convergence rates (ex: many 100's of iterations for small problems)
    - NPHASE combines SIMPLE-like outer iteration with coupled mass-momentum solve
  - All current work-horse T-H codes (RELAP5, TRAC, TRACE, CATHARE, RETRAN) use operator-split algorithms

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HYDRA-TH: model formulation

(5*N*)-conservation equations, *N*-field formulation

- Mechanical & thermal non-equilibrium
- Pressure equilibrium
- Multiple-bulk-pressure
- Hyperbolic (easily provable when *N*=2 fields)
- Can implement both acoustically-filtered and fully-compressible forms
- EOS: generic; for water – IAPWS-IF97 Standard
- Multiphase closures: from NPHASE methods, Lahey, Podowski, et al.
- [ILES, LES/DES, κ-ε and k-ω models in the future]
- [Interfacial area transport (IAT) in the future (from NPHASE/NEPTUNE)]

Application Focus

1. Subcooled boiling
2. Departure from nucleate boiling (DNB)
3. Loss-of-coolant accidents (LOCA)
4. Reflooding

} In the future

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HYDRA-TH: governing equations

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot (\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k) = \boxed{\Gamma_k}$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k]) = (\boxed{p_{ki}} - \boxed{\tau_{ki}}) \nabla \alpha_k + \boxed{\mathbf{M}'_k} +$$
$$+ \nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k} \right] \right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}^m_{ki}} \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t} \left(\alpha_k \bar{\rho}_k \tilde{e}_k \right) + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{e}_k + \bar{p}_k] \tilde{\mathbf{v}}_k) = \boxed{\mathbf{M}'_k} \cdot \tilde{\mathbf{v}}_k + (\boxed{p_{ki}} - \boxed{\tau_{ki}}) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k +$$
$$+ \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k} \right) - \boxed{\bar{\mathbf{q}}_k} - \boxed{\mathbf{q}^{Re}_k} \right] \right) +$$
$$+ \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k \right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} + \frac{\left(\boxed{v^e_{ki}} \right)^2}{2} \right) + \boxed{E_k} + \boxed{W'_k}$$

+ Turbulence equations

To close:

+ N equations of state, $\bar{p}_k \left(\bar{\rho}_k, \tilde{u}_k \right)$
+ Constitutive physics (for terms in boxes $\boxed{}$)
+ Compatibility condition, $\sum_k \alpha_k = 1$
+ Bulk pressure difference models, $\Delta \bar{p}_{(ij)} \left(\mathbf{U} \right), \; i \neq j, \; (i,j) = 0, \ldots, N-1$

HYDRA-TH: hyperbolicity/well-posedness

Wave/Eigen-structure

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot (\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k) = \Gamma_k$$

$\bar{p}$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k]) = (p_{ki} - \tau_{ki}) \nabla \alpha_k + \mathbf{M}_k +$$

$$+ \nabla \cdot \left(\alpha_k \left[\bar{\tau}_k + \mathbf{T}_k^{Re} \right] \right) + \alpha_k \bar{\rho}_k \tilde{\mathbf{b}}_k + \mathbf{v}_{ki}^m \Gamma_k$$

Total energy:

$$\frac{\partial}{\partial_t} \left(\alpha_k \bar{\rho}_k \tilde{e}_k \right) + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{e}_k + \bar{p}_k] \tilde{\mathbf{v}}_k) = \mathbf{M}_k \cdot \tilde{\mathbf{v}}_k + (p_{ki} - \tau_{ki}) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k +$$

$$+ \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\bar{\tau}_k + \mathbf{T}_k^{Re} \right) - \ldots \right] \right)$$

$$+ \alpha_k \bar{\rho}_k \left(\tilde{r}_k + \tilde{\mathbf{b}}_k \cdot \tilde{\mathbf{v}}_k \right) + \Gamma_k \left(u_k \ldots \right.$$

This is a non-physical model (used in TRAC/TRACE)

Non-hyperbolic IF

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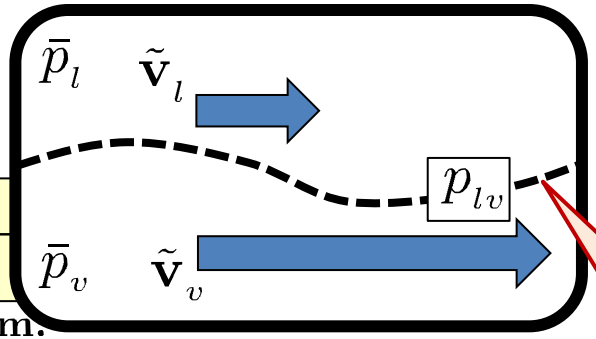
HYDRA-TH: hyperbolicity/well-posedness



Interfacial dynamic pressure:

$$\xi \hat{\rho} \Delta U^2$$

(Bernoulli effect, [Stuhmiller, 1977])

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} +$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(p_{ki} - \tau_{ki}\right) \nabla \alpha_k$$

$$\delta \alpha_l \alpha_v \frac{\bar{\rho}_l \bar{\rho}_v}{\alpha_l \bar{\rho}_l + \alpha_v \bar{\rho}_v}$$

$$+ \nabla \cdot \left(\alpha_k \left[\bar{\tau}_k + \mathbf{T}_k^{Re}\right]\right) + \alpha_k \bar{\rho}_k \tilde{\mathbf{b}}_k + \ldots \Gamma_k$$

[Bestion, 1990]

To

$$\frac{\partial}{\partial_t} \ldots \nabla \alpha_k +$$

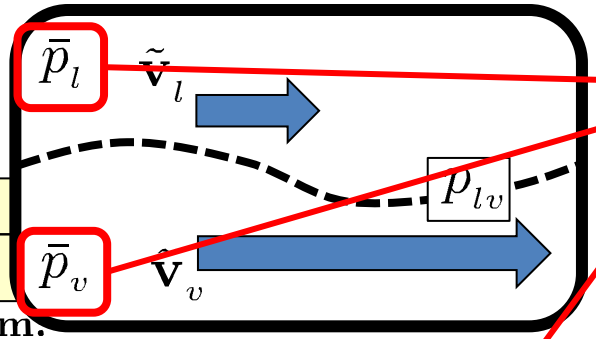
$$+ \alpha_k \bar{\rho}_k \left(\tilde{r}_k + \mathbf{b}_k \cdot \tilde{\mathbf{v}}_k\right) + \Gamma_k \left(u_{ki} \ldots\right.$$

Conditionally hyperbolic:

$$\delta \geq 1$$

CATHARE
NEPTUNE/OVAP

HYDRA-TH: hyperbolicity/well-posedness



Bulk pressure difference
(e.g., surface tension)

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \cdots$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(p_{ki} - \tau_{ki}\right) \nabla \alpha_k + \mathbf{M}_k' +$$

$$+ \nabla \cdot \left(\alpha_k \left[\bar{\tau}_k + \mathbf{T}_k^{Re}\right]\right) + \alpha_k \bar{\rho}_k \tilde{\mathbf{b}}_k + \mathbf{v}_{ki}^m \Gamma_k$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{e}_k + \bar{p}_k\right] \tilde{\mathbf{v}}_k\right) = \mathbf{M}_k' \cdot \tilde{\mathbf{v}}_k + \left(p_{ki} - \tau_{ki}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k +$$

$$+ \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\bar{\tau}_k + \mathbf{T}_k^{Re}\right) - \bar{\mathbf{q}}_k - \mathbf{q}_k^{Re}\right]\right) +$$

$$+ \alpha_k \bar{\rho}_k \left(\tilde{r}_k + \tilde{\mathbf{b}}_k \cdot \tilde{\mathbf{v}}_k\right) + \Gamma_k \left(u_{ki} + \frac{\left(v_{ki}^e\right)^2}{2}\right) + E_k + W_k'$$

HYDRA-TH: hyperbolicity/well-posedness

Added mass:

$$\mu \bar{\rho}_c \frac{\mathrm{d}_{\mathrm{d}} \Delta \vec{U}}{\mathrm{d}t}$$

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot \left(\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k\right) = \Gamma_k$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(p_{ki} - \tau_{ki}\right) \nabla \alpha_k + \mathbf{M}_k' +$$

$$+ \nabla \cdot \left(\alpha_k \left[\bar{\tau}_k + \mathbf{T}_k^{Re}\right]\right) + \alpha_k$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{e}_k + \bar{p}_k\right] \tilde{\mathbf{v}}_k\right) = \mathbf{M}_k' \cdot \tilde{\mathbf{v}}_k$$

$$+ \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\bar{\tau}_k + \right.\right.\right.$$

$$+ \alpha_k \bar{\rho}_k \left(\tilde{r}_k + \tilde{\mathbf{b}}_k \cdot \tilde{\mathbf{v}}_k\right) + \Gamma_k \left(u_{ki} + \frac{\left(v_{ki}^e\right)}{2}\right) + E_k + W_k'$$

RELAP5
NPHASE
NEPTUNE

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HYDRA-TH: hyperbolicity/well-posedness

Parabolic terms

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot \left(\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k\right) = \boxed{\Gamma_k}$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(\boxed{p_{ki}} - \boxed{\tau_k}\right) \nabla \alpha_k + \boxed{\mathbf{M}_k'} +$$

$$+ \nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}_k^{Re}}\right]\right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}_{ki}^m} \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{e}_k + \bar{p}_k\right] \tilde{\mathbf{v}}_k\right) = \boxed{\mathbf{M}_k'} \cdot \tilde{\mathbf{v}}_k + \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k +$$

$$+ \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}_k^{Re}}\right) - \boxed{\bar{\mathbf{q}}_k} - \boxed{\mathbf{q}_k^{Re}}\right]\right) +$$

$$+ \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} + \frac{\left(\boxed{v_{ki}^e}\right)^2}{2}\right) + \boxed{E_k} + \boxed{W_k'}$$

HYDRA-TH:

Solution algorithm
(preliminary design)

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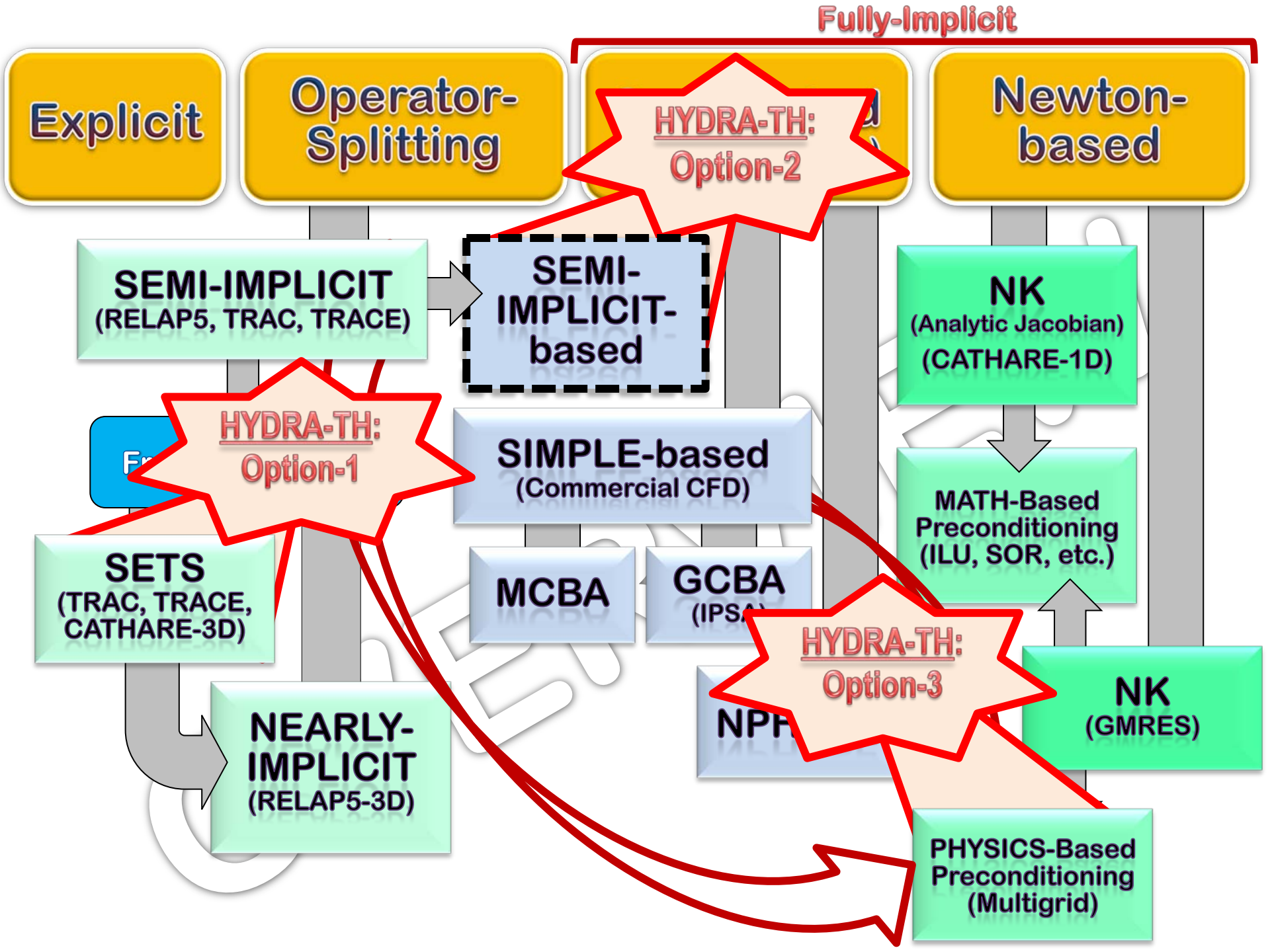

Fully-Implicit
Explicit
Operator-Splitting
Newton-based
HYDRA-TH: Option-2
SEMI-IMPLICIT (RELAP5, TRAC, TRACE)
SEMI-IMPLICIT-based
NK (Analytic Jacobian) (CATHARE-1D)
HYDRA-TH: Option-1
SIMPLE-based (Commercial CFD)
MATH-Based Preconditioning (ILU, SOR, etc.)
SETS (TRAC, TRACE, CATHARE-3D)
MCBA
GCBA (IPSA)
HYDRA-TH: Option-3
NK (GMRES)
NEARLY-IMPLICIT (RELAP5-3D)
PHYSICS-Based Preconditioning (Multigrid)

HYDRA-TH: solution algorithm, option 1

SETS-based operator-splitting (Fractional

No compatibility enforced

$$res_{\alpha} = 1 - \sum_{k} \hat{\alpha}^{\star\star}_{k_{(c)}} \neq 0$$

1. Volume fraction update ("mass stabilizer")

$$a^{(k)}_{c,c}\left(\mathbf{U}^{\star}\right)\hat{\alpha}^{\star\star}_{k_{(c)}} + \sum_{n}^{N} a^{(k)}_{c,n}\left(\mathbf{U}^{\star}\right)\hat{\alpha}^{\star\star}_{k_{(n)}} = b^{(k)}_{c}\left(\mathbf{U}\right.$$

Phasic mass

$$\tilde{\mathbf{v}}^{\diamond}_{k_{(c)}} = \frac{b^{(k)}_{c} + \sum_{m\neq k}^{K} c^{(k,m)}_{c}\tilde{\mathbf{v}}^{\star}_{m_{(c)}} - \sum_{n}^{N} a^{(k)}_{c,n}\tilde{\mathbf{v}}^{\star}_{k_{(n)}}}{a^{(k)}_{c,c} + \sum_{m\neq k}^{K} c^{(k,m)}_{c}}$$

ILU or AMG

2. Velocity update ("momentum stabilizer", SINCE-based)

No mass/energy conservation enforced

$$\hat{\tilde{\mathbf{v}}}^{\star\star}_{k_{(c)}} + \sum_{n}^{N} a^{(k)}_{c,n}\hat{\tilde{\mathbf{v}}}^{\star\star}_{k_{(n)}} == b^{(k)}_{c} + \sum_{m\neq k}^{K}\left[c^{(k,m)}_{c}\frac{b^{(m)}_{c} + \sum_{j\neq m,k}^{K} c^{(m,j)}_{c}\tilde{\mathbf{v}}^{\diamond}_{j_{(c)}} - \sum_{n}^{N} a^{(m)}_{c,n}\tilde{\mathbf{v}}^{\diamond}_{m_{(n)}}}{a^{(m)}_{c,c} + \sum_{j\neq m}^{K} c^{(m,j)}_{c}}\right]$$

$\tilde{b}^{(k)}_{c}$

...interfacial momentum coupling...)

3. Enthalpy update ("energy stabilizer")

$$a^{(k)}\left(\mathbf{U}^{\star}\right)\hat{\tilde{h}}^{\star\star} + \sum^{N} a^{(k)}\left(\mathbf{U}^{\star}\right)\hat{\tilde{h}}^{\star\star}_{k_{(n)}} = b^{(k)}_{c}\left(\mathbf{U}^{\star}\right)$$

Compressibility

Phasic energy conservation equations (ILU or AMG)

AMG

5. Turbulence Equations

...ion (mass/energy conservation + compatibility)

6. Other scalar transport equations

derivative of [Liles, Reed, 1978] "semi-implicit" (ICE-based) algorithm

HYDRA-TH: solution algorithm, option-2

Fully-Implicit, Segregated (Picard-iteration)

Fractional steps algorithm

1. Volume fraction update ("mass stabilizer")
2. Velocity update ("momentum stabilizer", SINCE-based)
3. Enthalpy update ("energy stabilizer")
4. Pressure-Helmholtz Equation
5. Turbulence Equations
6. Other scalar transport equations

Converged?

HYDRA-TH: solution algorithm, option-3

Fully-Implicit, NK (Physics-based preconditioning)

Fractional step algorithm
(preconditioning)

$$\mathbb{J}_{i,j} \equiv \frac{\partial res_i}{\partial \mathcal{X}_j}$$

Linear solve:

$$\mathbb{J}^{\mathrm{it}} \delta \vec{\mathcal{X}}^{\mathrm{it}} = -\vec{res}\left(\vec{\mathcal{X}}^{\mathrm{it}}\right)$$

Start Newton iteration

$$\vec{\mathcal{X}}^{\mathrm{it}+1} = \vec{\mathcal{X}}^{\mathrm{it}} + \delta \vec{\mathcal{X}}^{\mathrm{it}}$$

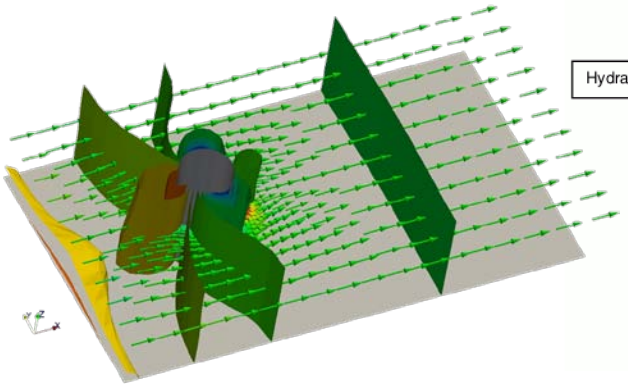
IF $\left\| \vec{res}\left(\vec{\mathcal{X}}^{\mathrm{it}}\right) \right\|_2 < \mathrm{tol}_{\mathrm{N}} \left\| \vec{res}\left(\vec{\mathcal{X}}^{0}\right) \right\|_2$ ELSE

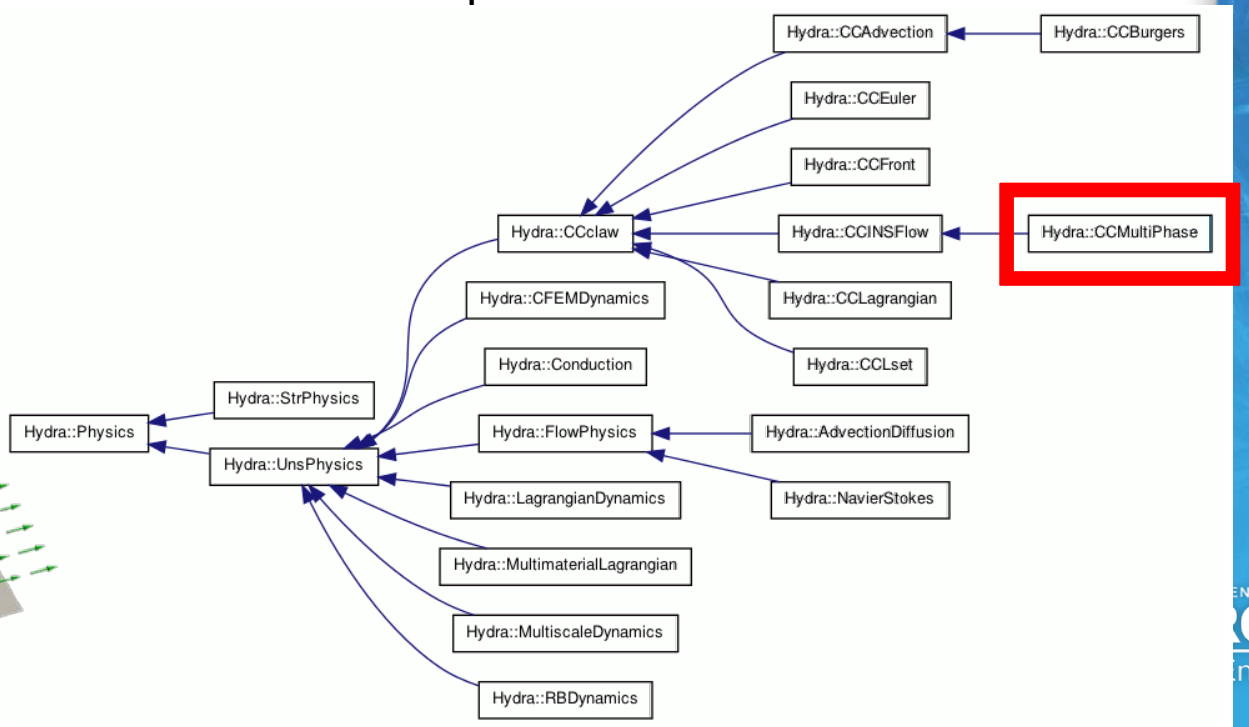
End Newton iteration

HYDRA-TH: Status

- **Prototype multiphase physics is in place**
  - Running simple problems and solving *N*-momentum equations w. single pressure
  - Volume fractions treated as passive scalars for now
  - All keywords, BC's, IC's inherited from the virtual incompressible physics

- **General development plan**
  - Re-use all existing BC's, IC's, materials, transport solvers, and turbulence statistics on a phasic basis
  - Implement both fully-coupled so
  - ***Segregated so physics-based***
  - ***Preserve exist for FSI***





Summary & Future Directions

- **The basic formulation is relatively well defined at this point**
  - Some questions remain on multiphase closures, e.g., the form of lift forces, mass exchange terms, etc.
    - ➢ May require some additional research to adequately define source terms
  - A number of questions/algorithmic decisions will be answered over the next 3-4 months

- **Prototype multiphase virtual physics is in place**
  - Able to solve multiple momentum equations with identical BC's and obtain correct solutions
  - Volume fraction transport (i.e., continuity) is in place
  - Extension for multiple energy equations appears straightforward
  - Additional effort required to integrate steam tables, additional constitutive and EOS models

- **On-track for L3:THM.CFD.P5.06 milestone**
  - Initial two-phase laminar test case to be based on DEBORA experiments is targeted – time permitting

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~ Backup Slides ~

NPHASE Solution Algorithm
a few general notes

- 2 approaches : segregated or coupled mass/momentum
- Coupled mass/momentum approach preferred approach
  - Better stability and robustness
- User routines for closure terms (drag force, lift interfacial force, wall interfacial force, turbulence dispersion interfacial force)
- Closure terms treated differently in segregated and coupled solver
  - Segregated algorithm: linearized drag force, other terms, other terms added as RHS terms held constant during iterations.
  - Coupled algorithm: linearized terms added to LHS and full model term added to RHS

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NPHASE Solution Algorithm (Coupled Solver) Coupled Mass/Momentum – Segregated Enthalpy

- Solve for velocity, pressure, volume fractions
  - Variables: (total variables is 5*Nfield)
    - Velocity (3), pressure (1) and volume fraction (1) per field
    - Density held constant → volume fraction equation
  - Equations:
    - Mass (continuity) (1 per field)
    - u, v, w momentum (3 per field)
    - Constraint – sum of volume fractions = 1 (1 total)
    - Jump equations – p_k-p=0 (P equilibrium) (Nfield-1)
- Solve enthalpy, turbulence k-e, species concentration
- Update density as function of T
- Iterate until convergence

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NEPTUNE (NURETH10 paper) Pressured-based method with mass/momentum/energy coupling

- predict velocities through partially linearized momentum equations (other variables are frozen and taken at previous time step)
- Mass/momentum/energy coupling
  - Momentum equation using predicted velocity (frozen convective/diffusive parts and pressure and volume fractions treated implicitly)
  - Coupled with mass and total enthalpy equation
  - Iterative solver for pressure, volume fraction, total enthalpy, velocity, density (function of p and h). Enthalpy, thermodynamic properties, volume fractions prediction, pressure equation correction, update velocities, iterate until convergence (convergence is sum volume fractions=1)
- Update other variables (turbulence, interfacial areas)

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NEPTUNE CFD V1.0
Interfacial momentum transfer terms

$$\vec{M}_{ki} = \vec{M}_k^D + \vec{M}_k^{MA} + \vec{M}_k^L + \vec{M}_k^{DT}$$

- Drag force

$$\vec{M}_g^D = -\vec{M}_l^D = -\frac{1}{8} a_i \rho_1 C_D \left|\vec{u}_g - \vec{u}_l\right| \left(\vec{u}_g - \vec{u}_l\right)$$

- Added mass (virtual mass)

$$\vec{M}_g^{MA} = -\vec{M}_l^{MA} = -C_{MA}\alpha \frac{1+2\alpha}{1-\alpha}\rho_l \left[\left(\frac{\partial \vec{u}_g}{\partial t} + \vec{u}_g \cdot \nabla \vec{u}_g\right) - \left(\frac{\partial \vec{u}_l}{\partial t} + \vec{u}_l \cdot \nabla \vec{u}_l\right)\right]$$

- Lift force

$$\vec{M}_g^L = -\vec{M}_l^L = -C_L \alpha \rho_l \left(\vec{u}_g - \vec{u}_l\right) \times \left(\nabla \times \vec{u}_l\right)$$

- Turbulent dispersion

$$\vec{M}_g^{DT} = -\vec{M}_l^{DT} = -C_{DT} \rho_l K_l \nabla \alpha$$

$C_{MA} = 0.5$

$C_L = 1$

$C_{DT} = 1$ (DEDALE)

$C_{DT} = 2.5$ (DEBORA)

Guelfi A. et al., NEPTUNE: A New Software Platform for Advanced Nuclear Thermal Hydraulics, Nuclear Science and Engineering, 156, 281-324, 2007

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NEPTUNE CFD V1.0
Interfacial heat and mass transfer terms

- Interfacial mass transfer

$$\Gamma_g = -\Gamma_l = \frac{-q_{li} - q_{gi} + q_e}{H_g - H_l}$$

- Liquid to interface heat transfer
  - Condensation
  - Evaporation

$$q_{li} = h_{li}\left(T_{sat} - T_l\right) \qquad h_{li} = \frac{\lambda_l}{d_S}\mathrm{Nu} \qquad \mathrm{Ja} = \frac{\rho_l C_{pl}\left(T_l - T_{sat}\right)}{\rho g L}$$

$$\mathrm{Ja} \le 0 \qquad \mathrm{Nu} = 2 + 0.6\,\mathrm{Re}^{0.5}\,\mathrm{Pr}^{0.33}$$

$$\mathrm{Pe} = \frac{d_s U_r}{a_l}$$

- Interface to vapor heat transfer

$$\mathrm{Ja} \ge 0 \qquad \mathrm{Nu} = \mathrm{Max}\left(\mathrm{Nu}_1, \mathrm{Nu}_2, \mathrm{Nu}_3\right)$$

$$\mathrm{Re} = \frac{d_s U_r}{\nu_l}$$

$$\mathrm{Nu}_1 = \sqrt{\frac{4Pe}{\pi}} \qquad \mathrm{Nu}_2 = \frac{12}{\pi}\mathrm{Ja} \qquad \mathrm{Nu}_3 = 2$$

$$\mathrm{Pr} = \frac{\nu_l}{a_l}$$

$$q_{gi} = \frac{\alpha \rho_g C_{pg}}{\delta t}\left(T_{sat} - T_g\right)$$

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NEPTUNE CFD V1.0
wall heat transfer terms

- Wall heat transfer

$$q_w = q_c + q_q + q_e$$

  - "single phase" like heat transfer through contact area A_c between the liquid and the duct wall

with heat transfer coefficient

$$q_c = A_c h_{\log}\left(T_w - T_l\right)$$

  - Quenching effect

$$h_{\log} = \rho_l C_{pl} \frac{u^*}{T^+}$$

  - Phase change heat flux (bubbles nucleated on the wall surface)

$$q_q = A_q t_q f \frac{2\lambda_l\left(T_w - T_l\right)}{\sqrt{\pi a_1 t_q}}$$

$$q_e = f \frac{\pi}{6} d_{nuc}^3 \rho_g L N$$

u^* wall friction velocity

T^+ non-dimensional temperature in the wall boundary layer

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NEPTUNE CFD V1.0 interfacial area equation

$$\frac{\partial a_i}{\partial t} + \nabla \cdot \left(a_i \vec{u}_i\right) = \frac{2}{3}\frac{a_i}{\alpha \rho_g}\left(\Gamma_{g,i} - \alpha \frac{d\rho_g}{dt}\right) + \pi d_{nuc}^2 \Phi_n^{NUC} + \Phi_{a_i}^{CO} + \Phi_{a_i}^{BK}$$

mass transfer and density change effect

nucleation

coalescence

breakup

Assume spherical bubbles

$$d_s = \frac{6\alpha}{a_i}$$

Sauter mean diameter

$$n = \frac{\alpha}{\pi d_s^3 / 6} = \frac{1}{36\pi}\frac{a_i^3}{\alpha^2}$$

Bubble number density

Mass Conservation Algorithm

- 1) estimate velocities – solve momentum equations implicitly using p^n (predictor step)
- 2) Find pressure correction δp_i
- 3) Update pressure, density, velocity

$$\rho^{k+1} \approx \rho^k + \left(\frac{\partial \rho_J}{\partial p}\right)^k \delta p_i + \left(\frac{\partial \rho_J}{\partial T}\right)^k \delta T_i$$

If weakly compressible

- 4) Solve continuity equation for volume fractions
  - Enforce sum of volume fractions to unity, by ((1-a), renormalization or under-relaxation
- 5) iterate until convergence

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Volume Conservation Algorithm (IPSA)

- 1) first estimate of volume fractions by solving implicitly continuity equation using u^n
- 2) first estimate of velocity by solving implicitly momentum equation
- 3) Find pressure correction using $\left(\alpha_1^k + \delta\alpha_1\right) + \left(\alpha_2^k + \delta\alpha_2\right) = 1$ to form equation for δp
- 4) Update pressure, volume fraction, velocity
- 5) iterate until convergence
- 6) if energy equation, solve for T, update density

$$\rho^{k+1} \square \rho^k + \left(\frac{\partial \rho_J}{\partial p}\right)^k \delta p_i + \left(\frac{\partial \rho_J}{\partial T}\right)^k \delta T_i$$ If weakly compressible

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CASL

The View from the Forrestal Building

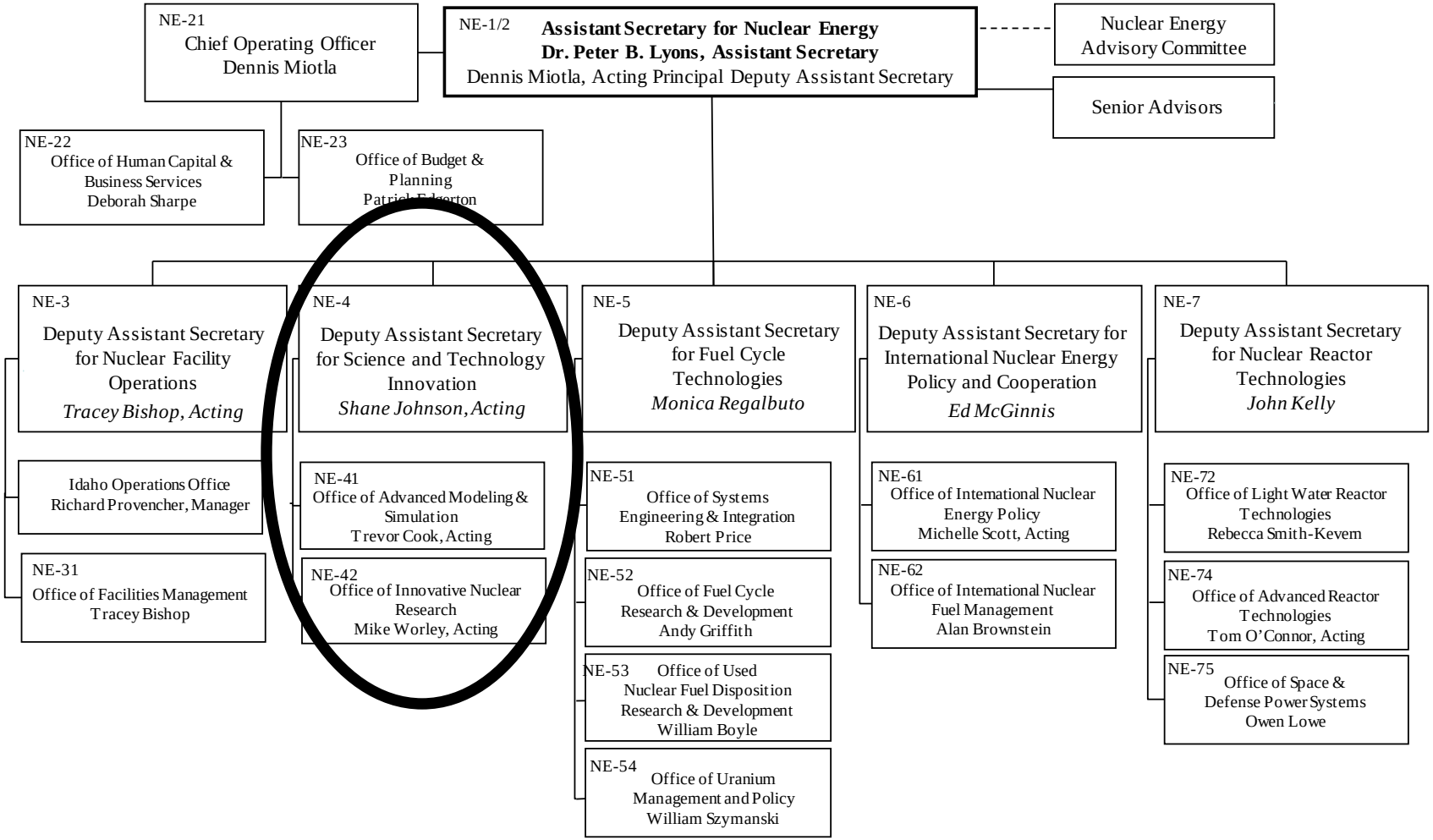
Alex R. Larzelere
Advanced Modeling and Simulation Office
Office of Nuclear Energy
U.S. Department of Energy

AMSO
ADVANCED MODELING & SIMULATION OFFICE

U.S. DEPARTMENT OF ENERGY

Nuclear Energy

Proposed NE Reorganization



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Application for CASL Renewal

Criteria

- Satisfying its goals and objectives
- Contribution to the overall missions of the Energy Innovation Hub

Draft Evaluation Factors

- Significance of milestones
- Milestone accomplished in significance ways
- Plans for the extension that contribute to the mission of the Hub and the missions of the Office of Nuclear Energy

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Application Timing (working backwards)

- **Award Notification**
  - July 1, 2014
- **Briefings to DOE Leadership**
  - May – June 2014
- **Merit Review**
  - March – April 2014
- **Application Submission**
  - March 1, 2014
- **Application Preparation**
  - December 2013 – February 2014
- **Application Request**
  - December 1, 2013
- **DOE Request Preparation**
  - October – November 2013
  - Coincides with DOE's FY-15 Budget Request Preparation

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Experiments for Modeling and Simulation

Challenges

- Separate effect observations
  - Filtering out other factors
  - Making highly resolved and detailed observations
  - Understanding “how” things happen to develop models of physical behaviors
  - More . . .
- Integrated effects observations
  - Boundary conditions
  - Observations at early and late times
  - 3D and high resolution (in time and space)
  - More . . .

Modeling and Simulation Responsibilities

- Understand and communicate requirements for experiments
- Examine existing experimental data and deficiencies
- Work closely with experimentalists
  - Develop new approaches to making experiments
  - Assist with modeling and simulation in making experiments better

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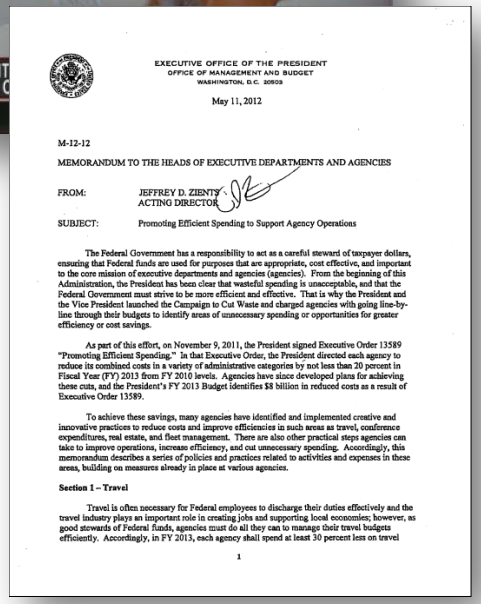
Why a Virtual Roundtable?



EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF MANAGEMENT AND BUDGET
WASHINGTON, D.C. 20503

May 11, 2012

M-12-12

MEMORANDUM TO THE HEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES

FROM: JEFFREY D. ZIENTS
ACTING DIRECTOR

SUBJECT: Promoting Efficient Spending to Support Agency Operations

The Federal Government has a responsibility to act as a careful steward of taxpayer dollars, ensuring that Federal funds are used for purposes that are appropriate, cost effective, and important to the core mission of executive departments and agencies (agencies). From the beginning of this Administration, the President has been clear that wasteful spending is unacceptable, and that the Federal Government must strive to be more efficient and effective. That is why the President and the Vice President launched the Campaign to Cut Waste and charged agencies with going line-by-line through their budgets to identify areas of unnecessary spending or opportunities for greater efficiency or cost savings.

As part of this effort, on November 9, 2011, the President signed Executive Order 13589 "Promoting Efficient Spending." In that Executive Order, the President directed each agency to reduce its combined costs in a variety of administrative categories by not less than 20 percent in Fiscal Year (FY) 2013 from FY 2010 levels. Agencies have since developed plans for achieving these cuts, and the President's FY 2013 Budget identifies $8 billion in reduced costs as a result of Executive Order 13589.

To achieve these savings, many agencies have identified and implemented creative and innovative practices to reduce costs and improve efficiencies in such areas as travel, conference expenditures, real estate, and fleet management. There are also other practical steps agencies can take to improve operations, increase efficiency, and cut unnecessary spending. Accordingly, this memorandum describes a series of policies and practices related to activities and expenses in these areas, building on measures already in place at various agencies.

Section 1 – Travel

Travel is often necessary for Federal employees to discharge their duties effectively and the travel industry plays an important role in creating jobs and supporting local economies; however, as good stewards of Federal funds, agencies must do all they can to manage their travel budgets efficiently. Accordingly, in FY 2013, each agency shall spend at least 30 percent less on travel

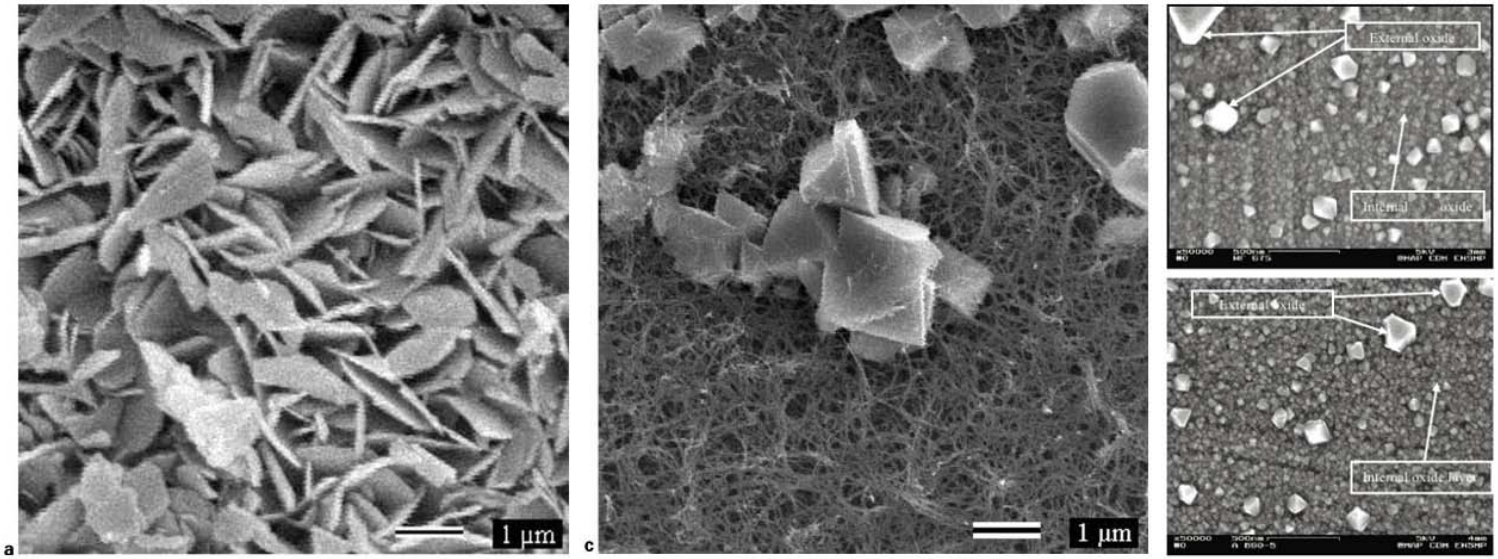
1

Statement of Essential Need

Impact of Denial

MAMBA-BDM Framework Fractal Material Models

- **Validate**: CRUD is a statistically self-similar fractalline porous solid
- Source term of CRUD is soluble/particulate matter from steam generator corrosion

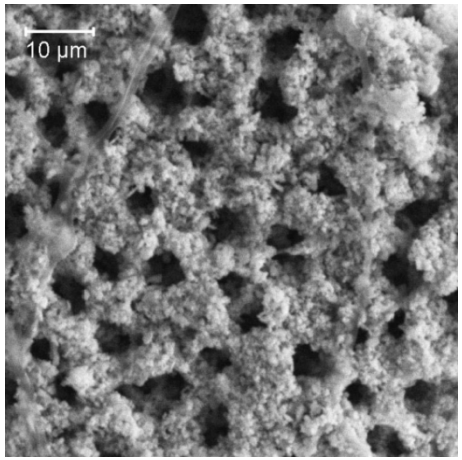


Oxides on the surface of alloy 600 after exposure to simulated PWR water

[1] P. Combrade et al. Oxidation of Ni base alloys in PWR water: Oxide layers and associated damage to the base metal. 12th Int. Conf. on Env. Degradation of Mater. in Nuc. Power Sys. TMS, 2005.
[2] C. F. C. Neves et al. Energy Materials, 3(2):126–131, 2008.

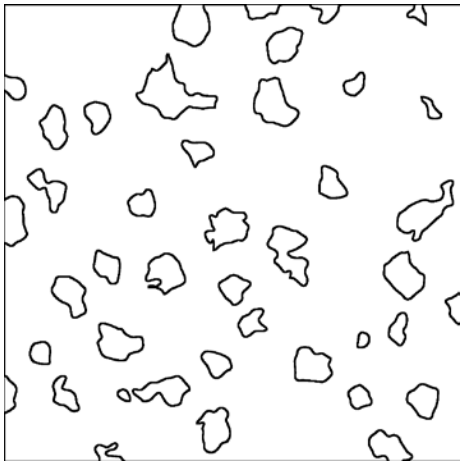
Modelling Real CRUD Scrapes

Acquire Microstructure

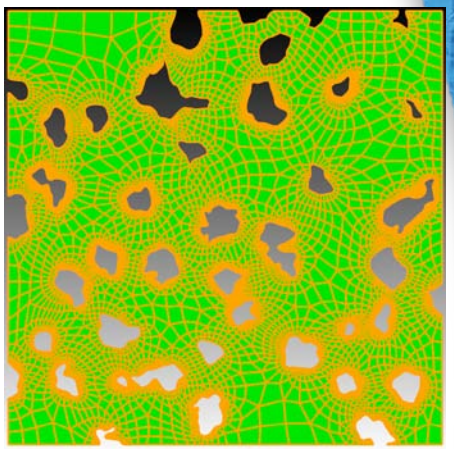


J. Deshon. "PWR Axial Offset Anomaly (AOA) Guidelines, Revision 1." EPRI Technical Report #1008102, p. 51 (2004).

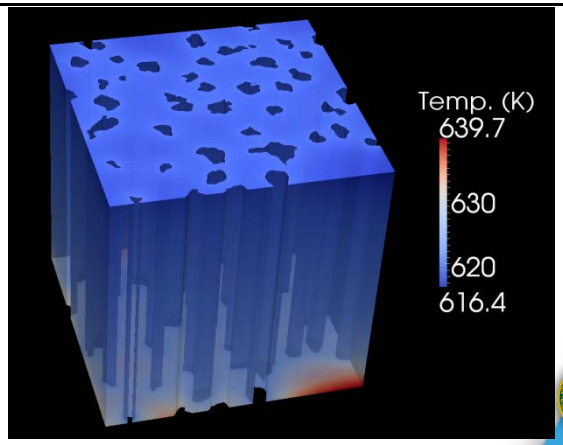
Extract Boundaries



Create CRUD Mesh

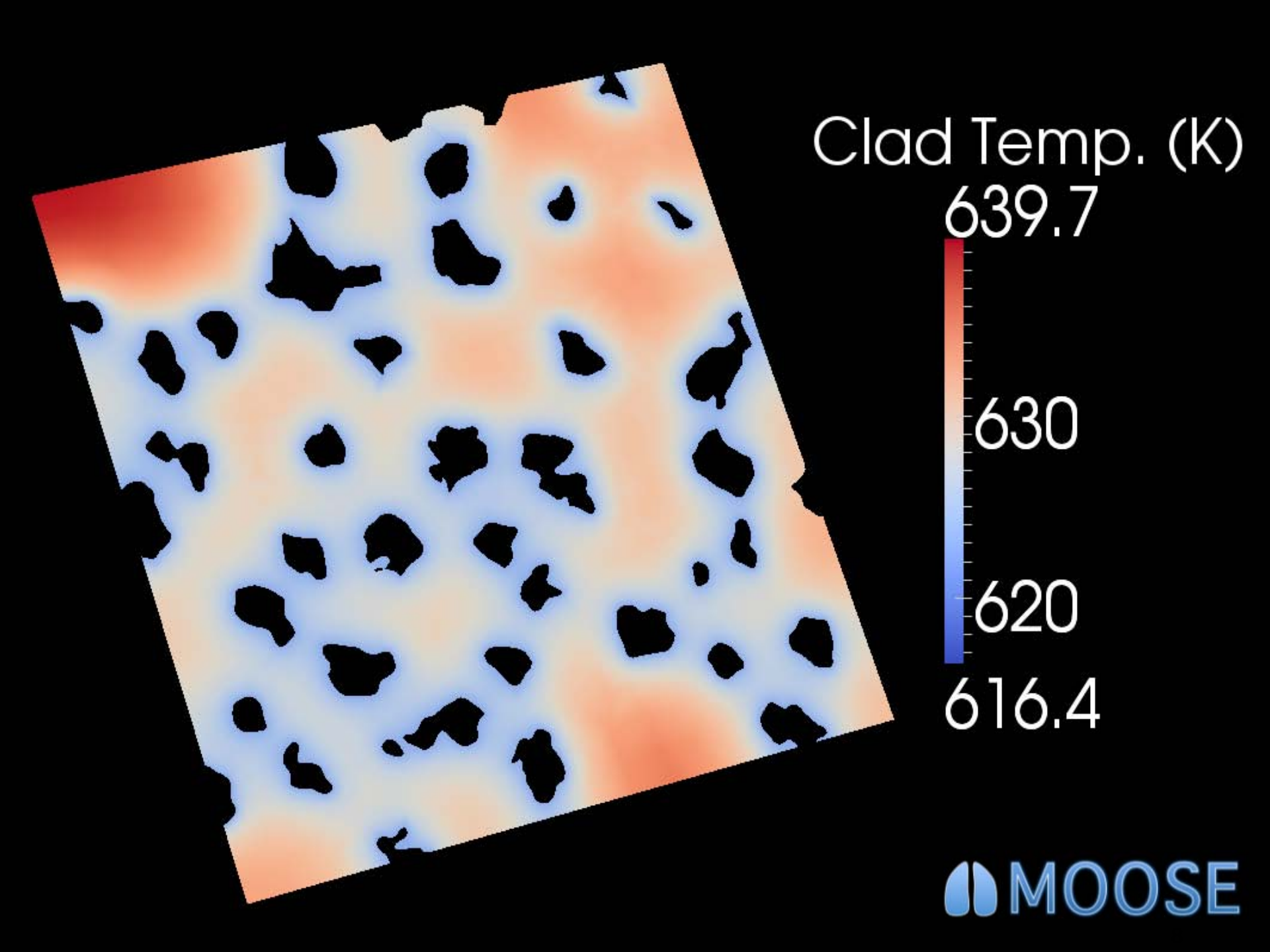


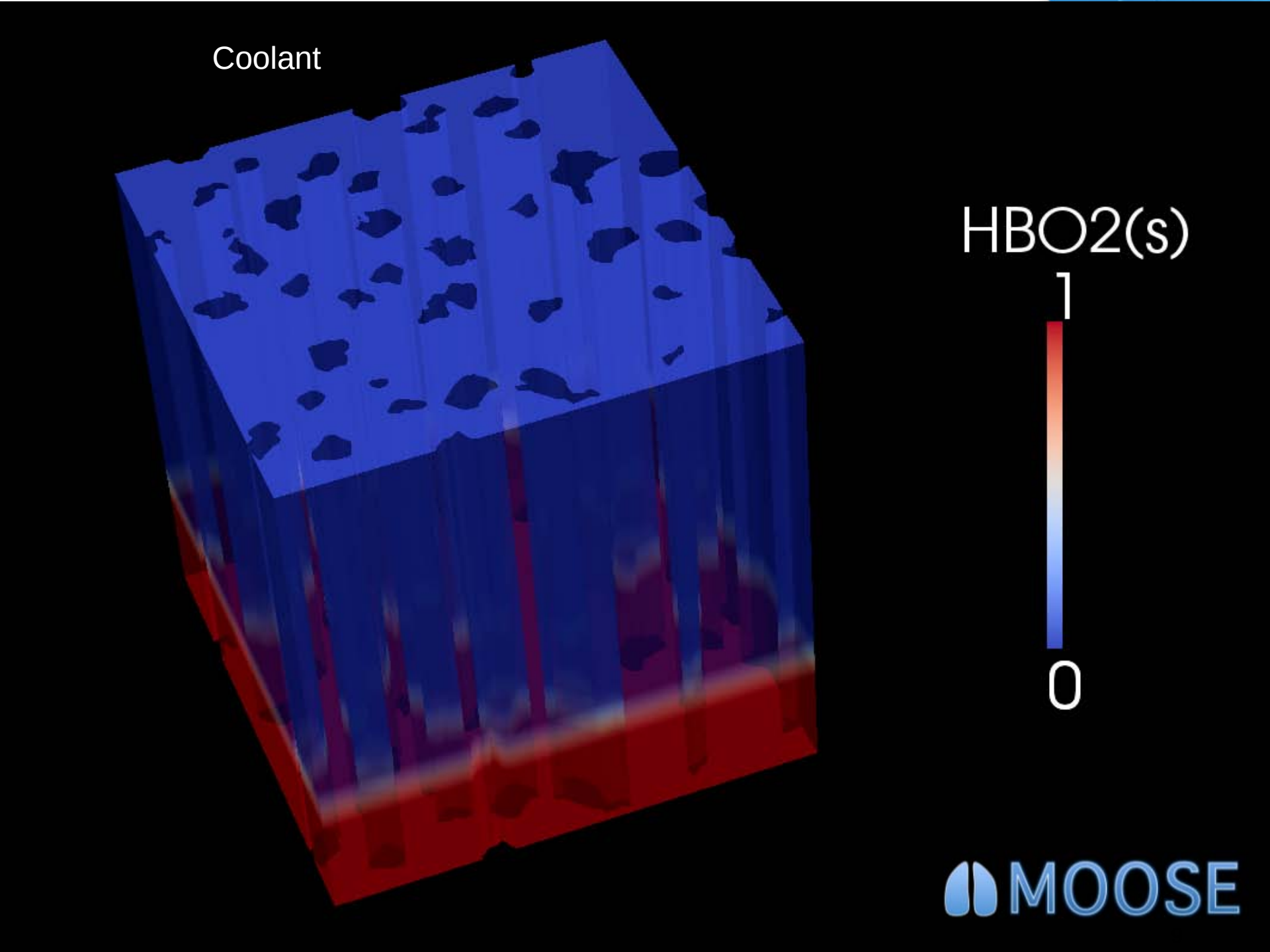
Simulate Real Microstructure



MOOSE

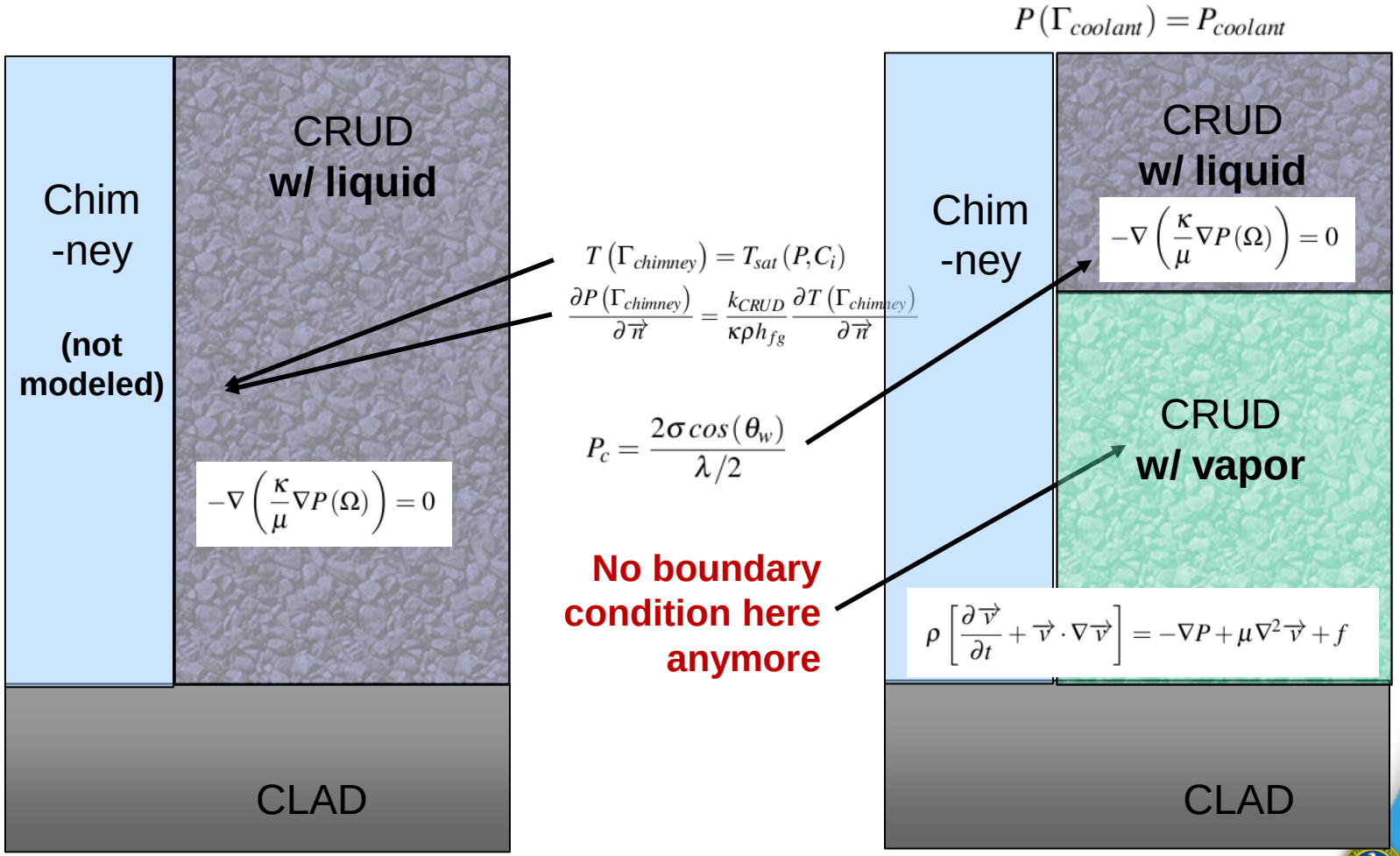
Develop Separate Physical Model


Clad Temp. (K)
639.7
630
620
616.4
MOOSE


Coolant
HBO2(s)
1
0
MOOSE

New Directions – Two Phase Flow

- P-H momentum balance with capillary forces
  - Acquired FALCON geothermal code from INL

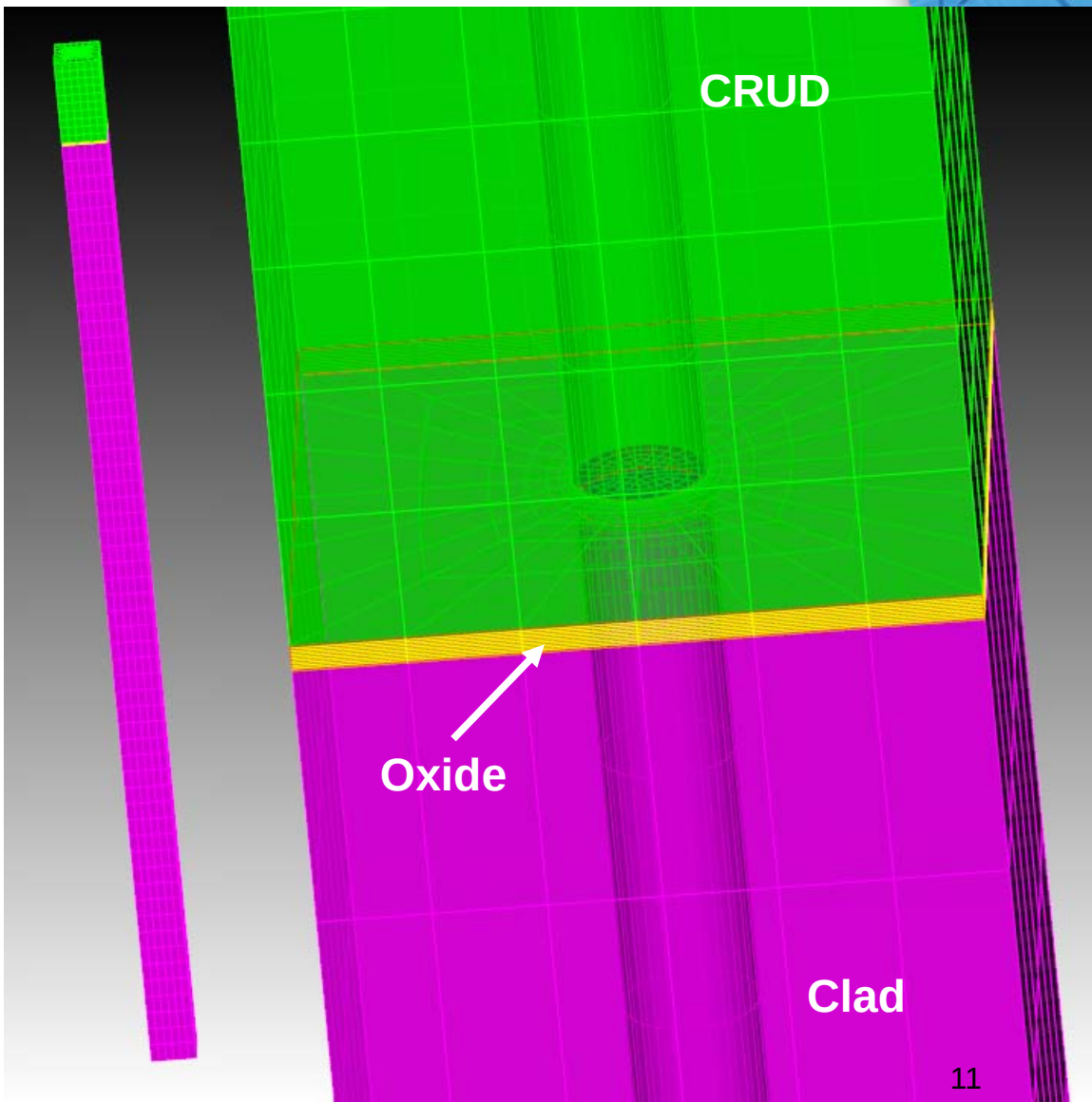


Old Model

New Model

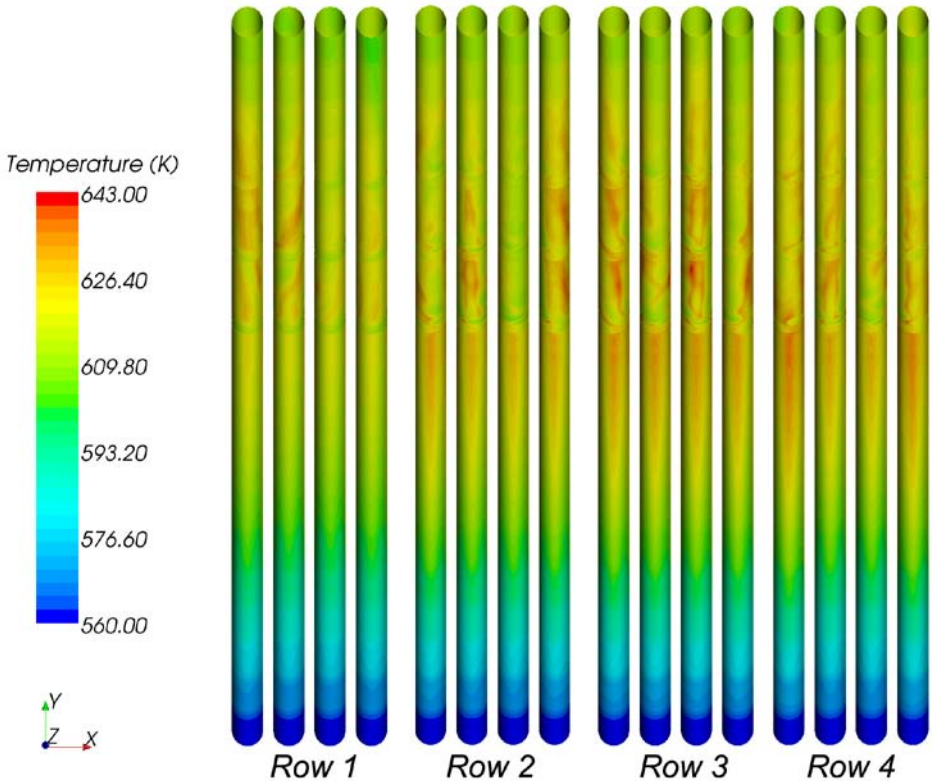
New Directions – Oxide/Clad Scope

- Oxide phase stability & transport
  - MPO models – **Yildiz et al.**
- Oxide growth & oxygen transport
  - MPO models – **Thornton, Aagesen**
- Heat transfer through oxide & cladding

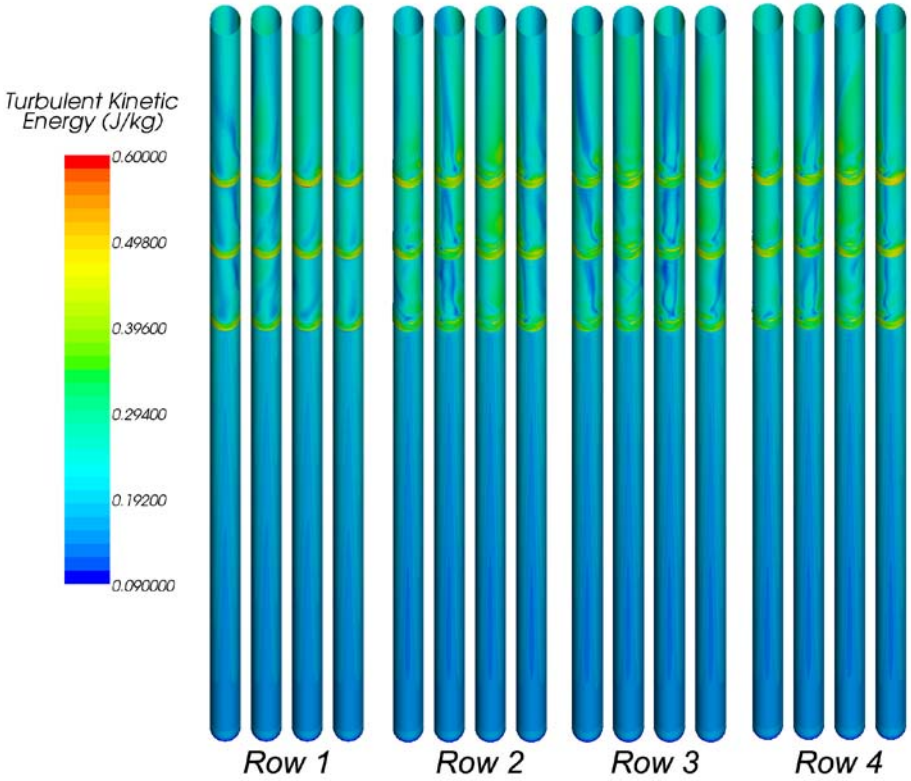


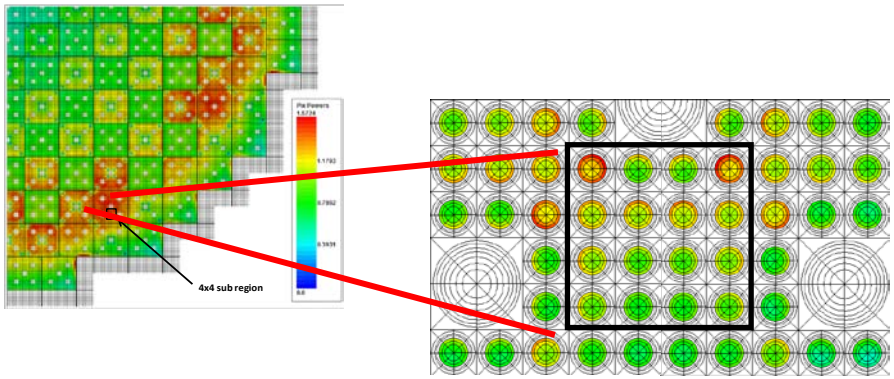
CFD Results – 4x4 subassembly

Cladding Temperature



TKE

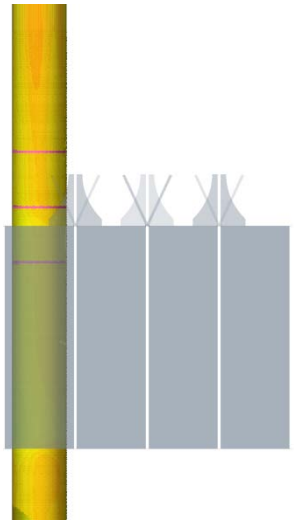


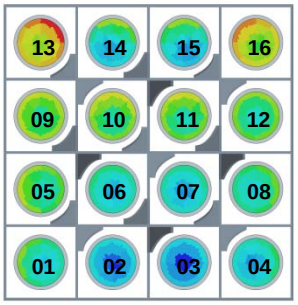


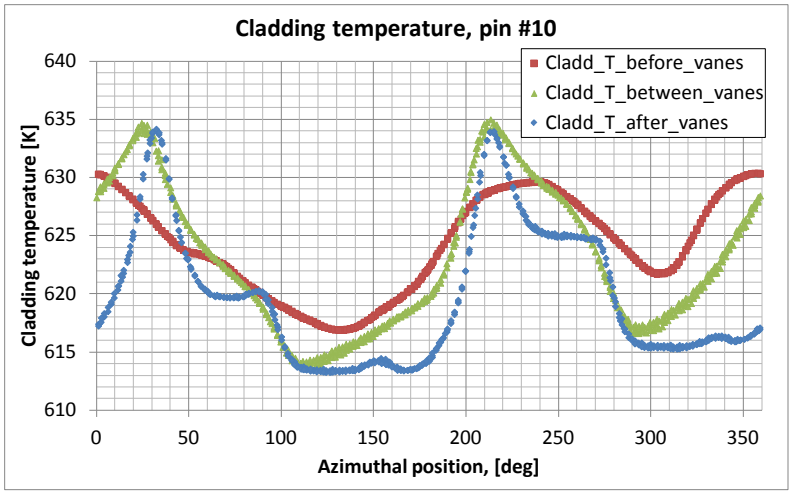
Parameters passed to MAMBA (1-way coupling):

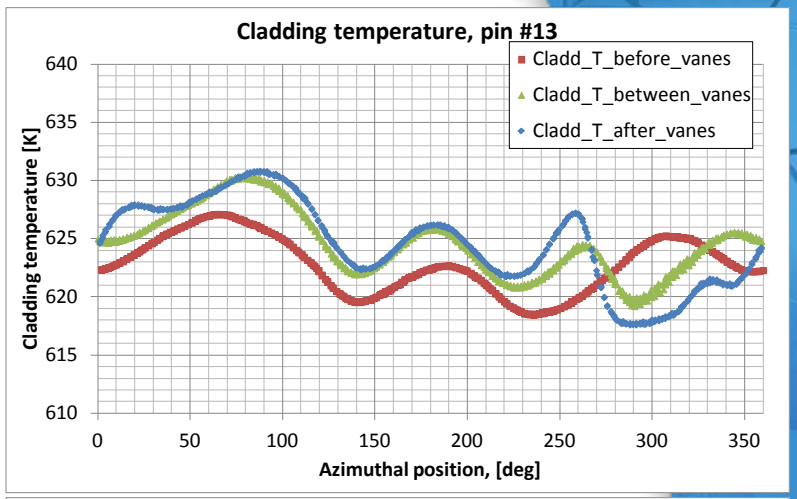
- Cladding Temperature (for crud deposition)
- TKE (for crud erosion)

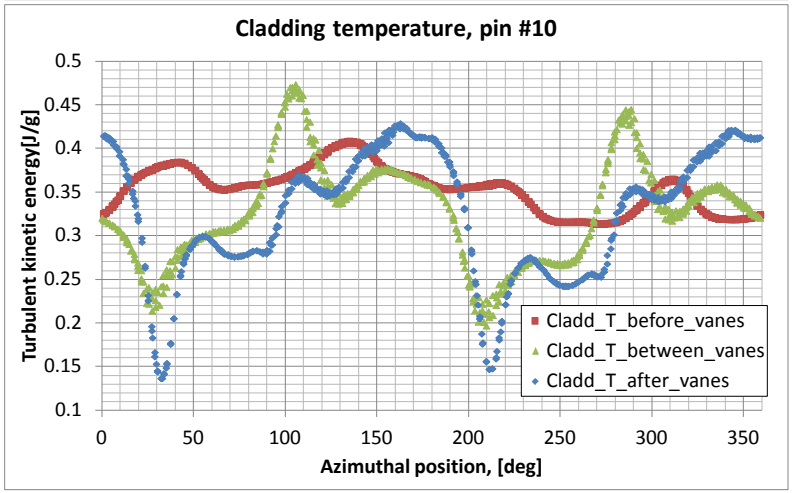
CFD Results – 4x4 subassembly

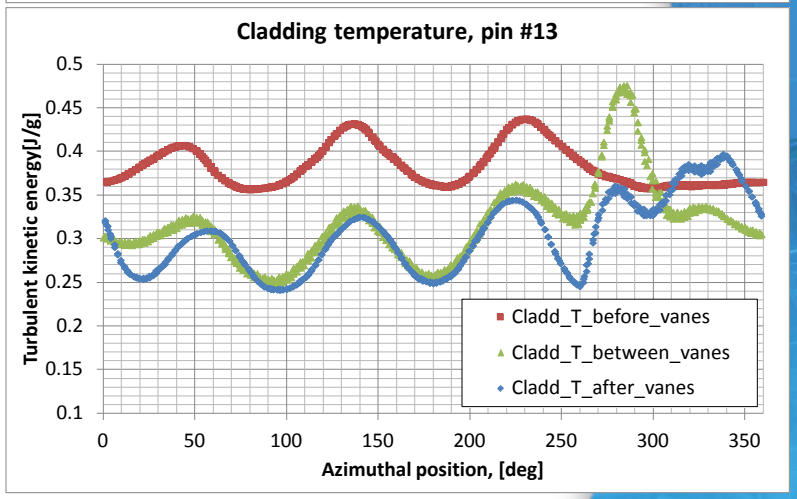






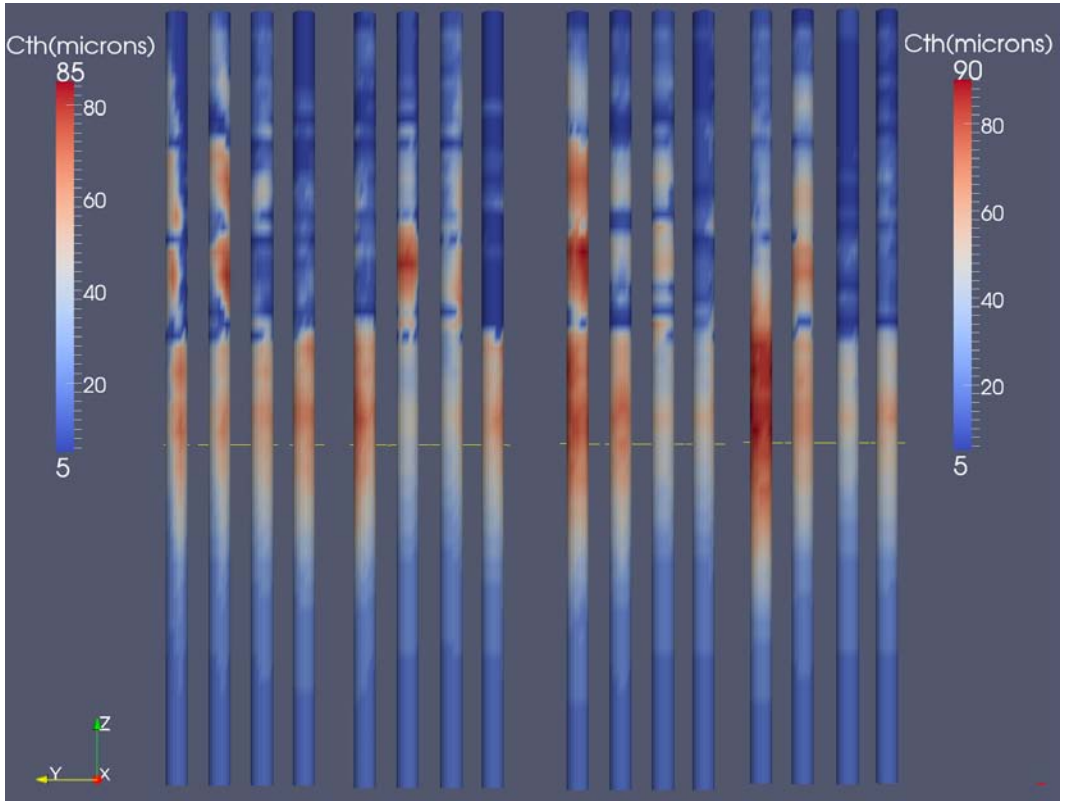




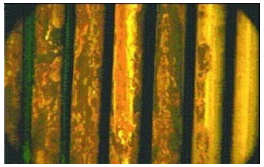


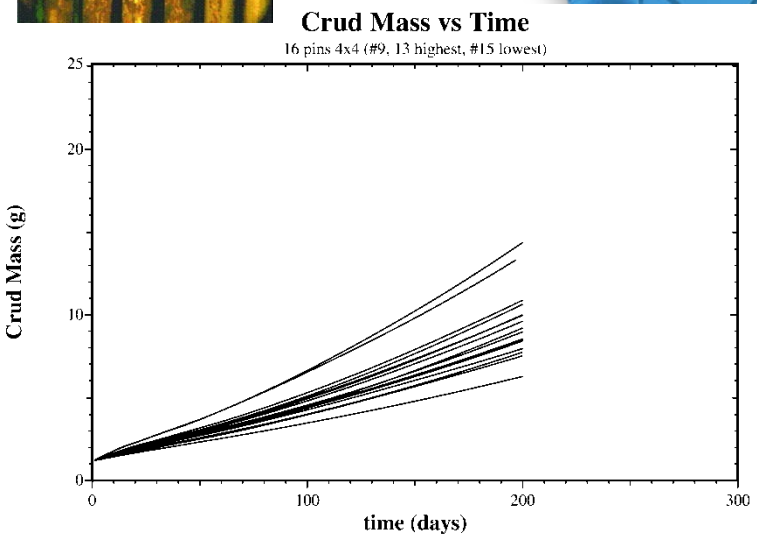
- Phase shift in cladding Temperature distribution along elevation (swirl)
- Maximum TKE (max crud erosion) at points with lowest T (lowest crud deposits)
- Hottest “hot spot” does not necessarily occur on pin with highest power (local effects)

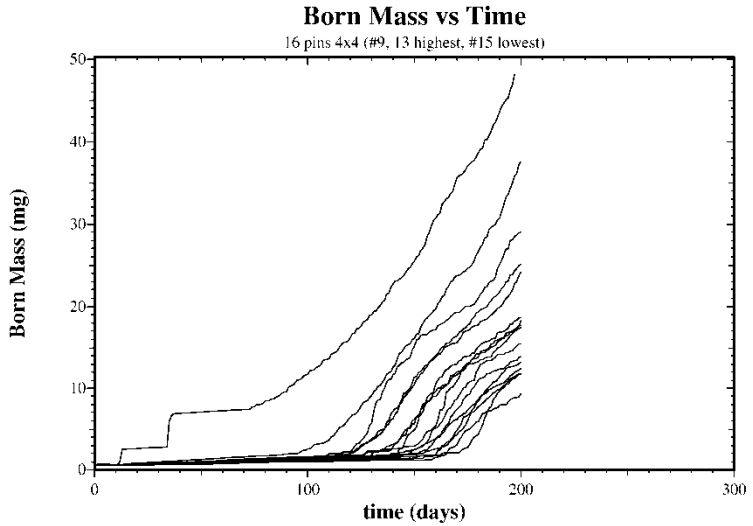
MAMBA results – with erosion rate

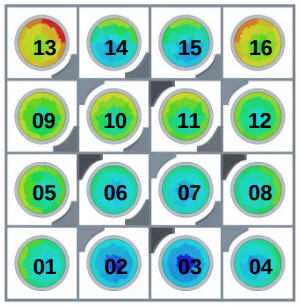


Row 1 Row 2 Row 3 Row 4









Lowest crud deposition does not necessarily occur on the pin with lowest power

VERA Core Simulator: VERA-CS

CASL Roundtable Meeting
June 11, 2012

Scott Palmtag
AMA/VRI

VERA-CS Description

- Code system used to model steady-state LWR conditions and depletion
- Direct inclusion of physics packages for: neutron transport, cross sections, thermal-hydraulics, fuel temperature, and depletion
- Linkage to other physics packages for: CFD, fuel performance, CRUD models, structural models, systems codes, etc.
- Provides reactor conditions and distributions needed to Solve Challenge Problems

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U.S. DEPARTMENT OF ENERGY Nuclear Energy

Examples of 3D Distributions Needed for Challenge Problems

General

- Instantaneous Power
- Instantaneous T/H
- Instantaneous Fuel Temperature
- Isotopic Distributions

GTRF

- Fluence in structural materials

CRUD

- Subcooled Boiling
- CRUD accumulation / dissolution

PCI

- Maximum Pin Powers
- Change in Pin Power
- “Conditioned” Pin Power
- Clad Stress
- Residual Gap

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Components of VERA-CS

1. Input processor with common geometry for all codes
2. T/H Solver (COBRA-TF)
3. Cross Sections (XSPROC, ESSM)
4. Neutronic Solver (DENOVO, MPACT)
5. Infrastructure (control rod movement, detectors, boron search, etc.)
6. Fuel Performance (temperatures, gap) (COBRA, PEREGRINE)
7. Depletion (including Xe/Sm) (ORIGEN)
8. Output processor to calculate pin powers, peaking factors, margins, etc.

More than Neutronics!

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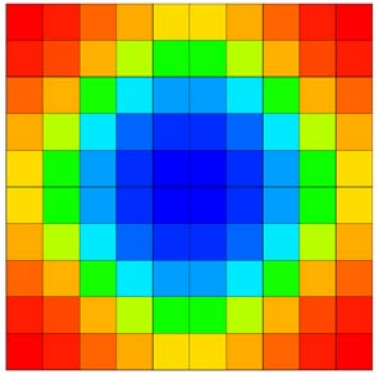
Parallel Development Paths in POR-5 (1) DENOVO/XSPROC/COBRA-TF

Develop full-core SN transport + cross sections + T/H on large computer clusters



Goals:

- Gain experience with LIME coupling
- Scale codes up to large problems
- Implement full-core modeling details
- Determine run-times on Jaguar – How big of a problem, and with what detail, can we realistically run?

Known Issues:

- Cross section accuracy (pin-cell models)
- Accuracy issues with Cartesian grid (IFBA, Gad)
- Large computing requirements – may need homogenization

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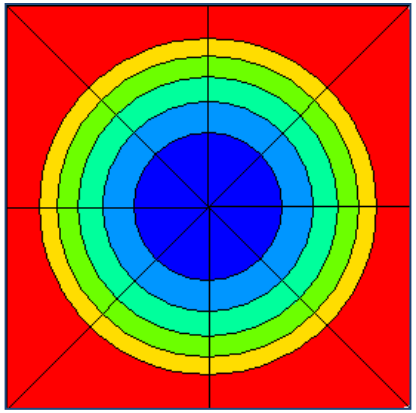
Parallel Development Paths in POR-5
(2) MPACT-MOC/ESSM/Depletion

Develop 2D full-core “slice” with MoC, ESSM cross sections, and ORIGEN depletion



Goals:

- Improved accuracy with geometrically resolved transport method (but limited to 2D)
- Improved resonance treatment in cross sections
- Implement capability to deplete core – all microscopic data will reside in MPACT “driver”

Known Issues:

- MoC currently limited to 2D
- ESSM has not been sufficiently tested

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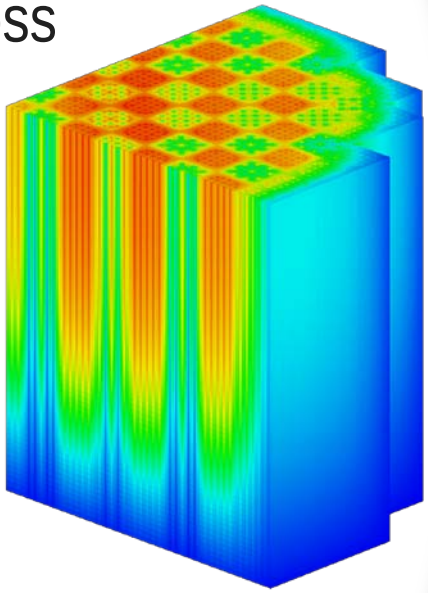
Methods Integration in POR-6

Bring development paths together in 2D/3D Coupling –

- MPACT generates flux-weighted macroscopic cross sections for 3D DENOVO
  - Flux weight each Cartesian grid volume
  - Multiple levels of homogenization possible
- DENOVO supplies axial leakage terms for 2D MPACT calculations
- Need to determine optimal method of parallel decomposition and passing data between codes



Alternate Method –

- Use the 2D/1D Coupling Methods of DECART

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Additional Projects

Projects that are not directly tied to VERA-CS, but will/may provide additional knowledge:

- Improve DECART stability for small axial mesh
- Improved DECART 2D/1D Methods (Larsen – Michigan)
- Coupling with DECART/STAR-CCM+ (AMA)
- Coupling with DECART/STAR-CCM+/MAMBA (MPO)
- Improved coupling with Data Transfer Kit (DTK)
- 3D MoC (RTM)

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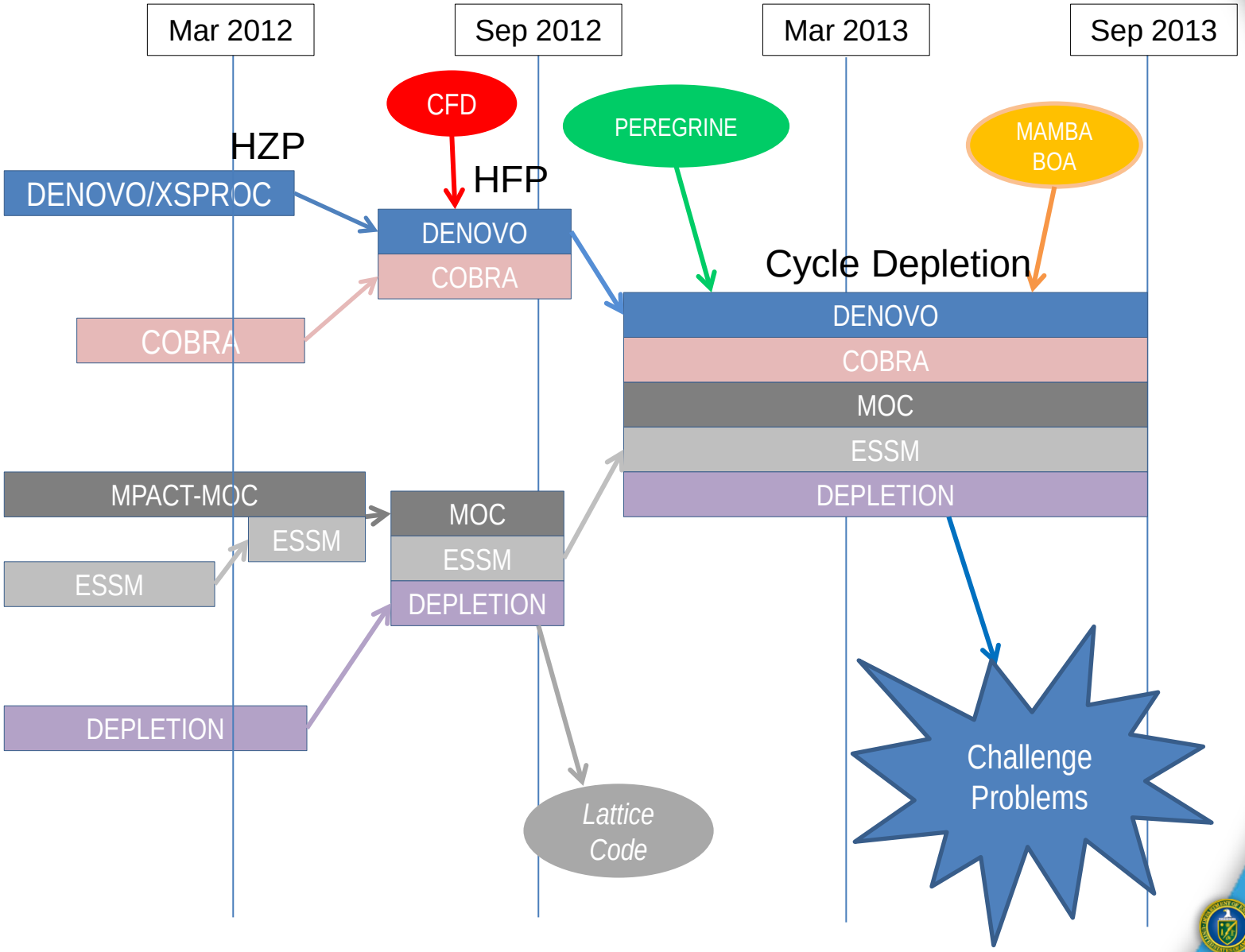
Integration Timeline



Capability Timeline

Jan 31	• #1 2D HZP Pin Cell	
Feb 29	• #2 2D HZP Lattice	
Mar 31	• #3 3D HZP Assembly	VERA 2.0
Jun 20	• #4 HZP 3x3 Assembly CRD Worth	
	• #5 Physical Reactor Zero Power Physics Tests (ZPPT)	RSICC Release 8/30/2012
	• #6 HFP BOL Assembly	
	• #7 HFP BOC Physical Reactor w/ Xenon	
	• #8 Physical Reactor Startup Flux Maps	
	• #9 Physical Reactor Depletion	
	• #10 Physical Reactor Refueling	
2013	• Start Challenge Problems!!	

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Current Status (Today)

• Input Processor	In progress
• DENOVO/XSPROC	Single-assembly (Benchmark #3) Multi-assembly + control in progress
• MPACT	Initial 2D Assembly with ESSM
• COBRA-TF	Standalone multi-assembly
• Depletion	Delayed until POR-6
• Output	Delayed until POR-6

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Risks

- We don't know how big of a problem we'll be able to run on Jaguar
  - Memory limitations – how many codes "in core" at one time?
  - Run-times – will the problems run in a reasonable time?
  - Queue limitations
  - Maximum problem size – Jaguar is not infinite

- Code Development
  - Estimating time is always hard, but even harder when you are doing new research
  - Funding does not always align with priorities.
  - We need to decide what the program goals are, what is "critical path", and fund accordingly

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Questions?

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ENERGY
Nuclear Energy

VERA Input and Analysis Capability

CASL Roundtable Meeting
June 11, 2012

Andrew Godfrey
AMA

Contents

- Why does VERA need I/O?
- What's been accomplished with Input?
- What does the simple ASCII input look like?
- What are the plans for Output?
- What types of analyses does AMA need now?

Success = (Input) Simulation (Output) + Analysis + Implementation

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VERA Input - Primary Goals

- Provide capability for reactor problem setup for SCALE/XSProc, DENOVO, COBRA, etc.
  - VERA-CS: assemblies, poisons, control rods, non-fuel structures, baffle, power, flow, depletion, etc.
- Eliminate inconsistencies between coupled physics codes through the use of a common geometry model
- Allow end users to create multi-physics models without being multi-physics experts
- Provide ability to create, archive, compare, and modify input similar to current industry workflows

Input to support full core, multi-cycle problems

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VERA Output - Primary Goals

- Produce combinatory results specific to reactor problems from non-reactor multi-physics codes
- Draw from input reactor geometry for calculation and presentation of typical reactor quantities
- Reduce large scale data down to human digestible format
  - Fine mesh results too large to process
  - Need average pin values and distribution statistics (max 3D pin power by assembly, max 2D integrated pin power by assembly, max 3D assembly power, etc)
- Provide results data for post-processing, visualization, and long term storage
- Provide an interface (GUI) for exploring problem setup and results in revolutionary ways

Output to support full core, multi-cycle problems

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VERA Input Timeline

- 10/12/2011: Small team formed to establish direction
- 11/11/2011: Recommendations made via report (CASL-I-2011-0156-000)
  1. Simple ASCII recommended for initial user input
  2. Common reactor geometry data structure
  3. Low-level, code specific interpreters
- 12/2011: Teuchos ParameterList (via XML) selected for the reactor geometry data structure. VERA-CS PL interface began development
- 1/17/2012: L3.VRI.VERA.P4.03 - DENOVO metadata implementation with python
- 2/1/2012: Development began on ASCII parser (via PERL)
- 3/30/2012: Ran VERA-CS full assembly with PL/XML input (VERA 2.0)
- 6/11/2012: ASCII Parser and VERA-CS PL nearly complete for full core BOC cycle 1 problem (i.e. no depletion or refueling)

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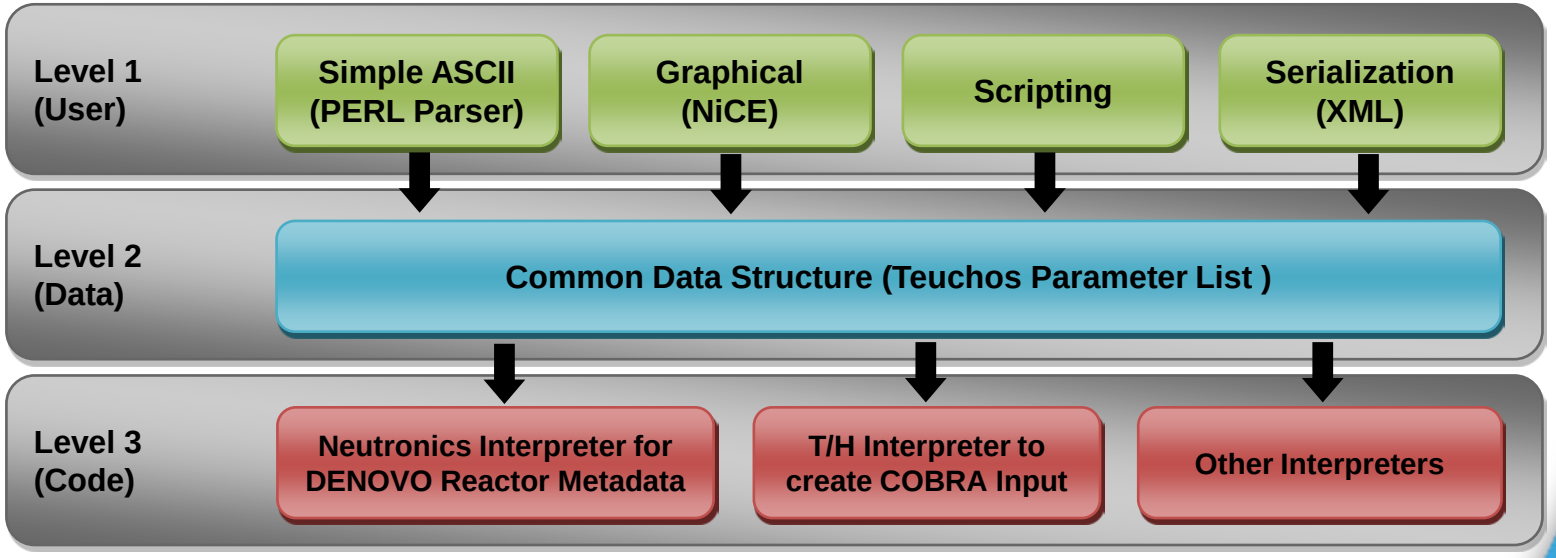
VERA Input Strategy

- **Level 1: High level user interface** – this is the level of user interaction.
- **Level 2: Middle level data storage** – a model-based common data structure for all codes in VERA. This is the priority for CASL at this time.
- **Level 3: Low level interpreters** – these are the PSS level code-specific interfaces to extract needed data from the data structure.



VERA ASCII Input

- Simple ASCII input for nuclear reactor fuel and components
- Consistent with current Industry core simulators
- Block-based schema extensible to other codes/physics
- Clean, concise, and human-readable
- Easy archival and comparisons (QA)
- Could be implemented relatively quickly

```
[ASSEMBLY]

  title "Westinghouse 17x17 Assembly"   ! assembly_title
  npin 17 1.260                         ! Assembly pins,pitch

  uo2    U21 10.257 / 2.11              ! 2.1% fuel

  cell 1   0.4096 0.418 0.475 / U21 he zirc    ! Fuel rod
  cell 2          0.561 0.602 / mod zirc       ! guide tube

  lattice REG1                          ! radial lattice
     2                                  ! arrangement
     1 1
     1 1 1
     2 1 1 2
     1 1 1 1 1
     1 1 1 1 1 2
     2 1 1 2 1 1 1
     1 1 1 1 1 1 1 1
     1 1 1 1 1 1 1 1 1

  axial A1  0.0  REG1 365.76  ! REG1 2.1%   ! Axial layout
```

```
[CORE]

  assm_map
    A1 A2 A1 A2 A1 A2 A1 A3    ! Assembly layout
    A2 A1 A2 A1 A2 A1 A3 A3
    A1 A2 A1 A2 A1 A2 A1 A3
    A2 A1 A2 A1 A2 A1 A3 A3
    A1 A2 A1 A2 A2 A2 A3
    A2 A1 A2 A1 A2 A3 A3
    A1 A3 A1 A3 A3 A3
    A3 A3 A3 A3

  insert_map
    P20 -   P20 -   P20 -   P24 P12 ! Poison layout
    -   P20 -   P24 -   P20 -   -
    P20 -   P24 -   P20 -   P24 P8
    -   P24 -   P20 -   P16 -   -
    P20 -   P20 -   P20 -   P16
    -   P20 -   P16 -   P24 -
    P24 -   P24 -   P16 -
    P12 -   P8  -

  crd_map
    4  0  1  0  4  0  3  0  ! Control banks layout
    0  0  0  0  0  6  0  0
    1  0  3  0  0  0  2  0
    0  0  0  1  0  7  0  0
    4  0  0  0  4  0  5
    0  6  0  8  0  0  0
    3  0  2  0  5  0
    0  0  0  0
```

Teuchos:ParameterList

- Simple and flexible hierarchal in-core object database
- Standard object control mechanism for all Trilinos and related software (e.g. Drekar)
- Accepts control options and other input at runtime from users and other clients
- Stores data completely in-core (i.e. does not touch the file system if desired)
- Can store any value-type and reference-type (through smart pointers) object
- Supports serialization to and from XML (OCP expandable). Current support includes int, double, float, string, as well as 1D and 2D arrays of these.
- Flexible full runtime validation of input parameter lists and high-quality user error feedback
- One point of definition of valid parameter lists, default values, documentation, and other features
- Supports various workflows dealing with user input and sending feedback
- Prototype QT-based graphical interface (Trilinos package Optika)

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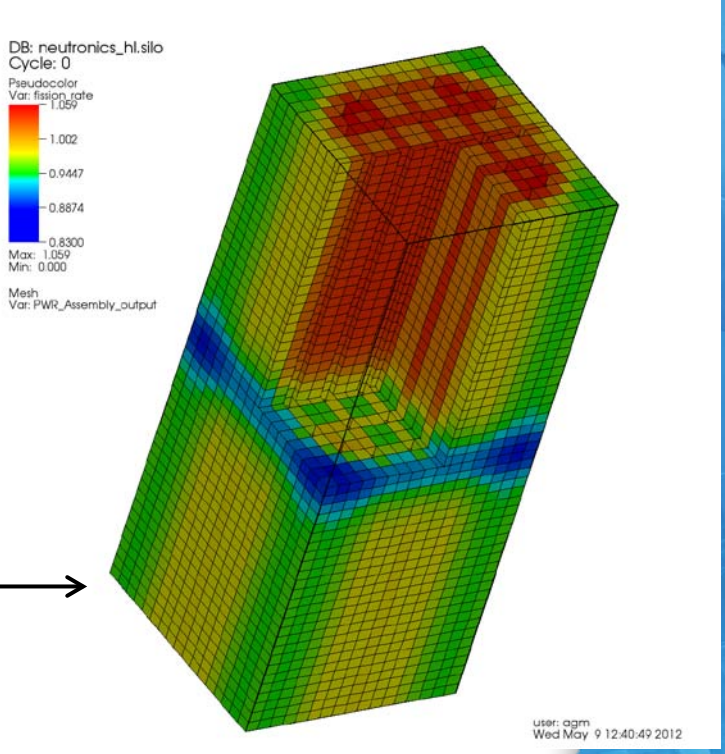
VERA Output and Analysis Status

- Currently a low priority – very little done
- Relative pin fission rate distribution calculation added to DENOVO
- No ASCII output file yet to coincide with input geometry
- Fission rate distribution written to HDF5/SILO files for visualization and post-processing
- Difficult to analyze results due to size of problems and lack of data and tools to process data

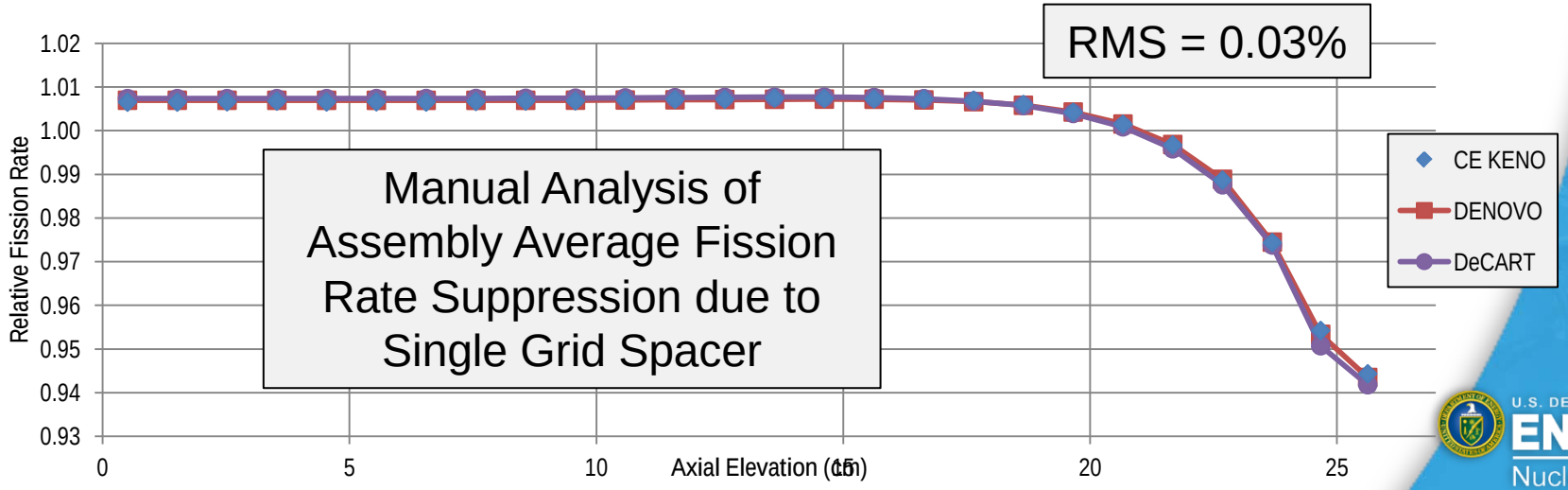


Fission rate distribution in a single grid span of a 17x17 assembly

Just now starting to put together a plan…

Current Output Plans

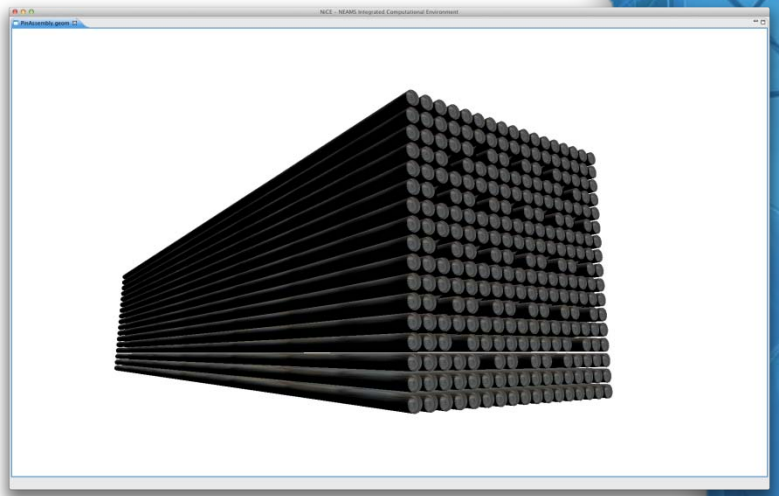
- Common ASCII output will provide for problem summary results
- Binary output (HDF5/SILO) will provide consolidated results for storage and post-processing (esp. VERA-CS)
  - Not the very large files fine mesh files.. Pin level or higher
- Short term: AMA will develop post-processors for analyses of fission rate distributions
- POR6: NiCE (leveraged from NEAMS) will provide more sophisticated visualization, analysis capability and data management

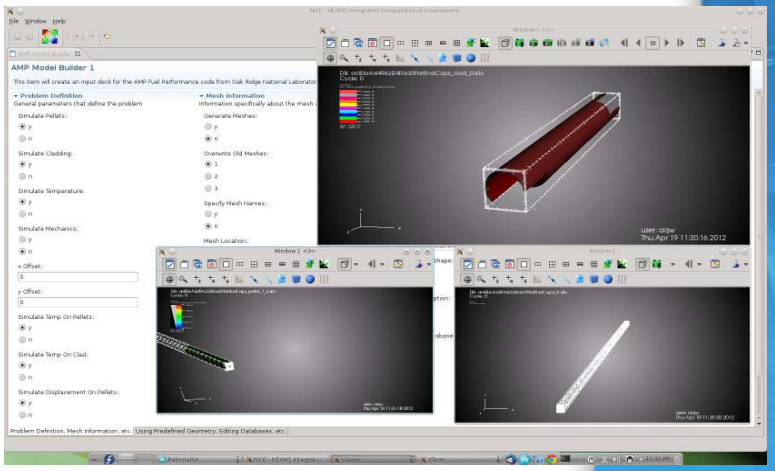


NiCE-ly Using and Collaborating with VERA

The NEAMS Integrated Computational Environment (NiCE) will help with all of those difficult chores…

- Managing inputs, geometry, materials, and meshing
- Job launch and monitoring
- Data analysis and visualization
- Data management for “Assets”
- Getting code into new software systems
- Creating applications from new software systems





The NiCE Geometry Editor (top) and VisIt embedded in NiCE analyzing AMP output (bottom)

Working with VRI and AMA in POR-6!

Short Term AMA Analysis Needs (Problem 5)

- ✗ Setup and execute quarter core reactor model at zero power
  - ASCII input (req. due to model complexity) and PL are nearly complete
- ✓ Output eigenvalue
- ✓ Output 3D relative reaction rate distributions
- ✓ Output 2D integrated reaction rate distributions
- ✗ Output assembly average 2D and 3D powers
- ✗ Output core average axial power and axial offset
- ✗ Ability to compare reaction rate distributions between codes
- ✗ Ability to calculate core critical soluble boron concentration
- ✗ Ability to move control rods and calculate control rod worths
- ✗ Ability to calculate core isothermal temperature reactivity coefficient

Long term: Need ability to create, store, and analyze fuel rod powers, T/H conditions, & fuel performance data for FULL CORE problems for dozens of statepoints per operating cycle!!

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Questions?

CASL Strategic Planning

Doug Kothe, Ronaldo Szilard, Paul Turinsky

CASL Round Table
June 12, 2012

Strategic Plan

- What?
  - A Strategic Plan determines where an organization is going, how it's going to get there, and how it'll know if it got there or not
- Why?
  - Define our purpose (mission)
    - With realistic goals and objectives consistent with that mission
    - In a time frame suitable for implementation
  - Communicate our goals and objectives
  - Develop ownership (shared fate) for our plan
    - Help to ensure that our resources are used effectively
    - By focusing these resources on the key priorities
  - Provide a baseline from which to measure our progress
    - Establish a mechanism for informed change
  - Build a consensus for our direction
    - By bringing together of everyone's best efforts

The CASL Strategic Plan serves as an initial cut at the 2nd 5-year proposal, due ~1.5 years from present

Urgency for a Strategic Plan

- CASL needs a shared vision that is consistent with and cognizant of the nuclear industry's needs and concerns moving forward
  - And our thinking has changed somewhat relative to our Jul 2010 start date
- CASL must be able to give compelling and reasonable answers to questions we are being asked
  - Are we relevant to safety?
  - What can we do to help on the "back end"?
  - Can we help with accident tolerant fuels?
  - What is our "sunset plan"?
  - What does success look like? What do we leave behind?
  - What does the tax payer get for $122M?
  - How does nuclear energy benefit?

A good strategic plan should answer these questions

Strategic Plan
Feedback Sought from our Board

- Descope & Rescope: 1st 5 years
  - A deep dive on all 10 Challenge Problems is not possible. Which ones should be descoped and/or given a relaxed schedule and which ones should have an increased emphasis and/or increased urgency?
  - Should safety (transients) and/or advanced fuels be emphasized more than planned within our current 10 challenge problem framework?
- Help define (narrow) 2nd Phase Options (2015-2020)
  - Easy choice: continue on with PWR in-vessel only. Compelling enough?
  - BWRs: increased emphasis on multi-phase, coupling, FSI, natural circulation; “simple’ extension?
  - iPWRs: same as BWRs; “simple” as well?
  - Plant System: containment structure, CFD/CMFD into RELAP7; energetic coolant/gas releases
  - Severe Accidents: aggressively evolve a RELAP-VERA-Severe Accident code; accident tolerant fuels
  - Advanced Fuels: manufacturing cause-and-effect, spent fuel behavior, advanced fuel performance
- Help us address safety centric Challenge Problems
- Define maturity concepts
- Realistic Sunset Plan
- Comment on Integration Plan

Strategic Plan
Feedback Received from our Board

- Phase 1 (1st 5 years)
  - Define metrics and success for each challenge problem within scope
- Phase 2 (2nd 5 years)
  - Choose a set of challenge problems now based on best knowledge and assessment
- View and call out currently out-of-scope problems as CASL "opportunities"
- Articulate a process in the plan for if and how opportunities are rolled into formal Phase 2 scope ("a process for prioritizing and capitalizing on these opportunities")
  - We have a year to settle on Phase 2 challenge problems so allow a process for change
- Include opportunities for DOE NE and industry as well
- Integration section is weak – focus especially on NRC. What about international?
- Be show to tout the fact that CASL is doing its job!
  - Chu calling on us; good 1st year Annual Review, milestones delivered, etc
- Carefully consider who should be the post-CASL steward of VERA
- Pare down to 20 pages – consider one document for the new Secretary and Under Secretary and another with Program Plan details (Roadmaps, etc.)
- Would like to see revised copy by Aug 1, with a detailed annotated outline in June

Strategic Plan: Current Thinking

- First Phase (what remains in FY13-FY14)
  - 3 safety CPs (DNB, Fuel-Clad/LOCA, Fuel-Clad/RIA): define scope
  - 5 operational CPs (GTRF, CIPS/CILC, PCI, FAD): define success
  - 2 lifetime extension CPs (vessel, internals): leverage capabilities
  - Advanced fuel concepts: benchmark/leverage M&S capabilities and assess concepts
  - Operational Reactor: aggressively evolve VERA-CS to support
  - Define and commit to specific Test Stand and Pilot Projects
  - VERA: !(code acquisition); physics enhancement, coupling, robustness, performance; 2-3 formal releases (2 external); support model; environment for prototype R&D
- Second Phase (FY15-FY19)
  - CPs: some carryover from first phase, some new (less than 10?)
    - Ex - BWRs: channel bow, CRUD, duty-induced fuel failure, hydriding, stability, dryout, high void modeling, debris fretting, vessels/internals integrity, RIA
    - Outside of vessel? SG tube vibration, SG corrosion
  - Continue advanced fuel concept support
  - More Test Stands and Pilot Projects; increased emphasis on V&V, licensing support?
  - VERA: environment already exists; “just” evolution and possibly some new integration

Ground the overall plan in budget realities. Do a better job in resource loading the work

Strategic Plan Timeline

- Nov 16, 2011
  - Kickoff strategic planning meeting
- Mar 31, 2012
  - Draft delivered to DOE
- May 1, 2012
  - Refined version delivered to CASL Board
- Jul 1, 2012
  - Board-modified version ready for graphic arts and technical editing
- Aug 1, 2012
  - First version for public consumption delivered to DOE as part of 2nd year Annual Review
- Mar 31, 2013
  - Next major revision

Target 2nd 5-year proposal being due end of Q2 FY14

Definitions

- Mission
  - Purpose: reason for existence
- Vision
  - Where we want to go; how we will operate in the future; how customers will benefit from our products and services
- Values
  - Overall priorities in how we will operate
- Goals
  - Overall accomplishments we should achieve (“what”)
- Strategies
  - Overall methods to achieve the accomplishments (“how”)
- Objectives
  - Still a goal, but on a smaller scale
  - Implementing a strategy typically involves implementing a set of tactics along the way – what we’re calling a “roadmap”

CASL 10 year Strategic Plan
Contents

1. INTRODUCTION

2. STRATEGIC PHILOSOPHY
   - 2.1 Mission
   - 2.2 Vision
   - 2.3 Values

3. GOALS
   - 3.1 Address Design, Operational and Safety Challenges for LWRs
   - 3.2 Develop and Effectively Apply Modern Virtual Reactor Technology
   - 3.3 Engage the Nuclear Energy Community through Modeling and Simulation
   - 3.4 Deploy New Partnership and Collaboration Paradigms

CASL 10 year Strategic Plan
Contents (continued)

4. STRATEGY
- 4.1 Challenge Problems
  - 4.1.1 First Phase: PWR Core Phenomena
  - 4.1.2 Second Phase
- 4.2 Virtual Environment for Reactor Applications (VERA)
- 4.3 Enabling R&D
  - 4.3.1 Radiation Transport
  - 4.3.2 Thermal Hydraulics
  - 4.3.3 Materials Science and Fuel Performance
  - 4.3.4 Validation and Uncertainty Quantification
- 4.4 Technology Delivery
  - 4.4.1 Release and Support of VERA
  - 4.4.2 Test Stands
  - 4.4.3 Pilot Projects
- 4.5 Education and Training
- 4.6 Collaboration and Ideation

5. OPPORTUNITIES
- 5.1 Other LWRs: Gen III+ PWRs, Gen II & III+ BWRs, iPWRs
- 5.2 Severe Accident Analyses
- 5.3 Current and Advanced Nuclear Fuel over Entire Fuel Cycle

CASL 10 year Strategic Plan
Contents (continued)

6. INTEGRATION
   - 6.1 Department of Energy
     - 6.1.1 DOE Office of Nuclear Energy
     - 6.1.2 DOE Office of Science
     - 6.1.3 DOE National Nuclear Security Administration
   - 6.2 Nuclear Regulatory Commission
   - 6.3 Research Community
   - 6.4 Nuclear Industry

7. SUSTAINED SUCCESS
   - 7.1 Community Support of CASL M&S Technology
   - 7.2 Community Progression of CASL M&S Technology

APPENDIX A. CASL Management Structure
APPENDIX B. CASL Performance Measures
APPENDIX C. CASL Status
APPENDIX D. Modeling and Simulation Benefits and Challenges for LWRs

Strategic Philosophy

- Mission
  - *Provide coupled, high-fidelity, usable capabilities needed to address light water reactor operational and safety performance-defining phenomena*
- Vision
  - *Predict, with confidence, the performance of nuclear reactors through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics*
- Values
  - *Safety and Security*
  - *Agility and Innovation*
  - *Delivering Results*
  - *Excellence with Integrity*
  - *Customer Focus*
  - Staff Development

Our Strategic Philosophy is in pretty good shape

Challenge Problems Must Directly Support Key Nuclear Industry Drivers

Industry Driver	Industry Driver Performance Measures	Supporting CASL Challenge Problems	Success Metrics for Tangible CASL Support
Power Uprates	• Augment planned U.S. reactor fleet power uprates beyond current value of 2694 MW_e thru 2016 [19] • Increase proportion of stretch (>2%) and extended (>7%) power uprates in U.S reactor fleet	• CRUD, PCI, FAD, GTRF • Cladding Integrity (DNB, LOCA, RIA) • Reactor Integrity (vessel, internals) • Advanced Fuels	• Reduce or eliminate restrictions to uprates associated with current challenge problem • Contribute capability to support one or more license uprate applications
Lifetime Extension	• License remaining ~30% of U.S. reactor fleet to 60 years where appropriate before 2015 • Safely extend lifetimes of U.S. reactor fleet to 80 years where appropriate before 2020	• Reactor Integrity (vessel, internals) • Advanced Fuels	• Provide reliable estimates of reactor environment experienced over lifetime • Contribute capability to support one or more lifetime extension applications
Higher Fuel Burnup	• Increase maximum fuel assembly burnup of 55 GWd/MTU in U.S. reactor fleet • Increase allowable peak fuel rod burnup of 62 GWd/MTU in U.S. reactor fleet	• CRUD, PCI, FAD, DNB, GTRF • Cladding Integrity (LOCA, RIA) • Advanced Fuels	• Provide capability to support increase average fuel cycle length • Provide capability to support increase NRC fuel burnup limits • Facilitate advanced fuel design
Improved Safety	• Maintain coolable fuel geometry and minimize fuel hydrogen production during/after LOCA • Minimize fuel damage and fission gas release during accidents • Maintain fission product barriers during anticipated accidents	• CRUD, PCI, FAD, DNB, GTRF • Cladding Integrity (LOCA, RIA) • Reactor Integrity (vessel, internals) • Advanced Fuels	• Facilitate advanced fuel design • Improved understanding and quantification of margins

CASL Strategic Objectives for M&S Solutions to Nuclear Industry Challenge Problems

Challenge Problem	Predictive M&S Capability Maturity: 2015	Predictive M&S Capability Maturity: 2020
CRUD	• Reduce uncertainty in predictions of CRUD thickness and boron uptake • Inform PWR core CRUD risk assessment to support margin management decisions • Expose CRUD vulnerability and guide mitigation	• Inform CRUD-resistant fuel designs • Deliver reliable CRUD risk assessments • Guide coolant chemistry program and steam generator tube material selection decisions
GTRF/FAD	• Quantify fuel assembly spacer grid material and geometry relationship to fuel system performance • Provide insight into whole core fuel assembly dynamic response during LOCA/seismic event to assess fuel structural integrity and coolability • Provide insight into fuel assembly design change and fuel management decisions to mitigate GTRF / FAD	• Contribute to GTRF- and FAD-resistant designs • Replace current industry analysis standards
PCI	• Inform margins imposed under a power maneuver • Inform fuel pellet-clad geometry and materials ties to performance	• Contribute to revised fuel cladding material standards • Guide fuel pellet-cladding geometry design decisions • Develop relationship between lab tests and in-core PCI performance
DNB	• Improve DNB prediction for PWRs based on targeted validation experiments and advanced CFD results • Complete initial DNB analysis capability	• Improve and validate DNB predictive capability for safety analysis that supports fuel designs, operating space, and trip setpoints • Quantify uncertainties in key DNB analyses
Cladding Integrity (LOCA, RIA)	• LOCA: Complete initial assessment of fuel of performance • RIA: Assess relationship of reactivity insertion to fuel pellet-cladding response and fuel rod failure mechanicsm	• LOCA: Provide guidance or consultation on regulatory standards for fuel performance • RIA: Quantify relationship between reactivity insertion and fuel pellet-cladding response and improve predictive method for margin quantification in safety analysis
Reactor Vessel & Internals Integrity	• Estimate neutron fluences, thermal fatigue and mechanical performance experienced after 60 years	• Estimate neutron fluences, thermal fatigue and mechanical performance experienced up to 80 years
Advanced Fuels	• Provide actionable and defensible recommendations for down-select of candidate advanced fuel concepts	• Support reliable prediction of in-reactor performance for leading advanced fuel concept

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Sustained Success

The "sunset plan": what do we leave behind

- Community Support of CASL M&S Technology
  - Continued availability and limited support of stable (static) or beta (exploratory) versions of VERA through RSICC distribution at ORNL in accordance with practices established during active CASL execution
  - Periodic availability and full support of evolving, stable, industry-hardened, and user-friendly versions of VERA through distribution by a CASL core partner or a 3rd party entity.
- Community Progression of CASL M&S Technology
  - The CASL strategic vision sees VERA becoming the *nuclear enterprise community model* for nuclear reactor and power plant M&S technology

Supplemental Material

www.casl.gov

2nd Phase Options

Other LWRs: Within the context of analyzing the reactor vessel and contained components

- Generation III+ PWR designs;
  - Enhance first phase capabilities
- Generation II and III+ BWR designs; and
  - Two-phase flow thermal-hydraulics (including natural circulation), internals fluid-structure interactions, NSSS stability, channel box material performance, and tighter multi-physics coupling
- SMRs utilizing iPWR designs
  - Fluid dynamics under natural circulation, vibrational aspects of structural mechanics and associated mechanical fatigue, pump performance, and tighter multi-physics coupling

2nd Phase Options (cont.)

- Plant Systems
  - Replacement of component models within RELAP7 with advanced thermal-hydraulic M&S (3D CFD and eventually CMFD)
  - Development of multi-fluid and multi-phase thermal-hydraulic M&S in support of the analysis of containment behavior during energetic coolant and combustible gas releases
- Severe Accident Analysis
  - Form partnership with developers of RELAP and severe accident code to develop coupled RELAP-VERA-Advanced Severe Accident Code
- Current and Advanced Nuclear Fuel over Entire Fuel Lifetime (manufacturing through storage)
  - Manufacturing process effect on determining fresh fuel characteristics
  - Behavior of zirconium alloy-clad UO_2 spent nuclear fuel under normal and abnormal conditions while in wet and dry storage
  - Performance of selected advanced fuel system designs during all postulated operating conditions

Reactor Applications Roadmap (2010-2020)

CASL
Consortium for Advanced Simulation of LWRs

2010
PWR Current Methods and Initial Models

- ✓ Describe current tools
- ✓ Develop CASL plans
- ✓ Initial coupling of current tools
- ✓ Develop initial vessel CFD models and run

2011
PWR Model Development

- ✓ Build CAD & CFD Models
- ✓ Couple existing tools
- ✓ Develop 3x3 pin multiphysics models
- ✓ Develop initial material models

2012
PWR High Fidelity Capability

- ✓ Run high fidelity coupled existing tools
- ✓ Run vessel CFD & zoom in for challenge problems
- ✓ Perform initial UQ
- ✓ Identify data for validation

2013
PWR Coupled Physics

- ✓ Couple material multiphysics models
- ✓ Develop link to system code
- ✓ Run high fidelity coupled tools with multiphysics models

2014
PWR Validation

- ✓ Run tools for challenge problems
- ✓ Validate tools to data
- ✓ Perform final UQ
- ✓ Document
- ✓ Perform PCMM

2015
PWR Challenge Problem Analysis Capability

- ✓ Compare advanced tools to existing tools
- ✓ Tools for risk assessment, high burnup, uprates, margins
- ✓ Develop M&S plans for iPWR and BWRs

2016
iPWR and BWR Model Development

- ✓ Build CAD & CFD Models
- ✓ Develop material models
- ✓ Link to system code
- ✓ Implement two-phase models
- ✓ Identify validation data

2017
iPWR and BWR High Fidelity Capability and Coupled Physics

- ✓ Couple material multiphysics models
- ✓ Run high fidelity coupled multiphysics tools
- ✓ Perform initial UQ

2018
iPWR and BWR Validation

- ✓ Run tools for challenge problems
- ✓ Validate tools to data
- ✓ Perform final UQ
- ✓ Document
- ✓ Perform PCMM

2019
iPWR and BWR Challenge Problem Analysis Capability

- ✓ Compared advanced tools to existing tools
- ✓ Implement tools for risk assessment, high burnup, uprates and understanding margins

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

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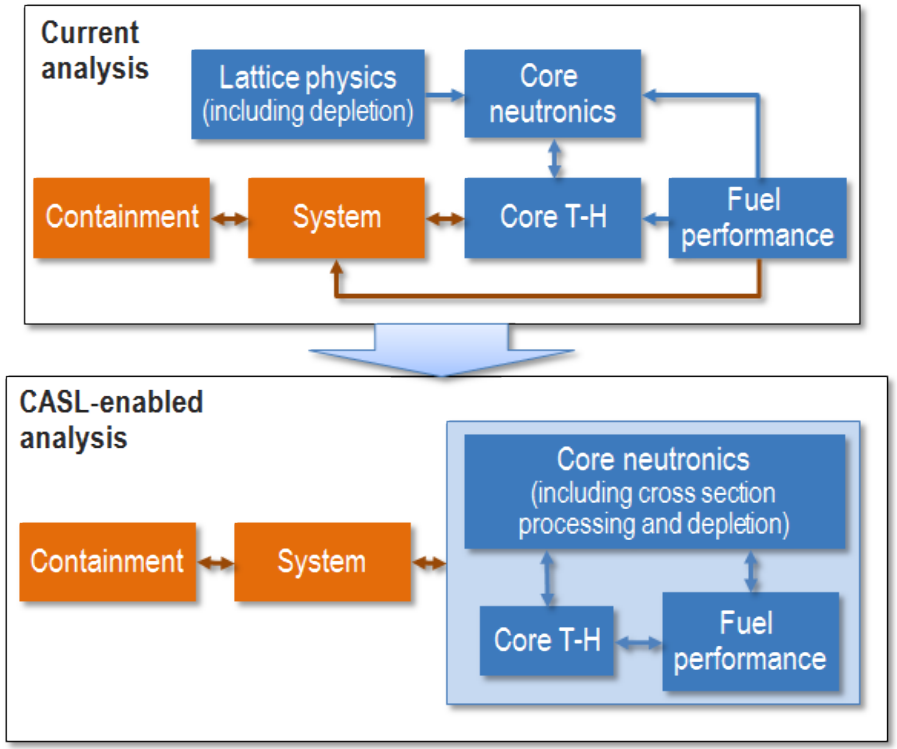
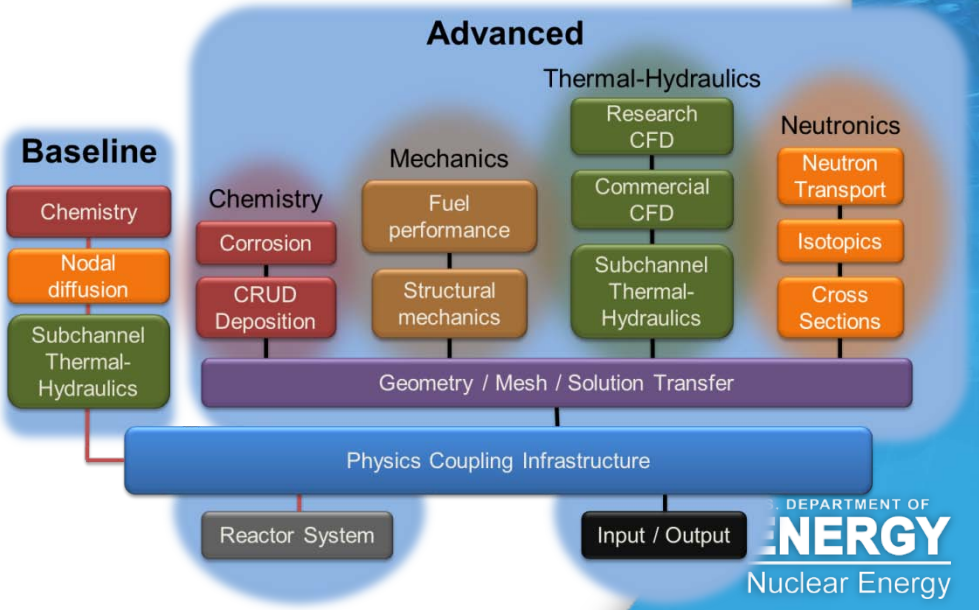
Virtual Environment for Reactor Analysis (VERA)

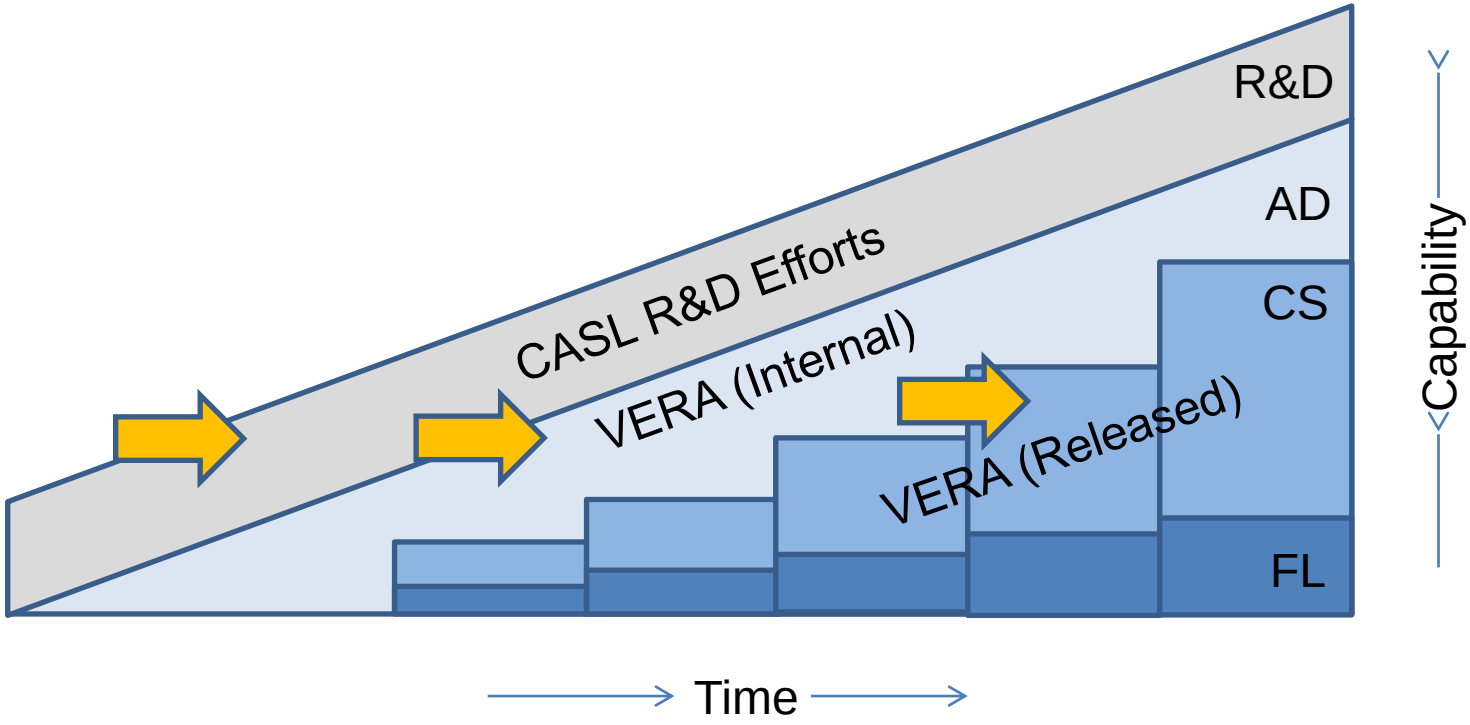


VERA capabilities have 3 levels of maturity:

1. Prototype
2. Functional
3. Robust



VERA Evolution Strategy



- What are the specific activities that need to be performed at “gate crossings”?
- What are the criteria for passage, e.g. V&V, Maturity Level?
- What documents are produced, e.g. code theory & users manuals, V&V report?

VERA Core Simulator Roadmap (2010-2020)

2010
Requirements Development

- ✓ Why, what, how, how well

2012
Verification and Benchmarking

- ✓ Validation with hot zero power and hot full power
- ✓ Develop advanced methods

2014
Application to Real-World PWR Operational Problems

- ✓ Challenge Problem applications

2016
Transient and Two-Phase Extensions for BWR and PWRs

- ✓ Develop transient and two-phase capabilities
- ✓ V&V for iPWRs and BWRs

2018
Advanced iPWR and BWR Applications

- ✓ V&V of transient applications

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

2011
Testing and Integration of Basic Components

- ✓ Power
- ✓ Thermal hydraulics

2013
Application to Typical Reactor Operating Cycles

- ✓ Advanced methods integration
- ✓ Integrate CFD and fuel performance models

2015
Deployment to PWR Industry

- ✓ Implement BWR and iPWR geometry models

2017
Safety Transient Applications

- ✓ Integration with system codes

2019
Application Support

Enabling R&D –
Computational Fluid Dynamics Roadmap (2010-2020)

2010
Assess Existing Capabilities

Develop Path Forward

2012
Prototype Multiphase Capability

Initial Multi-Physics Coupling

- ✓ Integration into VERA
- ✓ Intrusive UQ assessment
- ✓ LES & RANS turbulence models

2014
Robust Multiphase Capability

- ✓ Initial DNB capability
- ✓ Improved subcooled boiling

2016
Prototype Transient Capability

- ✓ Refined DNB
- ✓ Mature UQ approach for transients

2018
Robust Transient Capability

- ✓ Improved LOCA
- ✓ DNB best practices

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

2011
Single Phase Baseline

- ✓ Transient or steady state
- ✓ HPC ready
- ✓ 3D unstructured mesh

2013
Functional Multiphase Capability

- ✓ Bubbly flow model
- ✓ Subcooled boiling
- ✓ Transient or steady state

2015
Multi-Physics Transient Coupling

- ✓ Experimental development for DNB and LOCA modeling

2017
Functional Transient Capability

- ✓ Initial LOCA results
- ✓ Validated DNB

2019
Mature Transient Capability

- ✓ LOCA best practices

Enabling R&D –
Radiation Transport Methods Roadmap (2010-2020)

2010	2012	2014	2016	2018
Assess Existing Capabilities Develop Path Forward	Functional Homogeneous Pin Cell Transport Prototype Pin-Resolved Transport	Functional 3D Pin-Resolved Transport Prototype Monte Carlo Transport	Functional Hybrid Monte Carlo Transport	Robust General 3D Pin-Resolved Transport Robust Hybrid Monte Carlo Transport

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

2011	2013	2015	2017	2019
Prototype Homogeneous Pin Cell Transport	Robust Homogeneous Pin Cell Transport Functional Pin-Resolved Transport	Robust 3D Pin-Resolved Transport	Functional, General 3D Pin-Resolved Transport	Updates to Robust Capabilities

Enabling R&D –
Materials Science and Fuel Performance Roadmap

2010
Assess Existing Capabilities and Develop Framework for Advanced, 3-D Fuel Performance Models

- ✓ Initiate multiscale materials models of clad behavior

2012
Initiate Model Verification & Benchmarking activities

- ✓ Continue implementing fuel behavior phenomena
- ✓ Compare results to legacy codes and available test data

2014
Functional 3D Fuel Performance Predictions of in-core behavior

- ✓ Compare predictions to in-reactor performance
- ✓ Evaluate safety margins

2016
Model Burnup Limits & Assembly Distortion

- ✓ Refined models of hydrogen/corrosion enable high burnup assessment
- ✓ Benchmark predictions of transient behavior

2018
Validated BWR models assess fuel assembly distortion

- ✓ Validated models inform best practices to avoid FAD

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

2011
Initial Demonstration of 3D code capability

- ✓ Missing pellet surface simulation of pellet clad interaction
- ✓ Framework for thermal-chemical modeling of CRUD

2013
Refine strategy for physics coupling

- ✓ Improve coupling of fuel performance to neutronics and computational fluid dynamics
- ✓ Detailed uncertainty quantification of key variables

2015
Mature 3D Fuel Performance Capability

- ✓ Validated models inform assessment of fuel safety margin for PCI
- ✓ Validated CRUD models inform best operational practices

2017
BWR fuel performance models

- ✓ Validated models inform best practices to limit GTRF
- ✓ Benchmarking BWR fuel performance against experimental data

2019
Assess fuel utilization

- ✓ Expanded fuel performance modeling capabilities assess burnup limits & safety margins for fuel performance

Enabling R&D –
Advanced Fuels Roadmap (2010-2020)

2010
Assess Existing Capabilities
- ✓ Identify opportunities to improve predictive modeling

2012
Analysis of advanced fuel concepts
- ✓ Engage fuel development community
- ✓ Identify phenomena that control accident behavior

2014
Functional predictions of advanced fuel behavior
- ✓ Predict fuel degradation phenomena
- ✓ Recommended methodology for down-selection

2016
Model Advanced Fuel Performance
- ✓ Assess behavior of lead test assembly
- ✓ Assess accident behavior of advanced fuel concepts

2018
Predict advanced fuel behavior during transients
- ✓ Assess performance limits & accident performance of advanced fuels

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

2011
Demonstration of 3D fuel performance capability
- ✓ Verified steady-state modeling capability pre-requisite to advanced fuel/accident evaluation

2013
Initiate transient modeling capability
- ✓ Implement behavioral models for high power/temperature conditions
- ✓ Incorporate material data for advanced fuels

2015
Evaluate most promising advanced fuel concepts
- ✓ Recommended down select of advanced fuel concepts
- ✓ Initiate multiscale modeling to fill data needs

2017
Improved Fuel Models
- ✓ Refine materials phenomena models based on improved insight
- ✓ Assess operating safety margins of advanced fuels

2019
High Fidelity Assessment of Advanced Fuels
- ✓ Assess burnup limits & safety margins for advanced fuel performance

Enabling R&D –
Sensitivity, Uncertainty Quantification, and Data Assimilation Roadmap (2010-2020)

2010
Assess Verification, Validation, and UQ Workflows

2012
Integral-Effects Verification, Sensitivity, UQ, Data Assimilation
- ✓ GTRF application using Advanced VERA

2014
Extrapolation of Models for Predictions
- ✓ Selected CIPS, GTRF, and/or PCI quantities of interest

2016
Rapid Prototyping of VUQ Methodology
- ✓ New CASL challenge problems

2018
Coupled Optimization and UQ
- ✓ New fuel and/or reactor designs

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

2011
Separate-Effects UQ, Sensitivity, and Data Assimilation for T-H, Neutronics
- ✓ CIPS application using Baseline VERA

2013
Separate-Effects Sensitivity, UQ, Data Assimilation for Chemistry, Matls
- ✓ GTRF and CIPS applications

2015
Full-Scale Predictions with Dimension-Reduction Models
- ✓ CIPS, GTRF, and PCI applications

2017
Advanced Dimension-Reduction Capabilities
- ✓ Application to transients

2019
Adaptive Control of Uncertainty Budget
- ✓ Design prototyping to licensing

Technology Delivery: A Key Strategy for CASL

Proactive delivery of CASL technology to clients, customers, and users

- Release and support of VERA
  - Regular (annual) software releases of selected, ready (robust) portions of VERA to both CASL partners and the nuclear community at large
- Test Stands
  - Early deployment of VERA into an actual engineering/design environment at a core partner institution for assessment, use, and ultimate adoption of VERA in supporting real-world LWR applications
- Pilot Projects
  - Early demonstration of VERA and/or VERA simulation results to a problem of interest brought before the CASL Industry Council by a nuclear industry institution outside of the CASL consortium

Commit to early and regular delivery of our technology

- Following the CASL agile project and software management approach
- Amplifies learning through iterative development and refinement based on customer feedback and assessments

Integration –
DOE Office of Nuclear Energy (NE) R&D Programs

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Interact, coordinate, leverage

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- Light Water Reactor Sustainability (LWRS)
  - o RELAP7
  - o Material Properties
  - o Data
  - o Annual working meeting
- Nuclear Energy Advanced Modeling and Simulation (NEAMS)
  - o Fuels
  - o Systems
  - o Reactor Aware Infrastructure
- Small Modular Reactors (SMR)
  - o Industry Council participation

Other modeling and simulation activities

- Fuel Cycle R&D (FCRD)
  - o Accident Tolerant Fuel
- Advanced Reactor Concepts (ARC)
- Next Generation Nuclear Plant (NGNP)

Integration – DOE

DOE Office of Science

- Energy Frontier Research Centers (EFRC):
  - Center for Materials Science of Nuclear Fuel (INL)
  - Energy Frontier Center for Defect Physics in Structural Materials (ORNL)
  - Extreme Environment-Tolerant Materials via Atomic Scale Design of Interfaces (LANL)
  - Materials Science of Actinides (ND)
- Exascale Co-Design Centers:
  - Center for Exascale Simulation of Advanced Reactors (CESAR) (ANL)
  - Center for Materials in Extreme Environments (LANL)
  - Combustion Exascale Co-Design Center (SNL)

DOE National Nuclear Security Administration (NNSA)

- Advanced Simulation and Computing Program (ASC)
- Naval Reactors (NR)

Integration –

- Nuclear Regulatory Commission (NRC)
  - Annual meeting update with Commissioners
  - Quarterly interactions with RES
  - Share and Leverage: VUQ plans, Data, Benchmark Problems, Software Infrastructure
  - Share and evolve joint roadmaps

- Research Community
  - Dissemination of Research through publications, presentations, open source software releases, simulation results and datasets
  - Broad call for participation in CASL Round Table
  - Special issue of technical journals (e.g., JOM)
- Nuclear Industry
  - VERA Users Group
  - Test Stands
  - Industry Council
  - Workshops

CASL Challenge Problems 1st Phase

	Power uprate	High burnup	Life extension	Safety Relevance
Operational "Challenge Problems"				
CRUD-Induced Power Shift (CIPS)	×	×		CRUD influences both mechanical and reactivity behavior of the fuel, impacting operational performance and reactor safety response
CRUD-Induced Localized Corrosion (CILC)	×	×		
Grid-to-Rod Fretting Failure (GTRF)		×		Degraded fuel/clad mechanical integrity due to flow-induced vibrations during normal operations affect accident response
Pellet Clad Interaction (PCI)	×	×		PCI, a fuel failure mechanism during normal operations, can also occur during accident transients causing a local power increase
Fuel Assembly Distortion (FAD)	×	×		Distortion of fuel rods and fuel assemblies has the potential to inhibit control rod insertion, preventing timely reactor shutdown
Safety "Challenge Problems"	Full Scope-Current Focus		Full Scope-Future Focus	Partial Scope-Future Focus
Departure from Nucleate Boiling (DNB)	×			Quantify and prevent local vapor-induced clad surface overheating during certain accident scenarios
Cladding Integrity during Loss of Coolant Accidents (LOCA)	×	×		Predicting fuel response during a LOCA facilitates developing advanced fuel designs that minimize hydrogen production and maintain a coolable geometry
Cladding Integrity during Reactivity Insertion Accidents (RIA)	×	×		Predicting fuel response during an RIA-induced power excursion facilitates advanced fuel designs that minimize failures and fission product release
Reactor Vessel Integrity	×		×	Reactor vessel integrity is essential during normal operation and accident situations. Improved prediction (and models) of vessel irradiation and performance assure adequate fuel cooling
Reactor Internals Integrity	×		×	Operational condition of core internal components prior to an accident-induced transient impacts likelihood of safe shutdown

VERA Capability Roadmap (2010-2020)

2010
Requirements

- ✓ Requirements development
- ✓ Initial infrastructure development
- ✓ Software and quality process definition

2012
Initial Capability and Coupling

- ✓ Initial integration and coupling of core physics components
- ✓ Initial deployment of software infrastructure

2014
Mature PWR Capability

- ✓ Application to PWR operational issues
- ✓ Integration and coupling of advanced capabilities

2016
Transient Capability

- ✓ Initial transient and multiphase flow capability
- ✓ Integration with advanced reactor system capability

2018
Initial BWR Capability

- ✓ Refinement of capability for accident and SMR scenarios
- ✓ Initial extension to BWR analysis

2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

2011
Foundation Development

- ✓ Requirements development
- ✓ Infrastructure development
- ✓ Emphasis on core physics capabilities

2013
Coupling and Capability Development

- ✓ Additional core physics capabilities with improved coupling
- ✓ Initial deployment for educational use

2015
Deployment and Application

- ✓ Deployment to Test Stands for application to PWR challenge problems

2017
Initial Accident and SMR Capability

- ✓ Initial application to accident scenarios (DNB, RIA, LOCA)
- ✓ Initial extension to analysis of selected SMRs

2019
Deployment for BWR and SMR Application

- ✓ Deployment for application to BWR and SMR challenge problems

CASL Has 6 Principal Strategies

- Challenge Problems
  - First Phase: PWR Core Phenomena
  - Second Phase Options: Other LWRs, Plant System, Accidents, Fuel
- Virtual Environment for Reactor Applications (VERA)
- Enabling R&D
  - Radiation Transport
  - Thermal Hydraulics
  - Materials Science and Fuel Performance
  - Validation and Uncertainty Quantification
- Technology Delivery
  - Release and Support of VERA
  - Test Stands
  - Pilot Projects
- Education and Training
- Collaboration and Ideation

THM-GTRF: New Spider meshes, New Hydra-TH runs

J. Bakosi, M.A. Christon, M.M. Francois, R.B. Lowrie (LANL)

R.R. Nourgaliev (INL)

Contributors: R. Pawlowski, J. Shadid, T. Smith (SNL)

CASL Virtual Round Table Meeting, June 11-14, 2012

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THM-GTRF: New Spider meshes, New Hydra-TH runs

J. Bakosi, M.A. Christon, M.M. Francois, R.B. Lowrie (LANL)

R.R. Nourgaliev (INL)

Abstract: Progress is reported on computational capabilities for the grid-to-rod-fretting (GTRF) problem of pressurized water reactors. Numeca's Hexpress/Hybrid mesh generator is demonstrated as an excellent alternative to generating computational meshes for complex flow geometries, such as in GTRF. Mesh assessment is carried out using standard industrial computational fluid dynamics practices. Hydra-TH, a simulation code developed at LANL for reactor thermal-hydraulics, is demonstrated on hybrid meshes, containing different element types. A series of new Hydra-TH calculations has been carried out collecting turbulence statistics. Preliminary results on the newly generated meshes are discussed; full analysis will be documented in the L3 milestone, THM.CFD.P5.05, Sept. 2012.

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Overview

- Background
  - Our Dec. 2011 GTRF-milestone: *"Initial Assessment of Hydra-TH on GTRF Problems"* (THM.CFD.P4.01)
- Current work for L3 milestone THM.CFD.P5.05, Sept. 2012:
  - New hybrid meshes with Spider: 3x3, 5x5
  - New Hydra-TH runs, now collecting turbulence statistics
- Summary

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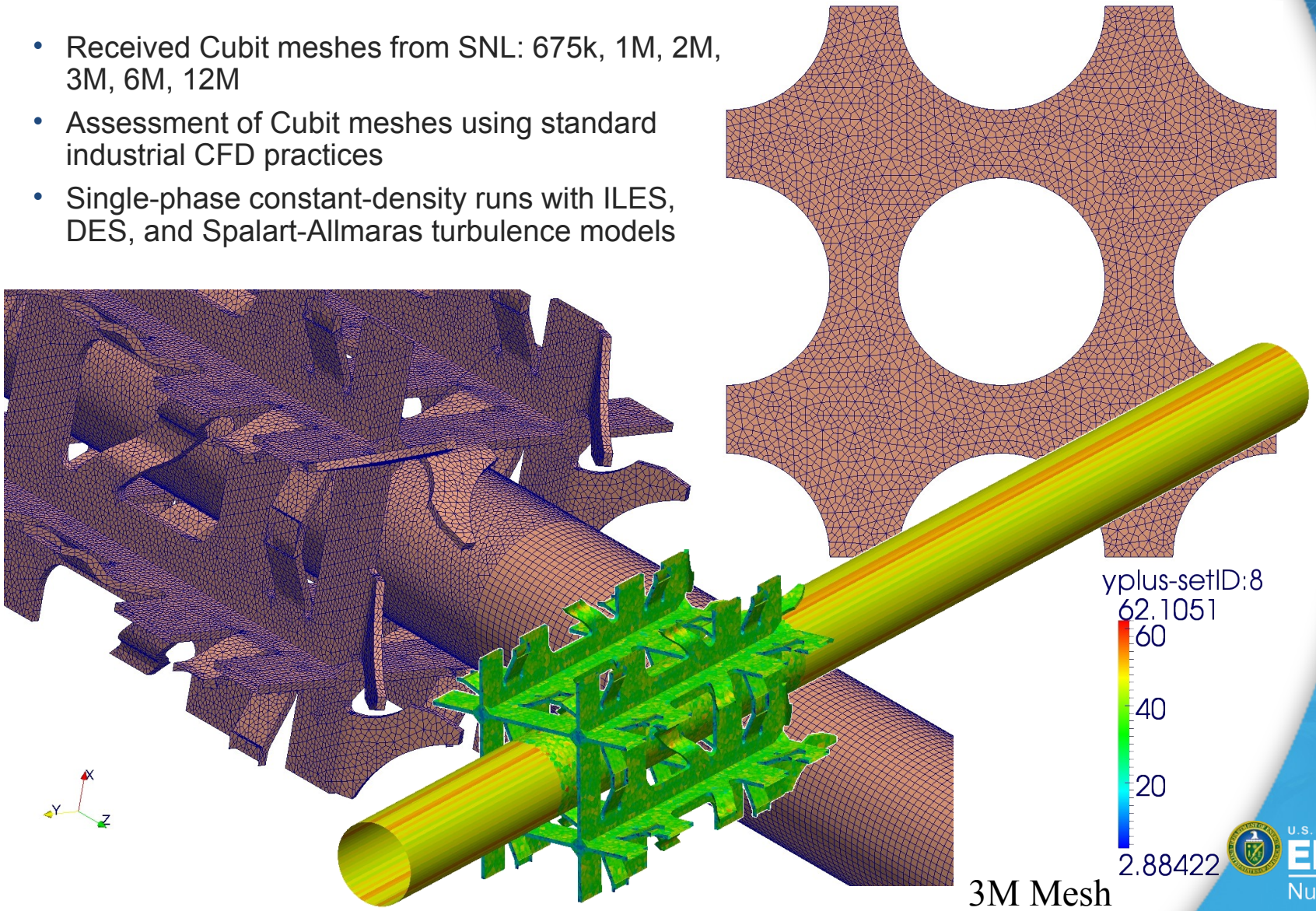
Background

Background

Snapshots from THM.CFD.P4.01 L2 milestone from Dec. 2011

- Received Cubit meshes from SNL: 675k, 1M, 2M, 3M, 6M, 12M
- Assessment of Cubit meshes using standard industrial CFD practices
- Single-phase constant-density runs with ILES, DES, and Spalart-Allmaras turbulence models

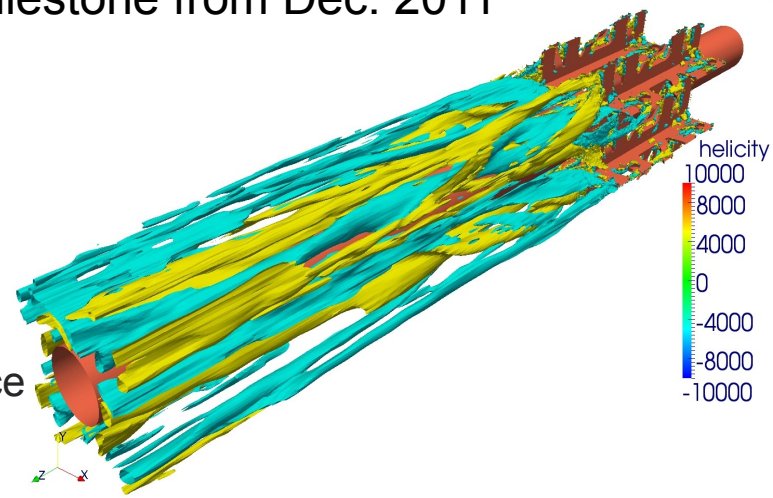


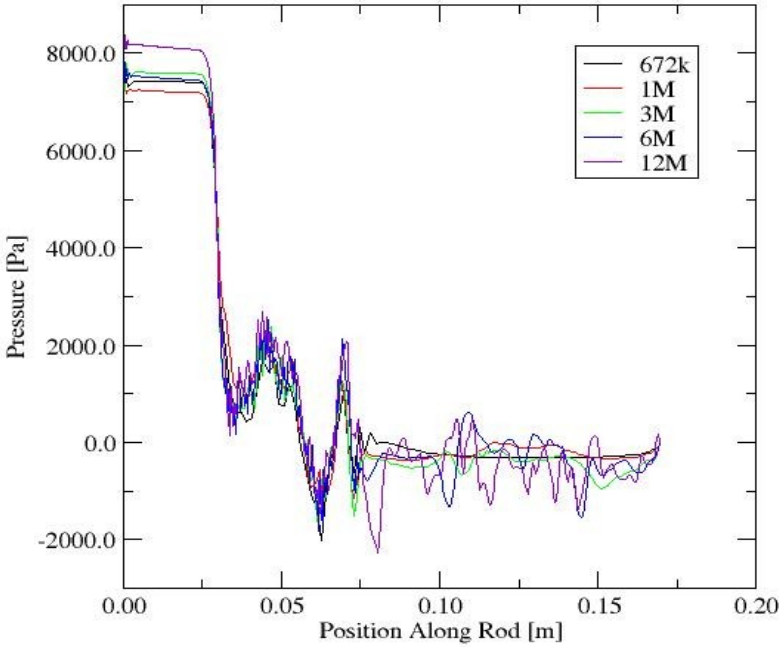
3M Mesh

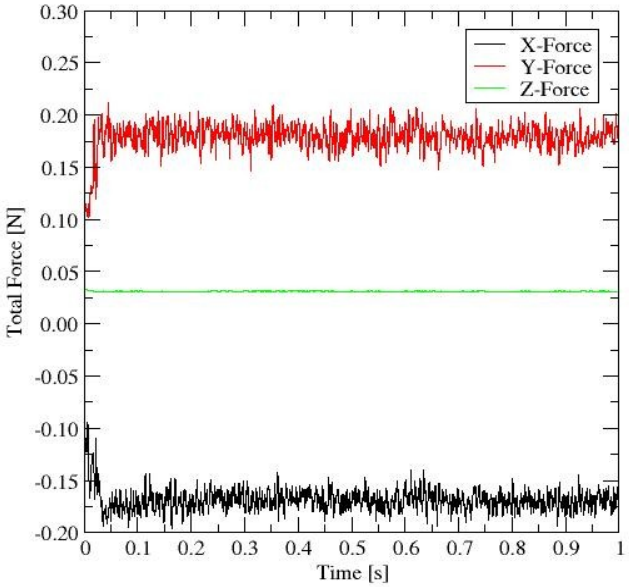
Background

Snapshots from THM.CFD.P4.01 L2 milestone from Dec. 2011

- Strong vortical structures captured
- Rod force time-histories suggest URANS may not be a good option for GTRF
- Largest Cubit mesh (at the time: 12M) suggests pressure drop not converged
- **Unresolved issues:** mesh quality, convergence, pressure drop, no turbulence statistics, which turbulence model to use, influence of periodic and outlfow BCs, domain length







New meshes for GTRF

Ongoing work toward new L3 milestone, Sept. 2012

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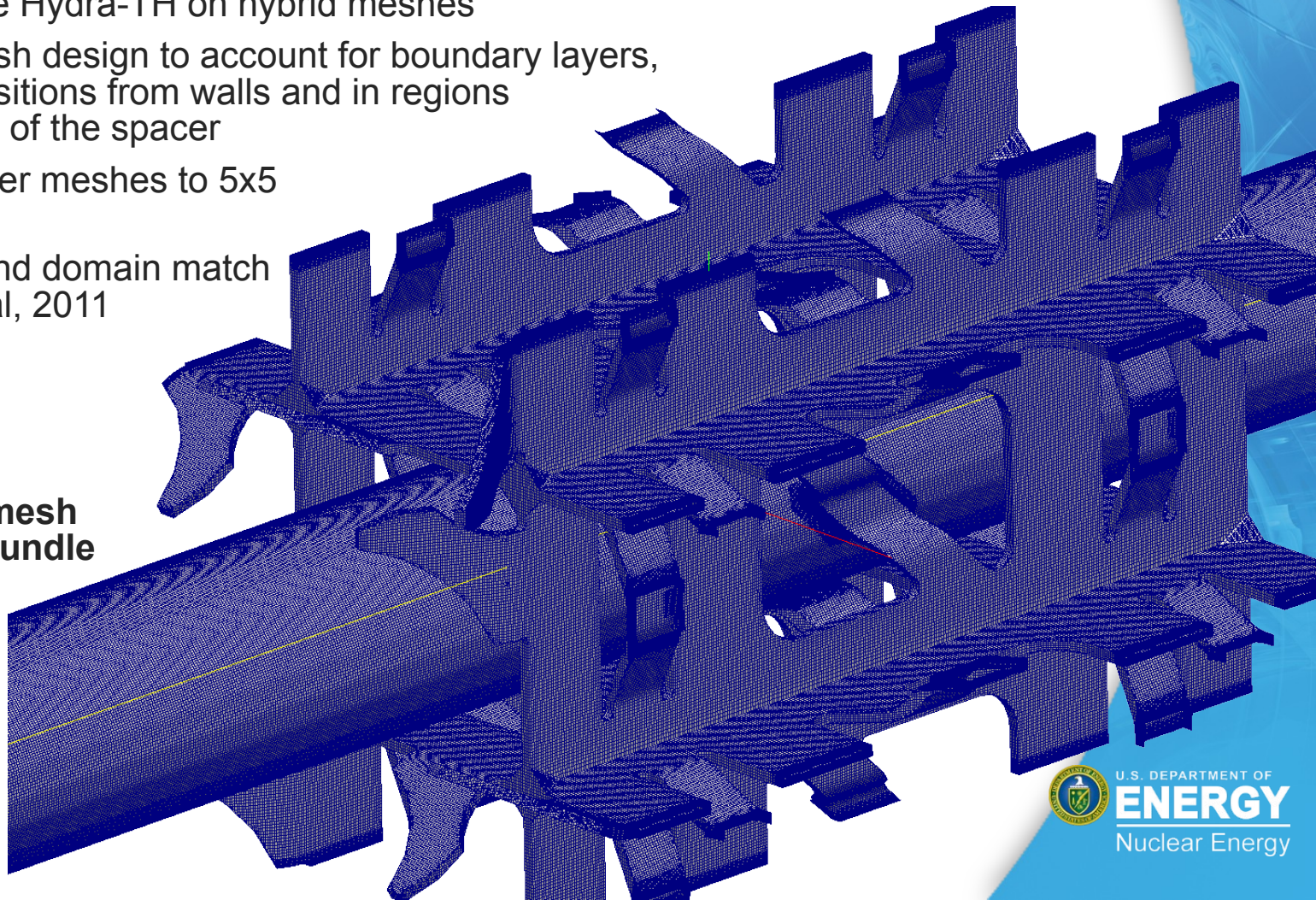
Meshing 3x3 rod-bundle with Spider

Goals:

- Demonstrate Numeca's Hexpress/Hybrid (a.k.a. “Spider”) automatic hybrid meshing technology on GTRF
- Demonstrate Hydra-TH on hybrid meshes
- Improve mesh design to account for boundary layers, smooth transitions from walls and in regions downstream of the spacer
- Extend Spider meshes to 5x5 rod bundle
- Geometry and domain match Elmahdi et al, 2011



47M Spider mesh for 3x3 rod bundle

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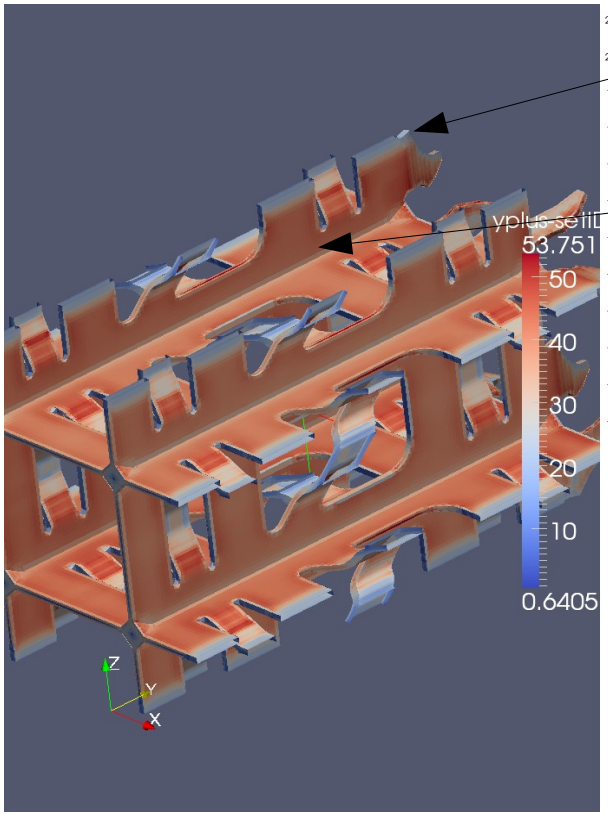
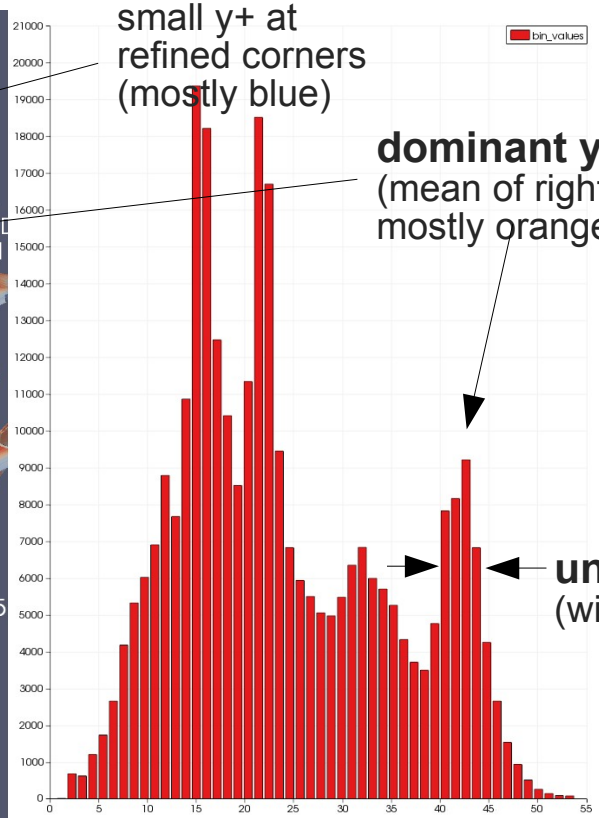
3x3 status

- Generated meshes for 3x3 with cell counts: 2M, 7M, 30M, 47M, 80M, 185M
- Initial runs with Hydra-TH to determine y+ on no-slip walls
- 2-47M ILES runs underway with 96-1920 compute cores at LANL

Mesh assessment using y+

$$y^+ = \sqrt{\tau_w/\rho}$$





small y+ at refined corners (mostly blue)

dominant y+ ~ 42 (mean of rightmost spike, mostly orange)

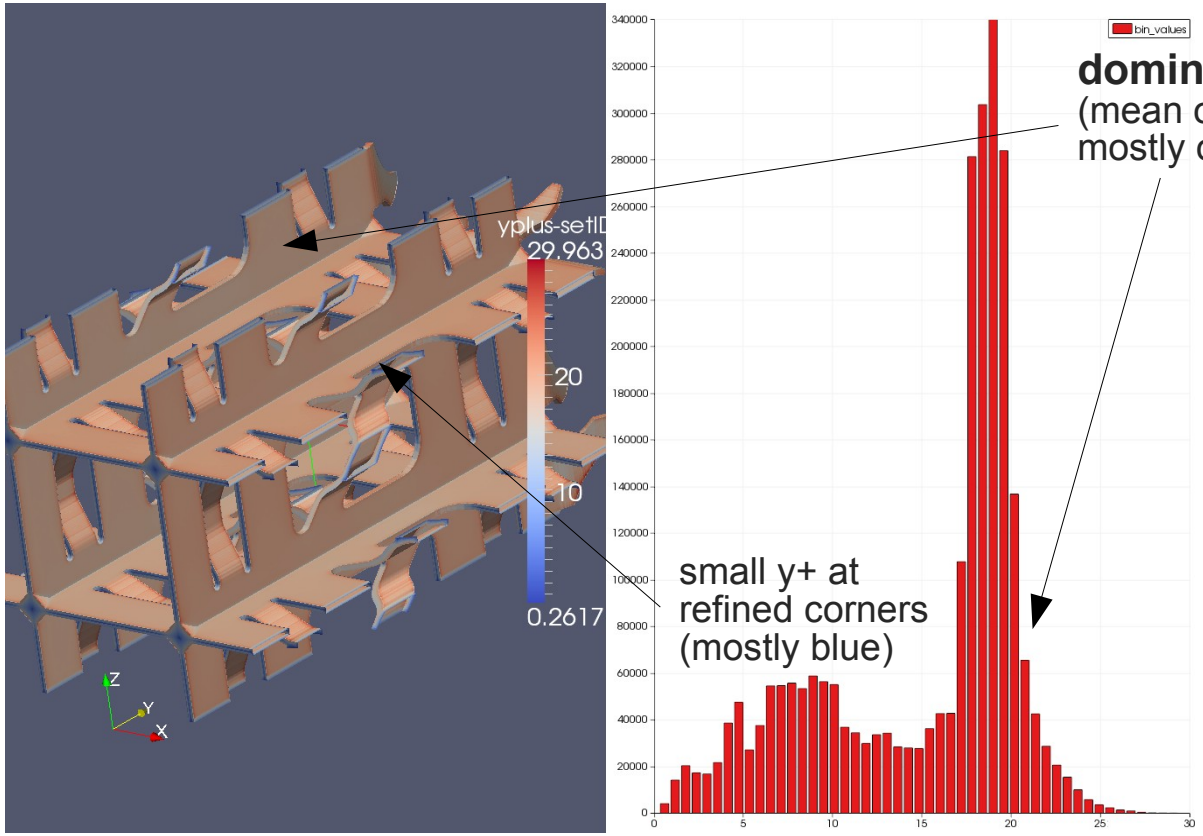
uniformity of y+ (width of rightmost spike)

y+ spatial distribution on 7M spacer

y+ histogram

Mesh assessment using y+

- Another example: 185M cells
- y+ = 1 required for full wall-resolution
- Mesh assessment:
  - **dominant y+** ~ How well the boundary layer is resolved?
  - **uniformity of y+** ~ How good is the mesh quality at walls?

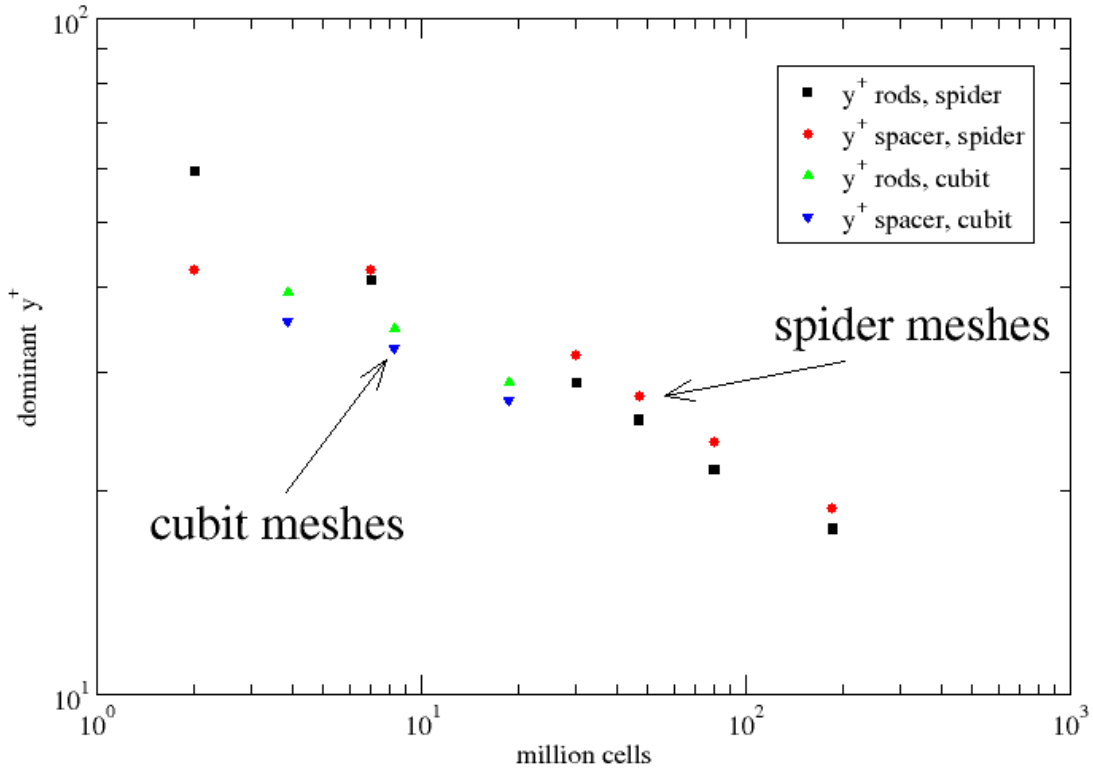


y+ spatial distribution on 185M spacer y+ histogram

Mesh assessment using dominant y+

Dominant y+ on spacer and rods vs. number of cells for

- Spider (2M, 7M, 30M, 47M, 80M, 185M)
- Cubit (3.9M, 8.3M, 18.6M)



- Both Spider and Cubit meshes exhibit monotonic decrease in y+ with increasing cell count
- Logarithmic trend: **None of these are boundary-layer meshes; trying to achieve y+~1 with this strategy would require 10^12 cells**
- Next step: add (power law) boundary layer refinement

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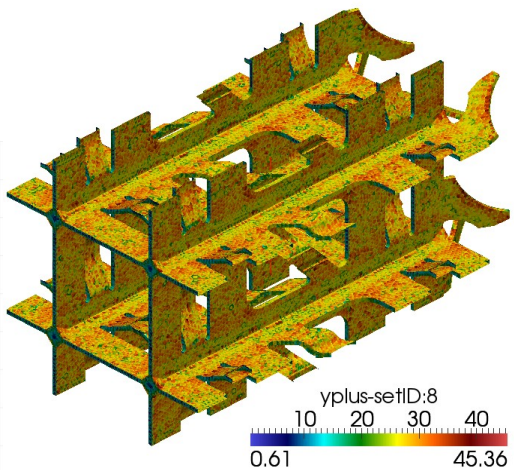
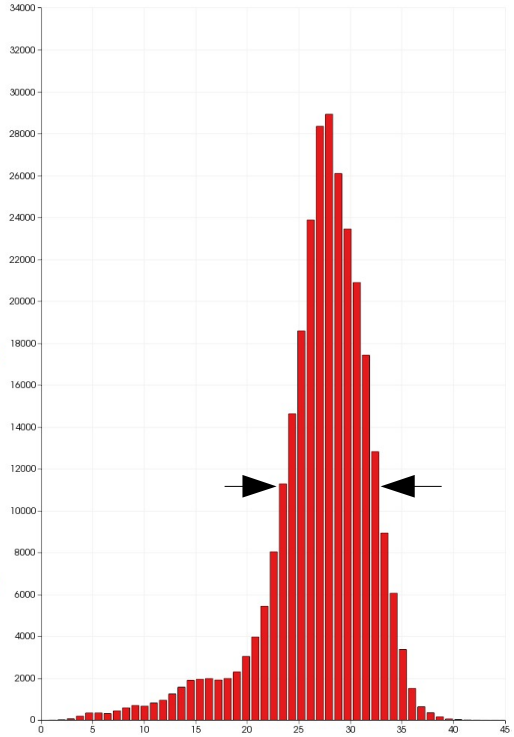
Mesh assessment using uniformity of y+

- Spider meshes on spacer are consistently more uniform
- A quantitative metric: entropy of the cell-area-weighted histograms (future work)

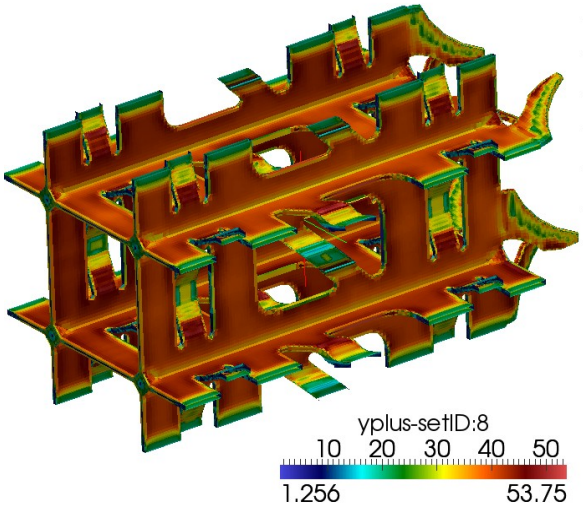
18.6M Cubit

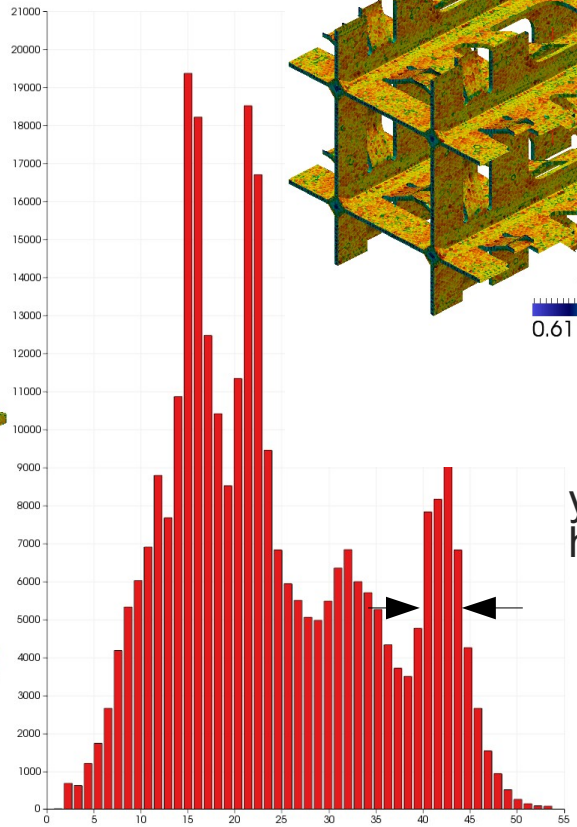




y+ spatial distribution and histogram on **18.6M Cubit** spacer

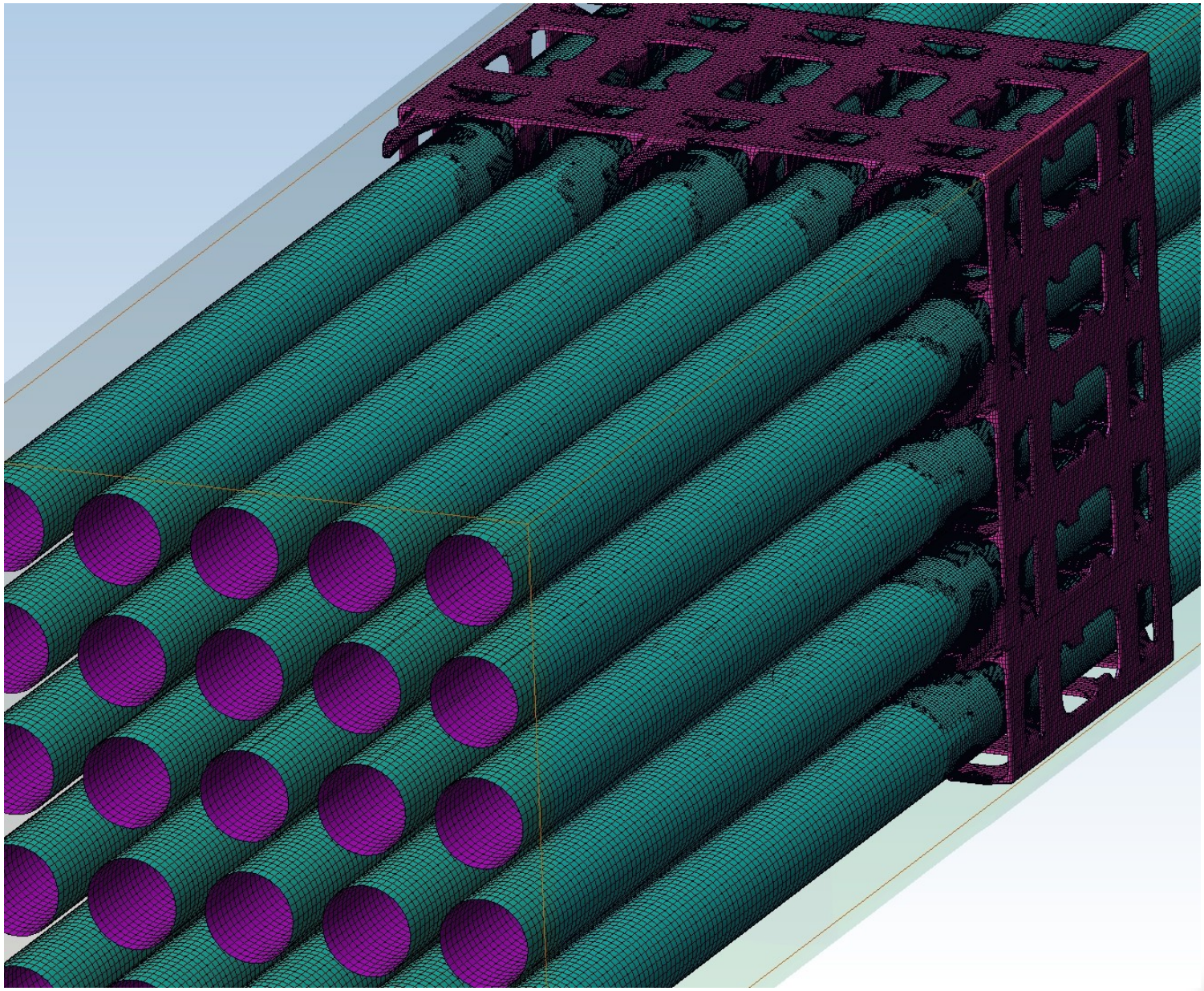
7M Spider





y+ spatial distribution and histogram on **7M Spider** spacer

Spider mesh for 5x5: 14M, (96M)



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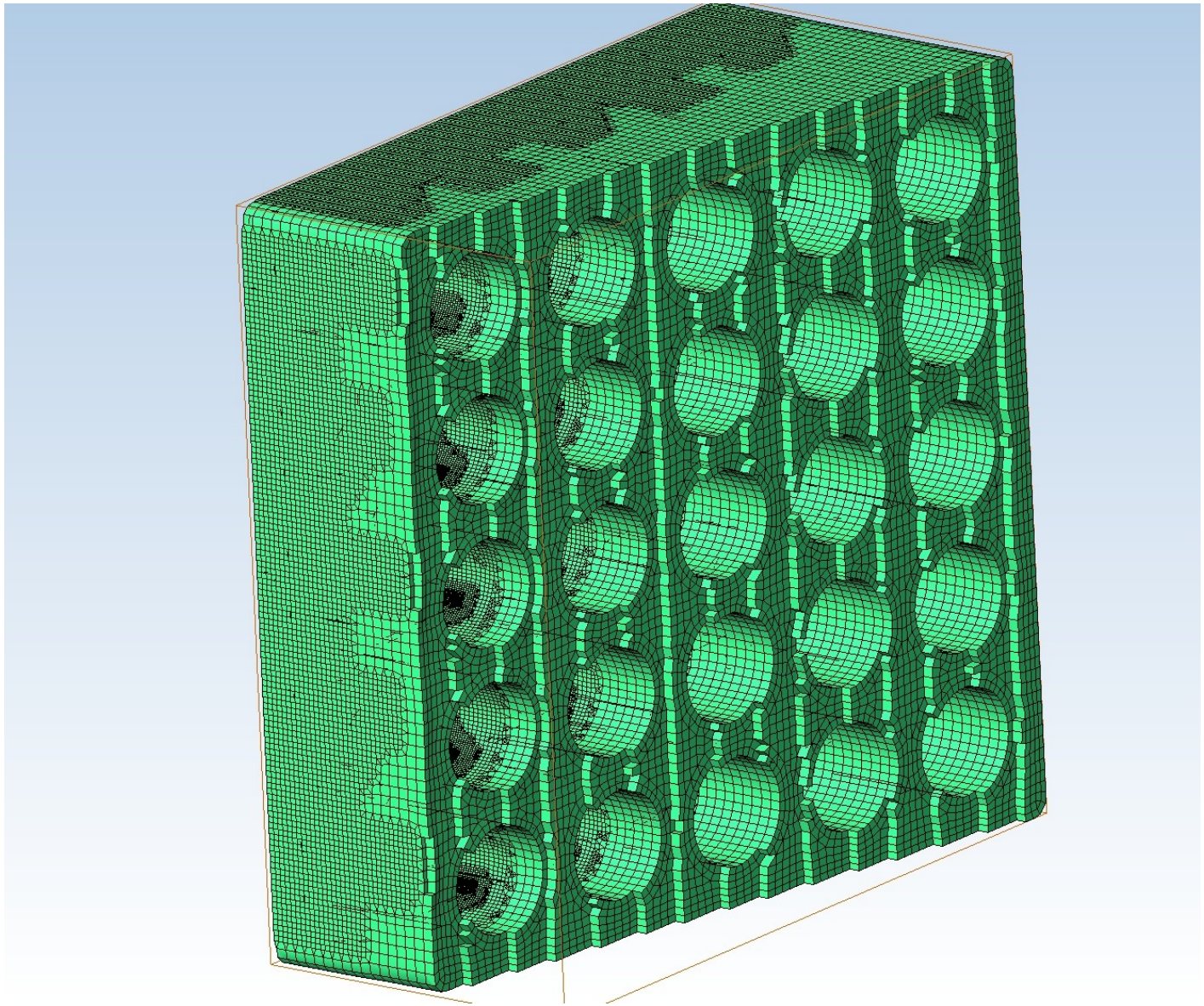
Spider mesh for 5x5: 14M, (96M)



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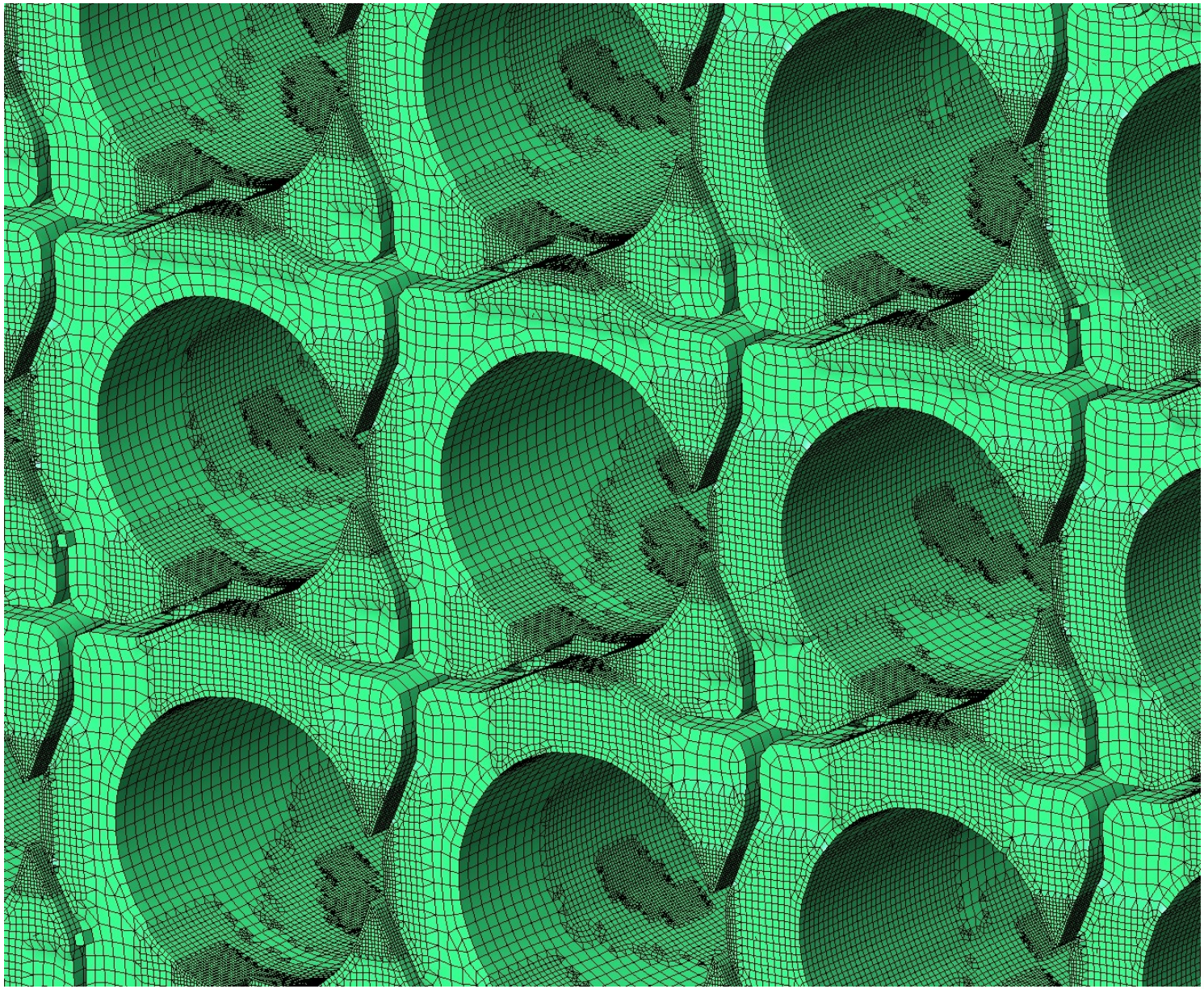
Spider mesh for 5x5: 14M, (96M)



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Spider mesh for 5x5: 14M, (96M)

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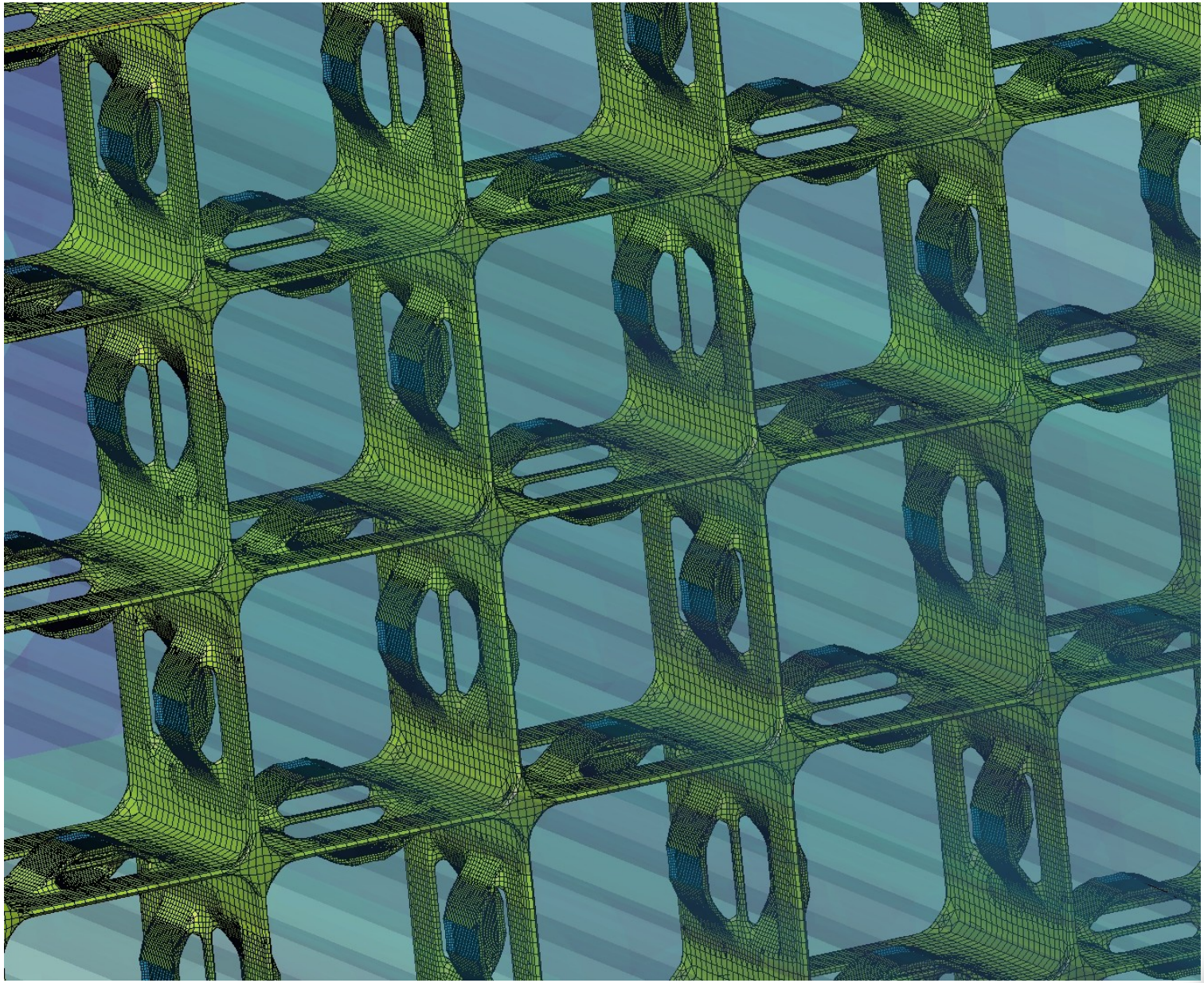

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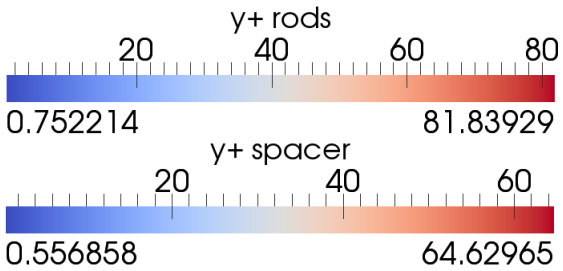
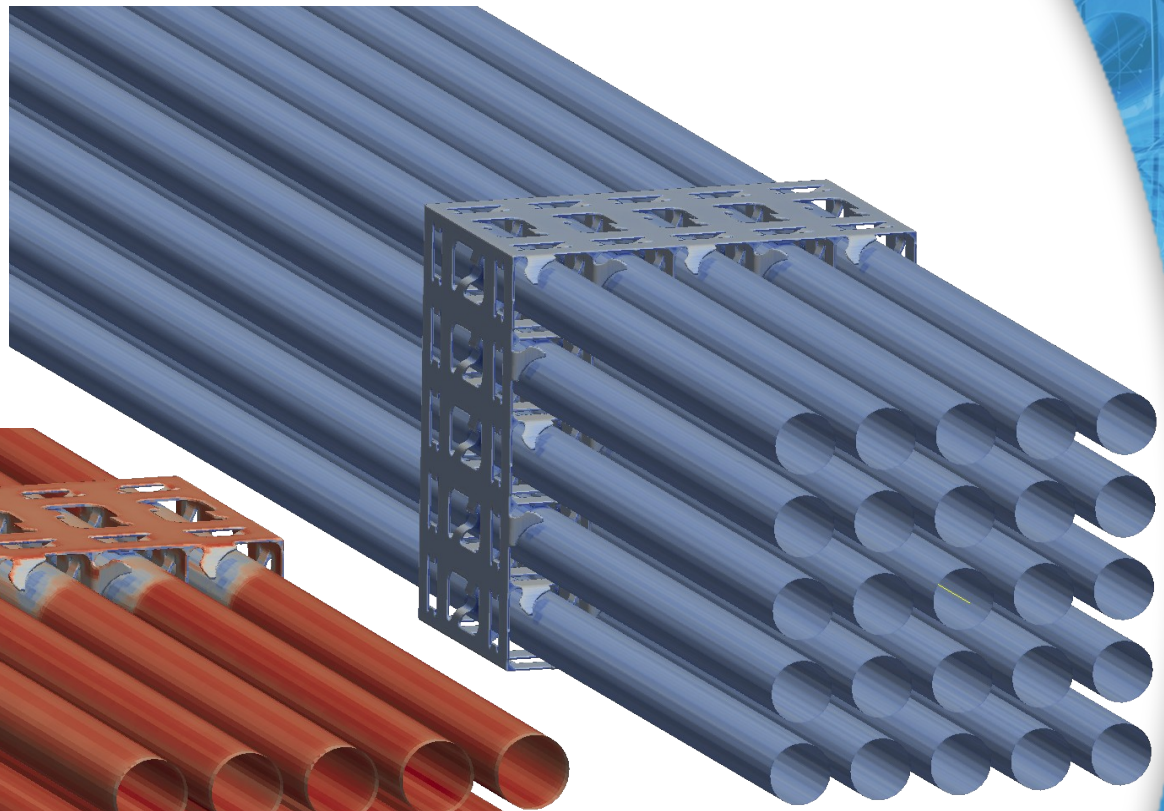
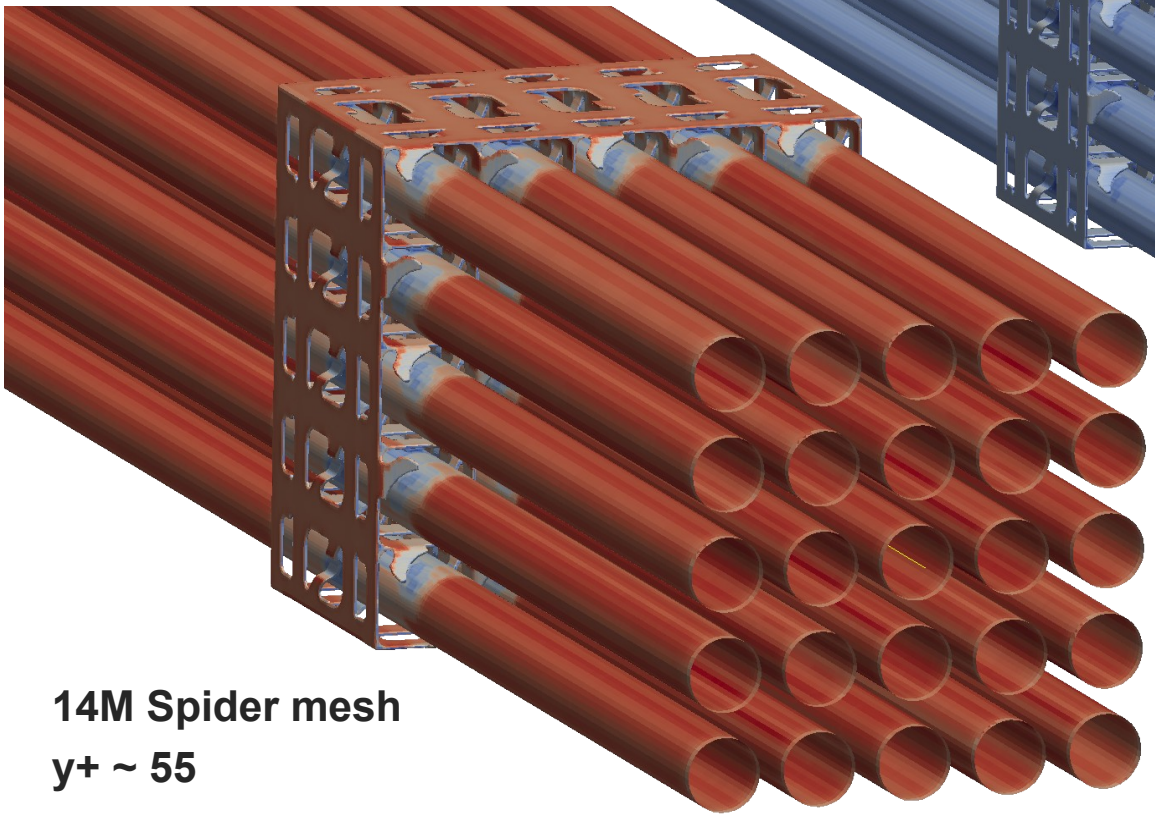
y+ on 5x5





96M Spider mesh

y+ ~ 18



14M Spider mesh

y+ ~ 55

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Numeca's Hexpress/Hybrid (a.k.a. Spider) meshing technology

- **Fully automatic** mesh generation; text config file; batch mode
- Unstructured, hex-dominant, conformal hybrid meshes
- High quality viscous layers
- Hole searcher in CAD geometry
- Shared-memory parallel
- Memory requirements: 0.5GB / million cells

5x5 status

- 5x5 meshes generated: 14M, 96M
- **96M mesh in 80 mins** on 8-core workstation with 48GB RAM
- Initial runs with Hydra-TH to assess y+
- 14M ILES run underway with 1200 compute cores at LANL

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New GTRF runs with turbulence statistics

Ongoing work toward new L3 milestone, Sept. 2012

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New GTRF runs with Hydra-TH

- Single-phase, incompressible NS
- ILES, collecting turbulence statistics
- Re-run 3x3 Cubit meshes: 672k, 1M, 2M, 3M, 6M, 12M
- 3x3 Spider meshes: 2M, 7M, (30M), (47M)
- 5x5 Spider mesh: 14M
- Larger meshes (80M, 185M, 96M): investigating memory allocation problems with PETSc using >5k cores

Ongoing work for Sept. L3 milestone

- Further assessment of mesh quality
- V&V of Hydra-TH with simpler turbulent flows: channel, lid-driven cavity, T-junction
- Turbulence models: ILES, DES, WALE, Spalart-Allmaras, Smagorinksy, k-ε
- Analyze turbulence statistics from GTRF runs
- Mesh convergence and HPC scaling study at LANL and Jaguar

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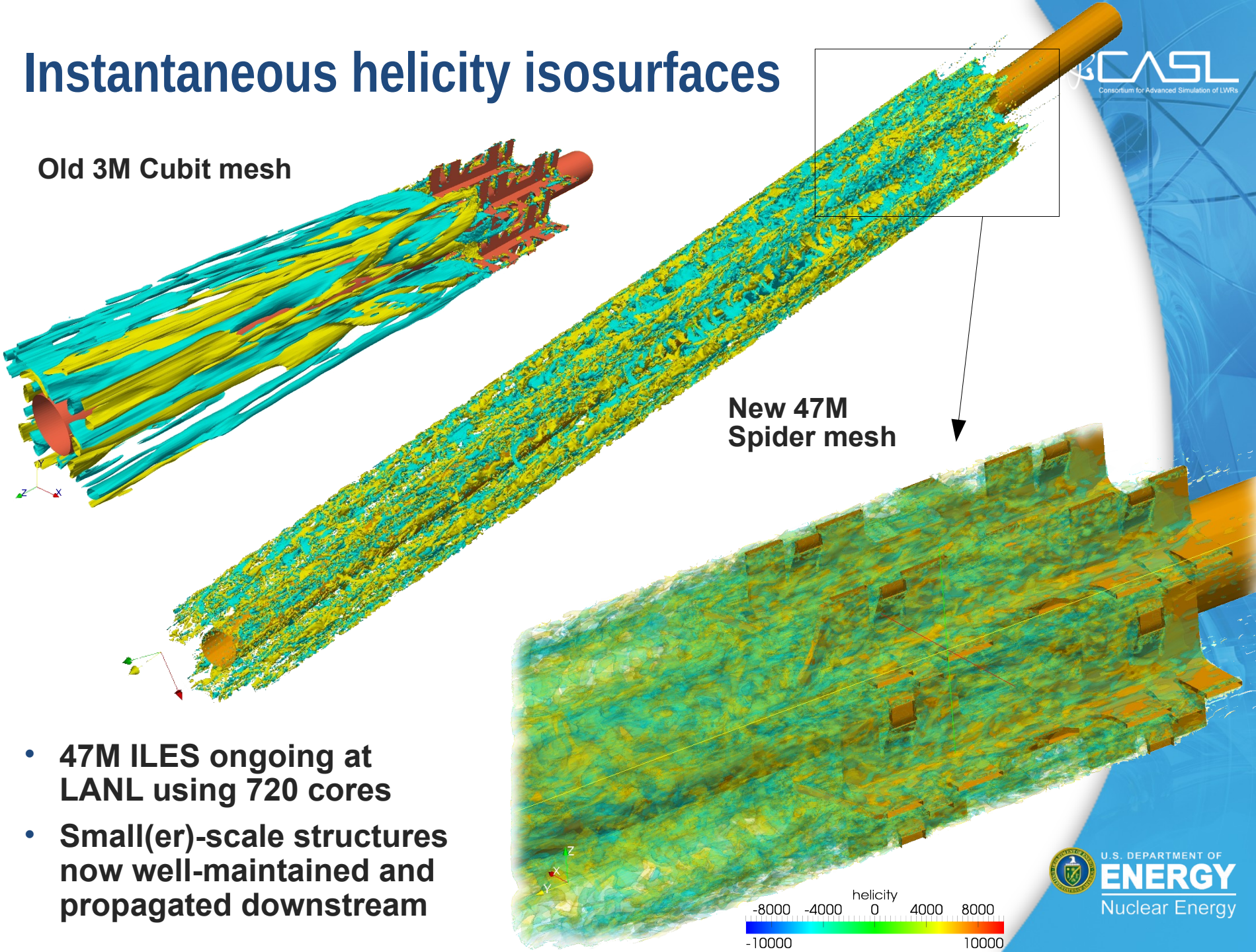
Instantaneous helicity isosurfaces



- 47M ILES ongoing at LANL using 720 cores
- Small(er)-scale structures now well-maintained and propagated downstream

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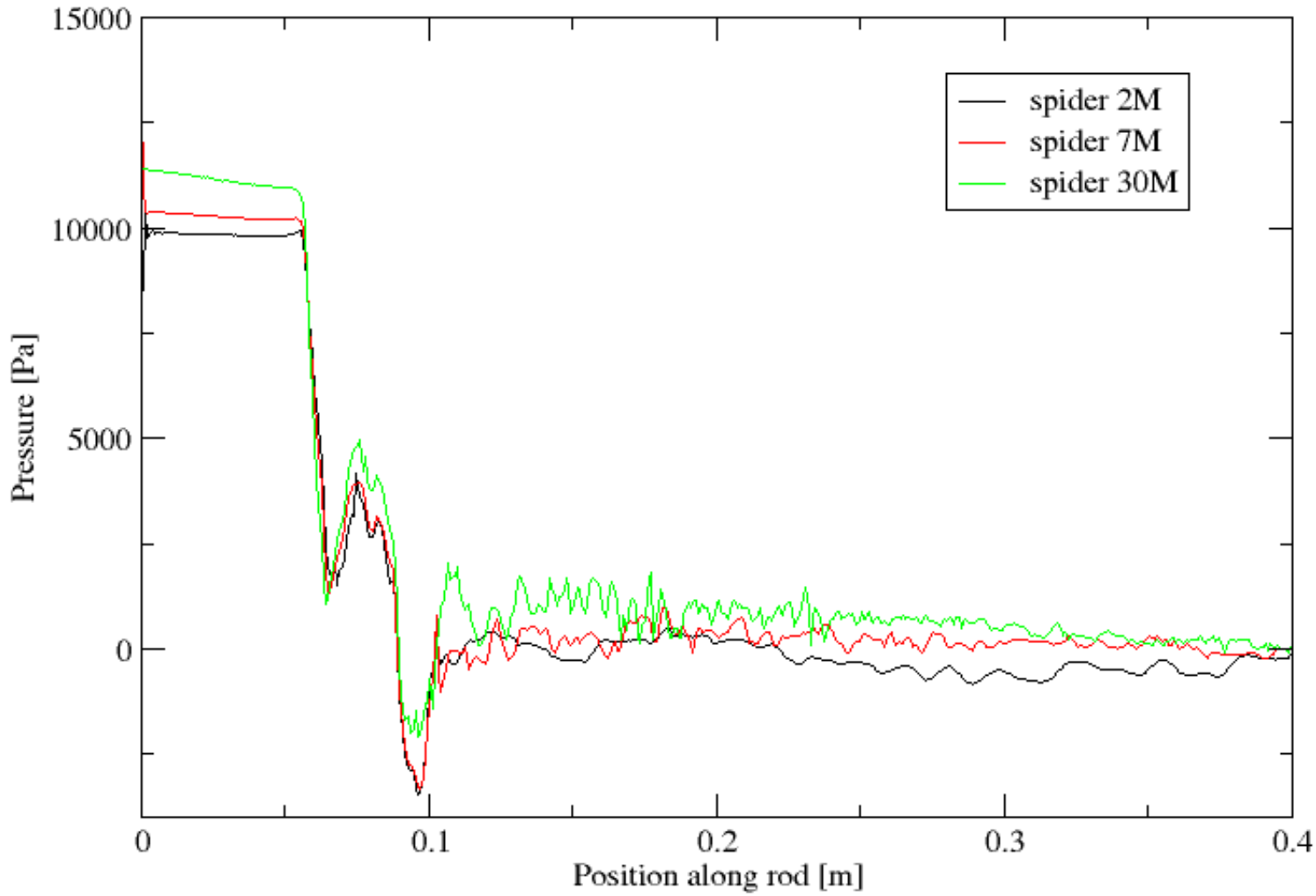
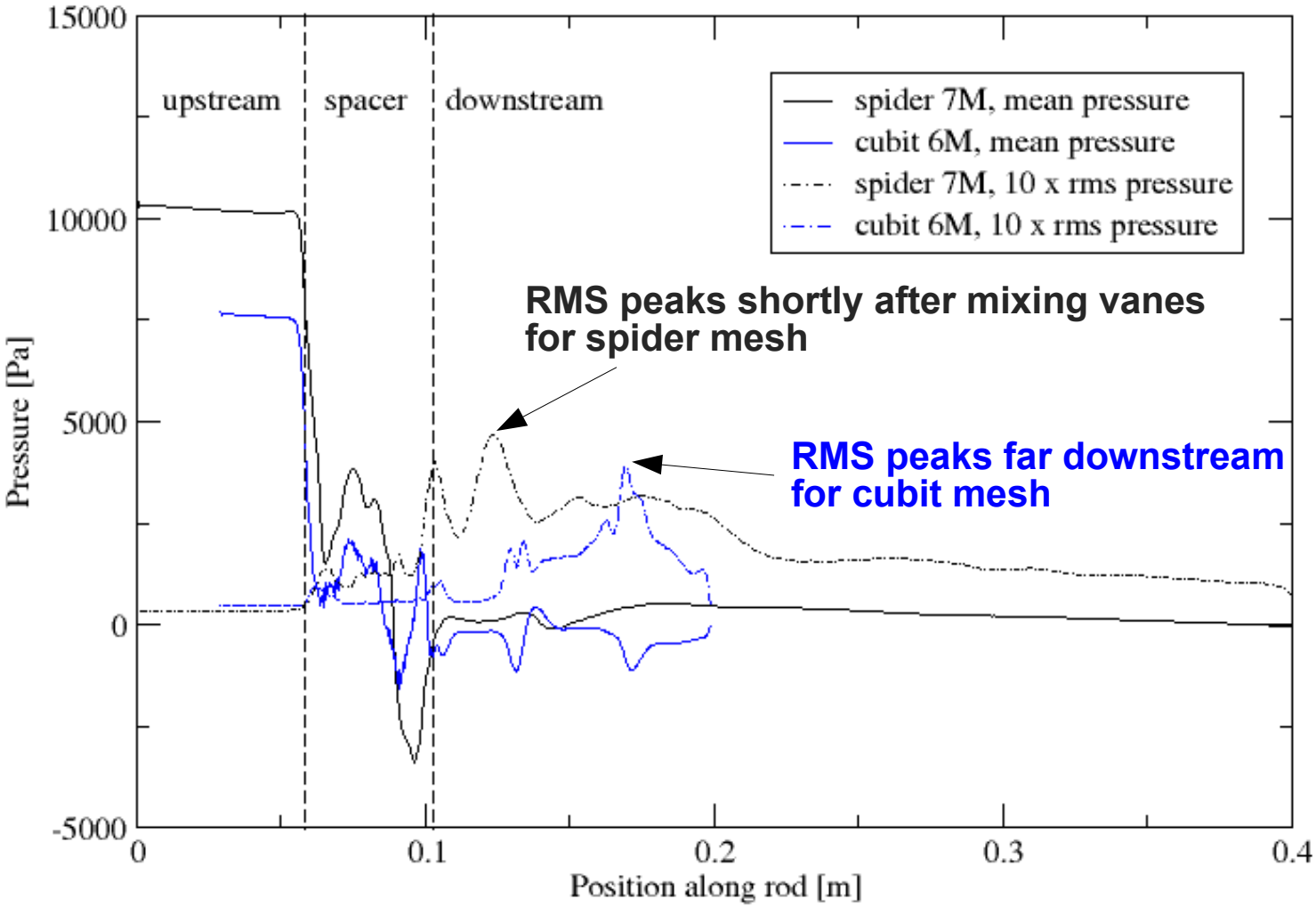
Instantaneous pressure along rod



- **47M running; 80M and 185M needs further work**
- **Pressure drop not yet converged**

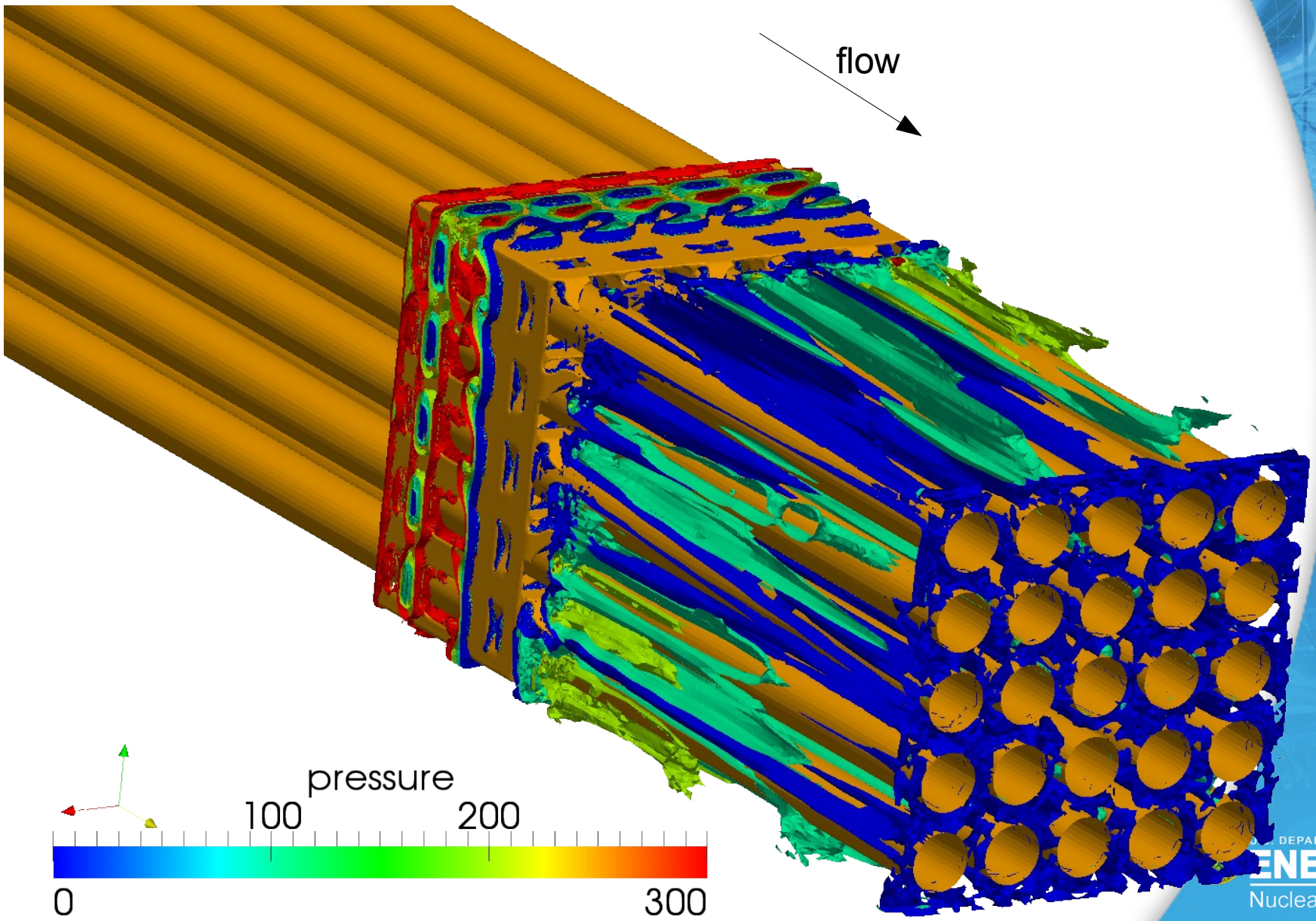
Mean and RMS pressure along rod

RMS pressure ~ "energy in pressure force"



Mean and fluctuation pressure very different for Cubit and Spider for similar mesh resolution

Instantaneous pressure on 14M 5x5



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Summary

- Numeca's Hexpress/Hybrid (“Spider”) is an excellent mesh generator for GTRF
- Automatic, simple to use

- Long domain, good quality mesh required for GTRF
- Next GTRF meshes: with boundary-layers, 0.5~1 billion cells

- Hydra-TH is (almost) ready for large-scale industrial CFD
- **More to come in L3.THM.CFD.P5.05, Sept. 2012**

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Pin Resolved 3D Transport: Full Core Capability

Thomas Evans

ORNL

CASL Roundtable 2012

Outline

- Objective
- Deterministic S_N Transport
- Solvers
- Whole Core Reference Problem
- Results

Objective

- Use consistent transport methods on 3-D, full core reactor problems
- Issues
  - Runtime
  - Memory
  - Setup
- Industry standard
  - High-order transport in 1/2D feeds low-order methods in 3D
  - Requires inconsistent coupling between low-order and high-order models to treat assembly boundaries, etc.
- Approach
  - Use regular, Cartesian grids to optimize runtime, setup, and memory for transport
  - Improve solvers
  - Better discretization/homogenization strategies

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Potential Deterministic Approaches

- 3D MOC
  - No theoretical barrier
  - Implementation and parallel scaling issues
  - Very high cost; may preclude use in medium term
- 2D/1D MOC
  - Consistency issues; research required
  - Axial resolution/behavior unclear
  - Best prospect for solving 3D IFBA/depletion in short term
  - Parallelization remains an issue
- Regular Grid S_N
  - Demonstrated for regular fuel pins
  - Will not work for IFBA (500×500 cells per pin required)
  - Limited utility for highly resolved depletion
- S_N w/embedded MOC
  - Potential for consistent 3D approach for all problems
  - No existing implementation yet; research required
  - May be too expensive to be practical
- Unstructured S_N
  - Meshing 3D IFBA/depletion layers problematic
  - High user setup costs
  - Memory/time intensive
  - Parallelization issues need to be researched
  - Not viable to meet Y3 Milestone

FY12 activities reveal another potential option – coupled MOC/S_N

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Discrete Ordinates Methods

- The S_N method is a collocation method in angle.
  - Energy is discretized in groups.
  - Scattering is expanded in Spherical Harmonics.
  - Multiple spatial discretizations are used (DGFEM, Characteristics, Cell-Balance).

$$\mathbf{L}\psi = \mathbf{MS}\phi + Q$$

$$\phi = \mathbf{D}\psi$$

- Dimensionality of operators:

$$t = N_g \times N_c \times N_u \times N_m$$

$$n = N_g \times N_c \times N_u \times N_a$$

$$(n \times n)(n \times 1) = (n \times t)(t \times t)(t \times 1) + (n \times 1)$$

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Degrees of Freedom

- Total number of unknowns in solve:

$$\text{unknowns} = N_g \times N_c \times N_u \times N_a \times N_m$$

- An ideal (conservative) estimate.

$$N_g = 238$$
$$N_c = 1 \times 10^9$$
$$N_u = 4$$
$$N_m = 16$$
$$N_a = 288$$

$$\boxed{\text{unknowns} \geq 4 \times 10^{15}}$$

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Eigenvalue Problem

- The eigenvalue problem has the following form

$$(\mathbf{I} - \mathbf{TMS})\phi = \frac{1}{k}\mathbf{TM}\chi\mathbf{f}^T\phi$$

- Expressed in standard form

$$\mathbf{A}x = kx$$

$$\mathbf{A} = (\mathbf{I} - \mathbf{TMS})^{-1}\mathbf{TM}\chi\mathbf{f}^T \quad x = \phi$$ Energy-dependent

$$\mathbf{A} = \mathbf{f}^T(\mathbf{I} - \mathbf{TMS})^{-1}\mathbf{TM}\chi \quad x = \mathbf{f}^T\phi$$ Energy-indepedent

- The traditional way to solve this problem is with *Power Iteration* (with CMFD or other acceleration methods)

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Advanced Eigenvalue Solvers

- We can use Krylov (Arnoldi) iteration to solve the eigenvalue problem more efficiently

$$y^k = \mathbf{A} v^k$$

Matrix-vector multiply and sweep $\quad z^k = \mathbf{TM}\chi\mathbf{f}^T v^k$

Multigroup fixed-source solve $\quad (\mathbf{I} - \mathbf{TMS}) y^k = z^k$

- Shifted-inverse iteration (Raleigh-Quotient Iteration) has been developed (using Krylov to solve the shifted multigroup problem in each eigenvalue iteration)

$$(\mathbf{I} - \mathbf{TM}\underbrace{(\mathbf{S} + \mu\mathbf{F})}_{\text{block-dense}})\phi = (\lambda - \mu)\mathbf{TMF}\phi$$

Multigroup Transport Problem

- Using Gauss-Seidel requires the solution of *G* within-group equations (using Krylov iteration) in each GS iteration
- Alternatively, the full energy system can be solved by Krylov iteration ($\mathrm{T}=\mathrm{DL}^{-1}$)

$$(\mathbf{I} - \mathbf{TMS})\phi = \mathbf{T}q$$

$$\left(\mathbf{I} - \begin{bmatrix} \mathbf{T}_0 & \dots & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \mathbf{T}_G \end{bmatrix} \begin{bmatrix} \mathbf{M} & \dots & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \mathbf{M} \end{bmatrix} \begin{bmatrix} \mathbf{S}_{00} & \dots & \mathbf{S}_{0G} \\ \vdots & \ddots & \vdots \\ \mathbf{S}_{G0} & \dots & \mathbf{S}_{GG} \end{bmatrix}\right) \begin{bmatrix} \phi_0 \\ \vdots \\ \phi_G \end{bmatrix} = \begin{bmatrix} \mathbf{T}_0 q_0 \\ \vdots \\ \mathbf{T}_G q_G \end{bmatrix}$$

Solver Taxonomy

The innermost part of each solver are transport sweeps

$$y = \mathbf{T}z = \mathbf{D}\,\underbrace{\mathbf{L}^{-1}z}_{\mathbf{L}\psi = z}$$

"It's turtles all the way down…"

Eigenvalue Solvers

Power iteration
Arnoldi
Shifted-inverse

↓

Multigroup Solvers

Gauss-Seidel
Krylov
Gauss-Seidel + Krylov

↓

Within-group Solvers

Krylov
Source iteration

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Solver Results

Solvers	Blocks	Sets	Domains	Solver Time (min)
PI + MG GS (2-grid preconditioning)	17,424	1	17,424	150.15
PI + MG Krylov	17,424	1	17,424	52.99
Arnoldi + MG Krylov	17,424	1	17,424	23.62
Arnoldi + MG Krylov	17,424	2	34,848	12.81

Total unknowns = 59,867,852,800
Number of groups = 2
k_{eff} tolerance = 1.0e-5

- The GS solver cannot use more computational resource for a problem of this spatial size
  - Simply using more spatial partitions will not reduce time to solution
  - Problem cannot effectively use more cores to run a higher fidelity problem in energy
- PI + MG Krylov will scale with sets similarly to Arnoldi, they just use different outer iteration strategies

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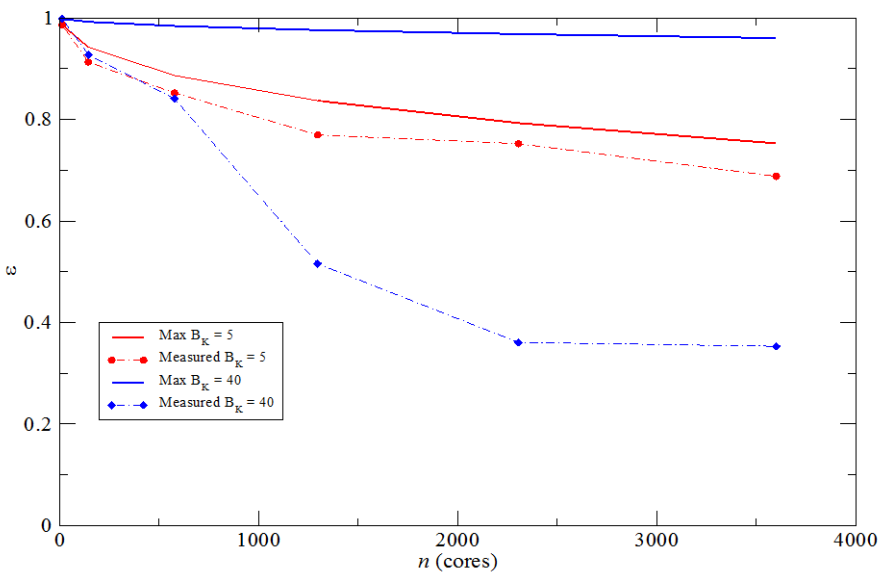
Space-Angle Parallellism

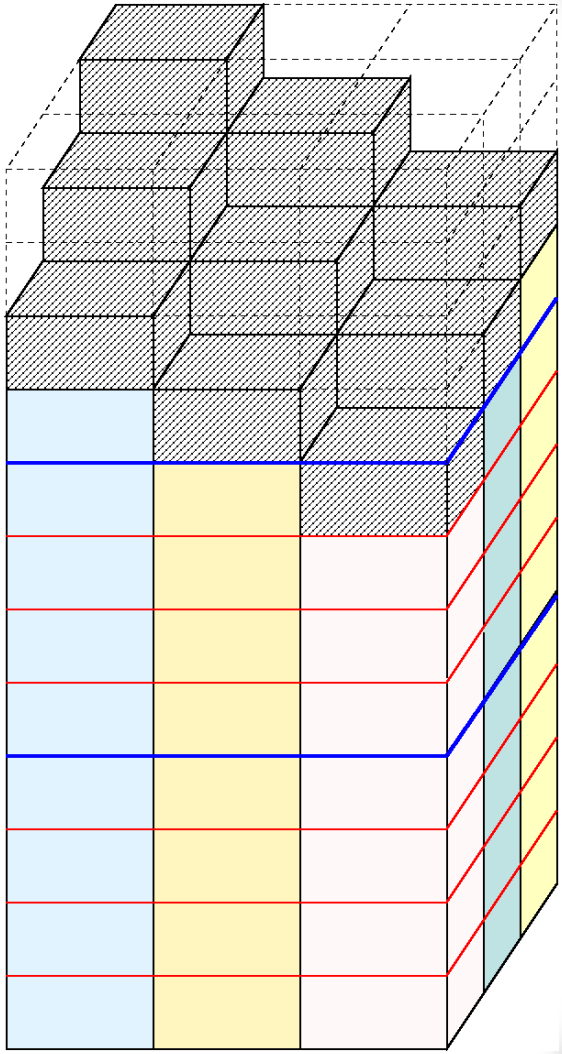
KBA Wavefront Method

- Angles in ± z directions are pipelined
- Results in 2×M pipelined angles per octant
- Quadrants are ordered to reduce latency

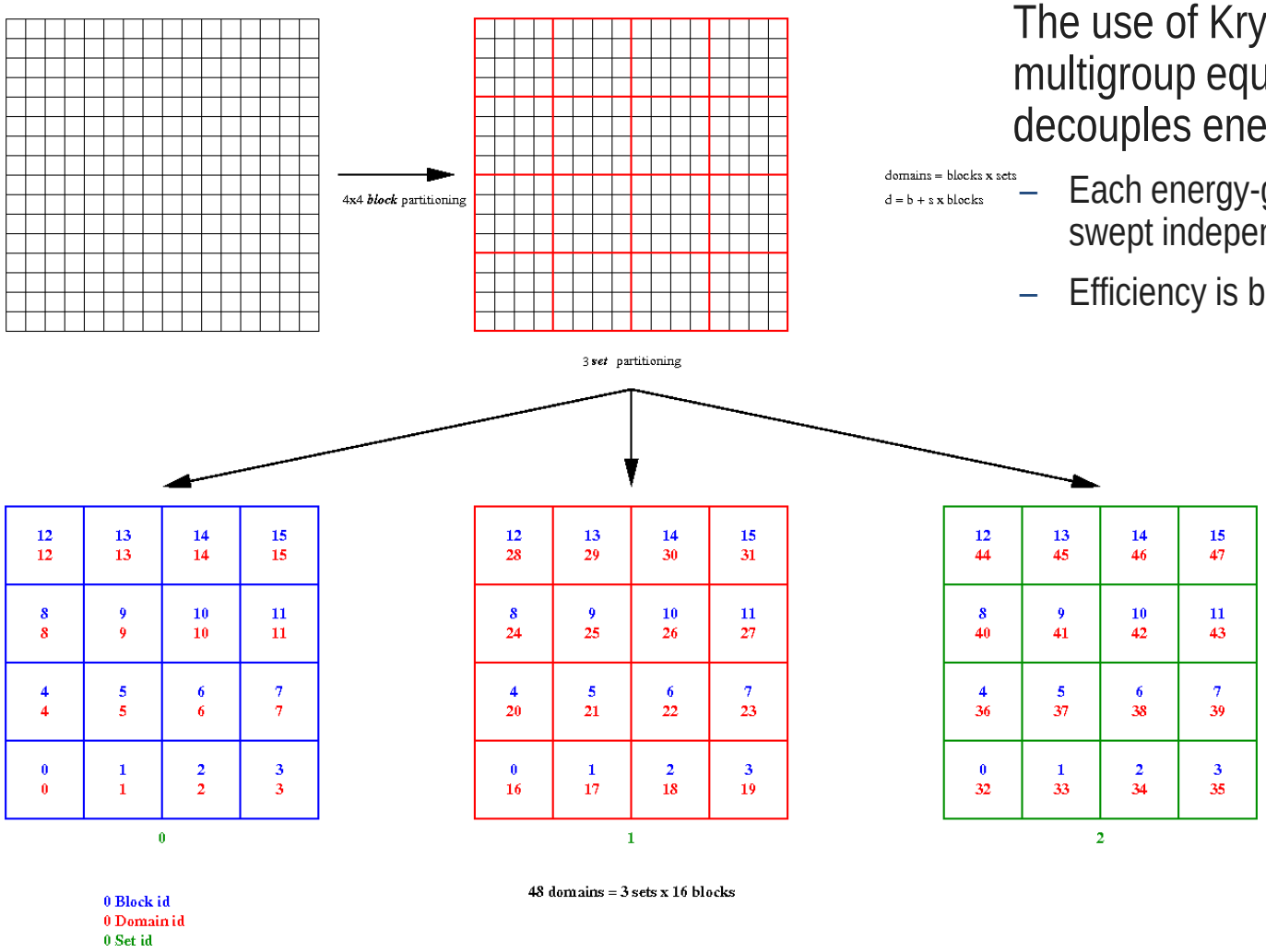
$$\epsilon_{\max} = \frac{2MB_K}{2MB_K + P_I + P_J - 2}$$



6 angle pipeline (S_4; M = 3)



Multilevel Energy Decomposition



The use of Krylov methods to solve the multigroup equations effectively decouples energy

- Each energy-group S_N equation can be swept independently
- Efficiency is better than Gauss-Seidel

Multilevel Summary

- Energy decomposed into sets.
- Each set contains blocks constituting the entire spatial mesh.
- The total number of domains is

$$\text{domains} = \text{sets} \times \text{blocks}$$

- KBA is performed for each group in a set across all of the blocks.
  - Not required to scale beyond *O(1000)* cores.
- Scaling in energy across sets should be linear.
- Allows scaling to O(100K) cores and enhanced parallelism on accelerators.

Whole Core Reactor Problem

- Problem Description
  - Generalized Westinghouse 3411 MWth PWR
  - Three different fuel enrichments
  - Burnable Poisons
  - 17x17 assemblies with a height of 12 feet
  - Boron concentration of 1000 ppm
  - Ignored spacer grids and control rod banks

	H	G	F	E	D	C	B	A
8	1.5	2.5 16	1.5	2.5 12	1.5	2.5 16	1.5	2.5
9	2.5 16	1.5	2.5 8	1.5	3.0 16	1.5	3.0 16	2.5
10	1.5	2.5 8	1.5	2.5 12	1.5	2.5 16	1.5	2.5
11	2.5 12	1.5	2.5 12	1.5	2.5 12	1.5	3.0 16	3.0
12	1.5	3.0 16	1.5	2.5 12	1.5	2.5 12	2.5	
13	2.5 16	1.5	2.5 16	1.5	2.5 12	2.5 8	3.0	
14	1.5	3.0 16	1.5	3.0 16	2.5	3.0		
15	2.5	2.5	2.5	3.0				

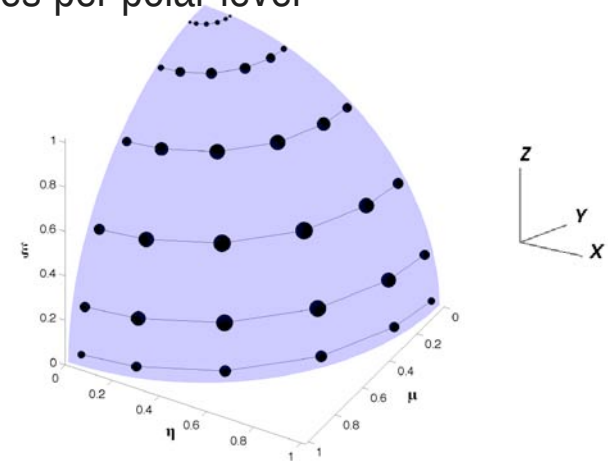
U-235 Enrichment (%)

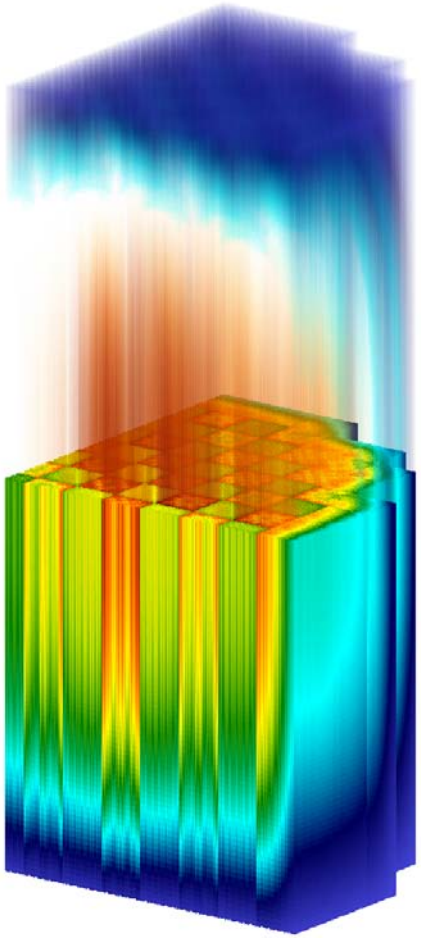
Number of BPs

Whole Core Reactor Problem

- P1 Scattering
- 8 group cross-sections (collapsed from 238 group structure)
- Spatial Methods
  - Step-Characteristics (SC)
  - Linear-discontinuous finite element (LD)
- Mesh
  - Radial (XY): 4x4 to 12x12 mesh per pincell
  - Axial(Z): 0.2 cm to 6 inch axial mesh size
- Quadruple Range quadrature
  - 2, 4, 6, and 8 polar levels
  - 4, 6, and 8 angles per polar level

QR 6x6





Power

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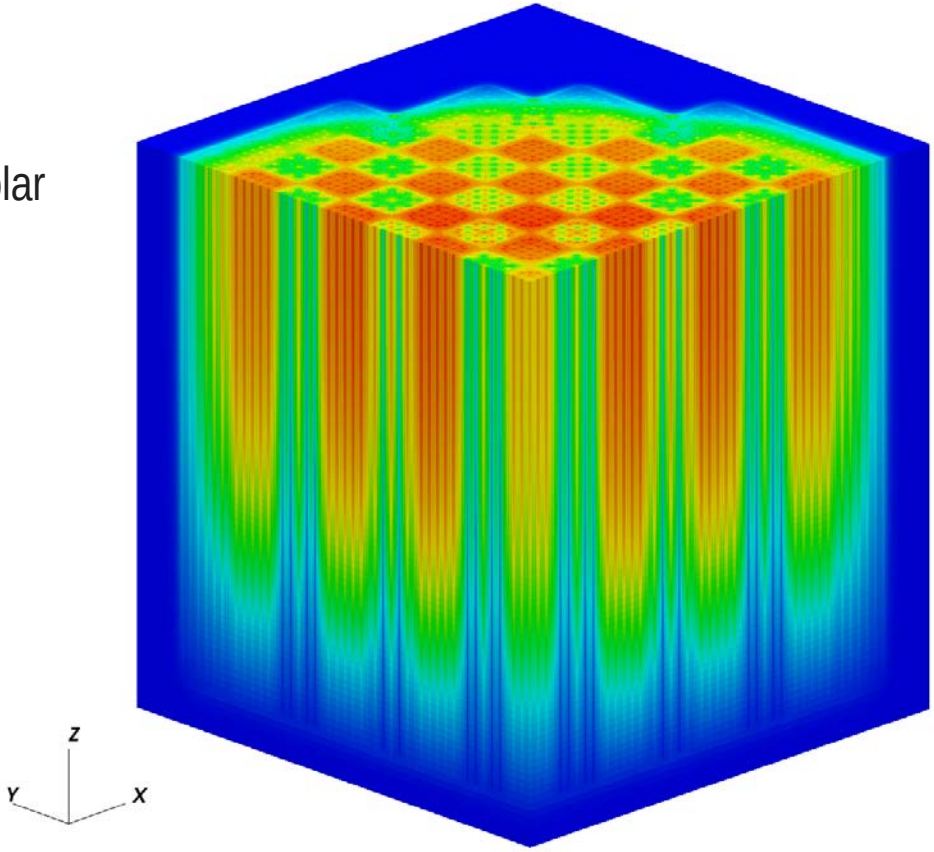
Whole Core Reference Case

- Reference Case
  - 0.2 cm axial mesh
  - 6x6 mesh per pincell
  - 1.6 billion cells
  - 4 polar levels and 6 angles per polar level (24 angles/octant)
  - Step-Characteristics



Thermal Flux

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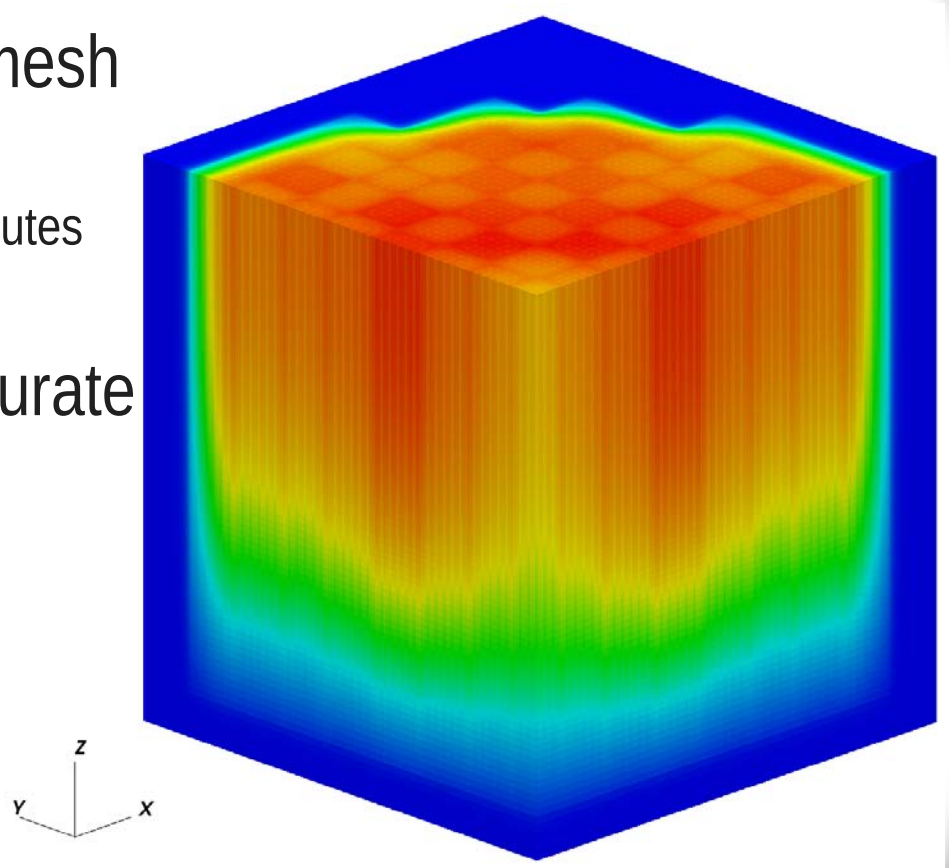
Eigenvalue Results

- 6 inch (15.24 cm) axial mesh
  - 21 million cells on 9600 cores
  - SC error of 960 pcm in ~17 minutes
  - LD error 9 pcm in ~24 minute
- LD was ~100x more accurate for a ~1.4x the time



Fast Flux

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Eigenvalue Results

- 1 inch (2.54 cm) axial mesh

Case ID	2D Mesh Discretization	Angles per Polar Level	Polar Levels per Octant	SC Error (pcm)	LD Error (pcm)
1	4	4	2	-204	-16
2	6	6	4	-113	33
3	6	6	8	-109	
4	8	6	4	-120	
5	10	6	4	-150	

- LD significantly more accurate (3-10x) for the eigenvalue

	SC			LD			
Case ID	Number of Processors	Runtime	CPU-hrs	Number of Processors	Runtime	CPU-hrs	SC Speedup
1	3000	19.9	995.4	4800	76.3	6101.2	6.1
2	5184	67.5	5832.9	19200	80.2	25651.2	4.4

- LD was ~4-6x slower and required ~4x more memory

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Eigenvalue Results

- 1 cm axial mesh

Case ID	2D Mesh Discretization	Angles per Polar Level	Polar Levels per Octant	SC Error (pcm)	LD Error (pcm)
6	4	4	2	90	
7	6	6	4	-5	35
8	6	6	6	-1	
9	12	8	4	-4	

- SC and LD are accurate at this mesh level
  - Reference Case is SC

	SC			LD			
Case ID	Number of Processors	Runtime	CPU-hrs	Number of Processors	Runtime	CPU-hrs	SC Speedup
7	28800	88.0	42250.4	96000	64.5	103240.0	2.4

- LD was ~2.4x slower and required ~4x more memory

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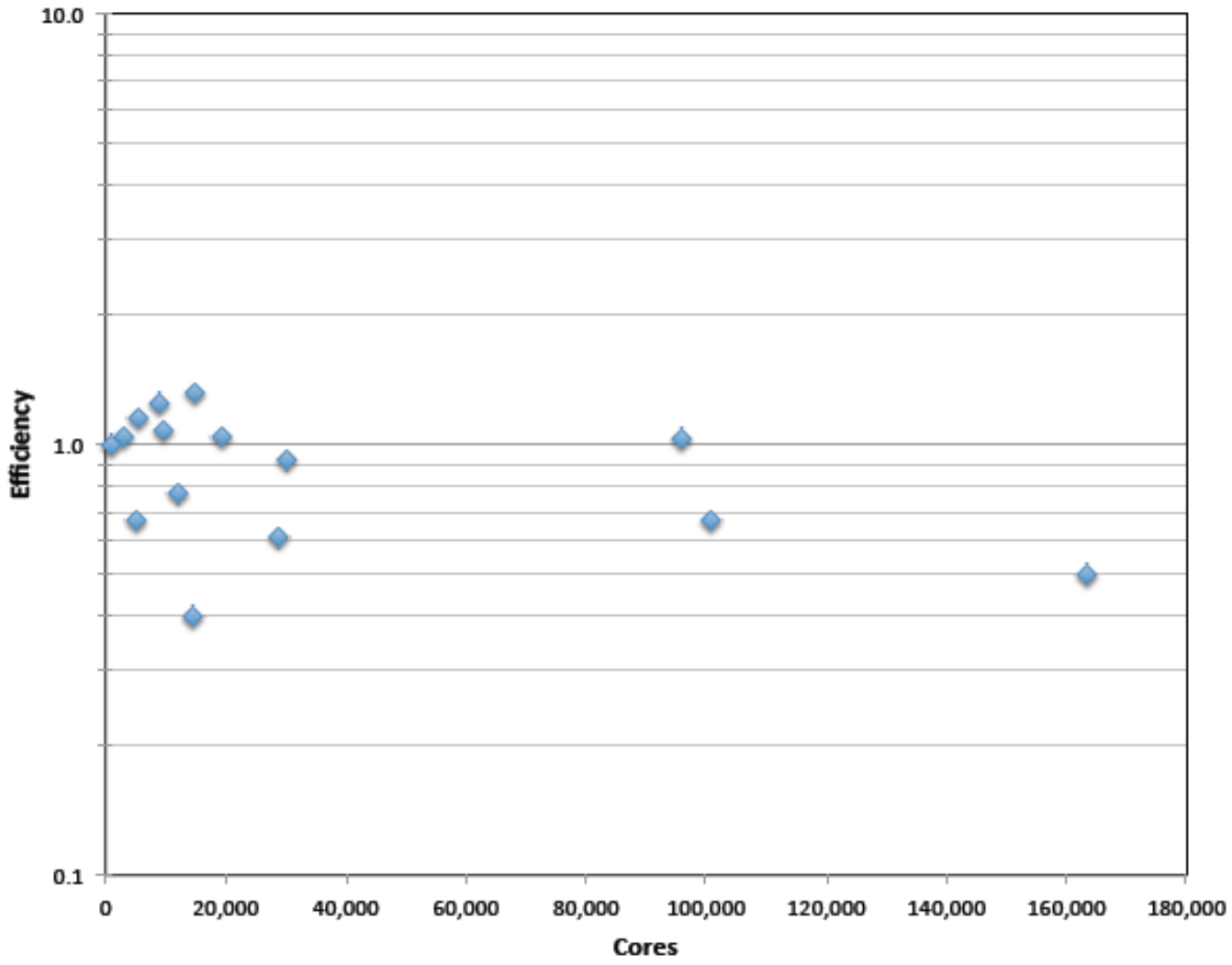
Weak Scaling on Jaguar XT5



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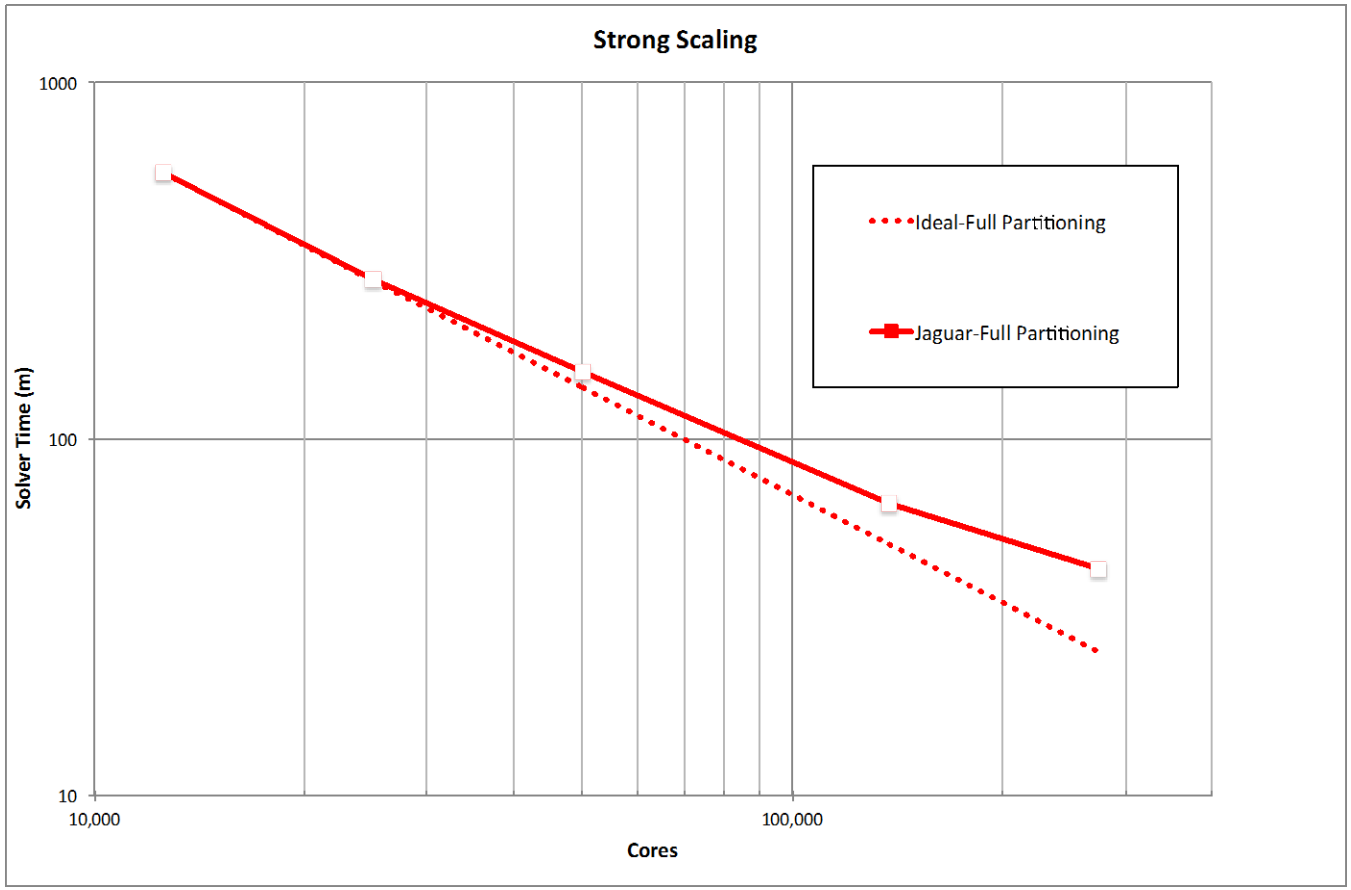
PWR900 Scaling on Jaguar XK6

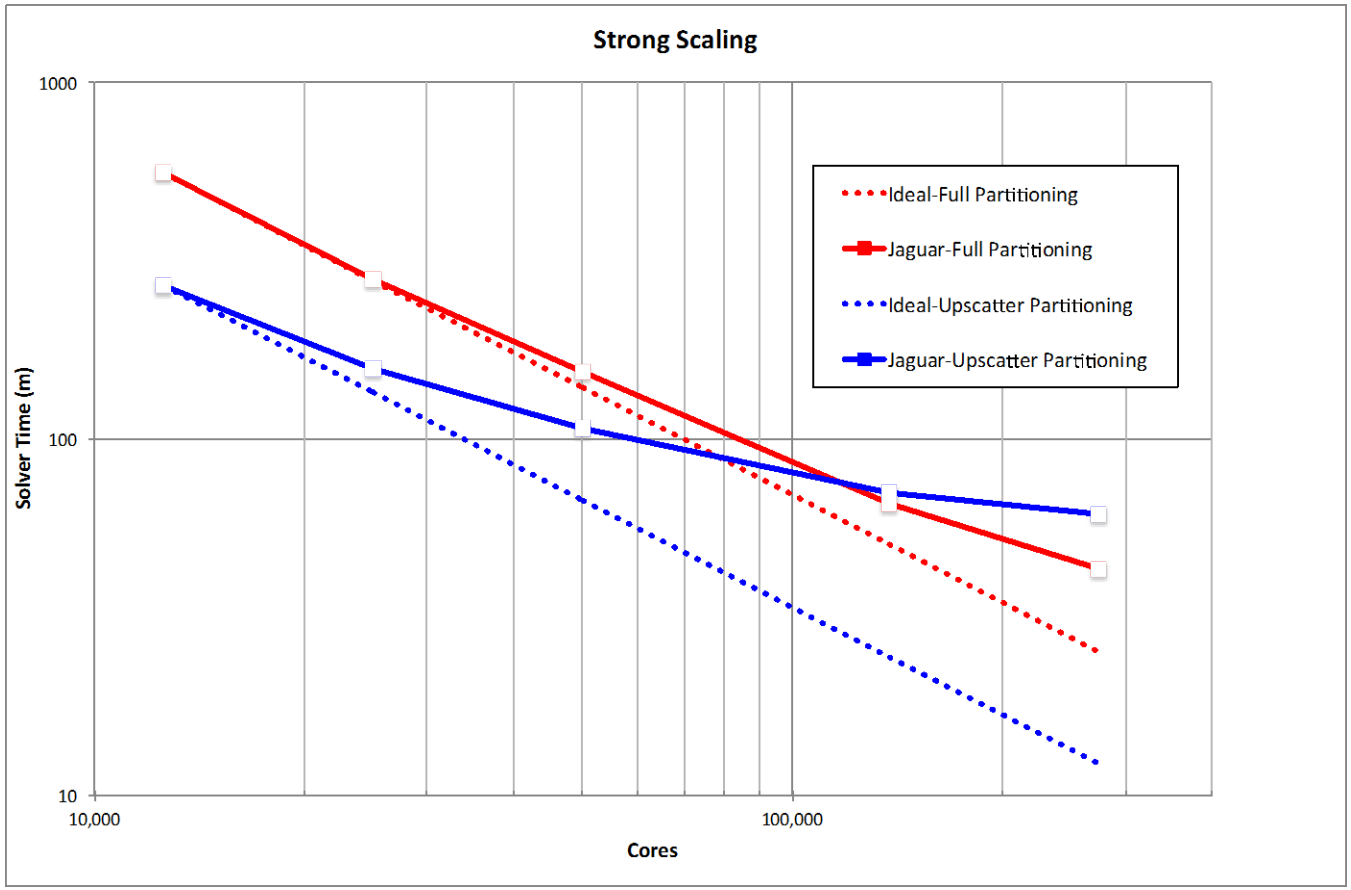


Full partitioning scales well to 275K cores

Improved interconnects + reduce-scatter have dramatically reduced global reduction cost

- Constant number of blocks = 12,544
- 44 total groups/22 coupled groups

PWR900 Scaling on Jaguar XK6



- Constant number of blocks = 12,544
- 44 total groups/22 coupled groups

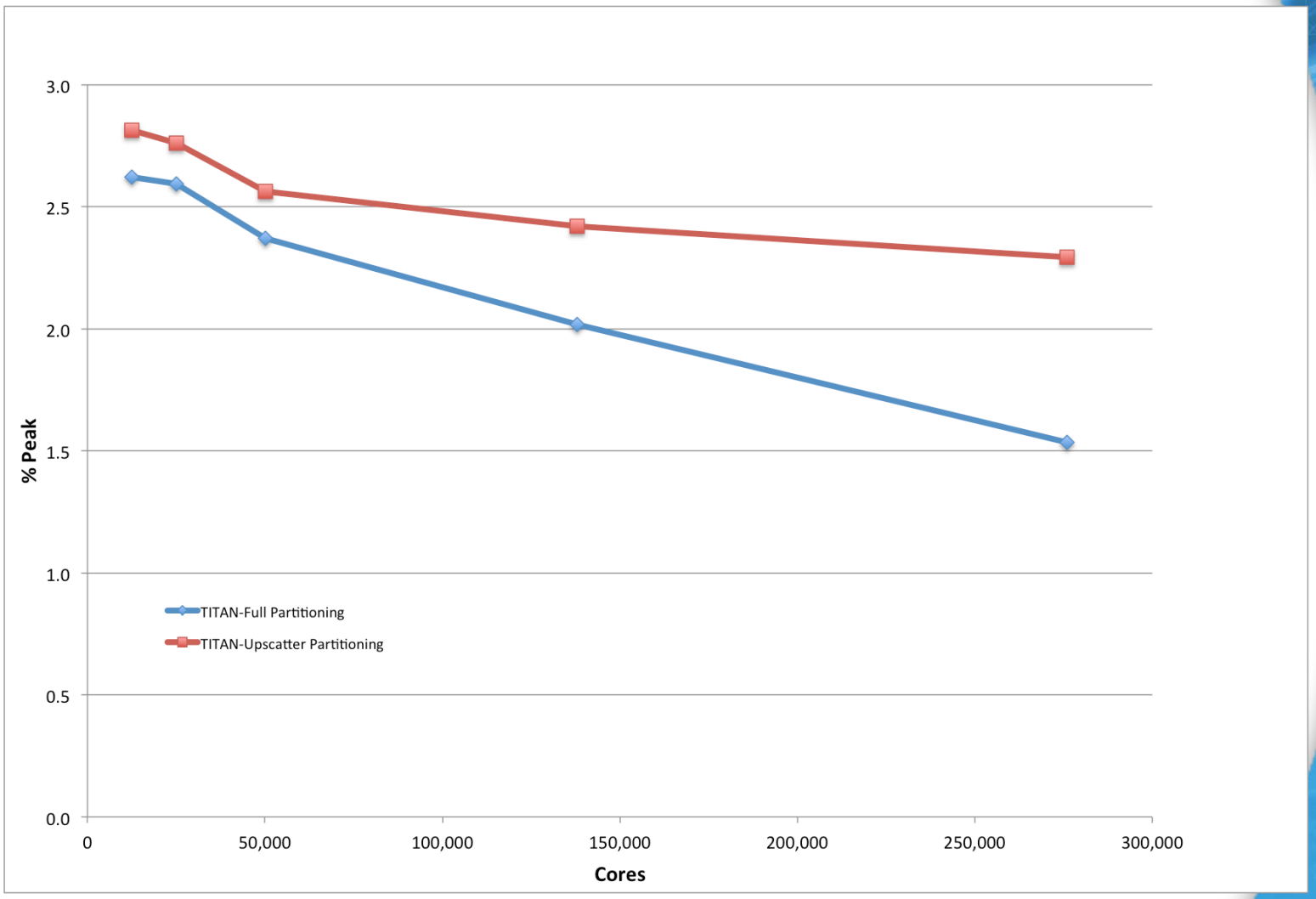
Full partitioning scales well to 275K cores

Improved interconnects + reduce-scatter have dramatically reduced global reduction cost

Upscatter partitioning more efficient at lower set counts

Roll-over occurs between 4 and 11 sets (5 and 2 groups per set) where serial work in GS solver dominates

Peak Performance on XK6



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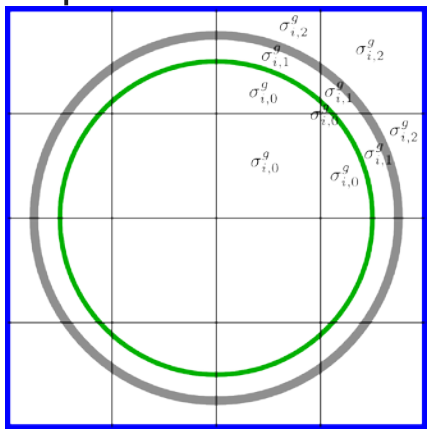
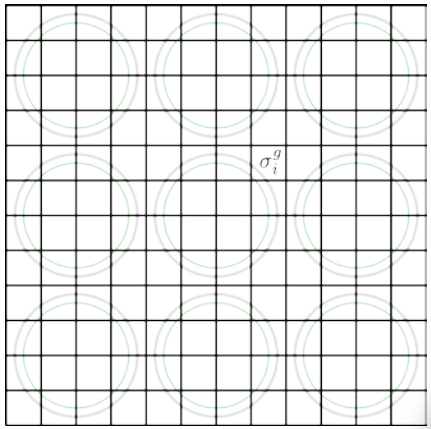
Discussion and Future Work

- We have demonstrated that the 3D transport problem can be solved, but…
  - Runtime is still an issue for practical engineering analysis
  - Depletion will create issues
  - IFBA pins require significantly more meshing, particularly as the energy-group structure is resolved
- Better coupling between 2 and 3D methods may be the short-to-medium term goal:
  - Depletion and cross section generation on highly resolved 2D models using MOC



Use fluxes from MOC to generate flux-weighted cross sections in each computational S_N cell



Denovo Framework

Thomas Evans
ORNL
CASL Roundtable 2012

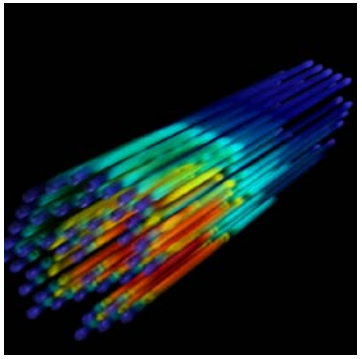
Outline

- Denovo Overview
- Denovo Architecture Features
  - Component-based design
  - Unit-Testing
  - Design-by-Contract ©
- Core-Simulator

Denovo Capabilities

- State of the art transport methods
  - 3D/2D, non-uniform, regular grid S_N
  - 2D MoC solver option
  - Multigroup energy, anisotropic P_N scattering
  - Forward/Adjoint
  - Fixed-source/*k*-eigenvalue
  - 6 spatial discretization algorithms
    - Linear and Trilinear discontinuous FE, step-characteristics, theta-weighted diamond, weighted diamond + flux-fixup
  - Parallel first-collision
    - Analytic ray-tracing (DR)
    - Monte Carlo (DR and DD)
  - Multiple quadratures
    - Level-symmetric
    - Generalized Legendre Product
    - Quadruple Range

- Modern, Innovative, High-Performance Solvers
  - Within-group solvers
    - Krylov (GMRES, BiCGStab) and source iteration
    - DSA preconditioning (SuperLU/ML-preconditioned CG/PCG)
  - Multigroup solvers
    - Transport Two-Grid upscatter acceleration of Gauss-Seidel
    - Krylov (GMRES, BiCGtab)
      - Multigrid preconditioning
  - Eigenvalue solvers
    - Power iteration (with rebalance)
      - CMFD acceleration (for MoC)
    - Krylov (Arnoldi)
    - RQI with multigrid preconditioning



Power distribution in a BWR assembly

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Denovo Capabilities

- Parallel Algorithms
  - Koch-Baker-Alcouffe (KBA) wavefront decomposition
  - Domain-replicated (DR) and domain-decomposed first-collision solvers
  - Multilevel energy decomposition
  - Parallel I/O built on SILO/HDF5

Core Neutronics Package in VERA Toolset
2012-13 INCITE Award
The Solution of 3D PWR Neutronics Benchmark Problems for CASL, 19 MCPU-HOURS
2010-11 INCITE Award
Uncertainty Quantification for Three Dimensional Reactor Assembly Simulations, 26 MCPU-HOURS
2010 ASCR Joule Code
2009-2011 2 ORNL LDRDs

- Advanced visualization, run-time, and development environment
  - multiple front-ends (HPC, SCALE, Python-bindings, core-neutronics)
  - Automated mesh generation from reactor metadata and combinatorial geometry
  - Direct connection to SCALE geometry and data (MG cross section processing)
  - Direct connection to MCNP input through ADVANTG
  - HDF5 output directly interfaced with VisIt
  - Built-in unit-testing and regression harness with DBC (353 separate tests)
  - Emacs-based code-development environment
  - Support for multiple external vendors
    - BLAS/LAPACK, TRILINOS (required)
    - BRLCAD, SUPERLU/METIS, SILO/HDF5 (optional)
    - MPI (toggle for parallel/serial builds)
    - SPRNG (required for MC module)
    - PAPI (optional instrumentation)

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Denovo Development Model

- Denovo is developed using an agile continuous-integration model
  - Each commit represents a stable version of the code base
  - Each commit is, in effect, a release of the code
    - all problems, except where otherwise documented, will run as expected
- Requirements for continuous-integration
  - Extensive unit-testing to insure code verification
  - Acceptance testing to verify numerics
  - Design-by-Contract© to enforce API correctness down to the functional level

Continous-Integration helps manage changing requirements that are common in scientific software projects

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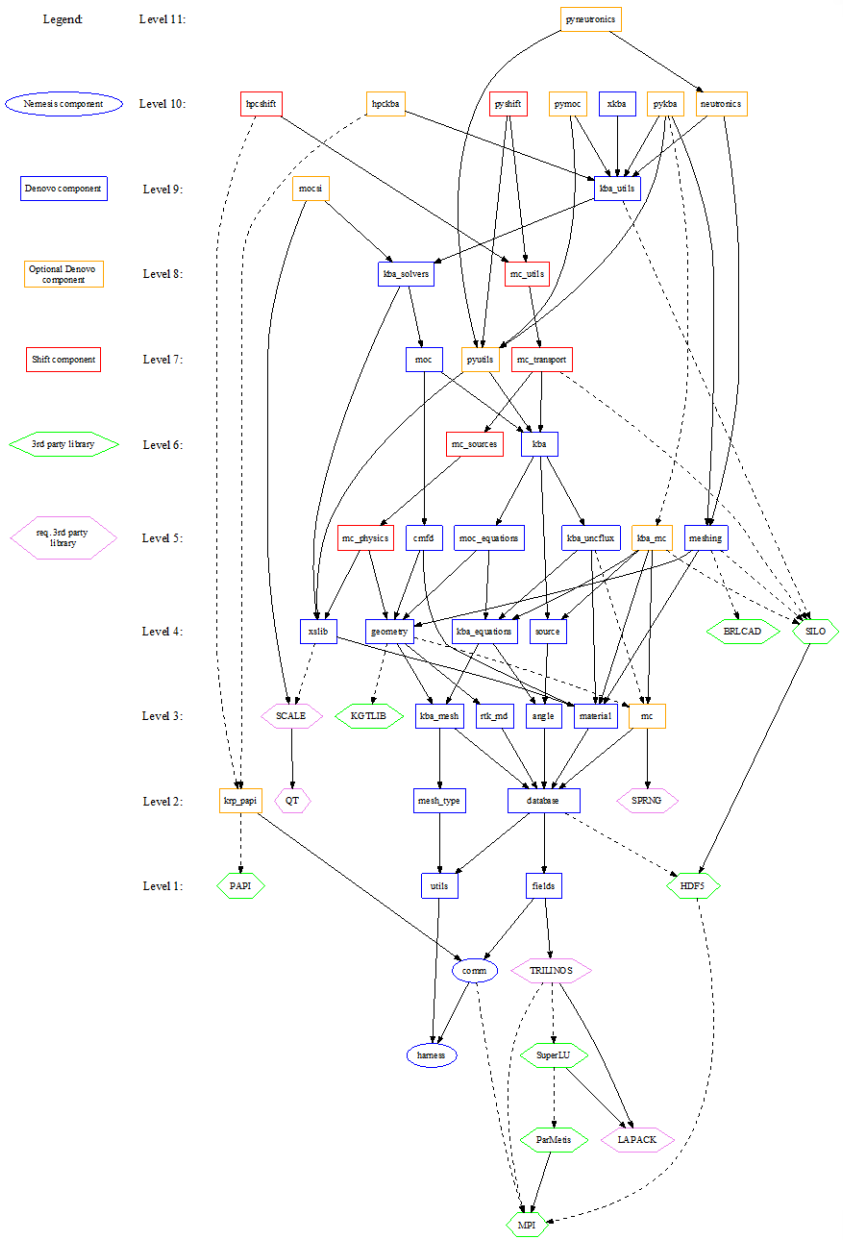
Component-Based Design

- dependencies are one-way (**acyclic design**)
- multiple front-ends use the same components
- most vendors can be toggled on/off (may limit some functionality)
- enables continuous-integration development model

Front-ends:

- neutronics
- pyneutronics
- pykba
- pyMOC
- hpckba
- xkba
- pyshift
- hpcshift



Multi-Language Architecture

- Optimize performance by dispatching as many operations as possible to BLAS
- Use of FORTRAN and C kernels provides highly optimizable code in deep loops
- Requires *contiguous* data containers at the top-level
- Use of templates and traits in C^{++} allows you to have your cake and it eat it too!

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Unit Testing

Unit Testing is a method of software verification

- It ensures that each part of the software performs its contracted task.
- The effectiveness of unit-testing is greatly enhanced by the following two code-design practices:
  - Acyclic code design
  - Design-by-Contract
- Enables continuous-integration development model

We practice a method of unit testing in which the unit test is written either before, or concurrently with, the executable code.

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Design-by-Contract©

- DBC enforces a function “contract” by testing the input, execution, and output of a function.
- In other words, DBC provides a software mechanism for enforcing a design contract on a function.
- DBC is also known as *Programming by Contract* and *Contract First Development*.
- See Meyer, Bertrand: *Design by Contract, in Advances in Object-Oriented Software Engineering*, eds. D. Mandrioli and B. Meyer, Prentice Hall, 1991, pp. 1-50 for more details.

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DBC Implementation

- Some languages (Eiffel, GNU C^2) have built in support for DBC.
- DBC is implemented in our codes using M4 (FORTRAN) or CPP (C/C^{++}).
- Types in C^{++} or FORTRAN modules are automatically checked by the compiler:
  - Require: input conditions
  - Check: execution conditions
  - Ensure: output conditions
- DBC macros can be toggled at compile time to avoid performance costs associated with in-code tests.

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Documentation

- Documentation in a code project can be classified in four general categories:
  - Algorithms, methods, and testing reports/manuals.
  - Configuration, build and development environment manuals.
  - User manuals.
  - Code-developer manuals.
- We use different tools depending upon the classification.
  - LaTeX/PDFLaTeX
    - algorithms, methods, testing reports/papers/manuals
  - Texinfo
    - configuration, build, IDE manuals
    - generate PDF, HTML, ASCII from same source
  - User Manuals
    - Sphinx
    - generate PDF and HTML from same source
  - Code-developer manuals
    - Doxygen

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Doxygen

```
/*!
 * \brief Calculate the even Spherical Harmonic.
 *
 * The \link http://www.gnu.org/software/gsl GSL (Gnu Scientific Library)
 * \endlink is used to calculate normalized associated Legendre Polynomials,
 * \f$\hat{P}_{lm}\f$ that are used to construct the even Spherical Harmonic,
 * \f$ Y^e_{lm}\f$.  The \f$\hat{P}_{lm}\f$ that are returned by the GSL are
 * defined:
 * \f[
    \hat{P}_{lm}(\cos\theta) = (-1)^m\sqrt{\frac{(2l+1)}{4\pi}
    \frac{(l-m)!}{(l+m)!}}
    P_{lm}(\cos\theta)
 * \f]
 * Thus, to calculate \f$ Y^e_{lm}\f$ requires the following:
 * \f[
    Y^e_{lm} = \sqrt{(2-\delta_{m0})}\hat{P}_{lm}\cos m\varphi
 * \f]
 *
 * \sa Spherical_Harmonics for the definition of \f$ Y^e_{lm}\f$.
 *
 * \param l \e l value of harmonic
 * \param m \e m value of harmonic
 * \param costheta \f$\cos\theta\f$
 * \param varphi \f$\varphi\f$
 */
double Spherical_Harmonics::Y_e(int    l,
                                int    m,
                                double costheta,
                                double varphi)
{
  // …
}
```

Comments are stored with code.

make autodoc

↓

documentation

Code Statistics

C++ Source Code	51,271
FORTRAN Source Code	1,209
Python Code	14,164
DBC Statements	8,329
Comments	103,280
Test Code	93,991

- Comments roughly 2-1 vs executable code
- 16% of the code is DBC contract statements
- Roughly 2x amount of code in individually compiled unit-tests as executable code

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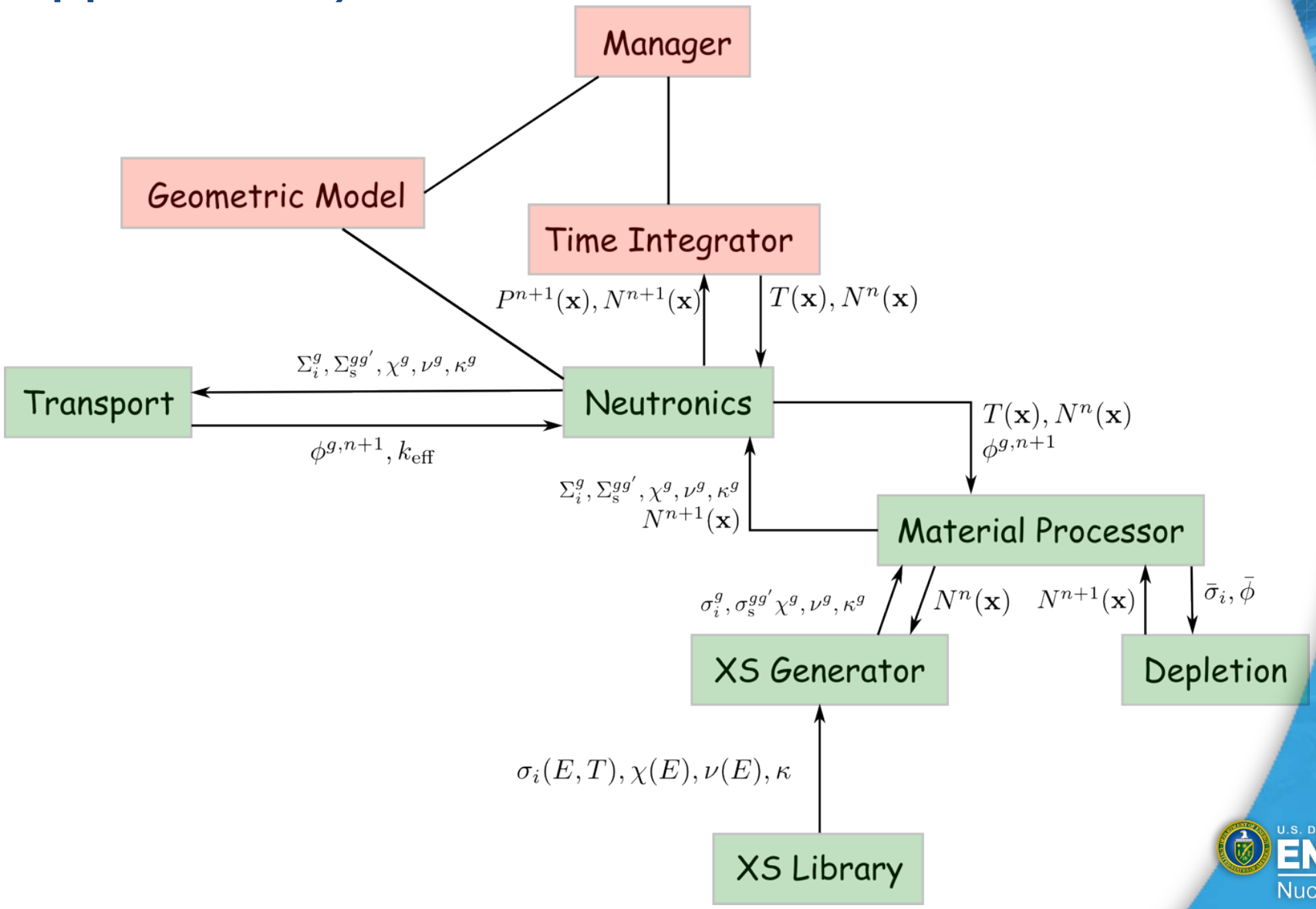
VERA (Virtual Environment for Reactor Applications)



Core-Simulator User Interface

ASCII Input (User)

```
STATE
  power 0.0
  flow  0.0
  xenon none
  boron 1000
  search 'boron' 1.0

CORE
  size 1
  apitch 21.5
  rated 17.673 557.7 2500 0.75
  boundary reflect

ASSEMBLY
  title "Westinghouse VANTAGE-5H Lattice"

  npin    17
  uo2    1 U21 10.257 / 2.110
  pitch  1.260
  cell 2  GT        0.561 0.602 / MOD ZR4
  cell 3  IT        0.559 0.605 / MOD ZR4
```

Preprocessor →

XML-Input


```
<ParameterList name="CASL_Problem_3">

<ParameterList id="10" name="Cell_1">
        <Parameter docString="" id="4" isDefault="false"
isUsed="true" name="id" type="int" value="1"/>
        <Parameter docString="" id="5" isDefault="false"
isUsed="true" name="mats" type="Array(string)" value="{uo2,
he, zirc}"/>
        <Parameter docString="" id="6" isDefault="false"
isUsed="true" name="mesh" type="int" value="8"/>
        <Parameter docString="" id="7" isDefault="false"
isUsed="true" name="num_rings" type="int" value="3"/>
        <Parameter docString="" id="8" isDefault="false"
isUsed="true" name="radii" type="Array(double)"
value="{0.4096, 0.418, 0.475}"/>
        <Parameter docString="" id="9" isDefault="false"
isUsed="true" name="type" type="string" value="fuel"/>
      </ParameterList>
      <ParameterList id="17" name="Cell_100">
```


↓

Core-Simulator

1. User prepares engineering spec in an ASCII file
2. Preprocessor converts ASCII input into hierarchical XML file
3. Core-simulator reads XML file and runs problem

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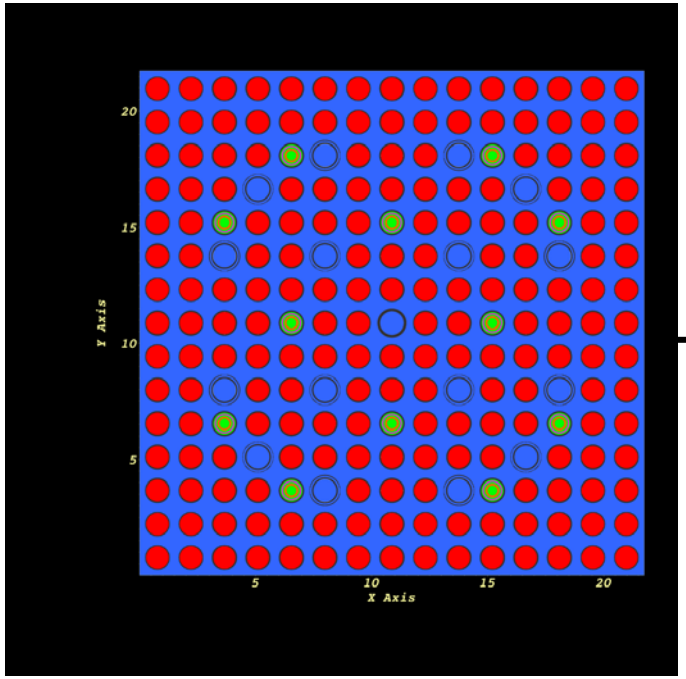
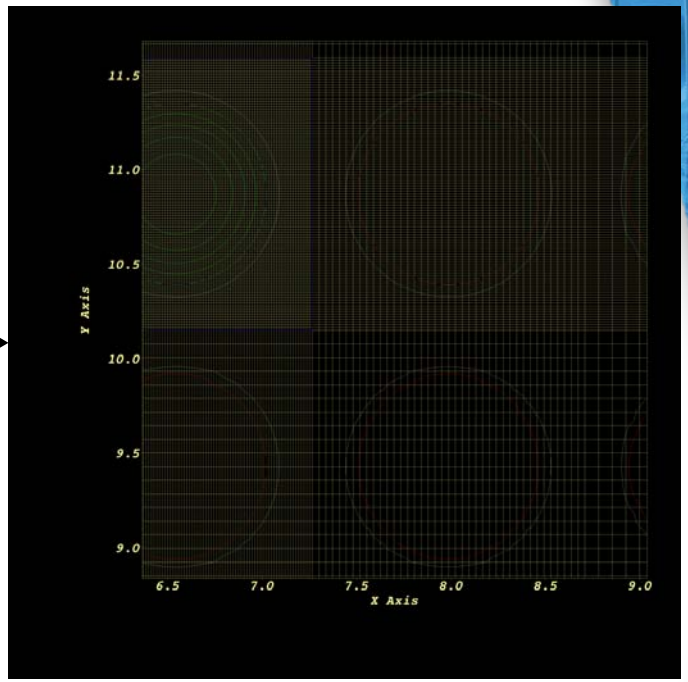
Core-Simulator Problem Initialization



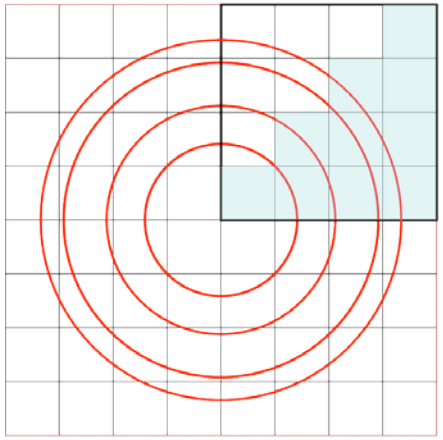
Mesh generation →



1. Setup mesh parameters
2. Partition problem (energy-space-angle)
3. Automatic mesh generation
4. Initialize material cross-section processor (XSProc)
5. Distribute cross-section data
6. Generate cross sections and assign to mesh
7. Transport
8. Output

Automated Mesh Generation

- Mesh generation and partitioning automated from meta-data description
  - Volume fractions of each material preserved to numerical precision
    - Analytic integration determines volume fractions of each unique region within a computational cell
  - Uses symmetry to reduce mesh-time



  - Each unique geometrical, parameterized pin is meshed only once
    - KD-trees used to store uniquely meshed geometric pins with specified mesh levels
  - For a full assembly with 92 axial cells, parallel mesh generation required 2.8 seconds
    - Cores should not require dramatically more time because there will not be many additional pins to mesh

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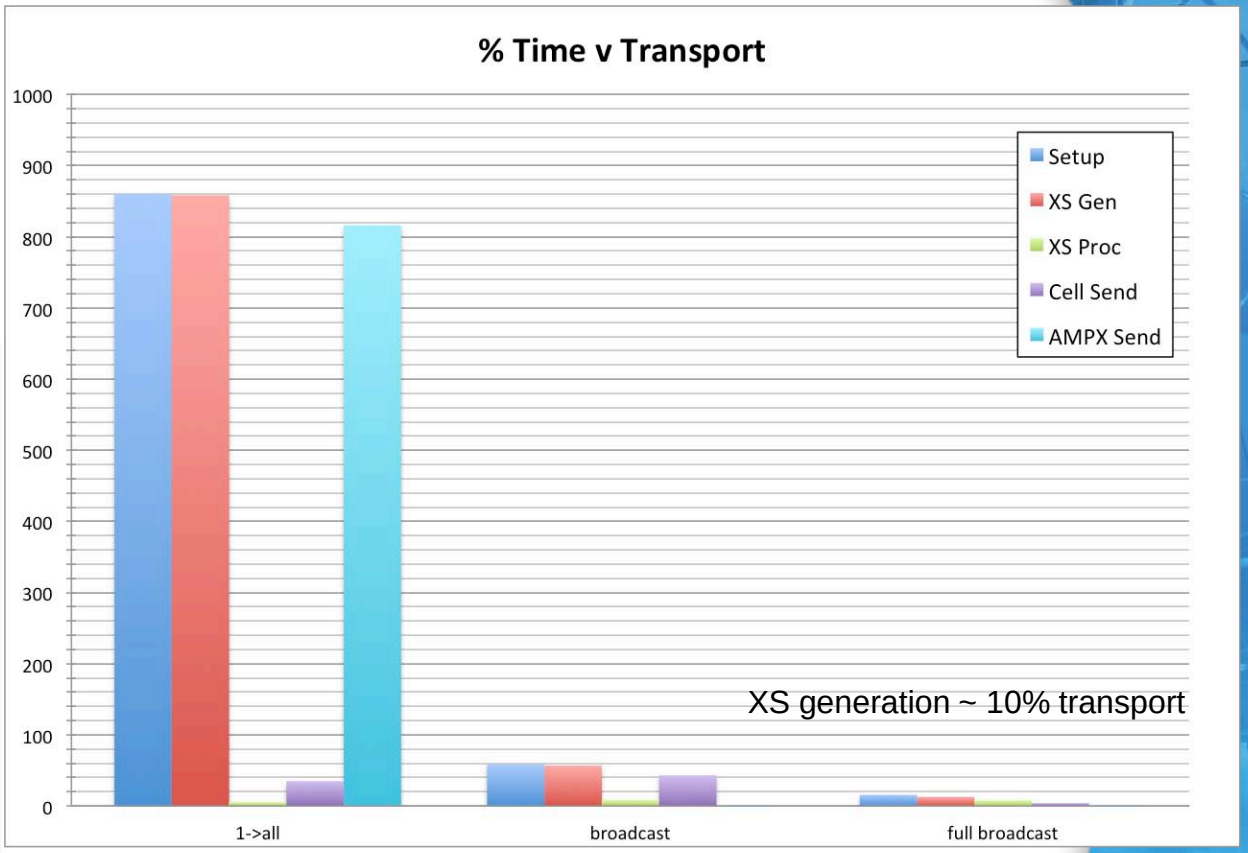
Runtime Parameters

Cores	69,632
Cells	1,752,048
Groups	238
Angles	256
DoF	106,748,780,544

```
                Routine   Max Fraction
========================================
          AMPX_broadcast     4.0206e-04
          AMPX_serialize     9.8271e-05
          Cell_broadcast     1.0068e-02
          Cell_serialize     1.0725e-05
                 Fulcrum     5.2216e-03
        Mesh_generation      1.0725e-03
                 Output      7.1948e-01
  Set_all_reduction_field    7.3006e-07
    Set_reduction_source     1.7976e-05
Set_sum_scatter_reduction    1.3686e-02
                 Setup       3.7898e-02
                 Sweep       1.8609e-01
     Sweep_Source_Build      1.5698e-02
  Sweep_Source_Initialize    2.5665e-02
             Transport       2.4262e-01
     Transport_Operator      1.9519e-01
                 XSProc      1.9774e-02
          XS_generation      3.0881e-02
            XS_message       1.0692e-02
========================================
```



Transport solve ~ 10 minutes

Output

0.946	0.935	0.937	0.947	0.959	0.969	0.967	0.967	0.971	0.967	0.967	0.969	0.959	0.947	0.937	0.935	0.946
0.935	0.929	0.938	0.959	0.982	1.014	0.987	0.986	1.013	0.986	0.987	1.014	0.982	0.959	0.938	0.929	0.935
0.937	0.938	0.969	1.022	1.046		1.033	1.030		1.030	1.033		1.046	1.022	0.969	0.938	0.937
0.947	0.959	1.022		1.065	1.055	1.011	1.006	1.036	1.006	1.011	1.055	1.065		1.022	0.959	0.947
0.959	0.982	1.046	1.065	1.043	1.054	1.013	1.009	1.039	1.009	1.013	1.054	1.043	1.065	1.046	0.982	0.959
0.969	1.014		1.055	1.054		1.043	1.040		1.040	1.043		1.054	1.055		1.014	0.969
0.967	0.987	1.033	1.011	1.013	1.043	1.010	1.008	1.039	1.008	1.010	1.043	1.013	1.011	1.033	0.987	0.967
0.967	0.986	1.030	1.006	1.009	1.040	1.008	1.007	1.037	1.007	1.008	1.040	1.009	1.006	1.030	0.986	0.967
0.971	1.013		1.036	1.039		1.039	1.037		1.037	1.039		1.039	1.036		1.013	0.971
0.967	0.986	1.030	1.006	1.009	1.040	1.008	1.007	1.037	1.007	1.008	1.040	1.009	1.006	1.030	0.986	0.967
0.967	0.987	1.033	1.011	1.013	1.043	1.010	1.008	1.039	1.008	1.010	1.043	1.013	1.011	1.033	0.987	0.967
0.969	1.014		1.055	1.054		1.043	1.040		1.040	1.043		1.054	1.055		1.014	0.969
0.959	0.982	1.046	1.065	1.043	1.054	1.013	1.009	1.039	1.009	1.013	1.054	1.043	1.065	1.046	0.982	0.959
0.947	0.959	1.022		1.065	1.055	1.011	1.006	1.036	1.006	1.011	1.055	1.065		1.022	0.959	0.947
0.937	0.938	0.969	1.022	1.046		1.033	1.030		1.030	1.033		1.046	1.022	0.969	0.938	0.937
0.935	0.929	0.938	0.959	0.982	1.014	0.987	0.986	1.013	0.986	0.987	1.014	0.982	0.959	0.938	0.929	0.935
0.946	0.935	0.937	0.947	0.959	0.969	0.967	0.967	0.971	0.967	0.967	0.969	0.959	0.947	0.937	0.935	0.946

Two SILO/HDF5 Files

Integrated Output

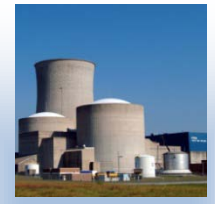
- Integrated 2D pin-power outputs
- Integrated 3D pin-power outputs
  - User-defined axial level

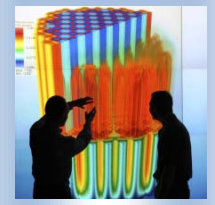
Fine-mesh output

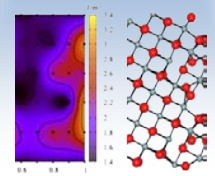
- Groupwise scalar fluxes
- Power (per computational cell)

AVOP

- AMA VERA output processor
- Library that enables AMA staff to interrogate integrated output files
- Enables custom comparisons between code outputs







CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

DeCART/STAR-CCM+ and MPACT

B Collins B. Kochunas
T. Downar et al.

University of Michigan

CASL
Consortium for Advanced Simulation of LWRs

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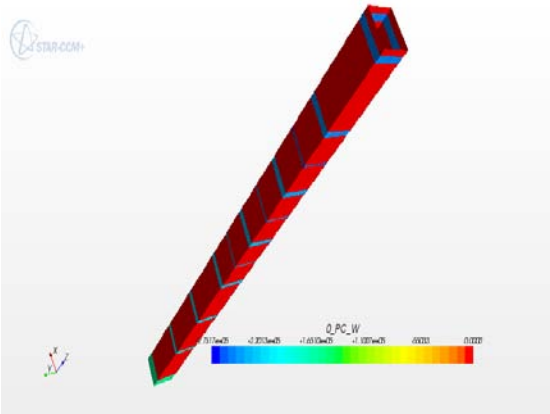
Outline

- Introduction
- Coupled CFD/Neutronics
- “Semi-Retirement” of DeCART
- MPACT
- Summary and Path Forward

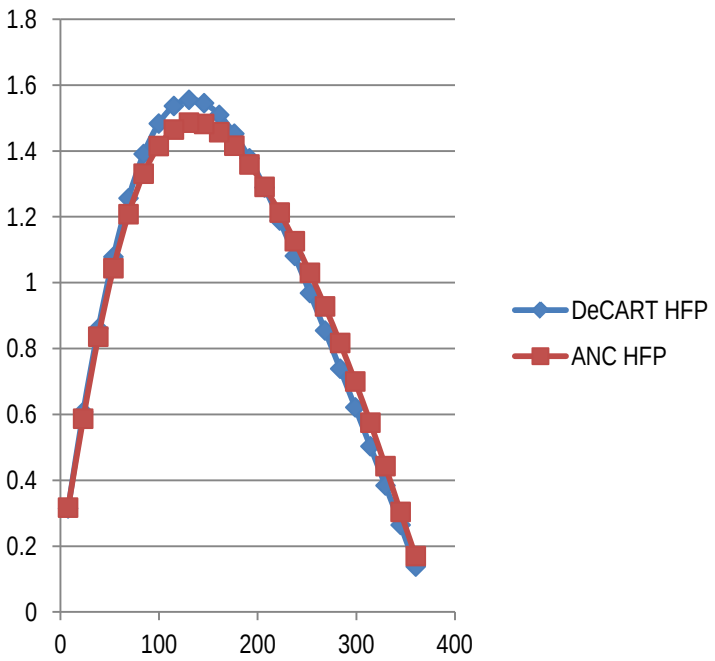
Fall 2010 L1: CASL.Y1.02

L1: CASL.Y1.02 - (12/31/10)

Apply a baseline transport (e.g. DeCART) and CFD (e.g. STAR-CCM+) capability with loose coupling to a PWR sub-core scenario to demonstrate feedback coupling and contrast predictions with WEC coupled tool predictions.

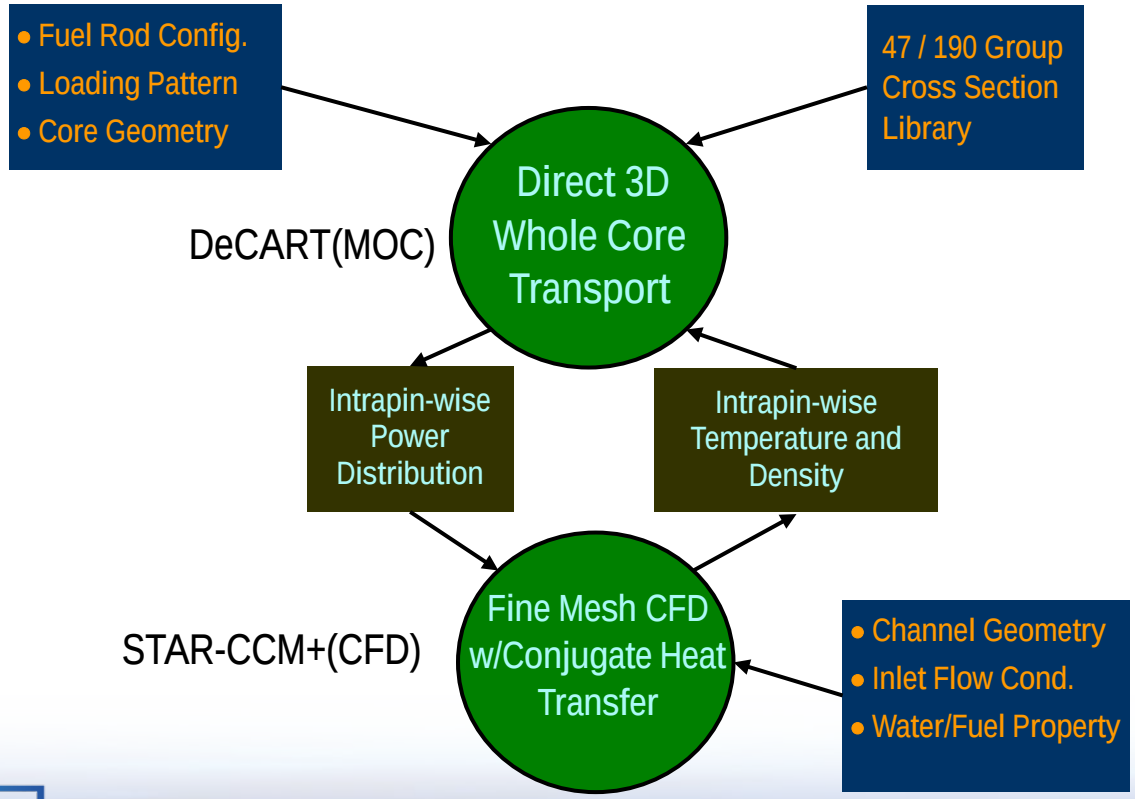


DeCART vs ANC Axial Power

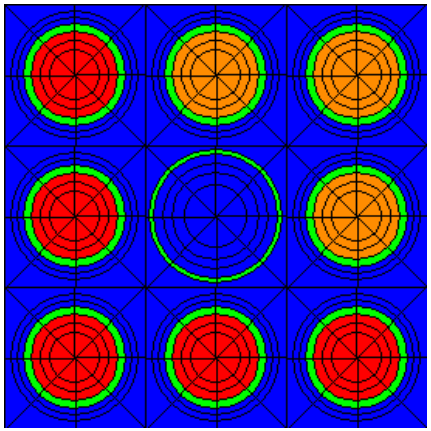


Coupling CFD / Neutronics

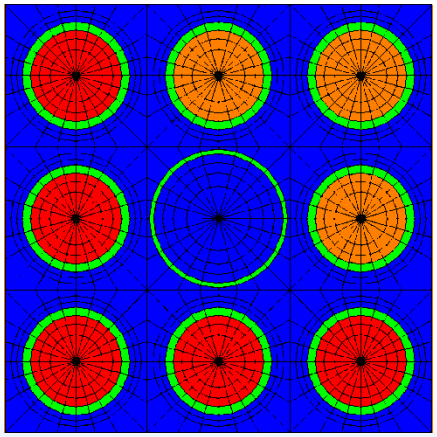
- Coupled using fixed point Gauss-Siedel iteration
- Parallel file I/O data transfers
- DeCART handles all mesh mapping via volume mapping



DeCART mesh

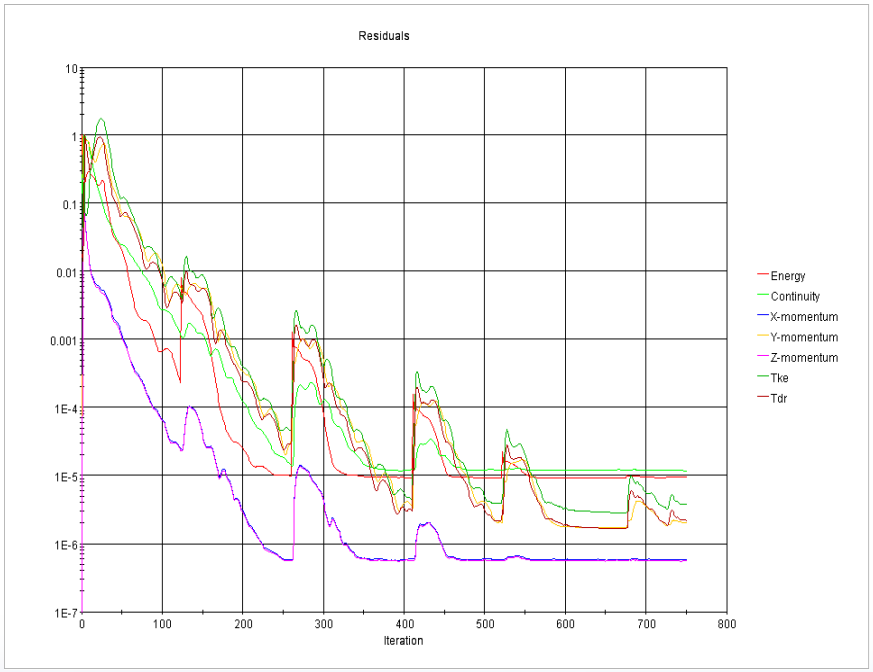


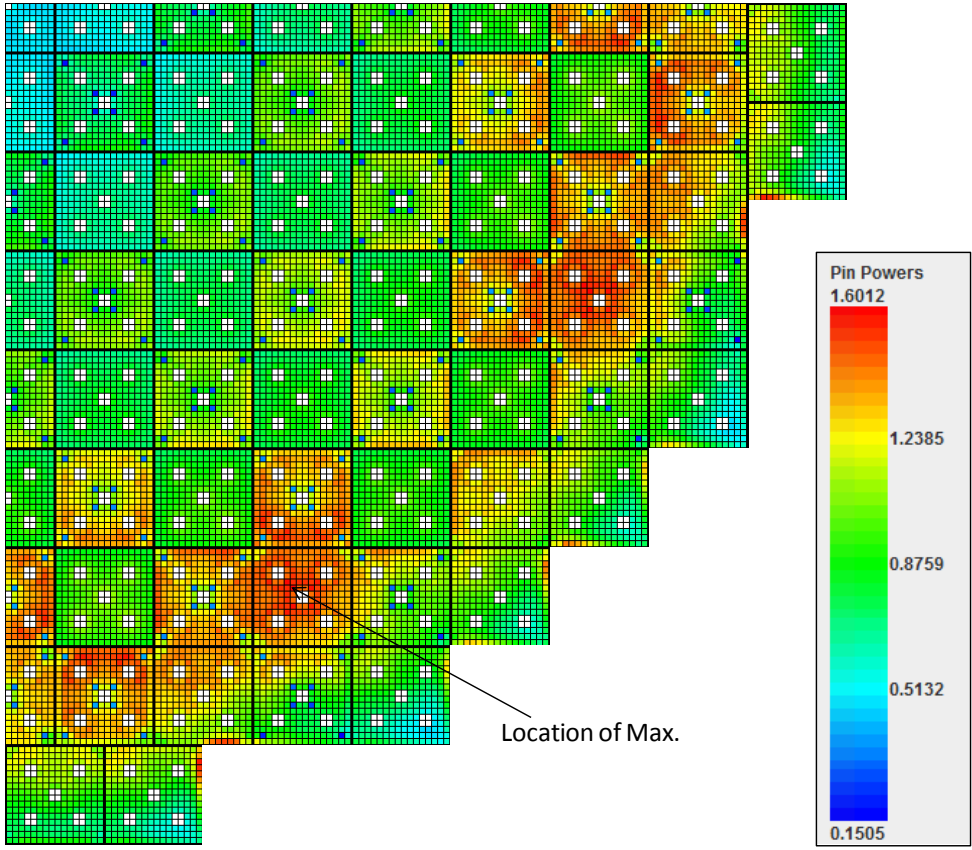
STAR-CCM+ mesh



Spring 2011 Ribbon-Cutting: Full-core 3D MOC transport (2D/1D, pin-resolved) DeCART coupled to STAR-CCM+

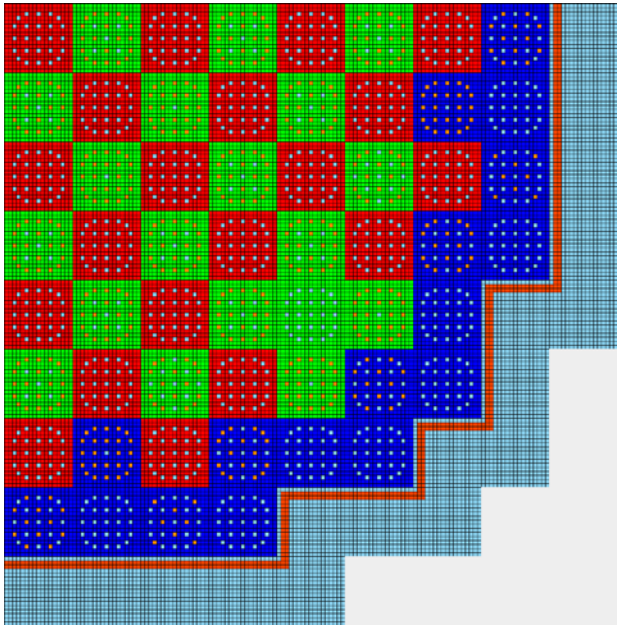
- STAR-CCM+ was run with 256 processors
- DeCART was run with 80 processors



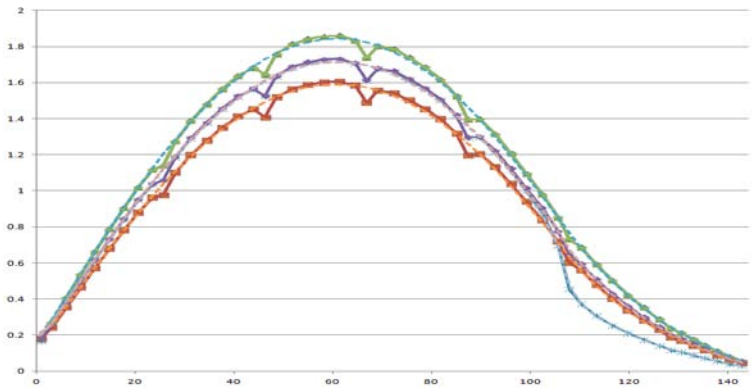


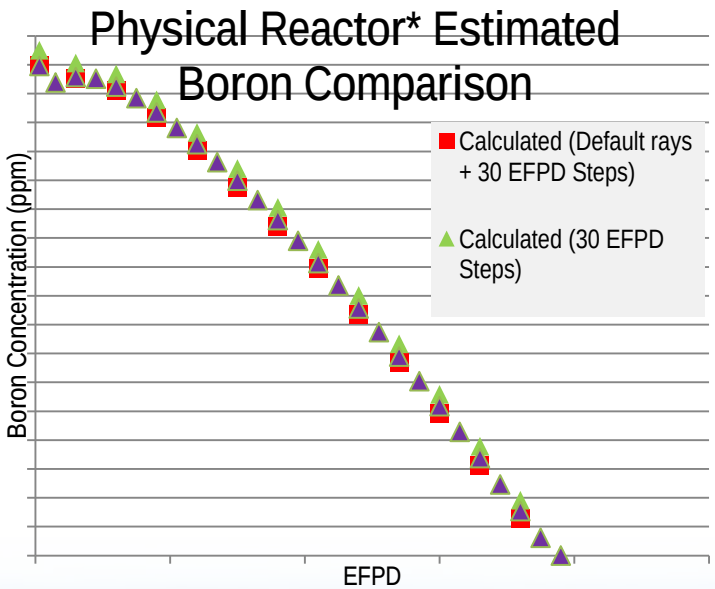
Winter 2012 Watts Bar I Depletion w/ DeCART

- Explicit Representation of Actual Core
- Cycle 1 Comparison w/ Plant Data

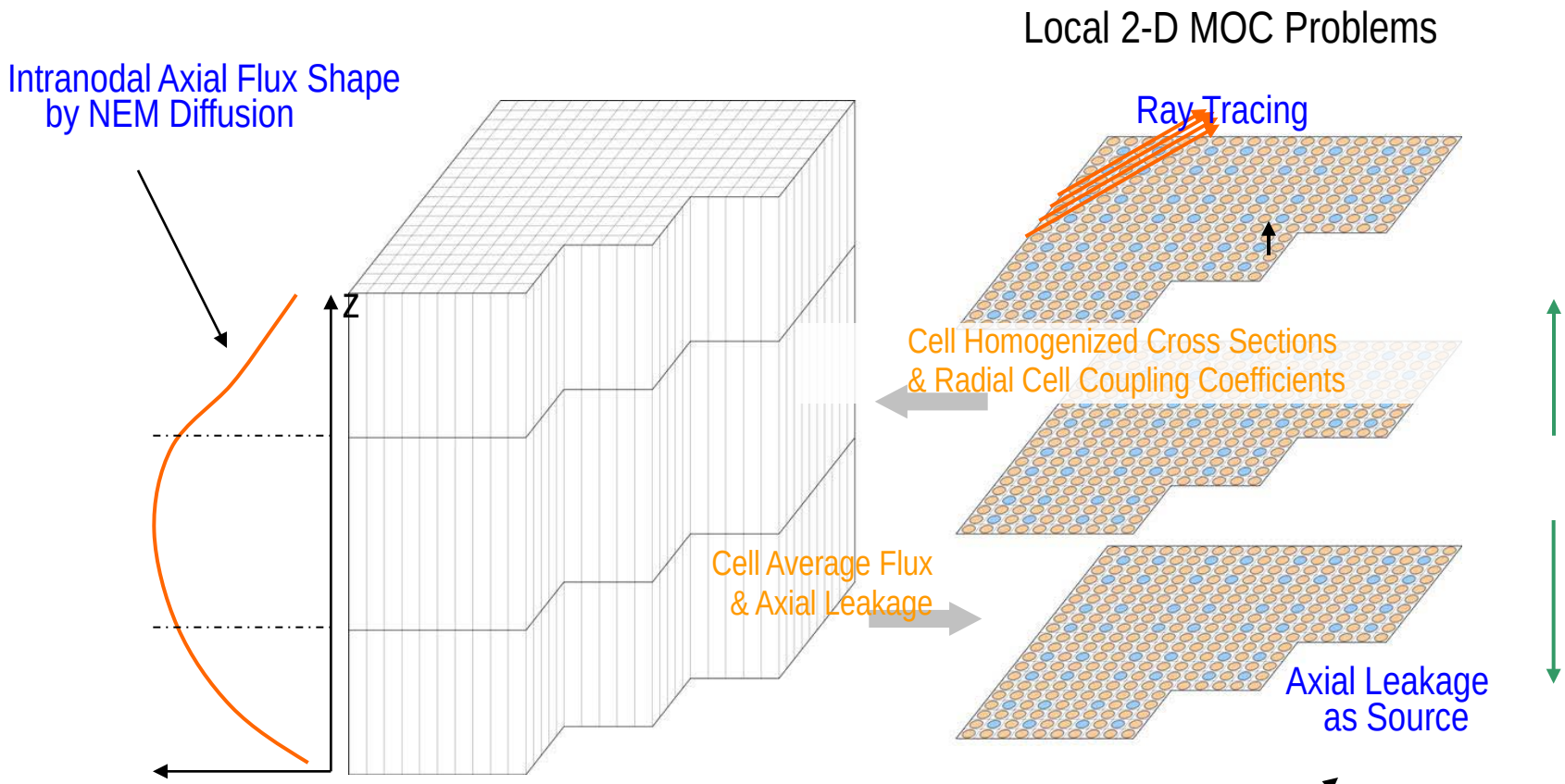


Axial Power Shape





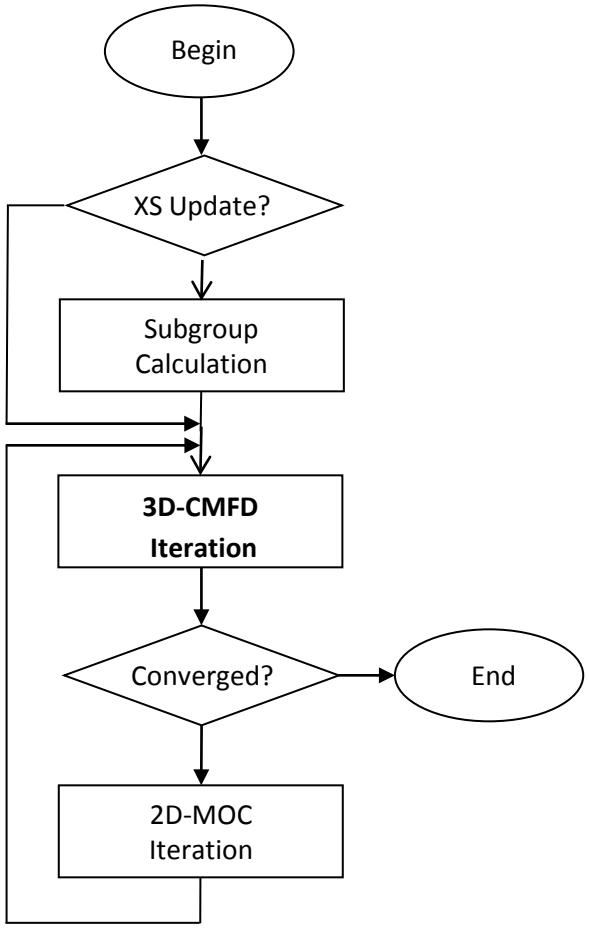
2-D / 1-D Convergence Issues: Axial Mesh Refinement



$$\left(\eta_m \frac{\partial \varphi_g^{m,n}}{\partial x} + \varepsilon_m \frac{\partial \varphi_g^{m,n}}{\partial y}\right) + \Sigma_{tg}\varphi_g^{m,n} = \frac{1}{4\pi}\left(\chi_g \psi^n + \sum_{g'=1}^{G} \Sigma_{gg'}\phi_{g'}^n\right) - \frac{\mu_m}{h_z}\left(\varphi_{gT}^m - \varphi_{gB}^m\right) + \frac{1}{4\pi} S_{tr}^{g,n}$$

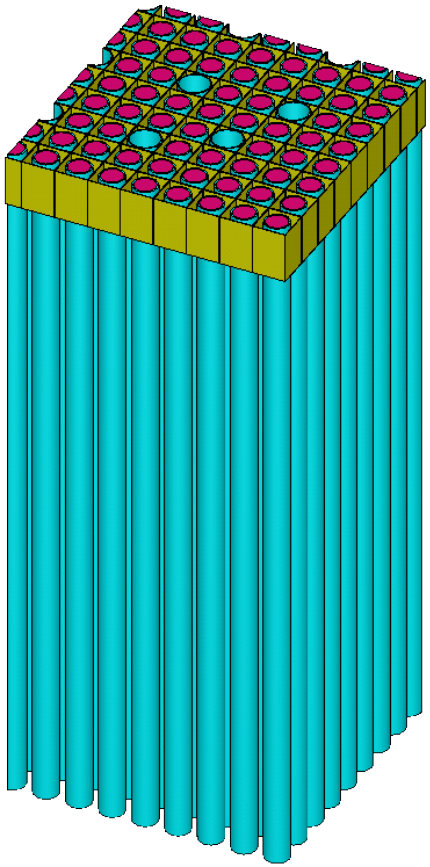
3D-CMFD - Overview

- Coarse Mesh Finite Difference (CMFD) used to accelerate multigroup eigenvalue problem by spatially homogenizing each pin
- Old CMFD version sweeps over planes (reduces memory requirements and improves parallelism, but limits refinement of axial mesh)
- New CMFD builds and solves the complete 3D matrix (increases memory requirements and reduces parallelism, but allows refinement of axial mesh).



Quarter Assembly with Grid Spacer

- Quarter-assembly (17x17) consisting of 24 planes in the fuel region with axial discretization of 1 cm each and 2 planes in the spacer grid at 0.9525 cm each.
- This problem did **not** run with standard CMFD in DeCART, but able to run with 3D-CMFD. (Results processed by AMA /A. Godfrey).



Results with New CMFD

Eigenvalue:

	Eigenvalue	Sigma	Difference
CE KENO v6	1.17573	11	---
DENOVO	1.17401	---	-172
DeCART	1.17729	---	327.5

Axially Integrated Pin Powers:

1.036	1.010							
1.036	1.010	1.011						
	1.036	1.037						
1.034	1.009	1.012	1.044	1.033				
1.031	1.006	1.009	1.044	1.051				
	1.025	1.027		1.036	1.017	0.974		
1.011	0.989	0.989	1.011	0.984	0.965	0.949	0.940	
0.977	0.973	0.972	0.974	0.965	0.956	0.947	0.943	0.949
Max	**1.051**		**Min**	**0.940**		**Avg**	**1.000**	

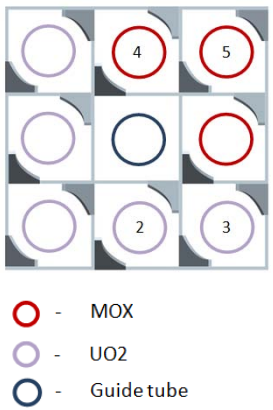
DeCART Powers

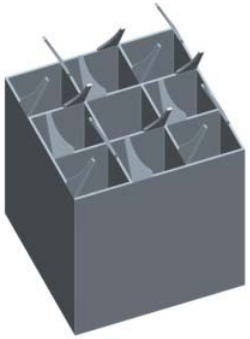
0.00%	-0.04%							
-0.02%	-0.01%	0.02%						
	-0.09%	-0.07%						
-0.01%	0.05%	0.02%	-0.05%	0.16%				
-0.08%	-0.04%	0.03%	-0.02%	0.11%				
	-0.02%	0.00%		0.15%	0.04%	0.02%		
0.07%	-0.02%	0.03%	0.00%	0.05%	-0.07%	0.02%	0.02%	
-0.05%	-0.02%	-0.02%	-0.13%	0.01%	-0.04%	0.00%	0.01%	0.06%
Max	**0.16%**		**Min**	**-0.13%**		**RMS**	**0.06%**	

DeCART-KENO

CRUD Challenge Problem: Coupled Crud/TH/Neutronics simulation required to capture feedback mechanisms

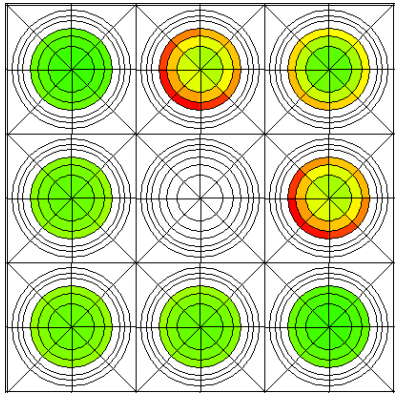
Test case: 3x3 fuel assembly (DeCart/STAR-CCM+)*





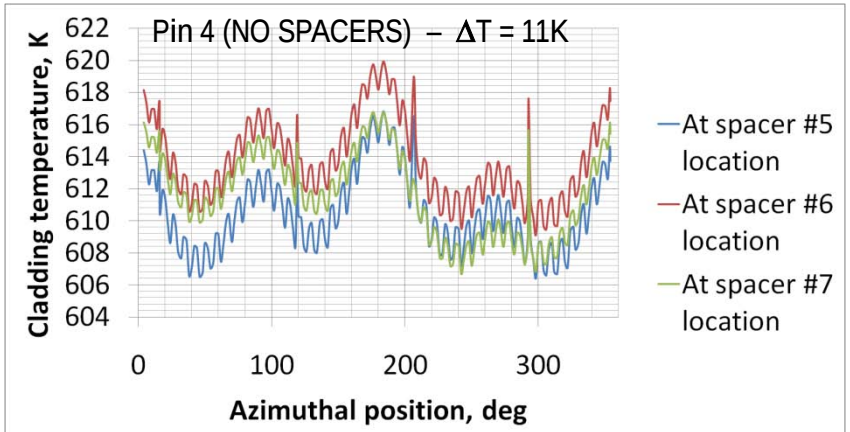
Spacer with mixing vanes

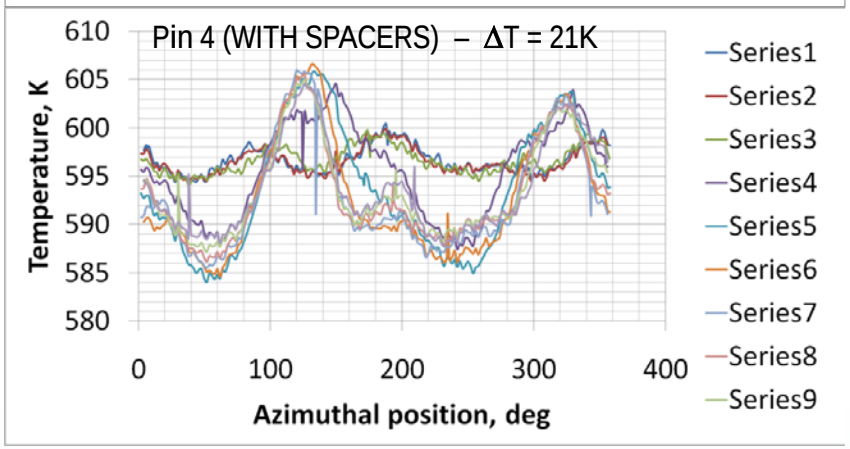
DeCart
power distribution



Large azimuthal and pin-by-pin variation of power

STAR-CCM+
Azimuthal cladding temperature profiles

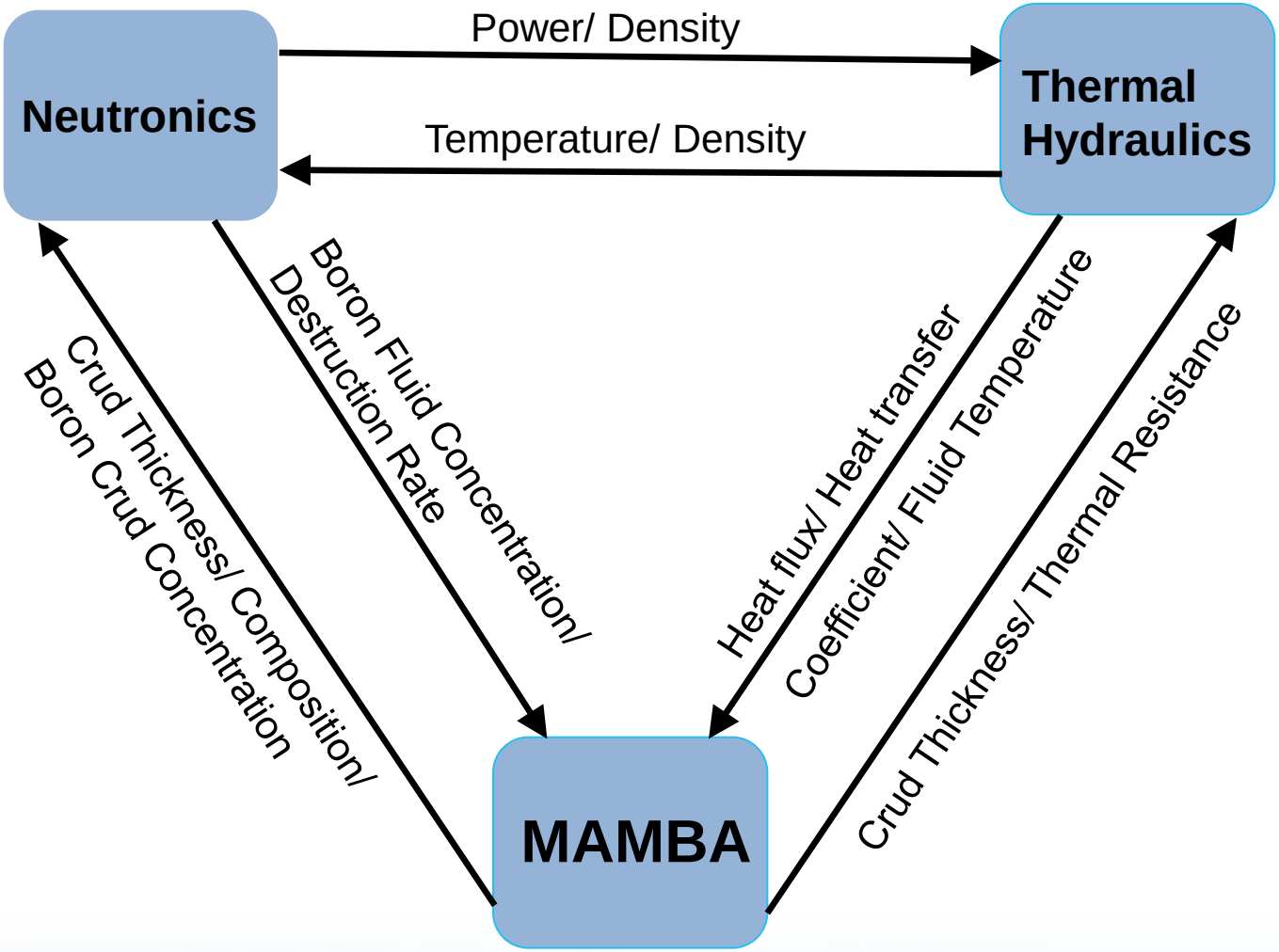




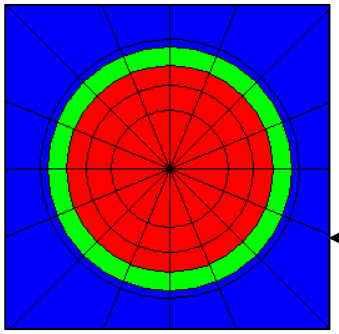
Large azimuthal variation in fluid/cladding temperature enhanced by presence of fuel spacers

* CASL THM Workshop Sandia National Laboratory December 14-15, 2011

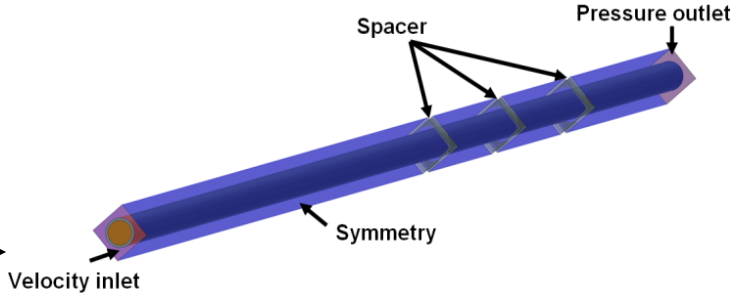
Interfaces were defined for coupling MAMBA with STAR-CCM+ and DeCART



CRUD Challenge Problem Results: Single Pin Analysis

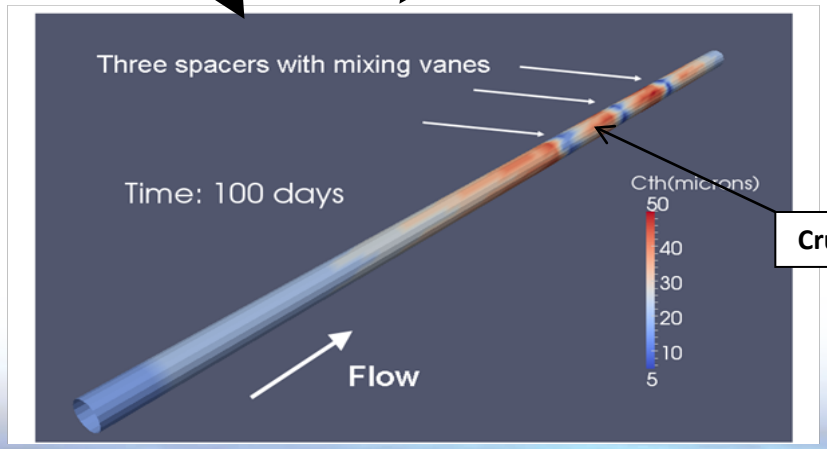


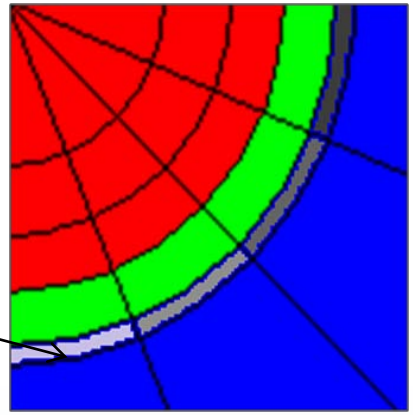
5000 Spatial Mesh
47 groups
128 angles
200 depletable isotopes
15-30 day timesteps



1.7M Spatial Mesh
~4.5M with all grids
7 unknowns
No temporal dependence

25000 Spatial Mesh
5 micron radial
20 degree azimuthal
5 cm axial
15 day timesteps





MPACT

- Introduction
- Code Architecture
- MPACT by the numbers
- Software Development Process
- Features
  - User Interface
  - Geometry and Ray Tracing
  - Transport
  - Cross sections
- Near Term Development Plan

Introduction

- **MPACT** Michigan Parallel Characteristics based Transport
  - Started development in Fall 2011
- 8 active developers and 3 Faculty
  - 5 PhD students
  - 1 Masters, 1 Post-MS & 1 Post-doc
  - Professors Downar, Martin, Larsen
- Written in FORTRAN 2003
  - Developed using GCC 4.6.1 and Intel 12.1 for Linux and Windows
- Modern software practices
  - Version control with Git
  - CMake based build system
  - Automated testing
  - Development process managed with Trac
  - Doxygen generated documentation
- Releases at least every 3 months

MPACT Code Layout

MPACT

Functional Control
Currently has power iteration routine

MPACT_UI

Process input
Output writing
Visualization

MPACT_MOC

3D MOC
2D MOC

MPACT_XS

Subgroup
ESSM
AMPX M/W Library
HELIOS Library
Benchmark Library

MPACT_REACTOR

Reactor Geometry
Decompose domain
Ray tracing routines

MPACT_UTIL

MPI
Timers
File I/O
Error Handling
BLAS Interface

MPACT Statistics

Metric		MPACT v0.1.0 January, 2012	MPACT 0.1.2 March, 2012	MPACT Current
Lines of Code	Source Code	21,212	31,072	40,819
	Unit Test Code	20,970	25,586	36,403
	Comments	12,635	17,528	25,581
	Blank Lines	2,373	2,949	4,290
	Total	57,190	77,135	107,093
Unit Tests		28	29	34
File Coverage		88.89%	95.92%	96.36%
Function Coverage		93.65%	94.13%	96.11%
Block Coverage		88.44%	87.74%	91.33%

MOC Basics

Propagation of flux along a characteristic segment

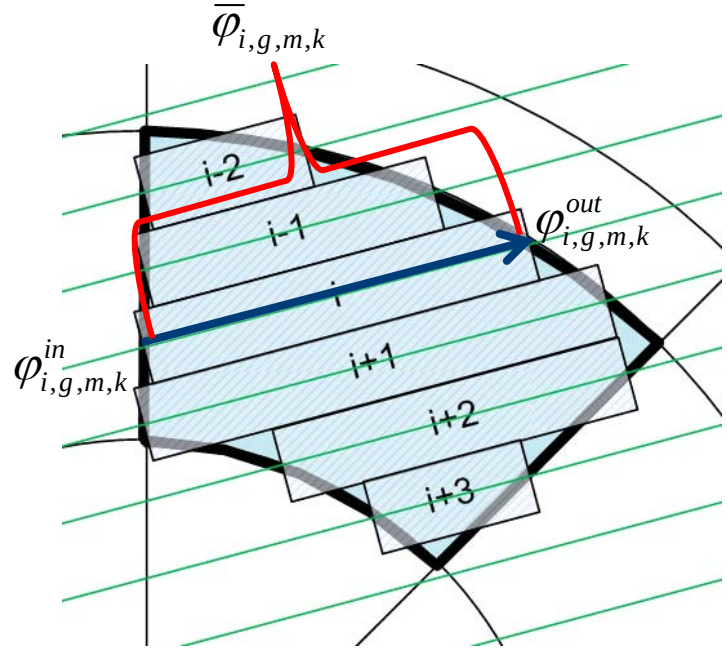
$$\varphi_{i,g,m,k}^{out} = \varphi_{i,g,m,k}^{in} \exp\left(-\Sigma_{t,i,g} s_{i,k,m}\right) + \frac{q_{i,g,m}}{\Sigma_{t,i,g}}\left[1 - \exp\left(-\Sigma_{t,i,g} s_{i,k,m}\right)\right]$$

Segment average angular flux

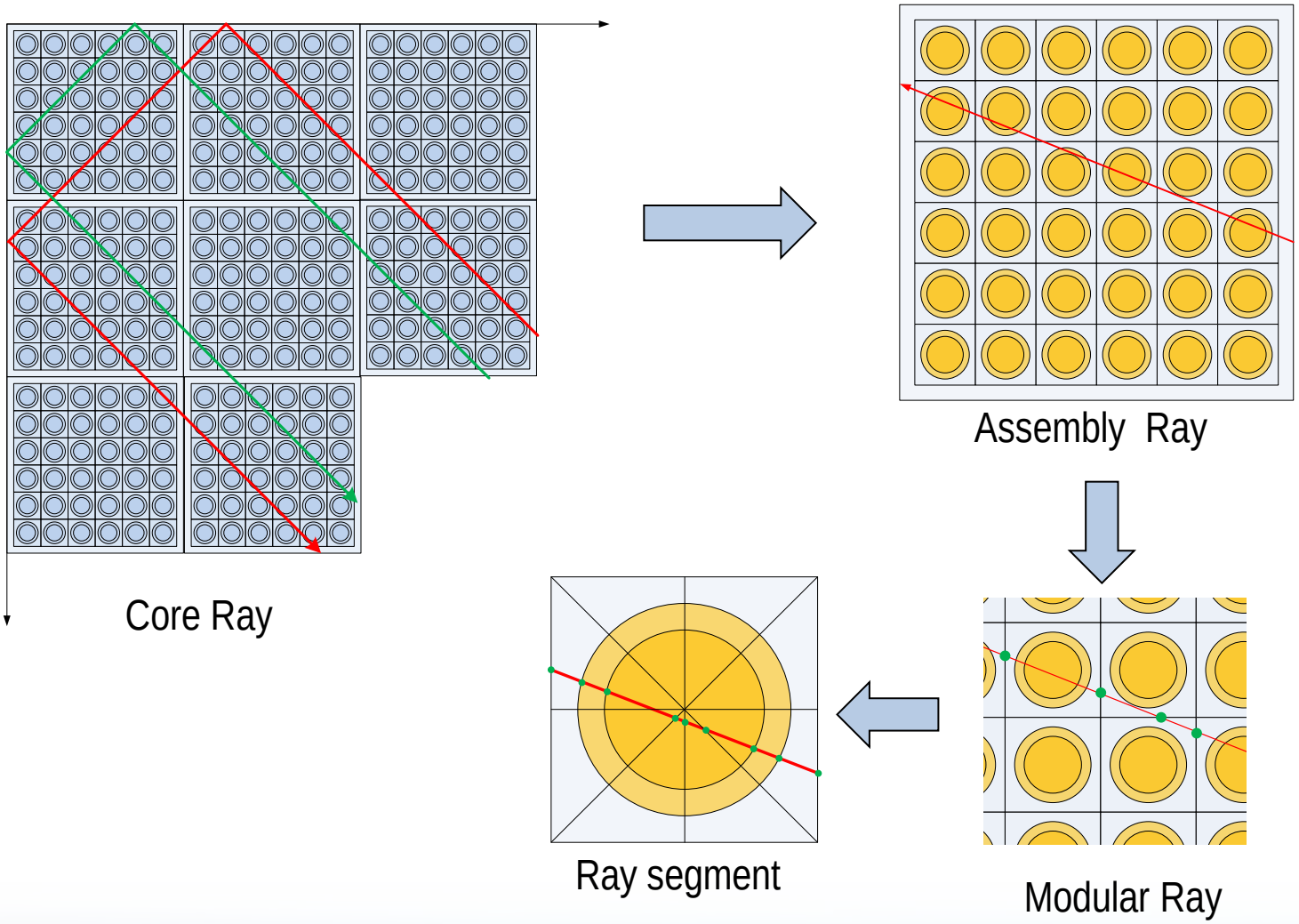
$$\overline{\varphi}_{i,g,m,k} = \frac{\varphi_{i,g,m,k}^{in} - \varphi_{i,g,m,k}^{out}}{\Sigma_{t,i,g} s_{i,k,m}} + \frac{q_{i,g,m}}{\Sigma_{t,i,g}}$$

Region average angular flux

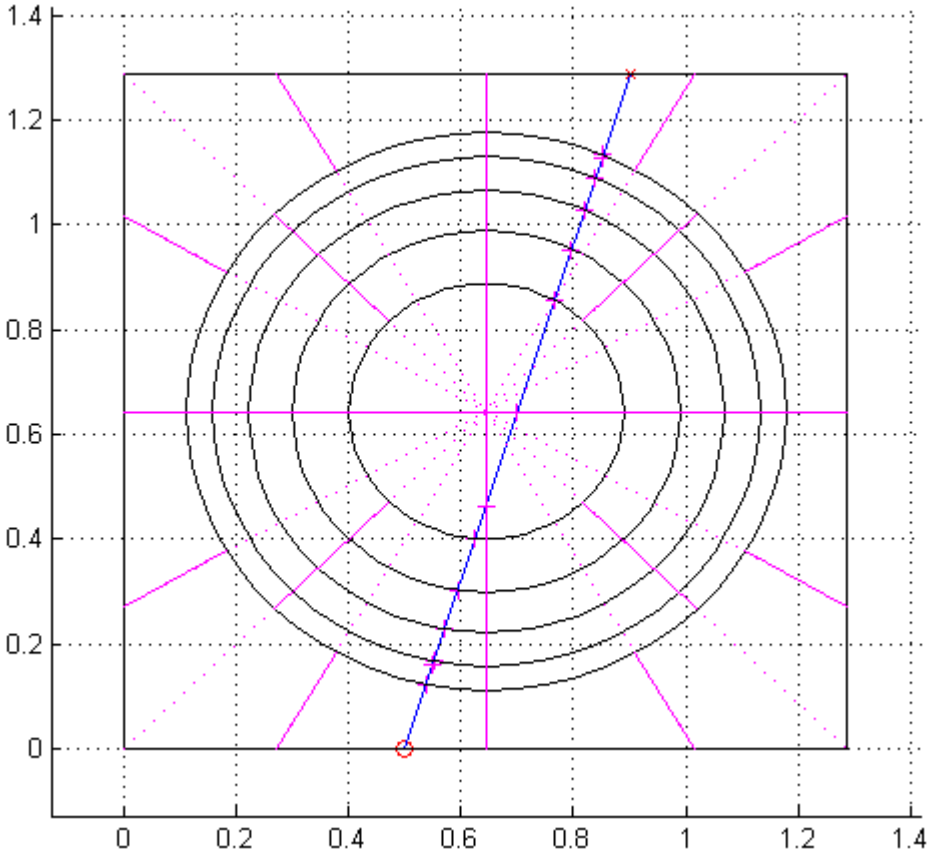
$$\overline{\varphi}_{i,g,m} = \frac{\sum_k \overline{\varphi}_{i,g,m,k} s_{i,k,m} \delta A_{k,m}}{\sum_k s_{i,k,m} \delta A_{k,m}}$$

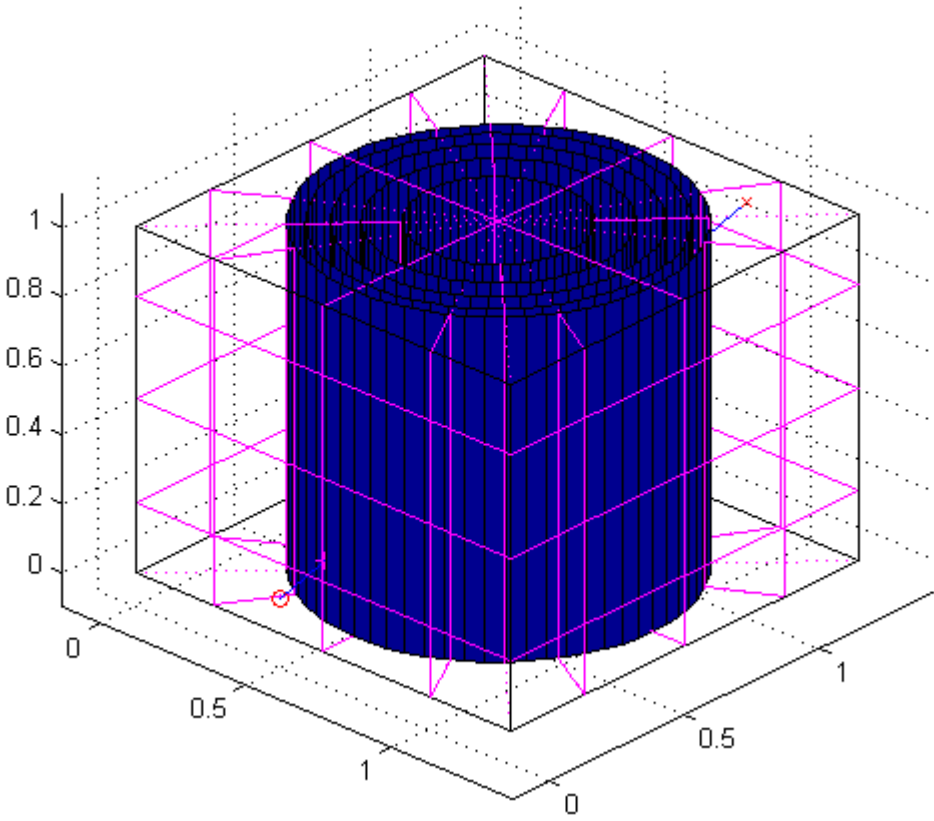


2D Modular Ray Tracing

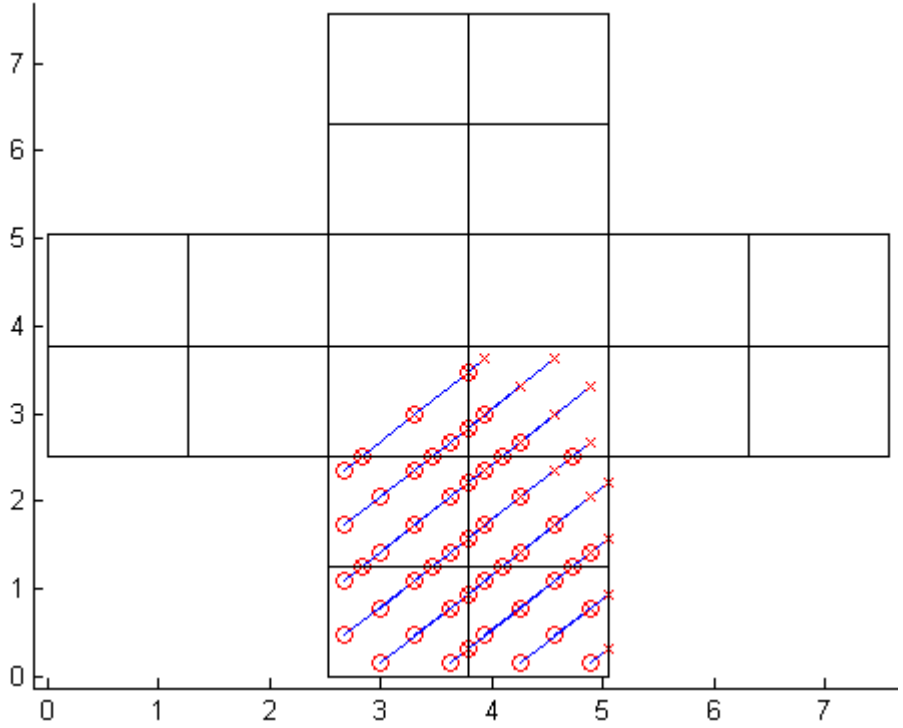


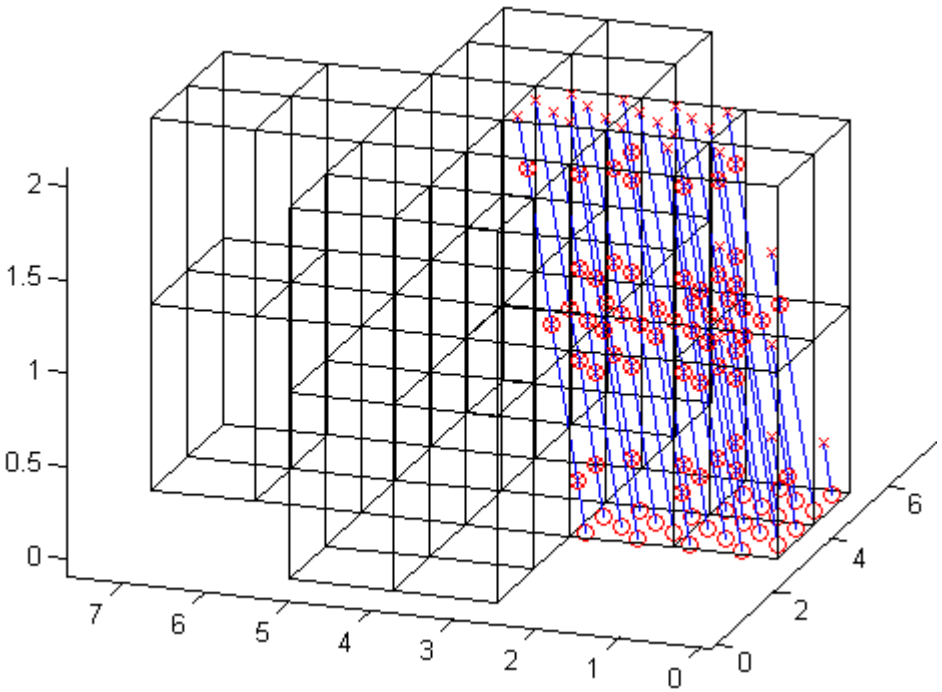
3D Circular/Cylindrical Ray Tracing



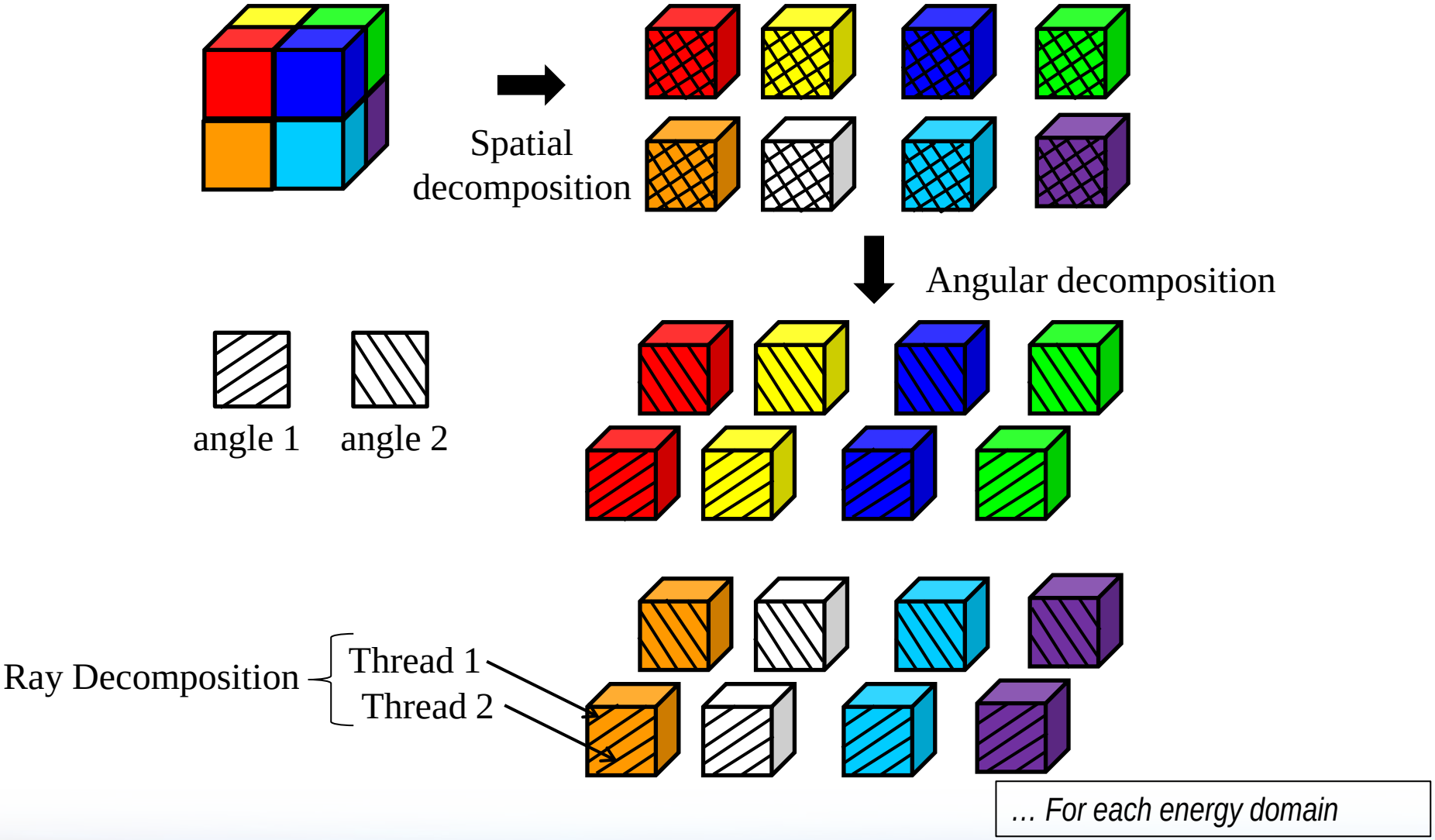


3D MOC: Long Rays through Core



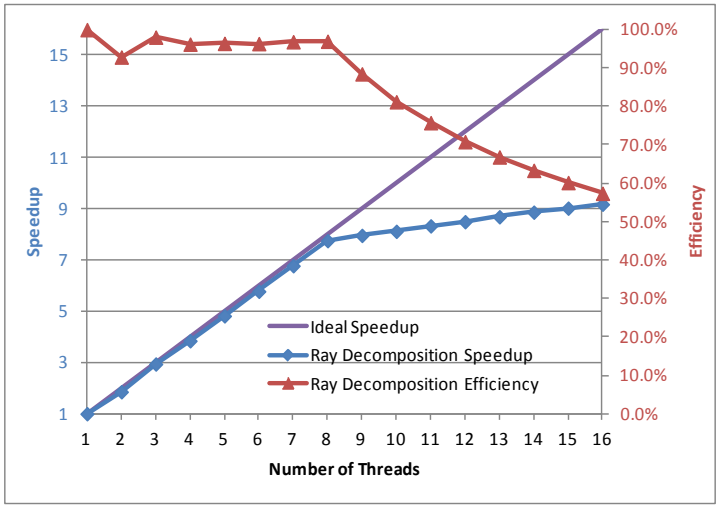


Parallel Decomposition

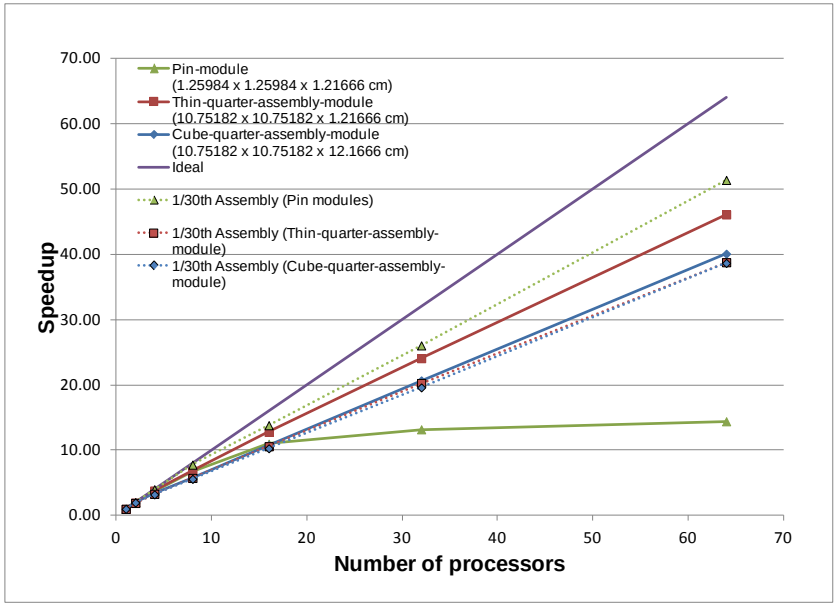


Parallel Decomposition

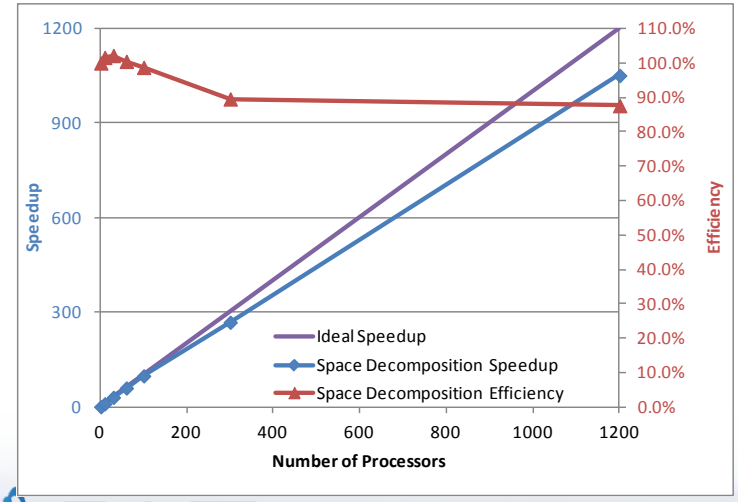
Rays



Angles

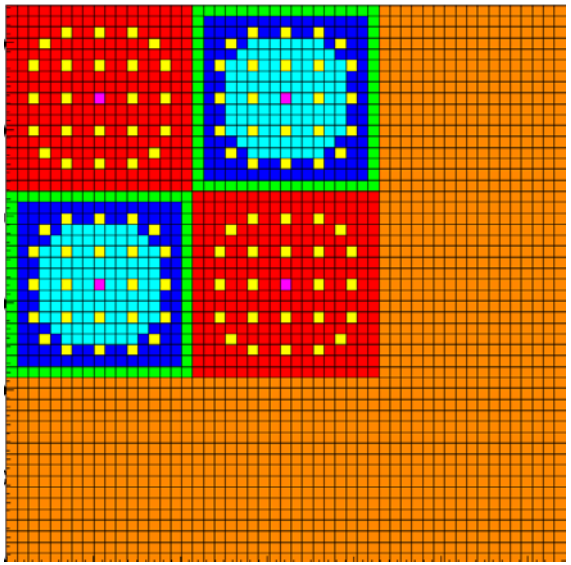


Spatial

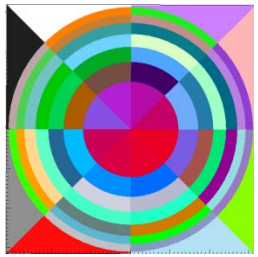


- Spatial Decomposition scaled very well
- Angular Decomposition scaled modestly
- Ray Decomposition scaled very well up to hardware limit
- Parallel MOC Sweep algorithm should be feasible for full core problems

Initial MPACT Benchmark Results: C5G7-2D

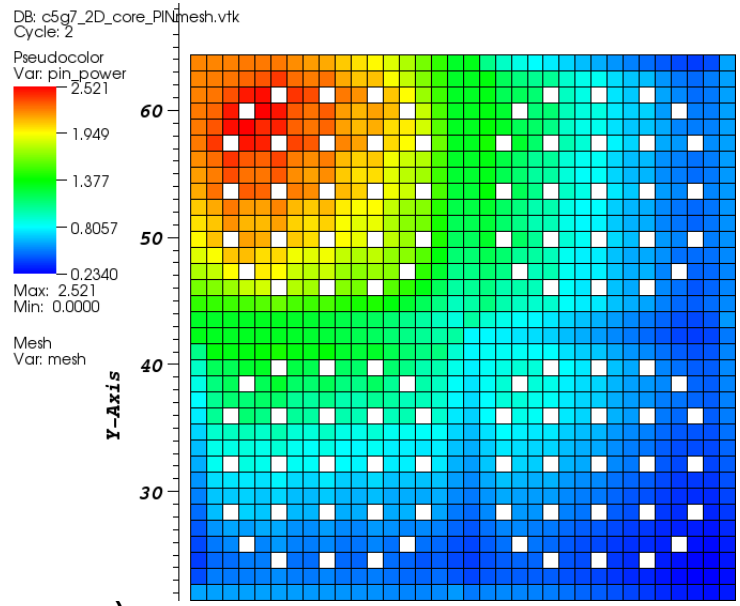


Core Pin Layout



Flat Source Regions

FSR = 97,104
#nseg = 26,736,000 (coarse rays)



Relative Pin Powers

#Procs	Avg. Sweep Time (s)	Speedup
1	0.930	1
8	0.131	7.08
16	0.094	9.91
32	0.054	17.10

Case	K-eff	Δk (pcm)
Reference	1.186550	---
Coarse Rays	1.186115	43
Fine Rays	1.186720	17

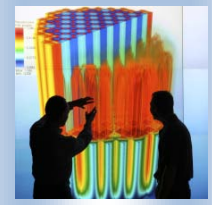
MPACT XSEC Capability

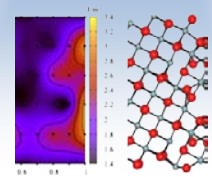
- Processing tools implemented for user defined benchmark cross-sections and AMPX working library
- Subgroup method based on HELIOS methodology
  - Can utilize DeCART HELIOS library
  - Can utilize library generated by Kim and Jessee at ORNL
- Work ongoing to implement ESSM Method based on M. Williams white paper

MPACT Role in CASL

- Functional libraries allow MPACT features to be used in DENOVO
  - MPACT_XS can provide cross-sections
  - MPACT_MOC can provide capability to do 2D and 3D MOC sweeps for 2D-1D or 2D-3D
- MPACT will provide MOC for Challenge Problems
  - 2D-1D sweeps to capture all DeCART functionality
  - 3D MOC

Questions?





VERA Strategy and September Limited Beta Release

John Turner (ORNL), Lead
Randall M. Summers (SNL), Deputy Lead

CASL
Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Virtual Environment for Reactor Applications (VERA)

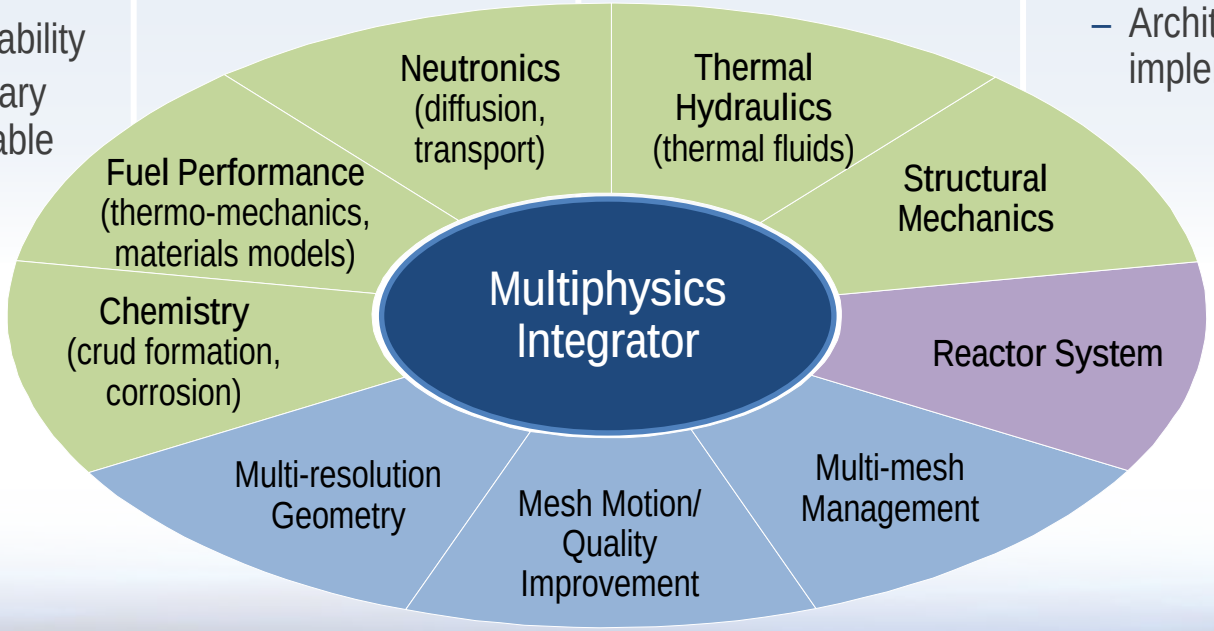
A suite of tools for scalable simulation of nuclear reactor core behavior

- Flexible coupling of physics components
- Toolkit of components
  - Not a single executable
  - Both legacy and new capability
  - Both proprietary and distributable

- Attention to usability
- Rigorous software processes
- Fundamental focus on V&V and UQ

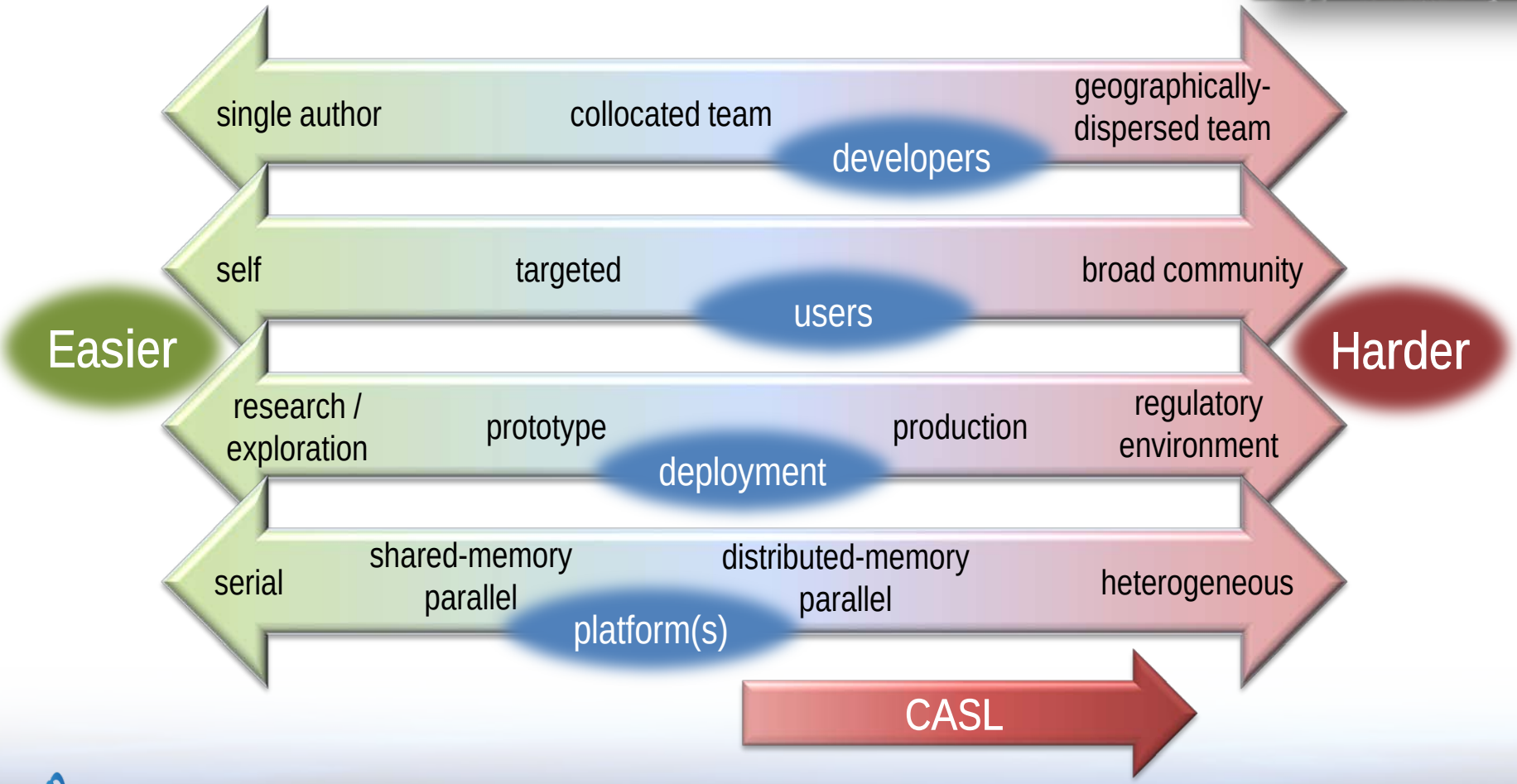
- Development guided by relevant challenge problems
- Broad applicability

- Scalable from high-end workstation to existing and future HPC platforms
  - Diversity of models, approximations, algorithms
  - Architecture-aware implementations



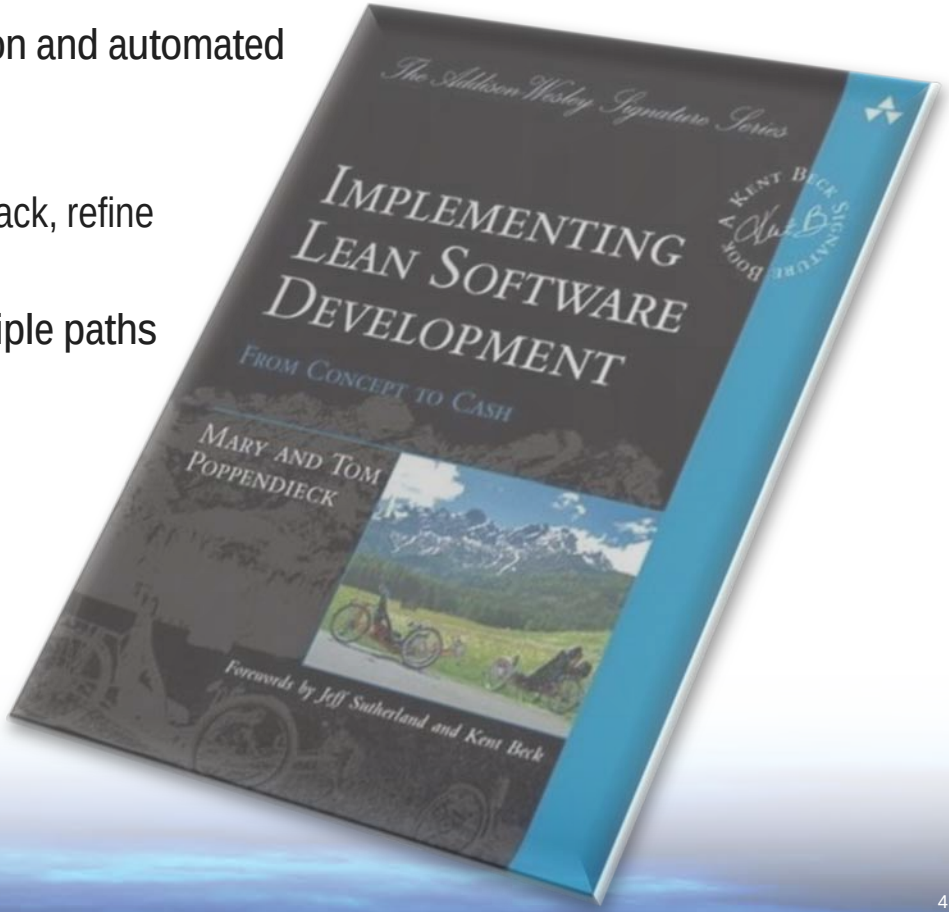
Writing software is easy

- Writing great software is hard.



Lean Software Development

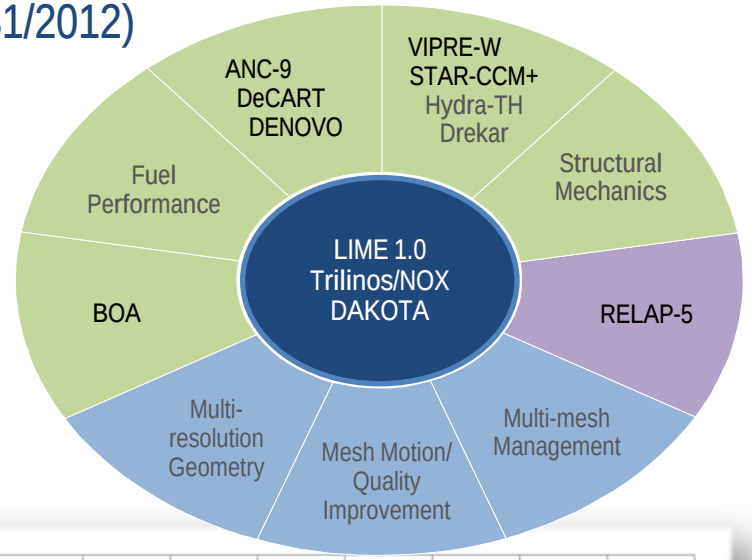
- Motivation for Lean Software Methods:
  - Lean Manufacturing (e.g. Toyota Production System)
- Seven Principles of Lean:
  1. eliminate waste
     - for software, waste is partially completed work, churn due to changing requirements, extra features, etc.
  2. build quality in
     - test-driven development, continuous integration and automated testing
  3. amplify learning through iterative development
     - sketch design, prototype, assess, customer feedback, refine
  4. defer commitment
     - delay irreversible decisions and/or follow multiple paths
  5. deliver fast
     - short release cycles, limit work in progress
  6. respect people
     - team should design and refine processes
     - no single "Best Way"
  7. optimize the whole
     - for CASL this means the entire analysis workflow

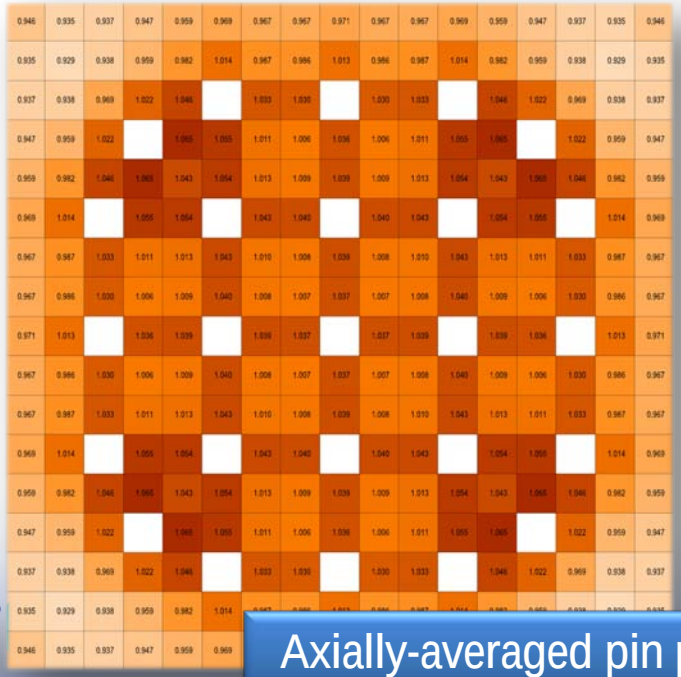


Virtual Environment for Reactor Applications (VERA)

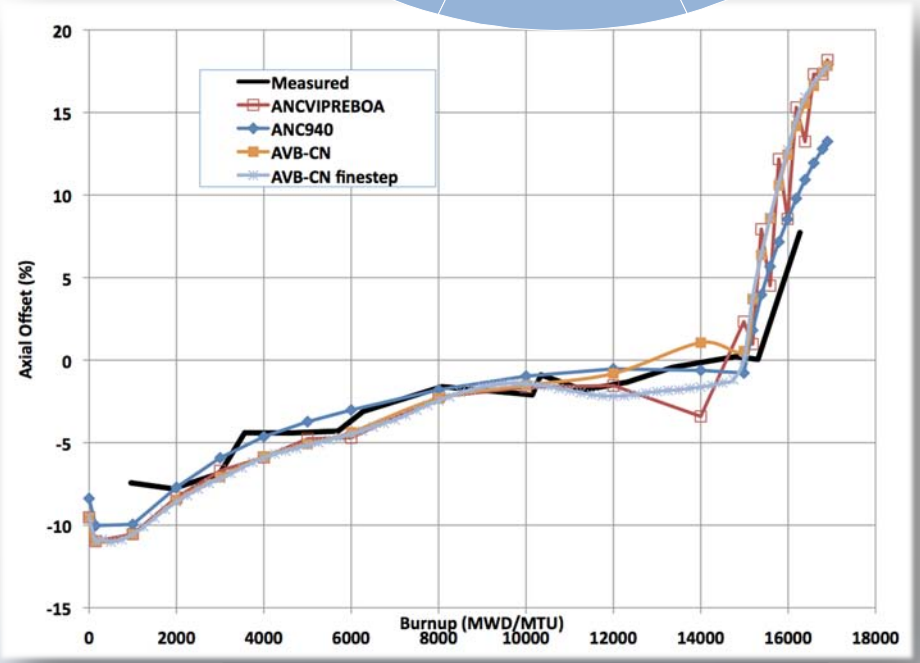
v1.0 (3/31/2011), v1.1 (9/30/2011), v1.2 (12/15/2011), v2.0 (3/31/2012)

- software foundation
  - based on widely-used advanced open numerical software
  - strong emphasis on continuous integration and testing
  - initial integration with optimization, sensitivity analysis, and uncertainty quantification
- baseline industry capability
  - based on Westinghouse and EPRI codes
- initial advanced capability
  - National Lab, University, and Commercial components
- initial coupling to reactor system capability



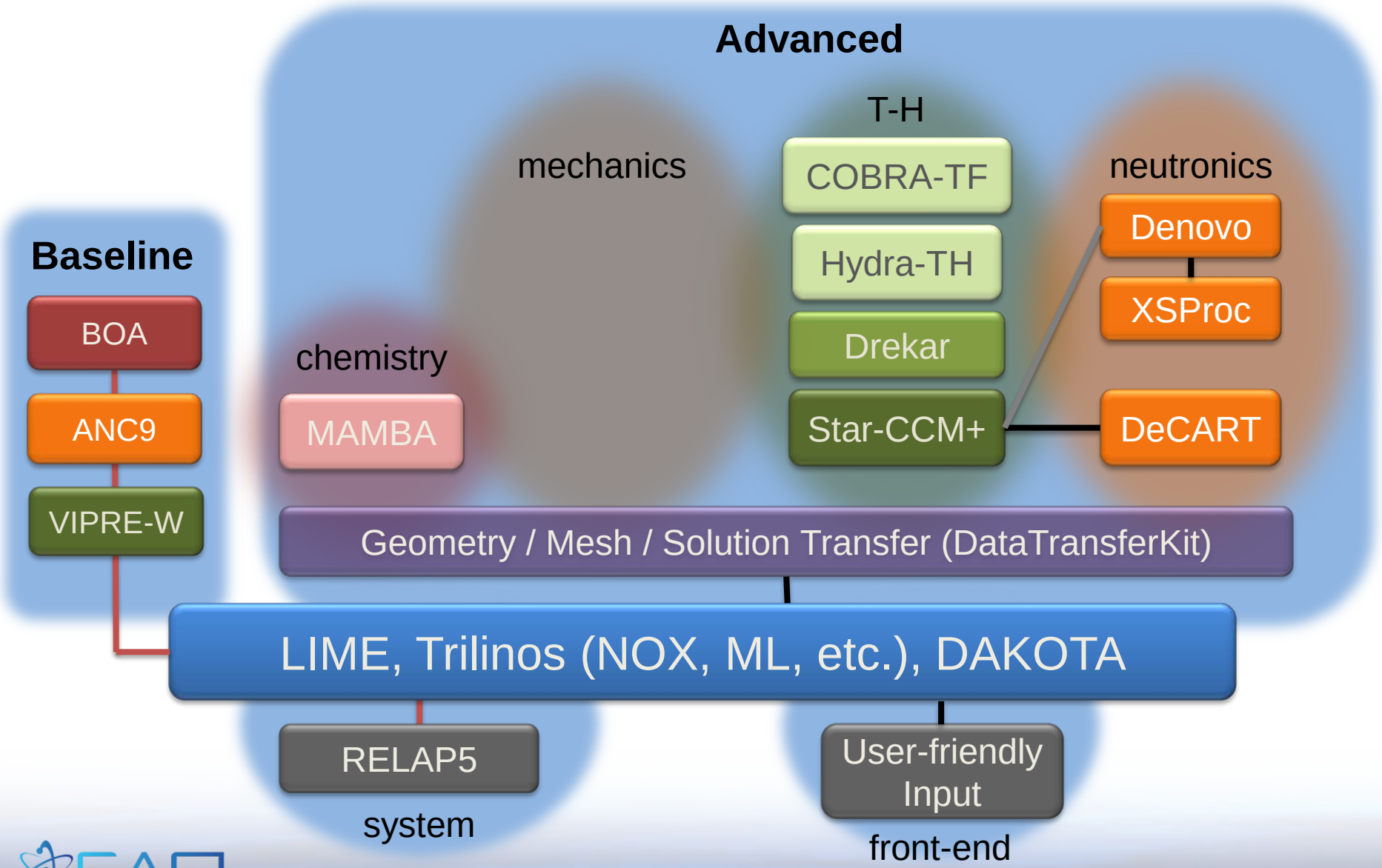


Axially-averaged pin powers



Axial offset for 4-loop PWR

VERA 2.0 snapshot (03/2012)



VERA constituents

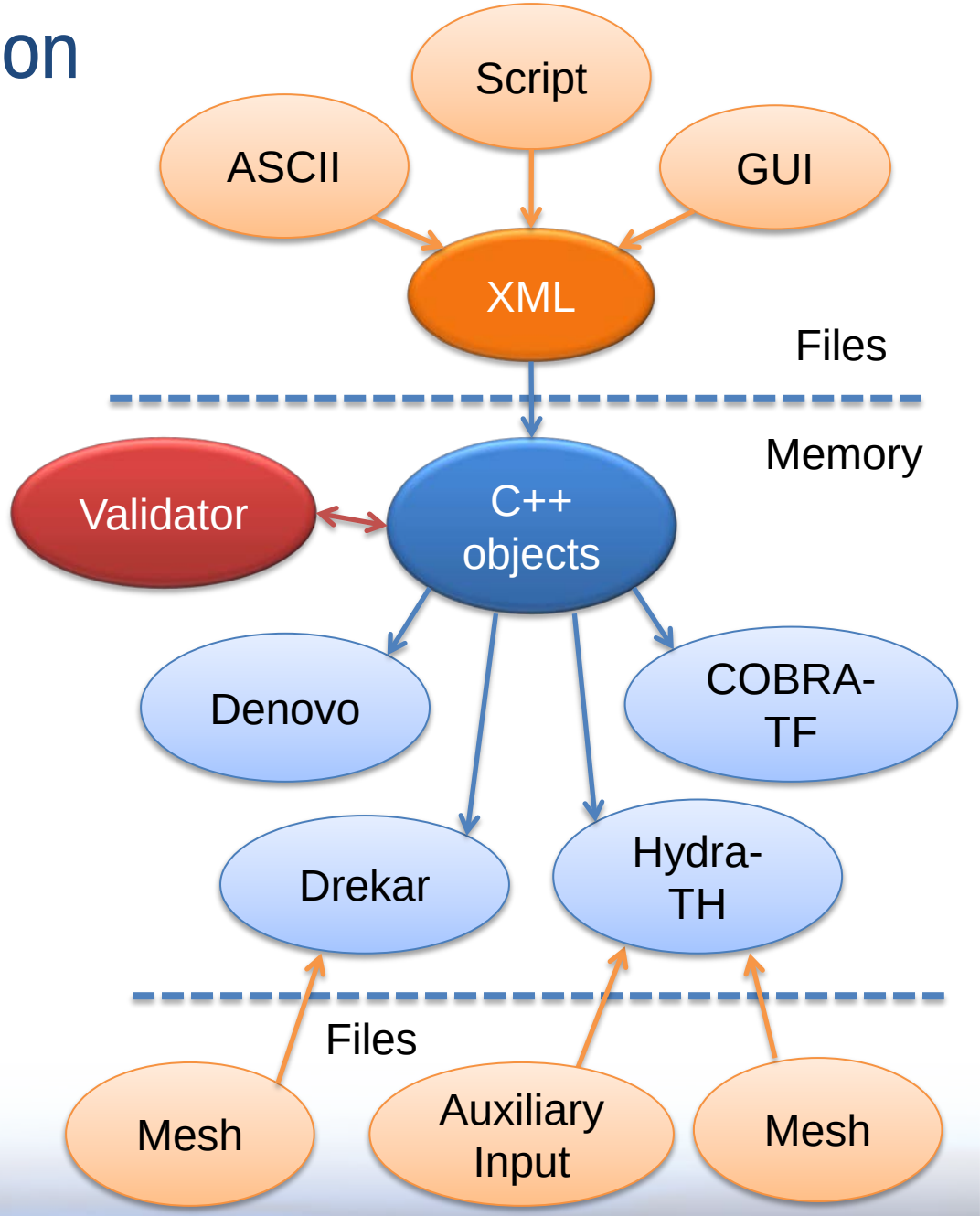
Now
Denovo + XSProc
DeCART
DeCART + Star-CCM+
Drekar
Hydra-TH
COBRA-TF
ANC + VIPRE-W
ANC + VIPRE-W + BOA

Under development
Denovo + XSProc + COBRA-TF
Denovo + XSProc + Drekar
MPACT
Denovo + MPACT
ANC + VIPRE-W + BOA + VABOC
DeCART + Star-CCM+ + MAMBA
Denovo + XSProc + ORIGEN

- number of repositories: 15
- number of TriBITS VERA packages: 187
- total repository source code statistics: 30K files, 5M source lines
- number of tests (not unit tests) in a VERA build: 167
- number of nightly build cases: 7 + 2 experimental (Intel 12.0.8)
- multiple compilers/platforms tested nightly
  - pure GCC 4.6.1 (official CI build), pure Intel 12.0.4, pure Intel 12.0.8, hybrid GCC 4.5.1 + Intel 11.1.064, hybrid GCC 4.5.1 + Intel 12.0.4,

Common input description

- provide capability for reactor problem setup for SCALE/XSProc, DENOVO, COBRA, etc.
  - VERA-CS: assemblies, poisons, control rods, non-fuel structures, baffle, power, flow, depletion, etc.
- eliminate inconsistencies between coupled physics codes through the use of a common geometry description
- provide ability to create, archive, compare, and modify input similar to current industry workflows
- doesn't have to be all-singing, all-dancing from the outset
  - can evolve as appropriate



VRI Priorities for PoR-5 (Mar-Sept 2012)

Highest Priorities

continue to push core simulator capability as rapidly as possible
- COBRA-TF integration
- neutronics / T-H feedback/coupling
- common input

expand usability push beyond input
- output and workflow

get CFD capabilities into AMA's hands, e.g.
- Hydra-TH
- Drekar

DOE-reportable milestones
- 6/30: VERA 2.0
- 7/15: infrastructure release
- 9/15: limited beta release via RSICC

fine-mesh ANC / VIPRE-W / BOA

Other Highest Priorities

integrate other new capabilities
- MAMBA
- Hydra-TH
- PEREGRINE
- MPACT

coupling and solution transfer
- Denovo / COBRA-TF
- Denovo / Drekar

capability development
- structural mechanics (FAD, GTRF)

common properties, etc.

GPU implementations

“Integration” is an overloaded and ambiguous term

what VRI means by integration is a process – not “delivery”

- while it requires source code access, it does not require “delivery” in a polished, release sense
- it does not preclude further development – quite the contrary
- VRI would like integration with build/test environment as early as possible in the development of CASL capabilities

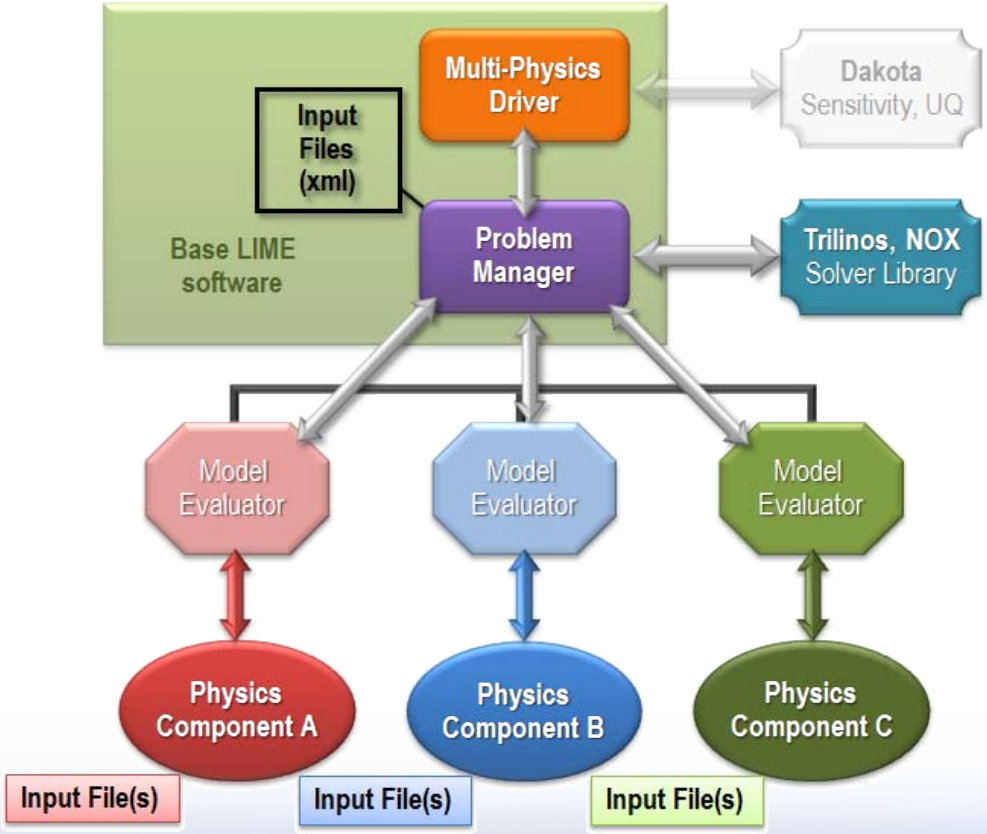
Rough steps in “integration”	Involvement
licensing / use agreement	owners / developers, legal
access / transmittal	developers, VRI
port to dev platform(s), confirm test probs	developers, VRI
evaluate w.r.t. Software Acquisition Process [*] • existing CI tests or test suite • communication path (direct access to repo?)	QA, VRI, developers, VUQ?, AMA?
port to TriBITS (both build and test infrastructure) • at this point development continues	developers, VRI
initial model evaluator (standalone)	developers, VRI
use VERA input	developers, VRI
improved model evaluator(s) for feedback / coupling / SA / UQ	developers, VRI

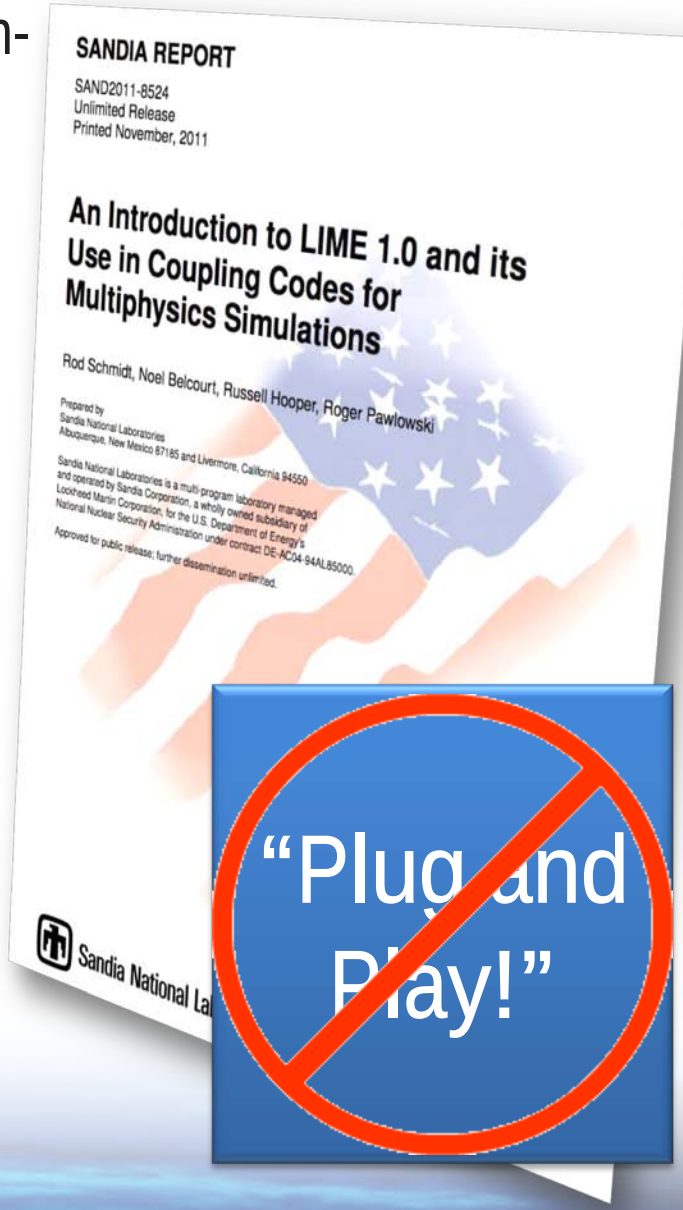
[*] https://casl-dev.ornl.gov/wiki/index.php/Software_Acquisition_Process

Public Release of CASL Infrastructure Software

LIME has been publicly-released under an open-source license:

- http://sourceforge.net/projects/lime1/





September Limited Beta Release

- primary goal is to exercise release process through Radiation Safety Information Computational Center (RSICC)
  - limited to CASL partners only – precursor to future more broad releases
  - components of the Virtual Environment for Reactor Applications (VERA)
  - initial documentation, limited user support
- schedule:
  - 06/13: “Go / No go” decision on components
    - license issues resolved, platform(s) defined, demo problems selected, draft documentation
    - full integration into VERA development environment to ensure stability via test infrastructure
  - 07/25: Dress rehearsal for release

September Limited Beta Release

- candidate components/capabilities

Physics Area	Application Area(s)	Component(s)	Probability	Note(s)
Coupling	All	LIME + DAKOTA	High	coupling software infrastructure + UQ
Neutronics	Multiple	Denovo	High	pin-homogenized transport
Neutronics	Multiple	DeCART	High	pin-resolved transport
Neutronics + CFD	Multiple	LIME-coupled DeCART and Star-CCM+	Medium	model evaluator for Star-CCM+ only
Thermal-Hydraulics	Multiple	COBRA-TF	Medium	stretch goal - using VERA input
Thermal-Hydraulics	Multiple	COBRA-TF + DAKOTA	Medium	leverage earlier VUQ work with VIPRE-W
CFD	GTRF, CRUD	HYDRA-TH	Medium	including mesh(es) for specific problem(s)
CFD	GTRF, CRUD	Drekar	Medium	including mesh(es) for specific problem(s)
Chemistry	CRUD	MAMBA	Low	must resolve BOA license issues
Neutronics + T-H	Multiple	Denovo + COBRA-TF	Low	probably next release

Beyond FY12

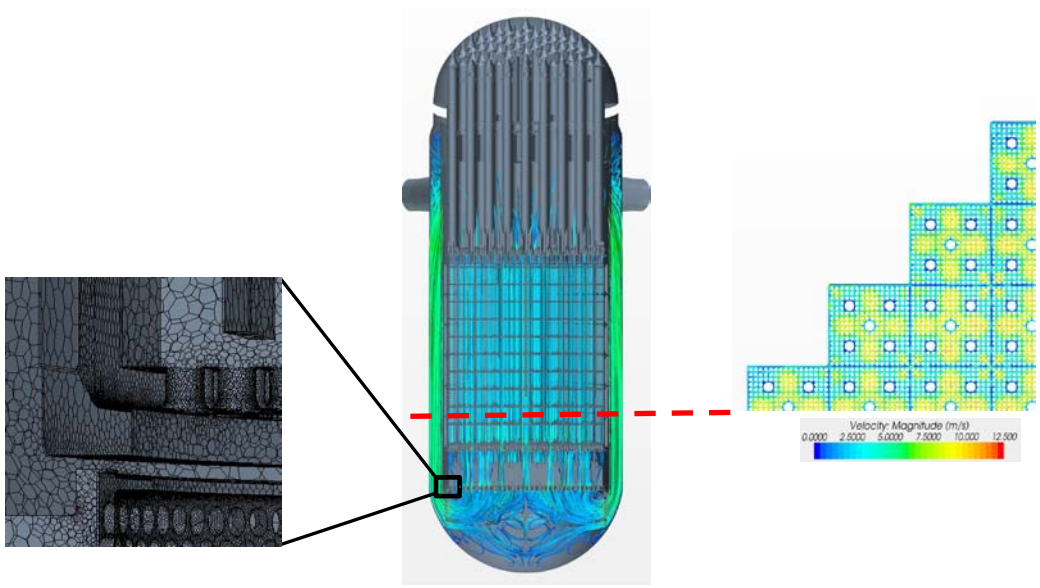
- continued VERA snapshots
  - 12/12, 03/13, etc.
  - capability integration and development driven by challenge problems
- deploy Test Stands and Pilot Projects
  - selected VERA components for targeted challenge problems and demonstrations
- broader release through RSICC

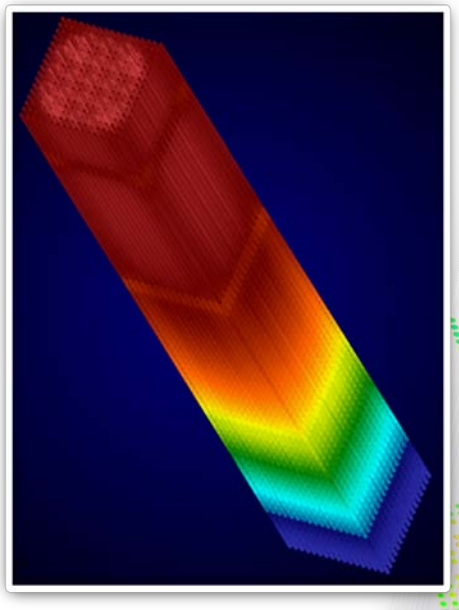
VERA deployment options and considerations

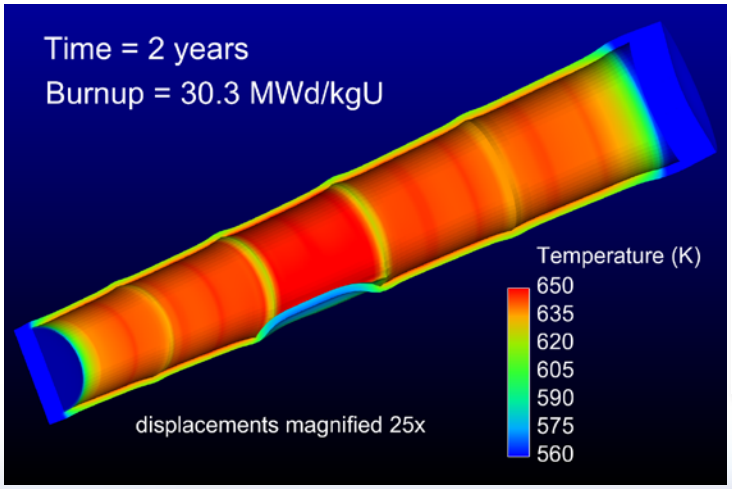
- related to the Test Stand concept
- platform options
  - laptops, workstations, clusters, HPC systems (current vs. future)
  - includes entire software ecosystem (OS, compilers, etc.) - Linux, Windows, Mac
- deployment mechanisms
  - source code
    - IP/export control
    - platform support
  - libraries/executables
    - can reduce both IP/export control and platform support issues
  - application server(s), e.g. via web-based interface
    - could further reduce IP/export control and platform support issues
    - can provide access to larger-scale systems
    - many issues/questions, but investigating

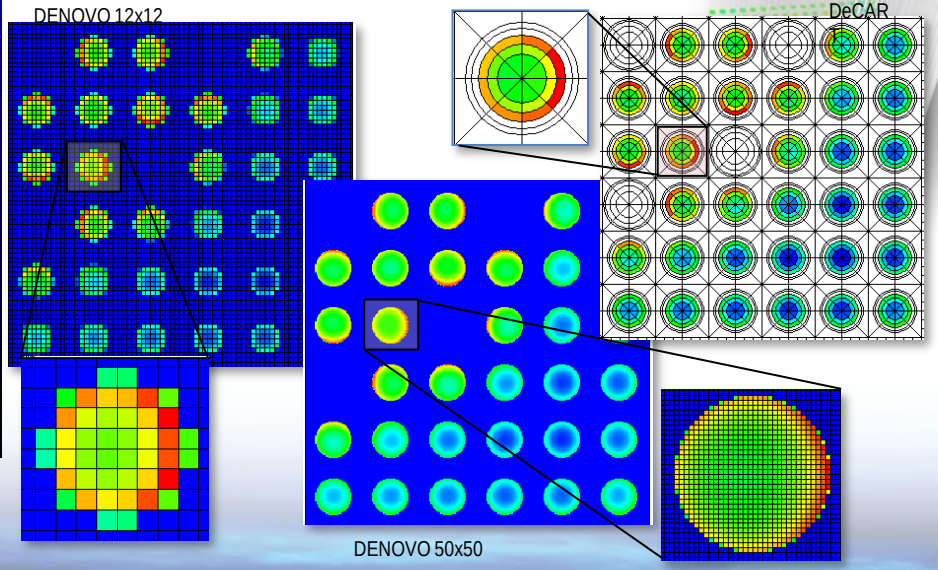
Questions?

www.casl.gov or *info@casl.gov*

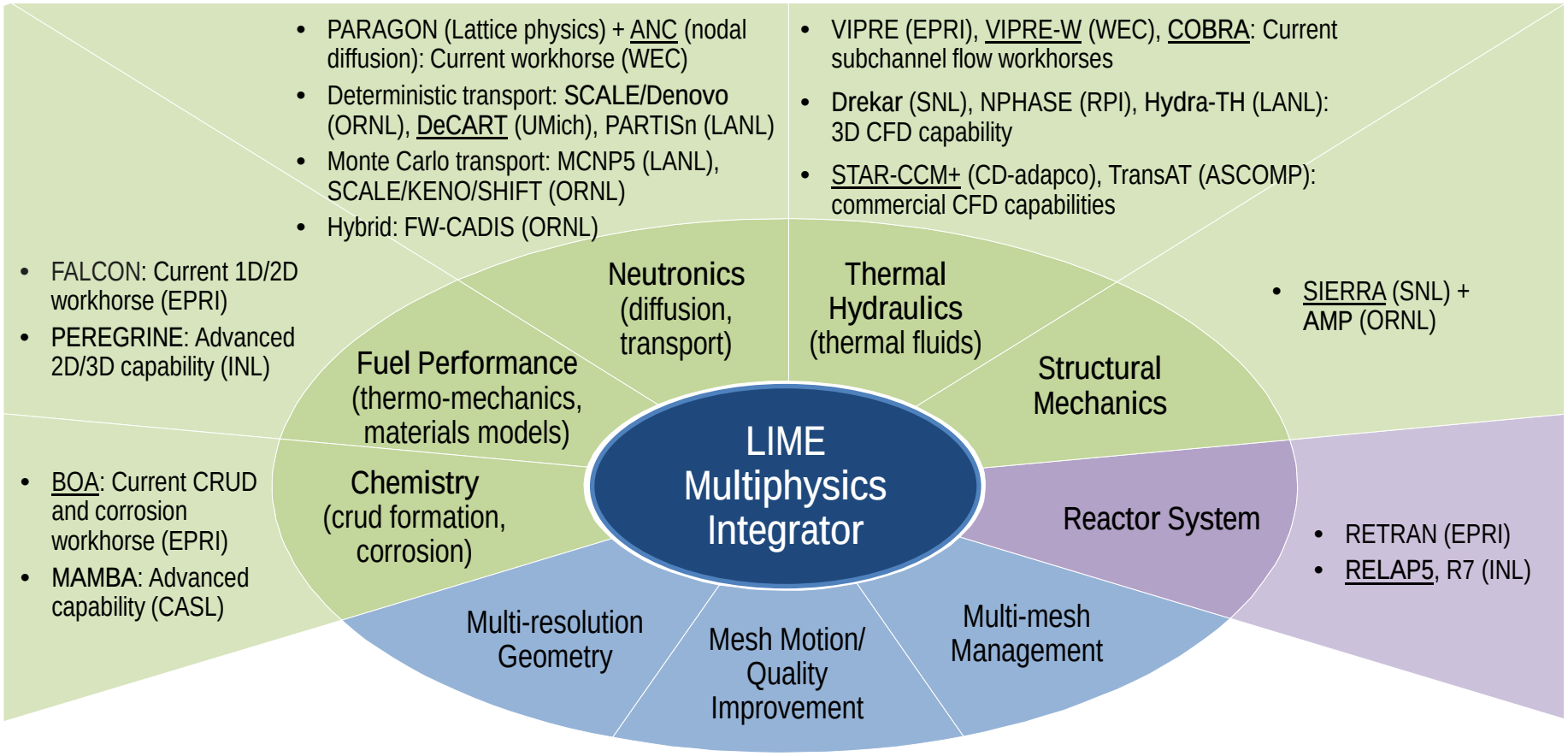








VERA (Virtual Environment for Reactor Applications) combines advanced capabilities with mature, validated, widely-used codes.



Core Simulator Description

- code system used to model quasi-steady-state LWR conditions and depletion
- included physics:
  - neutron transport, cross sections, thermal-hydraulics, fuel temperature, and depletion
- linkage to other physics:
  - CFD, fuel performance, CRUD models, structural, systems codes, etc.
- provides reactor conditions and distributions needed to solve challenge problems

Core Simulator Components

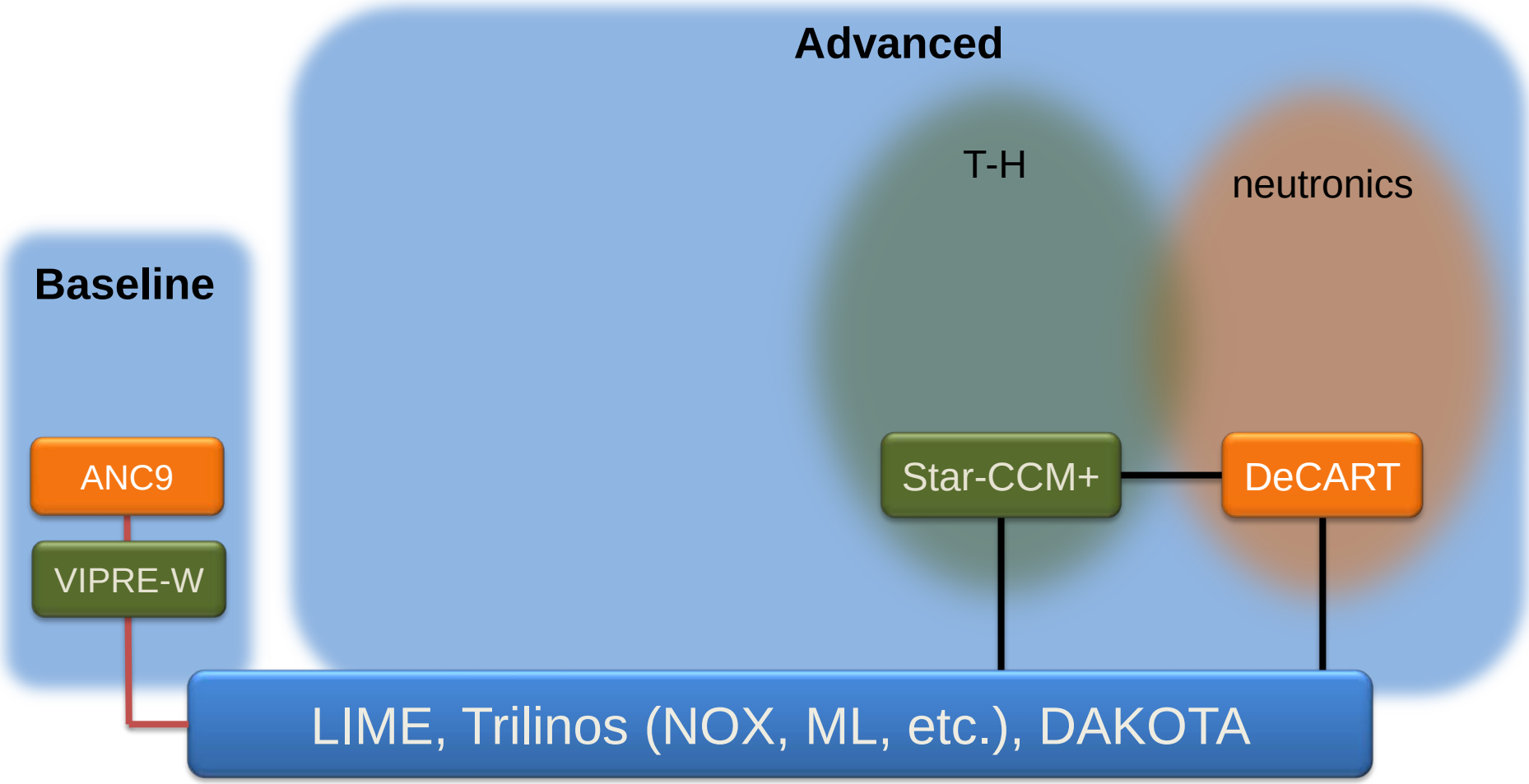
1. Input processor with common geometry description
2. T/H Solver (COBRA-TF)
3. Cross Sections (XSProc, ESSM)
4. Neutronic Solver (DENOVO, DeCART)
5. Infrastructure (control rod movement, detectors, boron search, etc.)
6. Fuel Performance (fuel temperatures, gap)
7. Depletion (including Xe/Sm) (ORIGEN)
8. Output processor to calculate pin powers, peaking factors, etc.

Same Components, Evolving Details

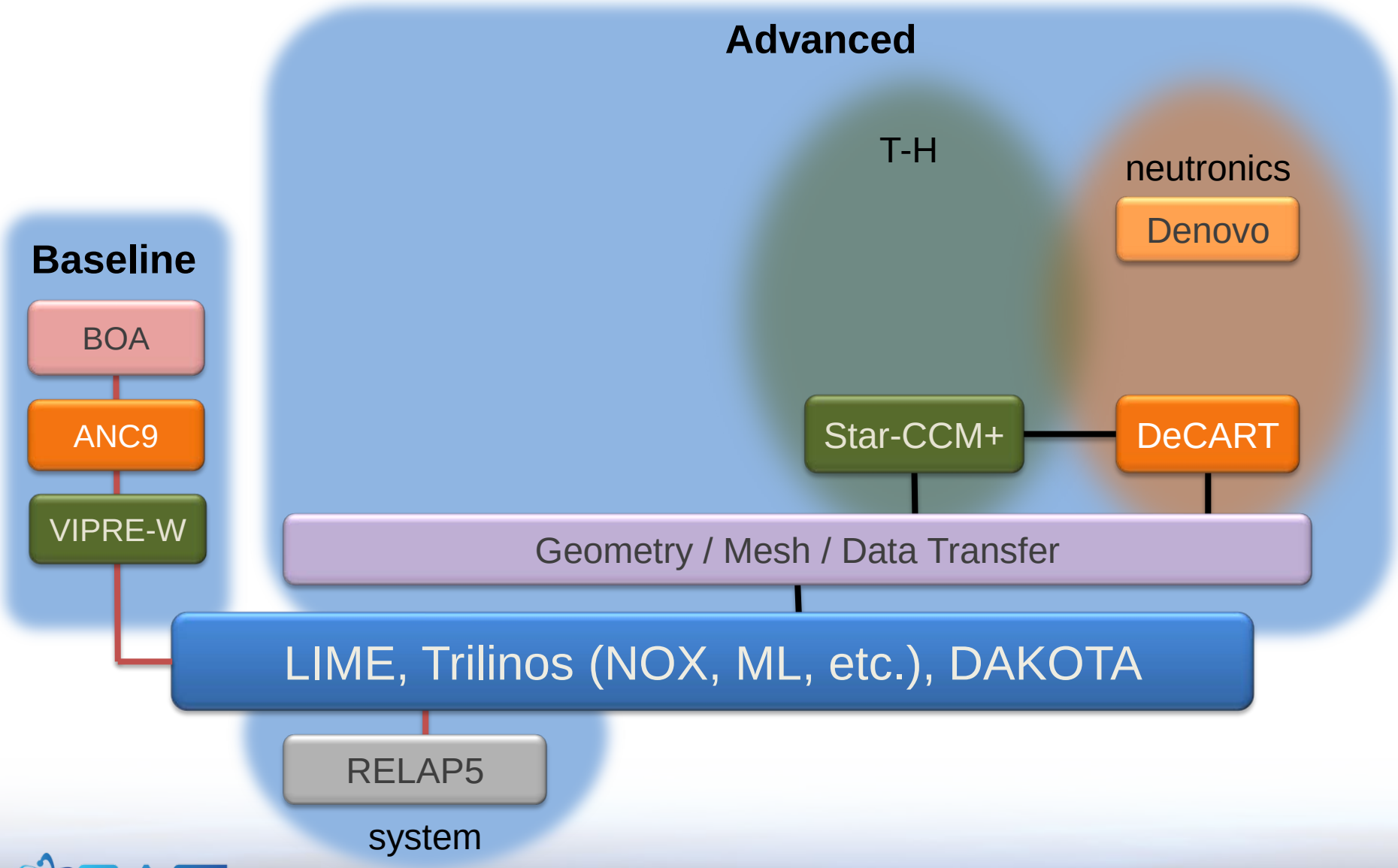
AMA "Benchmark problems"

- SCALE cross-section processing for DENOVO in VERA
- DENOVO pin cell capability with SCALE in VERA
- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- Mar 31 — #3 3D HZP Assembly — VERA 2.0
- #4 HZP 3x3 Assembly CRD Worth
- Sep 15 — #5 Physical Reactor Zero Power Physics Tests (ZPPT) — Limited Beta Release 9/15/2012
- #6 HFP BOL Assembly
- #7 HFP BOC Physical Reactor w/ Xenon
- #8 Physical Reactor Startup Flux Maps
- #9 Physical Reactor Depletion
- #10 Physical Reactor Refueling
- Integrate with Challenge Problem components

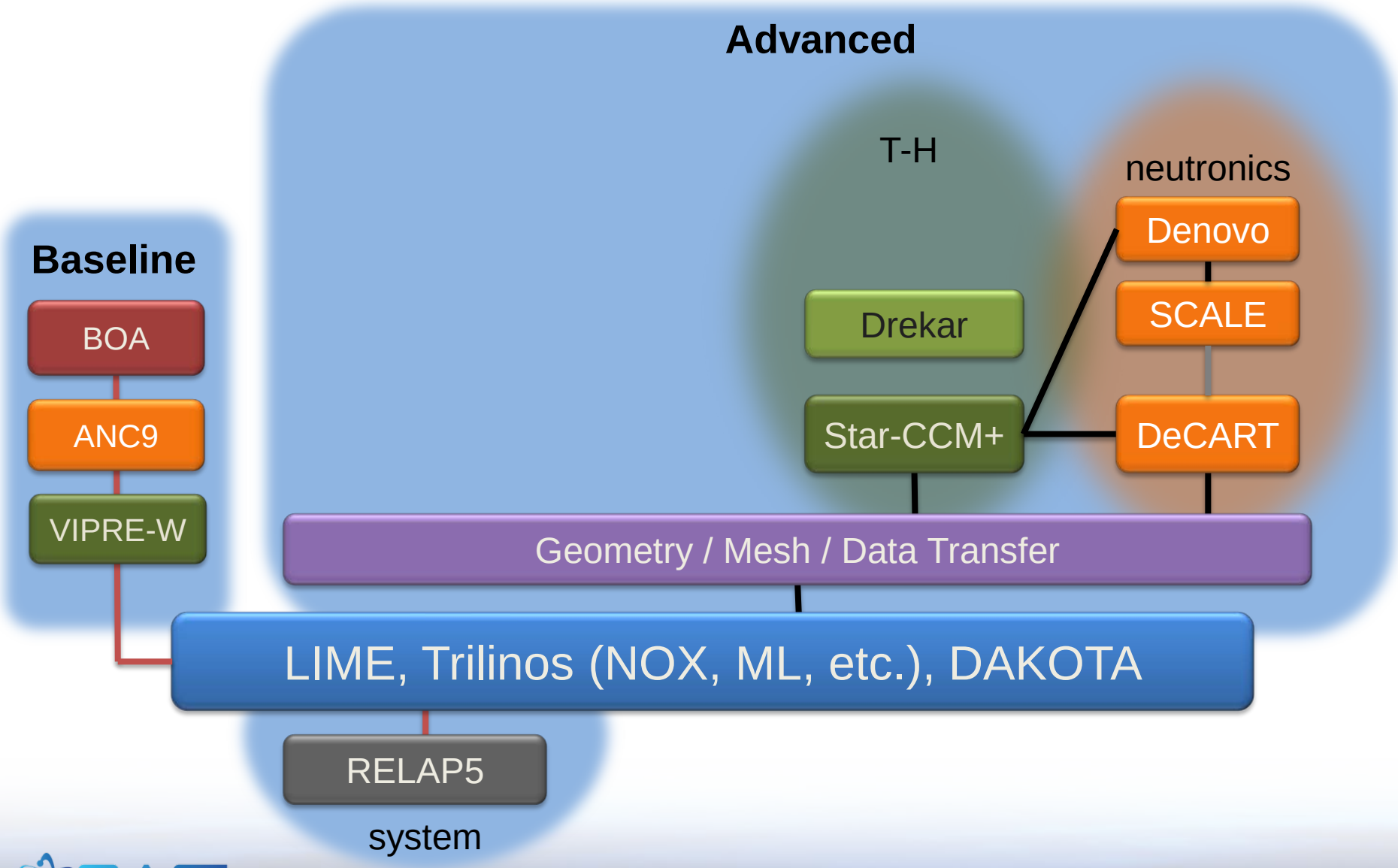
VERA 0.5 (12/2010)



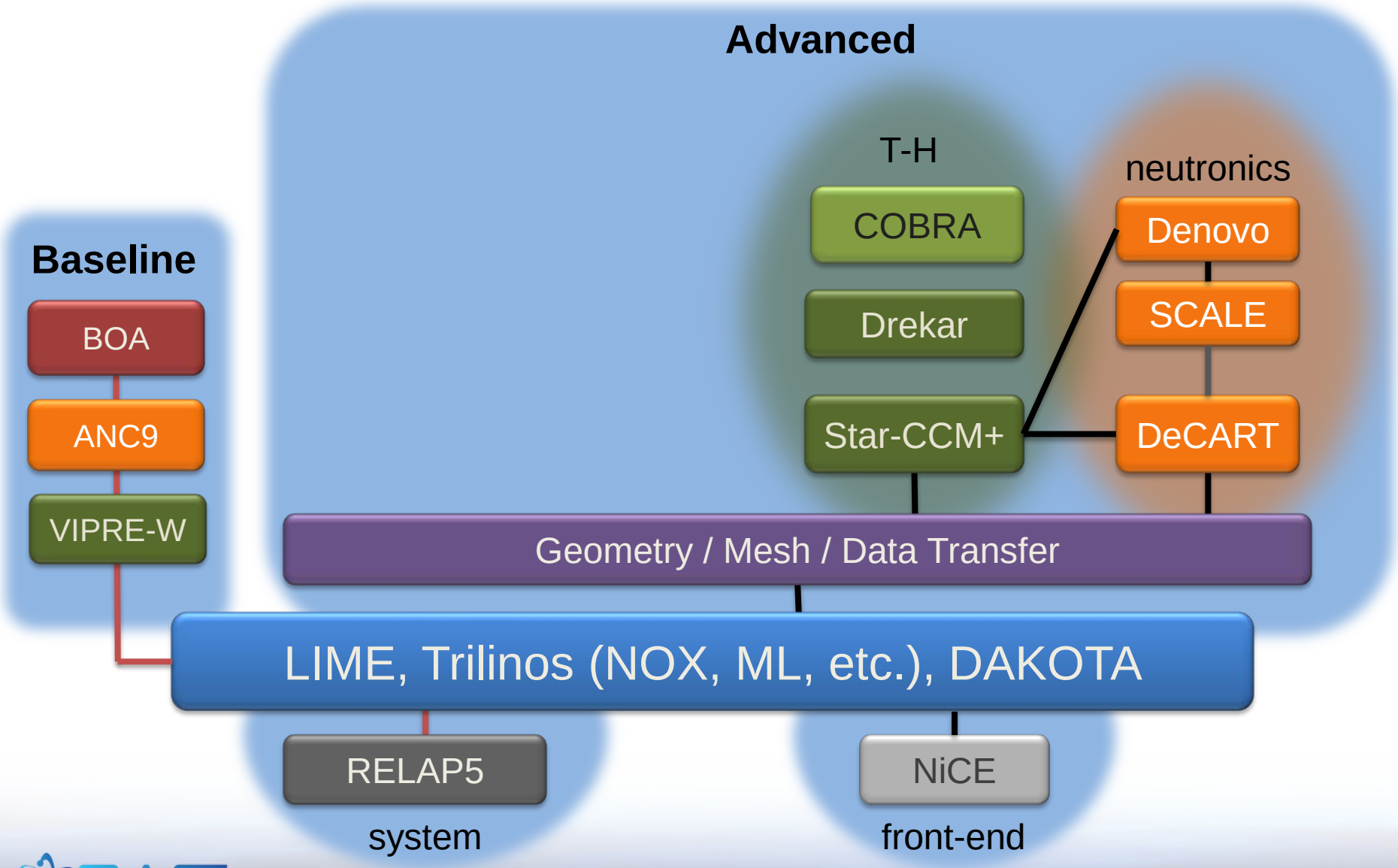
VERA 1.0 (03/2011)



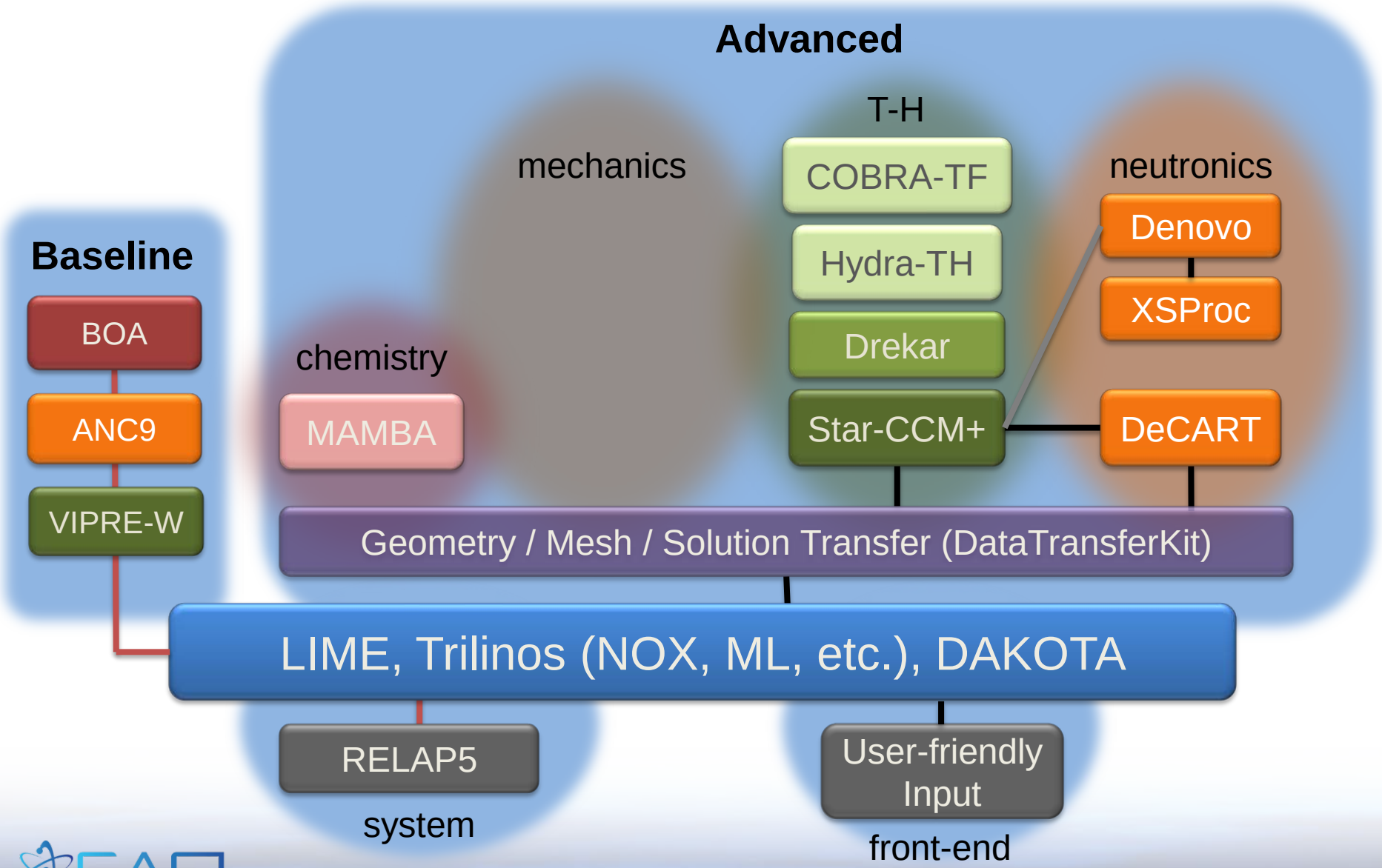
VERA 1.1 (09/2011)



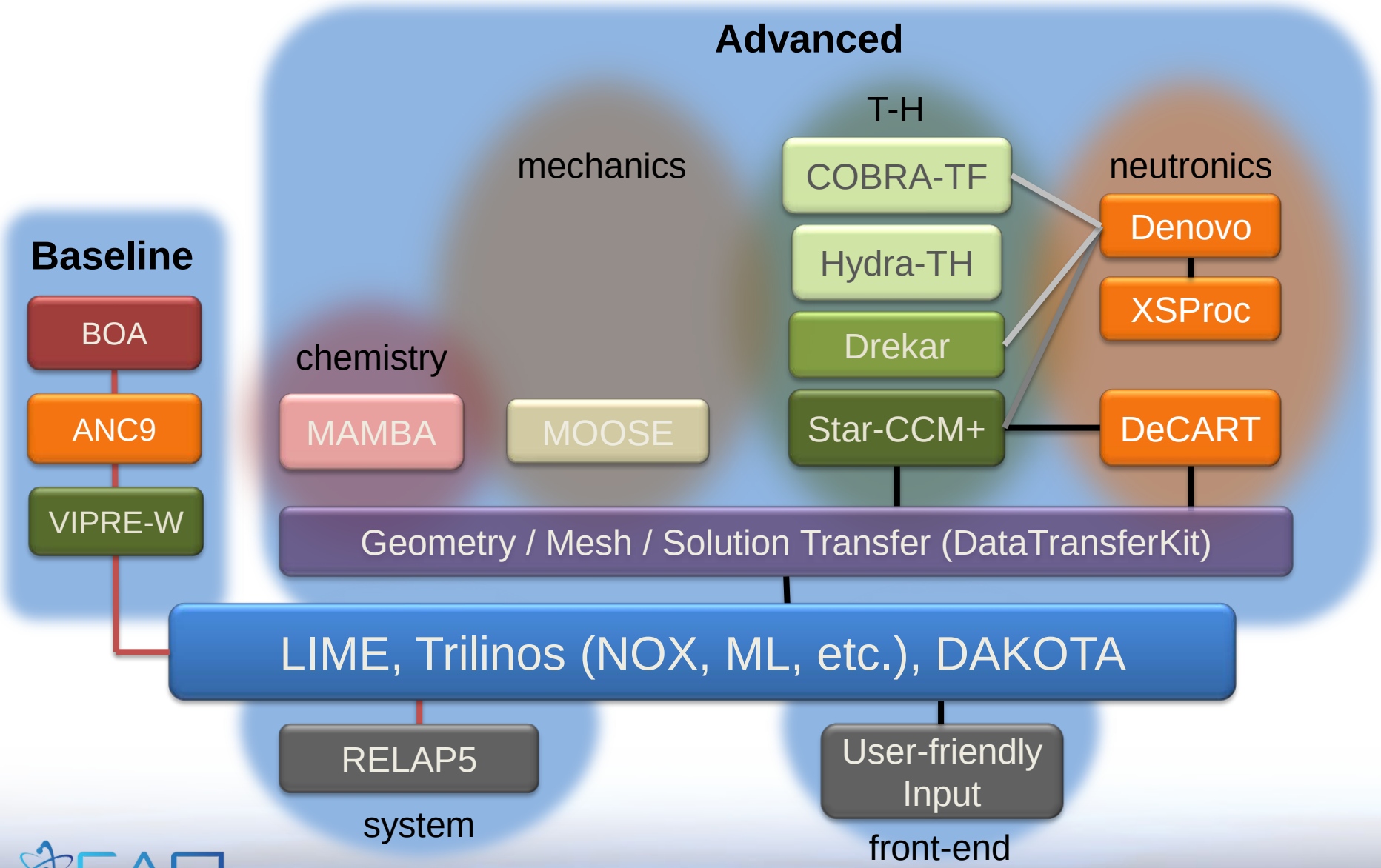
VERA 1.2 (12/2011) – projected



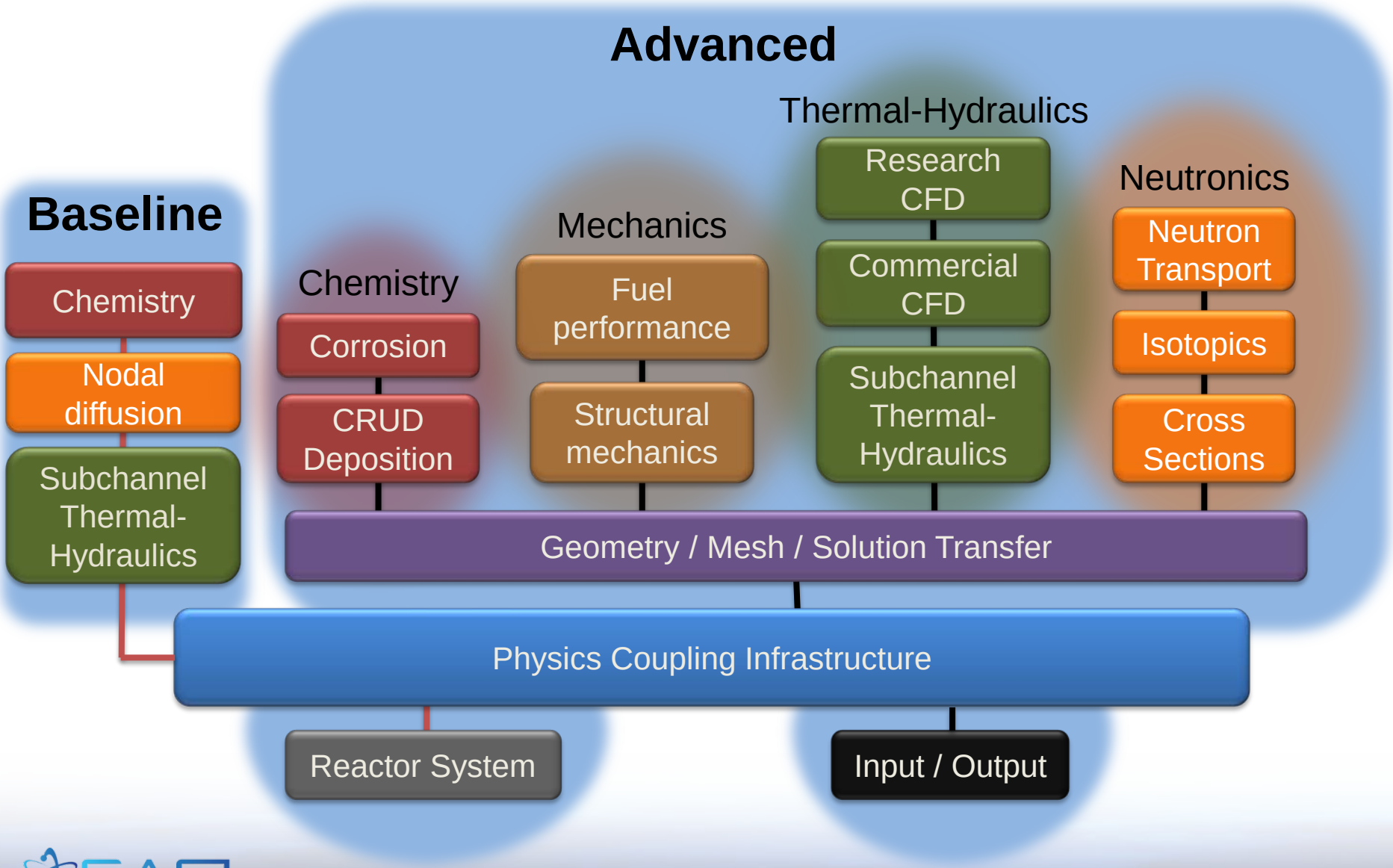
VERA 2.0 snapshot (03/2012)



VERA 2.1 snapshot (06/2012)



VERA


Advanced
Baseline
Chemistry
Nodal diffusion
Subchannel Thermal-Hydraulics
Chemistry
Corrosion
CRUD Deposition
Mechanics
Fuel performance
Structural mechanics
Thermal-Hydraulics
Research CFD
Commercial CFD
Subchannel Thermal-Hydraulics
Neutronics
Neutron Transport
Isotopics
Cross Sections
Geometry / Mesh / Solution Transfer
Physics Coupling Infrastructure
Reactor System
Input / Output

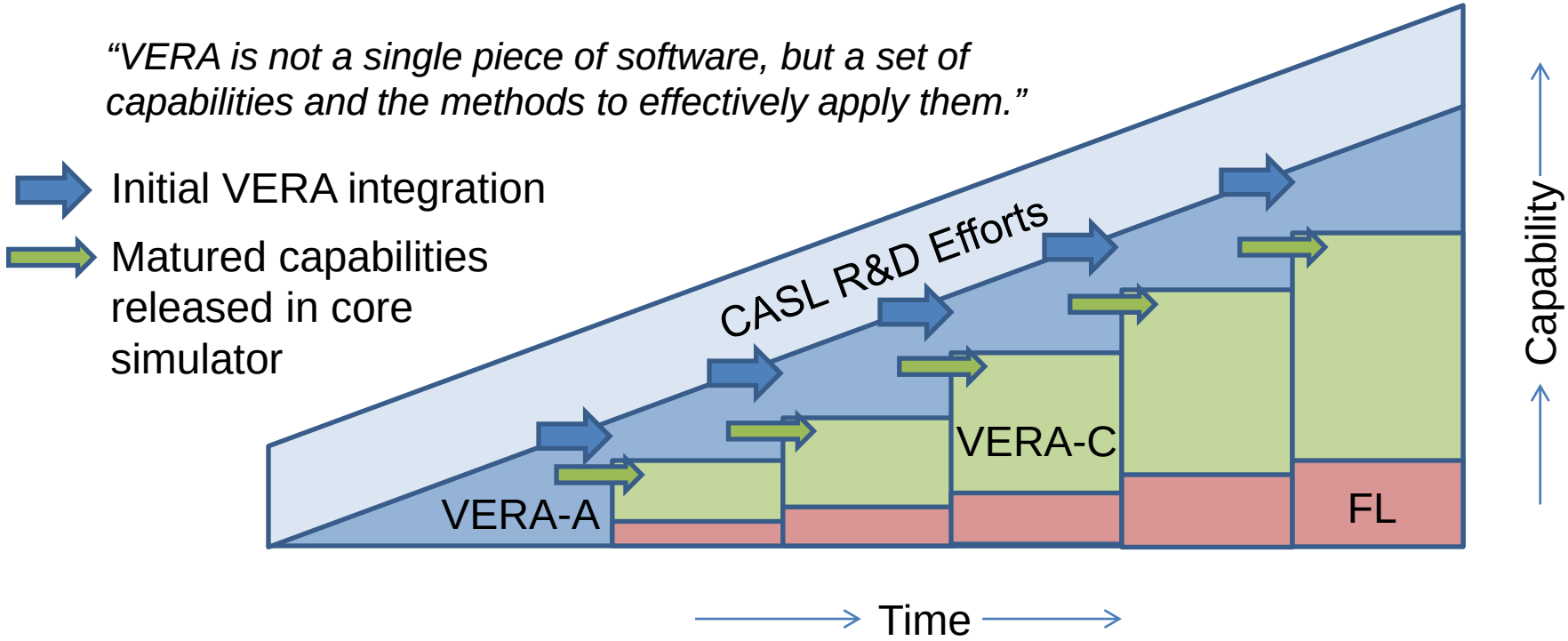
Missing…

- geometry
  - goal is a common geometry database, but long way to go
- material properties
  - similar to geometry goal/status
- mesh generation
  - looking at multiple options
- common input / user interface
  - reactor-aware, data-aware
- analysis / design / optimization

VERA Evolution Strategy

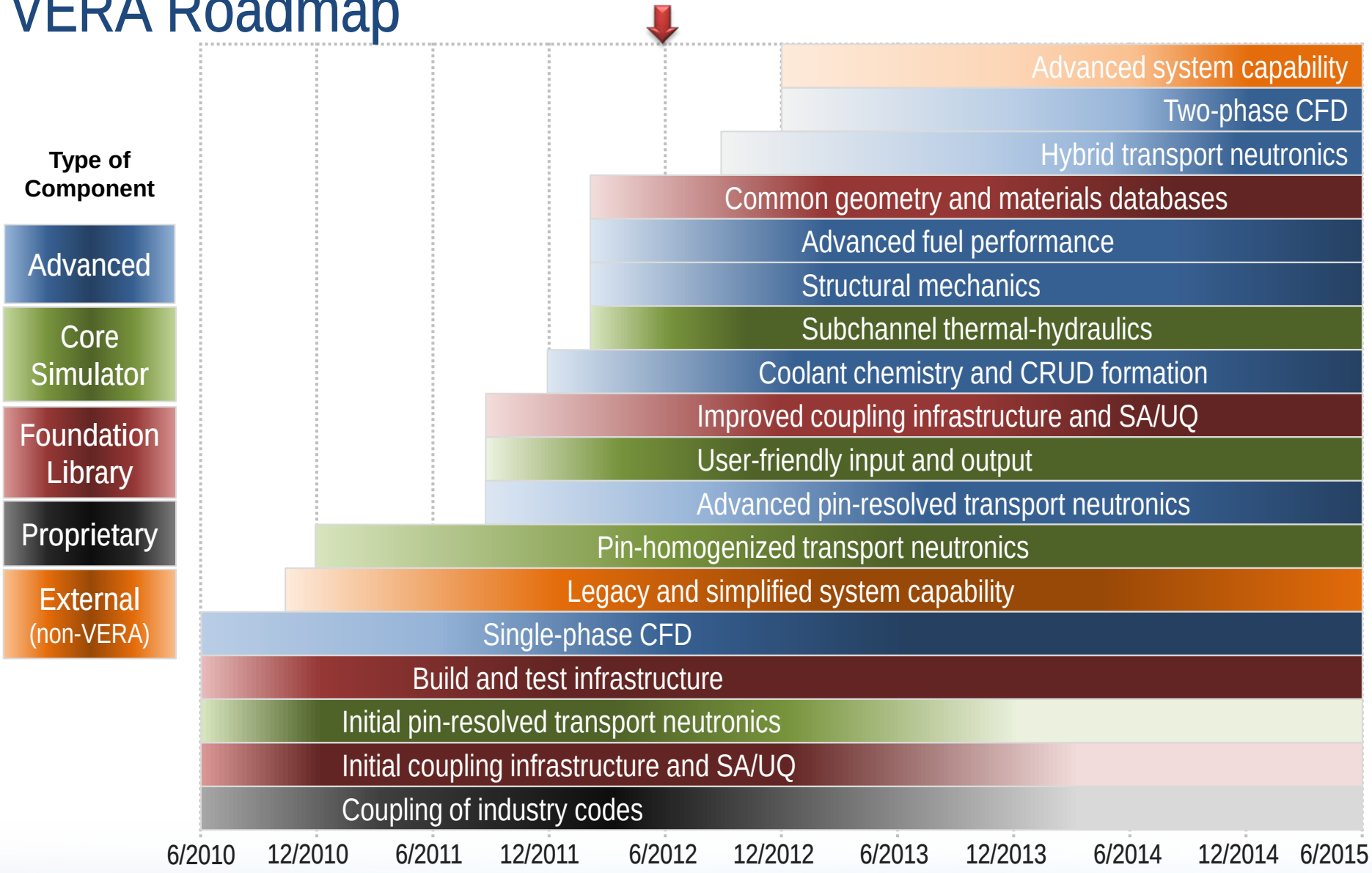
Migrating Advanced Capabilities to the Nuclear Industry

"VERA is not a single piece of software, but a set of capabilities and the methods to effectively apply them."

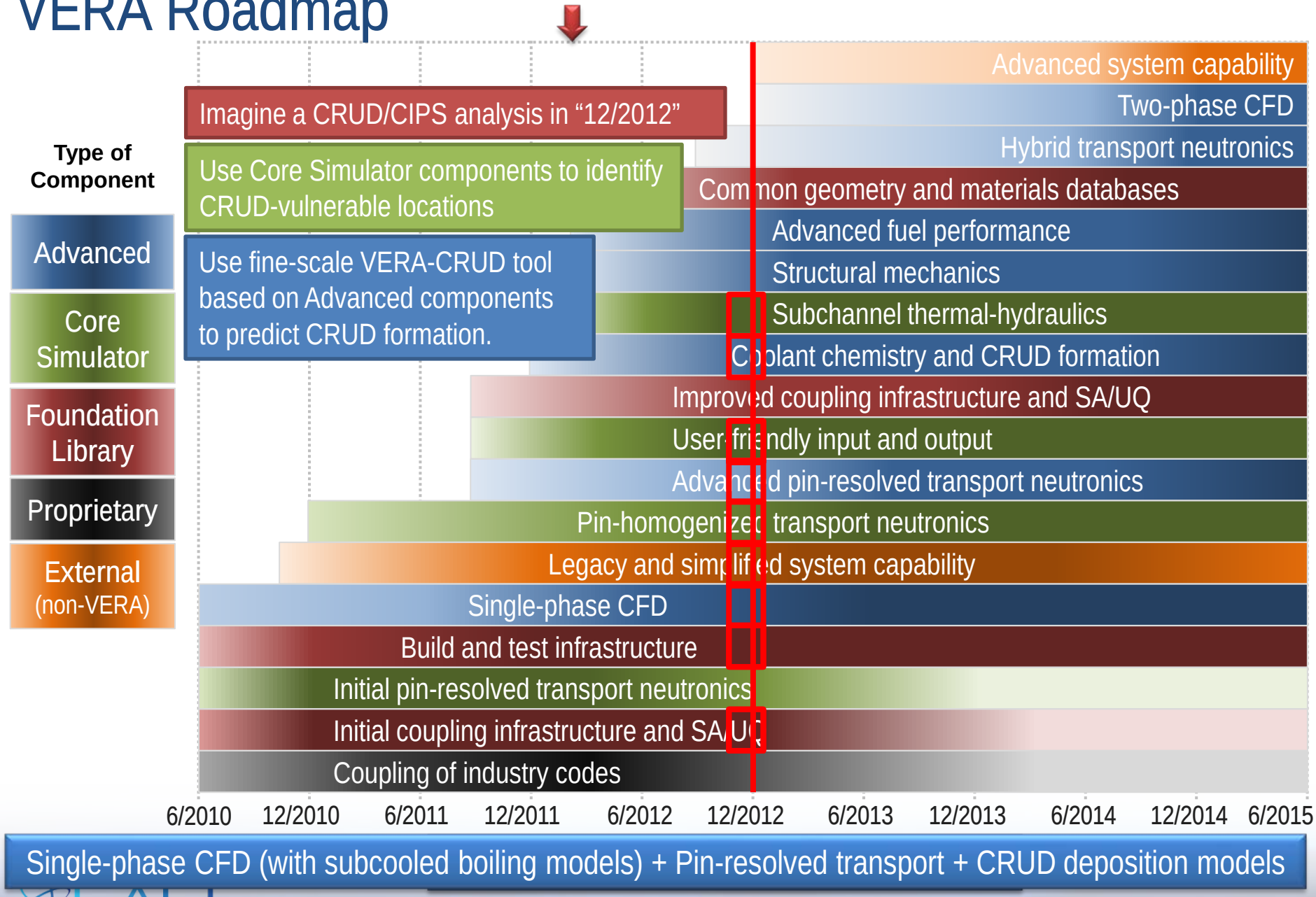


CASL-FL (Foundation Library)	VERA-C (Core Simulator)	VERA-A (Advanced)	CASL R&D
• Foundational components • Open source (non-EC) • Deployed to industry & academia • Annual releases	• Industrial class computing in 5-10 years • Mature capability • Driven by baseline problems • Deployed to industry & academia • Annual releases	• Leadership-class computing • Advanced capability • Driven by challenge problems • Use in collaboration w DOE • Continually developed	• Leadership-class computing • Cutting-edge capability • Driven by research problems • Initial development

VERA Roadmap



VERA Roadmap



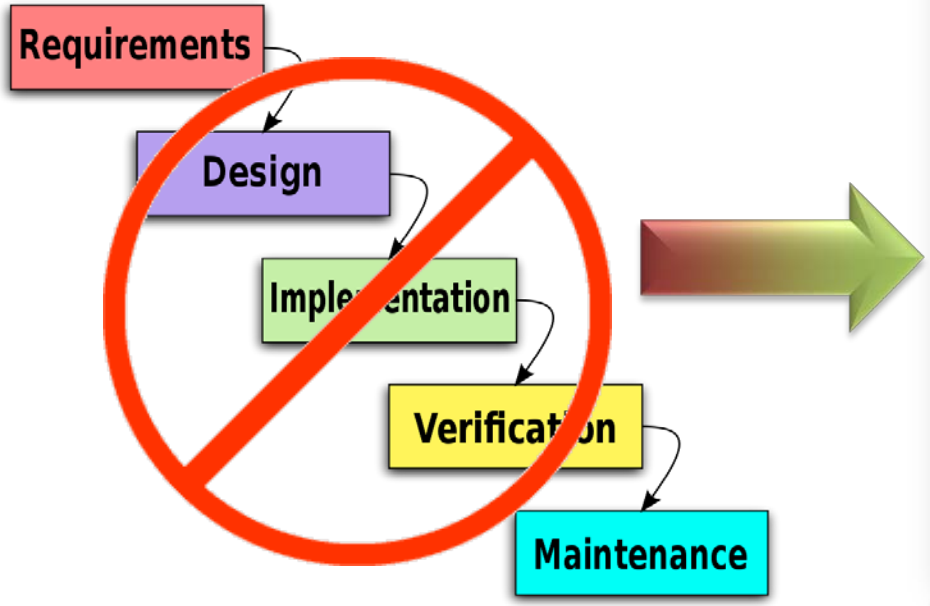
Single-phase CFD (with subcooled boiling models) + Pin-resolved transport + CRUD deposition models

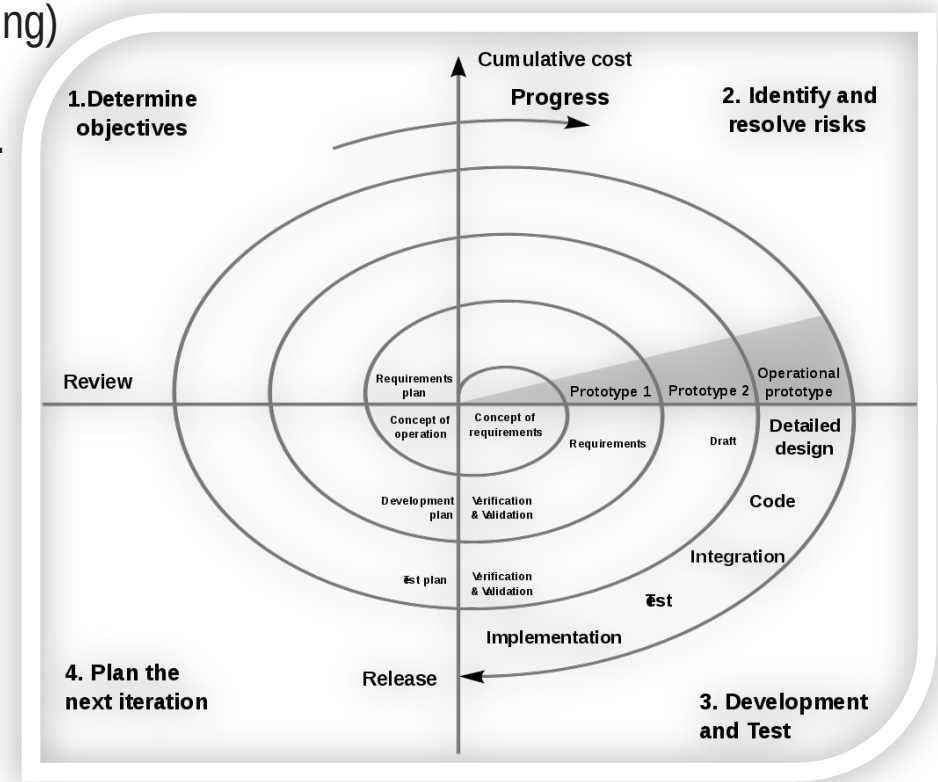
Summary of VERA-based CRUD/CIPS analysis

- overall workflow (initial)
  - use tool composed of Foundation and Core Simulator components, along with simplified system capability, to identify CRUD-vulnerable locations
  - use tool composed of Foundation, Core, and Advanced components to predict CRUD formation
  - use tool composed of Foundation and Core Simulator components to analyze CIPS
- potential improvements
  - automate process (single automated analysis rather than 3-stage)
  - design optimization
  - sensitivity analysis and UQ

CASL is using Agile software development processes

- software development processes:
  - processes, practices and activities that drive software development
  - customer interactions (e.g. requirements gathering)
  - contract models
  - planning, day-to-day coordination, releases, etc.





Traditional waterfall approach is unable to accommodate changing requirements and research-driven projects.

Agile methods fix Time (fixed iterations, fixed releases) and Effort (fixed team size) and vary Scope (functionality) based on iterative feedback with customer(s).

The CASL Quality Management System

- maps three major Quality standards to our internal processes
  - DOE O 414.1C
  - ISO 9001-2008
  - NQA-1-2008 & Part II Subpart 2.7
- supported by a dedicated Quality Manager who reports to the CASL Director
- documented in a Quality Manual, continually revised and published yearly
- reviewed yearly for continuing suitability

The CASL QA Program Strategy is Built on Process Maturity Levels

Level 1 (Initial)
- Undocumented
- Constantly changing
- Driven by personal heroics

Level 2 (Repeatable)
- Established process, but inconsistent
- No rigorous discipline

Level 3 (Defined)
- Documented
- Standardized
- Improving with time

Level 4 (Managed)
- Measureable
- Controlled using metrics

Level 5 (Optimizing)
- Focus is on continuous improvement

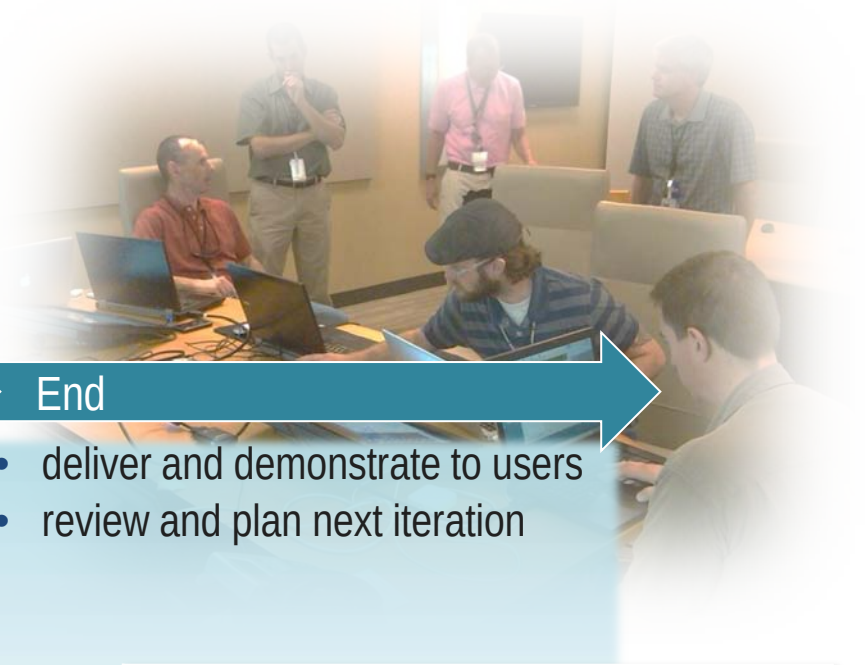
1. Identify the requirements of the quality standards
2. Identify the CASL processes that implement those requirements
3. Biannually assess the maturity of those processes
4. Identify areas for improvement, fold initiatives into POR cycle

CASL Process	Maturity Level (May 2011)
Assessment	1
Communication	1
Configuration Management	2
Defect Management	1
Design	1
Documents & Records	2
Infrastructure Management	1
Monitoring & Metrics	1
Planning	2
Procurement	3
Project Management	2
Quality Management	1
Release Management	1
Requirements Management	2
Software Acquisition	1
Training	1
Test, Verification & Validation	2
Work Processes	2

- Requirements of the standards are implemented by Processes.
- Processes are graded according to their maturity using a scale similar to that used by the CMM system.

CASL is using a modified Agile process

- based on widely-used methodologies
- customized for CASL and refined as needed
- enabled diverse team to be productive very quickly



Start

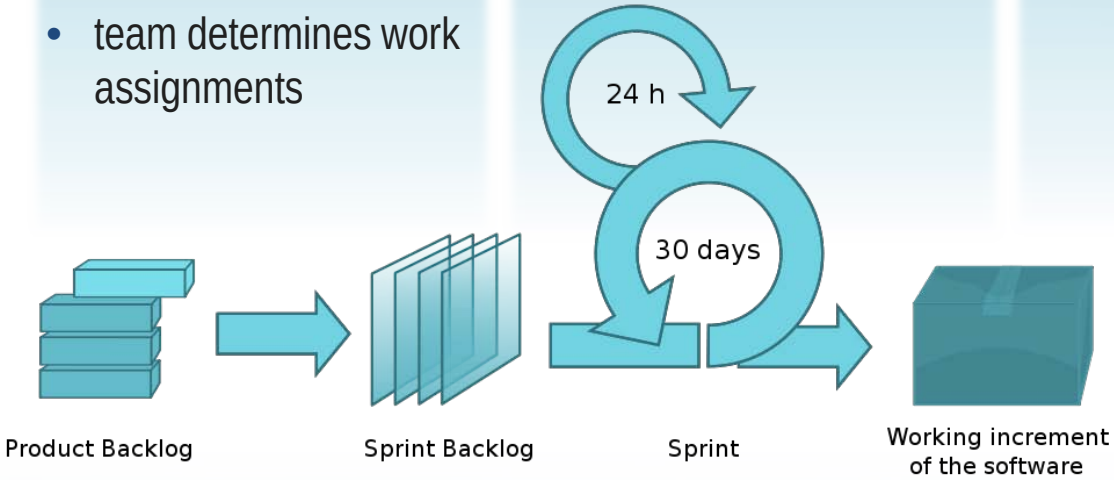
- users prioritize goals for next 4-week iteration
- team determines work assignments

Execute

- two 30-minute standup meetings each week

End

- deliver and demonstrate to users
- review and plan next iteration



Scrum: http://en.wikipedia.org/wiki/Scrum_%28development%29

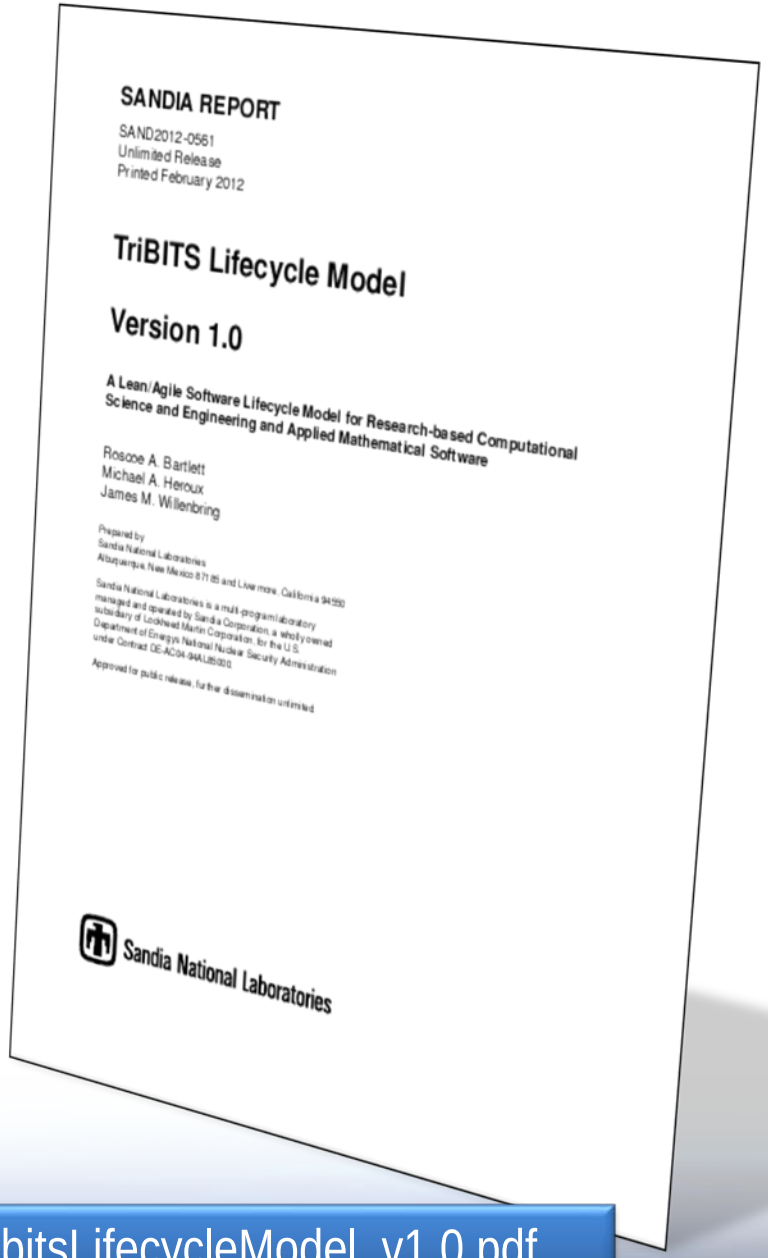
Desirable attributes

- emphasis on collaboration and adaptability
- constant communication / interaction
  - both within team and with user community
- accommodates changing requirements & unpredictability

Agility + Formality

Goals for the TriBITS Lifecycle Model

- allow exploratory research to remain productive
  - only minimal practices for basic research in early phases
- enable reproducible research
  - minimal software quality aspects needed for producing credible research
  - researchers will produce better research that will stand a better chance of being published in quality journals that require reproducible research.
- improve overall development productivity
  - focus on the right SE practices at the right times, and the right priorities for a given phase/maturity level
  - developers work more productively with acceptable overhead
- improve production software quality
  - focus on foundational issues first in early-phase development
  - higher-quality software will be produced as other elements of software quality are added
- better communicate maturity levels with customers
  - clearly define maturity levels so customers and stakeholders will have the correct expectations



SANDIA REPORT

SAND2012-0561
Unlimited Release
Printed February 2012

TriBITS Lifecycle Model

Version 1.0

A Lean/Agile Software Lifecycle Model for Research-based Computational Science and Engineering and Applied Mathematical Software

Roscoe A. Bartlett
Michael A. Heroux
James M. Willenbring

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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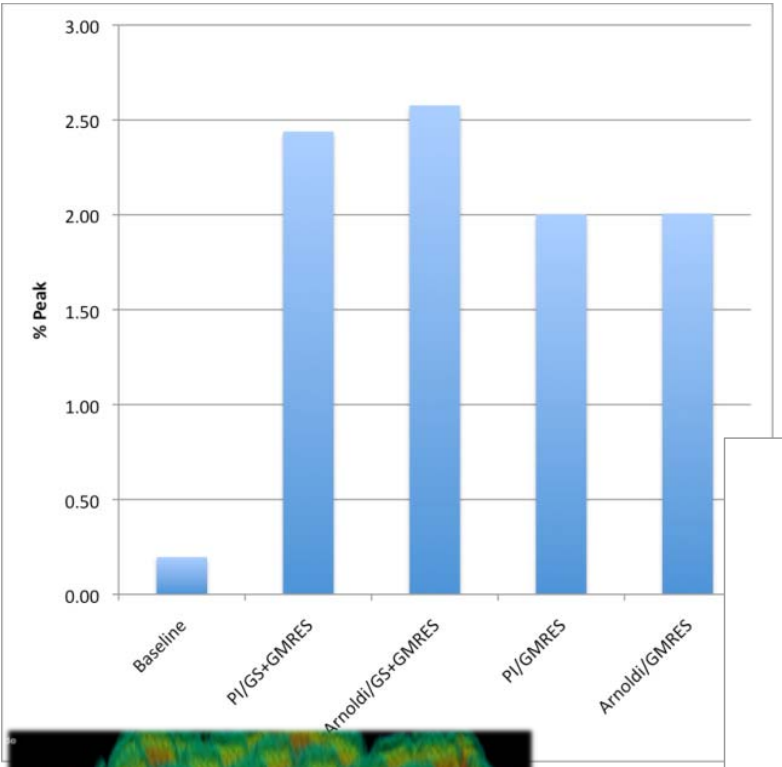
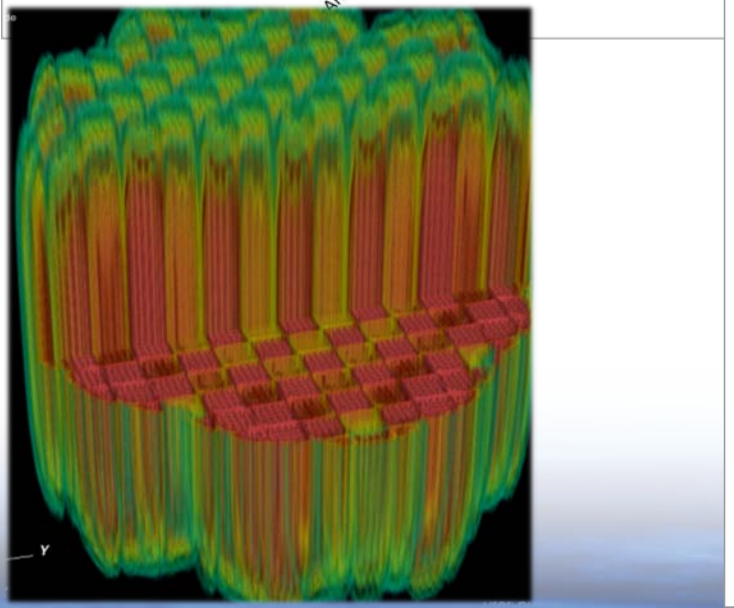
http://www.ornl.gov/~8vt/TribitsLifecycleModel_v1.0.pdf

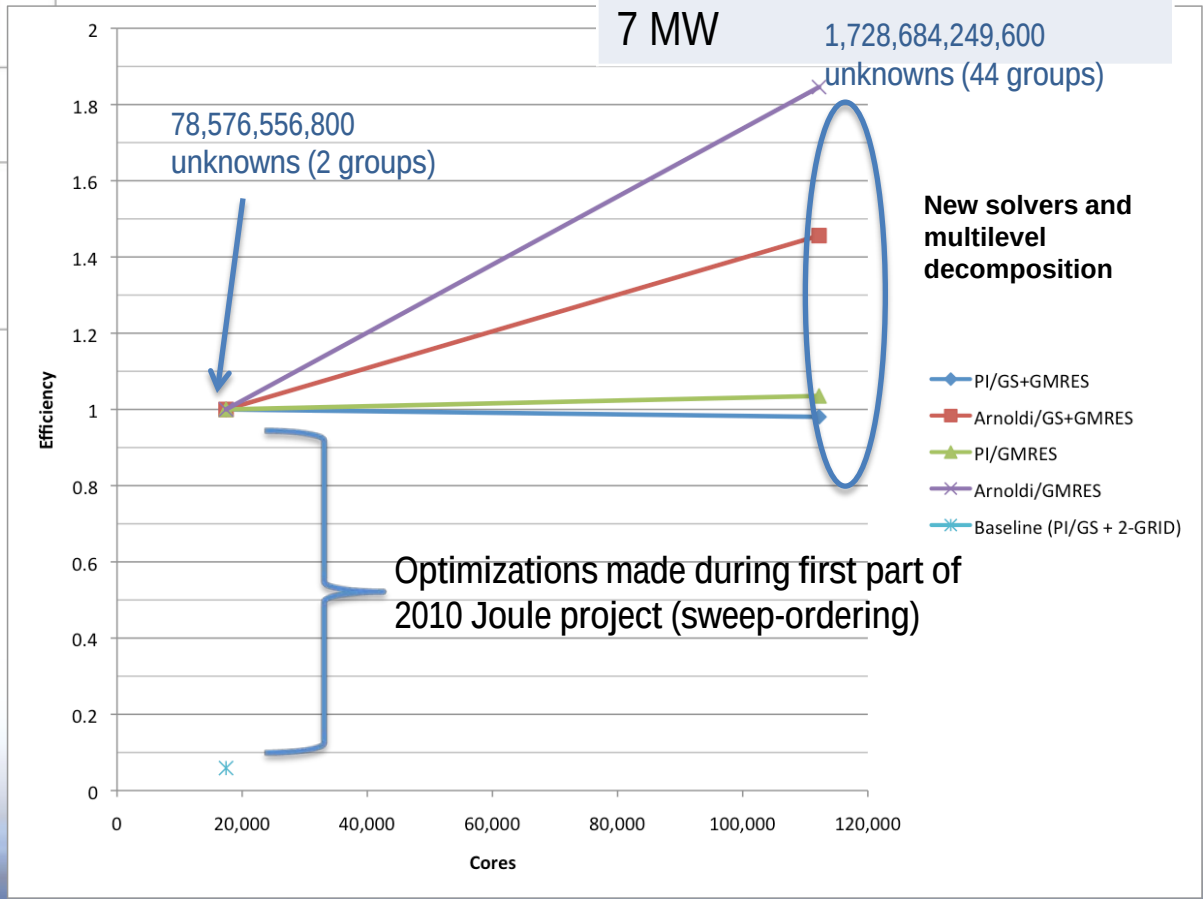
Denovo Parallel Performance



Factor of 10x increase in peak efficiency gained through Joule project + ASCR OLCF-3 project work

Jaguar Cray XT5
37,376 AMD Opteron CPUs (6-core, 2.6 GHz)
224,256 total compute cores
2.332 Petaflop/s peak perf.
1.759 PF/s sustained perf.
362 TB total system memory
7 MW





CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

Cross-Section Processing Tasks

June 12, 2012

Brad Rearden
Matthew Jessee
Mark Williams

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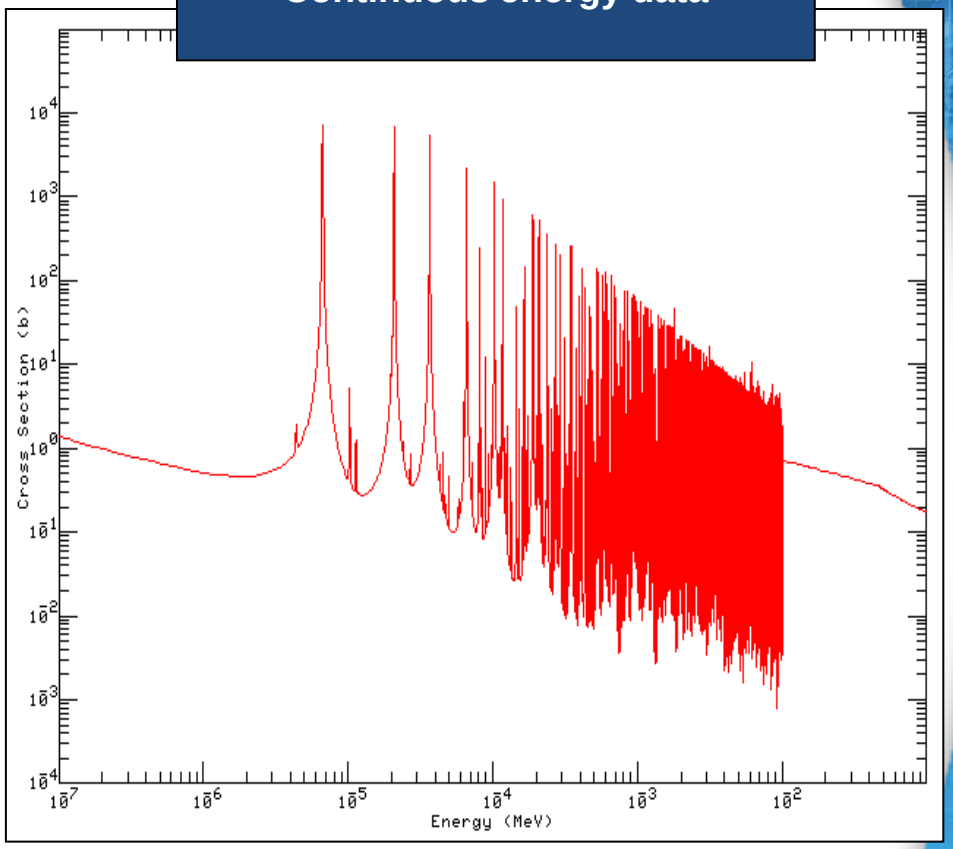
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Cross Sections 101

- Full-core simulation requires accurate computation of neutron flux distributions and power distributions
- Flux/power are spatial-, energy, and time- dependent variables,
- Different simulators for different applications => wide range of space/energy/time scales
- Energy-dependence governed by the representation of neutron cross sections, i.e. probabilities of interaction between a neutron and target nuclide.

Continuous energy data



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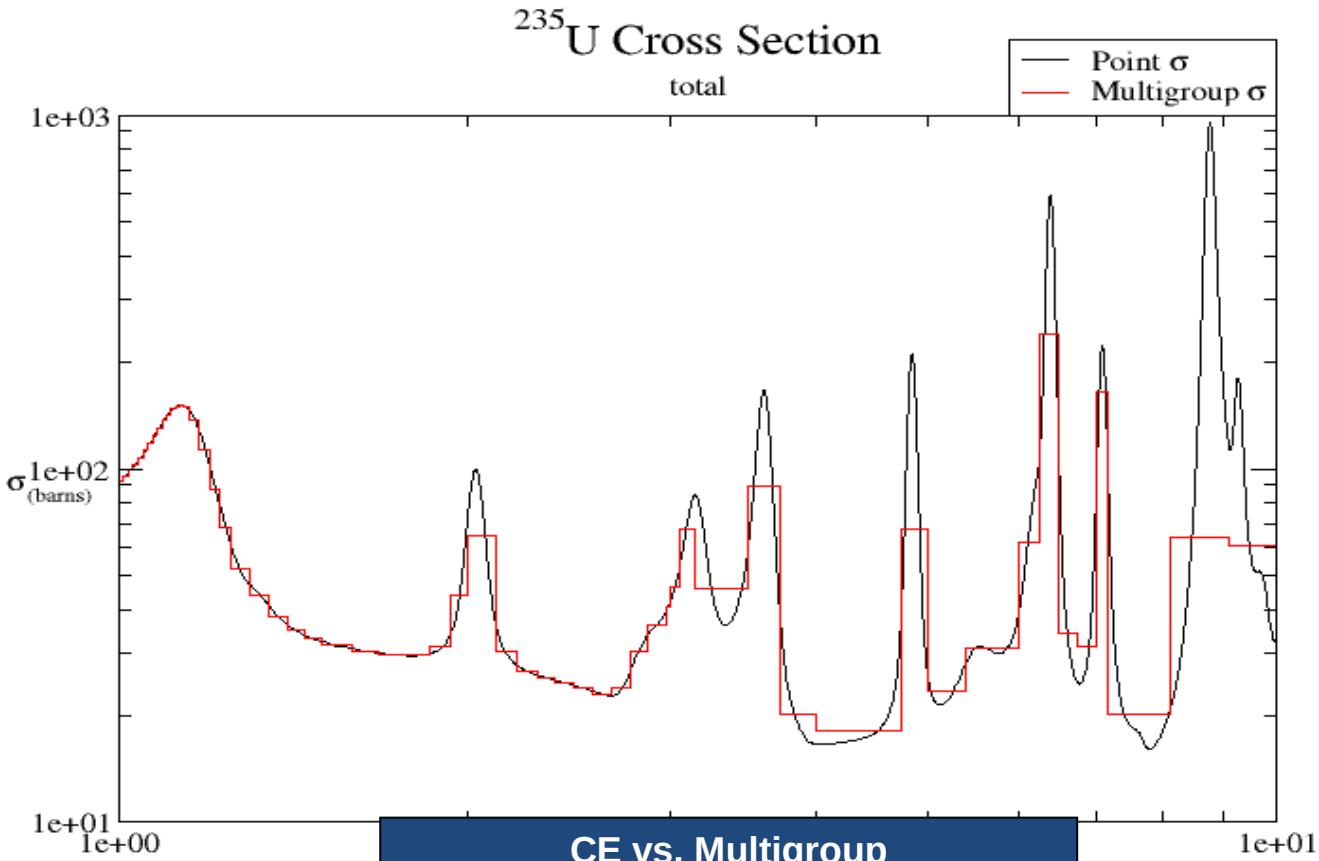
Cross Sections 101



CE vs. Multigroup

For full-core simulation, continuous-energy (CE) cross-sections are represented by multigroup (MG) cross sections.

Cross Sections 101

- Simulation accuracy depends on appropriate preparation of MG cross sections.
- MG cross section preparation a function of:
  - Number of energy groups
  - XS Methodology
    - Unit Cell
    - Subgroup
    - Embedded Self-Shielded Method (ESSM)
- All 3 methodologies under consideration for CASL core simulation

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Overview of Cross-Section Processing Tasks

- VRI – Cross-section Processing (XSPROC) Integration
  - Integrate current SCALE methodology for multigroup (MG) cross-section (XS) processing into Denovo (Unit-Cell)
- RTM –Subgroup Library Generation
  - Develop multigroup XS libraries for DeCart based on AMPX and SCALE code systems (Subgroup)
- RTM – Embedded Self-Sheilding Methodology (ESSM)
  - Develop ESSM methodology and integration plan into MPACT

Takeaway point

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XSPROC Integration into Denovo

VRI
Lead: Brad Rearden/Tom Evans (ORNL)

SCALE Contributors (ORNL):
Brad Rearden, Robert Lefebvre, Jordan Lefebvre, Lester Petrie, Ugur Mertyurek, Mark Williams

Denovo Contributors (ORNL):
Tom Evans, Greg Davidson, Josh Jarrell

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Example Layout: Title Only

Presenter

Objectives and Strategies

- Point 1
- Point 2
  - Subpoint A
  - Subpoint B
- Point 3

Requirements Drivers

- Point 1
  - Subpoint A
  - Subpoint B
  - Subpoint C
- Point 2

Outcomes and Impact

- Point 1
- Point 2
  - Subpoint A
  - Subpoint B
- Point 3

Subgroup Library Generation

RTM
Lead: Matthew Jessee (ORNL)
Contributors: Kang Seog Kim (ORNL)
Mark Williams (ORNL)
Ben Collins (UM)
Yuxuan Liu (UM)

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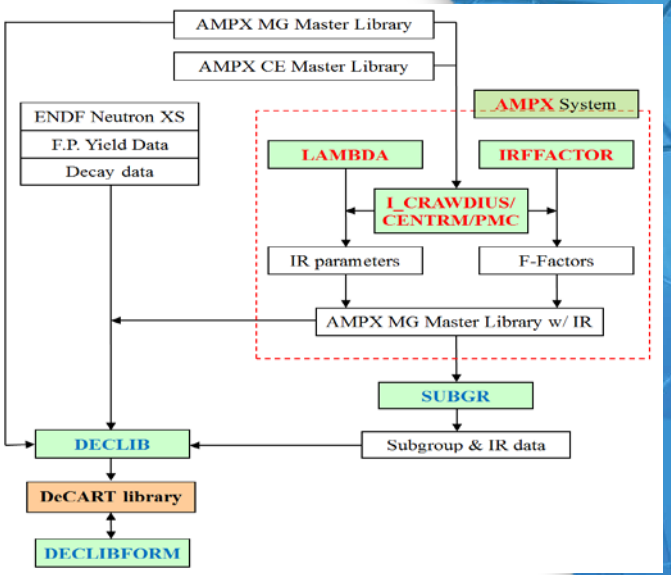
Nuclear Energy

Subgroup Library Generation (POR-4)

Presenter

Objectives and Strategies

- Development of library generation "process" using ORNL code systems (AMPX and SCALE)
  - Minimize user interaction in library development
  - Minimize cost associated with future library generation efforts
- Deliver Draft Subgroup Library for initial testing in DeCart
- Deliver Letter Report documenting AMPX/SCALE-based library generation procedure



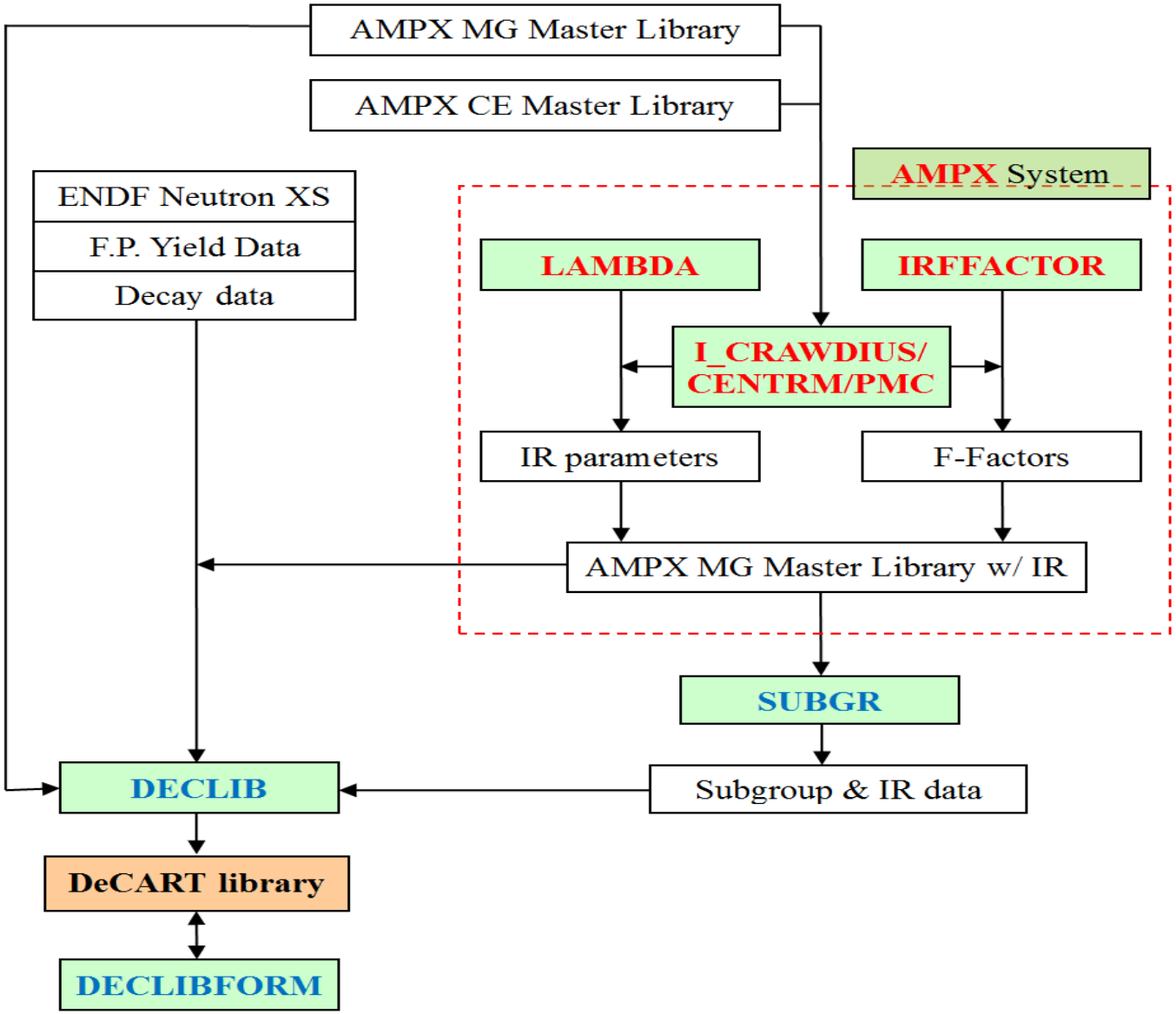
Requirements Drivers

- The DeCART core simulator uses the subgroup method to generate MG cross sections.
- Current library based on older evaluations (ENDF/B VI)
- Current library is not releasable
- New library based on public code systems (AMPX and SCALE)
- New library based on ENDF/B VII

Outcomes and Impact

- Established subgroup library generation process
- Delivered 81-group Draft library to UM for initial testing
- Draft library successfully tested with in-house transport code
- Delivered letter report documenting generation procedure
- Final library delivery planned for POR-5

Subgroup Library GenerationProcedure



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ENERGY
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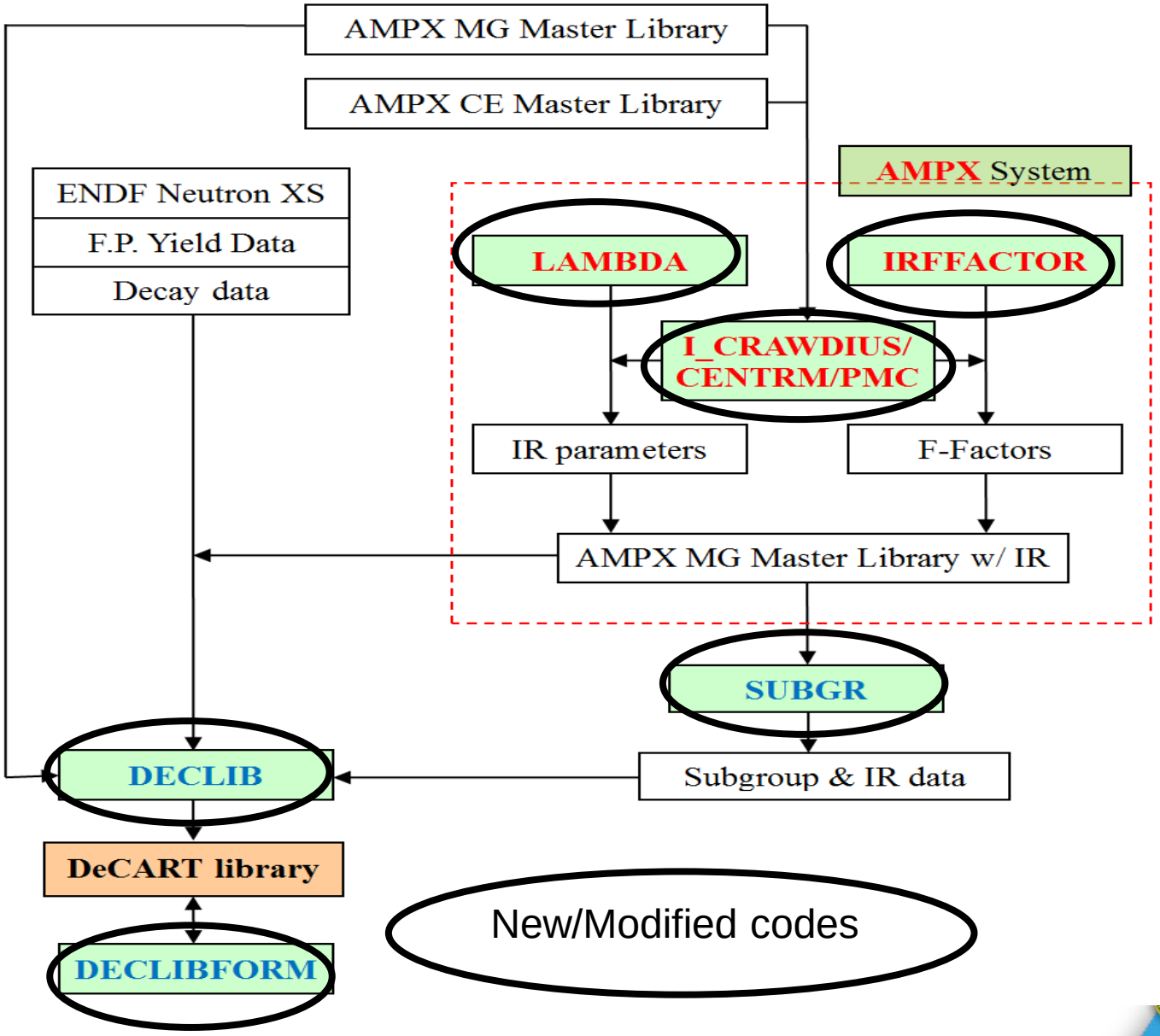
Subgroup Library GenerationProcedure



Inhouse Subgroup Library Testing

- CASL VERA Benchmark Problems: 2D PWR HZP Pin Cell

Zone	Radius (cm)	Material	Density (g/cm^3)	Remarks
Fuel Pellet	0.4096	UO_2	10.36	3.1% ^{235}U
Gap	0.4180	He	0.001	
Cladding	0.4750	Zr-4	6.56	
Moderator	1.2600	H_2O	0.743 (565K) 0.661 (600K)	1300 ppm 2250 psia

Case	1A	1B	1C	1D
Moderator	565 K	600 K	600 K	600 K
Cladding	565 K	600 K	600 K	600 K
Fuel	565 K	600 K	900 K	1200 K

Case		1A	1B	1C	1D
KENO		1.18699	1.18221	1.17163	1.16226
INHOUSE Code	without RS	1.19499	1.18949	1.17728	1.16680
	$\Delta\rho$(pcm)	564	518	410	334
	with RS	1.18867	1.18290	1.17132	1.16104
	$\Delta\rho$(pcm)	119	49	-23	-90

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Embedded Self-Shielding Method

RTM
Lead: Mark Williams (ORNL)
Contributors: Kang Seog Kim (ORNL)
Mark Williams (ORNL)
Ben Collins (UM)
Yuxuan Liu (UM)

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Nuclear Energy

Embedded Self-Shielding Method (POR-5)

Presenter

Objectives and Strategies

- ESSM
  - A new method to prepare MG XSs for full-core transport
  - Similar advantages and disadvantages as subgroup method
- Objective to develop new fine-group and broad-group libraries for ESSM method.
- Finalize subgroup library for DeCart

Requirements Drivers

- CASL funding development of new core simulator code MPACT (Univ. Michigan)
- MPACT Cross-section methodology will depend on AMPX/SCALE-based libraries, either ESSM or subgroup
- Broad-group library generation necessary for run-time requirements

Outcomes and Impact

- Published paper on ESSM method, with initial test results for pin-cell problems

Williams, Kim, "The Embedded Self-Sheilding Method", PHYSOR Conference, April 2012

- 252-group fine-group library currently under evaluation.
- 252-group subgroup library and broad-group libraries to be developed later in POR-5

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Title of Presentation
Date
Etc.

Example Layout:1_Title and side-by-side content with take-away

- Topic 1
- Topic 2
- Topic 3
  - *Subpoint A*
  - *Subpoint B*
- Topic 4
  - *Subpoint A*
    - *Subpoint A-1*
    - *Subpoint A-2*
  - *Subpoint B*

- Topic 5
  - *Subpoint A*
  - *Subpoint B*
    - *Subpoint B-1*
    - *Subpoint B-2*

Take-away point

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- Topic 3

Takeaway-point

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  - Subpoint B
- Point 3

Example Layout: 2_Title and Content

Topic 1:

- Subpoint A
- Subpoint B

Topic 2:

- Subpoint A

Topic 3:

- Subpoint A
- Subpoint B

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VOCC Project Update

April Lewis
CASL Collaboration and Ideation Officer(CIO)
6/12/2012, CASL Roundtable

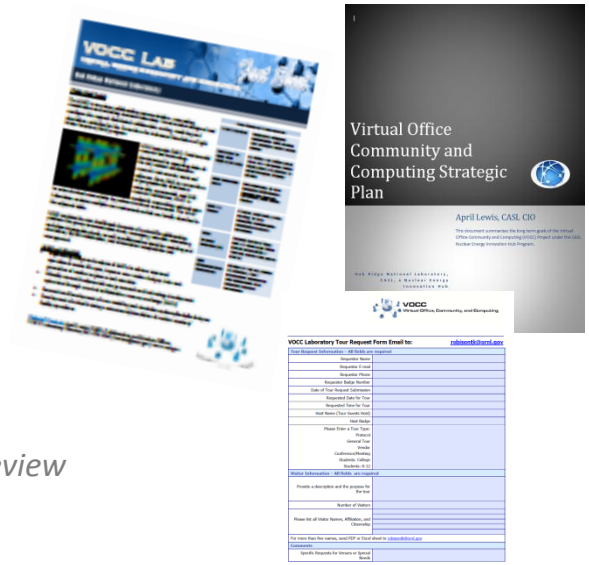
Talking Points

- Open Scope for VOCC
- Status of Activities
- Operations Status
- VOCC R&D
- Strategic Development
  - Growth and Future Support

Open Work Scope for VOCC

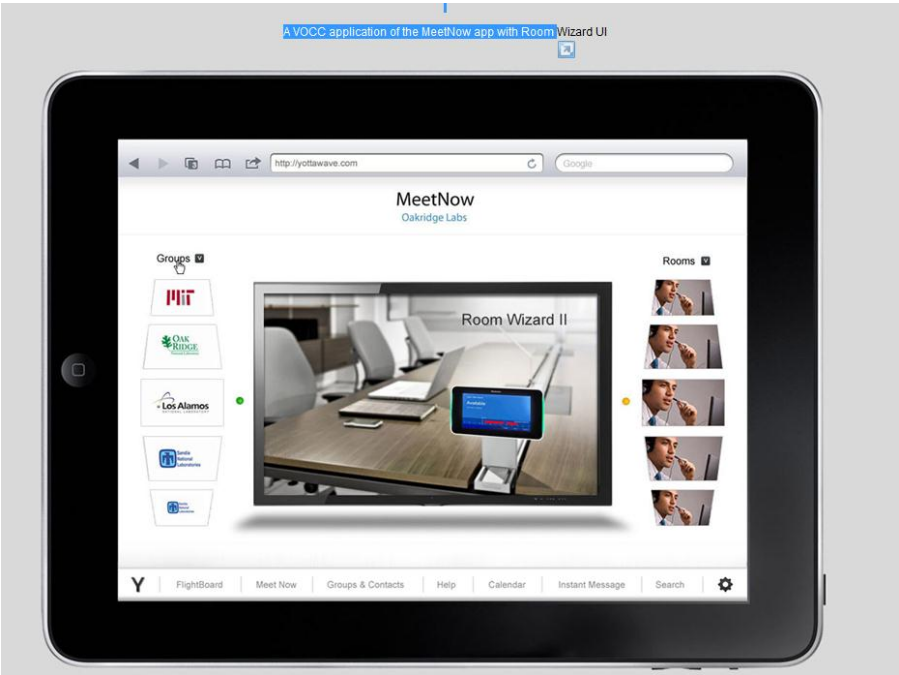
- VOCC Lab Operations/Support to CASL and ORNL
  - Lab management(space and instrument maintenance, personnel access, physical & cyber security, instrument development, equipment utilization, subcontracts, procurement, tours, user technical assistance, training, etc.)
  - > 235 users, utilization climbing, decreasing resources
  - Difficult to manage "goals", "time is managed by others"
- Tours: people count = "823" since July 2011 to 6/12/2012, FY12 so far = 89 formal & 26 informal
- VOCC Document Development
  - Fact Sheet, Tour Request Form, Vidyo Tips/FAQ
  - Strategic Plan, Governance Statement, etc…
- VOCC Inventions: Personal Immersive Device Patent,

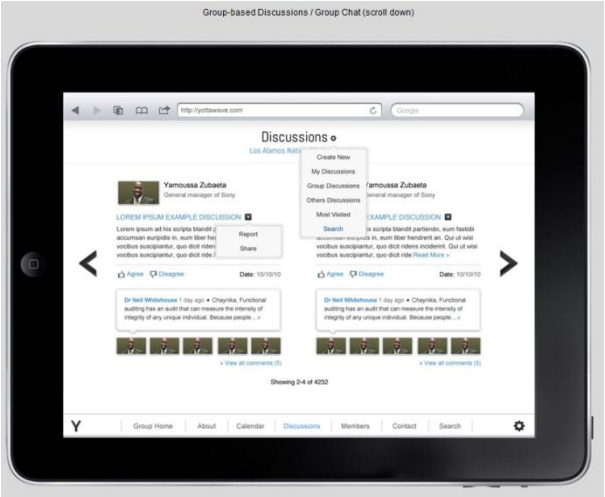
  Docket No. 2765.0, UT-Batelle, LLC. filed on 2/22/2012
- Design and Host VOCC "External" Web Site
  - ***www.voccnet.org***
- F-5 Telepresence Configuration
- Deploy Agile Collaborative Communication(ACC) Management Tool
- VOCC Broadcast Capability
- Metrics Collection and Database Development
- Semantic Analysis of CASL SharePoint
- *Migrate Immersion Room to ORNL network, Viz. support to Annual Review*
- Multi-tenant portal configuration
- *Ticketing system software*
- *Mentor Summer Students*
- *"unplanned scope": Review, Evaluate, Investigate, and Critique CDC Proposal*



VOCC Yottawave SW Development

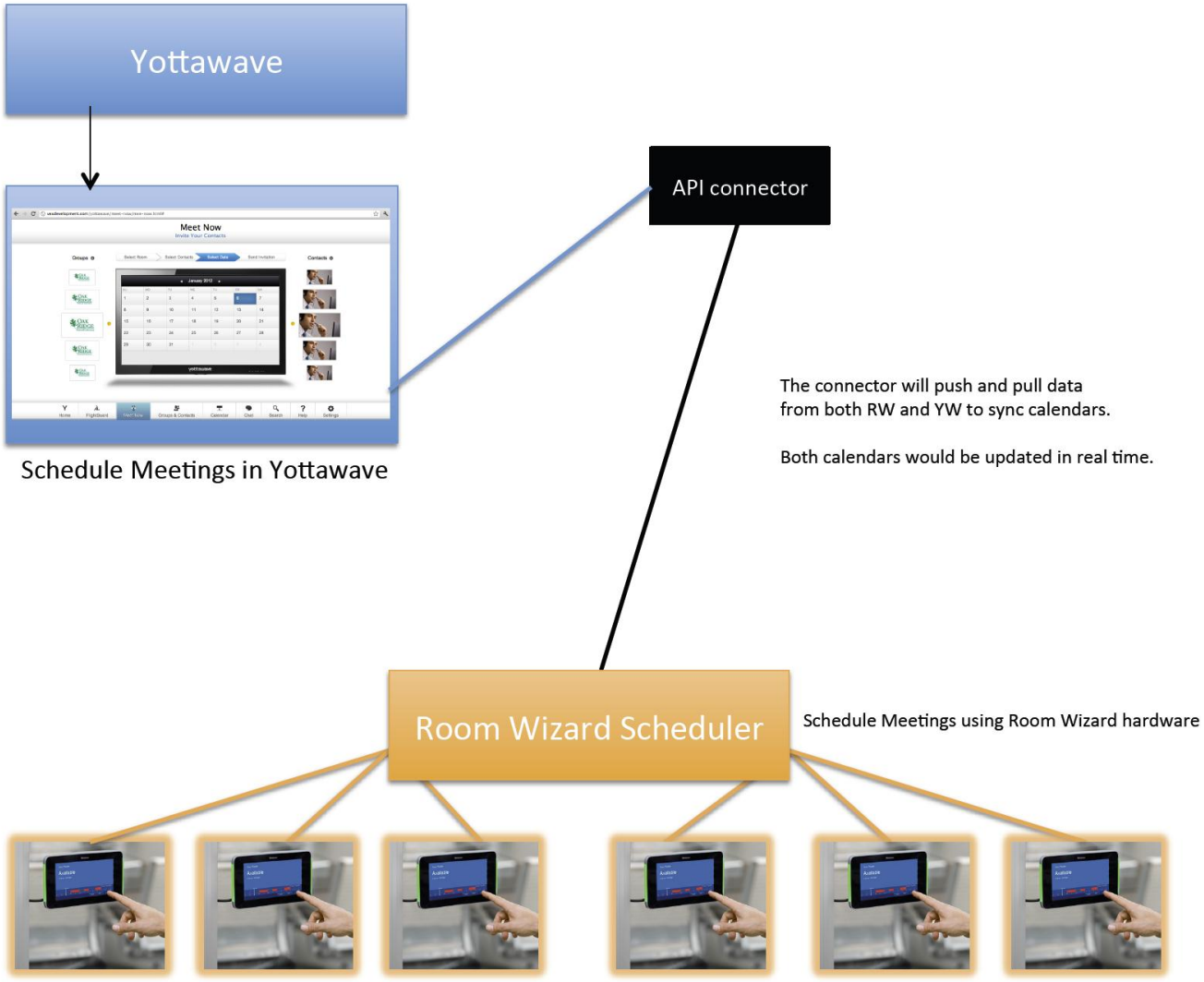
- A Web application, Java based, social network/”enterprise” collaborative communications scheduler/management tool





VOCC NET

VOCC Software Development



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VOCC Software Development

Yottawave

Schedule Vidyo Meeting

Each user has their Vidyo Room link added to their Yottawave Profile:

1. When setting up a meeting in Yottawave, the user will choose the meeting options from the wheel.
2. If My Vidyo Room is chosen, the Vidyo room link will be added to the meeting invitations
3. If a Room with a 220 is chosen, the meeting room URL can be added the same way as the individual room URL by manually adding from an admin account to Yottawave.
   The user will fill out the rest of the meeting invite information.
4. User sends out meeting request and participants join following the Vidyo Guest model.
5. Invitations are sent to primary emails, so they can be added to Outlook (or any other) Calendar.

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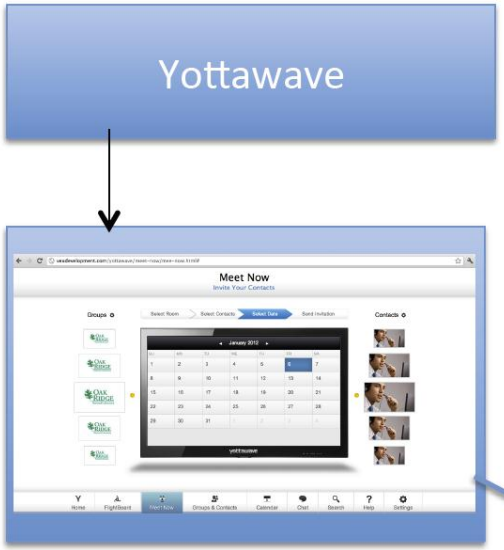
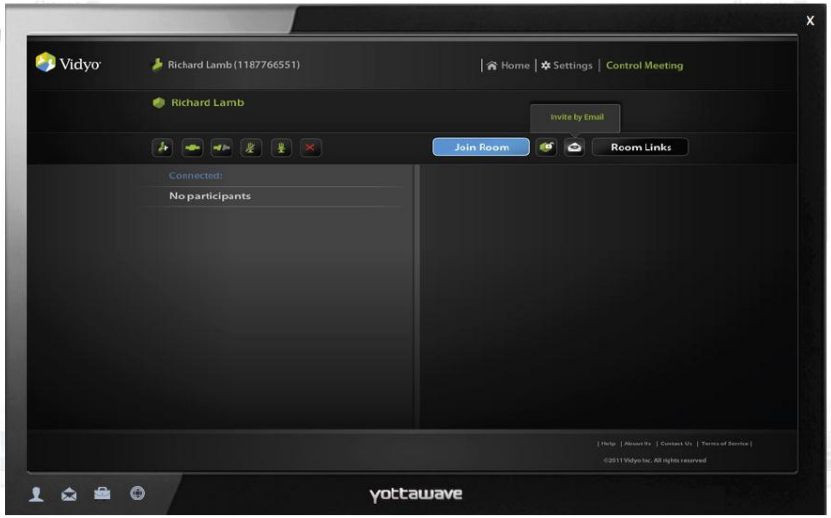
VOCC Software Development



Direct Vidyo Call

Direct calls (on the fly) can be initiated leveraging the current Vidyo directory through the Yottawave interface. This approach bypasses the Yottawave calendar system.



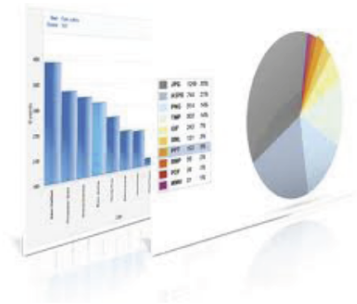
VOCC NET

VOCC Software Development

RW Reporting

The RW reporting tool should be able to pull analytics for all calendaring events utilizing the Room Wizard mapped meeting rooms. However, the Room Wizard meeting scheduler does not share the same meeting-based logic with Yottawave. Therefore, meeting locations that are not mapped to the Room Wizard directly, cannot be populated from Yottawave.

Room Wizard Reporting Tool

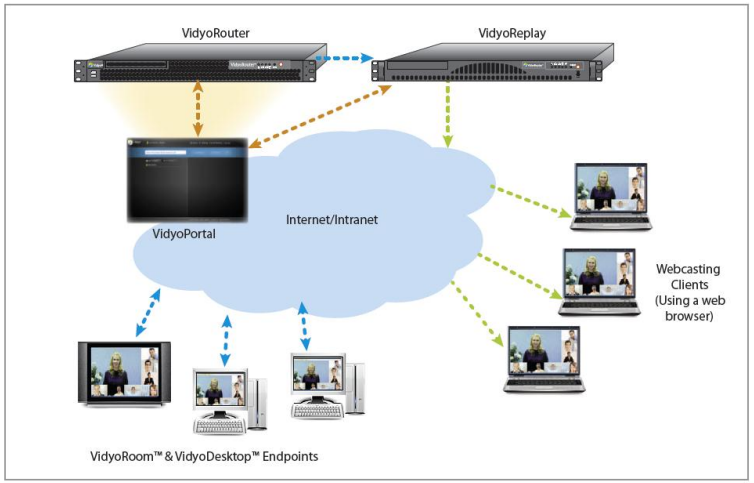


- "First steps to full automation of metric information collection, analysis, and reporting
- Support socialization of metric results/impacts via dashboards

VOCC NET

Recording CASL Video Exchanges for Webcasting

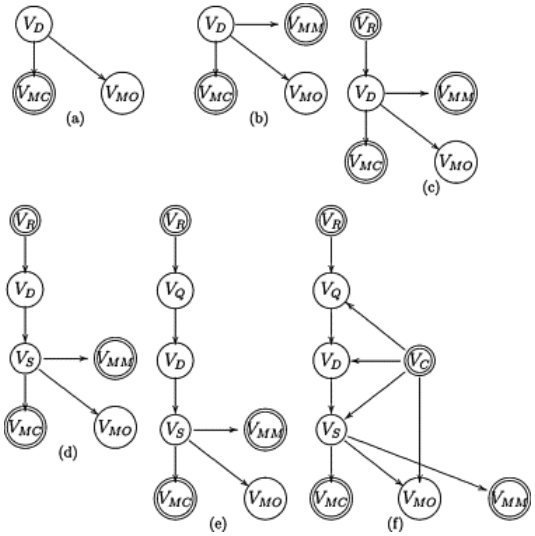
- Webcast conferences cost effectively to large audiences – no client download or Vidyo Line consumption to view
- Webcast and record in FLV Format
- Every Vidyo endpoint can become a Content Creation station
- Manage access and metadata of created content
- Standard web video file format – no proprietary player required to view recorded content

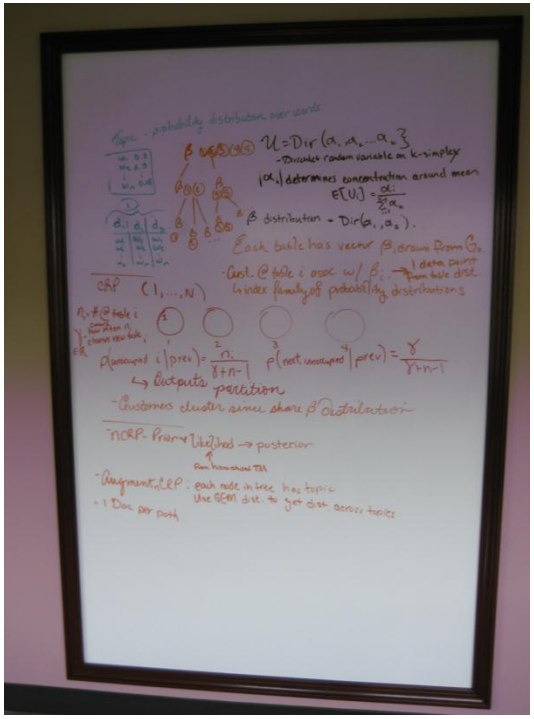


** Will require a VOCC developed information management/protection protocol*

Semantic Analysis of CASL SharePoint

- VOCC is evaluating the potential impacts of implementing a semiotics algorithm to aid in characterization of its collaborative information stores developed specifically for the CASL Program. VOCC hopes to use themes developed from the semiotic algorithms output to develop a more “natural” folksonomy for CASL information organization. The more natural folksonomy should provide a better way to store information in collaborative environments and therefore make it much easier for CASL team members to find information.





Reducing the time scientists look for information means there is more time for “innovation”!

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VOCC Metrics Dbase and Analysis

- VOCC is developing a “single relational data store” for all of its metrics collected.
  - Access logs, Cameras, RWizards, Visitor logs(VOCC/Collocation), Vidyo CDR, VidyoVoice, System Logs, lamp hours, PC log, error reports, etc.

*soon to include “population density”

- Multi-zone/directional traffic pedestrian traffic & occupancy.
- Combines shape recognition and motion detection technologies.

“Identify Trends and Optimize…
Collaboration Space/Resources Utility”

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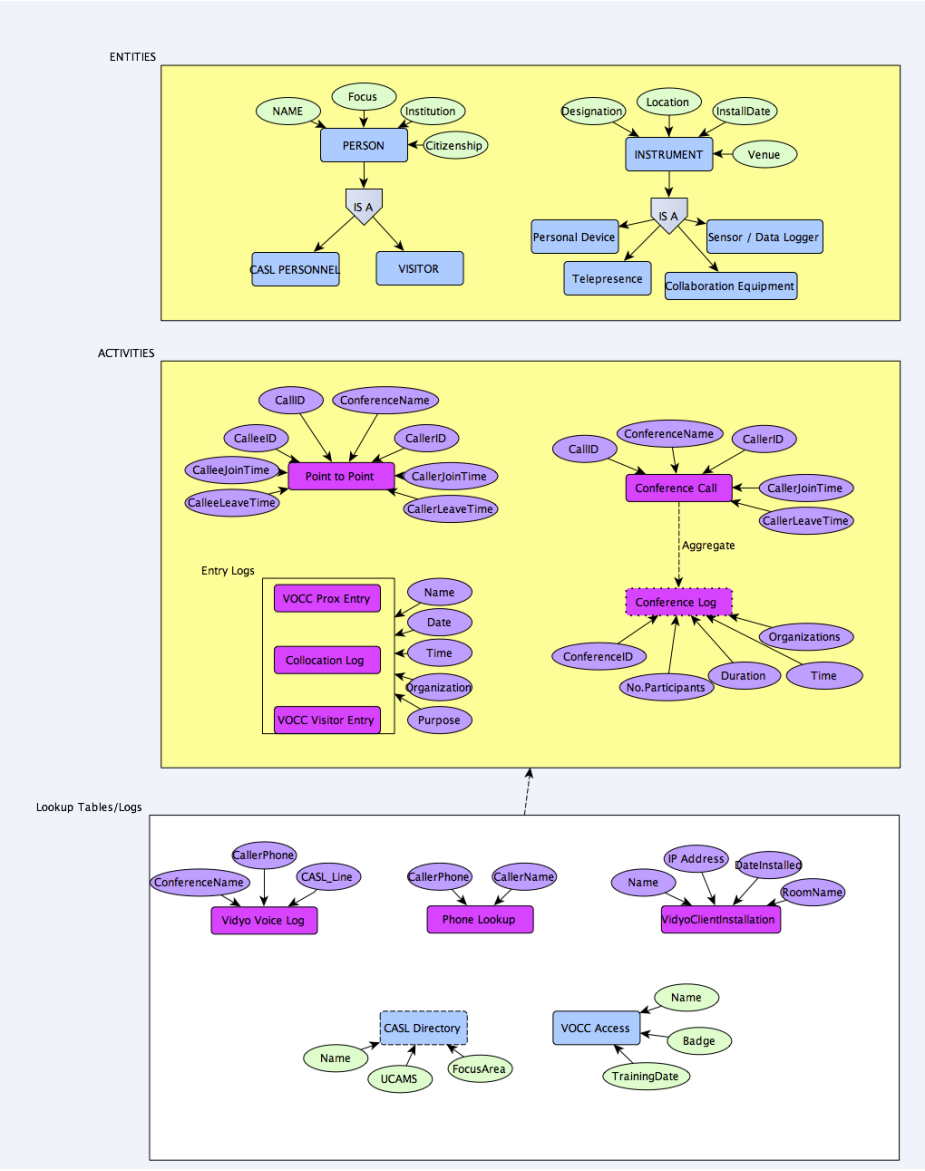
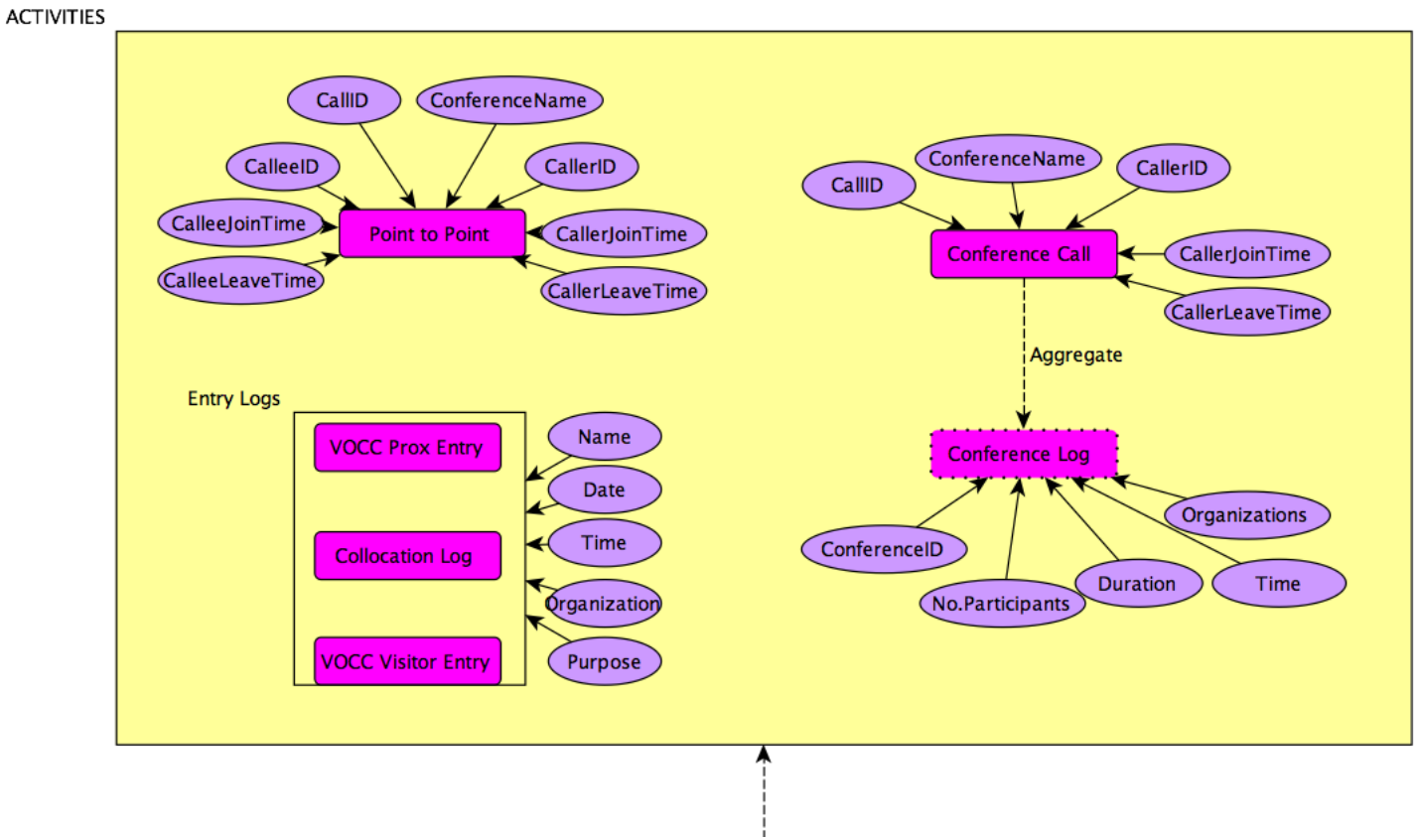
Metrics Initial Taxonomy

All final results "anonymized"



Sample- Taxonomy Fine View

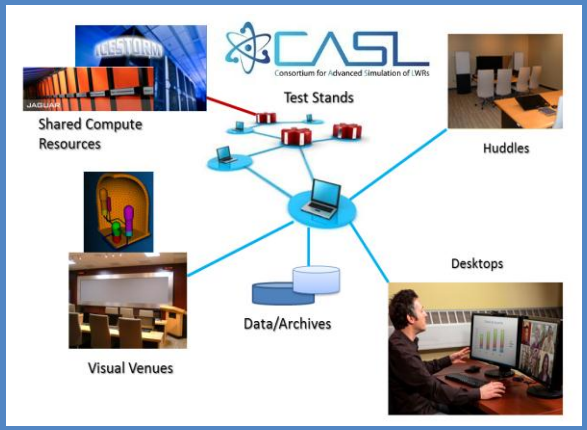


VOCC Strategic Plan

SHARED RESOURCES

SCIENTIFIC, SOCIAL CONNECTIVITY

Multi-Tenant Environment



Multi-Portal

IPC Software

"Enabling Energy Innovation Through Collaboration R&D"

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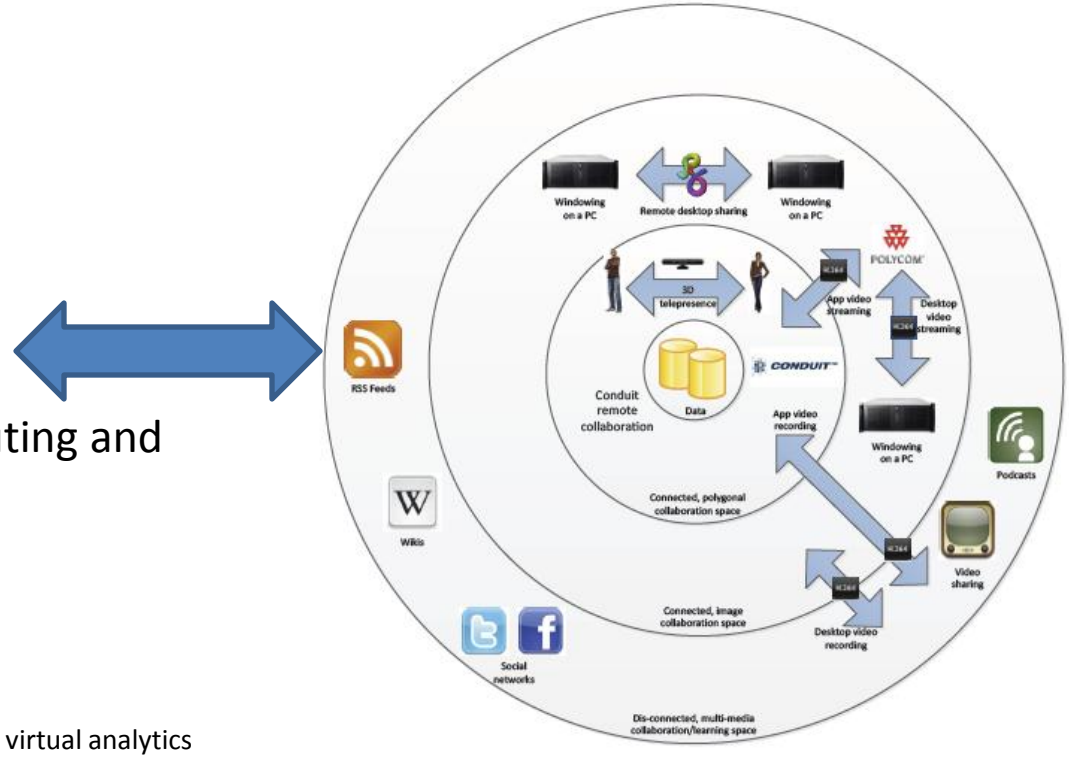
VOCC Developments

- VOCC will continue to have very lofty goals for improving collaborative communication in 3D environments. VOCC will seek research partners to solve problems with or to establish initial capability for:



- Personal Supercomputing and Visualization!

  - Collaborative, immersive 3D virtual analytics
  - 3D Telepresence or “Tele-immersion”
  - AV/IT/HP convergence towards a centralized dynamically managed collaboration resource paradigm.
  - Improved methods for collaborative group data storage, access, “findability”, and secure info sharing

VOCC NET

Challenge Problem Integration

Zeses Karoutas

AMA Deputy Lead

Westinghouse

CASL Roundtable Virtual Meeting

June 13, 2012

Outline

- Challenge Problem Integrators
- Description of Challenge Problem & Need for Model & Simulation
- What is Proposed Success for Addressing each Challenge Problem
- Next Steps

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Challenge Problem Integrators

- Observations & Concerns:
  - Current management structure built on Focus Areas (FAs) can lead to “Silos of Excellence”
  - Tasking and scheduling Focus Area activities in integrated fashion for Challenge Problems
- Potential Solution:
  - Introduce Product Integrators to work across FAs to assure above noted observations & concerns are addressed
  - Responsibilities include driving critical applications, products, & outcomes that cross FA boundaries
  - Have budget influence but not budget authority: work with the FA teams to set and define milestones, complete certain milestones as appropriate, and review milestones for which they are the customer
  - Overall Challenge Problem Integrator will oversee solutions to CPs
  - Individual Problem Integrator will be defined for each CP
  - Chief Scientist will provide guidance to Integrators

Integrators also Defined for Validation and Core Simulator

CASL Challenge Problems

		Power uprate	High burnup	Life extension
Operational				
CRUD-induced power shift (CIPS)	J. Secker	✕	✕	
CRUD-induced localized corrosion (CILC)	J. Secker	✕	✕	
Grid-to-rod fretting failure (GTRF)	K. Yueh		✕	
Pellet-clad interaction (PCI)	R. Montgomery	✕	✕	
Fuel assembly distortion (FAD)		✕	✕	
Safety				
Departure from nucleate boiling (DNB)		✕		
Cladding integrity during (LOCA)		✕	✕	
Cladding integrity during (RIA)		✕	✕	
Reactor vessel integrity		✕		✕
Reactor internals integrity		✕		✕

Other Integrators to be Defined

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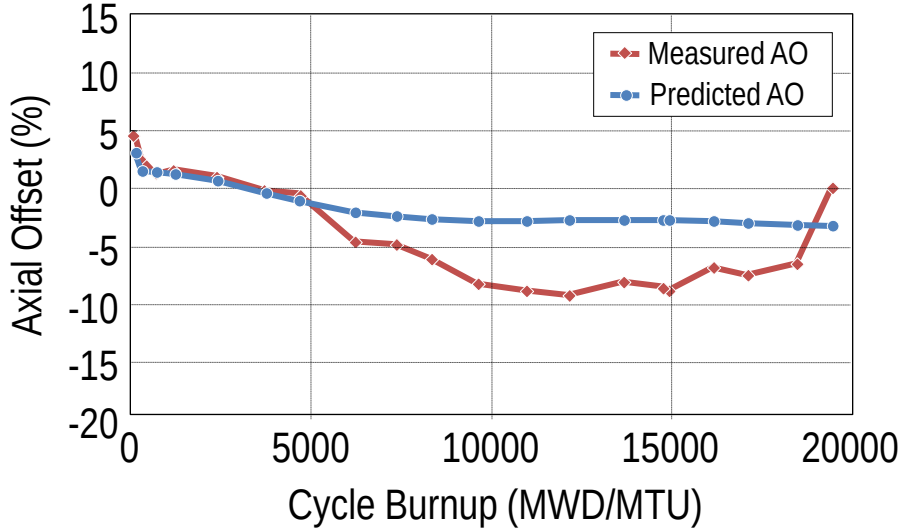
CRUD-induced power shift (CIPS)

- Problem:
  - High uncertainty in predicting CIPS due to uncertainty in crud source and boiling surface area affects fuel management and thermal margin in many plants

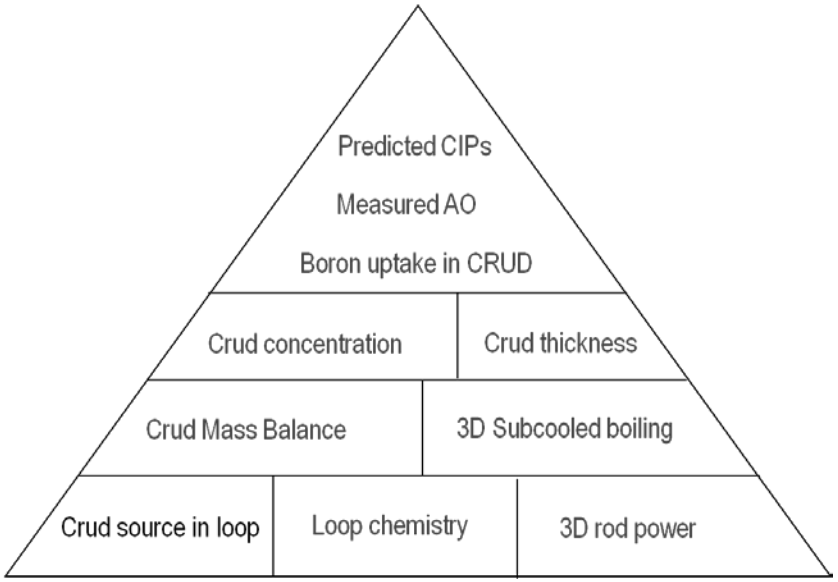


CRUD deposits

Need: multi-physics coupled tools with improved models and high fidelity to better predict CIPs plus quantifying risks via UQ.

CIPS – What is Success ?

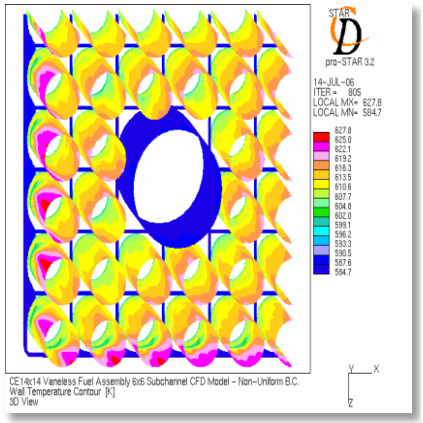
- Couple Baseline tools to include boron feedback in neutronics
- Apply VERA-CS in fine mesh (every pin in core) to get accurate boiling surface for crud mass balance and crud deposition
- Evaluate boron uptake and CIPs with reduced uncertainty
- Validate with available plant data (e.g.Vogtle)

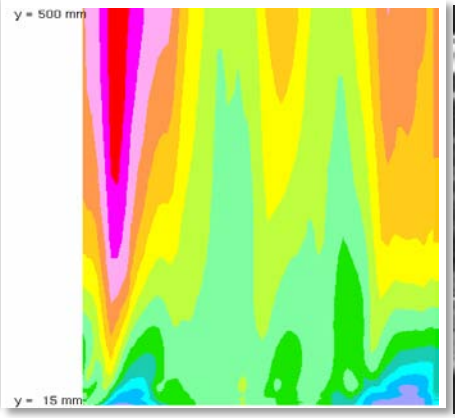


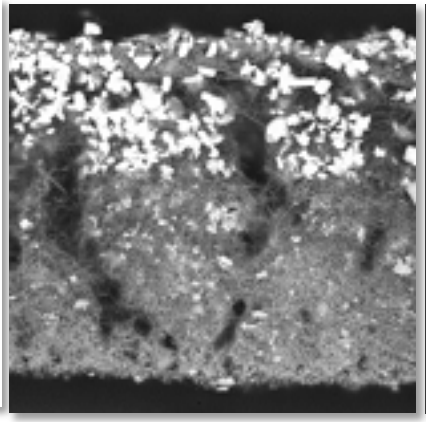
Reduce CIPS Uncertainty by accounting for boron feedback and more accurate calculation for crud and boron uptake

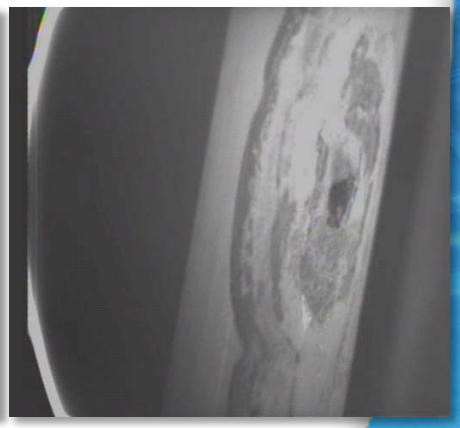
CRUD-induced localized corrosion (CILC)

- Problem:
  - Hot spots and excessive boiling with high CRUD concentration in coolant can lead to thick CRUD deposits, CRUD Induced Localized Corrosion and fuel leaker
  - Not understanding the real margin to CILC fuel rod leakers, limits fuel management for power uprates





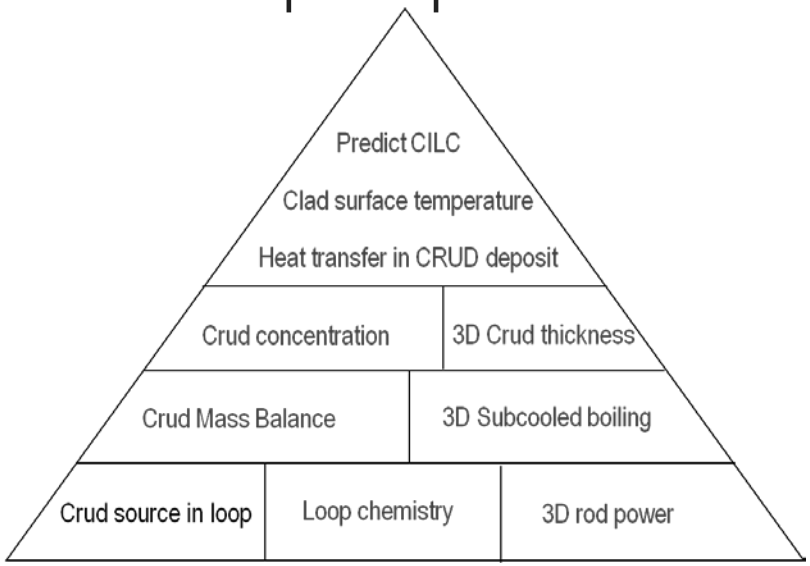




Need: High-fidelity, high-resolution capability to predict hot spots, localized crud thickness, and corrosion

CRUD CILC – What is Success ?

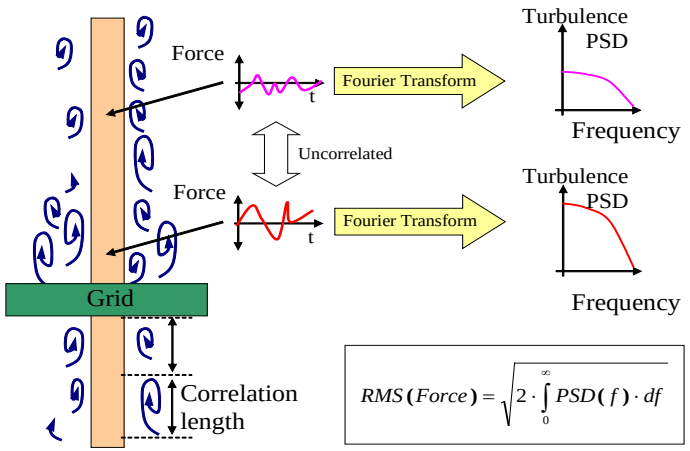
- Complete effort for CIPs to establish accurate crud mass balance
- Develop advanced CRUD tools to better estimate localized crud thickness, CRUD chemistry, clad temperature, accelerated corrosion and CILC
- Apply advanced tools for a plant with CILC leakers
- Validate tools to WALT loop and plant CRUD data (e.g. Seabrook)



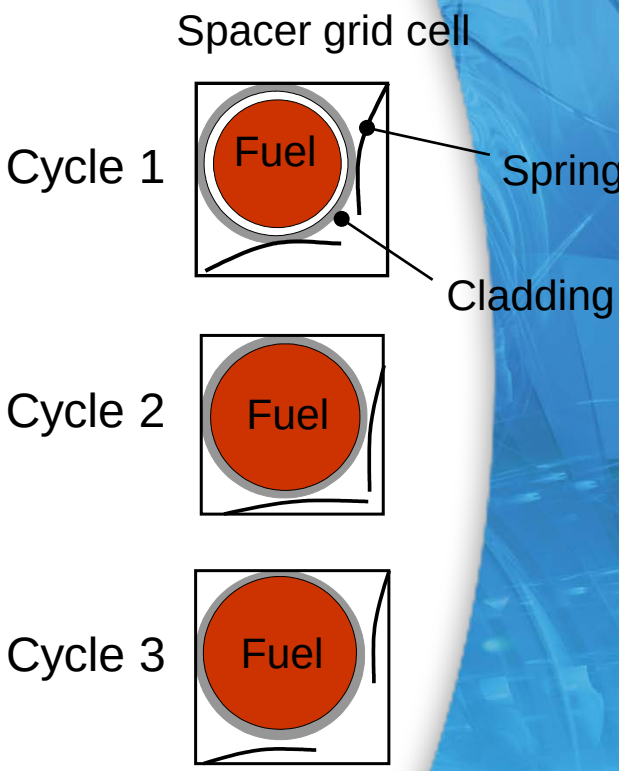
Develop Advanced Tools to Predict a CILC Leaker

Grid-to-rod fretting failure (GTRF)

- Problem:
  - Clad failure can occur as a result or rod growth changes, flow induced vibration, irradiation-induced grid growth and spring relaxation (Leading Cause of PWR fuel leakers)
  - Power uprates and burnup increase potential for fretting



$$RMS(Force) = \sqrt{2 \cdot \int_0^\infty PSD(f) \cdot df}$$



Need: High-fidelity flow induced vibration tool to predict grid to rod gap, turbulent flow excitation, rod vibration and wear

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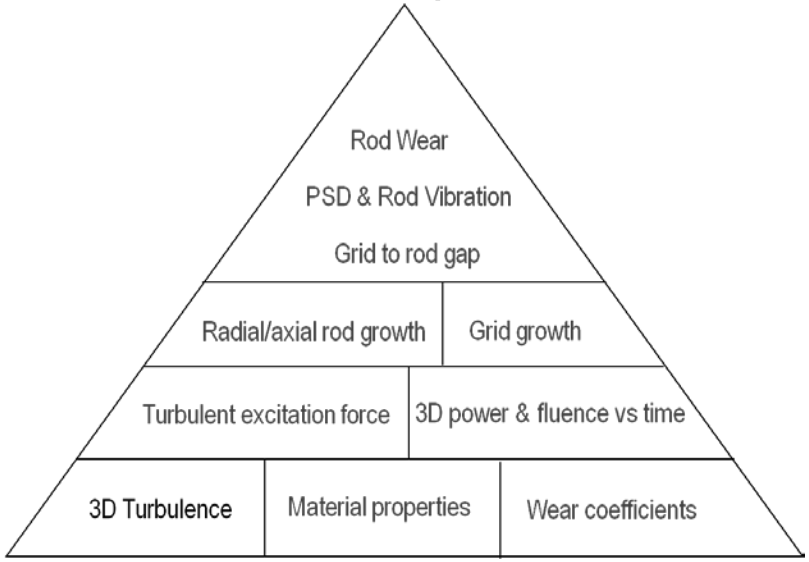
GTRF – What is Success ?

- Develop CFD tools to measure turbulent excitation force
- Develop tool to predict grid to rod gap
- Develop rod wear model accounting for different grid and rod surfaces
- Develop full length single rod tool to predict rod vibration and wear any time in life in core
- Benchmark tools to V5H test and plant wear data



Predict Rod Wear Margin for any Location in Core

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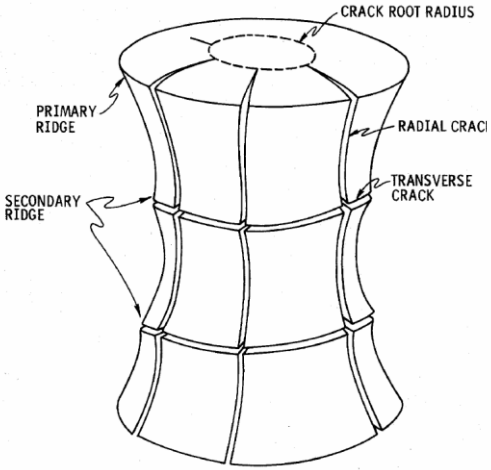
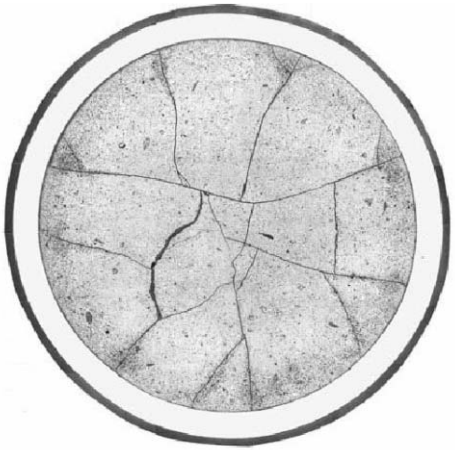
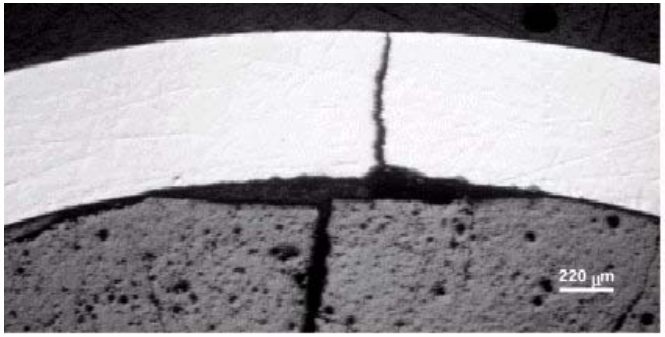
Pellet Clad Interaction (PCI)

- Problem:
  - Cladding "creeps down onto pellets after about one cycle of operation. During power maneuvers, pellet expands and creates stresses against cladding
  - Pellet imperfections such as Missing Pellet Surface (MPS) increase local stresses resulting in clad failure







Need: 3D FEA Fuel Rod Modeling of Rods in Core to Evaluate Clad Stresses From PCI

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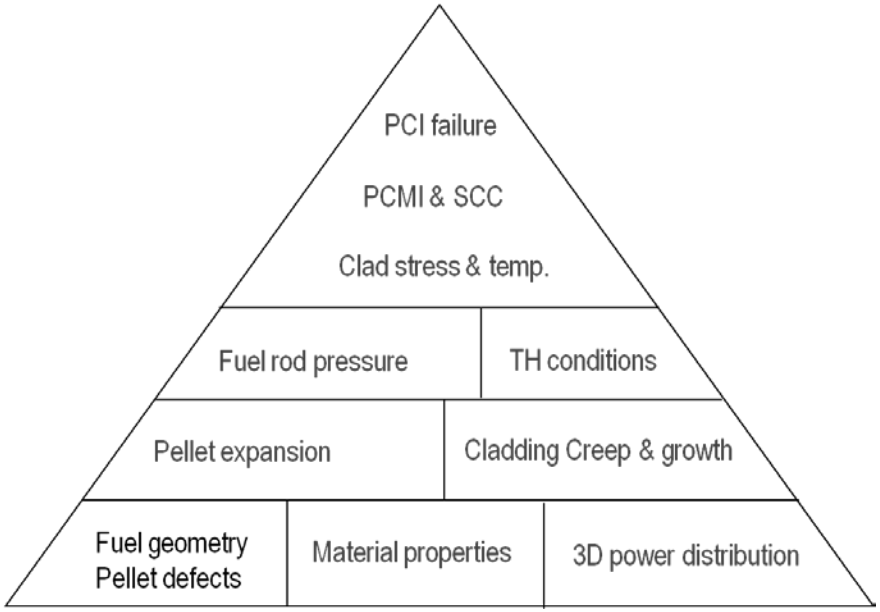
PCI – What is Success ?

- Develop advanced fuel rod (FR) performance tool
- Couple FR tool to Neutronics & TH and apply for core wide analyses (PCI, corrosion, hydrogen, creep, crud, clad strain, etc)
- Apply FR tool with detailed model for PCMI analyses and evaluate other high burnup issues (fuel pellet dispersal, etc)
- Benchmark tools to available FP data and PCI plant failures



Evaluate core wide PCI margin and predict PCI failure

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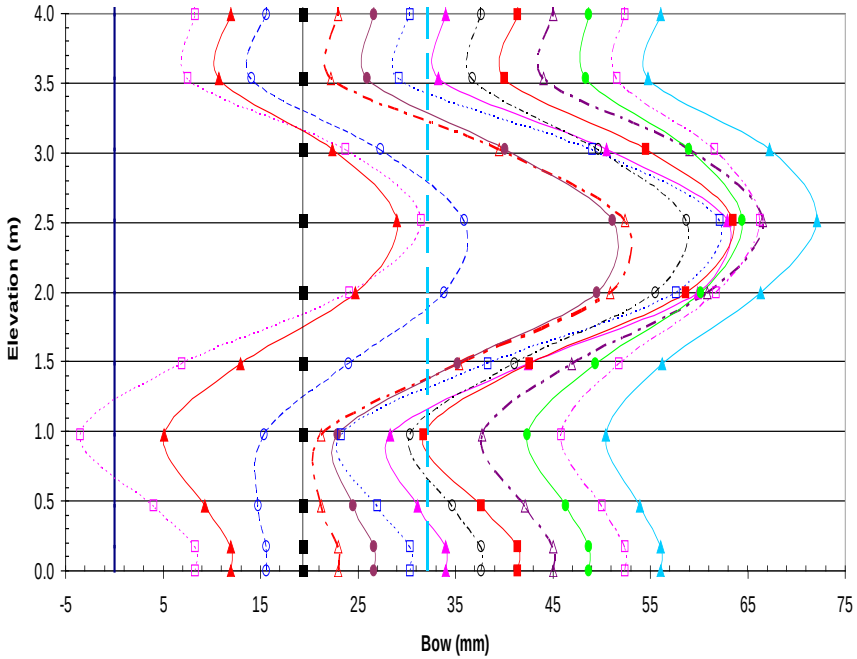
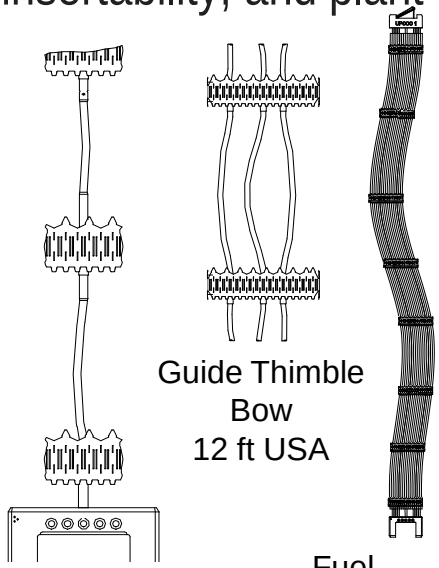
Fuel Assembly Distortion (FAD)

- Problem:
  - Excessive axial and lateral forces caused by radiation-induced swelling, flow, holddown springs and using new materials can lead to fuel assembly distortion
  - Power uprates and increased burnups can increase fuel distortions, alter core power distributions, fuel handling scenarios, control rod insertability, and plant operation





Guide Thimble Bow 12 ft USA

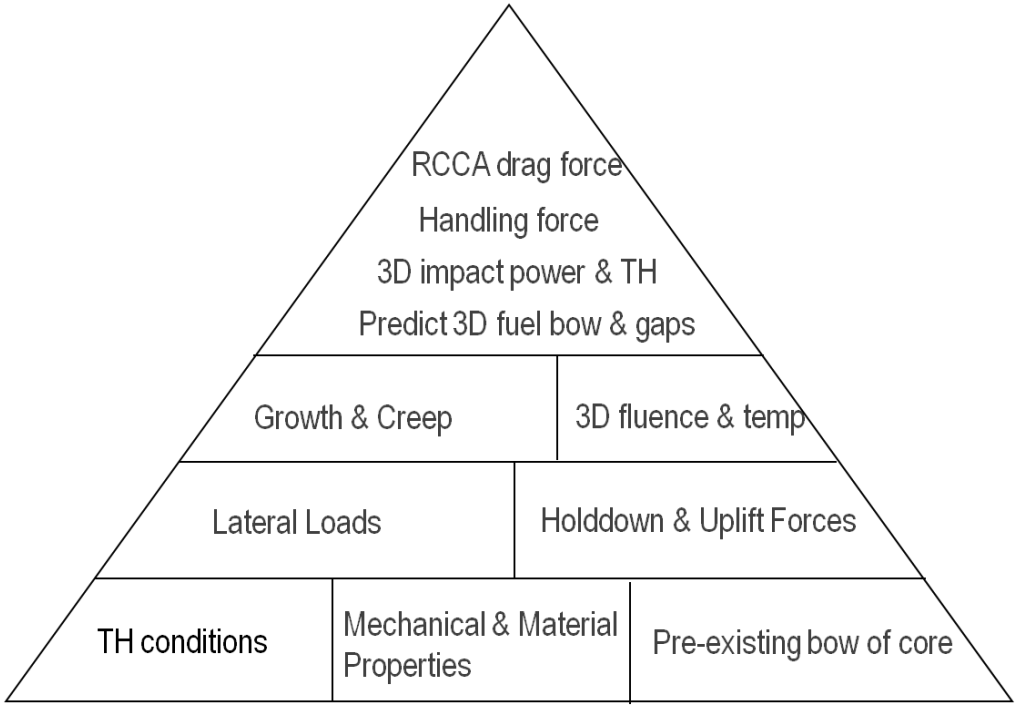
Bow in the Dashpot 14 ft USA

Fuel Assembly Bow 12, 14 ft Europe

Need: Tool to predict distortion and impact on power distributions, GTRF and safety analyses

FAD – What is Success ?

- Build 3D Structural Model of Fuel Assemblies in Core
- Evaluate fuel assembly distortion and compare to plant data
- Use same model to predict grid impact loads during LOCA/Seismic
- Investigate FSI impact on FAD (stretch goal)



Predict Fuel Assembly Distortion for Normal Operation & Grid Impact Loads during LOCA/Seismic Conditions for Entire Core

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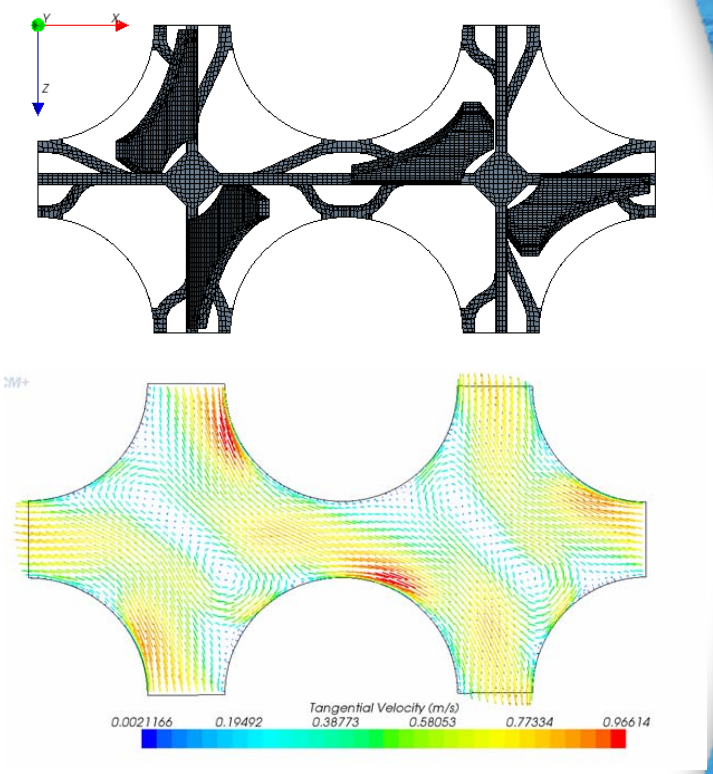
Departure from Nucleate Boiling (DNB)

- Problem:
  - Local clad surface dryout causes dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow)
  - Current limitations:
    - Absence of detailed pin modeling in coupled TH methods results in conservative analysis
    - Detailed flow patterns and mixing not explicitly modeled in single & two-phase flow downstream of spacer grids
  - Power uprates require improved quantification of margins for DNB or dryout limits



Need: High-fidelity modeling of complex flow and heat transfer for all pins in core downstream of spacer grids

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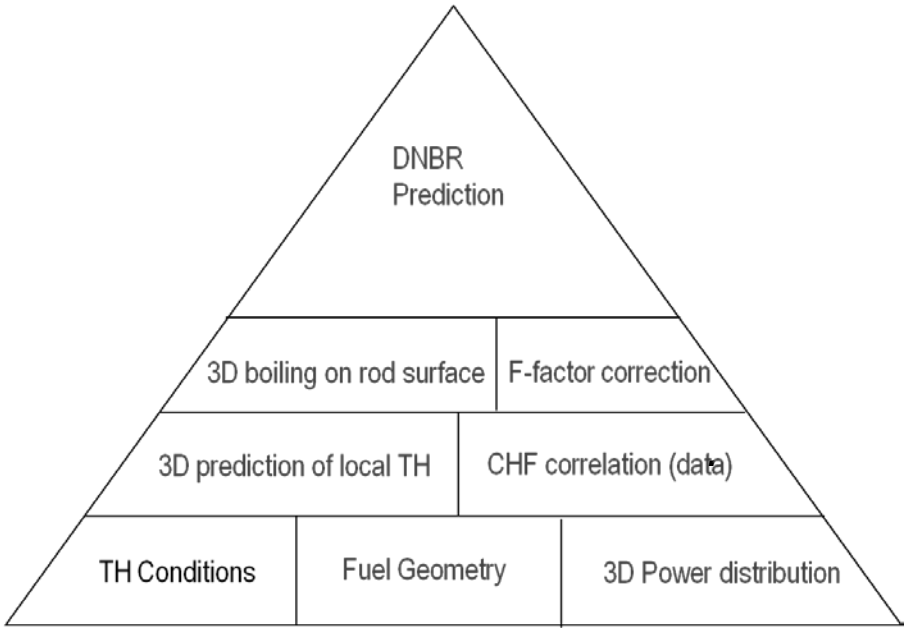
DNB –What is Success ?

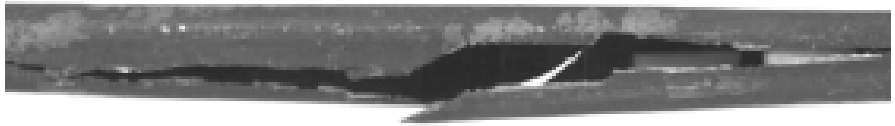
- Apply coupled baseline tools for all pins in core for selected DNB transients to improve DNB margin
- Develop improved mixing method downstream of mixing grids using CFD tools for single and two-phase flow.
- Benchmark to available single and two-phase flow data



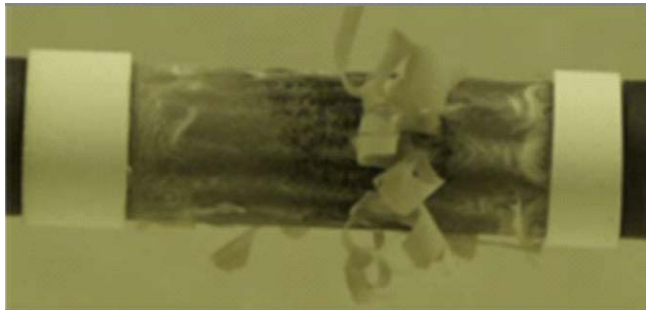
Improve DNB Margin to Support Power Uprates

Clad Integrity during RIA, LOCA & Post LTCC

- Problem:
  - Clad failure due to rapid heating of pellet, leading to pellet disintegration (Rod Ejection)
  - New limits developed by NRC which are hydrogen based account for effects of corrosion on ductility for RIA and LOCA
  - Demonstrate acceptable breakaway oxidation performance in LOCA
  - Demonstrate Post Long Term Core Cooling performance (GSI-191)
  - Use of advanced cladding materials to improve performance in severe accidents



Clad Failure in RIA test with Fuel Dispersal



Breakaway Oxidation During LOCA

Need: 3D Advanced Methodologies Coupling Space-time Neutronic, Fuel Rod, TH Calculations and Investigate Accident Tolerant Cladding

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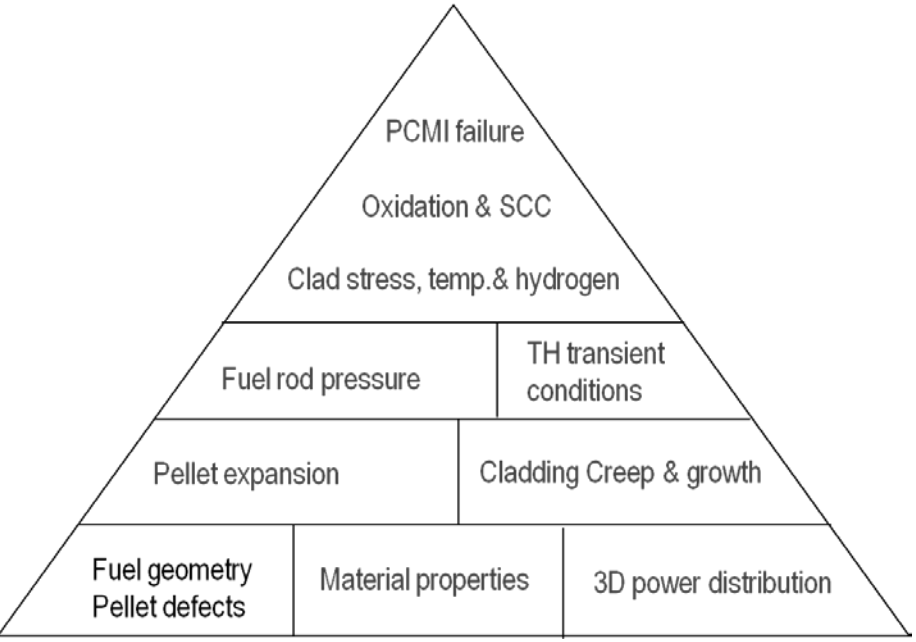
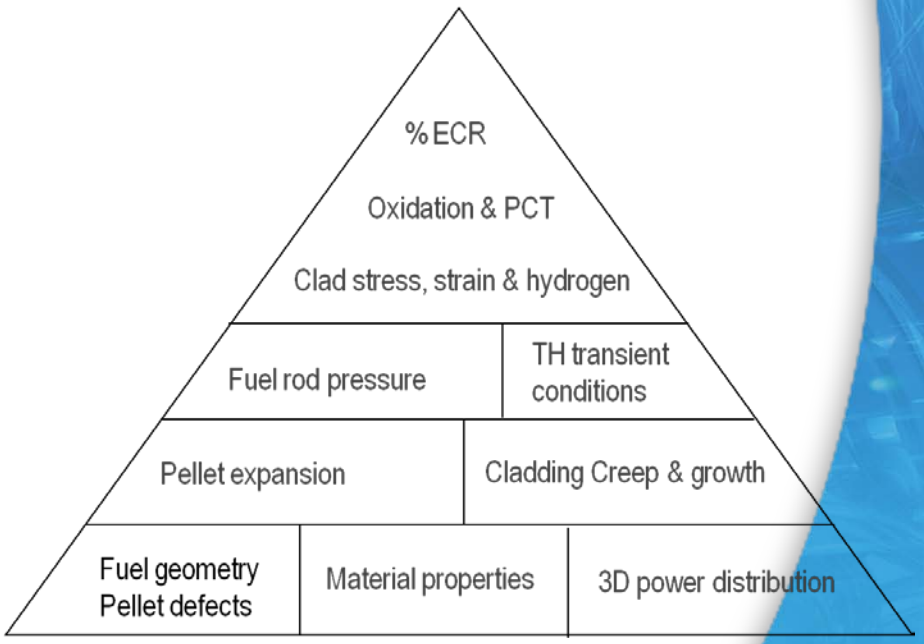
RIA, LOCA & Post LTCC – What is Success ?

- J. Gaertner to make presentation on Safety Challenge Problems



RIA

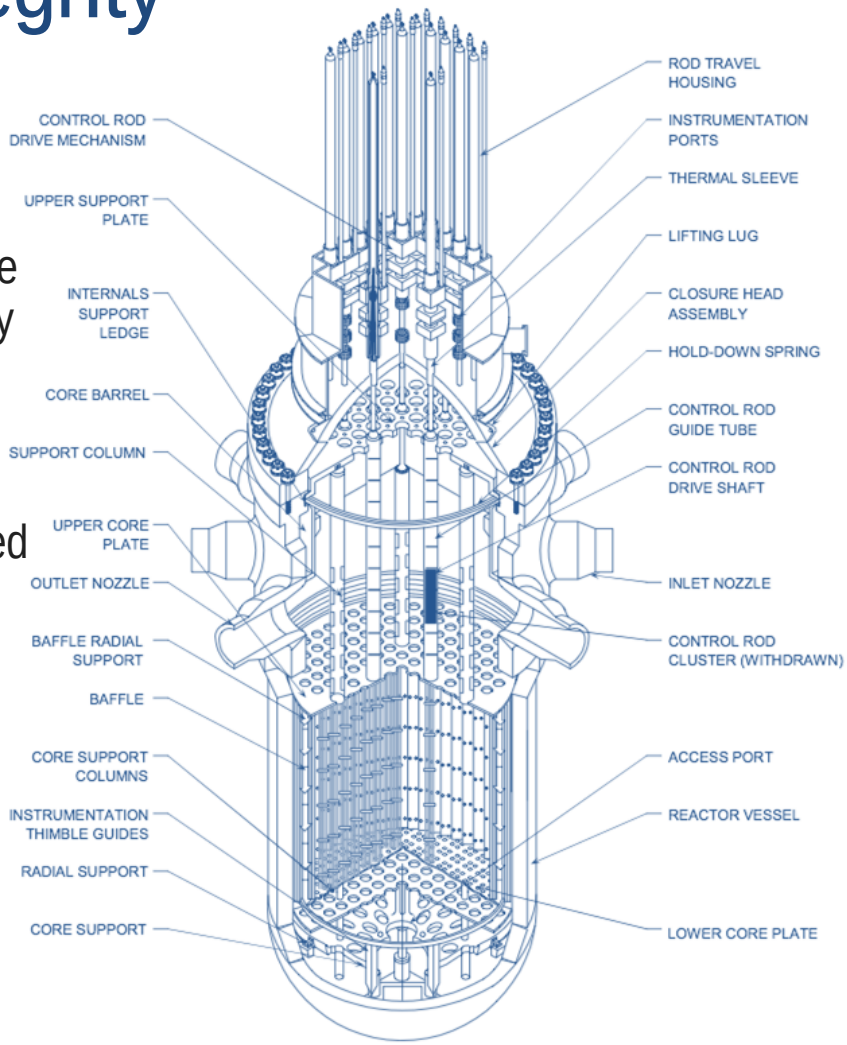


LOCA

3D Advanced Methods to improve RIA & LOCA Margin and evaluate benefits of ATF

Reactor Vessel & Internals Integrity

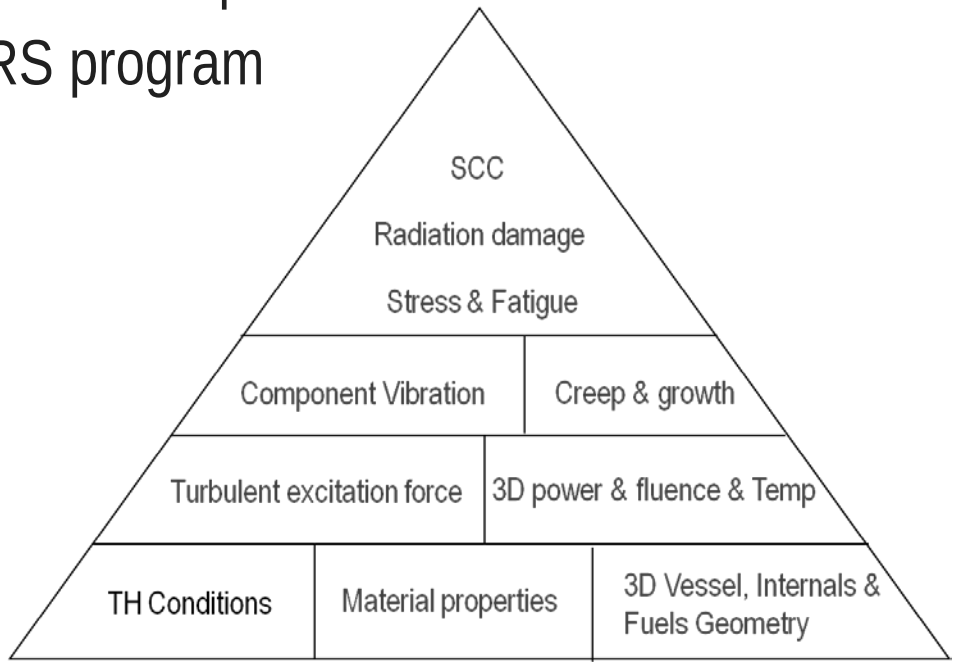
- Problem:
  - Reactor vessel:
    - Radiation damage results in increased temperature for onset of brittle failure, making failure more likely due to thermal shock stresses with safety injection
    - Increased power rating and lifetime both increase radiation damage to the vessel
    - Low leakage loading patterns and proposed revised NRC rule indicate expected vessel lifetime > 80 years for most PWRs
  - Internals:
    - Damage can be caused by thermal fatigue, mechanical fatigue, radiation damage, and SCC
    - Replacement cost of internals is high, making lifetime extension less economically attractive



Need: High-fidelity tool to predict temperatures, stresses, and material performance (fatigue and cracking) over long-term operation

RVI Integrity – What is Success ?

- 3D prediction of temperature, stress, fluence, and growth of fuel and reactor internal structures and vessel
- Predict fatigue, SCC and radiation damage
- Predict any component vibration
- Benchmark to available plant data
- Work with LWRS program



Predict Margins for SCC, Radiation Damage and Stress/Fatigue

Next Steps

- Identify Product Integrators (PI) for remaining Challenge Problems
- Have biweekly or monthly meetings with PI to monitor and coordinate progress
- PI to clarify what is success for their Challenge Problem
- PI to develop more detailed plan of what and when certain tasks will be completed

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U.S. DEPARTMENT OF ENERGY Nuclear Energy

PERCEPT

Tools for Verification

Kevin Copps

CASL Round Table Meeting

June 13, 2012

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

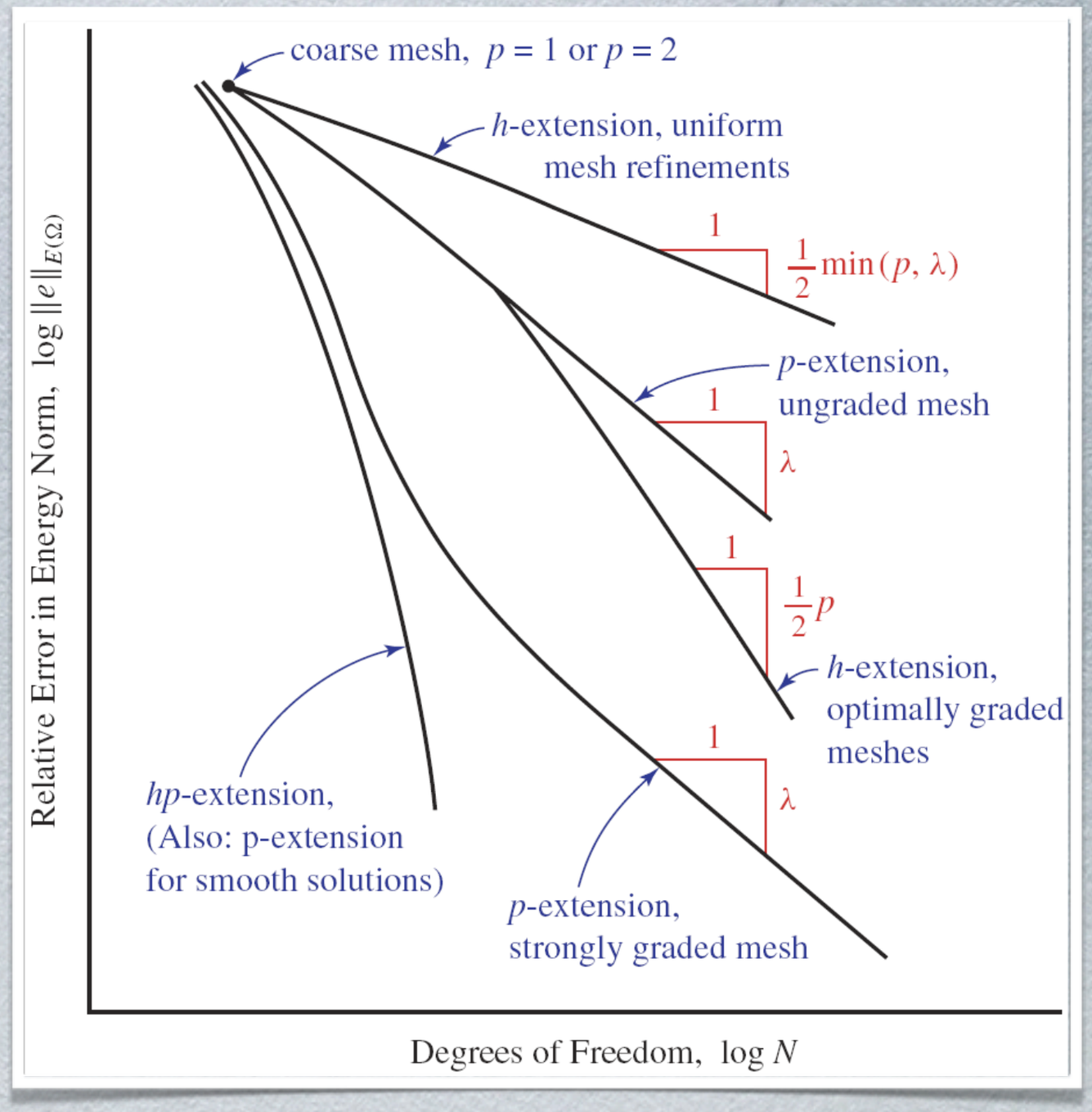
WORK SCOPE

- Objectives:
  - Implement a set of verification tools and capabilities for the CASL community. Enable open source integration with the VERA platform.
  - Demonstrate robust code and solution verification methods on GTRF.
- Contributors:
  - VUQ: Rider, Witkowski (SNL)
  - THM: Shadid, Tom Smith, Weber, Cyr, Pawlowski (SNL)
  - VRI: Turner, Rodriguez, Garcia, White (SNL)
  - MPO: Sham, Nath (ORNL), Crane (SNL)
  - Other: Steve Kennon (SNL contractor, ASC program)
- Completed Milestones:
  - L3.VUQ.VVDA.Y1-2.04
    Open source the Percept software and demonstrate verification of a Grid-to-Rod Fretting problem
    June 2011
  - L3.VUQ.VVDA.P3.01
    GTRF CFD-to-Mechanics Data Transfer Verification
    October 2011

SOLUTION CONVERGENCE

- The goal of a convergence mesh study is to hopefully achieve an asymptotic convergence rate.
- In the asymptote, we can easily and accurately estimate error by extrapolation.
- The rate of convergence is dominated by regularity (smoothness) of the solution, λ — usually the strongest singularity in a derivative of the solution.

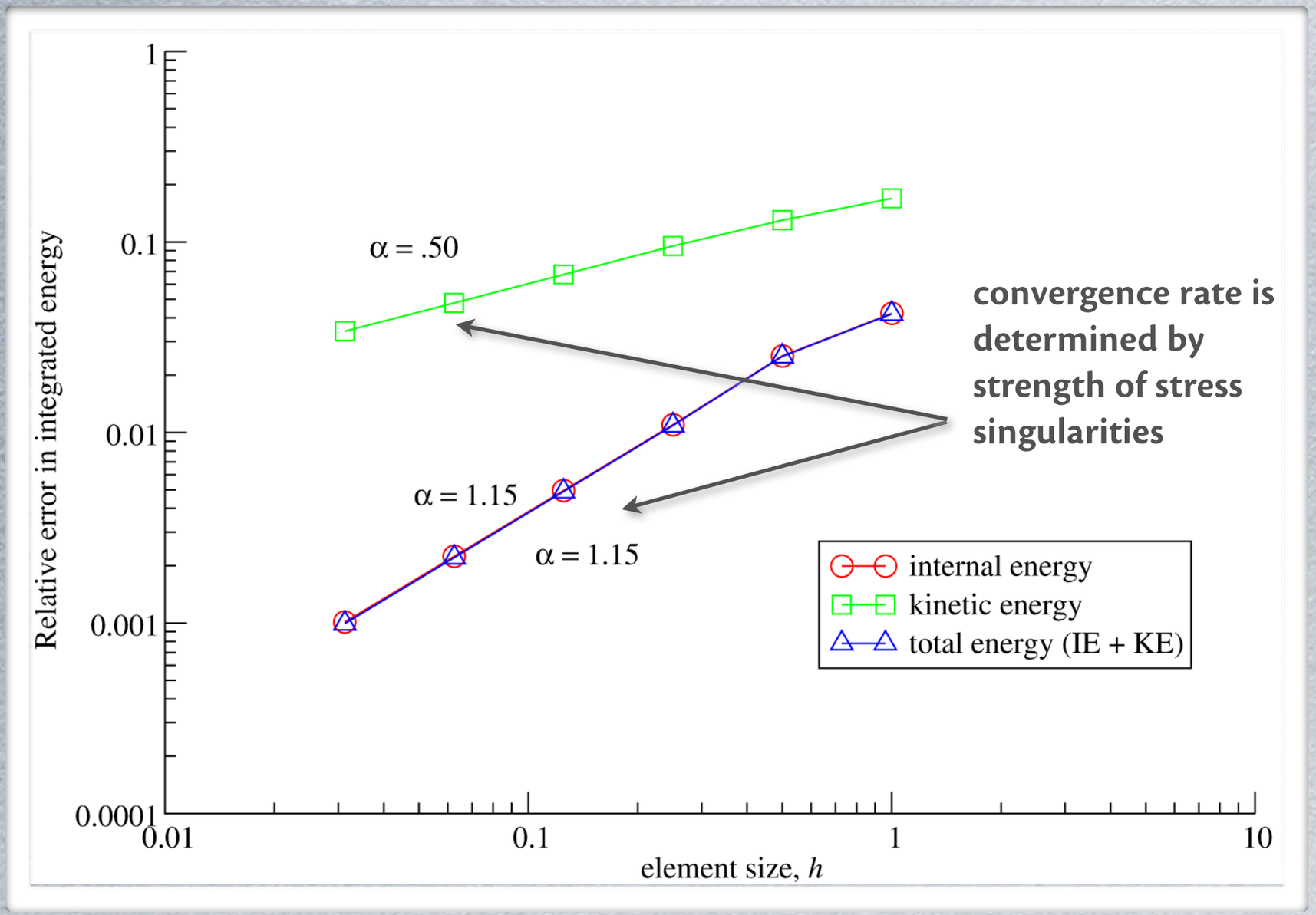
The type of mesh refinement, or adaptivity, determines the path of spatial asymptotic convergence (error) .

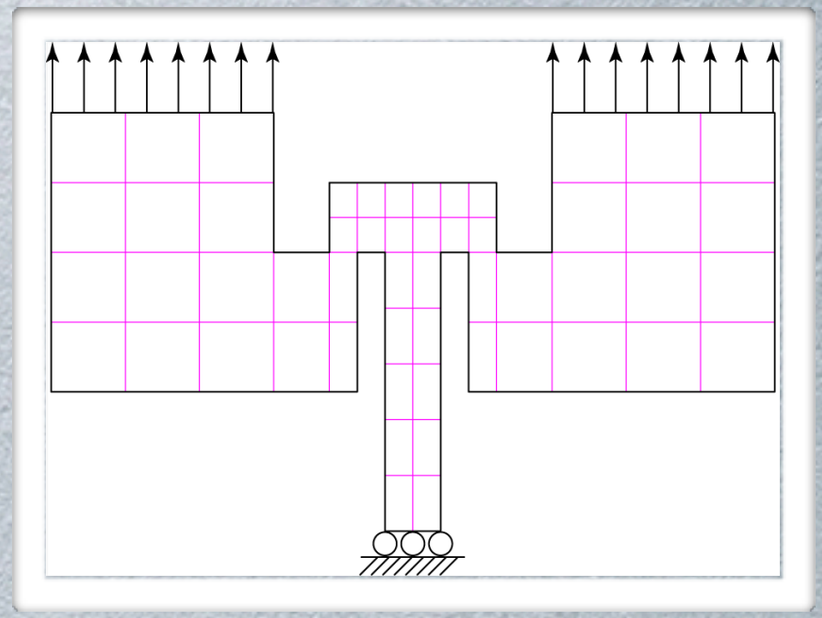


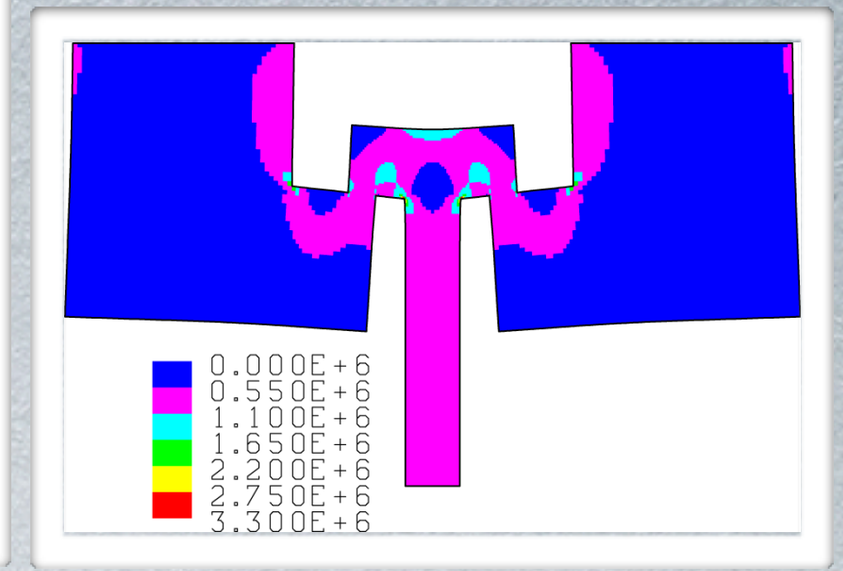
h ≡ element size

p ≡ polynomial degree of the basis (shape) functions

Global energies and energy balance are also an important quantity to be controlled on a sequence of finer meshes.

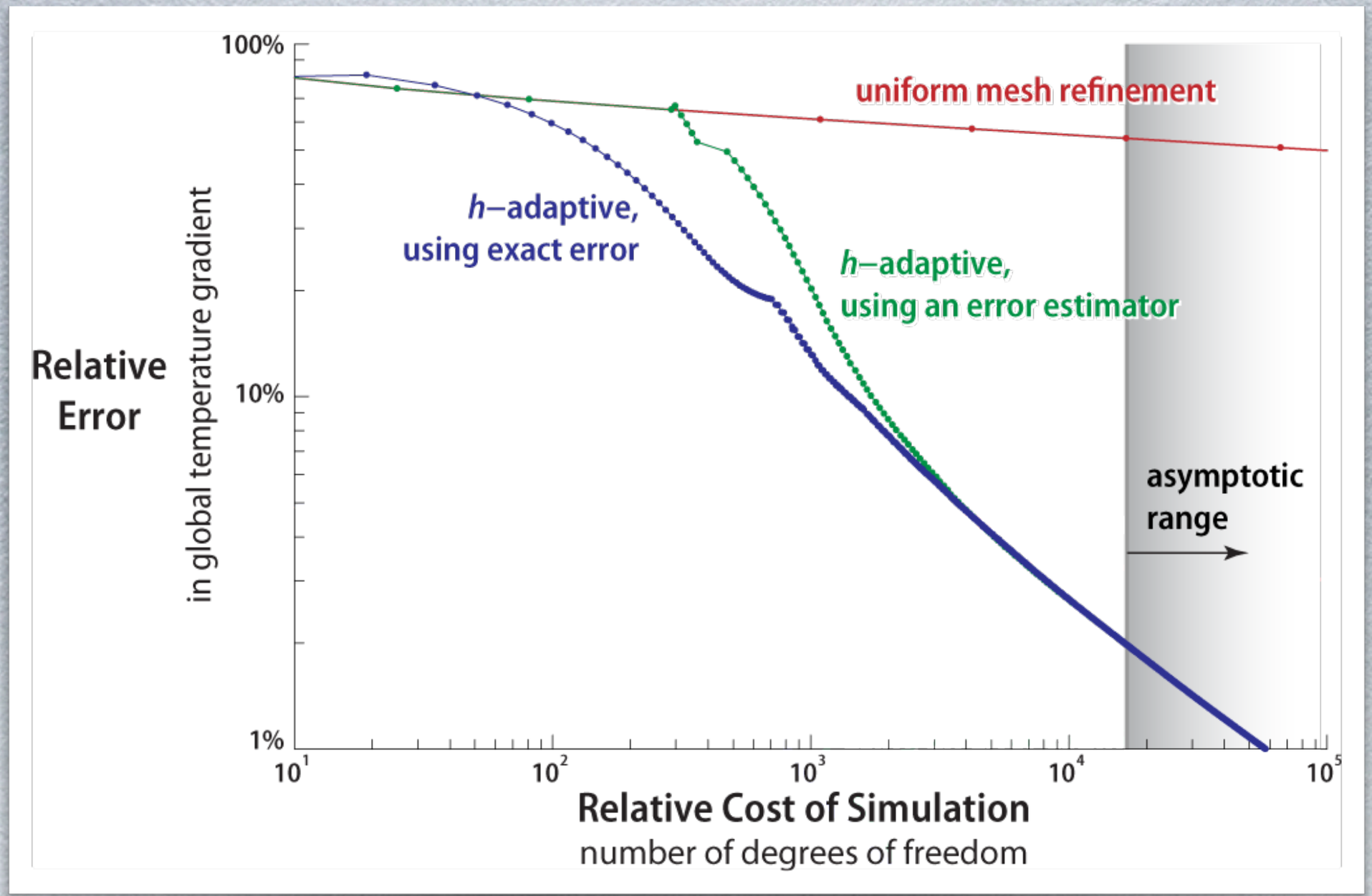






SOLUTION CONVERGENCE

In practical cases, *h*-adaptive refinement may dramatically outperform uniform refinement.
A subcomponent model of a Sandia thermal battery problem with a known exact solution, which exhibits a strong singularity in heat flux.



SOLUTION CONVERGENCE

LEGACY SOFTWARE DRIVERS

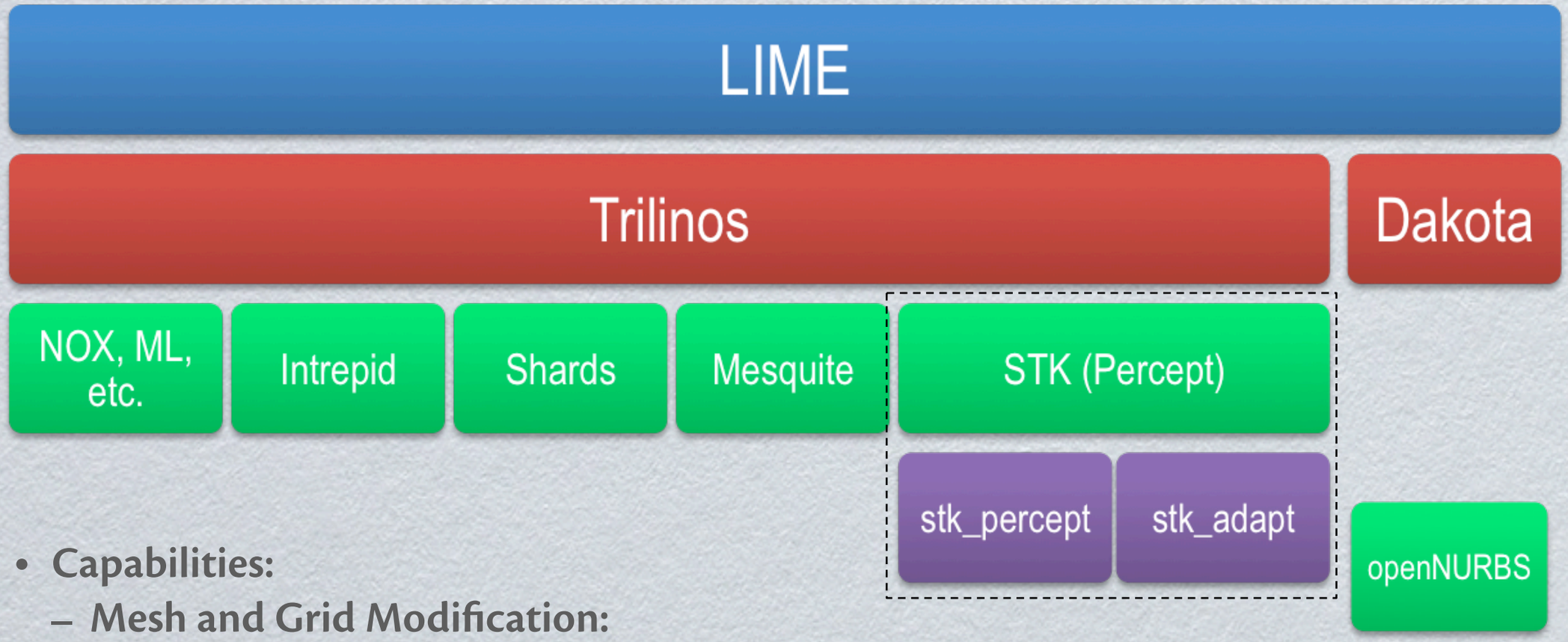
- Adjoint, higher order elements, hanging nodes, ghosting, are things to be designed into a physics code early in development cycle.
- Smoothness requirements too restrictive in practical models.
- CAD geometry.
- Control time/memory budget.
- Uniform refinement—the most robust extension—may still reveal a host of code issues (MPC contact, phase change)
- Sierra input file design inflexible and frustrating for verification: *Solution Control*.
- Error in quantities of interest questionable in presence of nonlinear instabilities.

DEVELOPMENT OF PERCEPT

- Problem: software tools for verification, when they do exist, are code specific, proprietary, or they do not scale.
  - Many simulation code development teams roll their own tools.
  - Postprocessing and visualization tools do not represent fields using the higher order continuous function spaces (polynomial representation) of fields.
  - Current mesh generation and refinement technology and tools do not scale to distributed parallel machines.

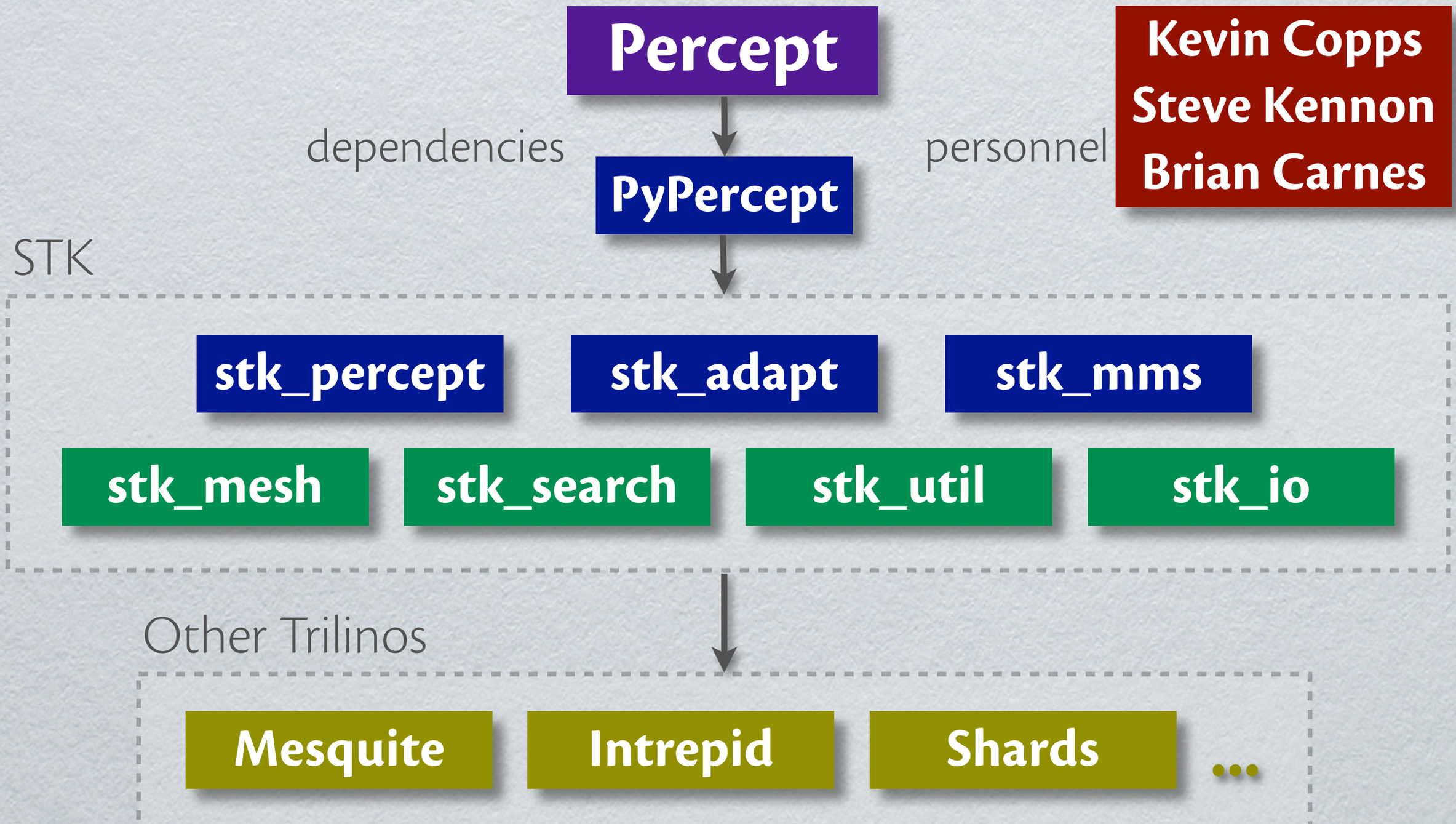
- Design Goals: a new set of verification tools for VERA: Percept
  - Open source licensed: part of the Trilinos package system
  - Massively parallel using the open source STK (Sierra Toolkit)
  - Take lessons learned from many simulation communities and the previous Sandia Sierra Encore effort.

DEVELOPMENT OF PERCEPT



- Capabilities:
  - Mesh and Grid Modification:
    - Uniform refinement of all common unstructured mesh cell types (using Shards library)
    - Adaptive refinement (edge based division of tetrahedra)
    - Mesh smoothing and element shape optimization (using the Mesquite library)
  - Other:
    - Postprocessing of quantities of interest (using the Intrepid element library)
    - Curved CAD geometry representation in parallel (using openNURBS library)
    - Scripting API using industry standard Python numpy and scipy modules.

STRUCTURE


Percept
dependencies
PyPercept
personnel
Kevin Copps
Steve Kennon
Brian Carnes
STK
stk_percept
stk_adapt
stk_mms
stk_mesh
stk_search
stk_util
stk_io
Other Trilinos
Mesquite
Intrepid
Shards
...

CAPABILITIES

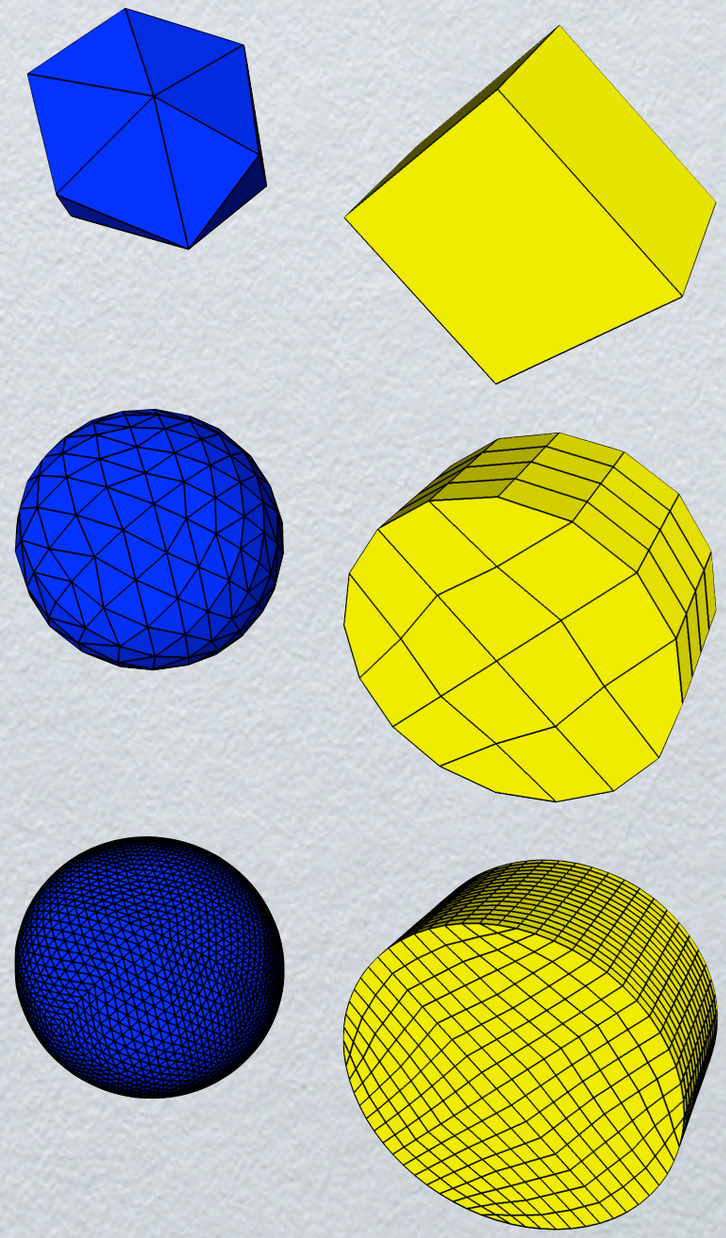
Code Verification	Solution Verification	
Exact fields, string functions (runtime)*	Fully STK based implementation	H-method adaptivity (triangles/tetrahedra)
Difference of fields and exact solutions*	Open source, Trilinos distribution	Directional adaptivity (triangles/tetrahedra)
MMS plugins (compiled)*	Uniform h-refinement*	
MMS automatic derivatives (compiled)	Out of core refinement	Richardson Extrapolation/Error Estimates
MMS plugins (dynamic language)	Refinement of pyramid elements	
	Cubit/openNURBS CAD geometry	User selected initial refinements*
	Virtual/Composite CAD geometry	H-method (adaptivity) Quads/Hexahedra*
	Arbitrary IGES/STEP CAD geometry*	Boundary layer grading
	Full element library with quadrature*	Spatial Error Indicators (least squares, jumps)*
	Convergence plots	R-method (mesh movement)
	Simple command line interface	P-method (polynomial extension)*
	Scripting through Python API	Non-linear dynamic error estimator [Bishop]
	Grid-to-Grid Transfers*	HP-method
	Workbench Integration	Adjoint based error estimators*

fully operational/tested/usable *nearly functional/need improvement* *activity has started* *not started*

** partial or full implementation in the SIERRA framework based Encore*

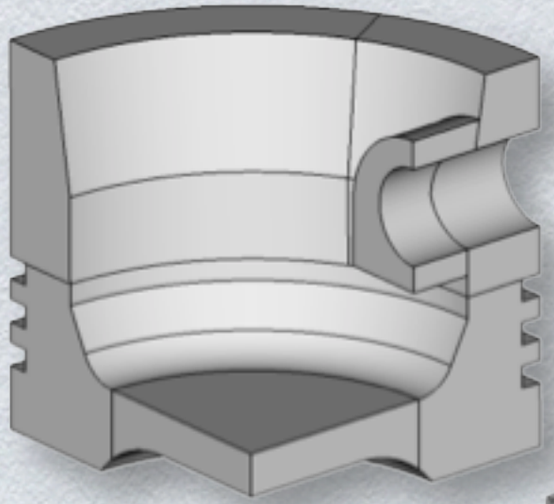
PETA/EXASCALE GRID REFINEMENT

- Problem: the most basic and robust verification methodology (h-method) requires a sequence of successively finer grids.
  - Must reach into the asymptotically converged regime.
  - 4 meshes of successively finer grid size.
  - Achieving a billion or more cells/nodes will be common.
- Capability: Percept provides scalable uniform and adaptive refinement in parallel
  - Start from serial unstructured mesh
  - Carry complex curved CAD geometry (openNURBS API and format) on to parallel processors
  - Limitations: Exodus format, CAD must be importable in CUBIT, maximum of 2.1 billion cells
- Practical Use: used in refinement of structural dynamics meshes for verification of single physics and coupled transfer GTRF simulations.
  - 318M cells (with CAD geometry) generated in 1 minute on 512 cores

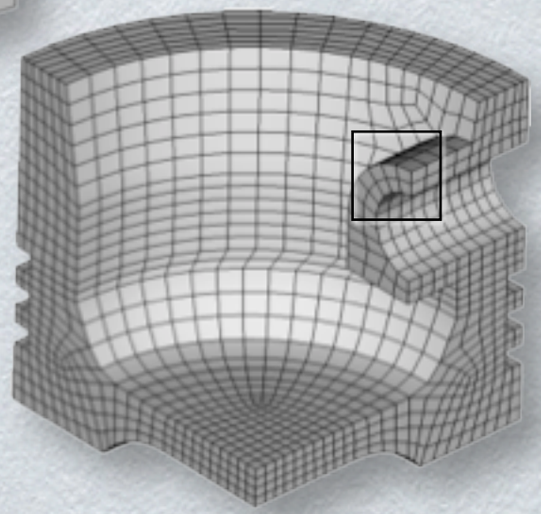


Example of uniform refinement from coarse grid from CAD geometry using Percept

GEOMETRY WORKFLOW

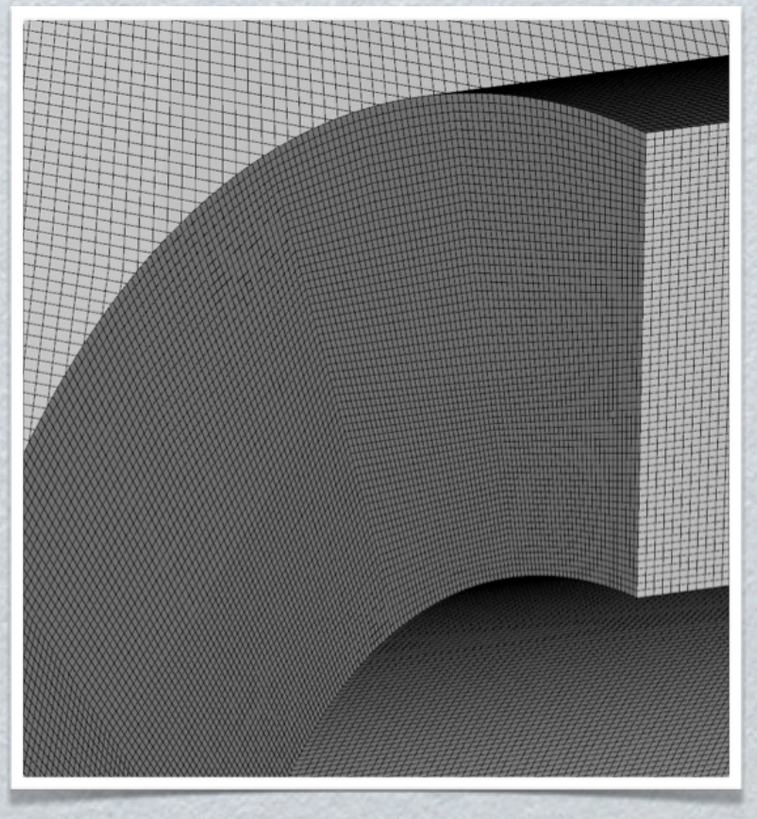


openNURBS
3DM file



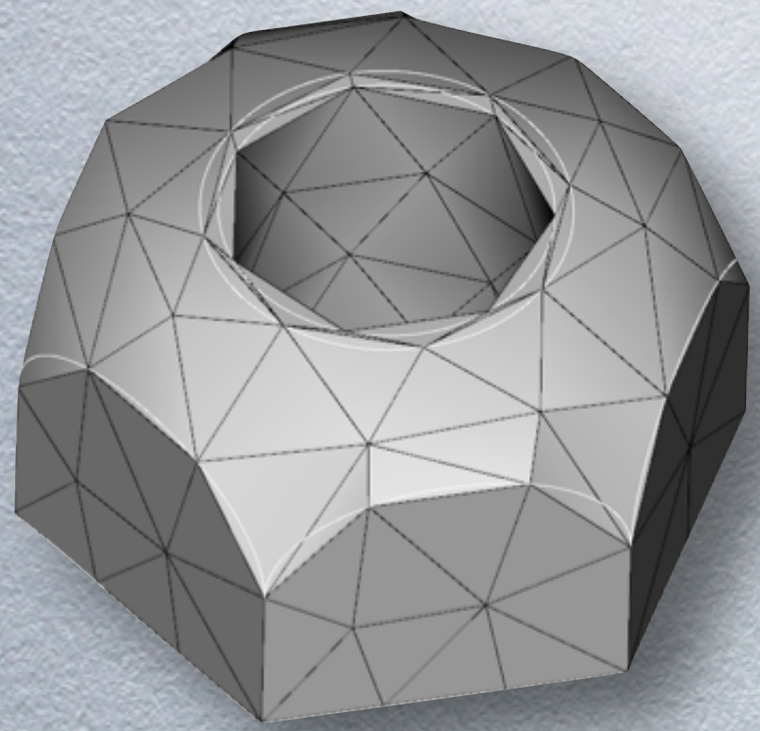
ExodusII Mesh
with metadata

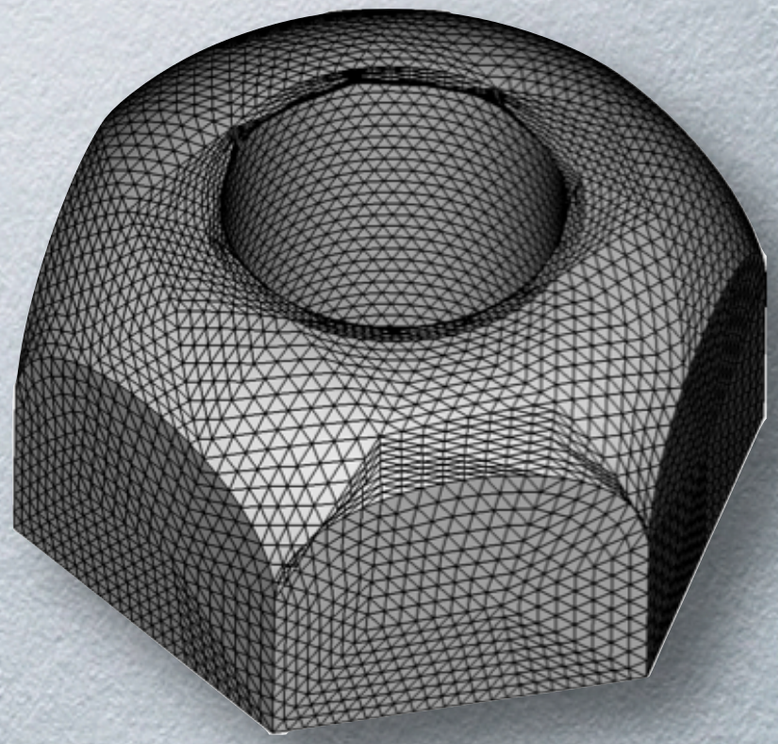
1. Cubit exports:
   openNURBS *.3dm file
   ExodusII *.exo file
2. Decomposition into one *.exo per process
3. Percept stk_adapt performs refinement in parallel
4. Mesh smoothing using *Mesquite*

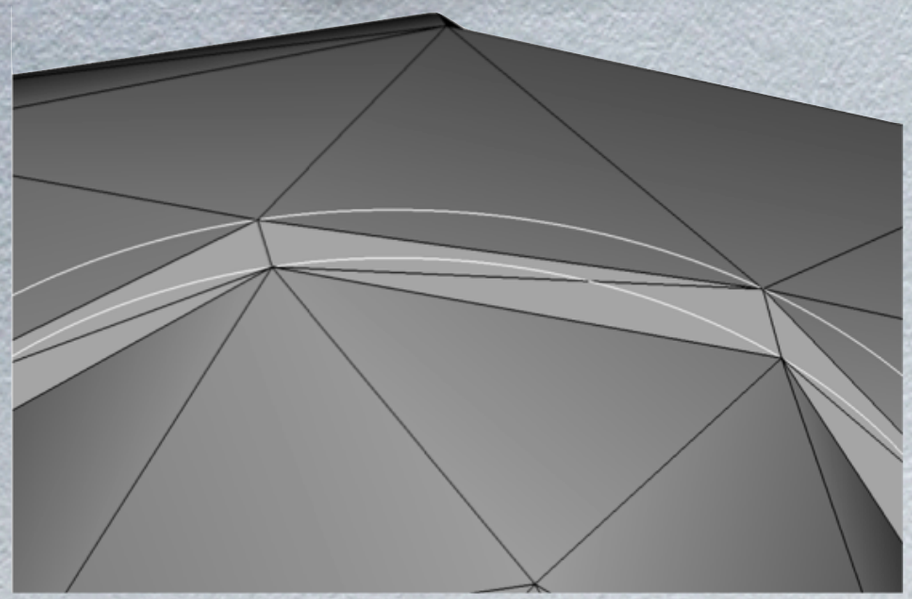


uniformly
refined
mesh

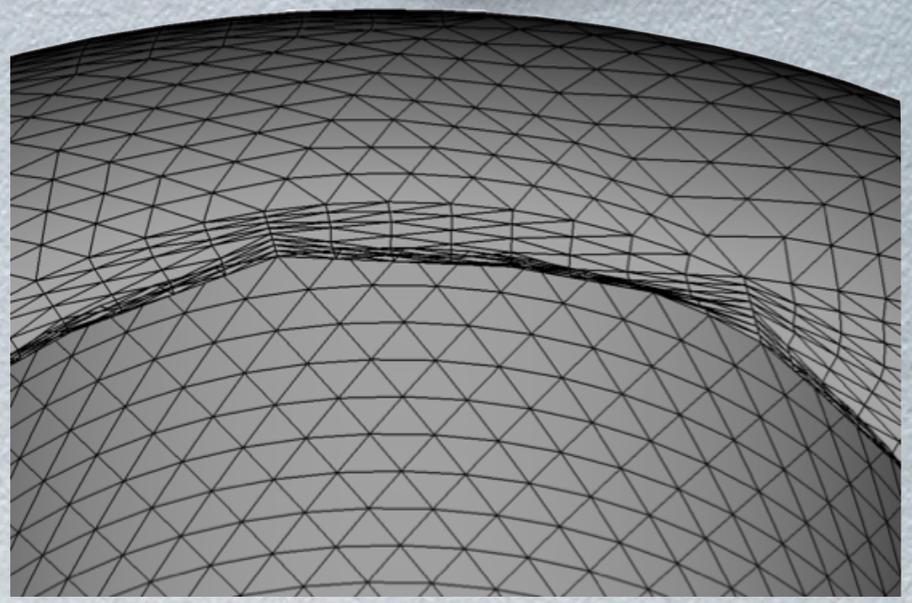
112M Hex
20 processes





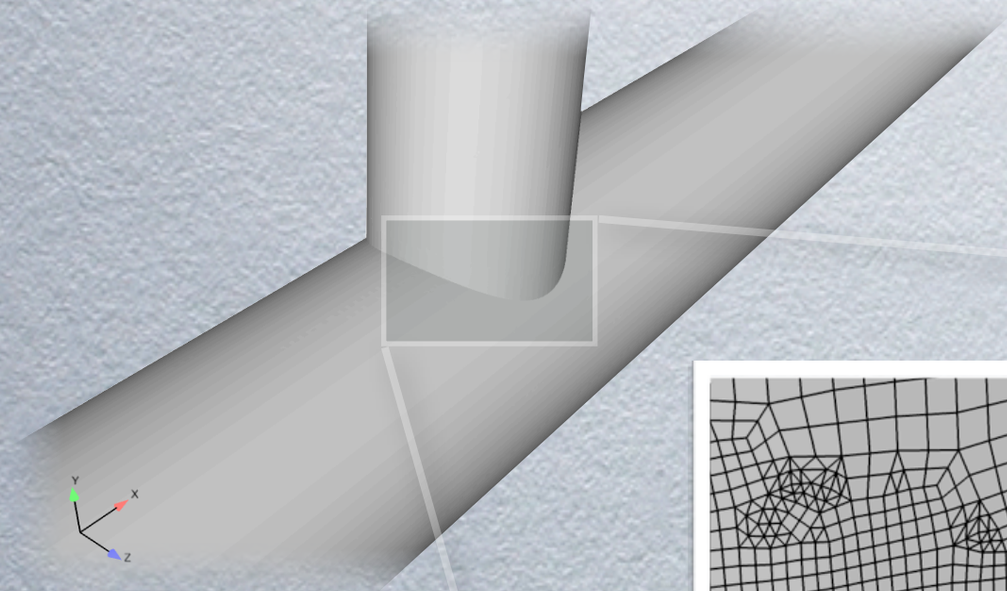


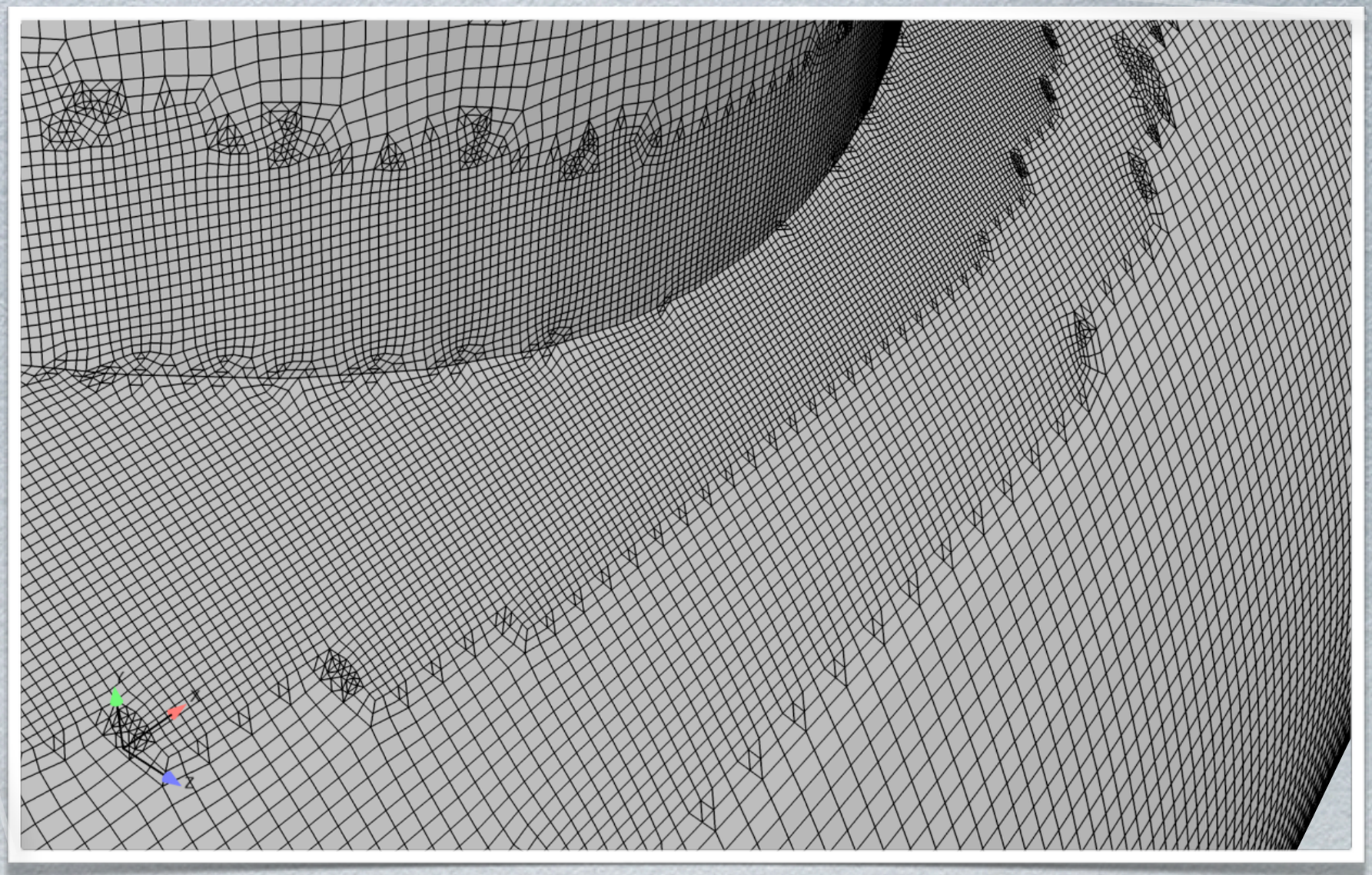
After refinement with geometry elements may be inverted.



MESH SMOOTHING

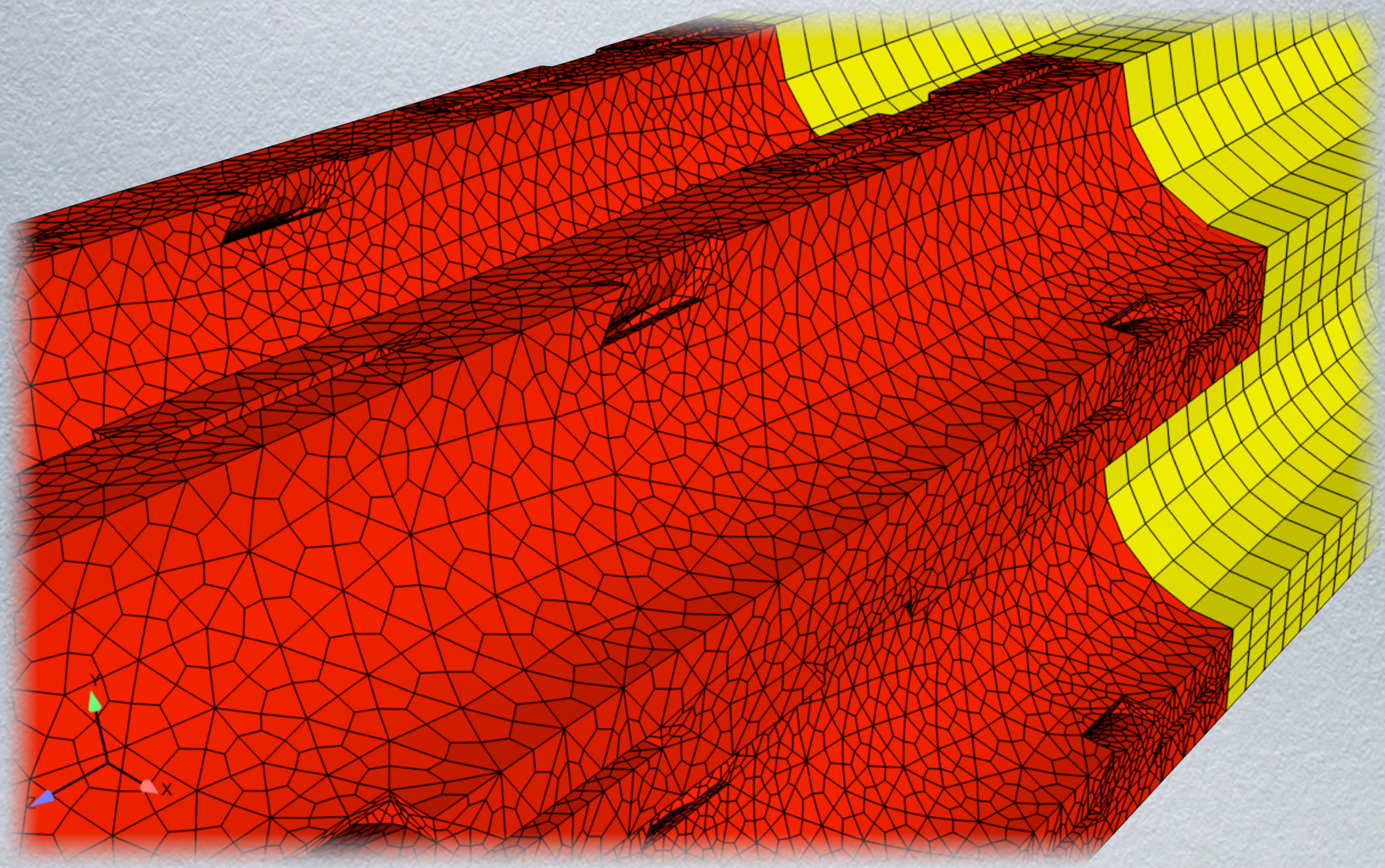
Meshes created by the **commercial Spider tool (used by Hydra)** also contain mixed **Pyramid** elements, now supported by ***Percept***.





SPIDER MESH SUPPORT

Refinement should conform to original curved surfaces. **GTRF fluid model** requires support for ***composite curves and surfaces***, which are present in the original representation.



GTRF FLUID SPACER GRID

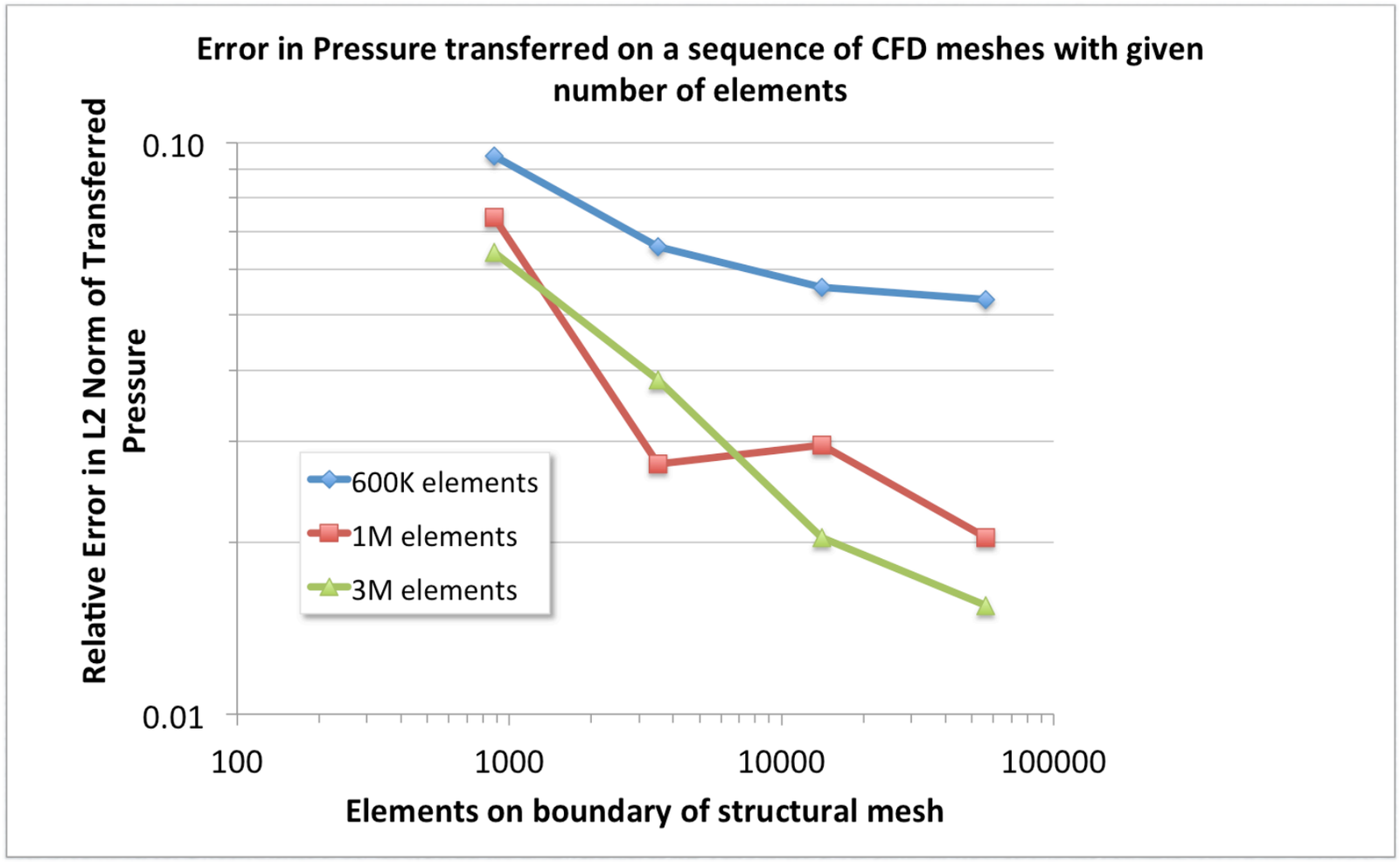
18.4K ELEMENTS / SECOND / PROCESS

Uniform refinement levels for the Sierra open-jet model. Percept refinement scales linearly.

Level	Code	Machine/Proc	Time mm:ss	Nnode	Nelem	Exo (Gzip) File Size
R1	-	-		278.9K	273.7K	?
R1R2	**Encore votd**	blade/4	**21:06**	2.2M	2.2M	?
R1R2	**Encore migrate**	blade/4	**15:20**	"	"	"
R1R2	**Percept**	blade/4	**00:26**	"	"	"
R2R3	**Encore votd**	blade/4	*out-of-mem*	17.6M	17.5M	1.2G
R2R3	**Encore migrate**	blade/4	*out-of-mem*	"	"	"
R2R3	**Percept**	blade/4	02:02	"	"	"
R3R4	**Percept**	blade/4	*out-of-mem*	140.4M	140.14M	9G (2.4G)
R3R4	**Percept**	Redsky/2K	00:06.4	"	"	"
R4R5	**Percept**	Redsky/2K/512/4*	00:26	1.12G	1.12G	72G (21G)

* 2048 processes running on 512 8-way nodes with only 4 cores/node active to allow for each process to have access to double the normal memory.

GTRF FLUID/SOLID TRANSFER



- **Problem:** loosely coupled data transfer of boundary condition in GTRF fluid/solid
- **Activity:** Verify the field data transfer.
  - Use a known exact nearby solution for fluid solution.
  - Execute the same data transfer.
  - Evaluate the error in the transfer on the solid mechanics grid.

- **Conclusions:**
  - Transfer error is kept under control when fluid/solid grids are refined together.
  - **Unsmoothness in transferred fields** results because of mismatched boundaries of the fluid/solid. This may slow or prevent convergence of solid mechanics model, although no *significant effect seen yet.*
  - **Transfer is not conservative.** Energy lost in the coupling may have dissipative effect on solid mechanics behavior and feedback to fluid once two-way coupled.

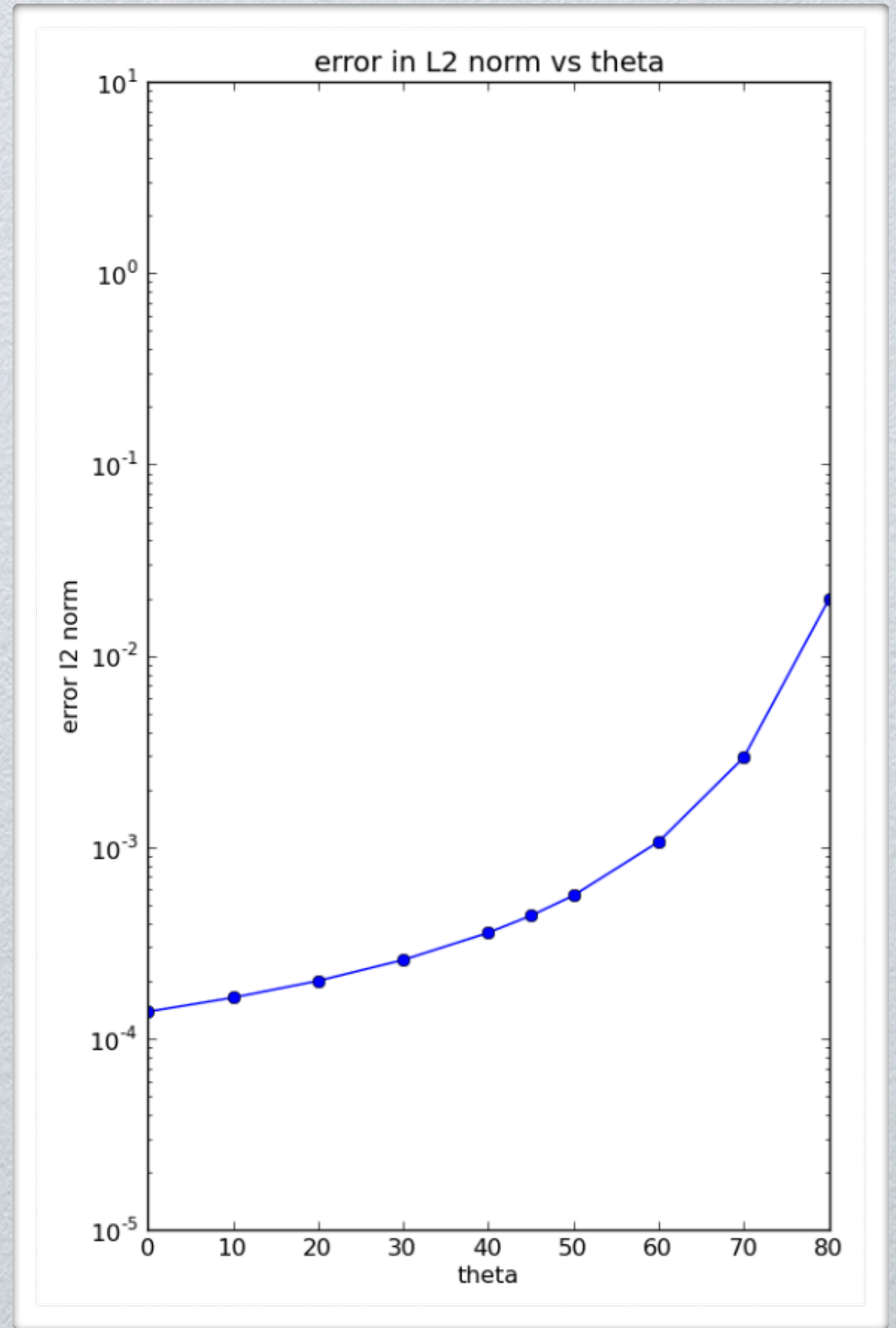
PROTOTYPE CONVERGENCE ANALYSIS

```python
# error analysis
pMesh = PerceptMesh(2)
pMesh.open("conduction_res_last.e")
pMesh.commit()

metaData = pMesh.getFEM_meta_data()
bulkData = pMesh.getBulkData()
coords_field = metaData.get_field("coordinates")
Tnd_field = metaData.get_field("Tnd")

ff_Tnd = FieldFunction("ff_Tnd", Tnd_field, bulkData, Dimensions(2), Dimensions(1), FieldFunction.SIMPLE_SEARCH)

cubDegree = 2
lInfNorm = LInfNorm(bulkData)
lInfNorm.setCubDegree(cubDegree)
l2Norm = L2Norm(bulkData)
l2Norm.setCubDegree(cubDegree)

#          TMMS = x**3 + y**2 + x*y
sf_exact = StringFunction("x*x*x + y*y + x*y", "sf_exact", Dimensions(2), Dimensions(1))
sf_diff = StringFunction("sf_exact - ff_Tnd", "sf_diff", Dimensions(2), Dimensions(1))
```

A prototype Python language file used to perform convergence analysis using the Percept Python API. This analysis was performed as part of the recent SIERRA/Fuego non-orthogonal correction studies.

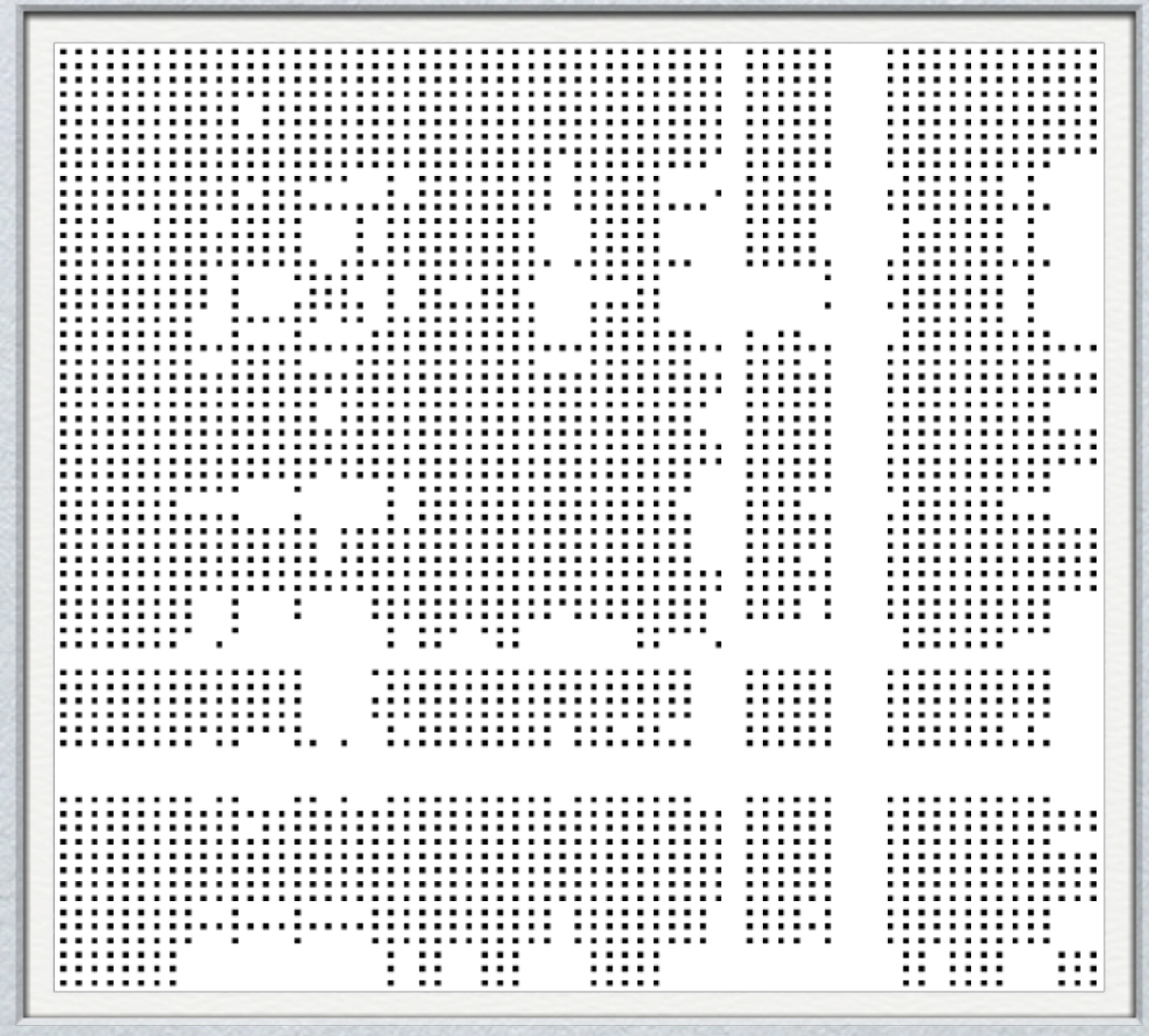
PROTOTYPE PLOTTING CAPABILITIES

```
ax1 = plt.subplot(121)
ax1.set_yscale("log")
ax1.set_xlabel("theta")
ax1.set_ylabel("error l2 norm")
ax1.set_aspect(1)
ax1.set_title("error in L2 norm vs theta")
ax1.plot(thetas, norml2, "o-")

ax2 = plt.subplot(122)
ax2.set_yscale("log")
ax2.set_xlabel("theta")
ax2.set_ylabel("error linf norm")
ax2.plot(thetas, normlinf, "o-")
ax2.set_aspect(1)
ax2.set_title("error in L-inf norm vs theta")

plt.draw()
plt.show()
```



FEATURE COVERAGE ANALYSIS

- Problem: collect and present evidence of code verification
  - Are the features of the simulation code used in my simulation correct?
  - What verification tests are actively running?
  - Are any two features used in my simulation tested together (2-way coverage)?
  - Subset of PCMM (predictive capability maturity model)
- Activity: demonstrated use of Sierra Feature Coverage Tool on GTRF solid mechanics
  - Report on verification tests actively being executed on the features of the GTRF simulation
- Conclusion:
  - Gaps identified in the verification of:
    - Tied Mechanical contact
    - Node set subroutines



The matrix resulting from a 2-way feature coverage analysis of a GTRF solid mechanics simulation. Some features are not tested together (empty off-diagonals), or not tested at all (empty diagonals).

FUTURE WORK PLANNED

- Expose and integrate mesh refinement capabilities more intrinsically within Drekar, a STK based code for the fluid modeling of GTRF.
- Provide verification evidence for the fully coupled fluid/solid GTRF calculations.
- Investigate providing feature coverage analysis for all VERA codes.
- Support a wider set of mesh and grid file formats.
- Provide easier to configure software and distribution mechanism for Percept and especially Python.
- Smoothing and graded boundaries for fluid boundary layers.
- r-method adaptivity
- Out-of-core streaming refinement on desktop, does not require “meshing box”.

WRAPPING UP...

- The Percept project is tightly focused on support for legacy and production codes.
- Percept developers are concentrating on robust, easy to use tools.
- All **Code verification** tools are close to maturity with a low barrier to entry.
- Uniform refinement with appropriate quantities of interest is a best practice for **solution verification**.
- Limited adaptive refinement with predictable controls maybe possible.
- **stk_samba** promises to be even faster and less memory.
- Open source licensing and membership in Trilinos pay off, including easy distribution to CASL (ORNL, SNL, soon LANL).
- Pull from analysts for scientific Python

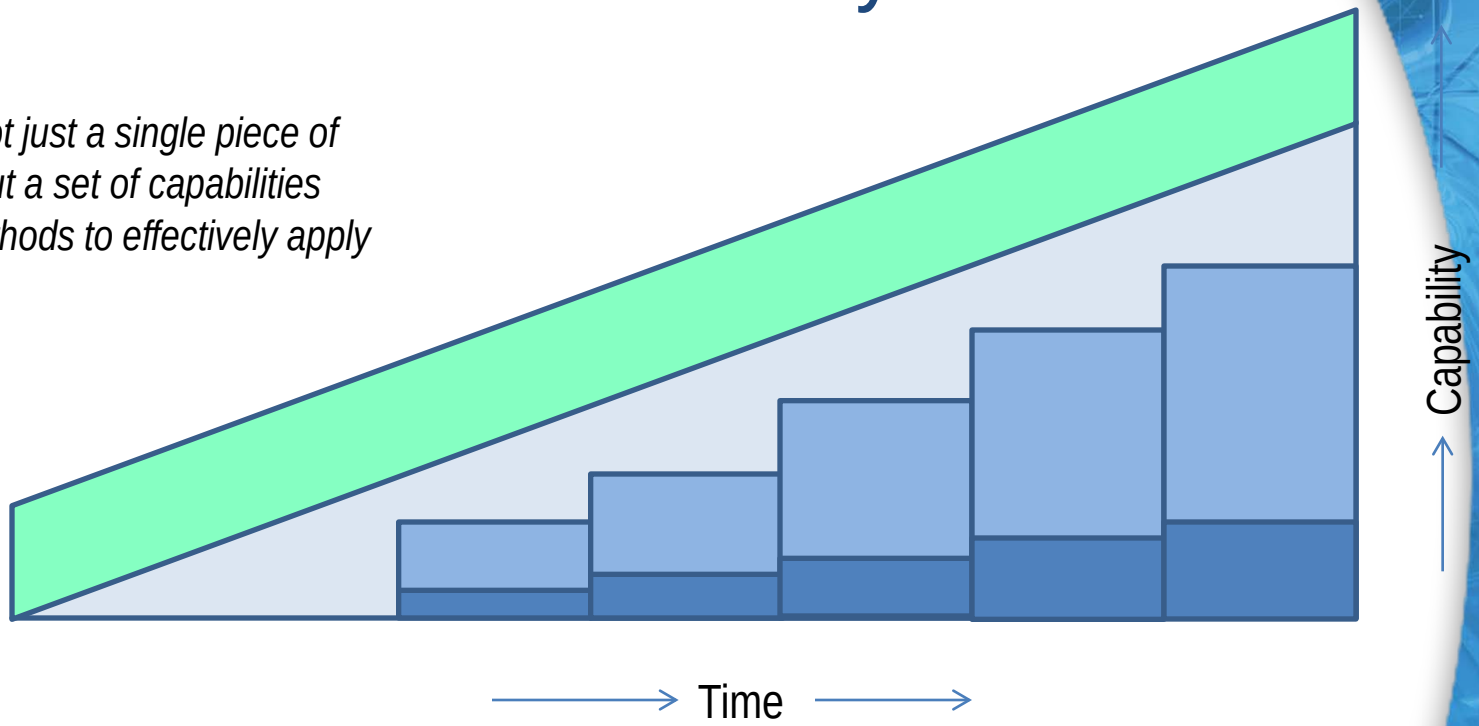
VERA Requirements Document (VRD) Revision

Stephen M. Hess (EPRI): CASL – AMA Deputy Focus Area Lead

CASL 2012 Roundtable
11 – 14 June 2012
Oak Ridge National Laboratory
Oak Ridge, TN

VERA Strategy: Migrating Advanced Capabilities to the Nuclear Industry

"VERA is not just a single piece of software, but a set of capabilities and the methods to effectively apply them."



CASL-FL (Foundation Library)	VERA-CS (Core Simulator)	VERA-A (Advanced)	CASL R&D
• Foundational components • Open source (non-EC) • Deployed to industry & academia • Annual releases	• Industrial class computing • Mature capability • Driven by baseline problems • Deployed to industry & academia • Annual releases	• Leadership-class computing • Advanced capability • Driven by challenge problems • Use in collaboration w COE • Continually developed	• Leadership-class computing • Cutting-edge capability • Driven by research problems • Unstable

CASL
Consortium for Advanced Simulation of LWRs
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

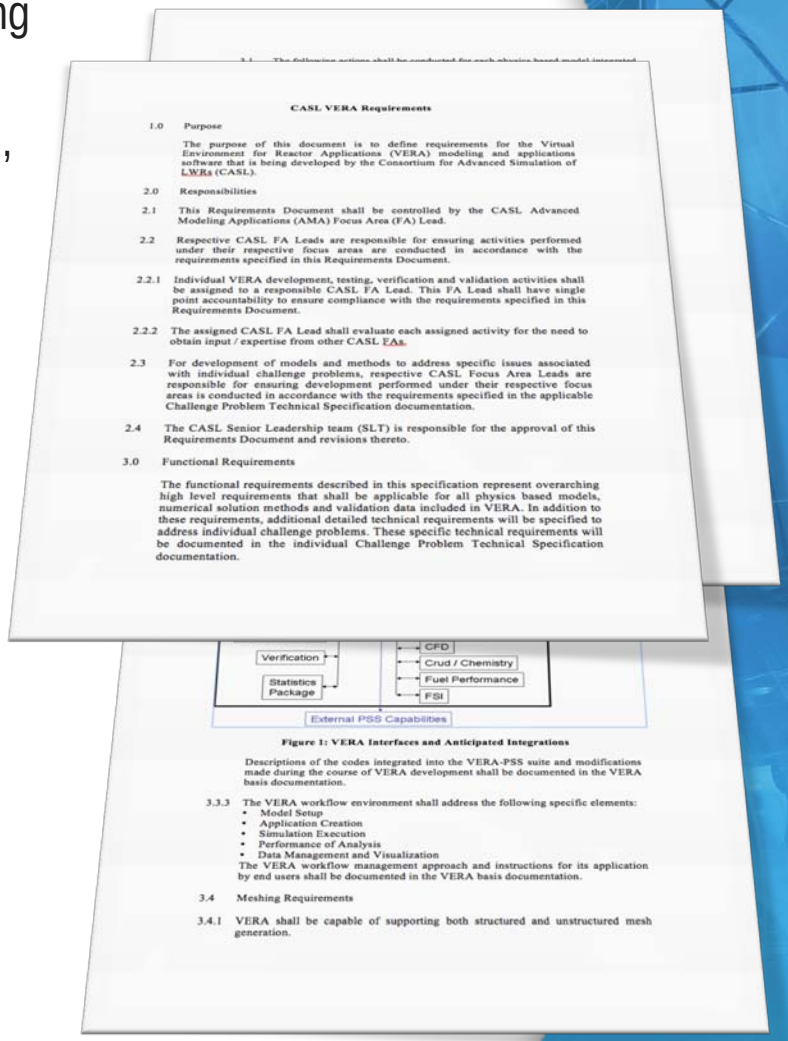
Primary Objectives of VRD Update

- Focus VERA development to achieve a foundational capability to function as a core simulator by end of CY 2013
  - Provide detailed technical requirements and corresponding benchmark problems to demonstrate capabilities
  - Permit testing / application of VERA by external stakeholders during first 5 years of CASL operation
- Provide better specification of QA requirements to align VRD with the CASL Quality Assurance Plan
- Add interfaces for CASL Challenge Problem Integrators

CASL Consortium for Advanced Simulation of LWRs
U.S. DEPARTMENT OF ENERGY Nuclear Energy

VERA Requirements and Assessments

- Purpose: Define high-level requirements for VERA modeling and applications software
- Provides connection between physical reactor applications, challenge problem applications, validation and VERA capabilities
- Outlines requirements: for
  - Function
  - Workflow Environment
  - Technical Capabilities
  - Data Management
- Status:
  - Initial Requirements Developed and approved February 2011
  - Initial assessment of VERA 1.2 completed December 2011
  - First VRD annual update input submitted to CASL Senior Leadership Team (SLT) for review and approval 3/30/2012



CASL VERA Requirements

1.0 Purpose

The purpose of this document is to define requirements for the Virtual Environment for Reactor Applications (VERA) modeling and applications software that is being developed by the Consortium for Advanced Simulation of LWRs (CASL).

2.0 Responsibilities

2.1 This Requirements Document shall be controlled by the CASL Advanced Modeling Applications (AMA) Focus Area (FA) Lead.

2.2 Respective CASL FA Leads are responsible for ensuring activities performed under their respective focus areas are conducted in accordance with the requirements specified in this Requirements Document.

2.2.1 Individual VERA development, testing, verification and validation activities shall be assigned to a responsible CASL FA Lead. This FA Lead shall have single point accountability to ensure compliance with the requirements specified in this Requirements Document.

2.2.2 The assigned CASL FA Lead shall evaluate each assigned activity for the need to obtain input / expertise from other CASL FAs.

2.3 For development of models and methods to address specific issues associated with individual challenge problems, respective CASL Focus Area Leads are responsible for ensuring development performed under their respective focus areas is conducted in accordance with the requirements specified in the applicable Challenge Problem Technical Specification documentation.

2.4 The CASL Senior Leadership team (SLT) is responsible for the approval of this Requirements Document and revisions thereto.

3.0 Functional Requirements

The functional requirements described in this specification represent overarching high level requirements that shall be applicable for all physics based models, numerical solution methods and validation data included in VERA. In addition to these requirements, additional detailed technical requirements will be specified to address individual challenge problems. These specific technical requirements will be documented in the individual Challenge Problem Technical Specification documentation.

Figure 1: VERA Interfaces and Anticipated Integrations

Descriptions of the codes integrated into the VERA-PSS suite and modifications made during the course of VERA development shall be documented in the VERA basis documentation.

3.3.3 The VERA workflow environment shall address the following specific elements:
- Model Setup
- Application Creation
- Simulation Execution
- Performance of Analysis
- Data Management and Visualization

The VERA workflow management approach and instructions for its application by end users shall be documented in the VERA basis documentation.

3.4 Meshing Requirements

3.4.1 VERA shall be capable of supporting both structured and unstructured mesh generation.

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VRD Update Approach / Actions

- VRD Update Kick-off Meeting at January 2012 co-location meeting
- Formed cross-FA team to work on VRD revision
  - Steve Hess – AMA (Lead)
  - Rose Montgomery – AMA
  - Andrew Godfrey – AMA
  - Scott Palmtag – AMA
  - Rod Schmidt – VRI
  - Bill Rider – VUQ
  - Matt Sieger – QA
- Review meeting conducted at February 2012 co-location meeting
  - Focus on identification of detailed technical characteristics required for VERA to function as a "core simulator"
  - Objective to achieve this capability by the end of calendar year 2013
- Numerous follow-up telecons / Vidyo presence meetings
- 3/22/2012: Steve Hess / Jess Gehin met in EPRI's Washington, DC office for final detailed review of proposed VRD revision
- VRD revision sent to SLT for review / approval 3/30/2012

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VRD R1 Major Changes

- Primary change is identification of foundational requirements that are contained in (new) Appendix A
  - Detailed set of technical requirements for core neutronics, thermal hydraulics, and fuel performance
  - Corresponding set of Benchmark Problems for neutronics, T-H, and fuel performance
- For capabilities identified as critical to achieving core simulator functional capability, added requirement for respective CASL FA Leads to develop an integrated plan / schedule for achieving the required level of functionality in the required timeframe.
- Include more comprehensive specification of QA requirements to align with the CASL QA Plan
- Added interfaces to Challenge Problem Integrators
  - Single POC for assigned Challenge Problem
  - Lead responsibility for developing Challenge Problem workflow

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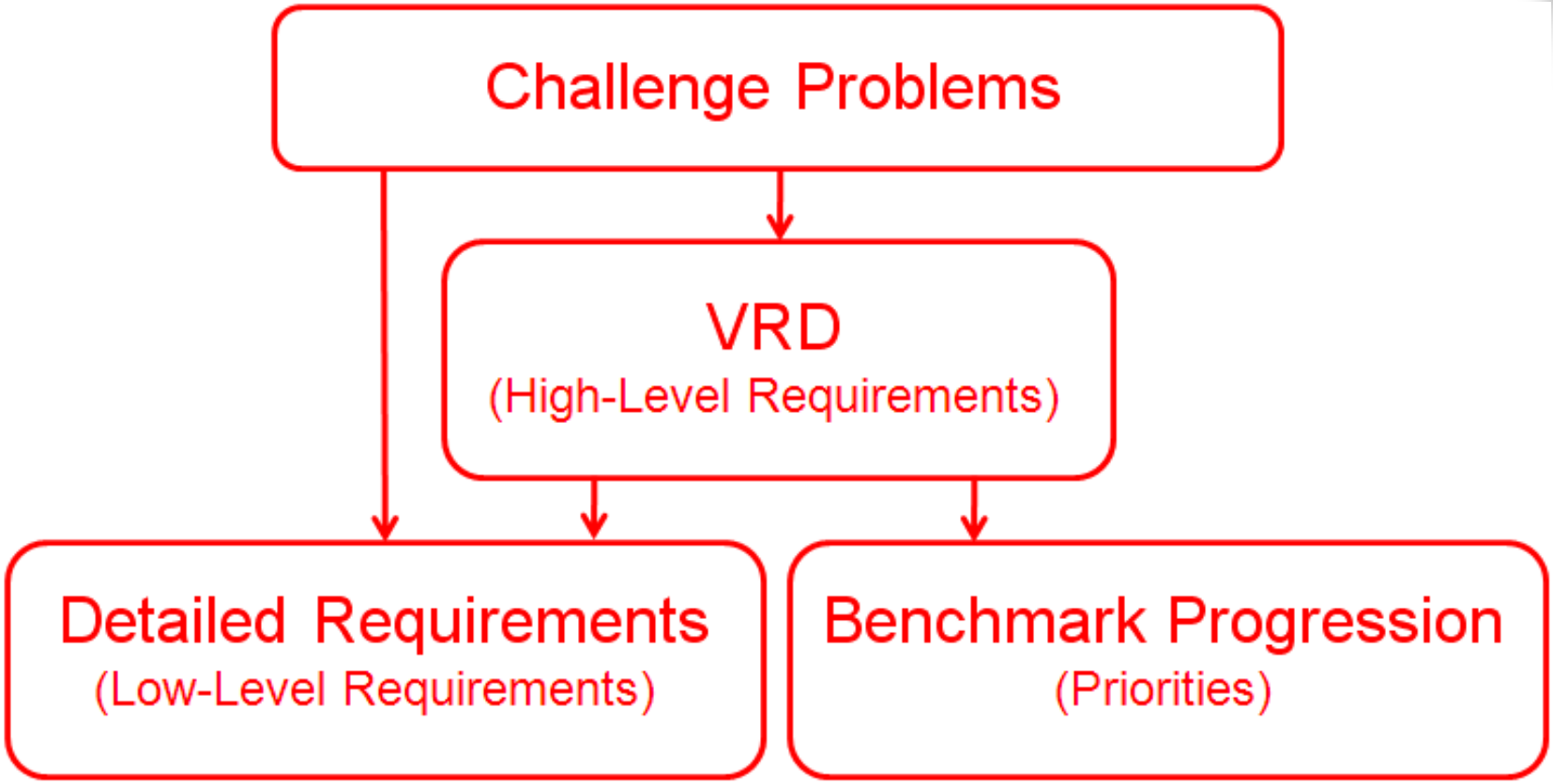
VERA Requirements Hierarchy in VRD – R0



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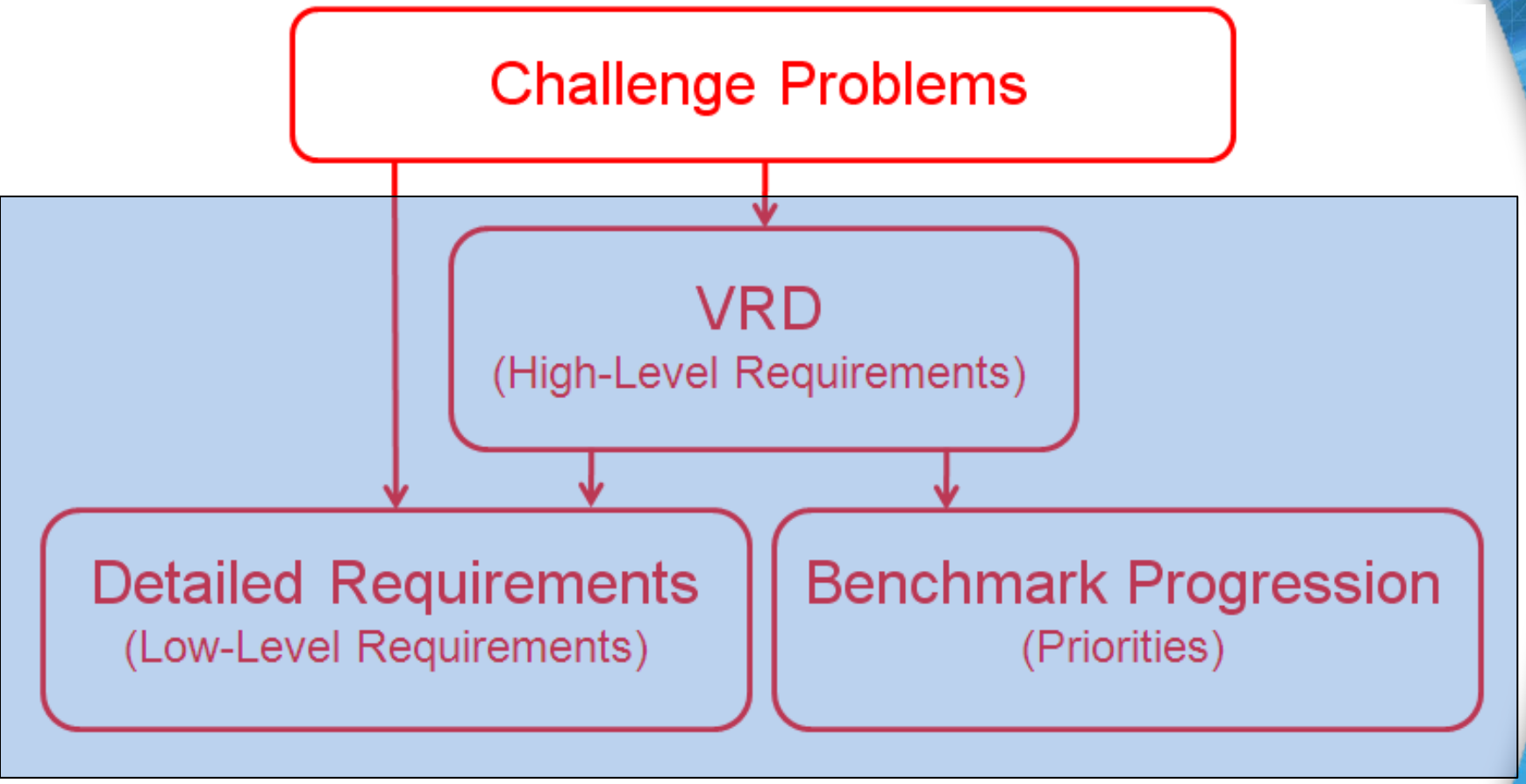
VERA Requirements Hierarchy in VRD – R1



VRD Rev 1 consolidates high level requirements / detailed technical requirements and benchmark progression problems

Core Physics Progressions Defined

Start with Single Physics Neutronics

- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #4 HZP 3x3 Assembly CRD Worth

Model Zero Power Physics Tests and Compare to Plant Data

- #5 Physical Reactor Zero Power Physics Tests (ZPPT)
- #6 HFP BOL Assembly
- #7 HFP BOC Physical Reactor w/ Xenon
- #8 Physical Reactor Startup Flux Maps
- #9 Physical Reactor Depletion

Continue to Coupled Physics Modeling of Reactor Operation

- #10 Physical Reactor Refueling

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Initial T-H Progression Defined

TH benchmark progression ordered to reflect planned development sequence through single phase flow up to / including sub-cooled boiling

Sequence modeled on benchmarks used in VIPRE qualification

Need to identify benchmarks for multi-phase flow and CFD

- #1 Single Phase Simple Channel Pressure Drop
- #2 Single Phase Bundle Pressure Drops / Flow Distributions
- #3 Single Phase Heat Conduction
- #4 Sub-Cooled Boiling Simple Channel Pressure Drop
- #5 Sub-Cooled Boiling Pressure Drops in Bundles
- #6 Single Channel / Lattice Sub-Cooled Boiling Void Fractions
- #7 Heat Conduction for Single Phase with Sub-Cooled Boiling

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Initial Fuel Performance Progression Defined

Currently high level – need to refine with information from FALCON capabilities and MAMBA development plan

- #1 Steady State Fuel Rod Operation
- #2 High-Burnup Fuel Rod Modeling
- #3 Transient Fuel Rod Modeling
- #4 3D Fuel Rod Modeling

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Detailed Technical Capabilities Specified

- Coupled Physics
- Individual Physics
  - Nuclear / Core Physics
    - Steady State
    - Cross Sections
    - Depletion
  - Thermal Hydraulics
  - Fuel Rod Thermo-Mechanics
  - Structural
  - Material Models and Properties
  - Uncertainty Quantification
  - Supporting Requirements
    - General Modeling
    - General Simulation
    - Input / Output
    - Usability

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Next Steps

- Incorporate comments / recommendations from SLT review and obtain approval for revision
- Specify more complete specification of thermal-hydraulics and fuel performance benchmarks (AMA POR-5 Level 3 Project)
  - First draft to be developed by early July
  - Planned meeting to review / modify at July co-location
  - L3 project report due 31 July 2012
  - Identified critical changes / additions will be incorporated into update to address SLT comments on VRD rev1
- Longer Term Items
  - Similar to core simulator (neutronics) benchmarks, TH and FP benchmarks are expected to evolve over time
  - Need to develop specific multi-phase and CFD benchmarks that are directly applicable to reactor application issues (including NPP safety)

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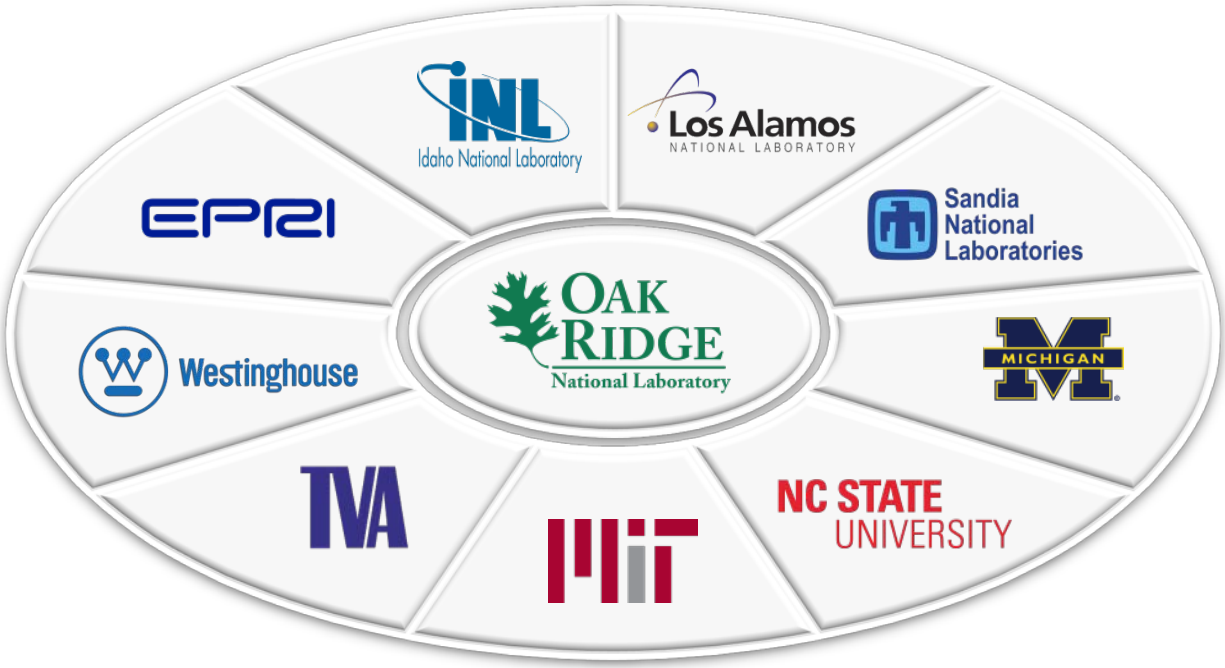
QUESTIONS?



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CASL Safety Analysis Strategy

Paul Turinsky
John P. Gaertner
Steve Hess

June 14, 2012

CASL Safety Issues Overview

- Objectives
  - Assure satisfactory progress on Safety Challenge Problems (CP) in Phase I
  - Define expected VERA capability for Safety CPs and transients in Phase I
  - Plan Safety CPs, VERA capability, and applications for Phase II

- Strategy
  - Identify resources for Safety CPs 2012-2015
  - Establish infrastructure to support work on Safety Analysis
  - Define milestones, schedule, and success for Phase I
  - Propose Phase II work scope

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CASL Challenge Problems

	Power uprate	High burnup	Life extension	Safety Relevance
Operational "Challenge Problems"	Full Scope-Current Focus			Full Scope-Future Focus / Partial Scope-Future Focus
CRUD-Induced Power Shift (CIPS)	×	×		CRUD influences both mechanical and reactivity behavior of the fuel, impacting operational performance and reactor safety response
CRUD-Induced Localized Corrosion (CILC)	×	×		
Grid-to-Rod Fretting Failure (GTRF)		×		Degraded fuel/clad mechanical integrity due to flow-induced vibrations during normal operations affect accident response
Pellet Clad Interaction (PCI)	×	×		PCI, a fuel failure mechanism during normal operations, can also occur during accident transients causing a local power increase
Fuel Assembly Distortion (FAD)	×	×		Distortion of fuel rods and fuel assemblies has the potential to inhibit control rod insertion, preventing timely reactor shutdown
Safety "Challenge Problems"				
Departure from Nucleate Boiling (DNB)	×			Quantify and prevent local vapor-induced clad surface overheating during certain accident scenarios
Cladding Integrity during Loss of Coolant Accidents (LOCA)	×	×		Predicting fuel response during a LOCA facilitates developing advanced fuel designs that minimize hydrogen production and maintain a coolable geometry
Cladding Integrity during Reactivity Insertion Accidents (RIA)	×	×		Predicting fuel response during an RIA-induced power excursion facilitates advanced fuel designs that minimize failures and fission product release
Reactor Vessel Integrity	×		×	Reactor vessel integrity is essential during normal operation and accident situations. Improved prediction (and models) of vessel irradiation and performance assure adequate fuel cooling
Reactor Internals Integrity	×		×	Operational condition of core internal components prior to an accident-induced transient impacts likelihood of safe shutdown

CASL Challenge Problems

	Power uprate	High burnup	Life extension	Safety Relevance
Operational "Challenge Problems"	Full Scope-Current Focus			Full Scope-Future Focus / Partial Scope-Future Focus
CRUD-Induced Power Shift (CIPS)	×	×		CRUD influences both mechanical and reactivity behavior of the fuel, impacting operational performance and reactor safety response
CRUD-Induced Localized Corrosion (CILC)	×	×		
Grid-to-Rod Fretting Failure (GTRF)		×		Degraded fuel/clad mechanical integrity due to flow-induced vibrations during normal operations affect accident response
Pellet Clad Interaction (PCI)	×	×		PCI, a fuel failure mechanism during normal operations, can also occur during accident transients causing a local power increase
Fuel Assembly Distortion (FAD)	×	×		Distortion of fuel rods and fuel assemblies has the potential to inhibit control rod insertion, preventing timely reactor shutdown
Safety "Challenge Problems"				
Departure from Nucleate Boiling (DNB)	×			Quantify and prevent local vapor-induced clad surface overheating during certain accident scenarios
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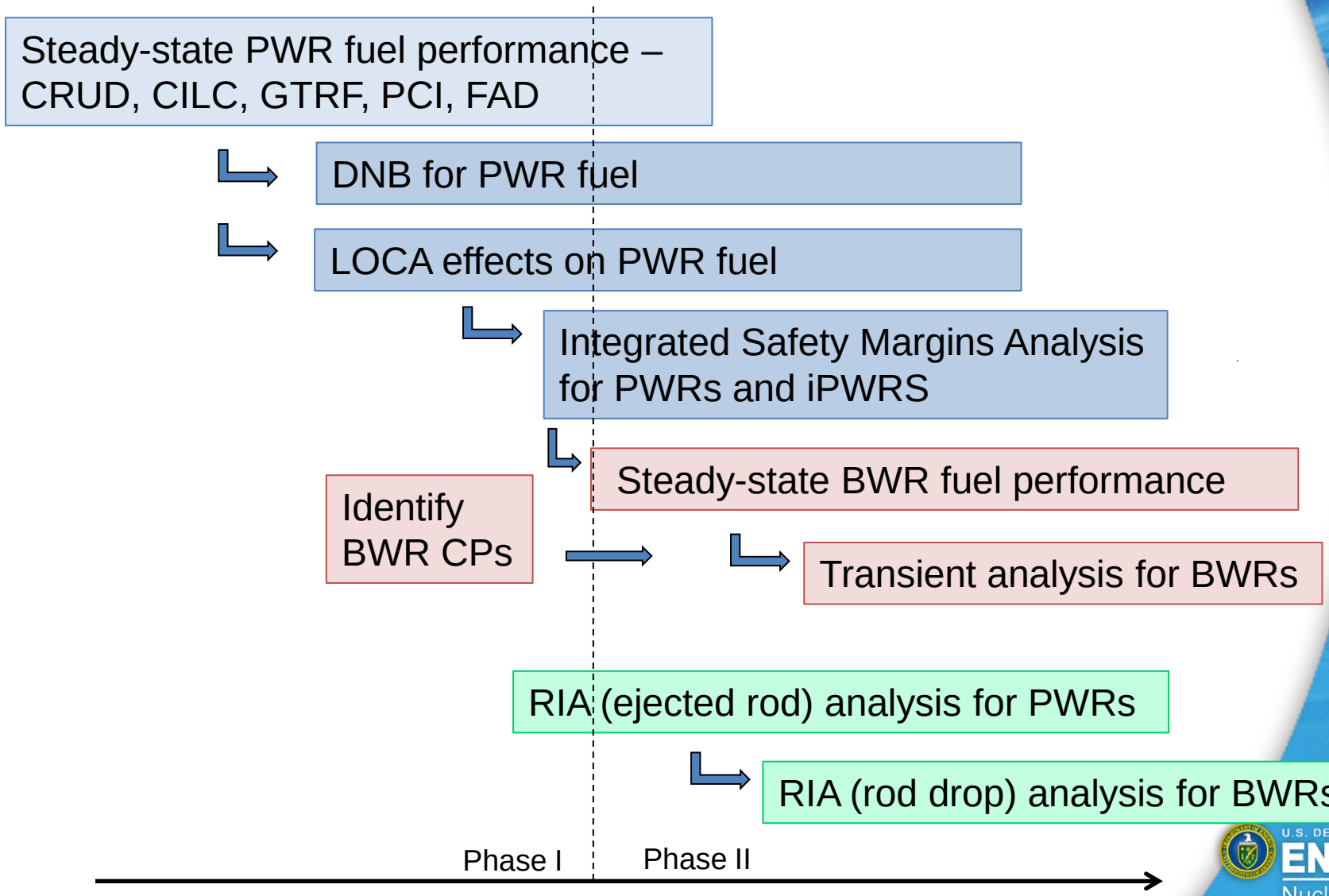
~~Reactor Vessel Integrity~~	×			Reactor vessel integrity is essential during normal operation and [illegible]ls) of vessel [illegible]ooling
Reactor Internals Integrity	×		×	[illegible] prior to an accident-induced transient impacts likelihood of safe shutdown

This plan does not include vessel and reactor integrity Challenge Problems at this time!

Evolution of VERA Safety Capability



Significant Issues for Success of Safety Plan

- Programmatic
  - Convene a working group and formulate CASL Safety Analysis Strategy
  - Identify Safety Challenge Problem Integrator
  - Define ramp-down of fuel performance CPs
  - Evaluate RELAP5-3D and COBRA-TRAC TF for LOCA system modeling
  - Develop detailed plans – including milestones, schedules, and resource needs – for the Safety CPs in Phase 1: DNB, RIA, LOCA
  - Work with BWR community, identify BWR CPs and applications for Phase 2
  - Identify application sponsors and collaborators

Significant Issues for Success of Safety Plan

- Technical
  - Select between Drekar and HYDRA-TH for transient analysis.
  - Prioritize work on tighter methods for coupling of neutronics and thermal-hydraulics models for transients.
  - Define roles of Peregrine and COBRA for fuel temperature modeling for transients.
  - Accelerate work on time dependence in radiation transport codes.
  - Set performance and run time metrics for safety CPs consistent with Work Flow needs
  - Define validation needs, sources, gaps

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Candidates where CASL Can Make a Difference –

- Analyze current safety issues contained within RPV (2012)
  - Analyze post-LOCA, in-vessel flow restrictions due to fibrous insulation
- Table-top exercises to identify and scope first CASL BWR uses (2013)
  - e.g, core instability; CHF due to dryout
- Limited benchmark of safety margins vs. use of current methods
  - Extended power up-rate or new plant design; e.g., AP-1000 (2014-2015)

Near-term to mid-term objectives

Candidates where CASL Can Make a Difference --

- RIA analysis of existing and new PWR fuel designs (2017)
- Safety Margins Benchmark for PWRs and iPWRS
  - Collaborative applications with vendors and other partners (2018)
- Safety Margins Benchmark for BWRs
  - Collaborative applications with vendors and other partners (2019)
- Large, integrated applications of VERA (2020)
  - Candidates
    - Large LOCA redefinition
    - Safety margins analysis for power up-rate
    - Design assist for new fuel design

Mid-term to long-term objectives

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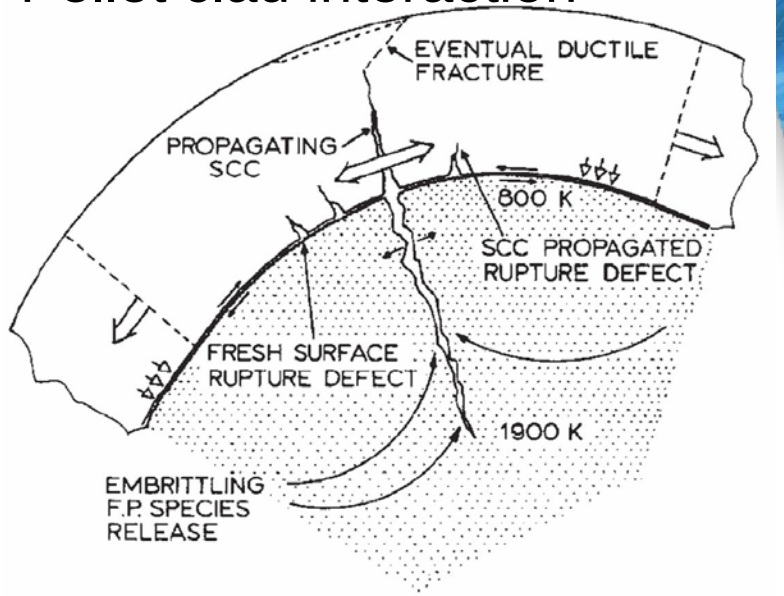
PWR fuel failure mechanisms

Grid Fretting

Crudding

Pellet clad interaction



Corrosion & Hydrogen pickup

- $2H_2O + 4e^- \rightarrow 2H_2 + 2O^{2-}$
- $2O^{2-} + Zr \rightarrow ZrO_2 + 4e^-$

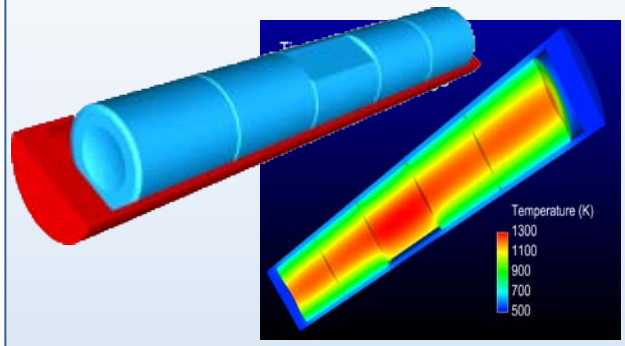
0.5 mm

* Edsinger, Stanek, Wirth, JOM **63, no. 8** (2011)

MPO delivers materials physics-based constitutive models to the virtual reactor for CASL challenge problems

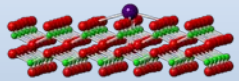
For CRUD, GTRF and PCI, identify 3-D, high resolution coupled physics simulation capability for interface with virtual reactor;

PCI

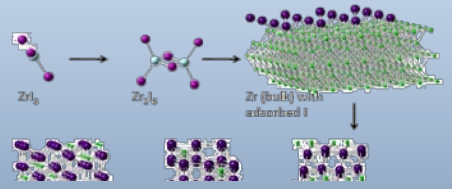


Peregrine

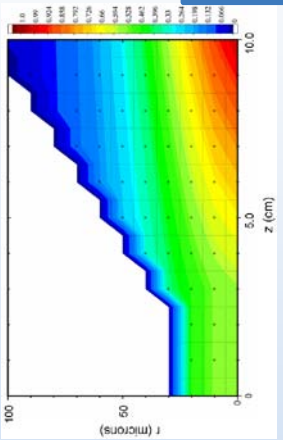
(Fuel Performance)

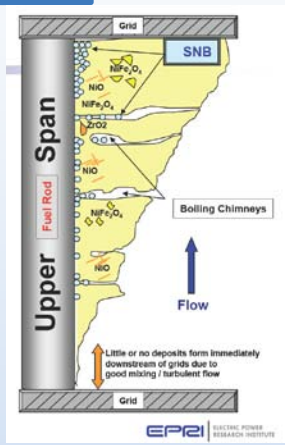


ZrO_2 / I_2 Interaction



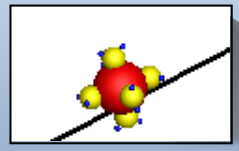
CRUD



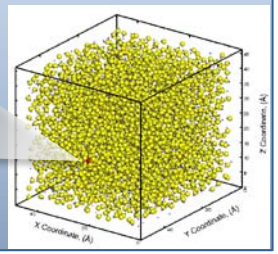


MAMBA

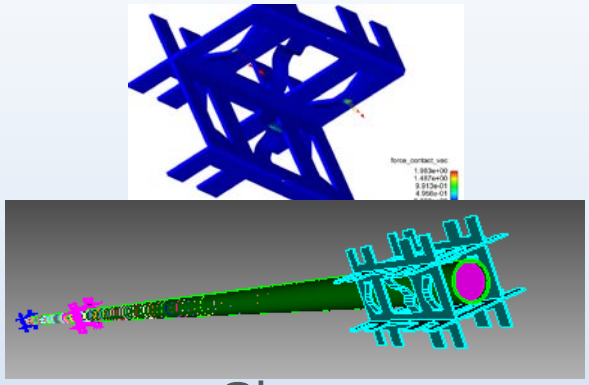
(MPO Advanced Model for Boron Analysis)



ΔH_{MD}

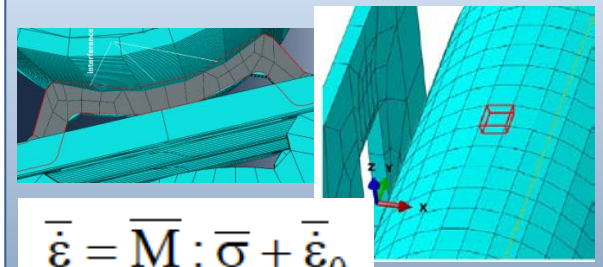


GTRF



Sierra

(Structural Mechanics)



$$\dot{\bar{\varepsilon}} = \bar{\bar{M}} : \bar{\sigma} + \dot{\bar{\varepsilon}}_0$$

Initiate a series of microscale activities to provide mechanistic/physical insight into complex degradation phenomena

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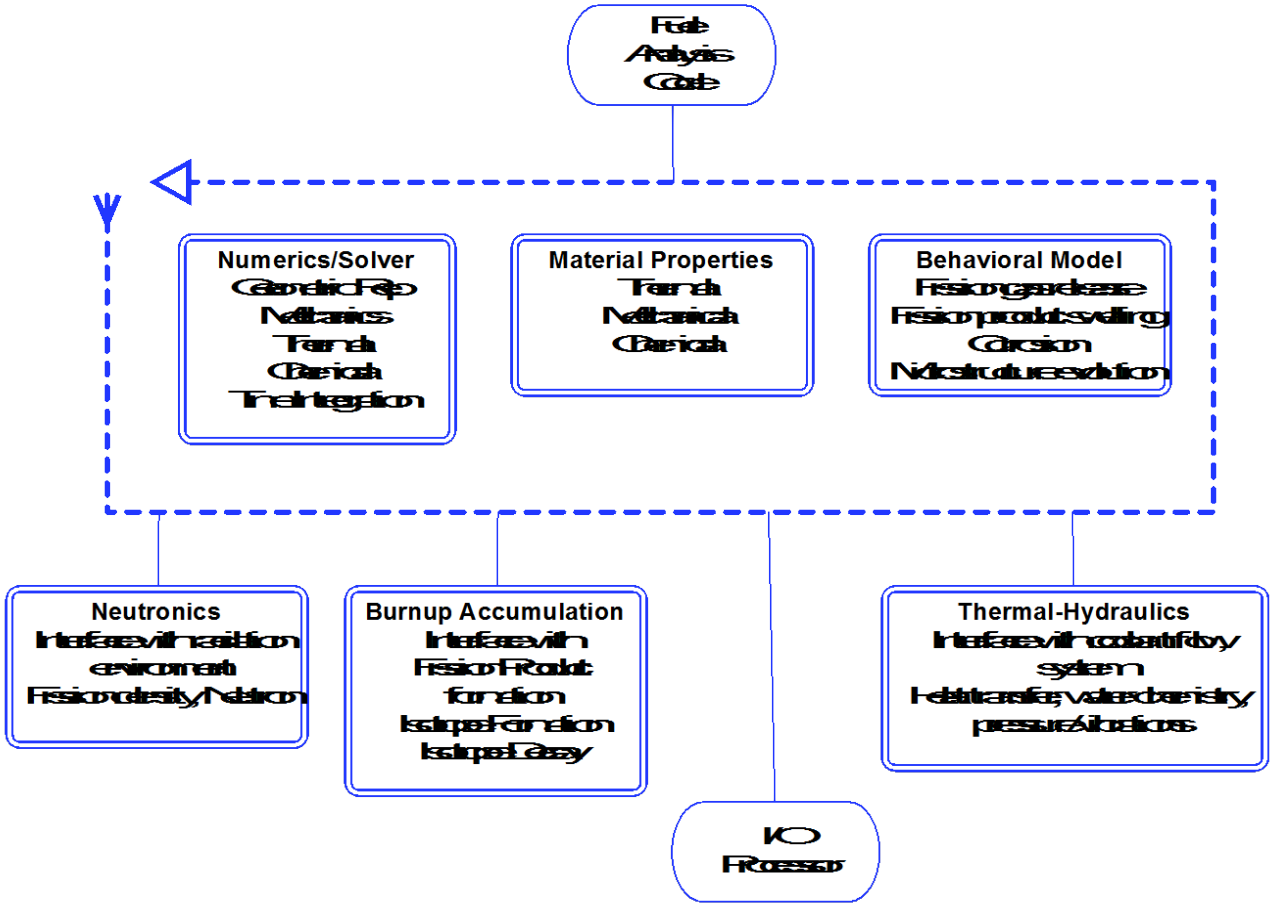
Fuel performance framework (inspired by Falcon & using Moose/Bison) to develop new, 3D model (PEREGRINE)

Major Components of Nuclear Fuel Modeling Capability



Inspired by Falcon & using Moose/Elk/Fox framework

Planned PEREGRINE Capability

Problem Setup ★
- Power Density
- Burnup Distribution
- Fast/Thermal Flux Dist.
- Thermal B/C
- Mechanical B/C

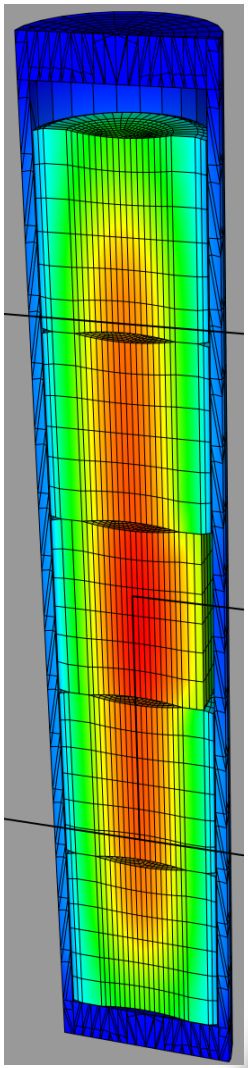
Material Properties
- Specific Heat
- Density
- Conductivity
- Elastic/Plastic Behavior
- Creep Rate

Behavior Models
- Swelling/Densification/Cracking
- Irradiation Creep/Growth
- Grain Growth
- Fission Gas Release
- Oxidation

Physics Solution ★
- Thermal Transport
- Mechanical Forces
- Chemical Transport

Global Parameters Integration
- Rod Pressure
- Fission Gas Composition
- Linear Power

Result Output ★
- Write global variables
- Shift Internal State Variables



★ - Elements provided by MOOSE/ELK/FOX systems

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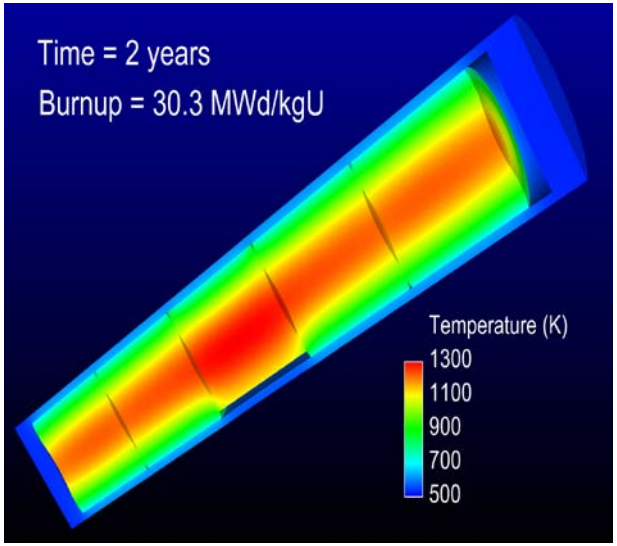
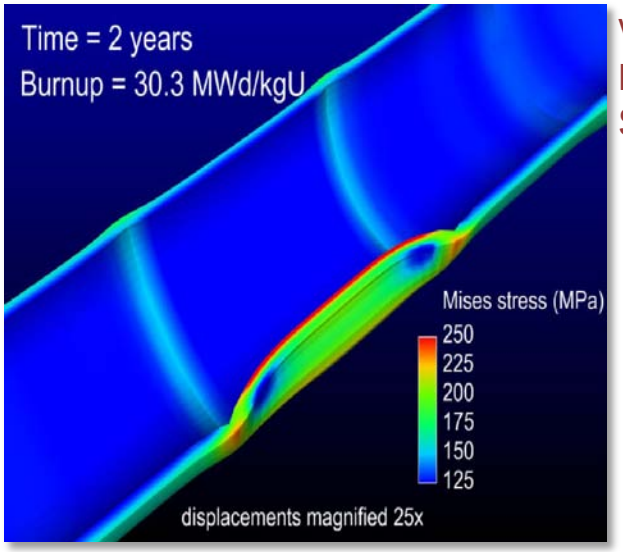
Peregrine simulation of missing pellet surface

3D multiphysics fuel performance capability to assess Pellet Clad Interaction (PCI)

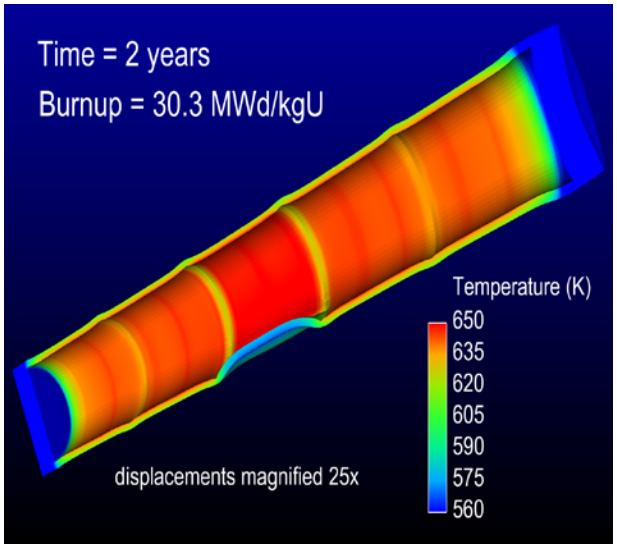
High resolution, 3D fuel performance calculation reveals the impact of a missing pellet surface on stress state, temperature profile, etc. (*i.e.* full nuclear fuel performance) as a function of fuel history.



Fuel Temperature



Von Mises Effective Stress



Clad Temperature

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PEREGRINE model development will enable evaluation of margin against PCI fuel failures

Outcomes and benefit to nuclear power industry

- HPC-scaling of the Peregrine fuel performance model will enable efficient consideration of complex phenomena

- Flexible framework will be used to systematically assess fuel performance during normal and transient operations and off-normal conditions:
  - *Evaluate effect of pellet irregularities on fuel performance*
  - *Optimize power maneuvers improving operational margins*

Peregrine fuel performance simulations will help eliminate PCI fuel failures

Next steps

- Building on BISON, develop Peregrine using industry standard, validated constitutive models & benchmark Peregrine versus FALCON

- Define and implement directed lower-length-scale modeling approaches to develop improved, physics based models of fuel and clad property evolution

- *Contribute to efficient evaluation of innovative fuel designs for normal and transient operation and best estimate of safety margins during reactor operation & accidents*

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Fuel Performance Requirements Span a Broad Range of Operating Conditions

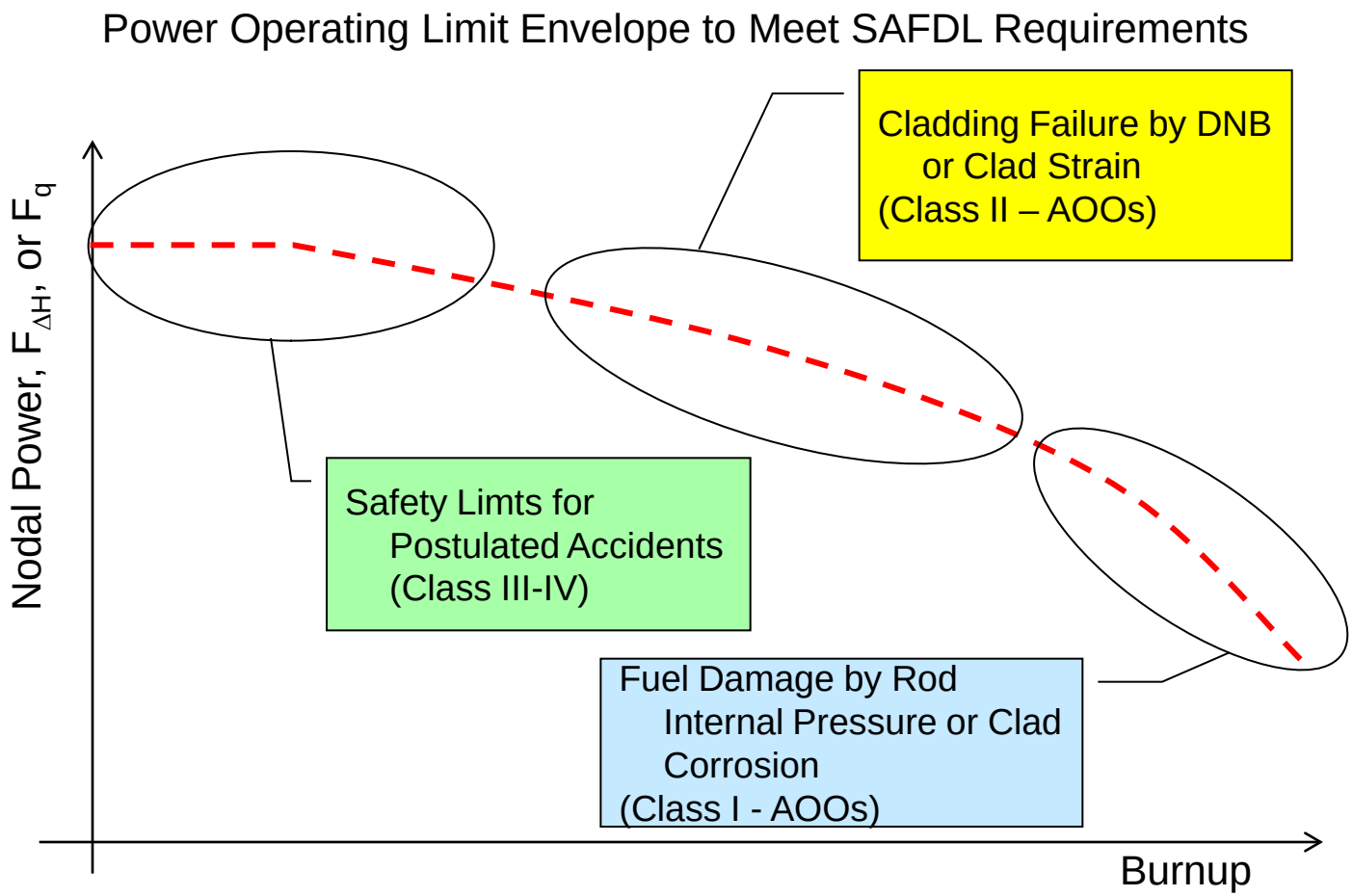
ANSI N18.2/ANS 51.1/52.1 Event Categorization	NUREG-0800 Rev. 3 Event Categorization	Example Events
Category I – Normal Operation and Operational Transients	Normal Operation and Anticipated Operational Occurrences (AOO's) (Events expected to occur once or more per reactor lifetime)	▪ Increase in feedwater flow ▪ Loss of feedwater heater ▪ Loss of external load ▪ RCCA withdrawal at power ▪ Complete loss of forced reactor flow ▪ Reactor Coolant Pump Shaft Break/Seizure ▪ Control Rod Ejection ▪ Control Rod Drop ▪ Small Break LOCA ▪ Large Break LOCA
Category II – Moderate Frequency (once per calendar year)		
Category III – Infrequent Incidents (once per reactor lifetime)		
Category IV – Limiting Faults (not expected to occur – consequences of significant radioactive release)	Postulated Accidents (not expected to occur – consequences of significant radioactive release)	

Normal Operation/AOOs – years of operation
Maintain hermeticity
No interference with reactivity control system

Design Basis Accidents – Seconds to hours
Structural integrity
Fission product retention

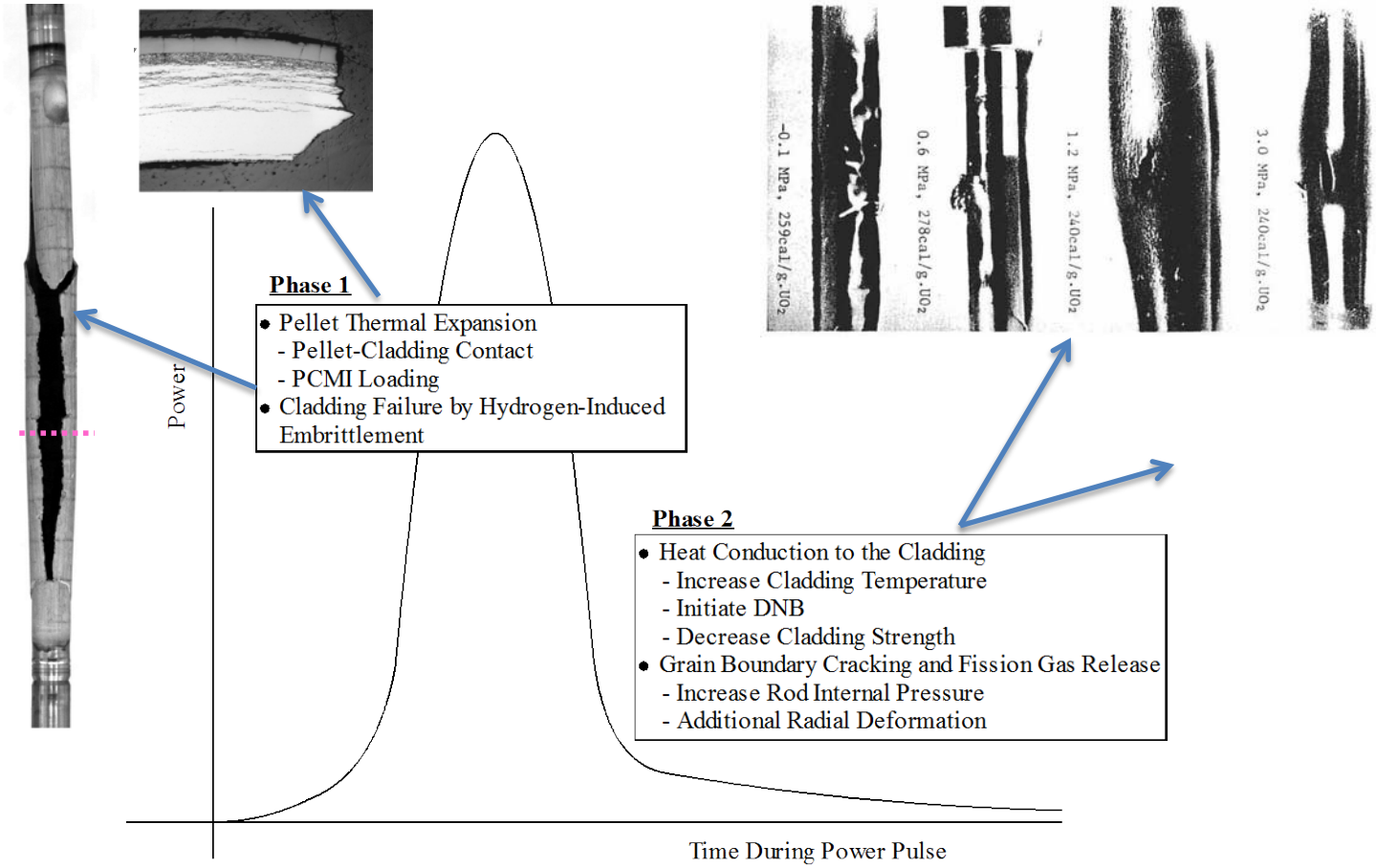
Severe Accidents – hours to days
Chemical stability ??

Fuel Performance Limitations: How do they apply?



Fuel Design Process is an Exercise in Compromise – Must balance many competing requirements and performance characteristics

Modeling Transient Behavior: Reactivity Insertion Accidents



Modeling allowed design of specific tests to address experimental observations and determine applicability to in-reactor behavior

UO_2-Zr based fuel degradation phenomena*

Dominated by System Response

Behavior of Fuel/Core Materials Affects Accident Progression

Focus on Radionuclide Retention

- Decline in core water level
- Fuel rods become exposed followed by limited heat conductance to steam
- Takes place in minutes to hours depending on the accident sequence

- Marks the onset of core degradation processes and fission product release
- Physical and chemical degradation in fuel and core components that lead to: i) further enthalpy production ii) hydrogen generation iii) partial deformation and relocation and iv) constrain coolability

- Marks the onset of significant core relocation and melting
- Initiate threats to RPV and containment
- Significant release of fission products
- Coolability is significantly hindered and cooling with water could become impractical

300ºC — Lead Up — 800ºC — Mid-Phase — (1500)ºC — Late-Phase

800°C
Melting of Ag-In-Cd alloy

950°C
Fe/Zr – Fe/Ni Eutectics

800-1100° C
Cladding Ballooning and Burst

1200° C
Onset of significant enthalpy production as a result of rapid Zr-steam reaction

1150°C
UO2/Zr reaction yields liquid U
B4C/Fe Eutectics

1300°C
Zr eutectics with Stainless Steel and Inconel

1450°C
Melting of Stainless Steel and Inconel

1750° C
Zircaloy melting and UO2 dissolution by molten metal

1975°
α-Zr(O) melting

2600-2700°C
U-Zr-O melting – ZrO_2 melting

2400°C
B_4C melting

2850°C
UO_2 melting

* K. Terrani, after Hofmann JNM (1999)

PEREGRINE Model Development & Data Needs for Transient Performance of New Fuel Forms

Key phenomena to model (Zr clad &/or advanced cladding)

- Clad phase change (T >~800°C for Zr), O/H reactions & diffusion, **hydrogen** uptake/**hydride precipitation**
- Oxidation kinetics & stability (inner & outer clad)
- Pellet – clad chemical/mechanical interactions (RIA)
- Thermal profiles, including axially dependent decay heats & thermal conductivity of fuel/clad
- Large strain plasticity & failure (including ballooning, secondary hydride cracking and **fragmentation of fuel & clad**)
- Post-quench flow & embrittlement

Data Needs (Thermo-Chemical-Mechanical, separate & integral)

- Temperature & state (BU, dpa, oxide)-dependent thermal (conductivity) & mechanical (creep, fracture) properties
- Temperature, pressure & steam quality dependent thermochemical reactions (oxidation kinetics, hydrogen fate, breakaway oxidation mechanisms?) & fuel-clad chemical interaction
- Thermal-mechanical processes (ductility/creep, fracture) at T & post-rewetting quench & as a function of state (dpa, oxide, H, …)
- Embrittlement mechanisms & integral performance

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CASL Validation Data Center

Nam Dinh
CASL-VUQ

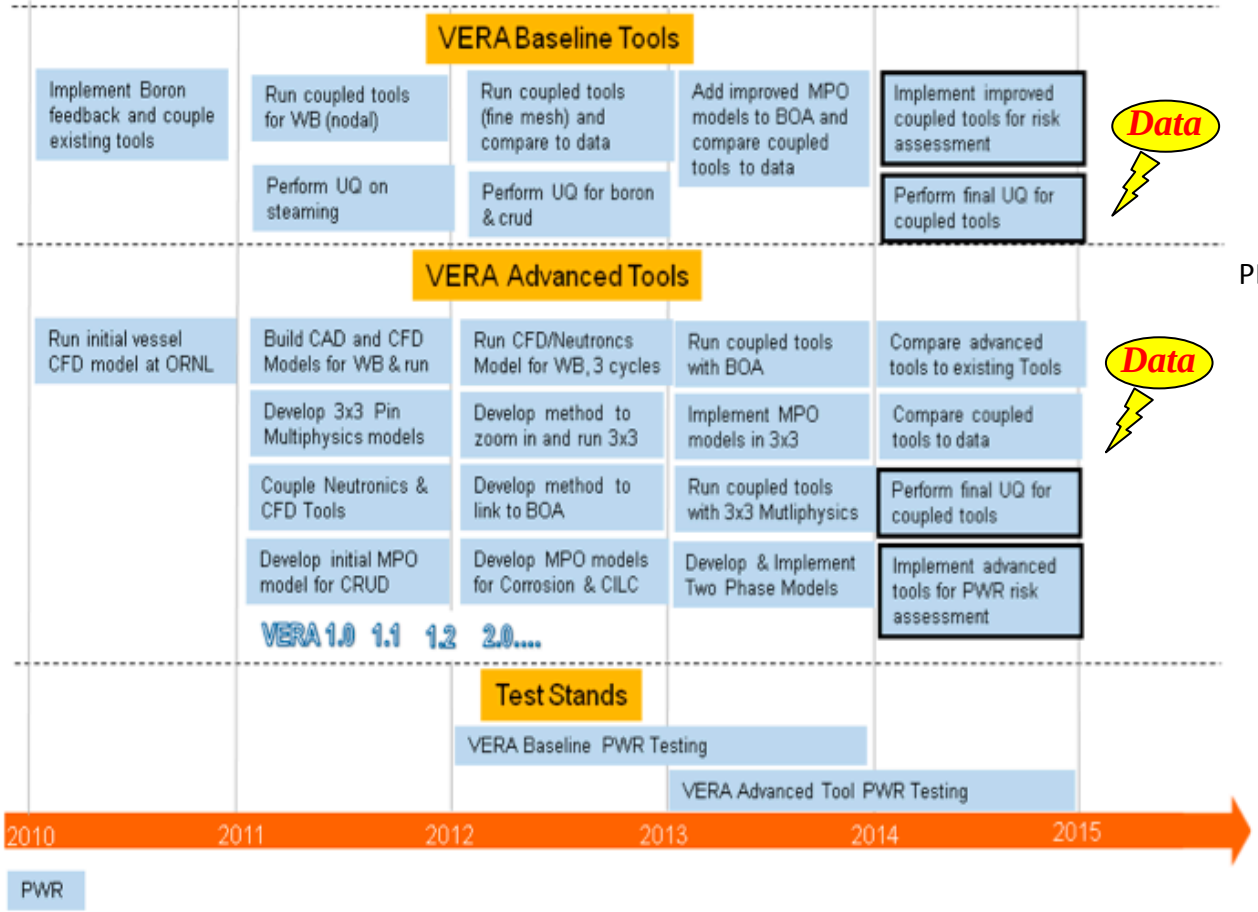
Hyung Lee
NE-KAMS

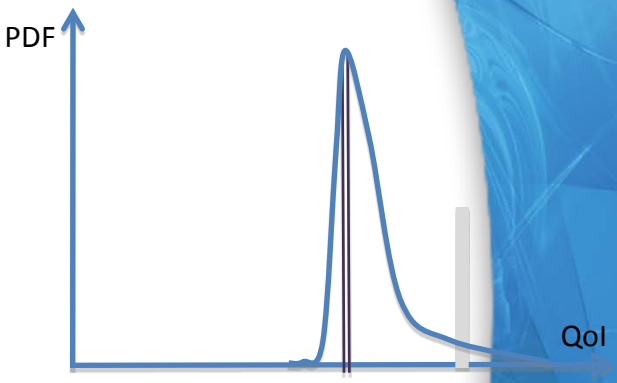
CASL Round Table
June 13, 2012

Contents

- VUQ Challenge
- Data
- CASL Approach to Validation Data
- CASL Validation Data Center

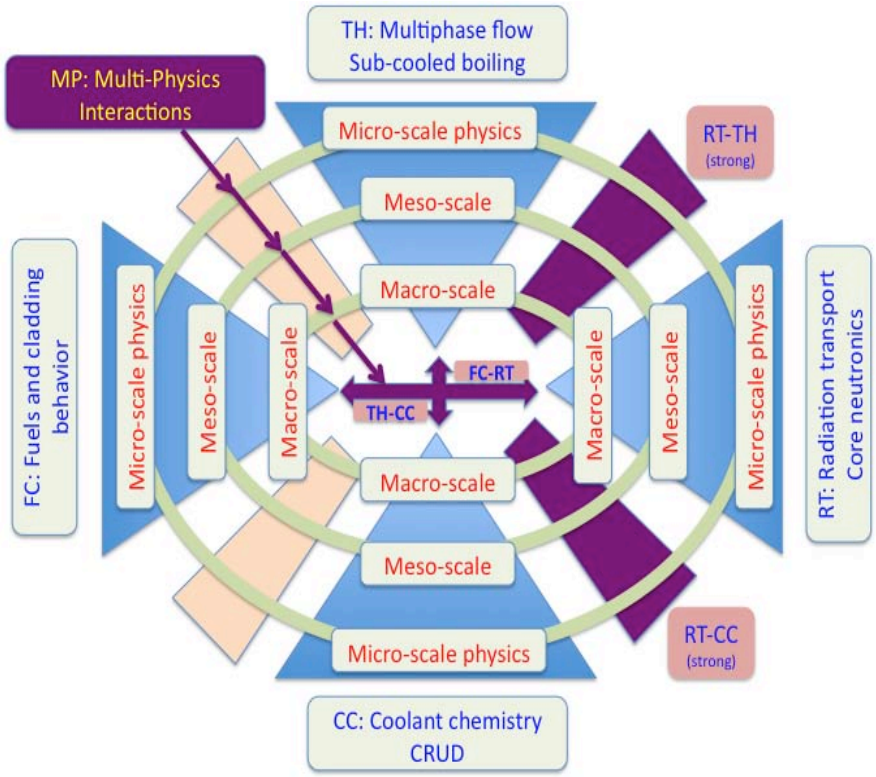
CASL Challenge: Quantitative Assessment of Calculation

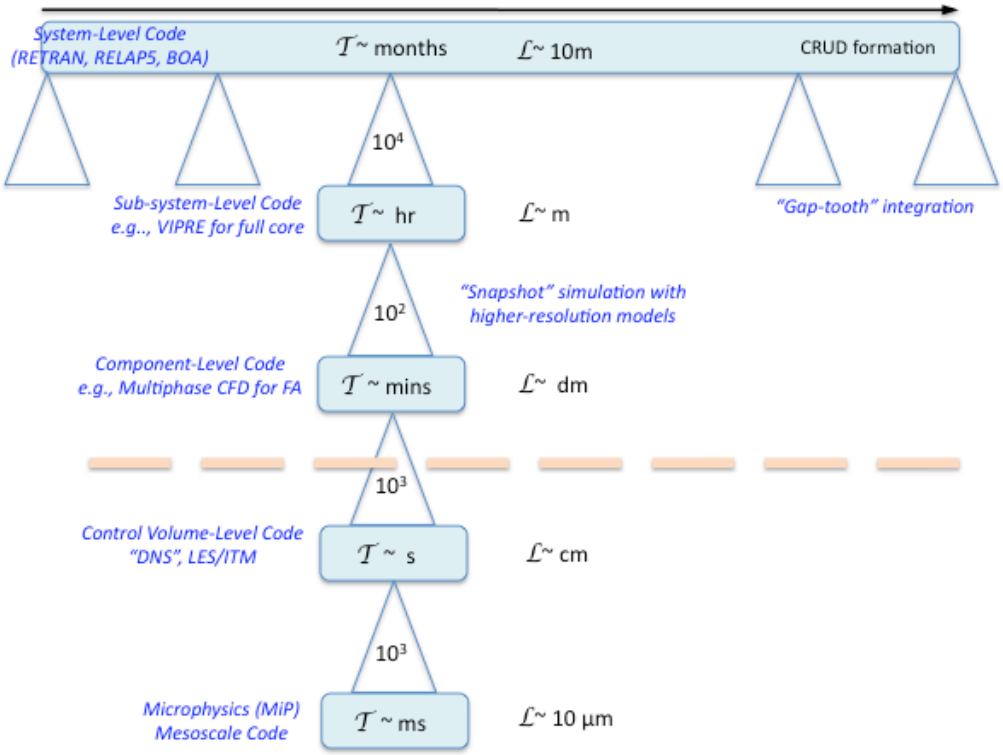




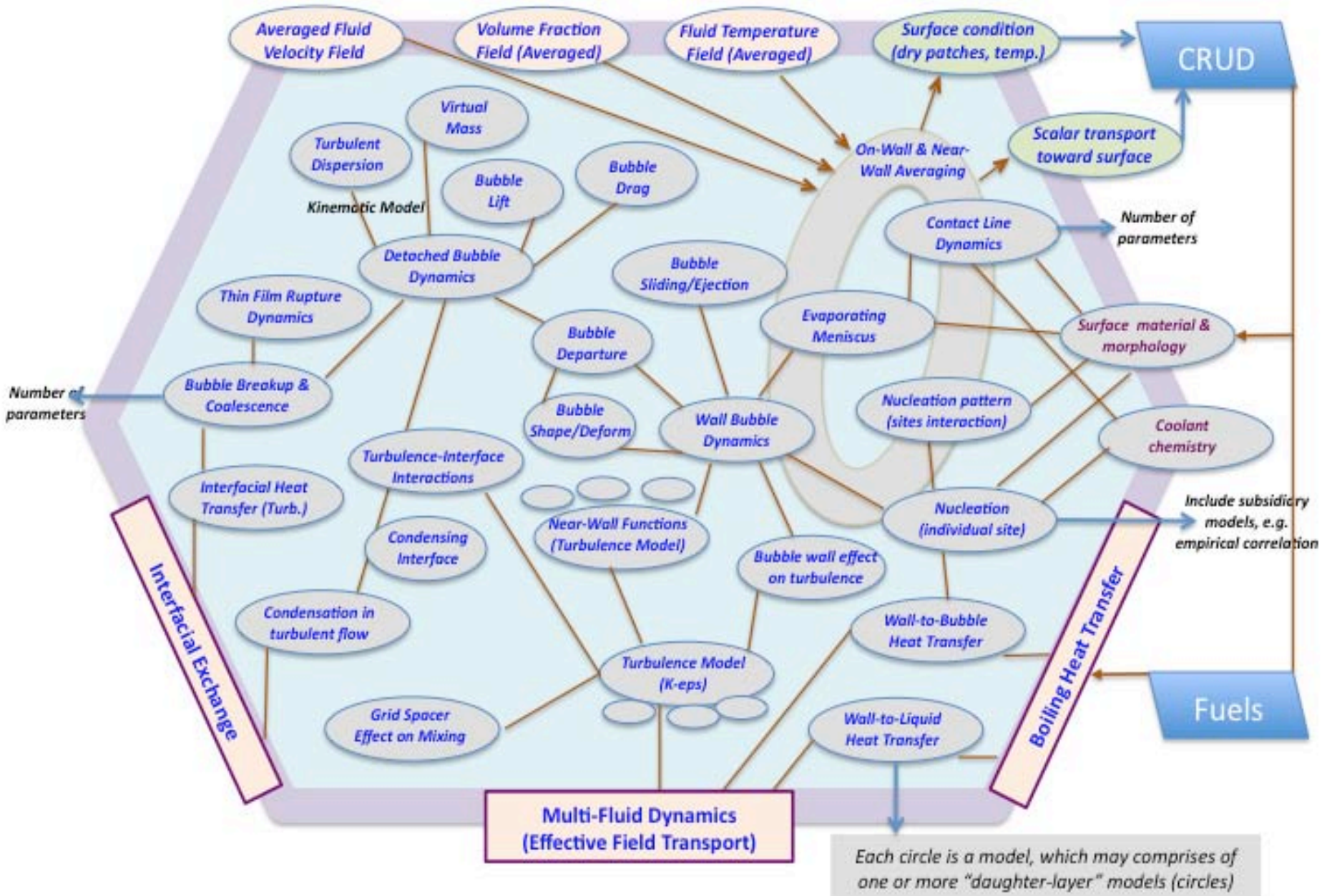
- Few experiments and plant data directly relevant to and usable for validation of high-fidelity mechanistic models
- Data that exist are not VUQ-grade (i.e. not compatible with modern VUQ methods)
- Severe lack of data to validate multi-physics, multi-scale capability,
- Long lead time are required for the acquisition of any new applicable experimental data. Limited amount of VUQ-grade data from prospective experiments over the next 3-5 years.

Multi-Physics, Multi-Scale Problems

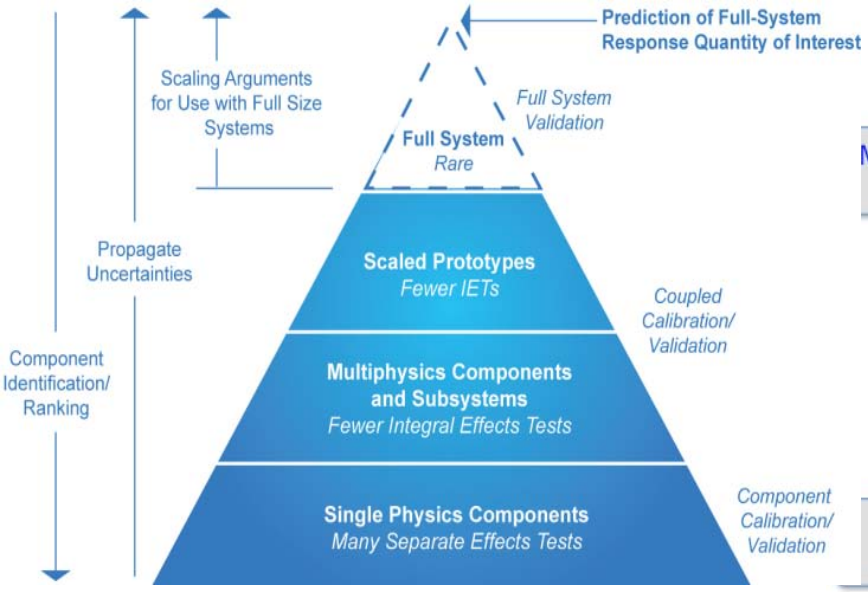


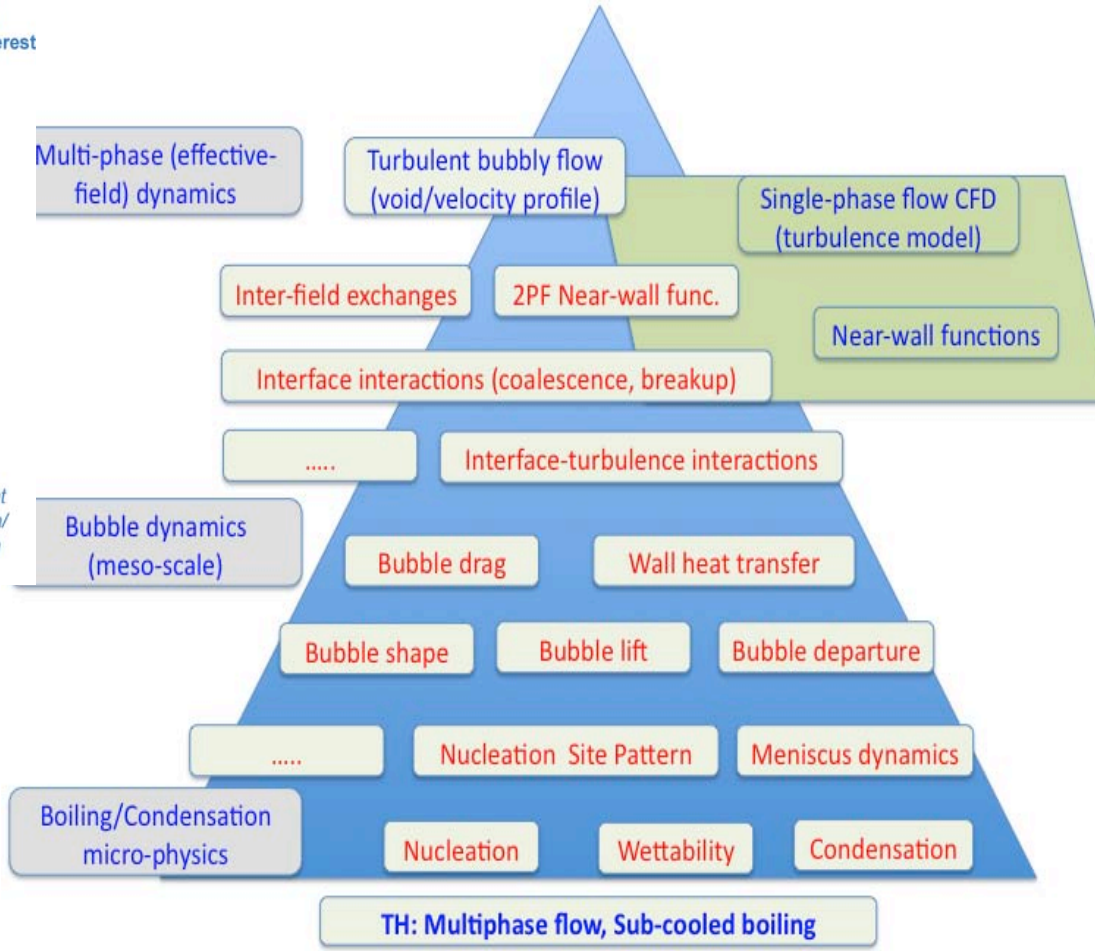


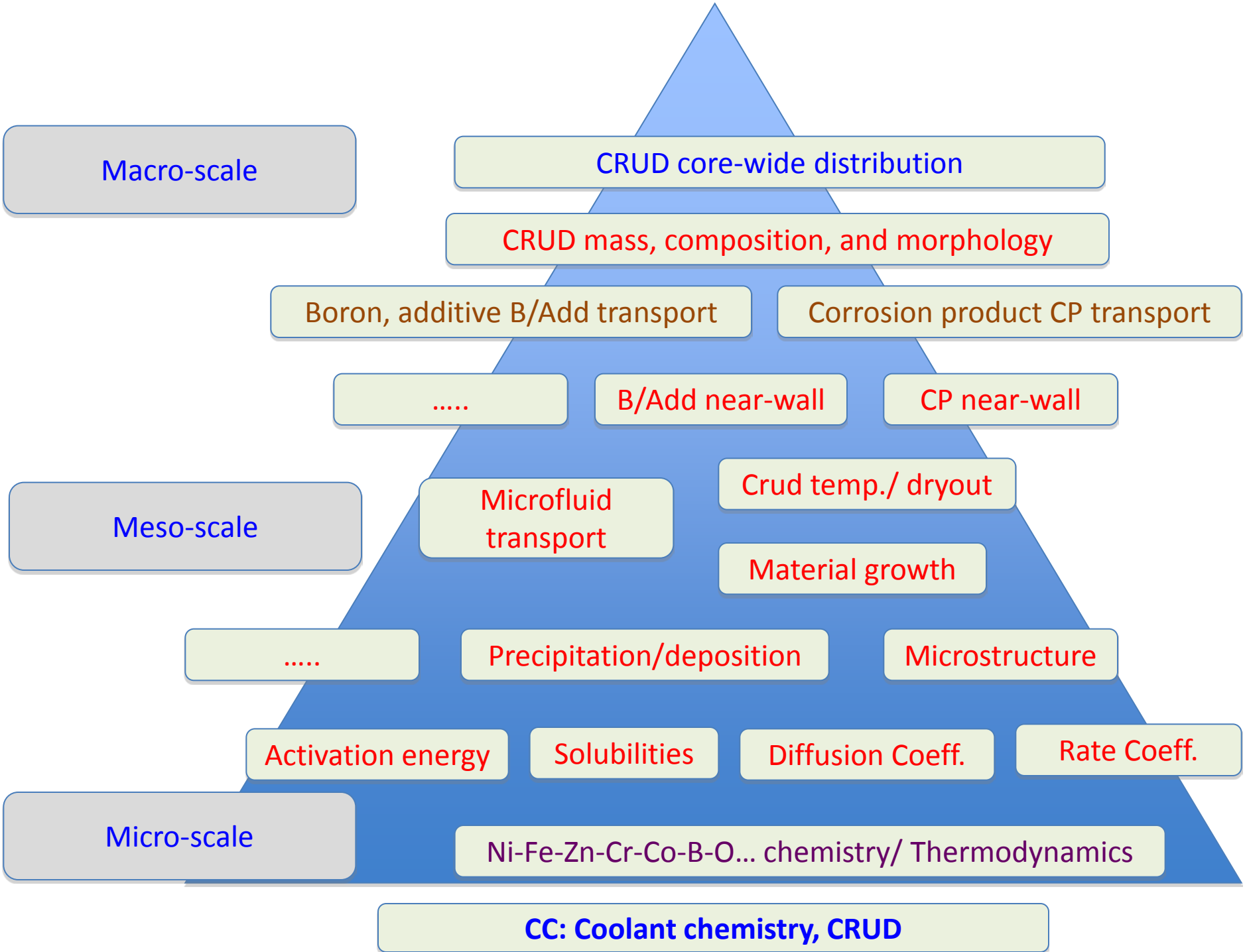
Sub-cooled Flow Boiling – Complex Modeling



Validation Hierarchy (Validation Pyramid)






Macro-scale
CRUD core-wide distribution
CRUD mass, composition, and morphology
Boron, additive B/Add transport
Corrosion product CP transport
.....
B/Add near-wall
CP near-wall
Meso-scale
Microfluid transport
Crud temp./ dryout
Material growth
.....
Precipitation/deposition
Microstructure
Activation energy
Solubilities
Diffusion Coeff.
Rate Coeff.
Micro-scale
Ni-Fe-Zn-Cr-Co-B-O... chemistry/ Thermodynamics
CC: Coolant chemistry, CRUD

CRUD Data

- Plant data
  - EPRI 1009951 (2004) catalogues the most comprehensive analysis of fuel deposits made in the U.S. commercial nuclear industry
  - International plant data
- In-pile data
  - Halden In-Reactor Test to exhibit PWR Axial Offset Anomaly
  - …
- Out-of-pile data
  - Westinghouse Advanced Loop Tester (WALT)
  - Studsvik CRUD tests
  - …

➢ A number of diagnostic methods employed with attendant capabilities and limitations

- ➢ Morphology
- ➢ Elemental composition
- ➢ Phase composition

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Data Realism & Data Heterogeneity

- Data (non)representativity
  - Issues in experimental conditions, design, procedure, diagnostics, processing
  - Relevance
  - Scaling

- Data quality… not “UQ-perfect” experiments
  - Past (pre-VUQ) experiments
  - Quality of data (in UQ grade)

- Not all experiment “born equal”
  - Over-kill model calibration by aligning with certain SETs

- Even within an experiment, not all data “born equal”
  - Measuring devices
  - Relevance of that parameters to FOM
    - P, T, VF, velocity…

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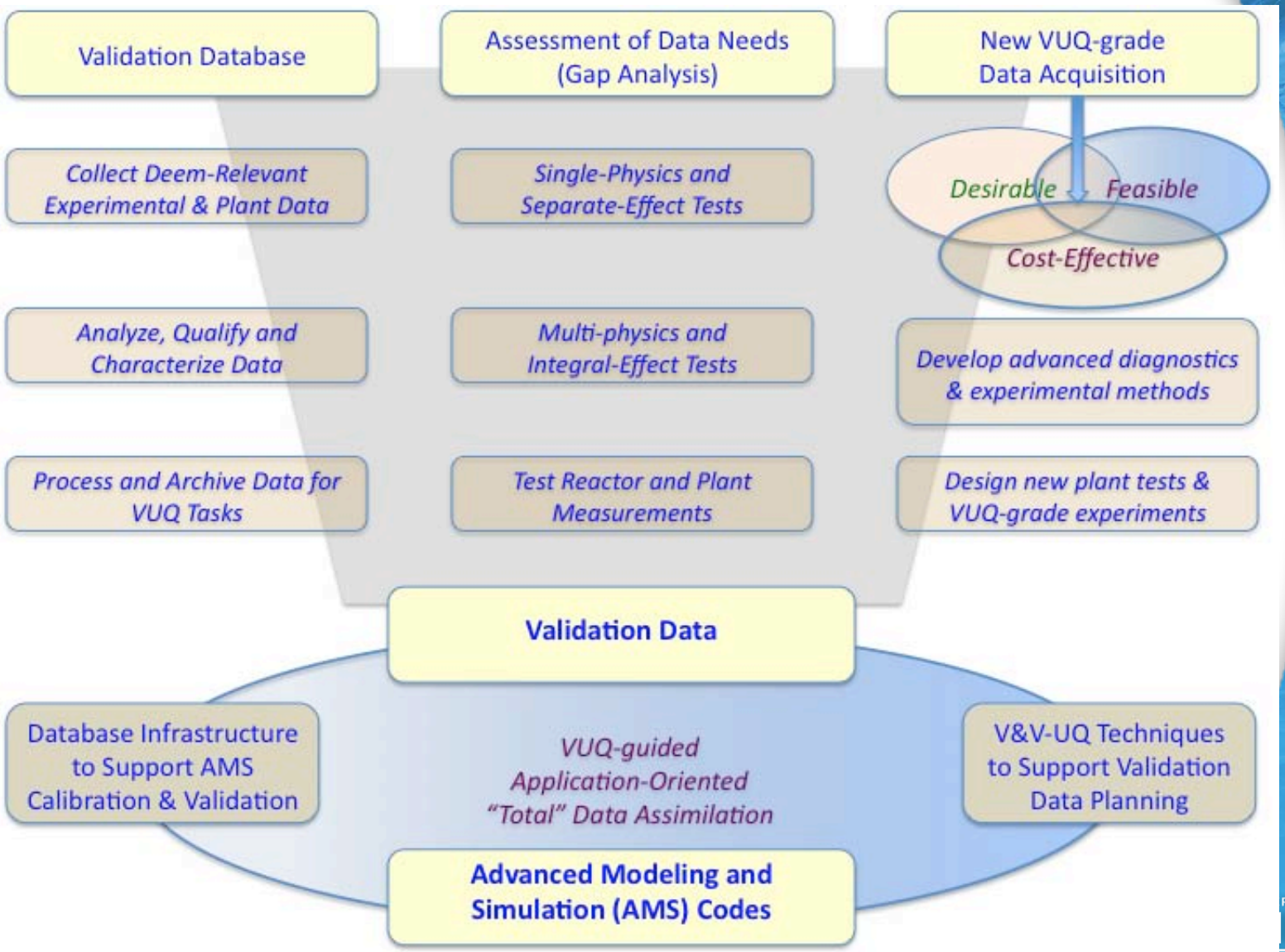
CASL Approach



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Data Qualification and Integration

- Data Identification
- Data Collection
- Data Review
- Data Characterization
- Data Assimilation

VUQ Quality	Grade				
	4	**3**	**2**	**1**	**0**
Relevance [R]	Very High (direct)	High	Medium	Low	N/A
Scaling [S]	Prototypic (full-scale)	Adequately scaled	Medium	Inadequately scaled (large distortions)	N/A
Uncertainty [U]	Well-Character-ized	Character-ized	Medium	Poorly-Characterized	N/A

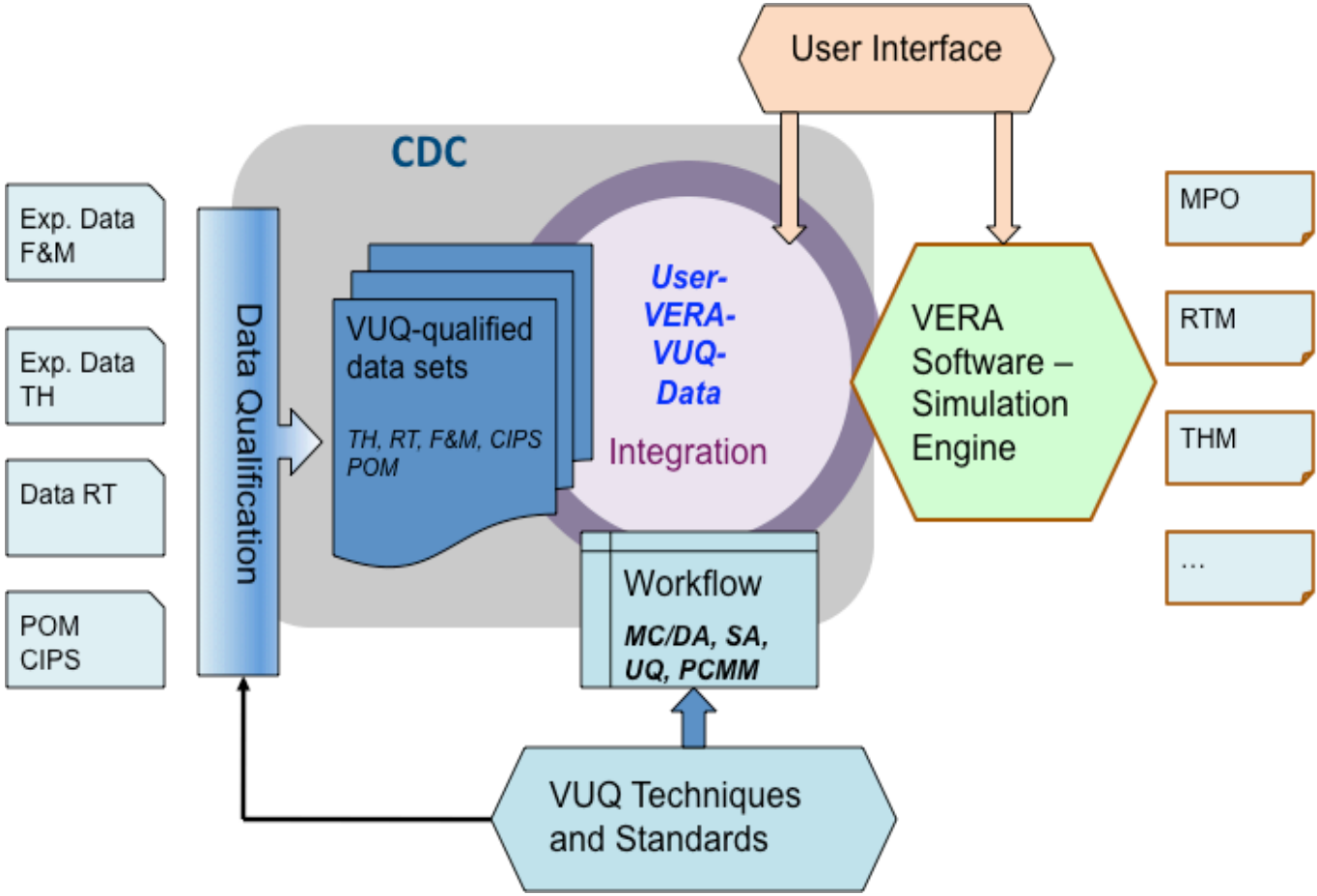
Data Sources

		Relevance	Scaling	Uncertainty
PMO	International Fuel Performance Experiments IPFE Recommendation: Low-to-medium priority	CRUD: 2 GTRF:2 PCI: 3	CRUD: 1 GTRF:1 PCI: 3	CRUD: 0 GTRF:0 PCI: 2
PMO	Data collected from operational plants Recommendation: High priority	CRUD: 4 GTRF: TBI	CRUD: 4 GTRF: TBI	CRUD: 0-2 GTRF:0-1
In-pile IET	Studsvik Cladding Integrity Project SCIP Recommendation: High priority	CRUD: 2 GTRF:3 PCI: 4	CRUD: 2 GTRF:2 PCI: 4	CRUD: 0 GTRF:0 PCI: 2
In-Pile IET	Halden Reactor Project Axial Offset Anomaly AOA Tests Recommendation: High priority	CRUD: 3 PCI: 2	CRUD: 2 PCI: 1	CRUD: 2 PCI: 1
Out-of-pile IET	Westinghouse Advanced Loop Tester WALT Recommendation: High priority	CRUD: 4 DNB: 3	CRUD: 2 DNB: 3	CRUD: 3 DNB: 1
Out-of-pile IET	New Experimental Studies of Thermal-Hydraulics of Rod Bundles NESTOR Recommendation: High priority	CRUD: 3 DNB: 3	CRUD: 2 DNB: 2	CRUD: 3 DNB: TBD
SET	Rod Bundle Heat Transfer RBHT : PSBT /BFBT (for PWR focus in Phase 1) Recommendation: High priority PSBT	CRUD: 3/1 GTRF:3/1 DNB: 4/1	CRUD: 3/2 GTRF:3/2 DNB: 3/2	CRUD: 3/3 GTRF:3/3 DNB: 3/3
SET	Subcooled flow boiling SFB: covering a range of SETs on participating phenomena (over 20 data sets) Recommendation: New, well-controlled, VUQ-grade SETs on SFB	CRD/GTRF/ DNB: range [2-4]	1 (low pressure) 3 (high P tests)	In range [1-2]
SET	Vibration Investigation of Small-scale Test Assemblies VISTA Fuel Assembly Compatibility Test System FACTS	GTRF: 4	GTRF: 4	GTRF: TBD

CASL Validation Data: An Initial Review, 2011

CASL Data Center – CDC

- The CDC functions include
  - (i) Validation data inventory and warehouse;
  - (ii) VUQ-guided data qualification, and
  - (iii) Data processing for interface with users' data operation, with VERA codes and with VUQ workflow, including data assimilation.



- Collaboration
  - VUQ
  - NE-KAMS
  - VOCC
  - AMA/VRI/…

CASL Data Center

- The three main components of the CDC will be
  - NE-KAMS – CASL Validation Data Management System (CVDMS)
  - VUQ – CASL VUQ methods, processes and workflows
  - VOCC – CASL data management / utilization infrastructure & collaboration and support services

- CDC will be an advanced information and data management framework to support M&S-V&V-UQ activities.
  - Support for validation data that are highly heterogeneous in their type, quality and origin
  - Provisions for identifying, collecting, documenting, processing, formatting, archiving, accessing and utilizing CASL validation data, both proprietary and public.
    - Relational databases and semantic storage systems
  - Provisions for CASL validation data qualification and classification
  - Offer software tools and utilities for V&V and UQ activity planning and implementation
  - Tight integration of CASL data assimilation methods to CVDMS
  - Tight integration of the VERA-BL and VERA-AC codes to the CVDMS

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Summary

- CASL Validation Data strategy is to be realized through design, implementation, demonstration, and operation of a CASL Data Center (CDC) that provides VERA developers, researchers and users with an effective support on validation data management and usage.

- The CDC functions include
  - (i) validation data inventory and warehouse;
  - (ii) VUQ-guided data qualification, and
  - (iii) data processing for interface with users' data operation, with VERA codes and with VUQ workflow, including data assimilation.
- Secure protection and access control (according to TCP protocols), partners-agreed policy for CDC sustainable operation will be in place and ensured from the get-go

- The CDC will be hosted, controlled and enabled by VOCC infrastructure.
- A CDC initial implementation will focus on basic functionality of (i)-(iii) above to demonstrate CDC operation in a high-priority development (*e.g.,* subcooled boiling, crud).

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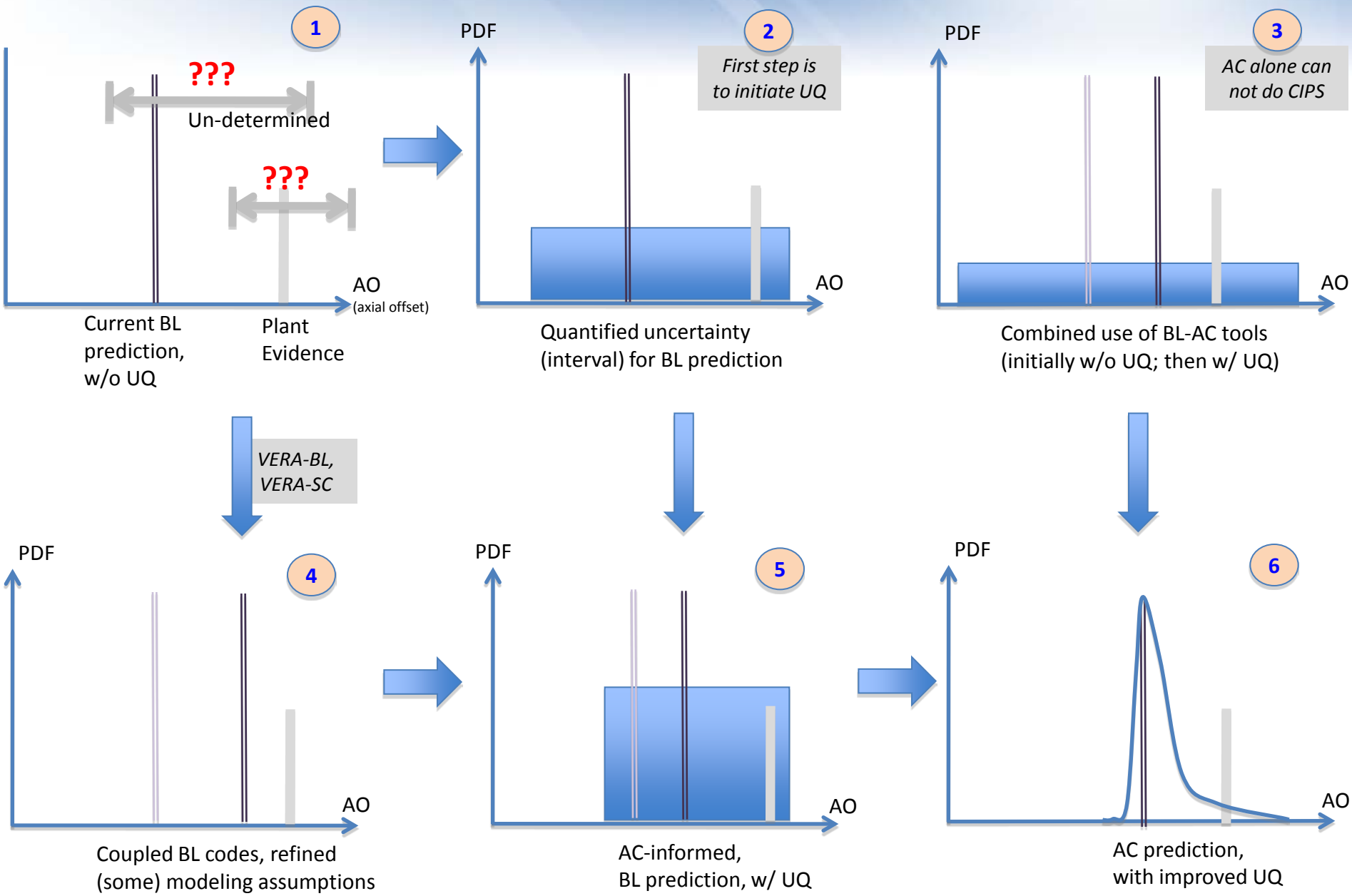
Back-up Slides

Interactions of Models and Uncertainties

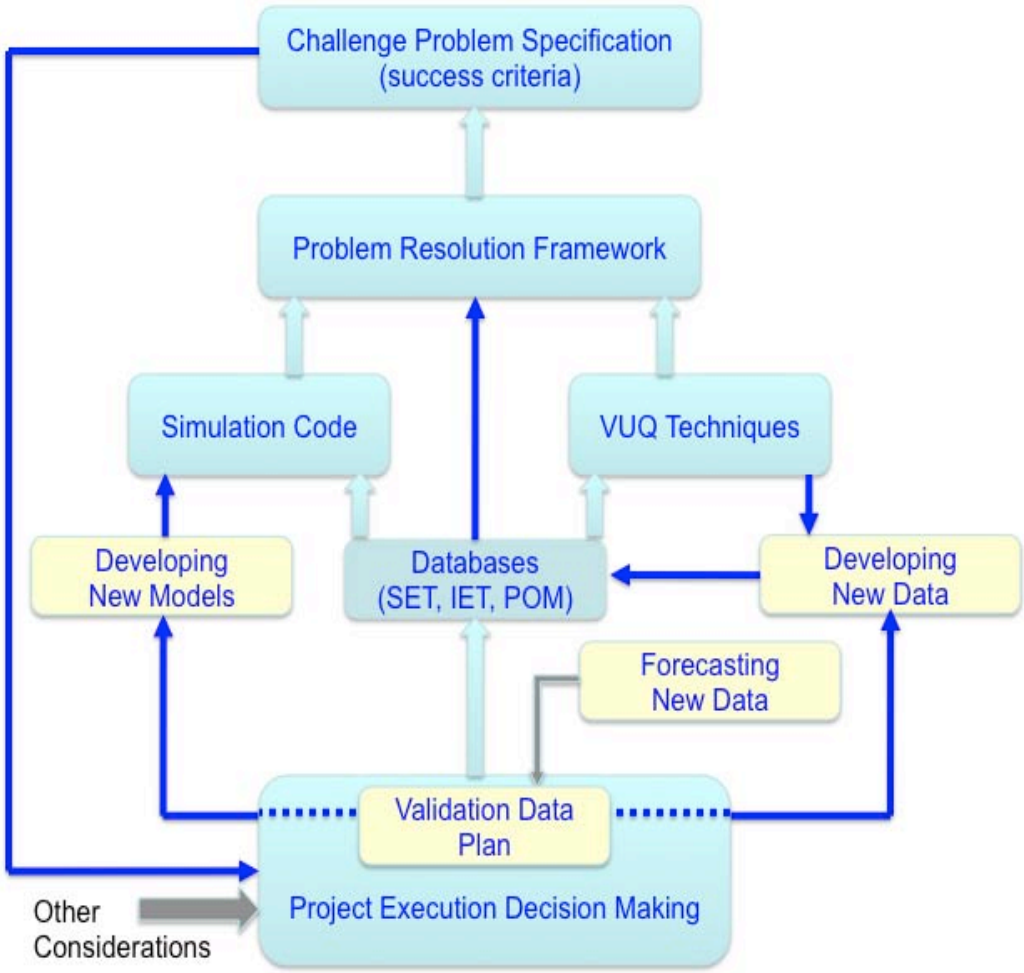


Trends & Challenges in Validation Data Support

- Mega-Trend: Quantitative Assessment of Calculations = UQ
- Higher fidelity modeling (physics detail)
  - Substantially increases the number of models and model parameters.
  - Requires advanced experimentation (e.g., isolating individual mechanisms that govern CRUD formation) under conditions of relevance.
- Higher resolution (temporal and spatial detail)
  - Requires advanced high-resolution diagnostics (typically, generating huge amount of data)
- Tight multi-physics coupling
  - Requires multi-physics system testing (often in-pile / research reactor testing, or actual plant's events)
- Coupling of models of different fidelity (in system simulation).
  - Requires integral experiments to test the coupling
- Multi-scale integration, *e.g*. "gap-tooth" scheme
  - Requires experiments with "multi-scale" diagnostics to obtain data for testing "conditioning" (from coarse-to-fine-scale) and "homogenization" (using fine-scale simulation to inform coarse-grain model parameters).

Validation Data Plan

- A practical validation data strategy that supports CASL's goal in applying modern V&V-UQ methods for assessing VERA predictive capability for the Challenge Problems
- Guide and enable the implementation of the CASL validation data strategy



- ❑ Knowledge of the modern view and capability in VUQ
- ❑ Knowledge of physical processes that govern the CIPS
- ❑ Knowledge of codes, models, and data available, used, potentially use accessible, and/or being developed in CASL

CASL Validation Data Strategy

- For CASL near- and medium terms, the validation data task is directed to support pragmatic decision-making in ***developmental assessment*** of CASL products during the VERA-AC's formative phase (… as opposed to a pursuit of validation of solidified products)

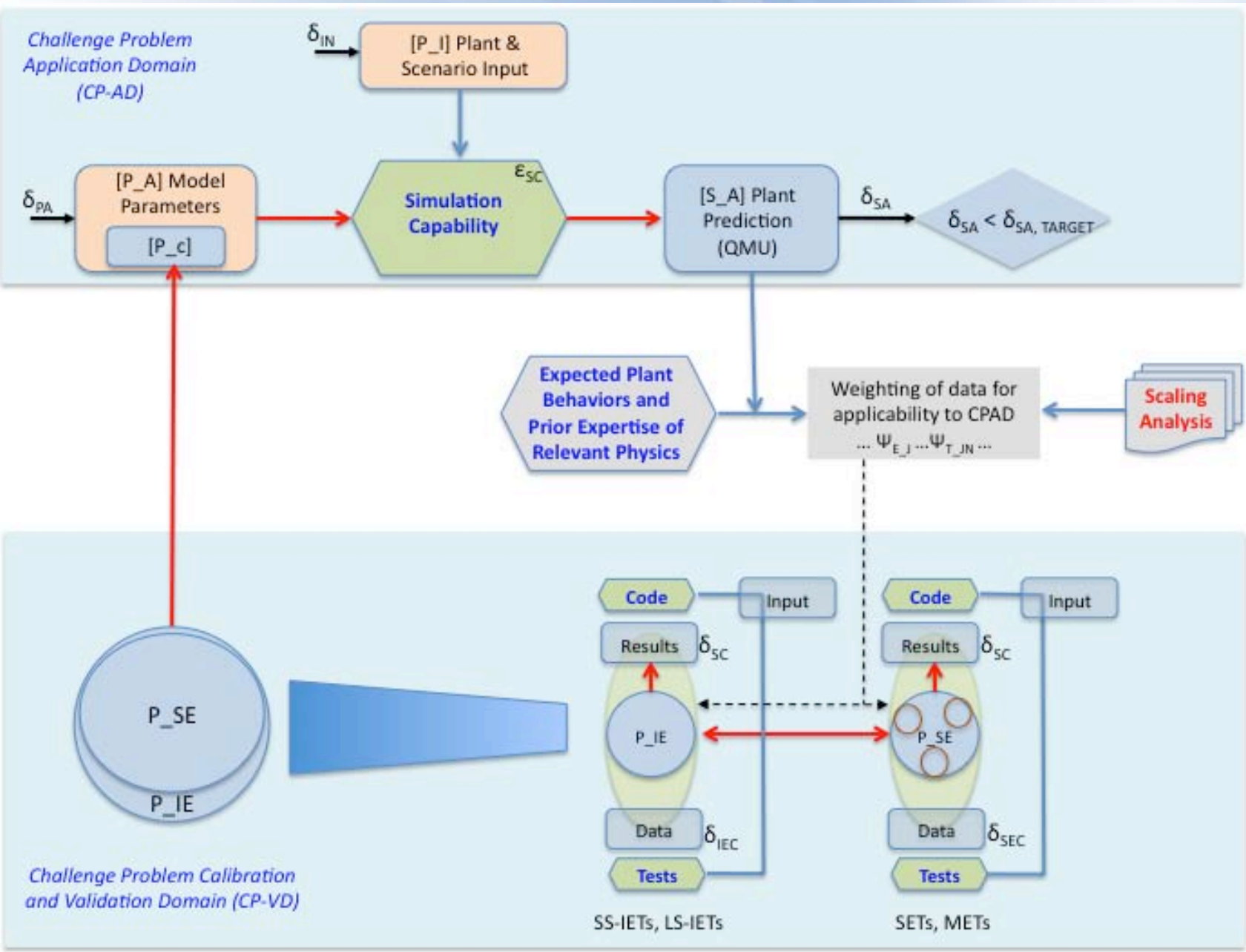
- ***"Data realism"*** (… as opposed to "data idealism"). The provision is that by using advanced data strategies and VUQ tools paramount information value can be extracted from community's knowledge base, including past experiments and legacy codes

- The **Validation Data Plan** that supports a structured, ***Bayesian inference framework for "total" data assimilation*** strategy that exploits the "the whole is much more the sum of parts" principle to enable multi-physics, multi-scale validation pyramid.

- Instrumental for VERA performance, data support is an organic part of the VERA capability and most effective when VERA software seamlessly integrates validation databases; ***CASL Data Center (CDC)*** is instrumental in implementing this position.

- Validation data support is a community-scale effort across and beyond CASL and DOE-NE Programs. The provision is that future VERA users greatly benefit from a systematic, collective and continually growing knowledge base and databases.

Bayesian Framework for Data Assimilation



NE-KAMS

- Multi-faceted KM resource supporting V&V and UQ of M&S for nuclear reactor design, analysis and licensing
- The primary goals of the NE-KAMS effort are to
  - Establish a comprehensive and web-accessible knowledge base to provide V&V and UQ expertise and resources for establishing confidence in the use of M&S for nuclear reactor design, analysis and licensing
  - Develop and implement standards, requirements and best practices for V&V and UQ that enable scientists and engineers to assess the quality of their M&S
  - Serve as an important resource for technical exchange and collaboration, enabling credible computational models and simulations for nuclear energy applications

NE-KAMS (Continued)

- Additional goals of NE-KAMS are to
  - Position DOE-NE programs to share the costs associated with development and application of M&S
  - Capture and preserve the V&V, UQ and M&S knowledge and data of the DOE-NE R&D programs
  - Provide value-added tools and utilities, leveraging the ability to share knowledge, to educate young scientists and engineers in government, industry and academia
- Being developed in partnership with INL, Bettis, and ORNL
- Collaborations and consultations with NRC, SNL, ANL, Utah State University, AREVA, Westinghouse, Enercon

NE-KAMS Status

- Developed NE-KAMS Five-Year Strategic Plan
- Developed High-Level Requirements for NE-KAMS
- Developed NE-KAMS V&V Data Standards and Requirements
- NE-KAMS demonstration in-progress, due in September 2012
  - Initial review and quality evaluation of CFD validation experimental datasets in progress
  - Designed initial database schema for CFD validation experimental datasets
  - Developed initial database metadata and documentation schema
  - Worked with ANL to obtain a subset of ANL MAX validation dataset for use in the NEAMS Pathways demonstration
  - Identified and secured hardware and software (ensuring low development costs) for the NE-KAMS database

Comments on Intrusive UQ for Thermal-Hydraulics

John Shadid, THM, SNL

THM: E. Cyr, R. Pawlowski, J. Shadid, T. Smith, P. Weber (SNL);

VUQ: T. Wildey (SNL);

VRI: R. Pawlowski (SNL);

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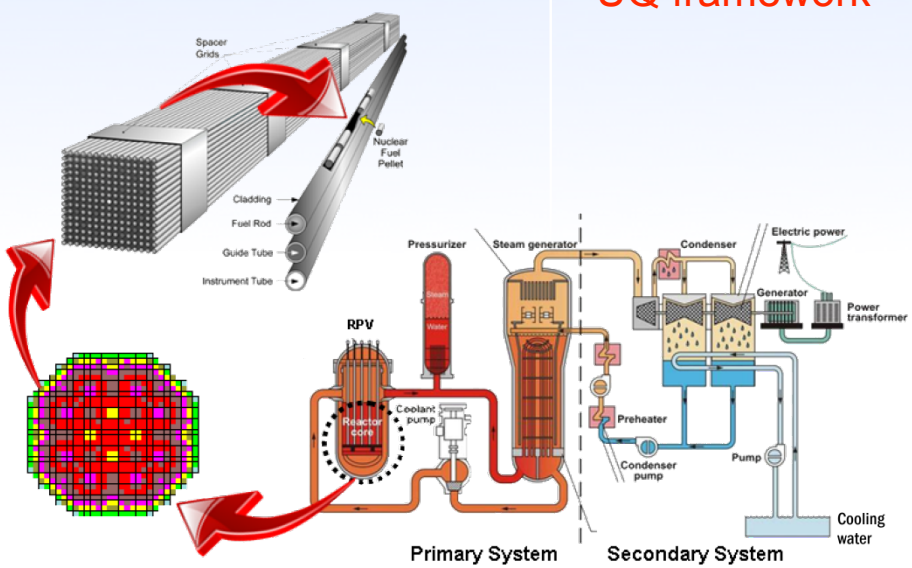
CASL vision: Create a virtual reactor (VR) for predictive simulation of LWRs

Drekar::CFD intended to contribute to VERA CFD in the areas indicated below.
UQ collaborative with VUQ; Coupling to VERA with VRI;

Leverage	Develop	Deliver
• Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications • Existing systems and safety analysis simulation tools	• New requirements-driven physical models • Efficient, tightly-coupled multi-scale/multi-physics algorithms and software with quantifiable accuracy • Improved systems and safety analysis tools • UQ framework	• Toolkit for predictive simulation of physical nuclear reactors • Architected for platform portability ranging from desktops to DOE's leadership-class and advanced architecture systems (large user base) • Validation basis against 60% of existing U.S. reactor fleet (PWRs), using data from TVA reactors • Base M&S LWR capability



Drekar::CFD Milestone Linkages (next 6 months!)

- L3:VUQ.VVDA.P4.03
  - Title: Advanced GTRF Verification
  - VUQ Milestone (Original due date: April 30, 2012, Expected delivery date: July 31,2012)
- L3:VRI.VERA.P5.02
  - Title: Go / no go decision on component release
  - VRI Milestone (Original due date: June 6, 2012, Expected delivery date: June 6, 2012)
- L3: THM.CFD.P5.01
  - Title: Demonstrate steady-state RANS and transient URANS solution to the THM CFD test cases #1 and #2 with Drekar
  - THM Milestone (Original due date: June 29, 2012, Expected delivery date: June 29, 2012)
- L3:VUQ.SAUQ.P5.02:
  - Title: UQ Algorithms for model-form uncertainty demonstrated for CIPS
  - VUQ Milestone (Original due date: June 30, 2012, Expected delivery date: June 30, 2012)
- L2:VRI.P5.03:
  - Title: VERA Snapshot 2.2
  - VRI Milestone (Original due date: Sept. 19, 2012, Expected delivery date: Sept. 19, 2012)
- L3:VRI.PSS.P5.07:
  - Title: DataTransferKit-based neutronics-TH coupling
  - VRI Milestone (Original due date: Aug. 29, 2012, Expected delivery date: Aug. 29, 2012)
- L3: THM.CFD.P5.02
  - Title: Complete an initial steady-state RANS validation study of the THM CFD test cases #1 and #2 with Drekar
  - THM Milestone (Original due date: Sept. 29, 2012, Expected delivery date: Sept. 29, 2012)
- L3:VUQ.VVDA.P5.05
  - Title: Parallel mesh refinement using Percept.
  - VUQ Milestone (Original due date: Sept. 30, 2012, Expected delivery date: Sept. 30, 2012)
- L3:VUQ.SAUQ.P5.05
  - Title: Initial Drekar Adjoint Development for Enabling New VUQ Capabilities
  - VUQ Milestone (Original due date: Sept. 30, 2012, Expected delivery date: Sept. 30, 2012)

Drekar::CFD critical aspect of future THM, VRI, VUQ Milestones

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Intrusive UQ Tools

- **Intrusive Stochastic Galerkin Expansions (SGE)**

  Possible Advantages

  - Under some assumptions embedded stochastic Galerkin methods can have an order of magnitude less unknowns then Smolyak sparse grids [Xiu and Hesthaven, SISC, 2005]
  - Embedded UQ allows exploration of advanced methods that require fine grain control of stochastic discretizations (see for example adaptive spatially varying UQ) that can result in massive decreases in total unknown count
  - Semi-Implicit linearizations and careful construction of preconditioners could be exploited to reduce the total cost of embedded UQ methods for nonlinear problems to better match the linear case and stochastic collocation [Le Maitre, Knio, Najm and Ghanem, J. Comp. Phys., 2001] and [Powell and Silvester, University of Manchester TR, 2012]
  - High density computations for embedded techniques can better exploit next-generation hardware (high concurrency nodes)
  - Drekar structure supports embedded stochastic Galerkin methods in addition to stochastic collocation (e.g. Dakota)

- **Adjoints**

  Possible Advantages

  - Produce Error estimates and sensitivities in specific scientific quantities of interest (QoIs).
  - Provides a means to identify error contributions from various components (spatial, temporal, quadrature, etc.): avoid over-solving the problem.
  - Well known to be advantageous when ratio of input parameters to output QoIs is large.
  - Couple with emerging black-box methods to efficiently build surrogate models and sample more efficiently. Focus effort where things are changing. Increase convergence rate and reduce function evaluations. (e.g. Dakota)
  - Can integrate with continuation methods for efficient sensitivity analysis along solution branches.
  - Adjoint methods can be used to study propagation of error in both strongly coupled (e.g. Drekar) and in loosely coupled solution methods (e.g. Loose coupling as in LIME coupling of Denova – Drekar [ASCR – Phipps et. al.], some work on operator splitting [ASCR - Estep et. al.])

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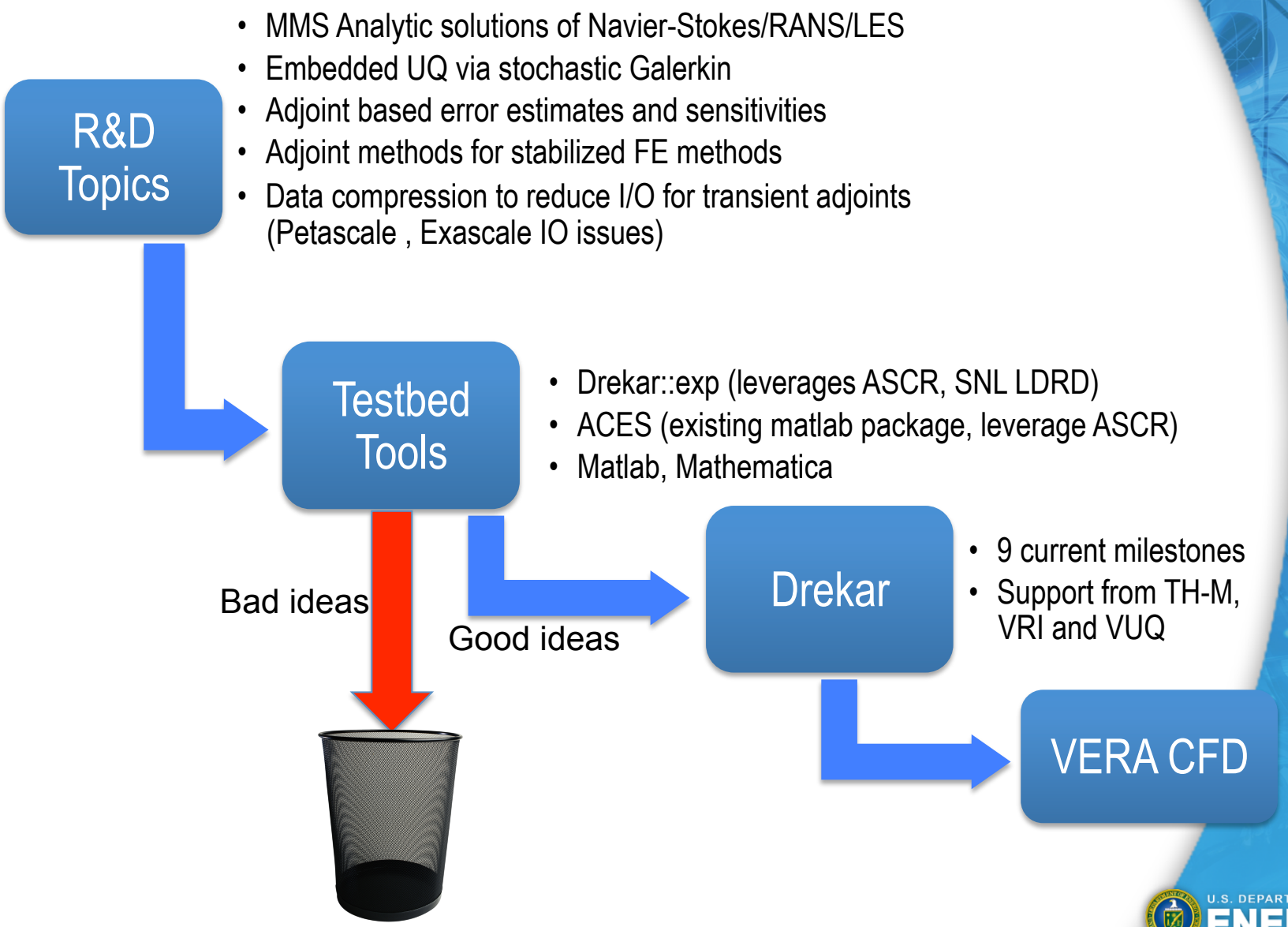
Overview of Recent Embedded UQ in Drekar



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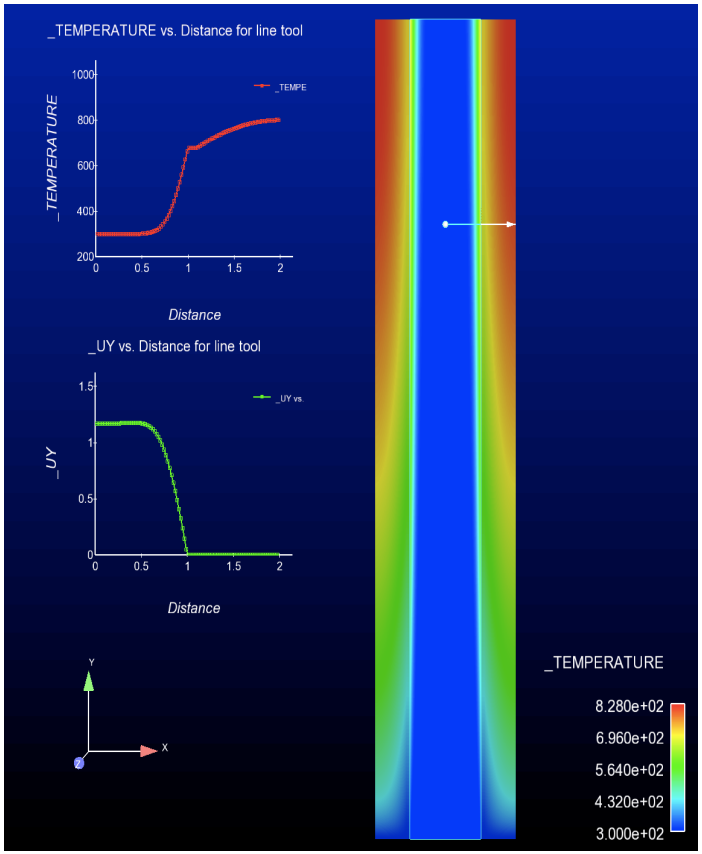
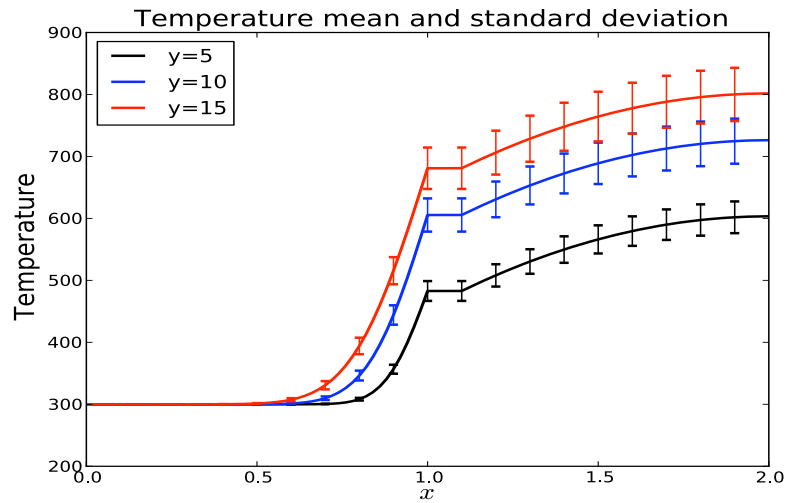
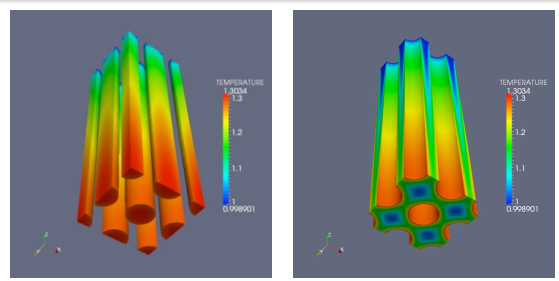
Leveraging of UQ tools underway (SGE) [from SNL LDRD and ASCR adjoint effort]



Idealized steady-state flow and heat transfer simulation. Conjugate heat transfer in cooling fluid, clad, and Fuel. Navier-Stokes Re = 1000

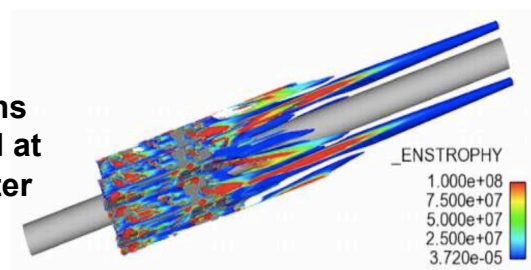


Stochastic Galerkin UQ analysis propagating uncertainty in the magnitude of the fuel source term and the inflow velocity.



Steady Temperature in solid (left) and fluid (right) in Drekar::CFD CHT simulation

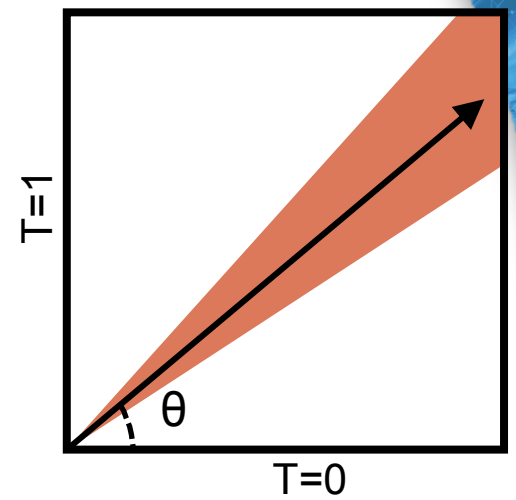
Enstrophy for a steady state RANS(SA) flow simulation; Demonstrated SS solutions for 1M, 3M, 6M; Integrated at up to CFL ~1e+4. Parameter continuation possible as well.



Demo Adaptive SGE: 2D Convection-Diffusion with a Boundary Layer (leveraging SNL LDRD)

Problem setup

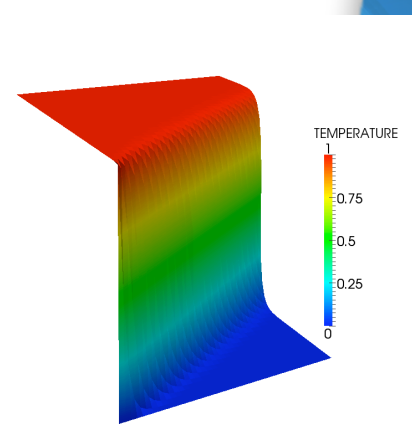
- Convection-Diffusion on unit square
- Strong Convection: Peclet Number=10^7
- Angle varies stochastically: $\mathcal{N}(40, 4)$
- Using SUPG stabilization



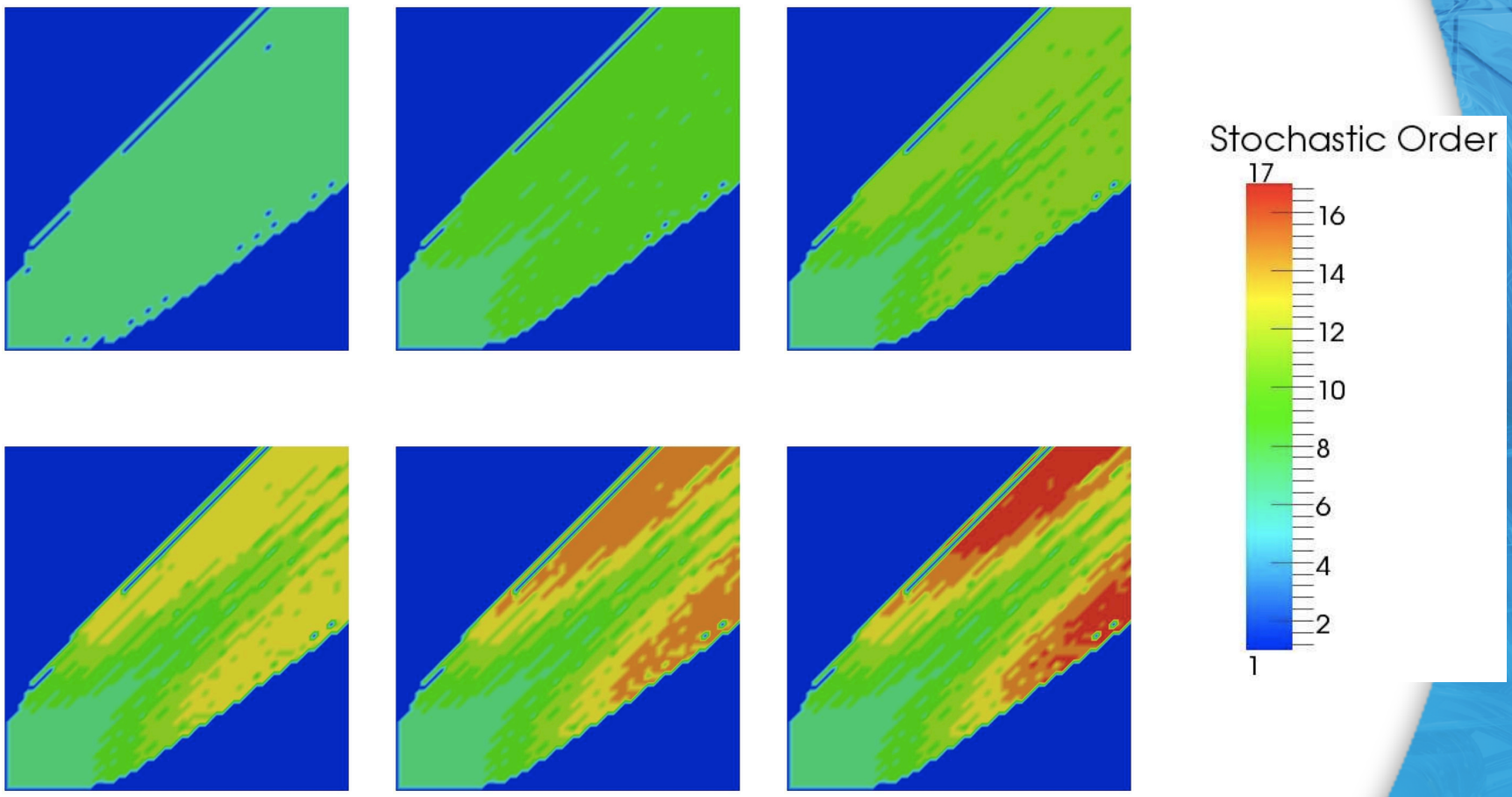
Deterministic Solution: θ=40

Compare uniform to adaptive refinement in UQ space

- Reference is 20th order uniform stochastic Galerkin
- Start from 2 term stochastic expansion
- Response quantities: Spatial average



2D Convection-Diffusion: Stochastic Order



Take Home: Refinement focuses high order where needed

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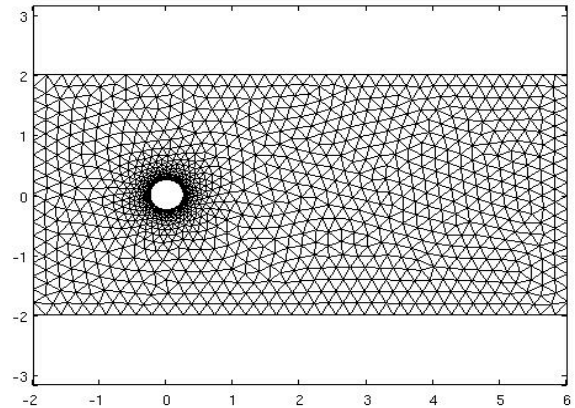
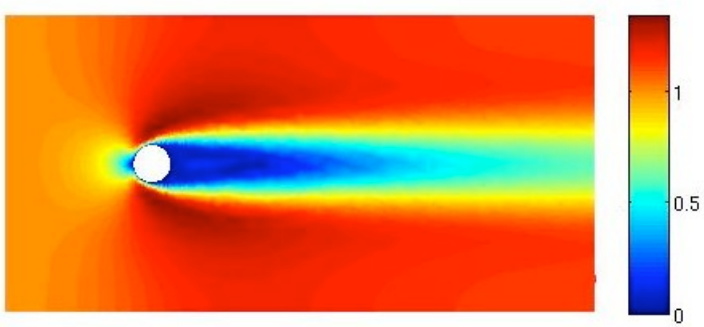
Example: Steady-state flow past a cylinder (Re = 50)
Forward solution

Forward prb.: Stabilized FE P1/P1
Adjoint prb.: P2/P2

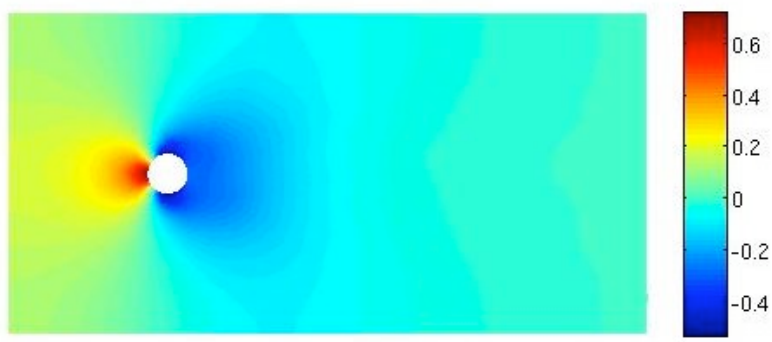
QoIs: 1) Average error in Vx
2) Error in Vx at point in wake
3) Average error in pressure



Error estimate compared with reference solution:
Higher-Order Taylor-Hood P3/P2

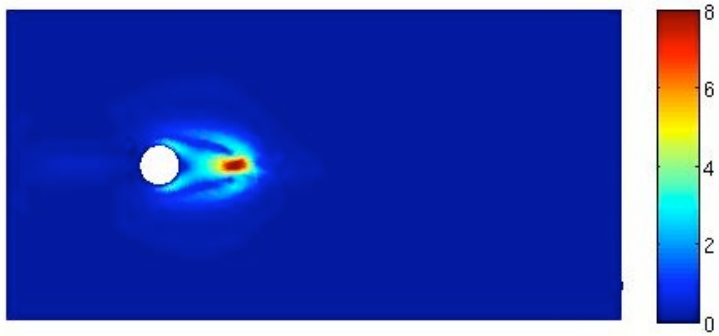


Magnitude of Velocity
(forward problem)

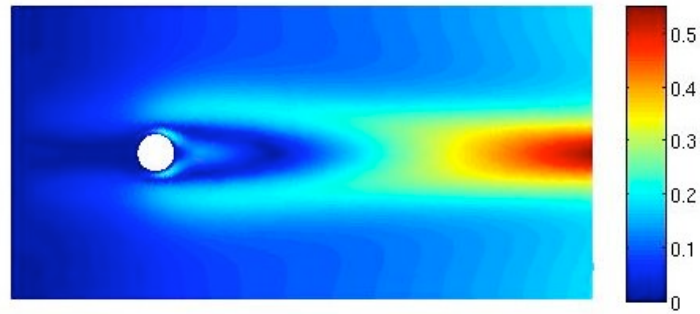


Magnitude of pressure
(forward problem)

Example: Steady-state flow past a cylinder (Re = 50) Adjoint solution



Magnitude of adjoint Velocity for QoI-2 (error in pt value of Vx in wake)



Magnitude of adjoint Velocity for QoI- 3 (average error in pressure)

ν	QofI	True Error	Eff-AofStab	Eff-AofStabC	Eff-StabofA
1E-1	1	1.48E-4	0.86	0.95	1.00
5E-2	1	-3.50E-4	0.97	1.12	1.00
1E-2	1	-6.88E-4	0.91	1.13	1.00
1E-1	2	-7.43E-3	0.98	0.99	1.04
5E-2	2	-2.25E-2	0.95	1.07	1.02
1E-2	2	-2.52E-2	0.93	1.07	1.11
1E-1	3	-1.08E-3	0.98	0.98	1.04
5E-2	3	-2.63E-3	0.96	0.96	1.01
1E-2	3	-5.68E-3	0.91	0.91	0.95

TABLE 4.5

Effectivity ratios for each of the three quantities of interest using the three adjoint approaches for various values of ν using SUPG-PSPG-LSIC stabilization.

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Verification of a Posteriori Error Estimates Using Analytic transient Multi-mode Forced Solution to N-S

Navier-Stokes Equations:

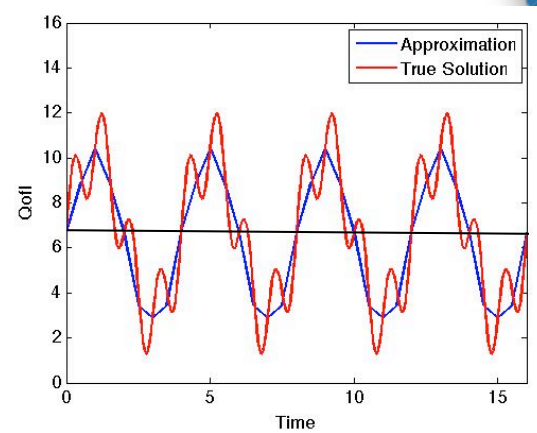
$$\rho \frac{\partial \boldsymbol{u}}{\partial t} - \nu \Delta \boldsymbol{u} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = f(\boldsymbol{x}, t),$$

$$\nabla \cdot \boldsymbol{u} = 0.$$

Taylor Hood (P2-P1) in space
Backward Euler in time

QofI is the value of the x-component of the velocity at $(0.5, 0.4)$.

We are interested in the time average of the QofI.



True – analytic Fn.

Approx. - FE solution on finite resolution spatial mesh and temporal under-sampling below Nyquist sample rate.

Exact time averaged value of QoI: 6.41
Exact error for FE computation of QoI: 3.24%

Verification of a Posteriori Error Estimates Using Analytic Solution

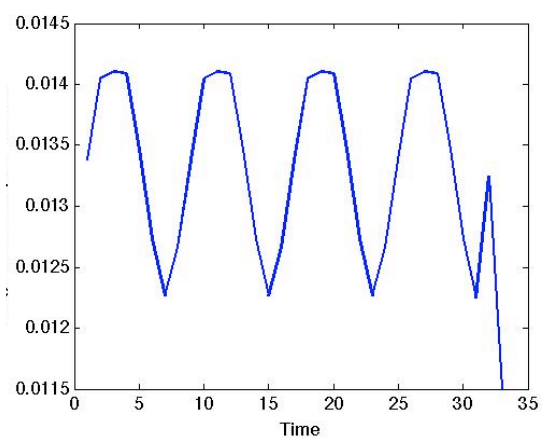
We solve the adjoint problem,

$$-\rho\frac{\partial\phi}{\partial t} - \nu\Delta\phi - \rho\boldsymbol{u}\cdot\nabla\phi - \rho\phi\cdot\nabla\boldsymbol{u} - \nabla z = \psi(\boldsymbol{x},t),$$

$$-\nabla\cdot\phi = 0.$$

where $\psi(\boldsymbol{x},t)$ is chosen based on the QofI.
The *linear* adjoint problem is solved using higher order Taylor Hood (P3-P2) in space and second order DG in time.

Estimated error in time averaged QofI: 0.206 (3.11%)



Magnitude of the adjoint velocity

$$\text{Effectivity} = \frac{\text{estimate}}{\text{truth}} \approx 0.96$$

Many successful applications of adjoints:
E.g. Estep, Rannacher, Oden, Suli,
Barth, Bangerth, ..

Issues Using Adjoints for Time-dependent Nonlinear Problems

- Original PDE is solved forward in time:

$$\frac{\partial u}{\partial t} + F(u) = 0, \quad 0 < t \leq T, \quad u(0) = u_0.$$

- Adjoint PDE is solved backwards in time:

$$-\frac{\partial \phi}{\partial t} + F'(u)^* \phi = \psi, \quad T > t \geq 0, \quad \phi(T) = 0.$$

- Requires significant I/O to retrieve forward solution for backward time integration and residual calculation.
- Check-pointing is often used to mitigate these difficulties.
  - ✦ Greatly reduces storage requirements by storing the forward solution at only a few points.
  - ✦ Provides the same error estimate / sensitivities as if the full forward solution were stored.
  - – Requires the re-solution of the forward problem over each subintervals (2x the work).
  - – May require additional storage if high-order BDF time integration methods are used.
  - – The choice of optimal check points/windows may be difficult.
- We consider alternative approaches based on compression of the forward solution to be used as linearization point.

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Question: Can adjoints be made efficient for highly transient / nonlinear problems?

Some reasons we believe this is likely possible

- **For nonlinear problems adjoints are already non-unique and approximate**
  - *Linearized about discrete solution routinely (numerical evidence this works)*
  - *Try alternate linearizations for backward-in-time adjoint about a reduced representation of the forward dynamics that captures important modes and attenuates high frequency spectrum (our initial ideas – use time-averaged forward problem, use ROM, data compression/reconstruction ideas,?)*
- **Specific nature of CASL TH-M problems**
  - *High frequency spatial/temporal fluctuations have limited effect on dynamics (mostly dissipative).*
  - *A large number of QoIs for performance modeling of reactor cores/sub-assemblies, are time-averaged quantities, low-frequency and macro-scale. These types of QoIs might not have significant sensitivity to high frequency modes.*
  - *Fluid turbulence has dominantly a cascade of length-scales from large to small. Effects of small sales are mostly dissipative and a reverse cascade not common. Implication is that propagation of error and stability of QoIs not sensitive to details of small scales.*

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Adjoints for Time Averaged Quantities of Interest
Define a steady adjoint and linearize about time-average.

- **Relatively new approach based on**

  Duality based a posteriori error estimation for quasi-periodic solutions using time averages. M. Braack, E. Burman, N. Taschenberger. SIAM J. Sci. Comp. 33 (2011), pp. 2199-2216.

- **To make a short story brief…**
  - Given a space-time variational formulation

$$\int_0^T (u_t, v)\ dt + \int_0^T A(u,v)\ dt = \int_0^T (f,v)\ dt.$$

  - Define the time-averages

$$\overline{u} = \frac{1}{T}\int_0^T u\ dt, \qquad \overline{A}(u,v) = \frac{1}{T}\int_0^T A(u,v)\ dt$$

  - Define a **stationary adjoint problem**,

$$A'(\overline{u_h})(v,\phi) = J(v).$$

  - Derive an error representation for the error in a time-averaged quantity of interest:

$$J(\overline{u} - \overline{u}_h) = E_1 + E_2 + E_3$$

  - The first term is a standard dual-weighted residual and is fully computable.
  - The second term is due to fluctuations of the operator in time and is difficult to compute.
  - The last term depends on the error at the initial and final times, and is also difficult to compute, but goes to zero as T increases.

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Adjoints for Time Averaged Quantities of Interest

- **Test case 1: Linear heat equation with analytic solution**
  - Solution is oscillatory in time
  - Quantity of interest is the time-average of the temperature at (1/3,1/3).
  - Coefficients do not depend on time ➔ the second term in error representation is zero.

T	True Error	Error Estimate	Percent Error (est)	Effectivity
1	6.06E-4	4.67E-4	10.9%	0.77
2	6.19E-4	4.52E-4	10.5%	0.73
4	6.14E-4	4.48E-4	10.4%	0.73
8	6.21E-4	4.47E-4	10.4%	0.72

- **Test case 2: Navier Stokes with multiscale periodic analytic solution**
  - Error estimates and effectivities only include E1
  - Quantity of interest is the time-average of the x-vel in the center of the domain (T interval for time average)

T	True Error	Error Estimate	Percent Error (est)	Effectivity
2.5	2.62E-2	2.49E-2	0.28%	0.95
5.0	1.91E-2	2.26E-2	0.26%	1.18
12.5	2.46E-2	2.52E-2	0.28%	1.03
25.0	2.32E-2	2.48E-2	0.27%	1.07

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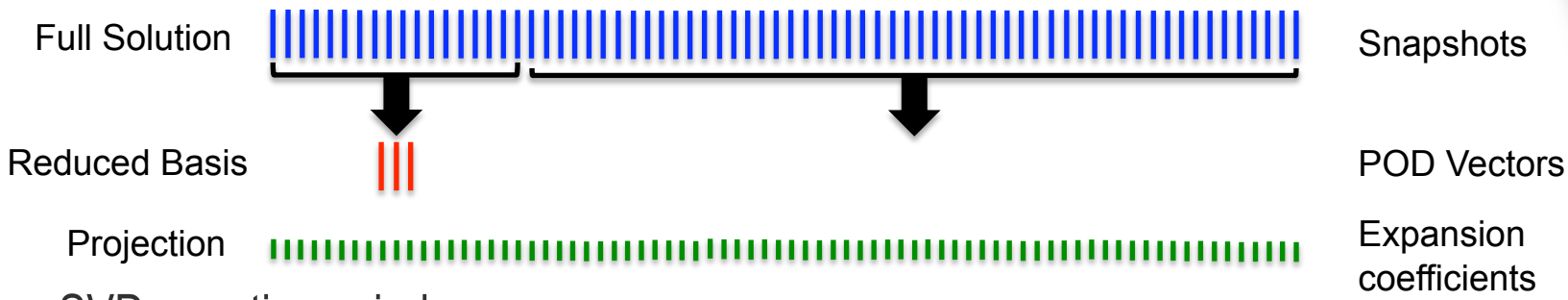
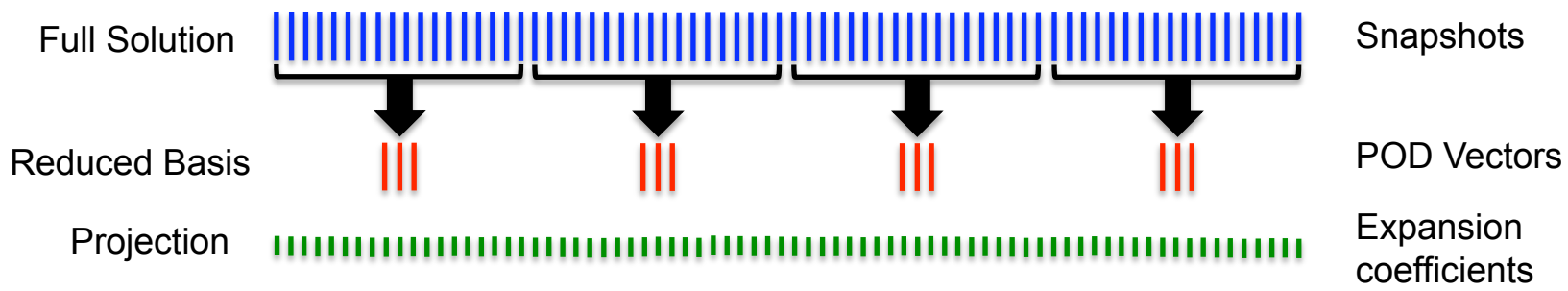
Strategies for Compression/Reconstruction of the Forward Solution Data

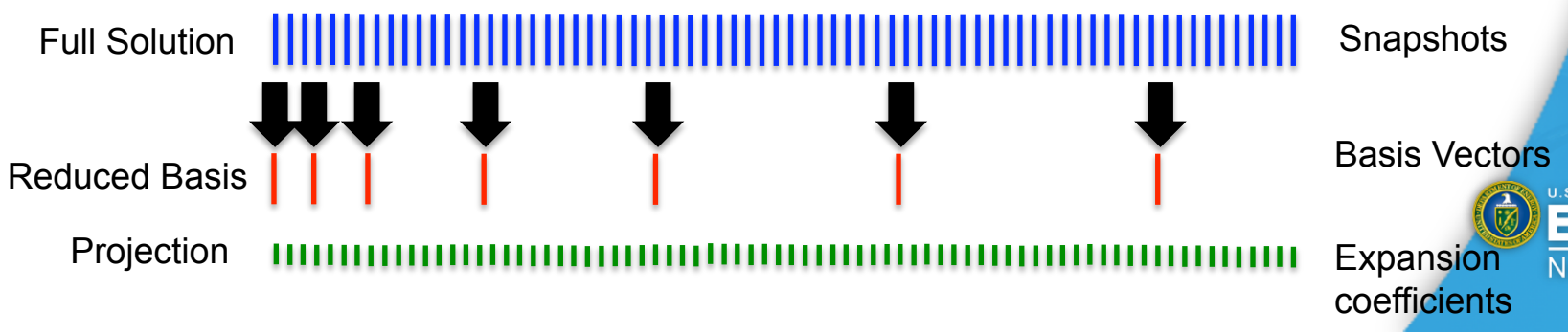
1. SVD over initial time window, then just projection



2. SVD over time-windows

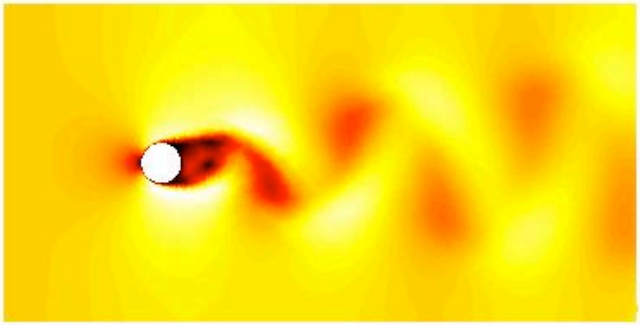


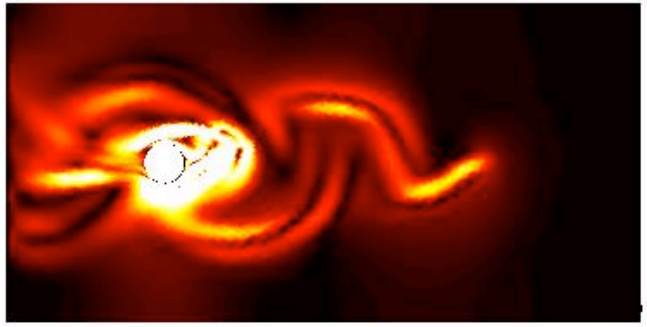
3. Gram-Schmidt orthogonalization (add basis vectors by user-defined norm and error criteria)



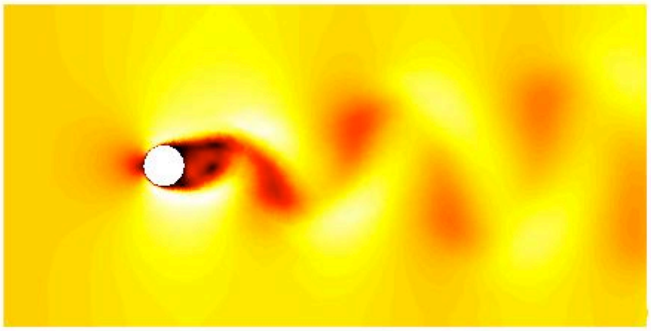
Von Karman Vortex Shedding

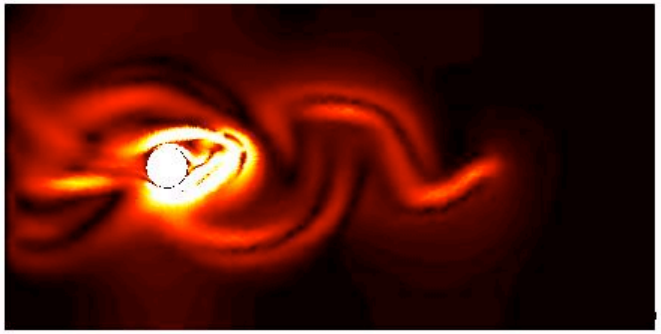
- Approximated using stabilized FEM and BDF time-stepping with Re = 500.
- Quantity of interest is the time-average of the x-vel at a point in the wake.
- Problem is restarted in periodic regime to reduce influence of initial condition.
- Full forward solution at t=T and corresponding adjoint at t=0:





- Compressed forward solution (5 basis vectors) at t=T and corresponding adjoint solution at t=0:





- The adjoint solution depends on the amount of compression.
- Too much compression may affect the a posteriori error estimate.

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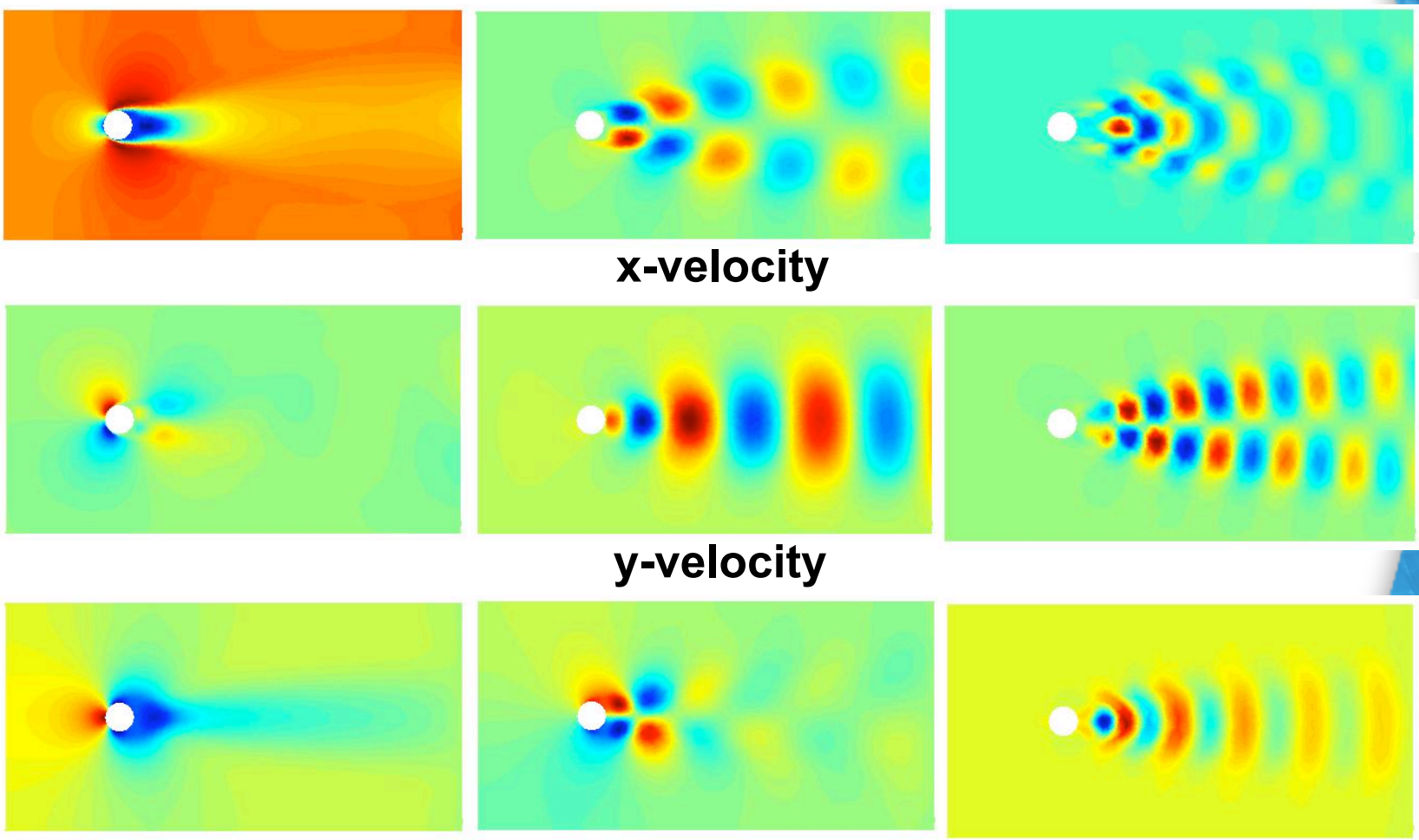
Von Karman Vortex Shedding: ROM Basis

- First, second and fifth basis vectors for the solution using SVD compression of the first 20 snapshots:



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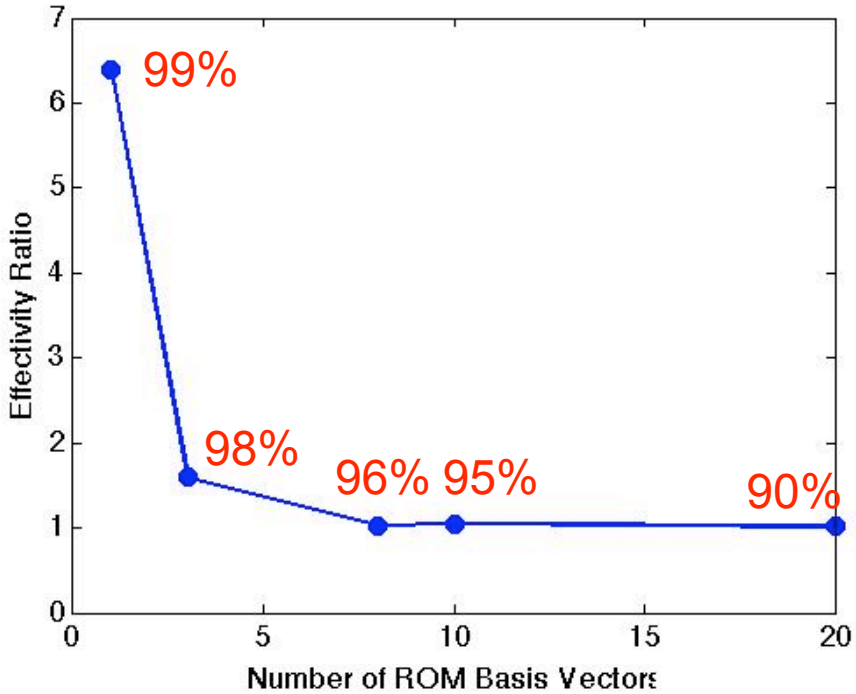
Von Karman Vortex Shedding

- The effectivity ratio (estimate/truth) converges to 1 as we increase the number of ROM basis vectors
- Percentages in red indicate amount of compression.



Increasing compression

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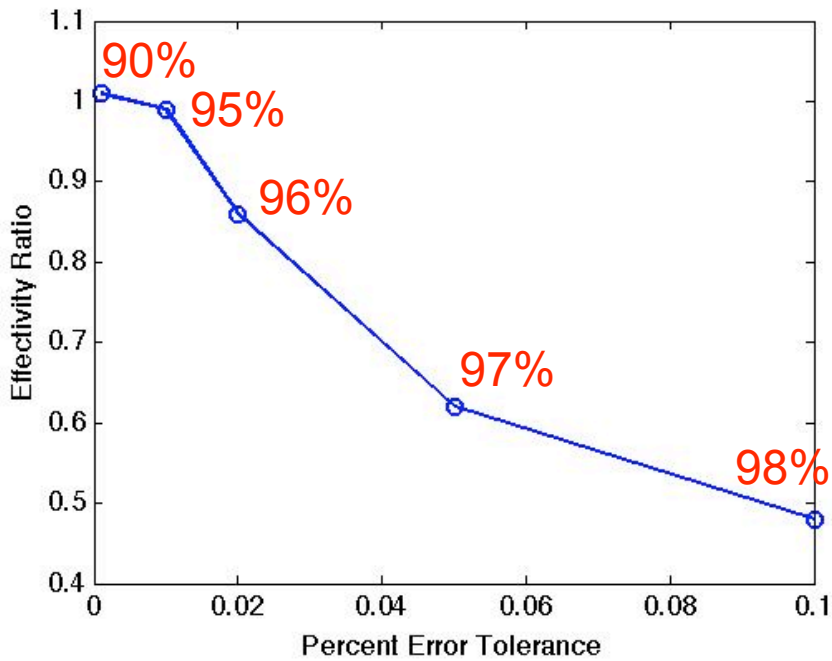
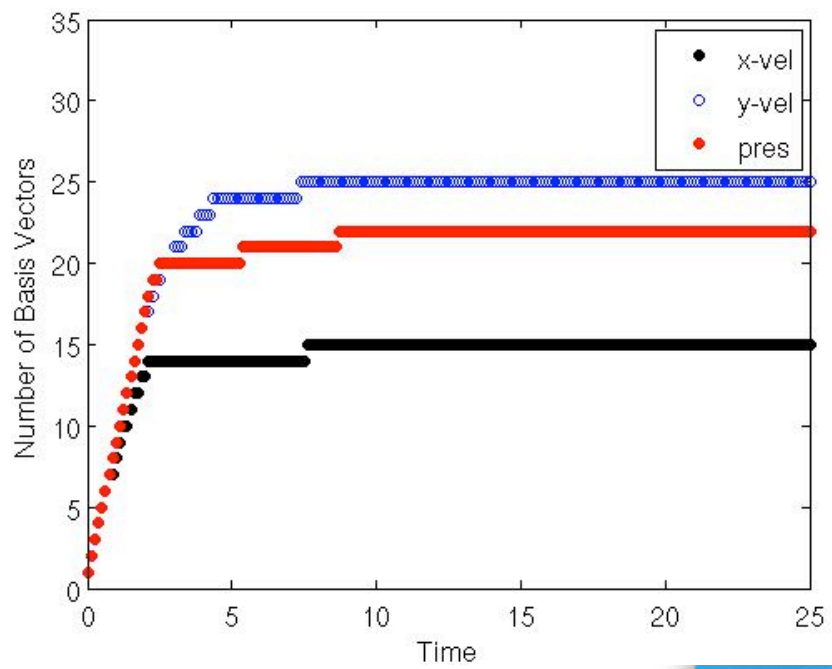
Von Karman Vortex Shedding

- The effectivity ratio (estimate/truth) converges to 1 as we decrease the tolerance criteria for adding a new basis vector with Gram-Schmidt.
- Percentages in red indicate amount of compression.



Increasing compression



Number of basis functions for each variable over time allowing 0.1% error

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Overview of Recent and Future Embedded UQ Development in Drekar

- This modest sized project is part of the Drekar::CFD CASL THM effort and is collaborative with VUQ. It also heavily leverages DOE ASCR and SNL LDRD.

- Development of analytical solutions for MMS verification [mathematica scripts with user defined profiles (u,v,w,P) generates sources; Also RANS – SA, k-e; LES- WALE]
- Application/demonstration of stochastic Galerkin for Navier-Stokes and conjugate heat transfer.
- Development of New approaches for variational adjoints of stabilized FE formulations.
- Evaluation of a steady-state adjoint approach for time-averaged QoI
- Application/demonstration adjoint capabilities for mixed integration and stabilized finite element formulations of convection-diffusion, Stokes and Navier-Stokes.
  [Note: FV methods have some associated analysis as mixed FE, DG - Estep, Barth]
- Adjoints using data compression/reconstruction of the forward solution to reduce I/O associated with solving backwards problem. (Petascale / Exascale issues)

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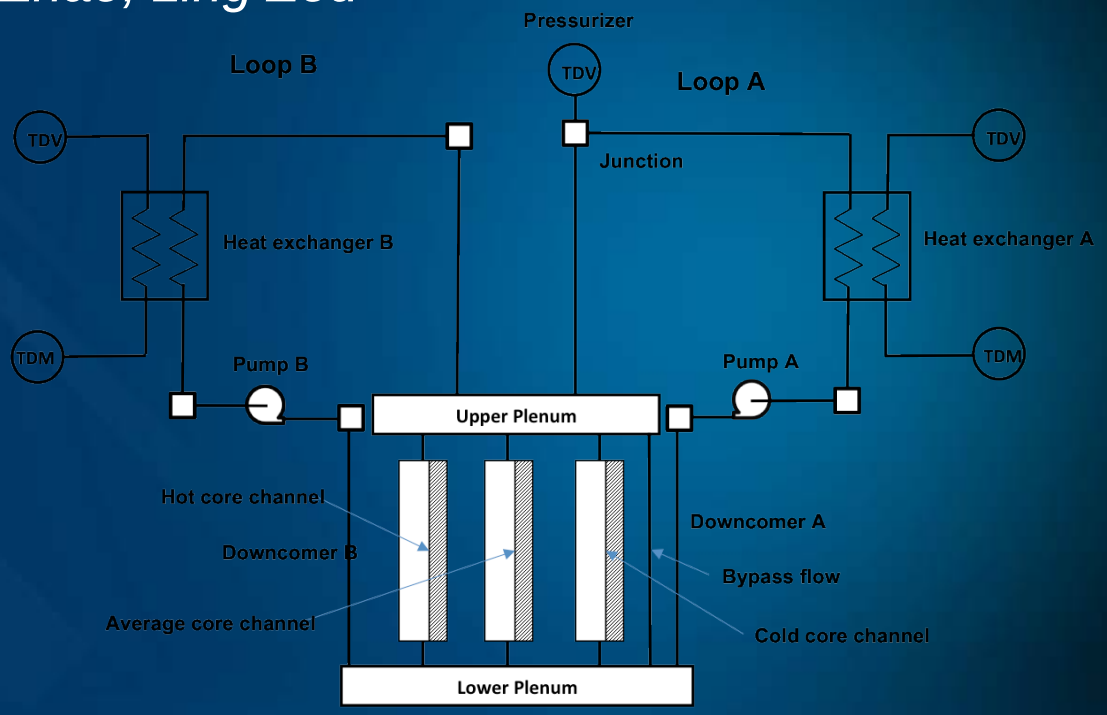
RELAP7: *The Next Generation Nuclear Reactor Systems/Safety Analysis Application*

Richard C. Martineau, David Andrs, Ray A. Berry, Derek Gaston, John Peterson, Hongbin Zhang, Haihua Zhao, Ling Zou



June 13, 2012

2012 CASL Roundtable Meeting

www.inl.gov

Idaho National Laboratory

RELAP7 Computational Team

Project Manager: Richard Martineau

Reactor Simulation Team: Haihua Zhao (PI), Ling Zou (developer) Hongbin Zhang (RELAP5 benchmarking, applications, neutronics), Paul Bayless (user requirement, validation and test)

Software Design Team: Derek Gaston (lead), David Andrs, John Peterson

Theory Team: Ray Berry (lead), Richard Martineau, Samet Kadioglu, Brandon M. Blackburn

Collaborators: EPRI (Steve Hess, Greg Swindlehurst, and Sherry Bernhoft), Argonne (Thomas Fanning and Rui Hu)

R7 is being re-factored into a MOOSE-based Application (RELAP7)

There were several considerations in this decision:

1. MOOSE allows faster development and delivery.
2. The ability to couple with other MOOSE-based physics applications, and codes from other DOE programs (such as NEAMS and CASL).
3. Restricting the focus of RELAP7 to systems analysis-type simulations.
4. Priority to retain and significantly extend RELAP5 capabilities.
5. To develop a flexible systems analysis capability for easier integration of industry requirements and RISMC needs.

What RELAP7 will be:

- A complete reactor safety/systems analysis application based upon the MOOSE development framework.
- The main reactor systems simulation toolkit of RISMC/LWRS.
- The next generation tool in the RELAP reactor safety/systems analysis application series (the replacement for RELAP5).
- Meet all NQA-1 requirements.
- The next generation reactor safety/systems analysis tool improving and extending RELAP5 capabilities. Nearly backward compatible with the RELAP5 input format.

Technical Guides:

1. *Desired Characteristics for Next Generation Integrated Nuclear Safety Analysis Methods an Software*, EPRI 1021085
2. *RELAP5/MOD3 Code Manual Volume III: Development Assessment Problems*

RELAP7 Major Design Aspects

- MOOSE-based application (linear FEM, implicit fully coupled components, mesh and time step adaptivity, parallel software, and more).
- Multi-Scale Time Integration:
  1. PCICE Scheme (pressure-based, operator split, second-order in time, stability limited by Material Courant). *Prototyped, not yet implemented into MOOSE.*
  2. JFNK Scheme (multiphysics coupling, solves stiff nonlinear dependencies for strongly coupled systems, first and second order in time). MOOSE's main solver.
  3. Point-Implicit Method (for slow, long duration transients and steady-state problems). *Prototyped, not yet implemented into MOOSE.*
- All-speed ($0 \leq Mach \leq 1$), all-fluid (two-phase, gas, liquid metal) flow.
- 1.5-D discretization (variable cross-sectional area piping) with 0-D system components.
- 2nd-order accurate temporal and spatial discretization (eliminate the traditional numerical errors).

Primary components finished and tested

- 1D components:
  - Pipes: isothermal and non-isothermal, gravity, wall heat transfer
  - Reactor core channel: coolant coupled with fuel rod, plate/cylindrical fuel (clad, gap, fuel), i.e. strongly coupled conjugate heat transfer
  - Heat exchanger: counter-current or co-current, conjugate heat transfer
- 0D components for setting boundary conditions:
  - TimeDependentVolume: set pressure and temperature boundary condition.
  - TimeDependentJunction: set velocity and temperature boundary condition (behaves like ideal pump at boundary).
  - TDM: time dependent mass flow rate boundary condition (behaves like ideal pump at boundary).

Primary components finished and tested (continued)

- 0D components for connecting 1-D components:
  - Branch, both isothermal and non-isothermal, any number of connections, with/without form losses.
  - IsoPump/Pump: one in one out, providing a head for positive flow and flow resistances for negative flow.
  - IdealPump: one in one out, providing fixed mass flow rate
- EOS: BarotropicEOS, Non-isothermalEOS

Primary components unfinished or not fully tested

- Point kinetics model: not coupled with thermal hydraulics yet
- Trip/control system (RAVEN)
- Valve, need control system (RAVEN)
- Flexible coupling fluid flow with 1D, 2D, or 3D heat structure

1-D, variable area (single phase) flow

$$\frac{\partial \rho A}{\partial t} + \frac{\partial \rho u A}{\partial x} = 0$$

$$f = \frac{\tau_w}{\frac{1}{2}\rho |u| u}$$

$$\frac{\partial \rho u A}{\partial t} + \frac{\partial A(\rho u^2 + p)}{\partial x} = p\frac{\partial A}{\partial x} - \frac{\rho |u| u f}{2}\frac{4A}{D_H}$$

$$D_H = \frac{4A}{perimeter}$$

$$\frac{\partial \rho E A}{\partial t} + \frac{\partial u A(\rho E + p)}{\partial x} = h\left(T_w - T\right)\frac{4A}{D_H} - u\frac{\rho |u| u f}{2}\frac{4A}{D_H}$$

$$E = e + \frac{u^2}{2}$$

$$p(\rho, e) = (\gamma - 1)\rho(e - q) - \gamma p_\infty \qquad e(\rho, T) = c_v T + \frac{p_\infty}{\rho} + q$$

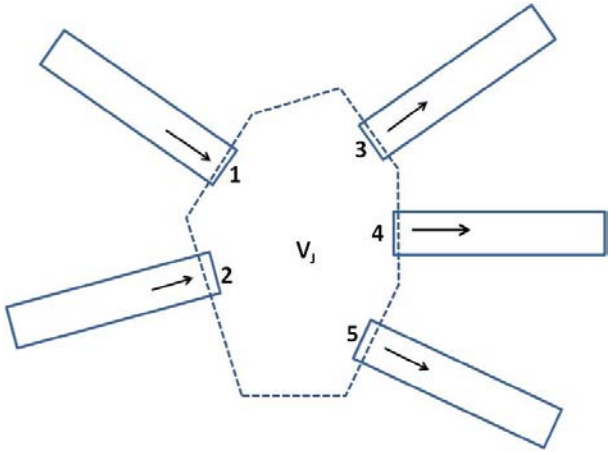
$$c^2(T) = \frac{\gamma\left(p + p_\infty\right)}{\rho} = \gamma(\gamma - 1)c_v T$$

(sound speed)

Governs all flow regimes and fluid types

New Flow Junction Model: based on fully implicit Mortar FEM

- Fully implicit with JFNK.
- Combines the method of Lagrange Multipliers with the FEM.
- Provides a strategy for finding the local maxima and minima of a function subject to set of inequality constraints.



Schematic of a flow junction

Single phase constraint system:

Mass

$$\sum_{e'} \rho_{e'} A_{e'} \vec{u}_{e'} \cdot \hat{n}_{e'} = 0$$

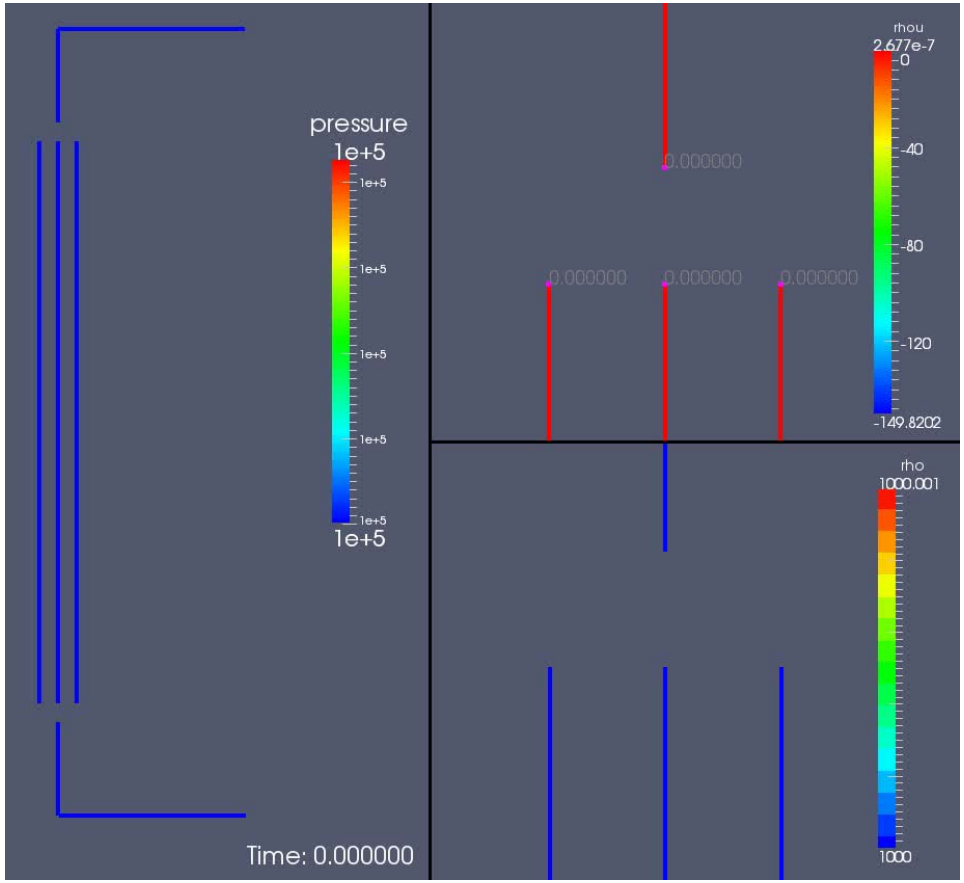
Mechanical Energy

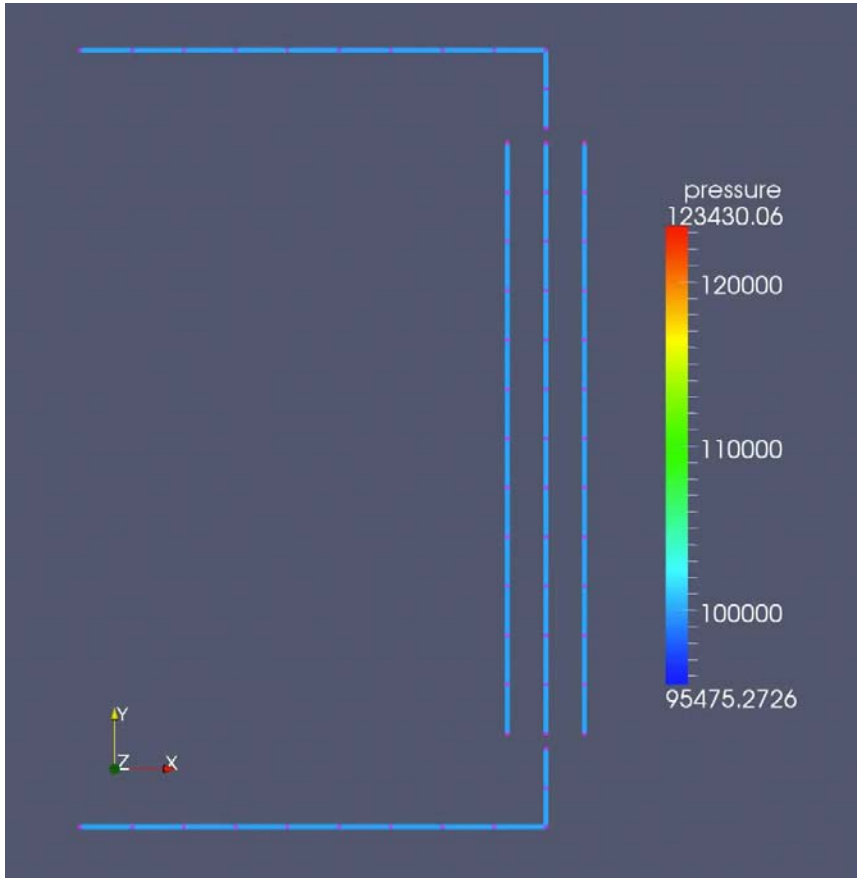
$$\sum_{e'} \left(\left(1 - K_{e'-e}\right) \frac{u_{e'}^2}{2} + \frac{p_{e'}}{\rho_{e'}} \right) \left(\rho_{e'} A_{e'} \vec{u}_{e'} \cdot \hat{n}_{e'} \right) = 0$$

Total Energy

$$\sum_{e'} \left(e_{e'} + \tfrac{1}{2} u_{e'}^2 + \frac{p_{e'}}{\rho_{e'}} \right) \left(\rho_{e'} A_{e'} \vec{u}_{e'} \cdot \hat{n}_{e'} \right) = 0$$

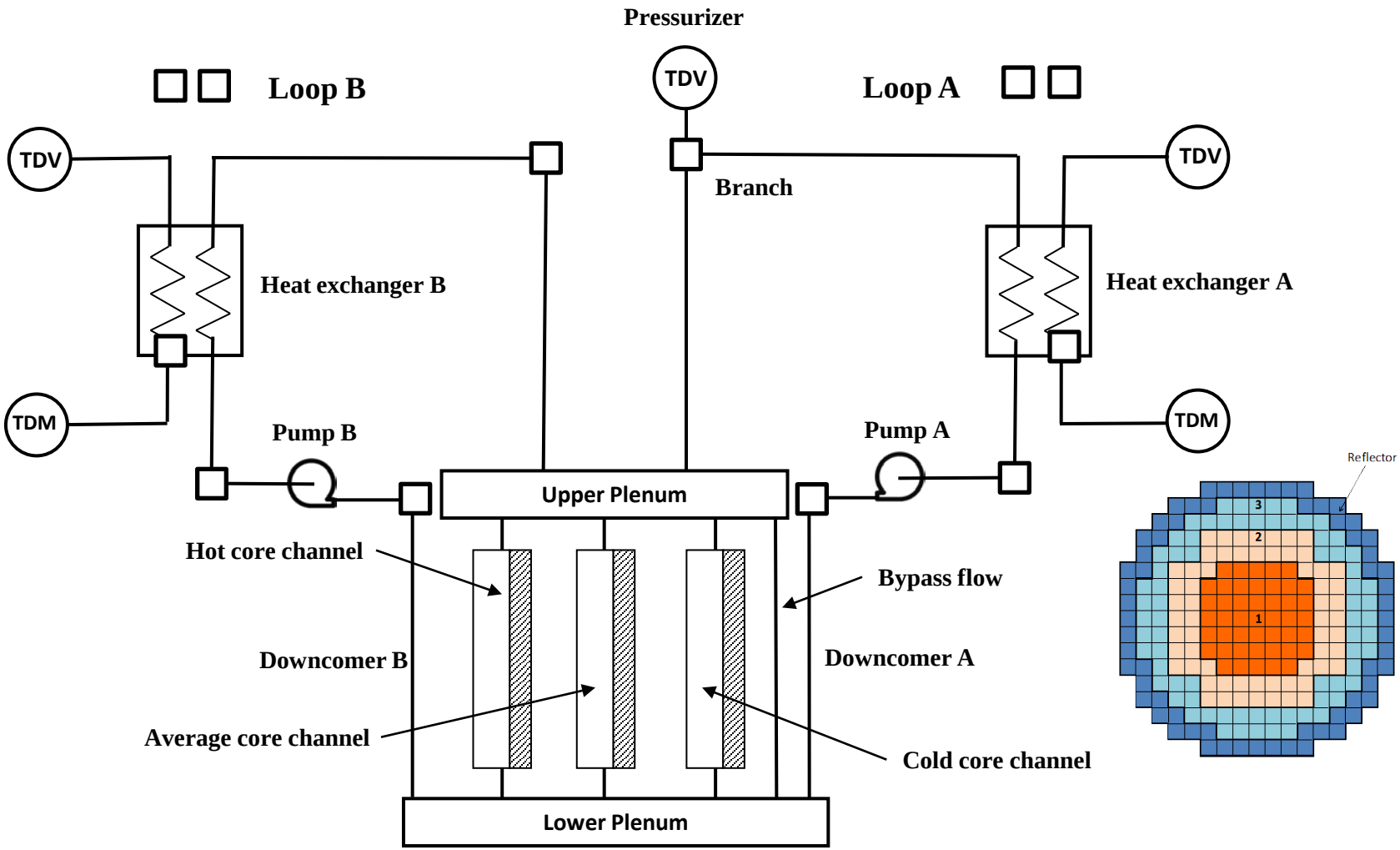
Pipe Network Examples





Time line		5/15/2012	11/15/2012	11/15/2013	11/15/2014
Major version release		RELAP7 α-0.1	α-0.2	α-0.6	β-0.1
Features	Software Design and structure	First working loop structure based on MOOSE, including major simplified physical components such as 1-D pipe, junctions, pump, heat structure and software structure for closure laws	Working loop structure for 2-φ flow, including several simplified major physical components for BWR primary and safety systems	Flexible software structure allowing scalable development of components; preliminary input/output	Complete software structure allowing rapid and scalable development; Easy to couple other moose based applications; methods for proprietary info; GUI
	Numerical methods	1st and 2nd order finite element methods for 1-D single phase flow; multi-physics coupling	1st and 2nd order methods for 1-D 2-φ flow; multi-physics coupling;	Large time steps for long transient; efficient preconditioning;	Efficient Parallel computing; multiple dimension coupling; multiple scale coupling
	Physics	1-D compressible single phase flow; point kinetics model; wall heat transfer and friction correlations; simple fluid and solid properties	2-φ flow with qualitative closure models for vertical flow regime; water properties; simplified models for reactor core, steam dome, dry well and wet well.	2-φ flow with some quantitative closure models; consistent choked flow; Single phase sub-channel model; 2-D or 3-D diffusion models; control/trip systems	More quantitative closure models for 2-φ flow; 2-φ sub-channel model; fuel burn-up model; interface to 3-D neutron transport model; more realistic physical component models
V&V		Verification: regression test packages; time and space steps convergence study; Validation: RELAP5 benchmark; few of phenomenological tests	Focus on verification; few of phenomenological tests for 1-D 2-φ flows; RELAP5 benchmark	Extensive verification; more phenomenological tests; RELAP5 benchmark	Extensive verification; phenomenological tests; some separate effect tests; RELAP5 benchmark
Demonstration cases		Typical single phase (PWR) reactor steady state simulation	Preliminary (simplified) BWR SBO analysis	Refined BWR SBO; ATR single phase transient or SFR transient or VHTR transient	Multi-scale BWR SBO (R7+BISON+others); PWR cases; one Gen-IV multiple dimensional transient demonstration

Simplified TMI-1 NPP Test (milestone)



Simplified TMI-1 NPP test (continued)

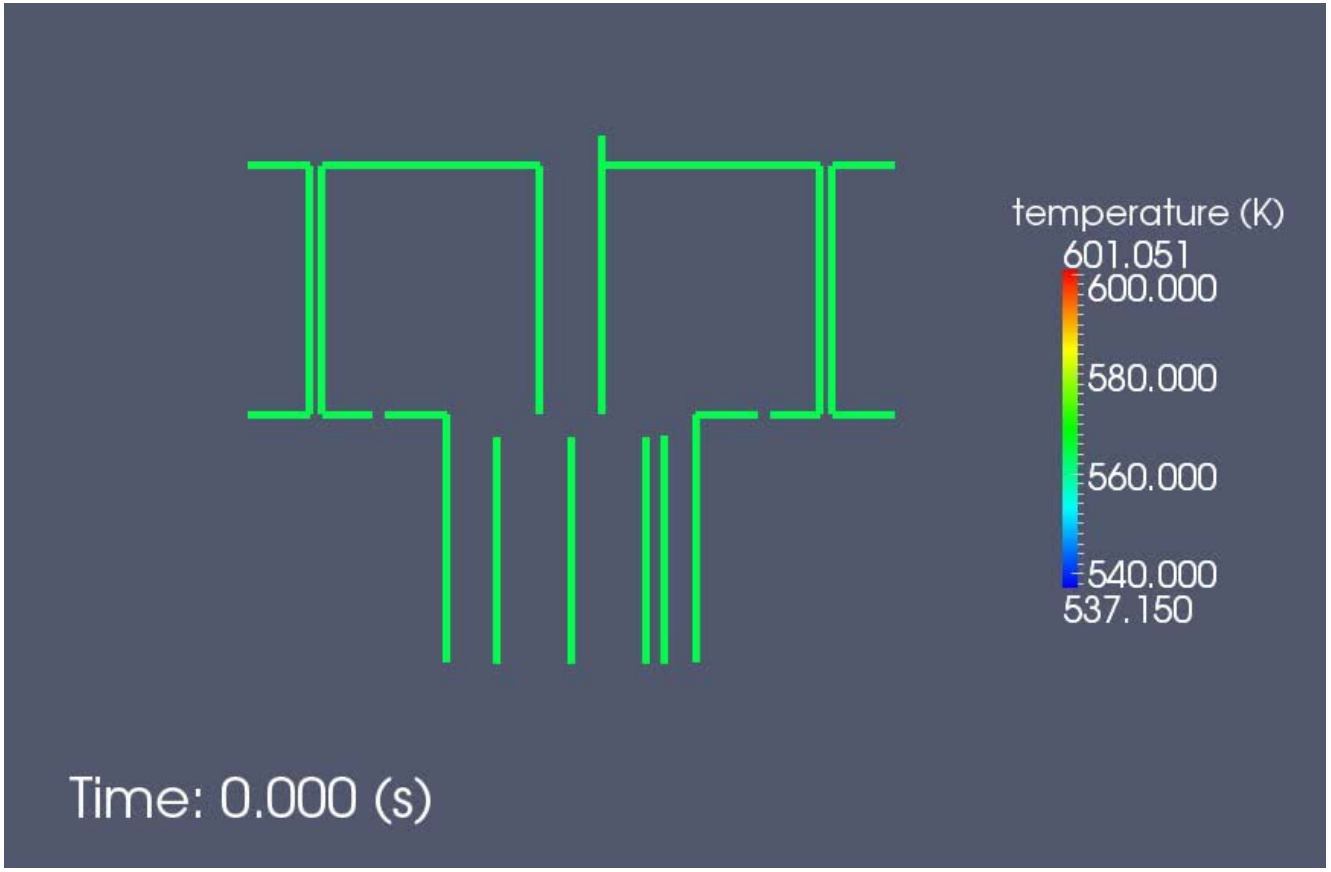
T/H Inputs:

- **Total thermal power: 2772 MW**
  - **33.37% for hot channel (CH1)**
  - **37.00% for average channel (CH2)**
  - **29.46% for cold channel (CH3)**
  - **Sine power shape**
- **Total core flow rate: 17602.2 kg/s**
  - **(2 loops, 8801.1 kg/s for each loop)**
- **Pressurizer pressure: 151.7 bars**

Component list (42 in total):

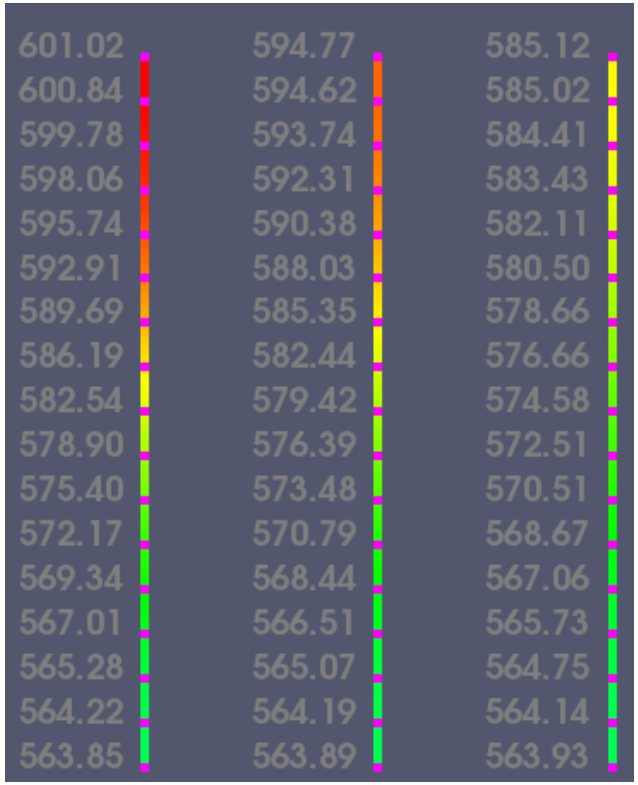
CH1 CH2 CH3 bypass_pipe LowerPlenum UpperPlenum
DownComer-A
pipe1-HL-A pipe2-HL-A
HX-A
pipe1-CL-A pipe2-CL-A
Pump-A
pipe1-SC-A pipe2-SC-A
MassFlowRateIn-SC-A PressureOutlet-SC-A
Branch1-A Branch2-A Branch3-A Branch4-A Branch5-A Branch6-A
pipe-to-Pressurizer Pressurizer
DownComer-B
pipe1-HL-B pipe2-HL-B
HX-B
pipe1-CL-B pipe2-CL-B
Pump-B
pipe1-SC-B pipe2-SC-B
MassFlowRateIn-SC-B PressureOutlet-SC-B
Branch1-B Branch2-B Branch3-B Branch4-B Branch5-B Branch6-B

Simplified TMI-1 NPP test (continued)

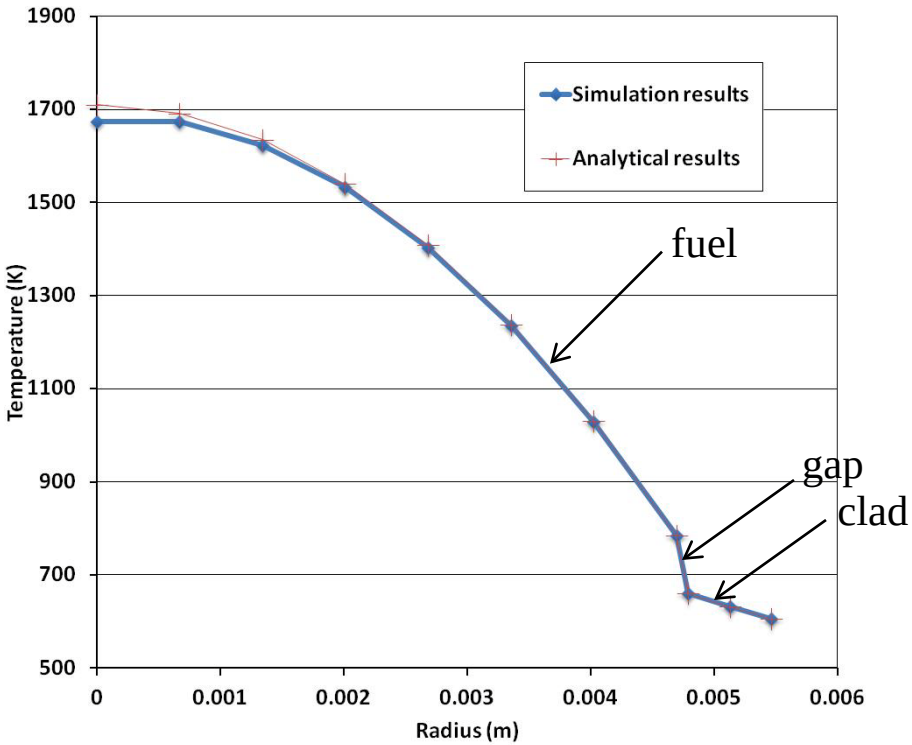


Expected core inlet/outlet temperature: 564.15K/ 591.15K
Calculated core inlet/outlet temperature: 564.05K/ 590.92K

Simplified TMI-1 NPP test (continued)



Fluid temperature in core region



Fuel temperature

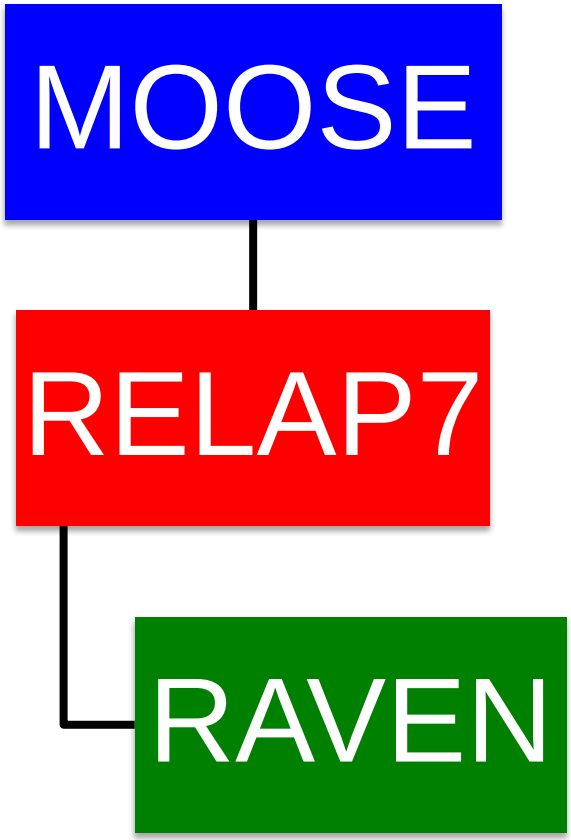
How will RELAP7 be used?

So how will RELAP7 engage in NEAMS/CASL/LWRS-RISMC activities? Answer: Build some more animals.

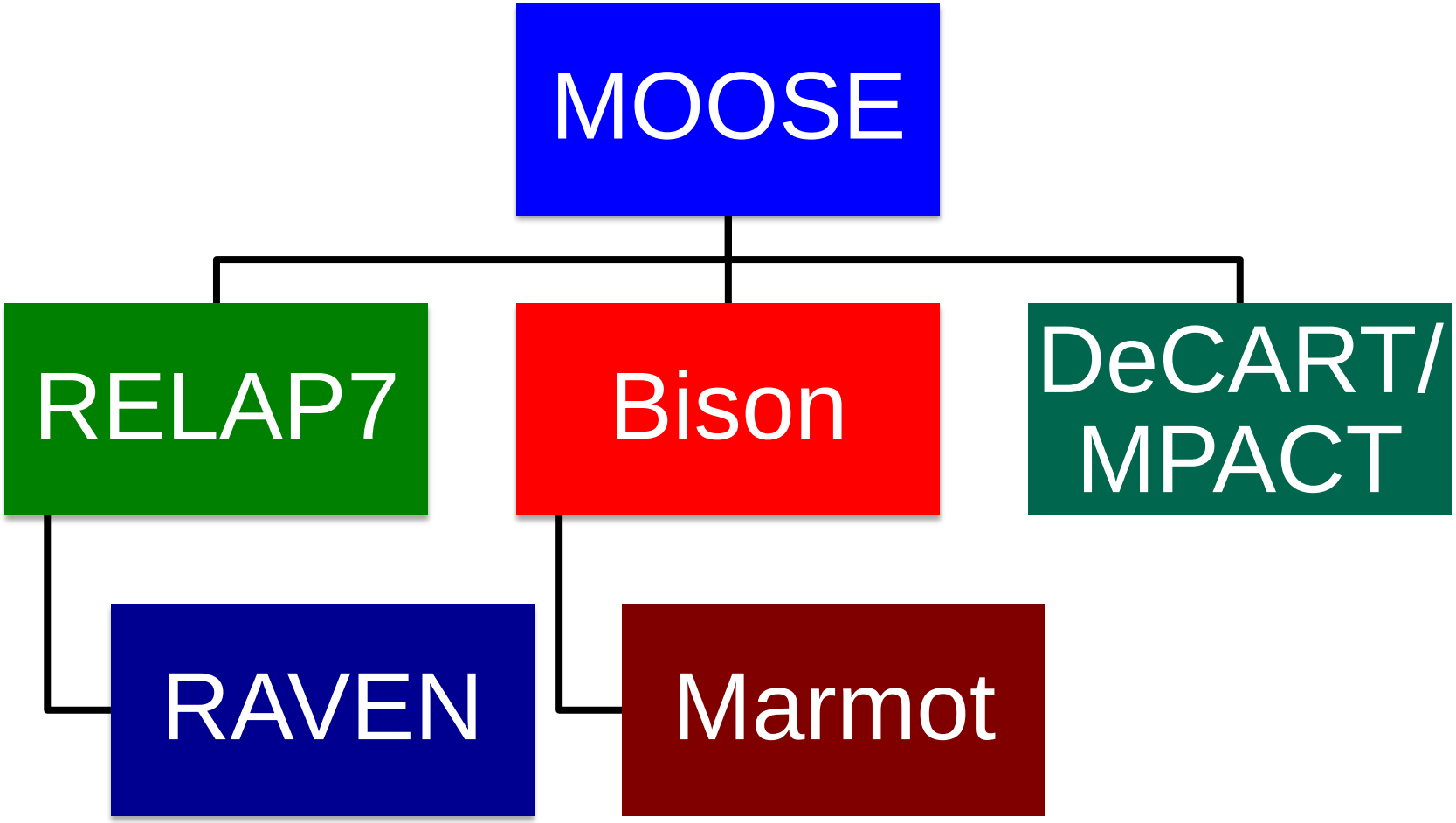
RAVEN (**R**eactor **A**nalysis and **V**irtual control **EN**vironment)

- Virtual reactor control room (historic/design basis event coordinator)
- Risk informed margin analysis (including PRA)
- Graphical front end (simulation controller, input and output)

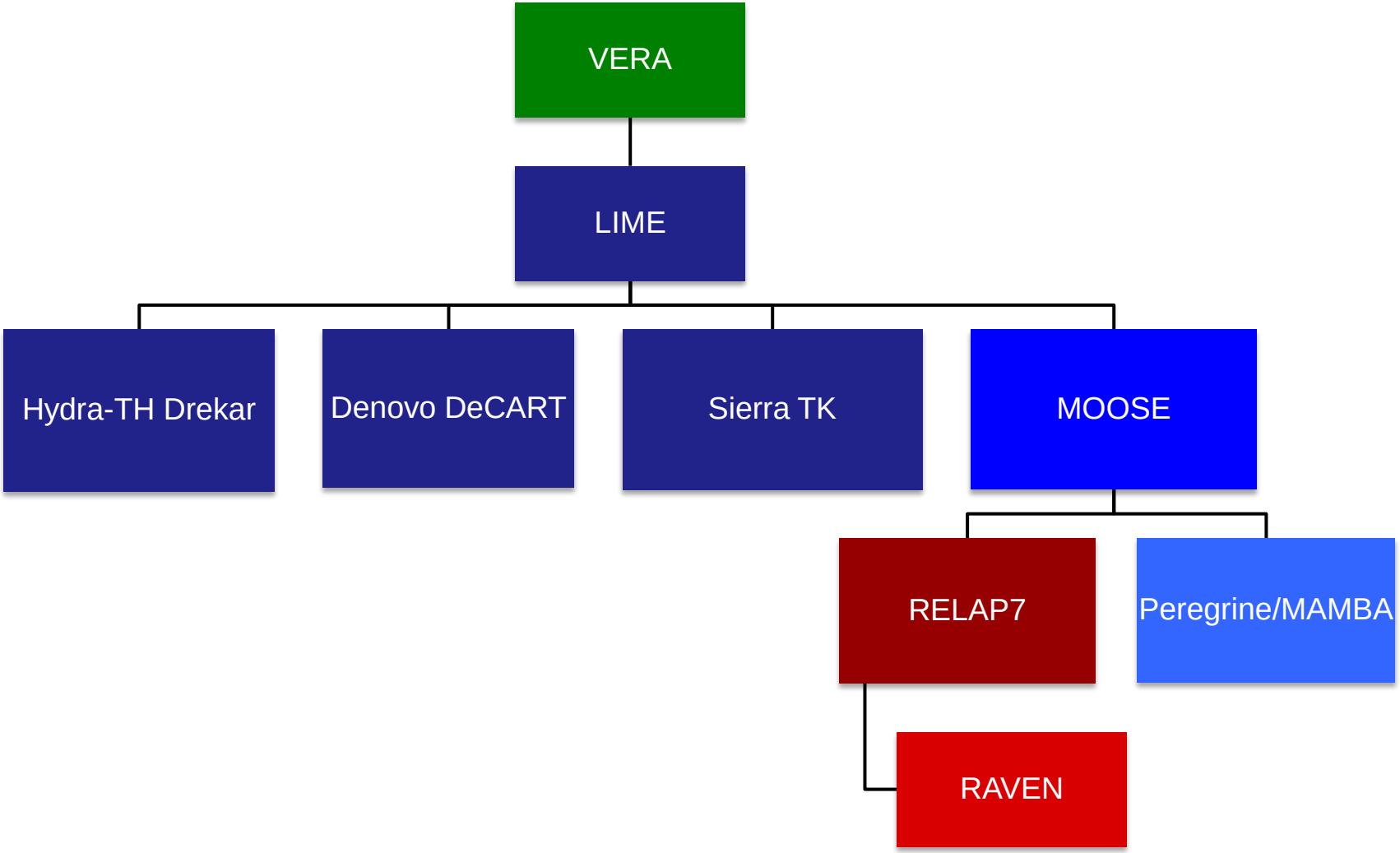
Systems Analysis



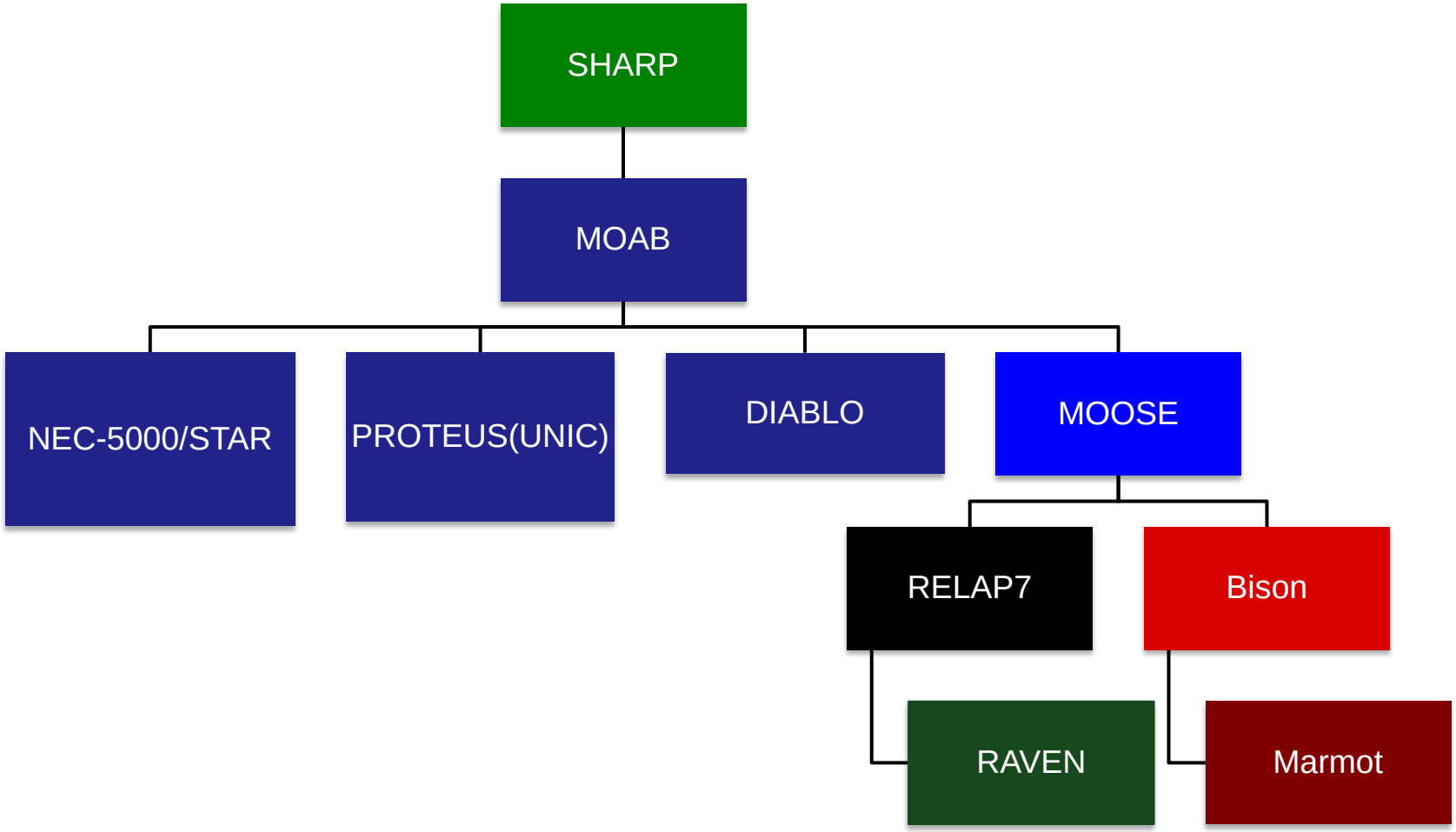
Coupled to LWR Fuels Performance (one option)



Coupled to VERA (balance of plant)



Coupled to SHARP (balance of plant)



Simulation Goal for the Next Phase of RELAP7 Development (11/15/2012)

Time line		5/15/2012	11/15/2012	11/15/2013	11/15/2014
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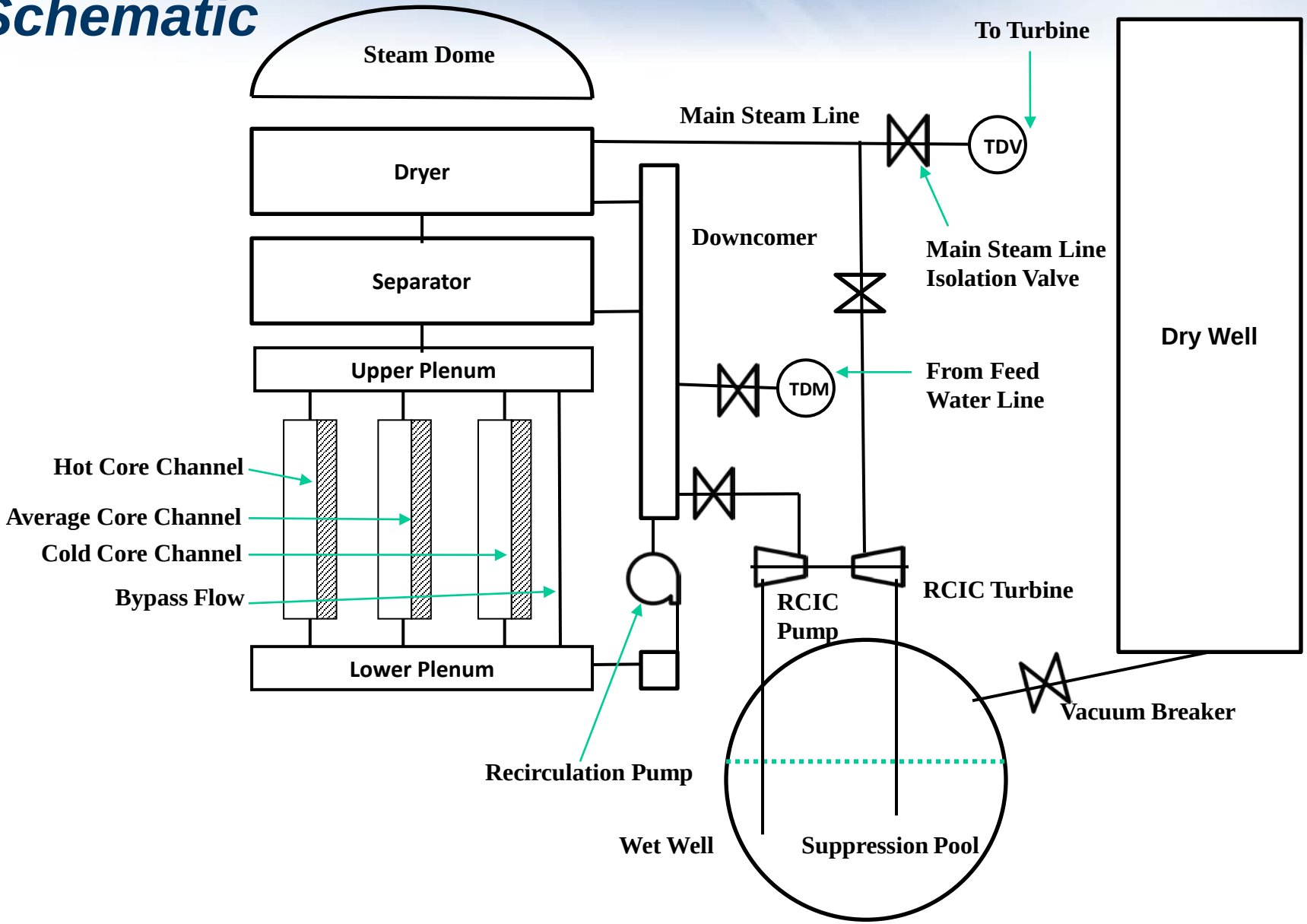
Simplified BWR SBO Schematic



Component Name	Descriptions	Phases
Pipe	1-D fluid flow within 1-D solid structure with wall friction and heat transfer	1Φ/2Φ
Core Channel	Simulating flow channel and fuel rod, including 1-D flow and fuel rod heat conduction	2Φ
Branch	Multiple in and out 0-D volume/junction, which provides form loss coefficients (K)	1Φ/2Φ
Separator/Dryer	Separating steam and water with mechanical methods, 1 in and 2 outs 0-D volume	2Φ
Steam Dome	0-D steam volume to provide pressure buffer for the whole primary system	1Φ steam
Downcomer	0-D volume to mix different streams of water	1Φ water and 1Φ vapor
Jet Pump	Simulating jet pump behavior, 0-D junction	1Φ water
Valve	Change flow rate by changing flow area, connected to control system, 0-D junction	1Φ water or vapor
Wet Well	0-D volume to simulate suppression pool and it's gas space	1Φ water and 1Φ gas
Dry Well	0-D volume to simulate dry well space	1Φ gas
RCIC Pump	Simulate Reactor Core Isolation Cooling (RCIC) pump which is driven by the RCIC turbine through a common shaft, 0-D junction	1Φ water
RCIC Turbine	Simulate Reactor Core Isolation Cooling (RCIC) turbine which drives the RCIC pump through a common shaft, 0-D junction	1Φ vapor
Time Dependent Volume (TDV)	Time Dependent Volume (TDV) to set pressure and temperature boundary conditions, no unknowns	1Φ water or vapor
TDM	Time Dependent Mass flow rate (TDM) to set mass flow rate and temperature boundary conditions, no unknowns	1Φ water or vapor

Major Simulation Sequences

- Initializing the simulation to steady state:
  - All the safety valves close, primary system valves open.
  - Recirculation pump on, reactor power on.
  - Run to steady state.
- Starting SBO to dry well overpressure or fuel damage temperature
  - All primary system valves close.
  - Recirculation pump trip, reactor trip.
  - RCIC valves on; steam begins to drive RCIC turbine, blow into suppression pool, and condense back to water; RCIC pump draws cooling water from the suppression pool back to the reactor core.
  - Temperature and pressure increase within the primary loop; the pressure at the wet well reaches the vacuum breaker setting point; gas flows into the dry well.
  - Other safety systems such as Isolation Condenser and High Pressure Coolant Injection are ignored (will be included in refined SBO analysis).

Thank you for your attention…questions?

Hybridization:

Path Forward for Immediate Deployment of UQ/SA/DA tools

Hany Abdel-Khalik
VUQ
North Carolina State University

June 13th, 2012

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NCSU VUQ Team

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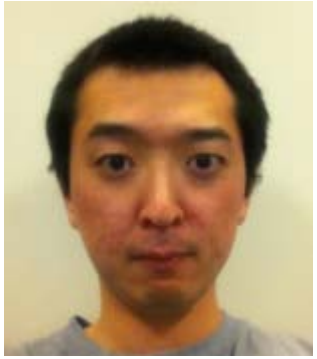
PhD Candidate

Congjian Wang,
PhD Candidate

Zeyun Wu,
Post-Doc

Jaeseok Heo,
Post-Doc

Mohammad Abdo,
PhD Student



Shota Soga,
MSc Student

Jason Hite,
Undergraduate

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Relevance

- Understanding uncertainties requires three essential exercises:
  - Uncertainty Quantification: propagation of various sources of uncertainties
  - Sensitivity Analysis: identify key sources of uncertainties
  - Data Assimilation: improve prediction via use of available experimental measurements

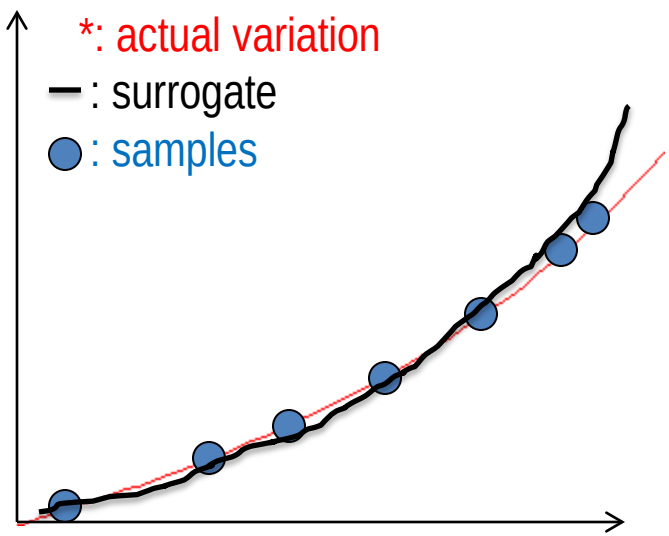
- This work aims to optimally utilize (via hybridization) state-of-the-art algorithms to enable their application to nuclear engineering models

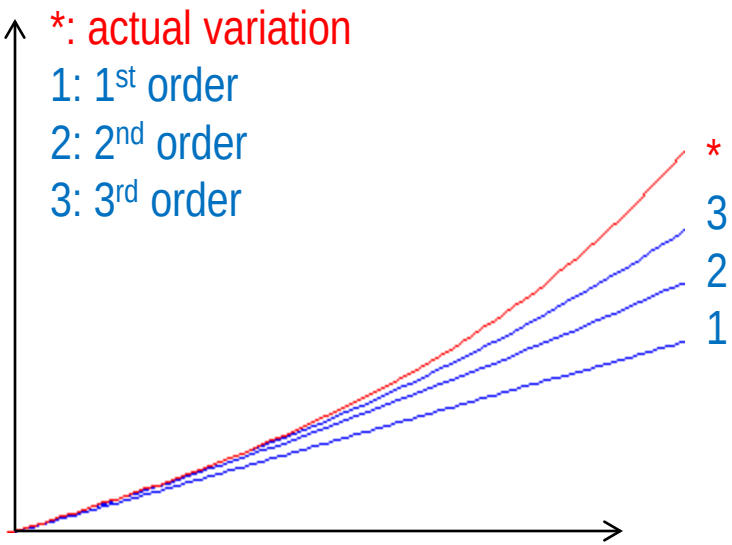
UQ/SA/DA Challenges

- Promoted use of advanced simulation tools overwhelms existing uncertainty management algorithms, e.g. UQ/SA/DA
- *Many many* model executions are required to understand uncertainties for a real-world model, expected to be:
  - Nonlinear
  - High dimensional (many parameters and many responses)
  - Multi-scale
  - Multi-physics
  - Some modeling components only accessible as black-boxes, or require unaffordable man-hours to modify
- 'High dimensionality'.
  - Number of afforded model executions (forward or adjoint) much less than number of input parameters and output responses.

State of the Art

- Forward (sampling) methods
- Variational (adjoint) methods





State of the Art

- Forward (sampling) methods
  - Easily implemented in existing codes
  - Captures entire PDFs for responses
  - Best for nonlinear models with few input parameters and many responses
  - Captures global effects of nonlinearity
  - Suffers from curse of dimensionality
  - Applicable to both probabilistic and deterministic codes
  - Applicable to single-physics and coupled codes

- Variational (adjoint) methods
  - Requires additional work to implement
  - Captures features (e.g. moments) of PDF
  - Best for linear models with many input parameters
  - Cost is proportional to number of responses
  - Captures nonlinear effects one order at a time
  - Computational cost becomes non trivial for nonlinear effects
  - Application currently limited to deterministic codes
  - Implementation difficult for coupled codes

Hybridize ……..

Advantages of Hybridization

- Realize benefits of both methods
  - Variational methods (although local) can be shown to reduce effective dimension of input parameters, with reduction error upper-bounded.
  - Forward methods, applied to reduced parameter, can then be used to propagate/understand uncertainties
- Immediate deployment
  - Only I/O manipulation of existing codes/methods is needed
- Significant reduction in computational cost, to enable routine execution

Hybridization: How?

- The hybridization framework is based on a surprising observation:
  - Behavior of most complex models is dependent on only small number of degrees of freedom, often much smaller than the problem dimensions
  - Reason: models are developed in the most general way but exercised in a very limited manner, e.g. assembly calculations
- Challenges:
  - The reduced DOFs are not known priori
  - There exists no clear way to quantify reduction errors
- Approach:
  - Use latest advances in reduced order modeling to identify reduced DOFs and rigorously quantify reduction errors
  - Once known, one can reduce associated computational cost for UQ/SA/DA analysis

Reduced Order Modeling

- The process of reducing a complex model into one that can be manipulated more efficiently is referred to here as ROM.
  - Using simplified physics (associated errors are difficult to evaluate).
  - Surrogate models construction (more theoretical basis is available for error control but still open problem)
  - Reducing the dimensionality of the data streams via Subspace Methods, e.g. parameters, state variables, and quantities of interest (recent research shows that this error can be potentially controlled)

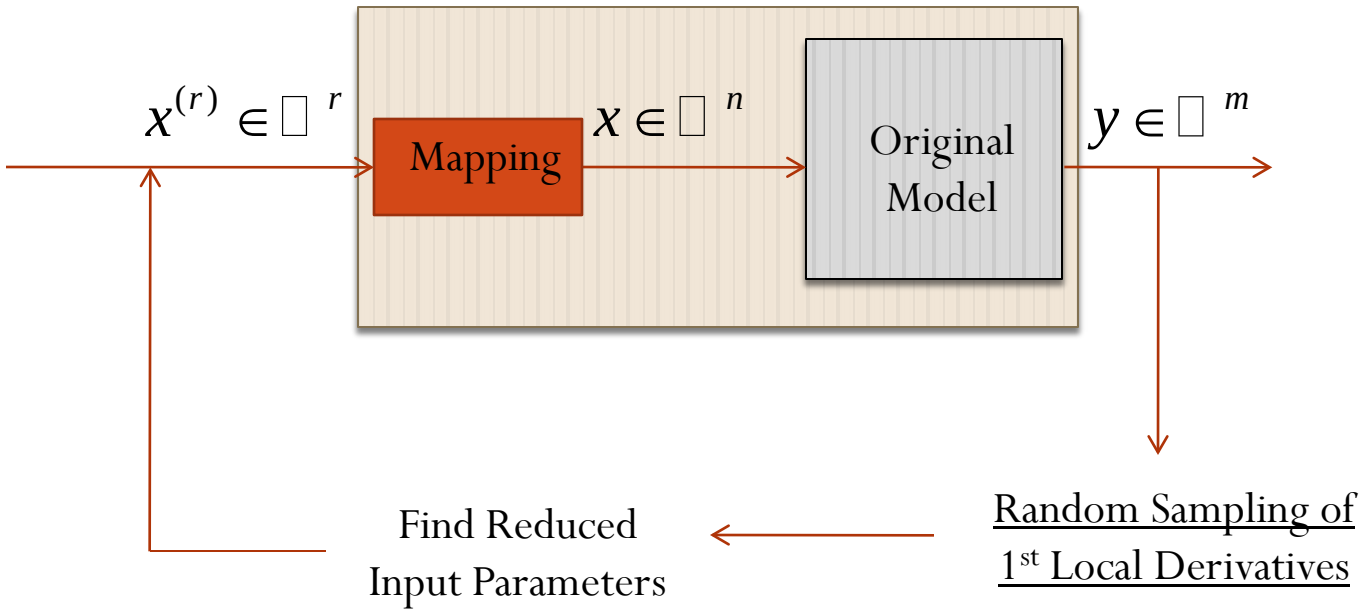
Subspace Methods

- Given the complexity of physics model, multi-scale strategies are employed to render practical execution times
- Multi-scale strategies are motivated by engineering intuition; designers often interested in capturing macroscopic behavior
- Multi-scale strategies involve repeated homogenization/averaging of fine-scale information to generate coarser information
- If codes are already written, why not reduce them first before tightly/loosely coupling them, and to perform UQ/SA/DA
- Why not design our solution algorithms to take advantage of lost degrees of freedom?

Subspace-Based Hybridization

Approach #1

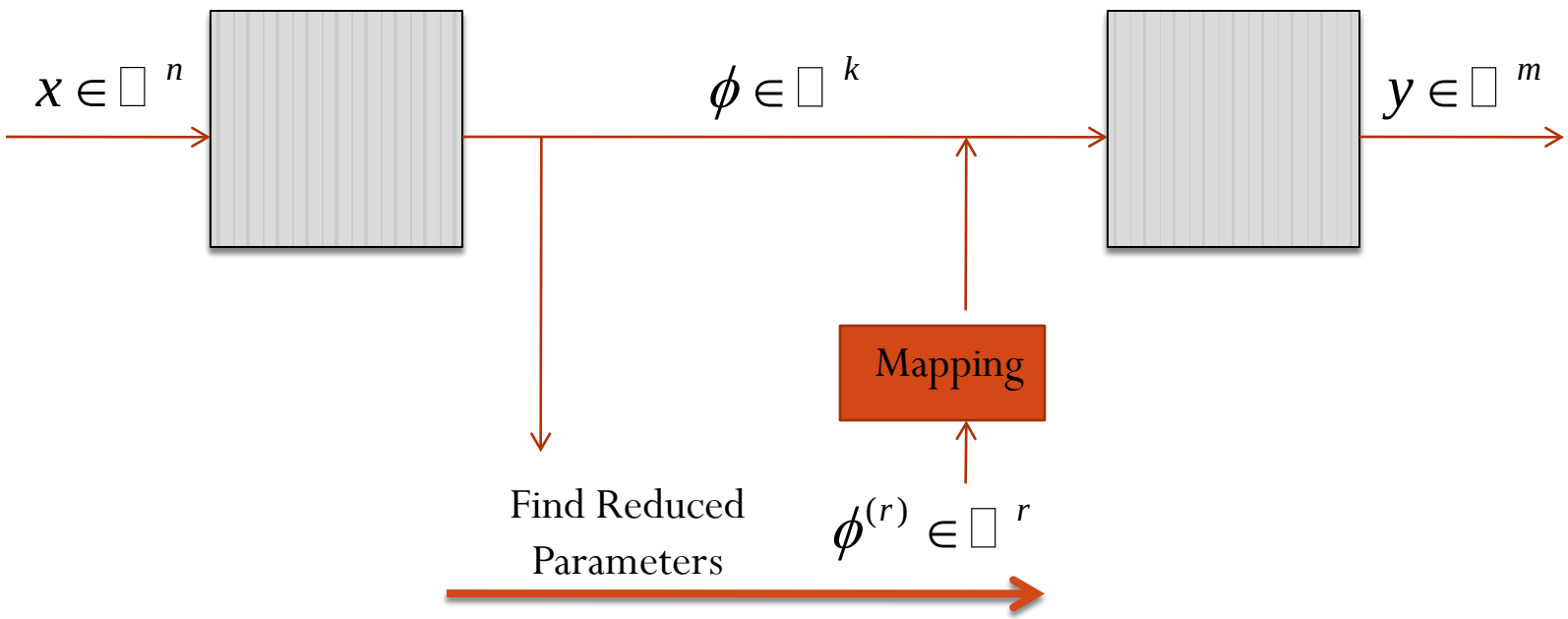
- Methods Hybridization inside each components
- Reduce subspace first, then employ forward method to sample the reduced subspace



Subspace-Based Hybridization

Approach #2

- Hybridization across components
- Employ different method(s) for each components, and perform subspace reduction across components interface



New Capabilities

- Year 1:
  - Hybrid Variational-Deterministic Framework (*demonstrated for neutronics models*)
  - Verification guidelines for UQ/SA results

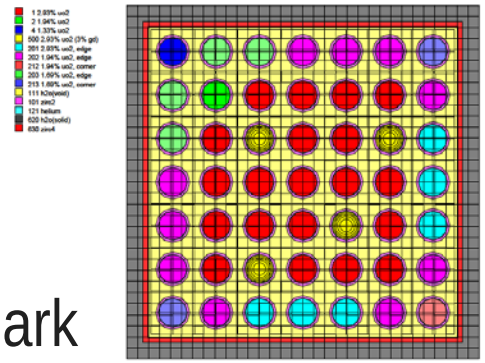
- Year 2:
  - Exact-to-Precision Generalized Perturbation Theory (E_pGPT) for high order Sensitivity Analysis (*for construction of surrogates)*
  - GPT-free Sensitivity Analysis for Monte Carlo Models
  - Hybrid MCMC-ESM for DA

Hybrid Variational Deterministic Framework
(By Youngsuk Bang and Jaeseok Heo)

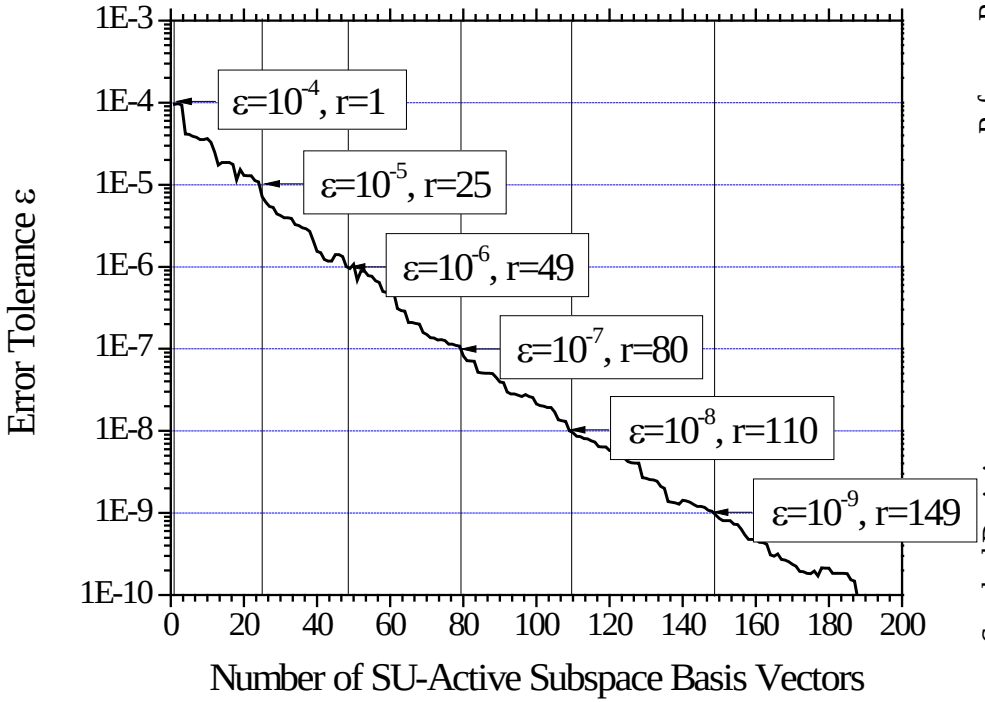
- FY12: Generate neutronics uncertainties for demonstration in VERA's WEC code system
  - Effort lead by Brian Adams to aggregate various sources of uncertainties, incl. neutronics and thermal-hydraulics, using ANC-VIPER-BOA
  - Due Date: Extended from June 30 to Sept 31, 2012.

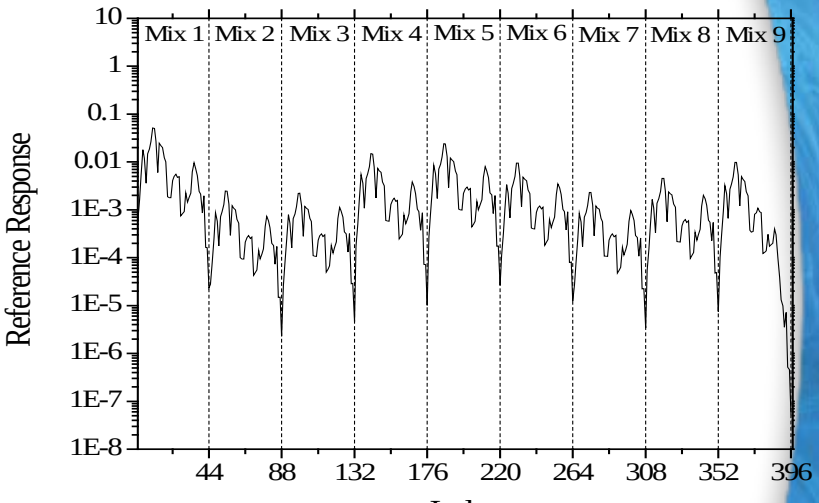
Hybrid-based UQ

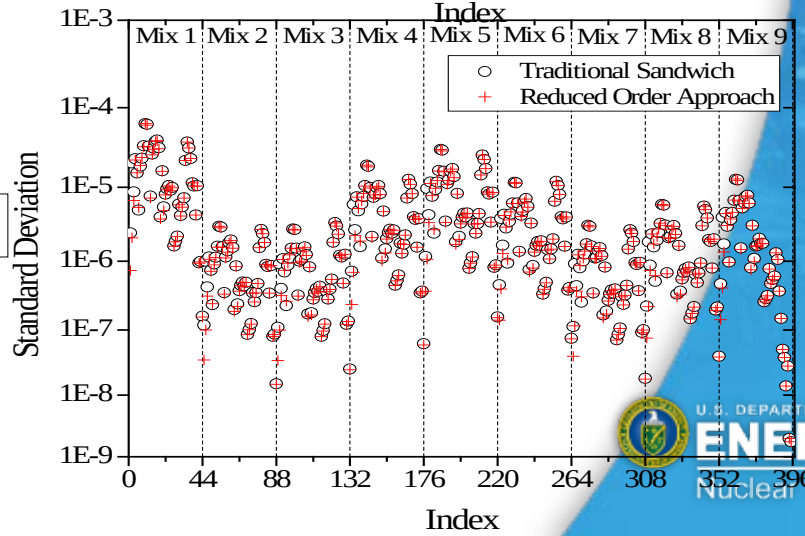
Based on Work by Youngsuk Bang



- BWR 7x7 Assembly Benchmark
  - Responses: 396 Group Fluxes
  - Parameters: 704 cross-sections







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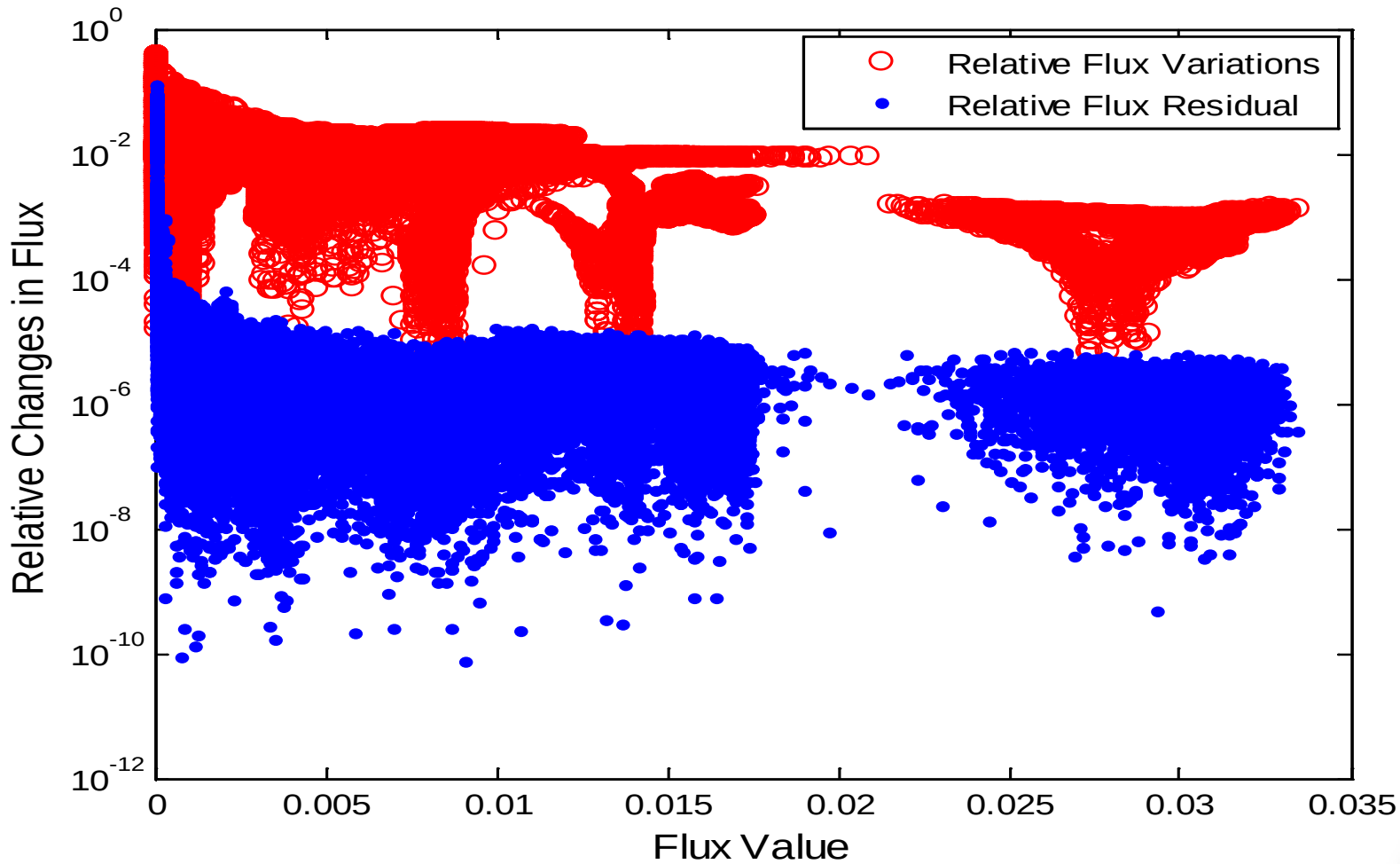
Exact-to-Precision Generalized Perturbation Theory (By Congjian Wang)

- Use of first-order GPT to capture all higher order effects
- Precision is user-defined
- Improve performance of hybrid framework by reducing reliance on forward approach to capture nonlinear effects
- Demonstrate capability using prototypical radiation transport models
  - Congjian Wang and Hany Abdel-Khalik, "EpGPT for Source Driven Problems," Nucl. Eng. Design, September 2011.
  - Youngsuk Bang, Congjian Wang, and Hany Abdel-Khalik, "State-Based Adjoint Approach for Reduced Order Modeling," Transport Theory and Statistical Physics, January 2012.
- Scheduled for FY2013 in support of extending hybrid framework to multi-scale multi-physics UQ

E_pGPT-estimated Flux Variations



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Current Focus
(By Jason Hite)

- Hybrid Subspace Implementation of Monte Carlo Markov Chain Approach for Data Assimilation
  - Use adjoint methods to reduce dimensionality of input parameter space
  - Apply MCMC on the reduced input parameters.
  - Application #1: TRITON fuel pin cell model
  - Application #2 (time permitting): Denovo assembly model

Future Work

- In collaboration with C. Webster, B. Williams, R. Smith, proposed a framework for completing DA in multi-physics models.
- UQ may be viewed as forward propagation of uncertainties; while DA as inverse propagation to identify key sources of uncertainties.
- Proposed for:
  - Improvement of predictive capability of core simulators using real plant data
  - Better simulation of challenge problems, e.g. CIPS (represents the initial focus).

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Thanks

- Thanks to Brian Adams, Jim Stewart, Jeff Banta, Zeses Karoutas, and Paul Turinsky for resolving the NDA issues with NCSU.
- Thanks to ORNL's Matthew Jessee and Mark Williams for hosting two students in support of CASL initiatives.
- Thanks to Linda Weltman for 'zero uncertainty performance'

Questions

For additional discussions/ideas, please contact me at:

abdelkhalik@ncsu.edu

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Industry Achievements

AMA Focus Area

J. Yan, J. Gehin, Z. Karoutas, R. Montgomery

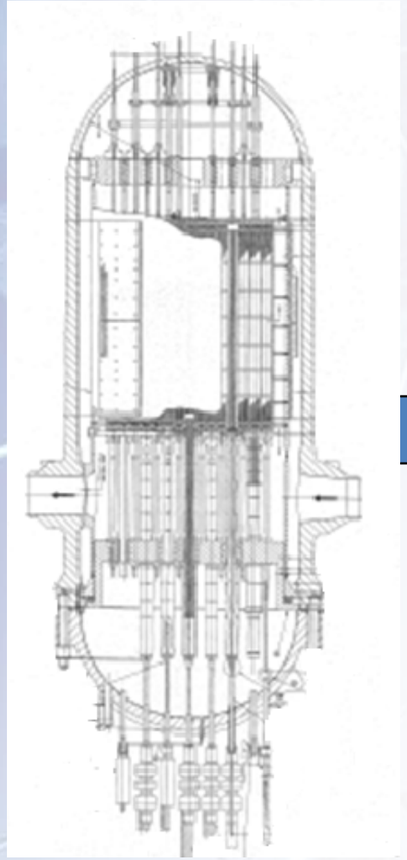
AMA team members

Content

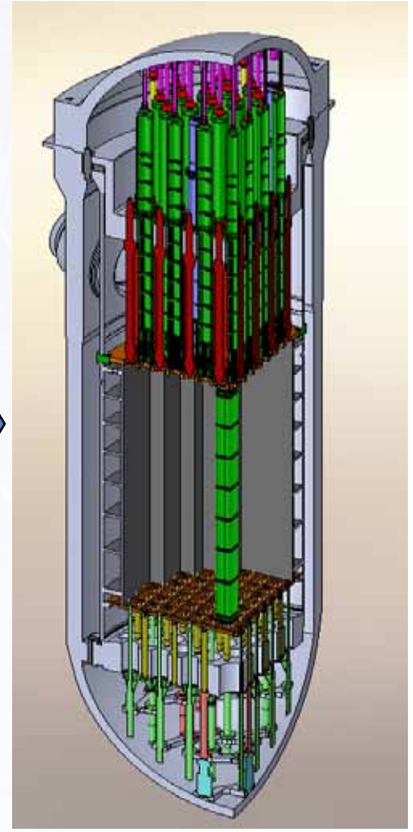
- 4 Loop Westinghouse PWR Multi-Physics Model Development
- TH Validations
- Thermal Hydraulics & Neutronic Coupling
- Industry Pilot Project: GSI-191

4 Loop Westinghouse PWR Multi-Physics Model Development

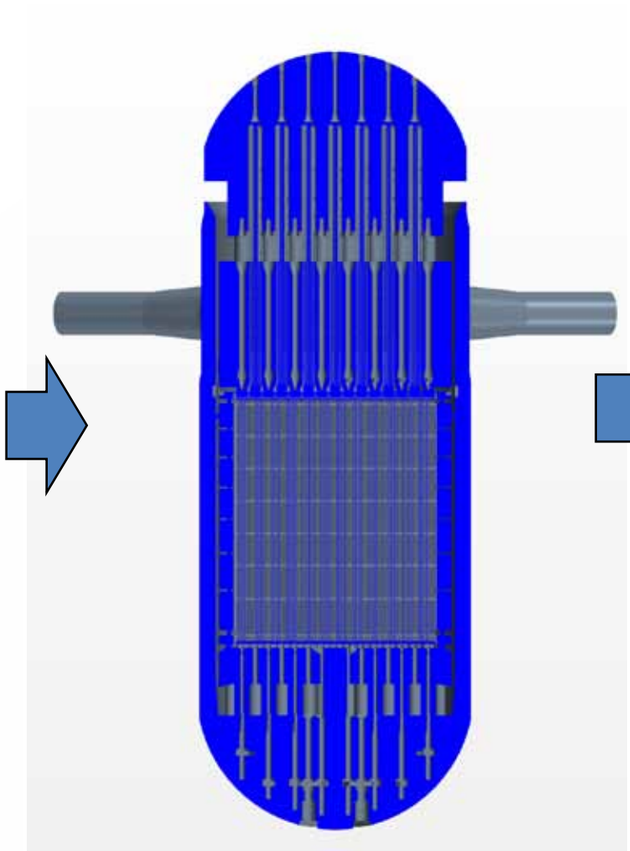
- RPV ID 173”, 193/4 Fuel Assemblies,13,944 fuel rods (fuel pellets, helium gap), 434 spacers, 148,224 mixing vanes; 1.2 billion cells



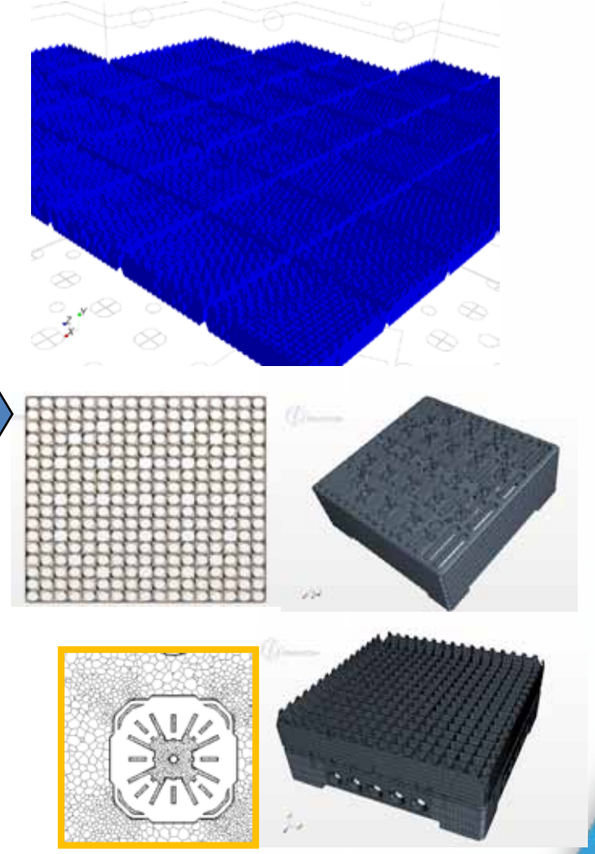
DRAWINGS



3D CAD



CFD

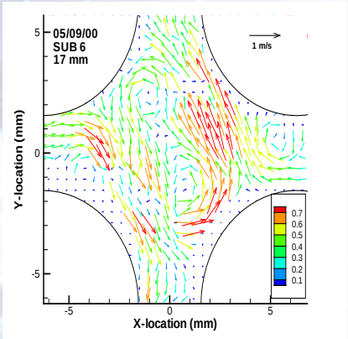


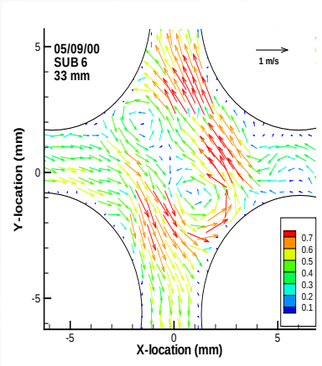
Mesh

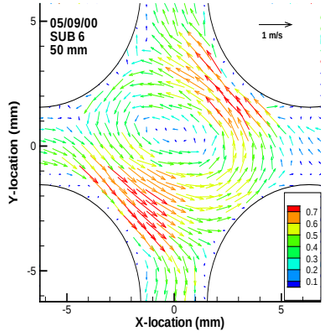
4 Loop Westinghouse PWR Multi-Physics Model Development

- Comparison of time-averaged flow fields at axial location of 17, 33, and 50 mm downstream of grid
- Fuel center line temperature prediction is validated against Westinghouse licensed code: PAD

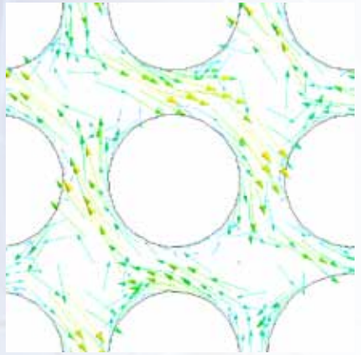
TEST

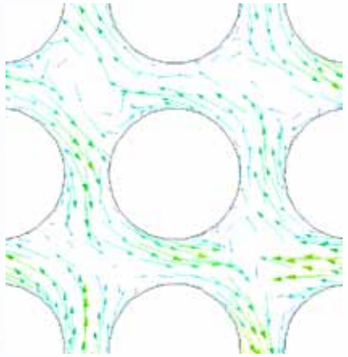


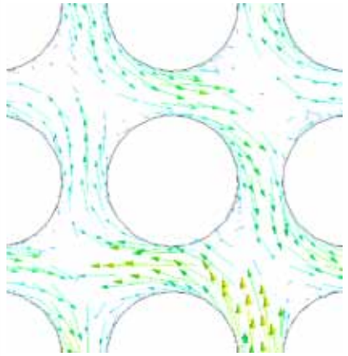


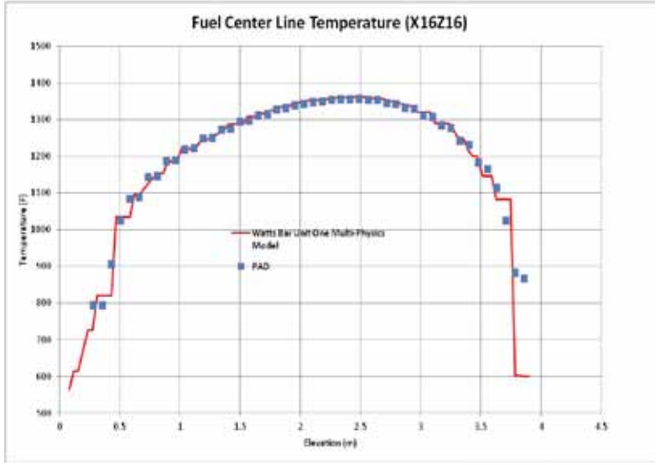


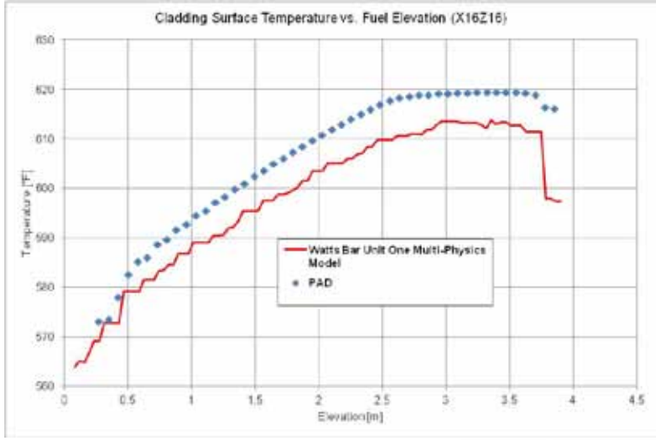
WBM2







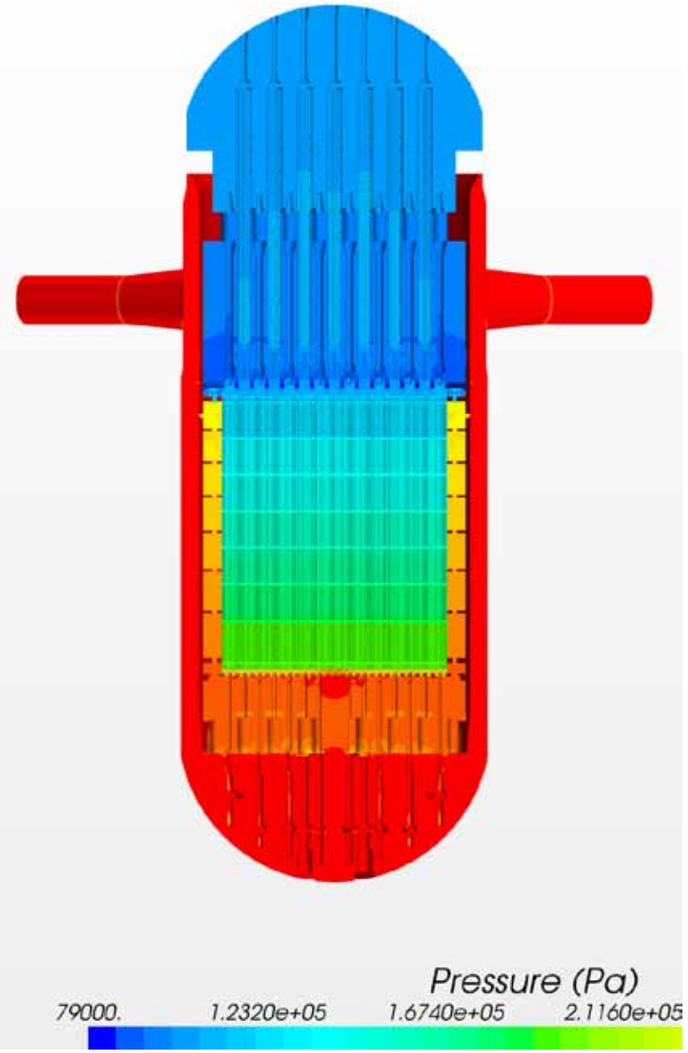


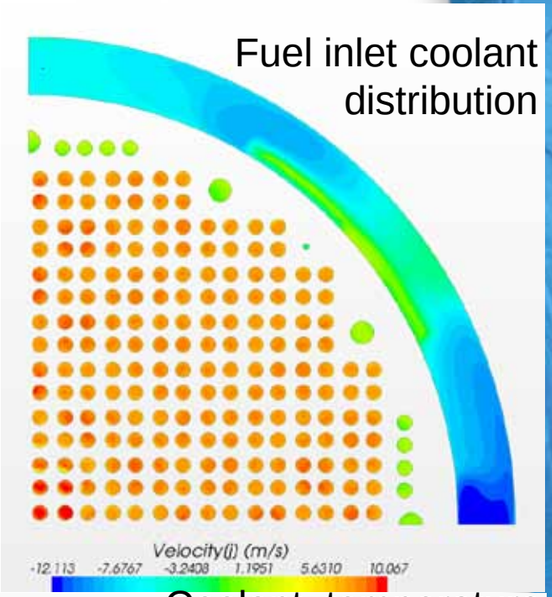


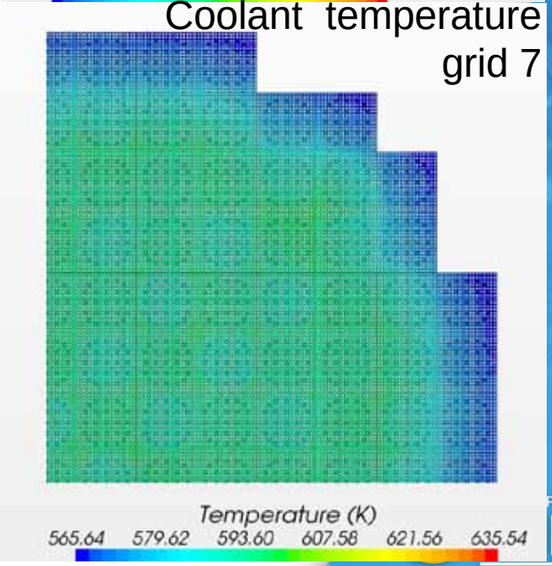
4 Loop Westinghouse PWR Multi-Physics Model Development

Benefits

- Local T&H conditions such as pressure, velocity, cross flow magnitude can be used to address challenge problems:
  - o GTRF
  - o FAD
  - o GSI-191
- The design TH questions under normal operating and accident conditions such as:
  - o Lower plenum flow anomaly
  - o Pressure drop
  - o Turbulence mixing coefficients input to channel code
  - o Lift force
  - o Cross flow between fuel assemblies
  - o Bypass flow
- The local low information can be used as boundary conditions for micro scale models.
- Local thermal conditions such as temperature and two phase flow can be used to address challenge problems:
  - CRUD
  - PCI
  - DNB
  - Cladding integrity during LOCA
  - AOA (Axial Offset Anomaly, boron hide out in crud)
- The normal design question can also be addressed:
  - Fuel center line temperature
  - Cladding hot spot
  - Gray rod center temperature
  - Thermal mixing at hot leg
- Provide Thermal boundary conditions for Micro scale models

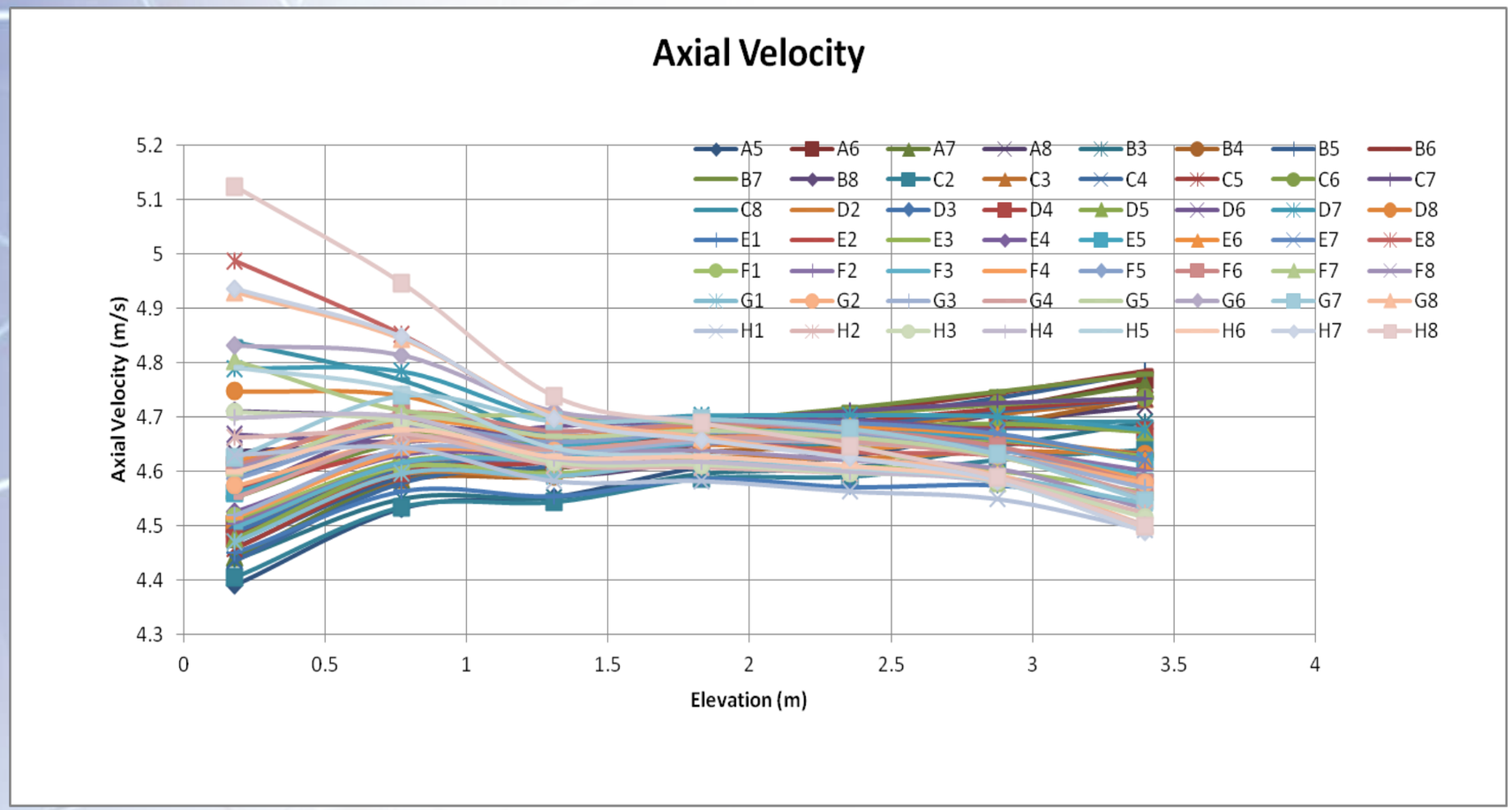




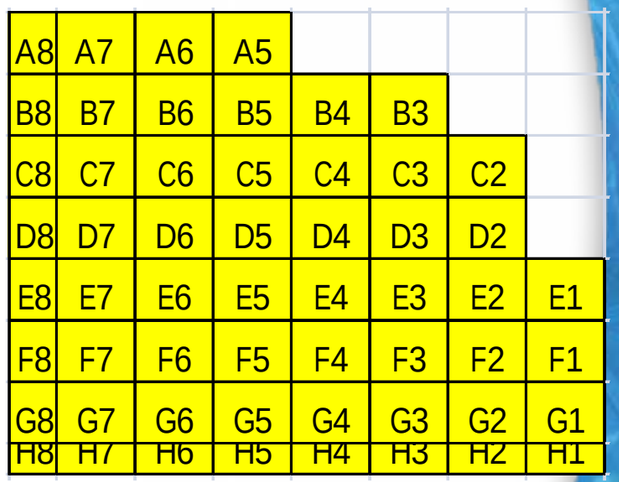


4 Loop Westinghouse PWR Multi-Physics Model Development

Automated assembly based average

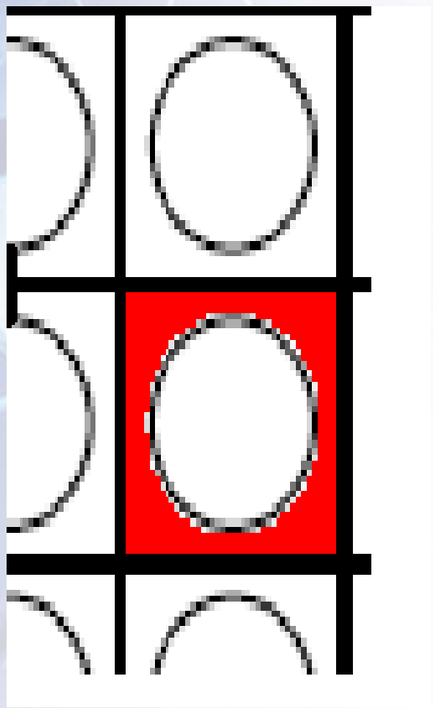


Core map



4 Loop Westinghouse PWR Multi-Physics Model Development

Automated rod based average cross flow evaluation for GTRF



	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1
A	0.56	0.60	0.73	0.59	0.71	0.72	0.66	0.70	0.71	0.65	0.61	0.65	0.65	0.69	0.60	0.72	0.52
B	0.72	0.88	0.80	0.75	0.82	0.76	0.75	0.78	0.75	0.75	0.84	0.79	0.75	0.77	0.78	0.81	0.68
C	0.79	0.81	0.89	0.76	0.73	0.73	0.84	0.74	0.73	0.75	0.81	0.71	0.83	0.76	0.70	0.81	0.72
D	0.77	0.80	0.81	0.72	0.70	0.83	0.77	0.67	0.82	0.75	0.65	0.76	0.77	0.73	0.75	0.79	0.59
E	0.78	0.86	0.78	0.70	0.84	0.86	0.74	0.81	0.81	0.73	0.77	0.83	0.62	0.74	0.79	0.75	0.68
F	0.83	0.85	0.68	0.84	0.80	0.73	0.83	0.86	0.76	0.86	0.81	0.70	0.78	0.79	0.72	0.80	0.65
G	0.79	0.71	0.83	0.76	0.70	0.81	0.78	0.63	0.80	0.78	0.67	0.81	0.78	0.62	0.72	0.79	0.62
H	0.79	0.81	0.88	0.72	0.81	0.85	0.74	0.79	0.86	0.76	0.79	0.83	0.73	0.81	0.83	0.75	0.67
I	0.90	0.82	0.75	0.85	0.87	0.76	0.85	0.79	0.75	0.83	0.89	0.73	0.84	0.82	0.71	0.80	0.72
J	0.78	0.76	0.86	0.79	0.70	0.81	0.77	0.70	0.84	0.78	0.64	0.79	0.79	0.63	0.78	0.80	0.54
K	0.77	0.83	0.82	0.66	0.76	0.81	0.73	0.80	0.84	0.71	0.78	0.82	0.72	0.76	0.78	0.72	0.71
L	0.84	0.84	0.75	0.84	0.77	0.75	0.80	0.80	0.76	0.87	0.81	0.71	0.77	0.80	0.70	0.82	0.69
M	0.85	0.70	0.81	0.77	0.59	0.83	0.80	0.65	0.78	0.81	0.73	0.83	0.81	0.68	0.77	0.87	0.65
N	0.73	0.80	0.82	0.71	0.76	0.78	0.70	0.76	0.84	0.72	0.76	0.83	0.73	0.74	0.76	0.79	0.67
O	0.90	0.84	0.74	0.80	0.86	0.72	0.86	0.85	0.77	0.82	0.85	0.69	0.85	0.80	0.86	0.81	0.72
P	0.74	0.81	0.91	0.77	0.78	0.82	0.82	0.67	0.84	0.78	0.72	0.79	0.87	0.75	0.79	0.85	0.61
Q	0.49	0.77	0.89	0.73	0.79	0.80	0.79	0.73	0.97	0.84	0.75	0.82	0.82	0.66	0.86	0.63	0.47

	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1
A	3.62	3.85	4.22	4.28	4.14	4.21	4.21	4.25	4.06	4.23	4.11	4.24	4.15	4.42	4.11	4.07	3.59
B	4.20	5.03	4.83	4.86	4.75	4.63	4.81	4.76	4.54	4.74	4.74	4.67	4.81	4.82	4.86	4.62	3.66
C	4.53	5.01	5.04	4.83	4.73	4.14	4.89	4.66	4.08	4.79	4.74	4.15	4.75	4.71	4.87	4.71	4.25
D	4.61	5.03	4.80	4.05	4.66	4.72	4.92	4.96	4.76	4.99	4.95	4.75	4.60	4.00	4.71	4.80	4.15
E	4.50	4.98	4.85	4.74	4.90	4.79	4.96	5.02	4.91	4.96	4.96	4.83	4.84	4.66	4.75	4.75	4.25
F	4.58	4.83	4.21	4.80	4.81	4.24	4.83	4.75	4.22	4.80	4.83	4.20	4.89	4.69	4.13	4.65	4.13
G	4.61	4.89	4.83	4.99	5.01	4.85	4.98	4.99	4.79	4.98	5.00	4.83	5.00	4.94	4.78	4.78	4.30
H	4.59	4.99	4.84	4.93	4.95	4.77	4.94	4.88	4.73	4.90	4.95	4.87	4.94	4.95	4.88	4.78	4.15
I	4.43	4.79	4.18	4.78	4.86	4.28	4.83	4.74	4.31	4.95	4.73	4.18	4.83	4.73	4.23	4.70	4.22
J	4.70	4.91	4.81	4.97	4.96	4.80	4.91	4.93	4.82	4.96	4.94	4.82	4.90	4.92	4.71	4.78	4.21
K	4.54	4.91	4.81	4.93	4.88	4.79	4.97	4.95	4.77	4.89	4.97	4.80	4.95	4.99	4.71	4.76	4.22
L	4.55	4.82	4.22	4.68	4.79	4.19	4.80	4.71	4.25	4.77	4.80	4.15	4.77	4.76	4.14	4.68	4.14
M	4.56	4.94	4.88	4.63	4.78	4.82	4.96	4.94	4.85	4.93	4.96	4.79	4.93	4.62	4.70	4.78	4.25
N	4.65	5.06	4.85	4.14	4.63	4.73	5.00	4.91	4.76	4.95	4.93	4.79	4.73	4.08	4.75	4.87	4.11
O	4.54	5.00	5.00	4.81	4.72	4.15	4.81	4.81	4.26	4.82	4.77	4.13	4.79	4.89	5.01	4.93	4.32
P	4.22	4.90	5.06	5.01	4.87	4.79	4.94	4.92	4.87	4.89	4.94	4.79	4.95	4.99	5.03	5.10	4.25
Q	4.03	4.37	4.63	4.64	4.64	4.53	4.58	4.59	4.57	4.59	4.63	4.56	4.61	4.58	4.58	4.05	3.57

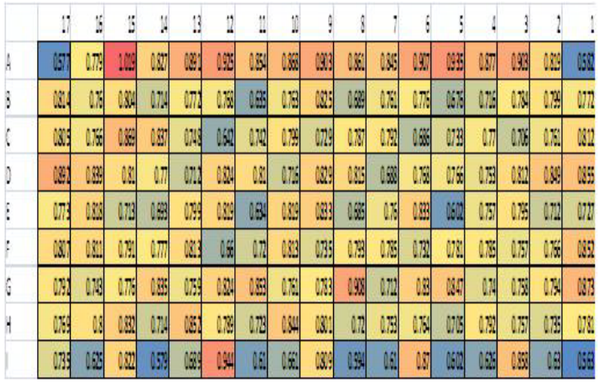
Fuel Assembly downstream of Mid-Grid 5

4 Loop Westinghouse PWR Multi-Physics Model Development

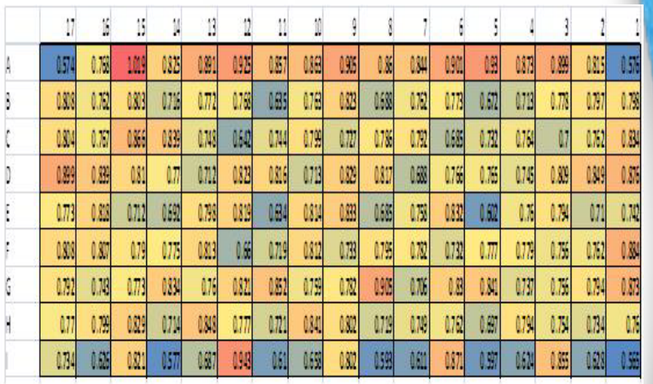
- **By evaluating the averaged cross flow magnitude, the high cross flow rod is identified in pink area.**

Rod_id	Elevation				Averaged Cross Flow	Maximum Cross Flow	Pressure	
H6_A15	2.876	-0.408	4.388	-0.106	1.019	1.819126321.5	0	
H2_A15	2.876	-0.417	4.407	-0.108	1.019	1.817126174.4	0	
H5_A15	2.876	-0.409	4.386	-0.106	1.018	1.819126287.7	0	
H3_A15	2.876	-0.409	4.39	-0.106	1.018	1.818126203.8	0	
H7_A15	2.876	-0.417	4.433	-0.11	1.016	1.821126341.1	0	
H4_A15	2.876	-0.41	4.404	-0.107	1.016	1.819126243.6	0	
A8_Q03	3.398	0.438	4.668	0.28	1.007	1.874114902.7	0	
B8_O09	2.876	-0.045	4.021	-0.621	1.006	2.219125705.2	0	
C8_O09	2.876	-0.04	4.009	-0.619	1.005	2.232125961.6	0	
B8_Q03	3.398	0.405	4.594	0.258	1.002	1.887115196.4	0	
A8_Q07	3.398	0.399	4.613	0.126	1.001	1.934115034.1	0	
D8_O09	2.876	-0.038	3.988	-0.614	0.999	2.226126273.8	0	
H1_A15	2.876	-0.404	4.413	-0.13	0.994	1.814126235.3	0	
E8_O09	2.876	-0.041	3.955	-0.611	0.991	2.198126591.9	0	
C8_Q03	3.398	0.4	4.525	0.256	0.988	1.876115716.6	0	
C8_A07	3.398	-0.373	4.453	-0.21	0.988	1.765115251.6	0	
B8_Q07	3.398	0.409	4.571	0.163	0.985	1.906115311.4	0	
F8_O09	2.876	-0.045	3.927	-0.605	0.982	2.164126847.2	0	
D8_A07	3.398	-0.366	4.386	-0.206	0.981	1.731115788.8	0	
H8_A03	1.31	-0.472	4.673	-0.057	0.98	1.893154313.4	0	

- High cross flow fuel assemblies



Fuel Assembly H2 downstream of Mid-Grid 5



Fuel Assembly H6 downstream of Mid-Grid 5

	10	9	8	7	6	5	4	3	2	1
A		0.514	0.855	0.921	0.811	0.785	0.795	0.829	0.78	0.587
B		0.604	0.743	0.868	0.762	0.759	0.832	0.862	0.809	0.885
C		0.892	0.82	0.866	0.786	0.769	0.843	0.774	0.835	0.918
D		0.71	0.791	0.738	0.843	0.768	0.794	0.852	0.816	0.831
E		0.584	0.759	0.865	0.826	0.563	0.815	0.808	0.709	0.908
F		0.897	0.85	0.819	0.727	0.842	0.834	0.731	0.809	0.92
G		0.621	0.835	0.741	0.829	0.797	0.684	0.807	0.787	0.832
H		0.616	0.725	0.854	0.789	0.761	0.824	0.853	0.64	0.881
I		0.871	0.807	0.858	0.787	0.841	0.833	0.719	0.854	0.869
J		0.733	0.82	0.776	0.805	0.775	0.684	0.847	0.798	0.887
K		0.56	0.723	0.85	0.824	0.663	0.808	0.735	0.647	0.847
L		0.894	0.802	0.846	0.756	0.803	0.839	0.709	0.793	0.931
M		0.624	0.897	0.761	0.822	0.824	0.699	0.751	0.784	0.895
N		0.609	0.715	0.824	0.737	0.755	0.722	0.791	0.768	0.874
O		1.006	0.791	0.822	0.753	0.751	0.823	0.857	0.824	0.872
P		0.731	0.824	0.809	0.732	0.813	0.824	0.828	0.761	0.795
Q		0.66	0.843	0.979	0.886	0.816	0.85	0.881	0.637	0.658

Fuel Assembly B8 of downstream Mid-Grid 5

	10	9	8	7	6	5	4	3	2	1
A		0.551	0.887	0.978	0.892	0.92	0.868	0.959	0.832	0.564
B		0.515	0.698	0.804	0.712	0.67	0.728	0.827	0.772	0.808
C		0.785	0.796	0.799	0.651	0.724	0.781	0.702	0.795	0.923
D		0.663	0.772	0.718	0.758	0.858	0.617	0.77	0.793	0.881
E		0.53	0.746	0.779	0.774	0.564	0.761	0.757	0.675	0.891
F		0.794	0.739	0.697	0.577	0.814	0.761	0.638	0.733	0.929
G		0.625	0.824	0.69	0.785	0.754	0.624	0.777	0.808	0.895
H		0.623	0.667	0.768	0.764	0.697	0.784	0.771	0.636	0.89
I		0.844	0.781	0.701	0.667	0.731	0.773	0.584	0.793	0.869
J		0.682	0.808	0.707	0.737	0.781	0.715	0.822	0.804	0.931
K		0.543	0.682	0.779	0.777	0.637	0.79	0.761	0.637	0.889
L		0.818	0.743	0.74	0.633	0.753	0.761	0.561	0.695	0.928
M		0.558	0.834	0.719	0.764	0.791	0.655	0.712	0.738	0.974
N		0.542	0.611	0.77	0.705	0.706	0.59	0.737	0.742	0.922
O		0.711	0.7	0.716	0.615	0.732	0.766	0.828	0.733	0.92
P		0.562	0.799	0.75	0.727	0.762	0.756	0.792	0.731	0.867
Q		0.687	0.904	0.985	0.912	0.919	0.906	1.002	0.608	0.597

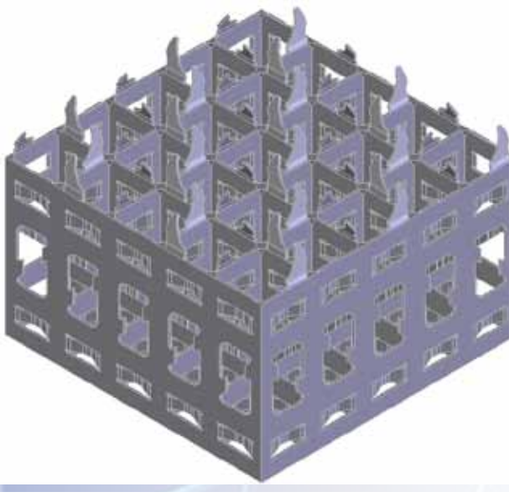
Fuel Assembly B8 downstream Mid-Grid 6

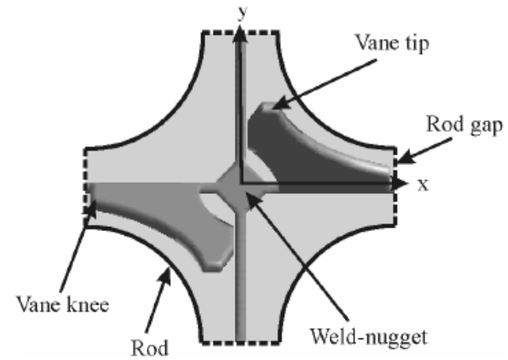
TH Validations

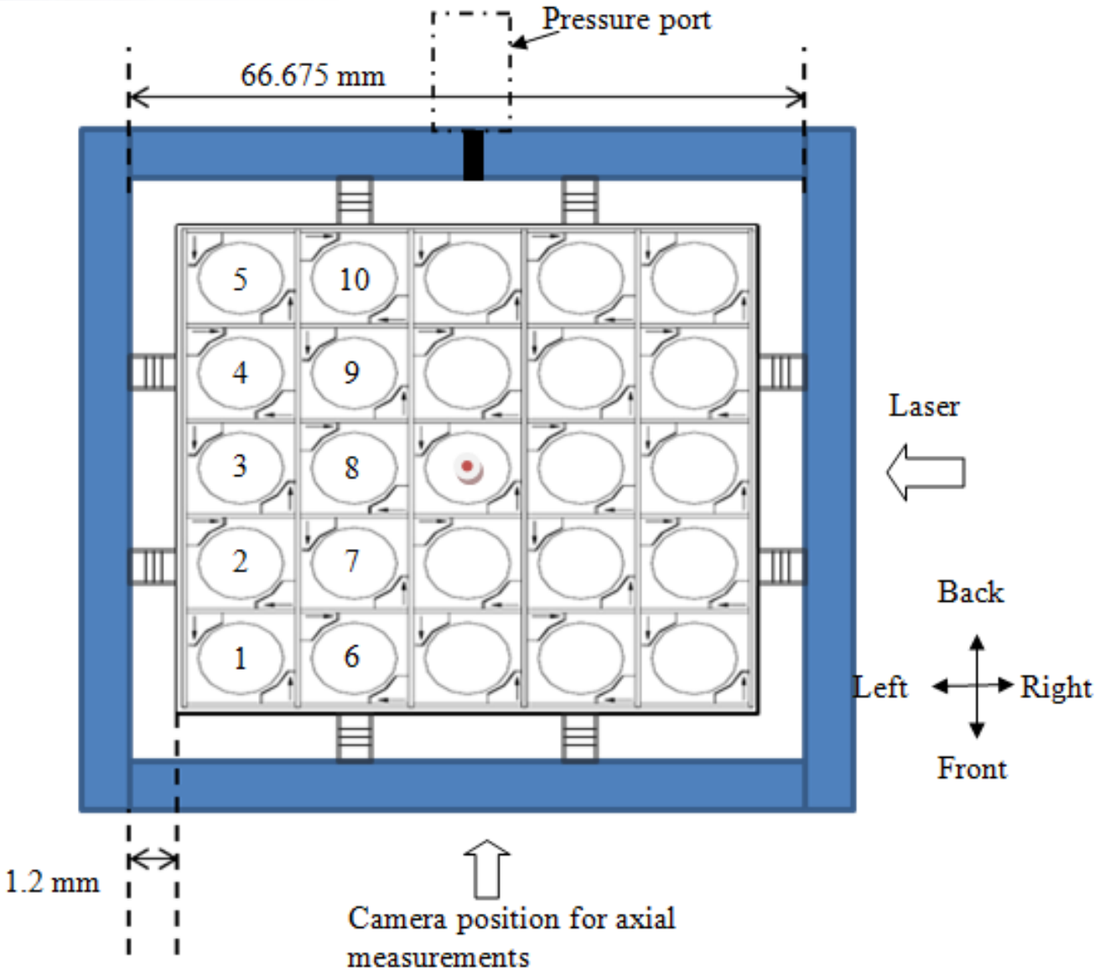
- Team
  - AMA: E. Popov (ORNL), B. Brewster (CD-Adapco), H. Zhang (INL), E. Baglietto (MIT)
  - THM: R. Lowrie (LANL), Y. Hassan (Texas A&M), E. Dominguez-Ontivero (Texas A&M), S. Pannala (ORNL), A. Stagg (ORNL)
- Four validation cases have been performed:
  - Case 1: Turbulent Pipe Flow (ORNL).
  - Case 2: Turbulent Flow in a U-bent Channel (ORNL).
  - Case 3: Flow in a 5 × 5 Rod Bundle with Spacer-Grids (WEC).
  - Case 4: Flow Passing Through a Heated Rod Bundle (INL).

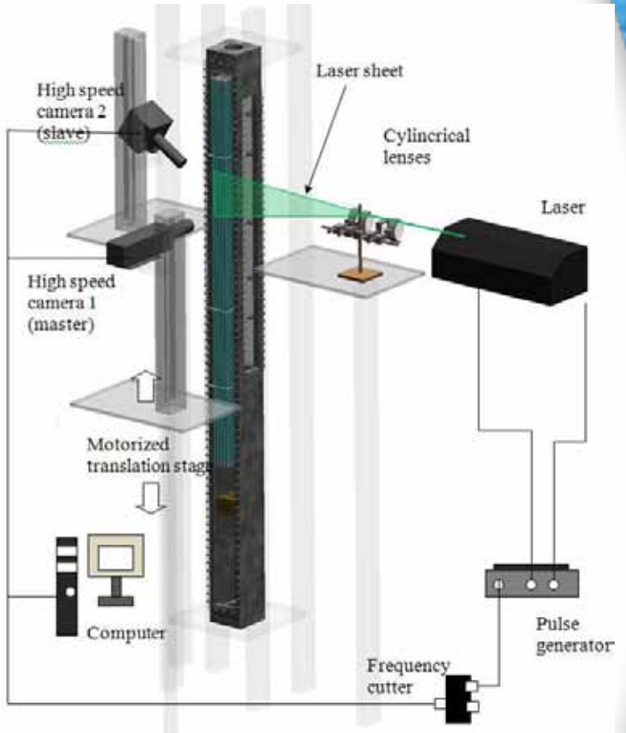
TH Validations

Texas A & M 5x5 Fuel Assembly Test



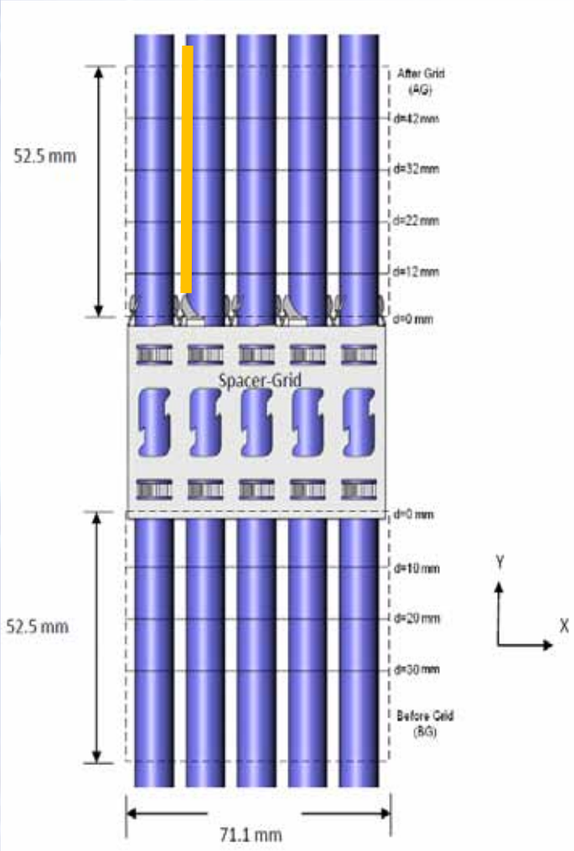


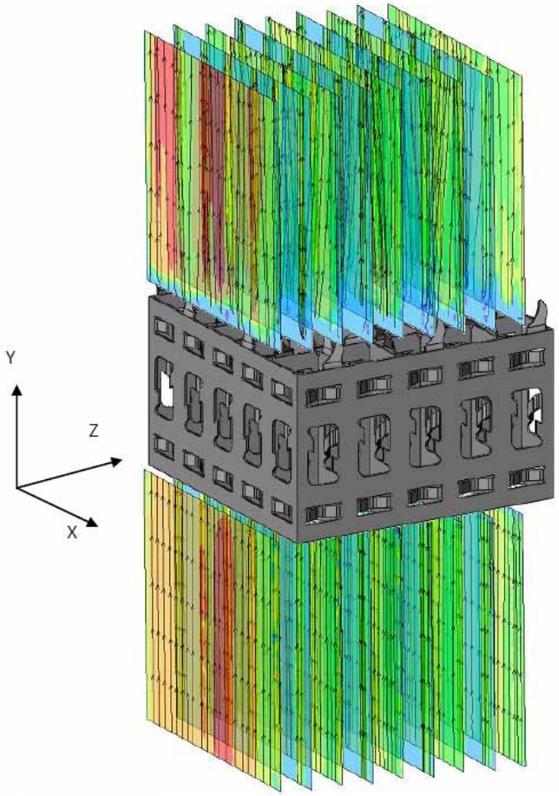


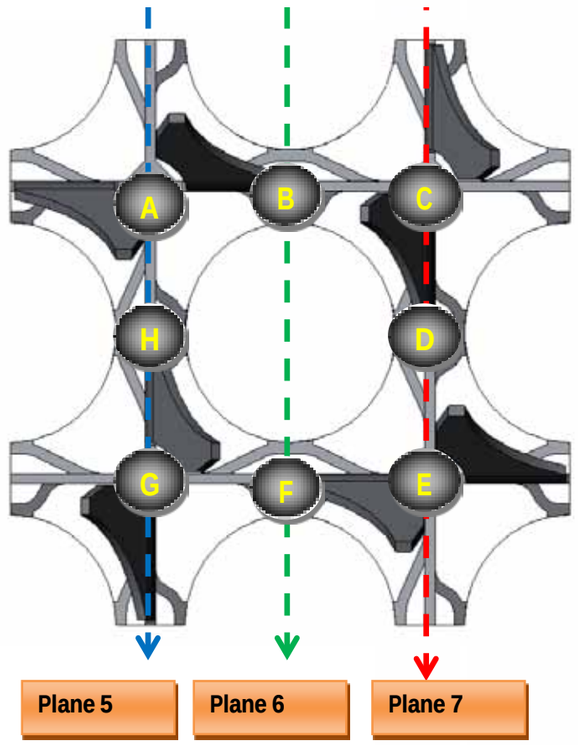


- **Motorized stages for measurements along the full span**
- **High repetition laser (20 KHz, l=527 nm, 10 mJ).**
- **High speed cameras: 800x600 pixels & 150,000 fps max., 14 bit.**

TH Validations



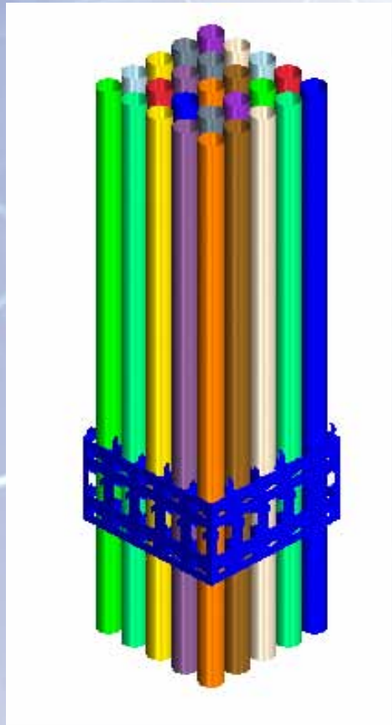


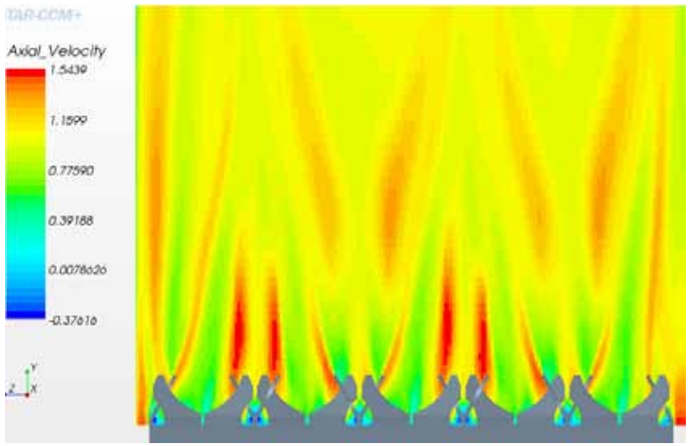


- PIV unsteady hydraulic measurement has been carried out on a spacer grid. The data is used to benchmark CFD models.

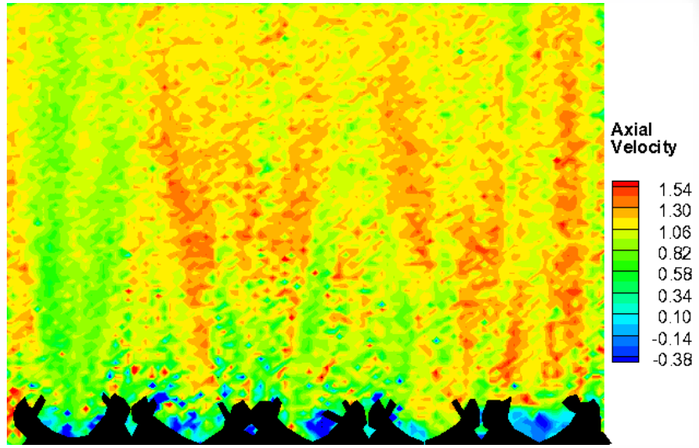
TH Validations

- CFD model and results comparisons

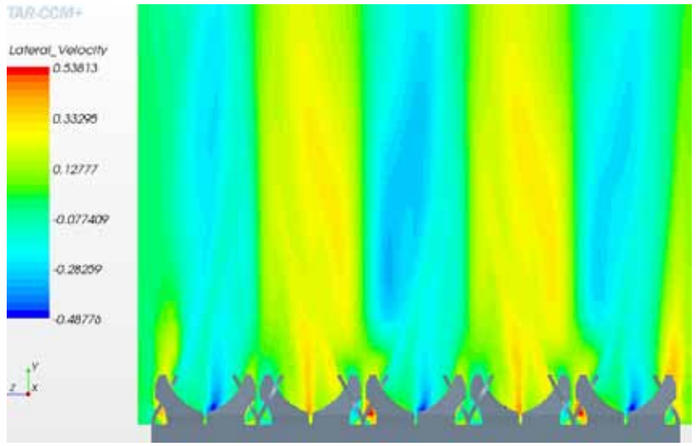




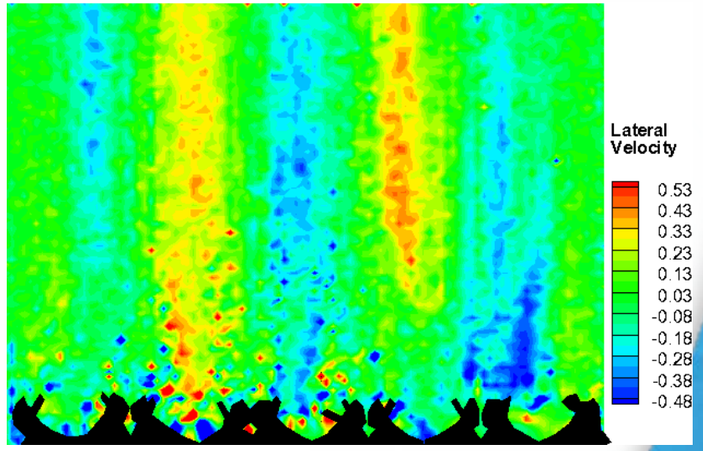
Axial velocity CFD. Plane 5 Re=28,000



Axial velocity Measured. Plane 5 Re=28,000



Lateral velocity CFD. Plane 5 Re=28,000



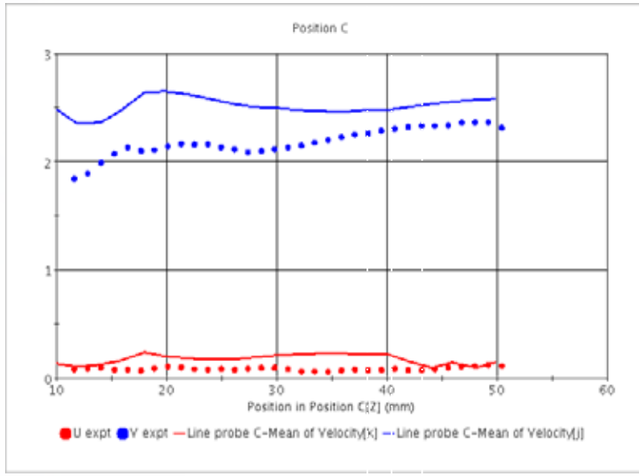
Lateral velocity Measured. Plane 5 Re=28,000

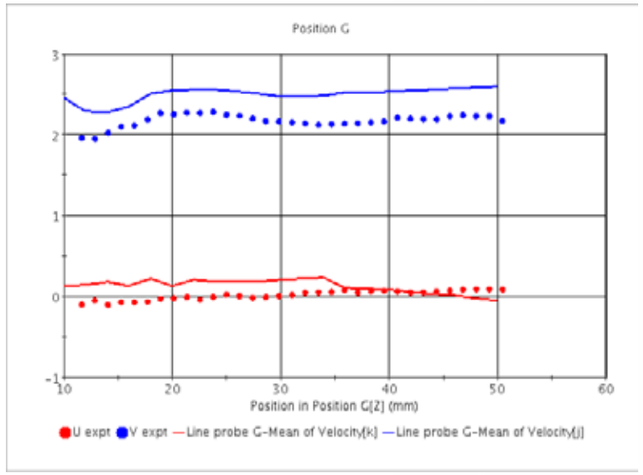
EDO

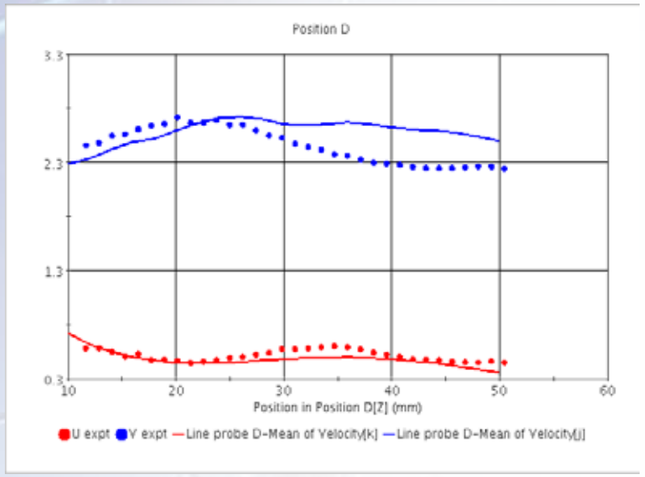
EDO

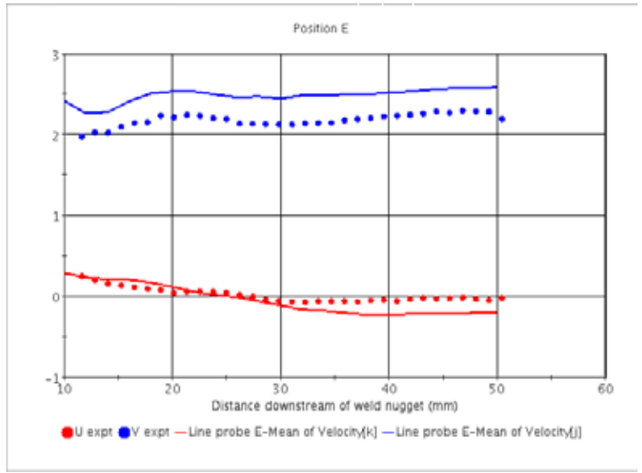
TH Validations

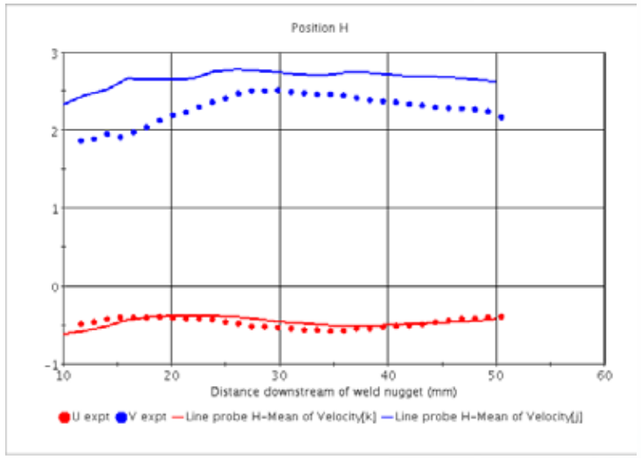
Time averaged line data comparisons





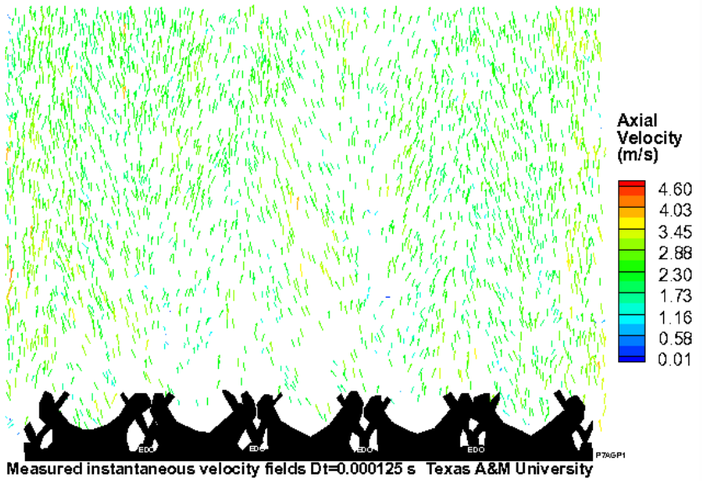




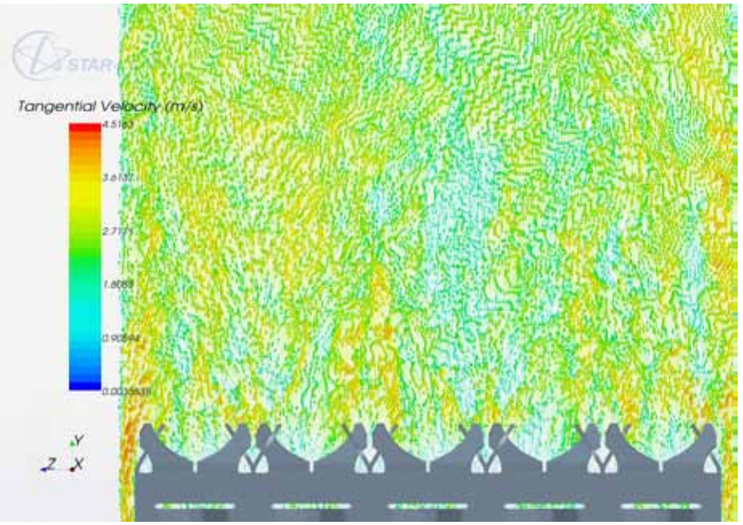


TH Validations

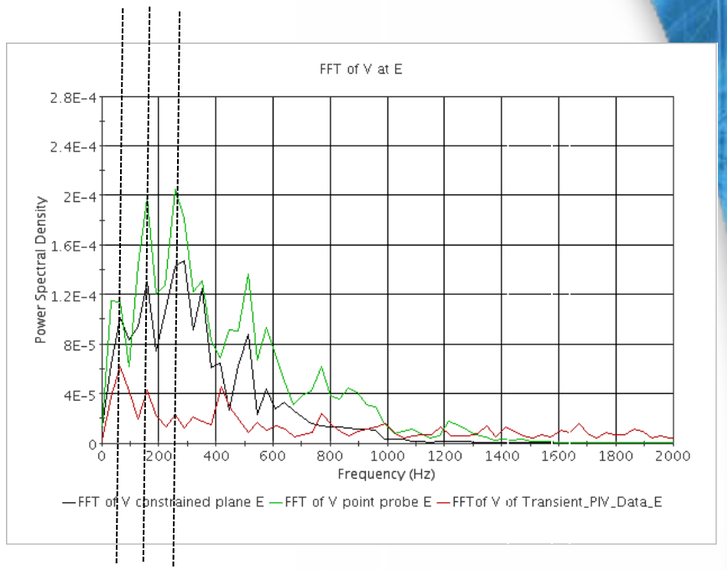
Transient data comparisons



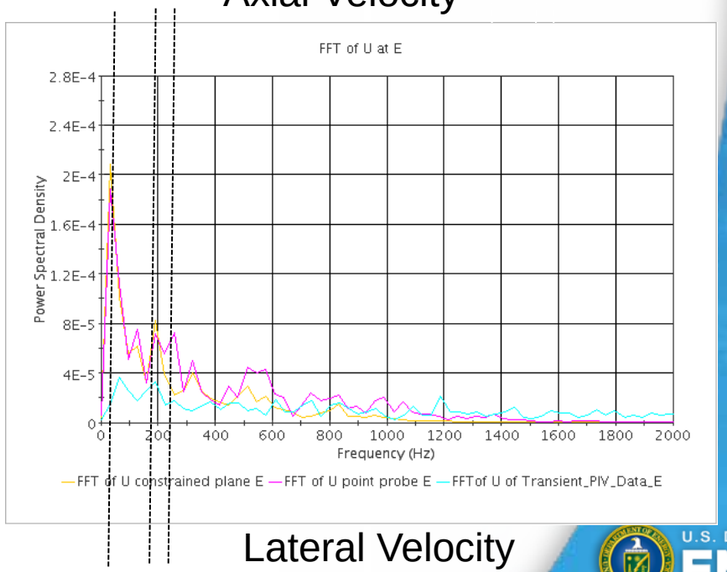
PIV data



CFD



Axial Velocity

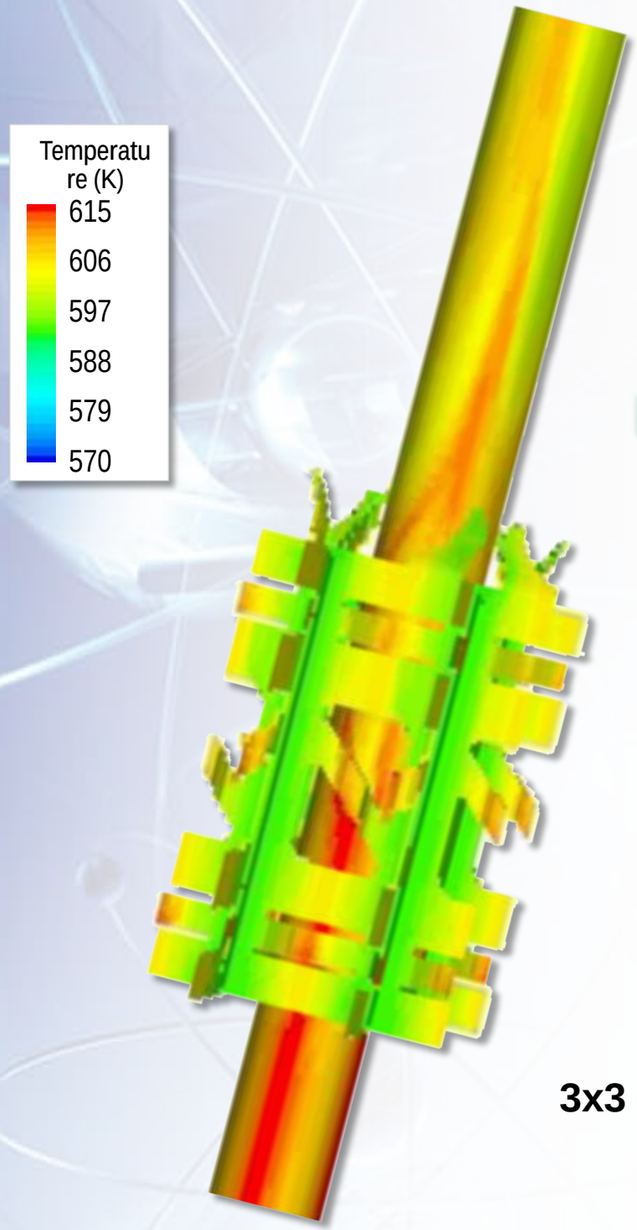


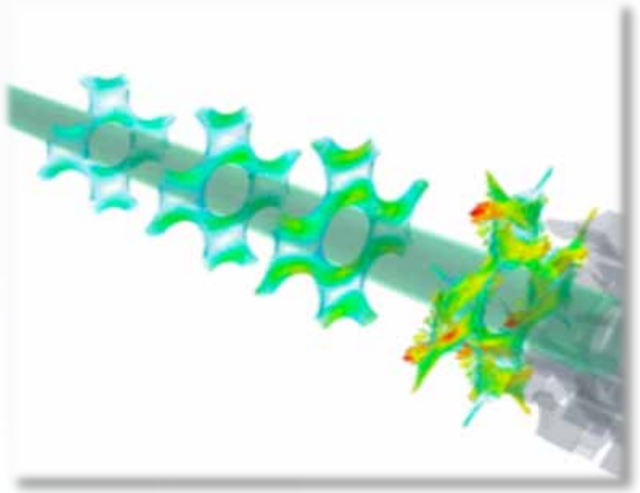
Lateral Velocity

Thermal Hydraulics & Neutronic Coupling

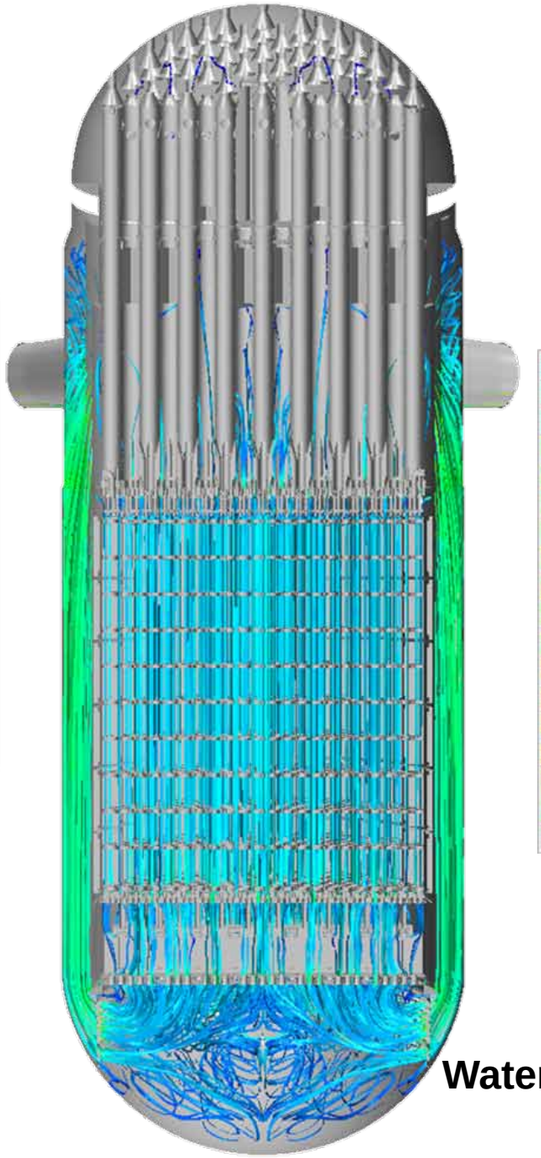
- Initial Development of StarCCM+ & DeCART coupling was carried out by AMA and UM. The coupling has also been implemented in VERA through LIME by VERA team.
- StarCCM+ & DeCART coupling on a state point has been accomplished based on Waterford quarter reactor and 3x3 fuel assembly.
- ANC & StarCCM+ coupling for a complete depletion cycle with 14 state points being performed.
- A quarter assembly CFD model and the corresponding DeCART model are ready for a state point coupling.

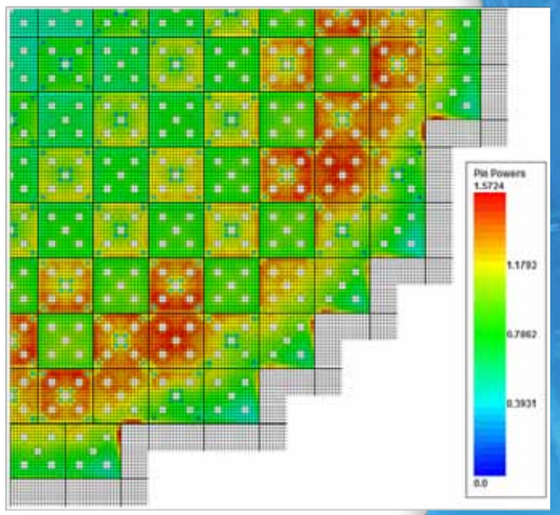
Thermal Hydraulics & Neutronic Coupling





3x3 coupling results

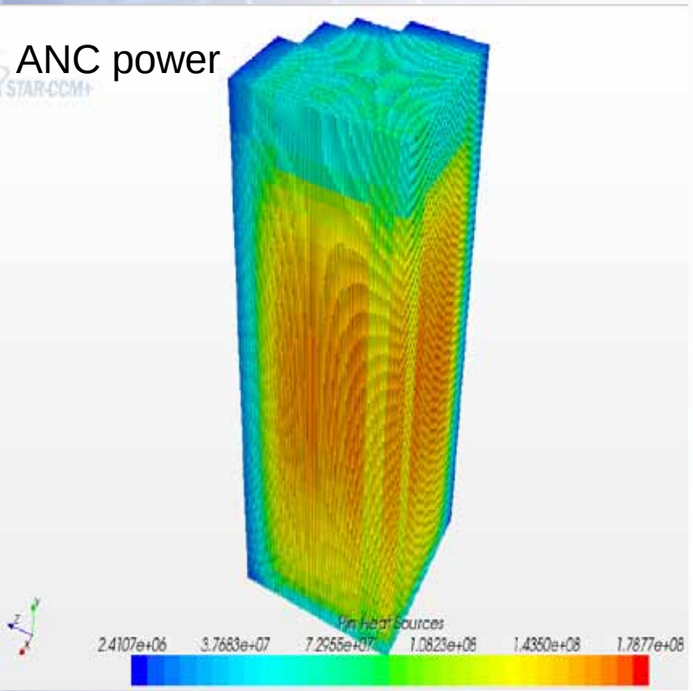


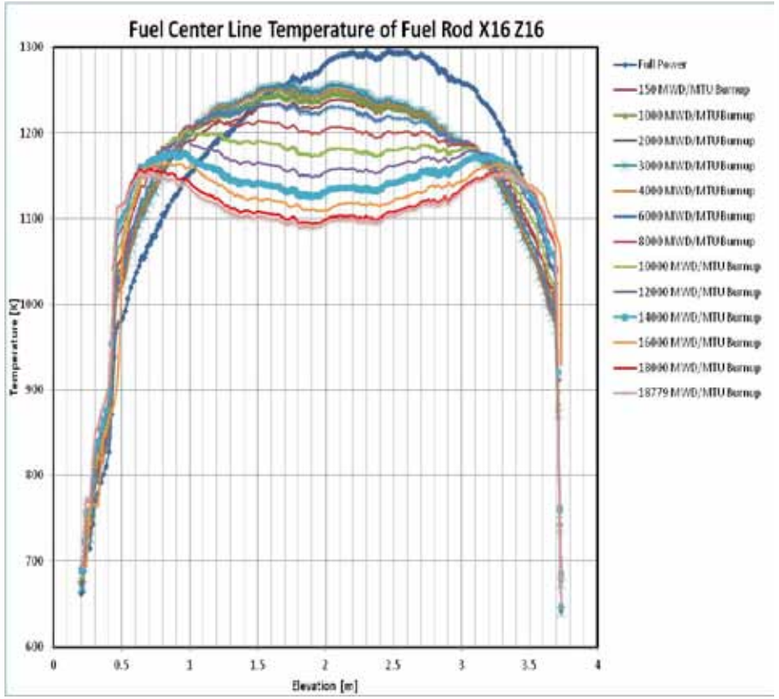


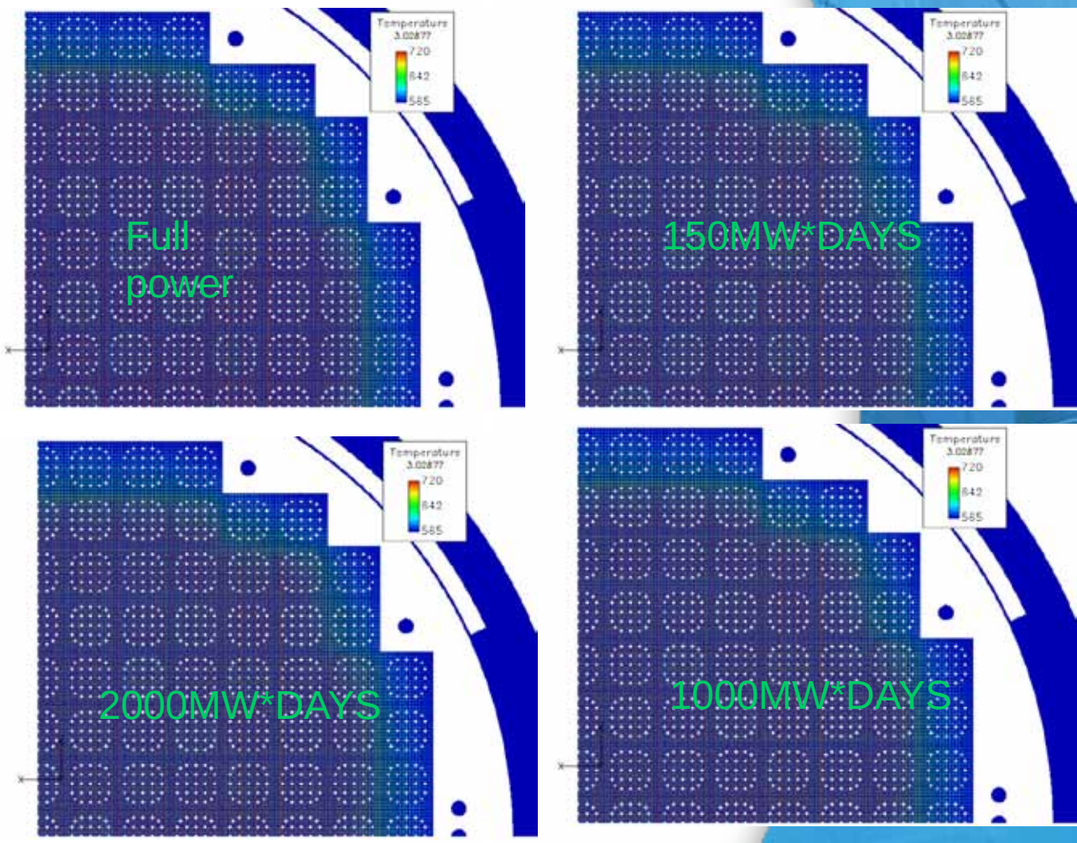
Waterford quarter core coupling results

Thermal Hydraulics & Neutronic Coupling

ANC & StarCCM+ full depletion cycle simulation: 14 state points, total time required for a complete depletion cycle: 44 hours on 1028 cores.







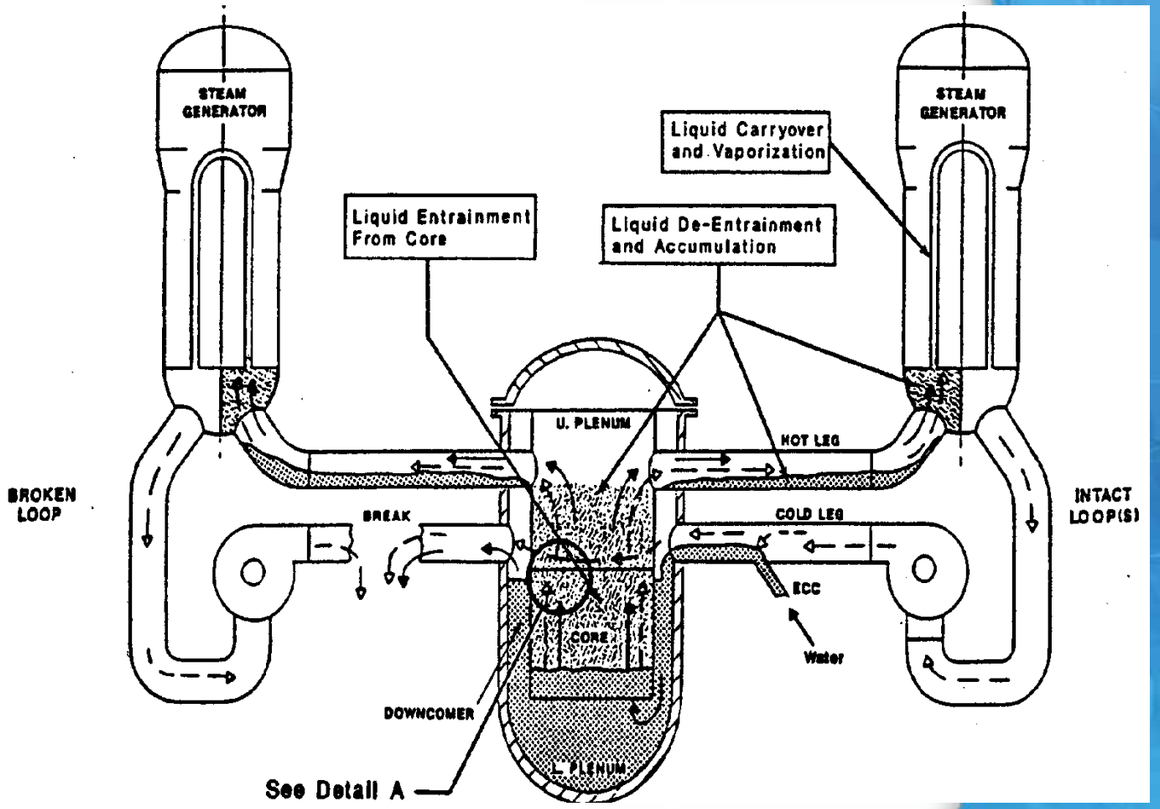
44 hours /per depletion-cycle **proves that high fidelity CFD & Neutronic coupling is practical for engineering design. The results will provide hot spot, boiling areas for CILC and crud simulation, fuel center line temperature, peak cladding temperature, and cross flow for GTRF.**

Thermal Hydraulics & Neutronic Coupling

- StarCCM+ & DeCART coupled depletion run
  - A Quarter fuel assembly StarCCM+ & DeCART coupled depletion run. Both the CFD and DeCART model has been ready for a month. However, VERA is not available on Fission or Jaguar. AMA is waiting for VERA to be installed on either system so that the coupling can be carried out for a state point. Then a depletion run may be carried out as soon as the new model is available in DeCART.
  - 3x3 assemblies StarCCM+ & DeCART coupled depletion run.
  - Watts Bar quarter core StarCCM+ & DeCART coupled depletion run.
- The Watts Bar quarter core TH & Neutronic coupling project has been delayed. At the current stage, the risk of NOT meeting the milestone this year is high!

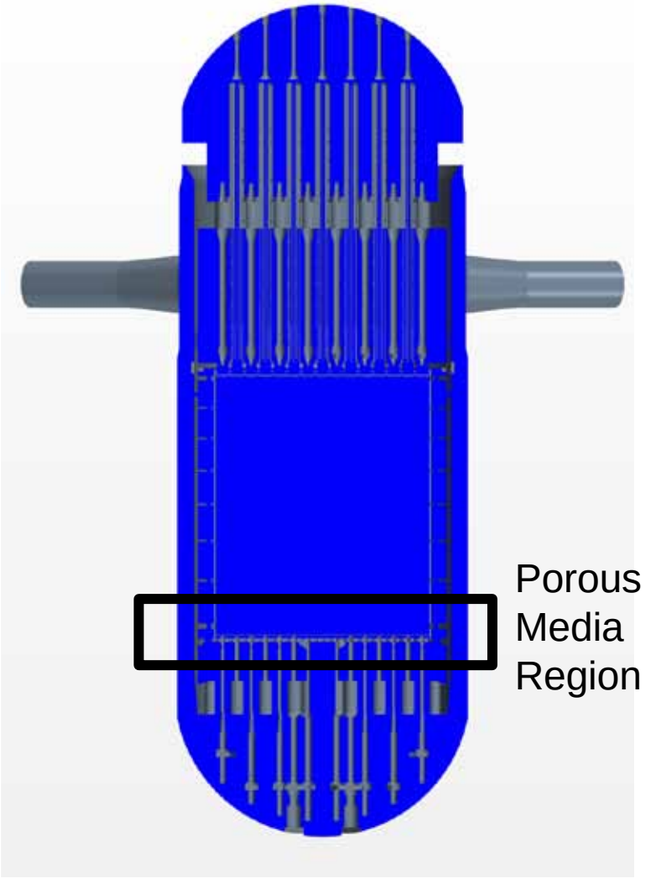
Industry Pilot Project: GSI-191

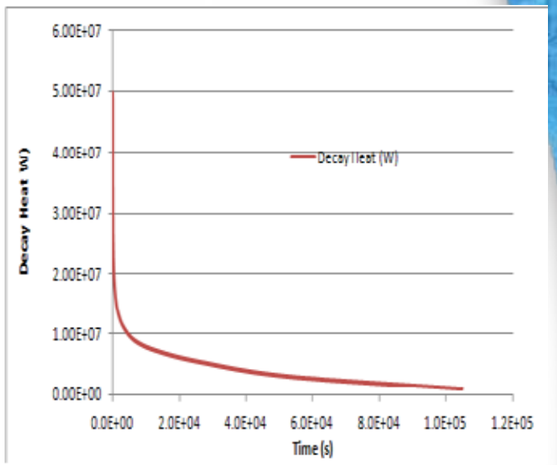
- LOCA: *Postulated accidents that result from the loss of reactor coolant at a rate in excess of the capability of the reactor coolant makeup system from breaks in the reactor coolant pressure boundary, up to and including a break equivalent in size to the double-ended rupture of the largest pipe of the reactor coolant system.*
- Long term cooling requirement:
  - Decay Heat Removal/Fuel Clad Oxidation: Maximum cladding temperatures maintained during periods when the core is covered will not exceed a core average cladding temperature of 800°F.
  - There is sufficient flow to replace core boil-off (Most important, if this is met, the above point will be met).



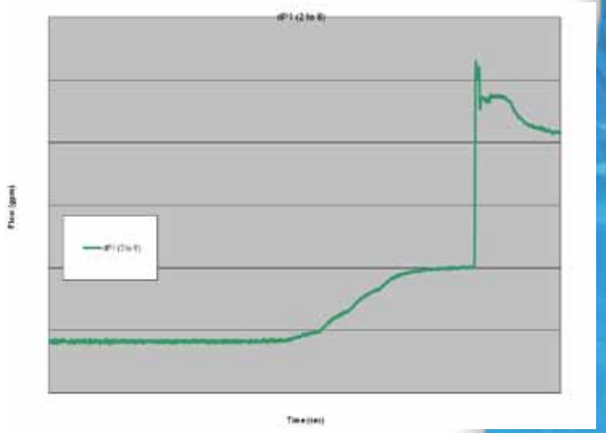
Industry Pilot Project: GSI-191

- Significant amount of effort has been spent in looking for the correct boundary conditions.
- An initial model has been constructed to test the ability of the software in modeling nature circulation.
- A full reactor model is under construction.





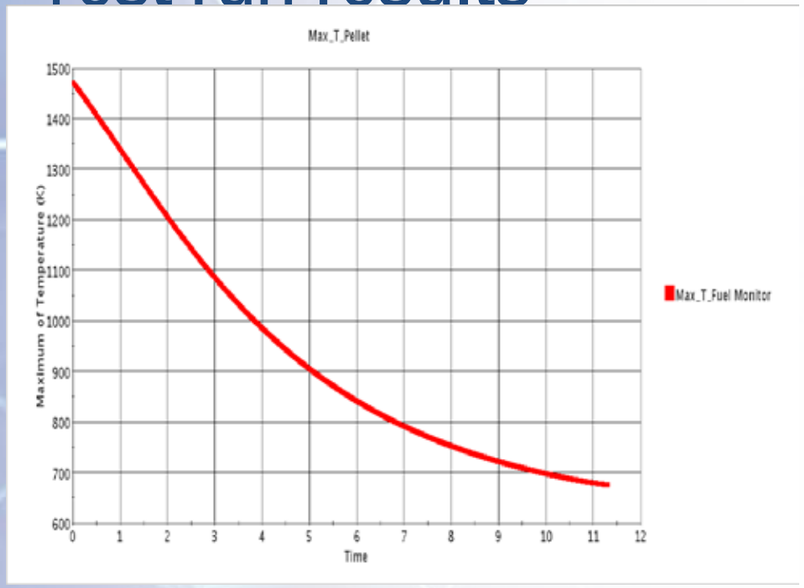
Decay heat

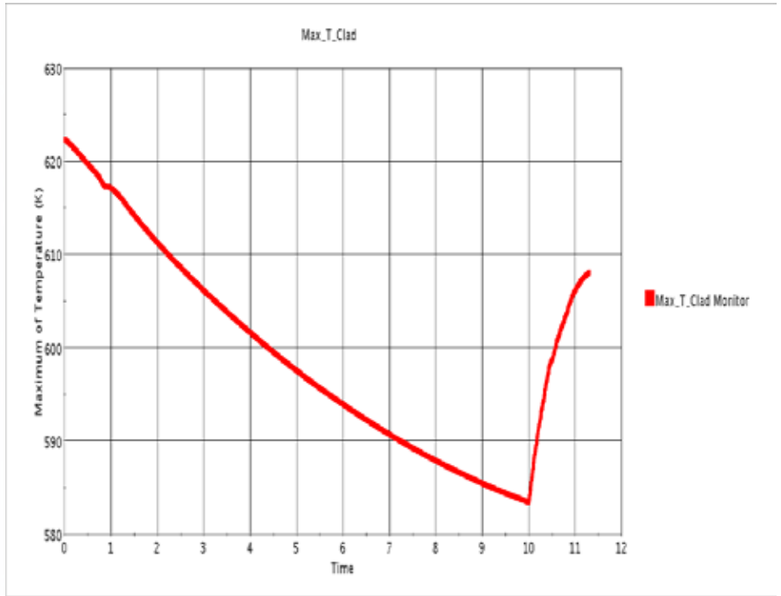


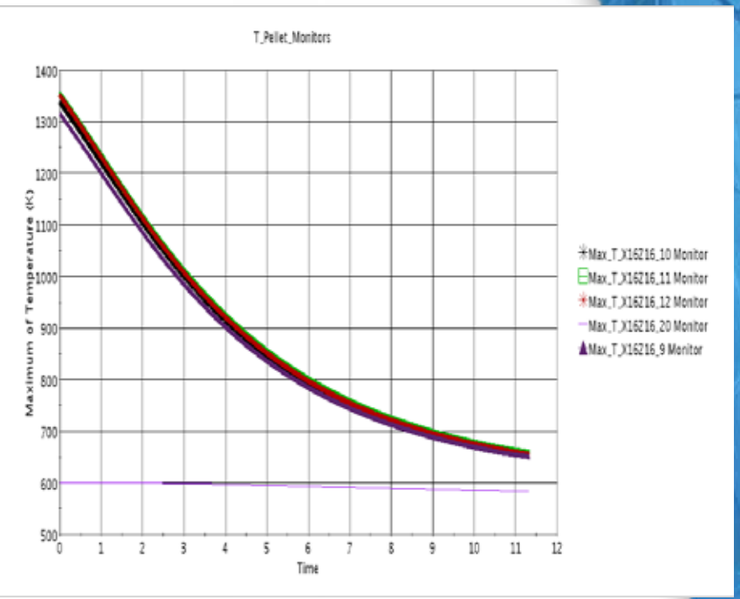
Pressure loss caused by debris

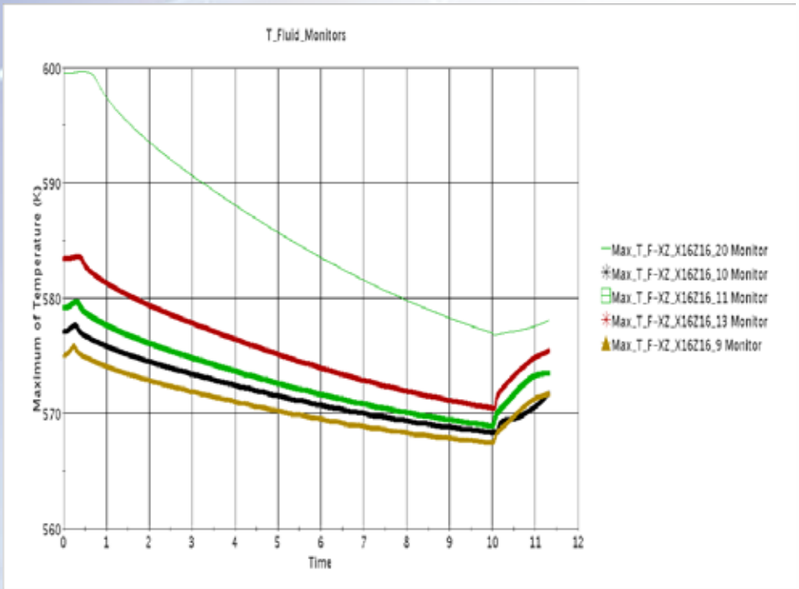
Industry Pilot Project: GSI-191

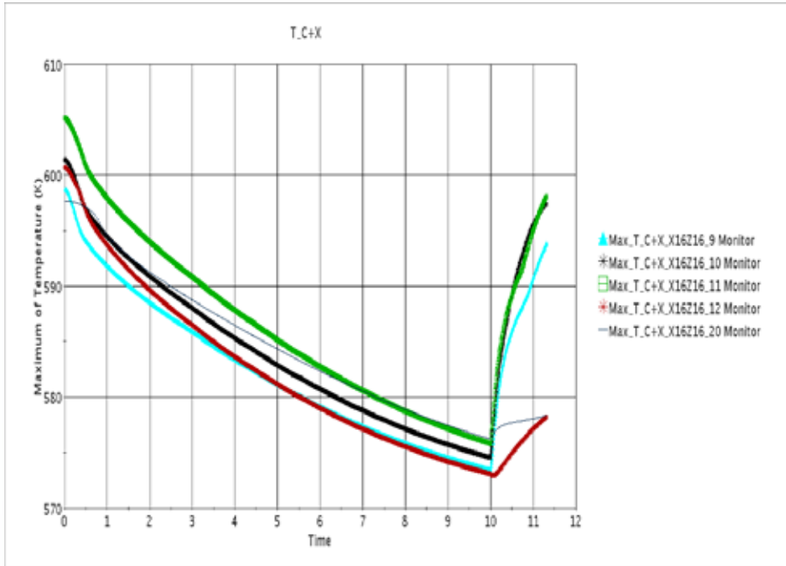
Test run results

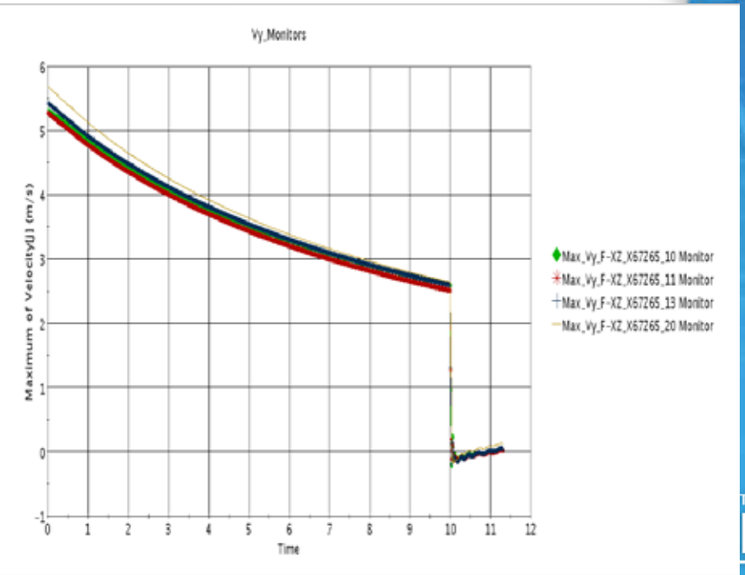












Summary

- AMA has completed many large scale industry focused projects by overcoming technical challenges and limit on resources
- Good progress made on Vessel Model CFD Development and running on HPC
- Is it feasible to perform fine mesh ¼ core multi-physics coupled analyses with full depletion using detailed vessel CFD model then zoom in to perform more detailed analysis ??
- TH validation is moving forward however need more data for two-phase flow validation
- Vessel CFD analysis for GSI-191 will be our first two-phase flow application supporting the Safety Challenge problem

PCMM Assessment for CASL

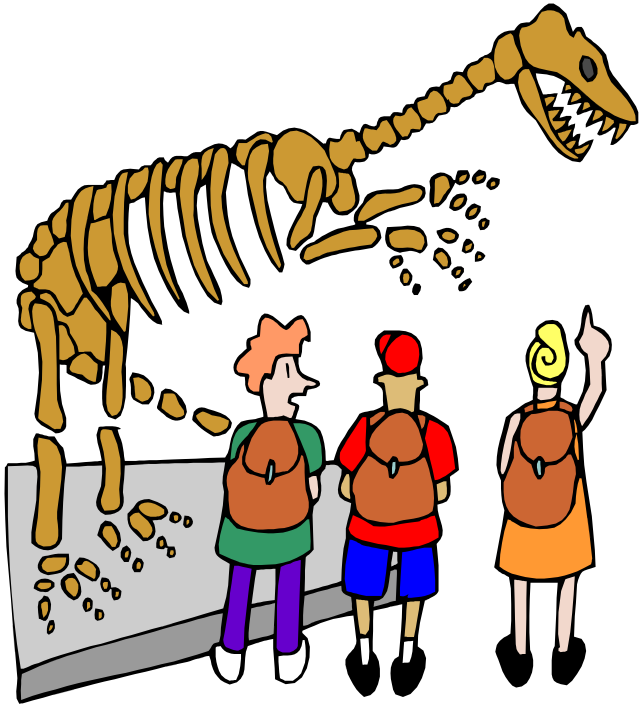
Bill Rider

2012 CASL Roundtable

June, 15 2012

"Progress, far from consisting in change, depends on retentiveness. Those who cannot remember the past are condemned to repeat it."

–George Santayana



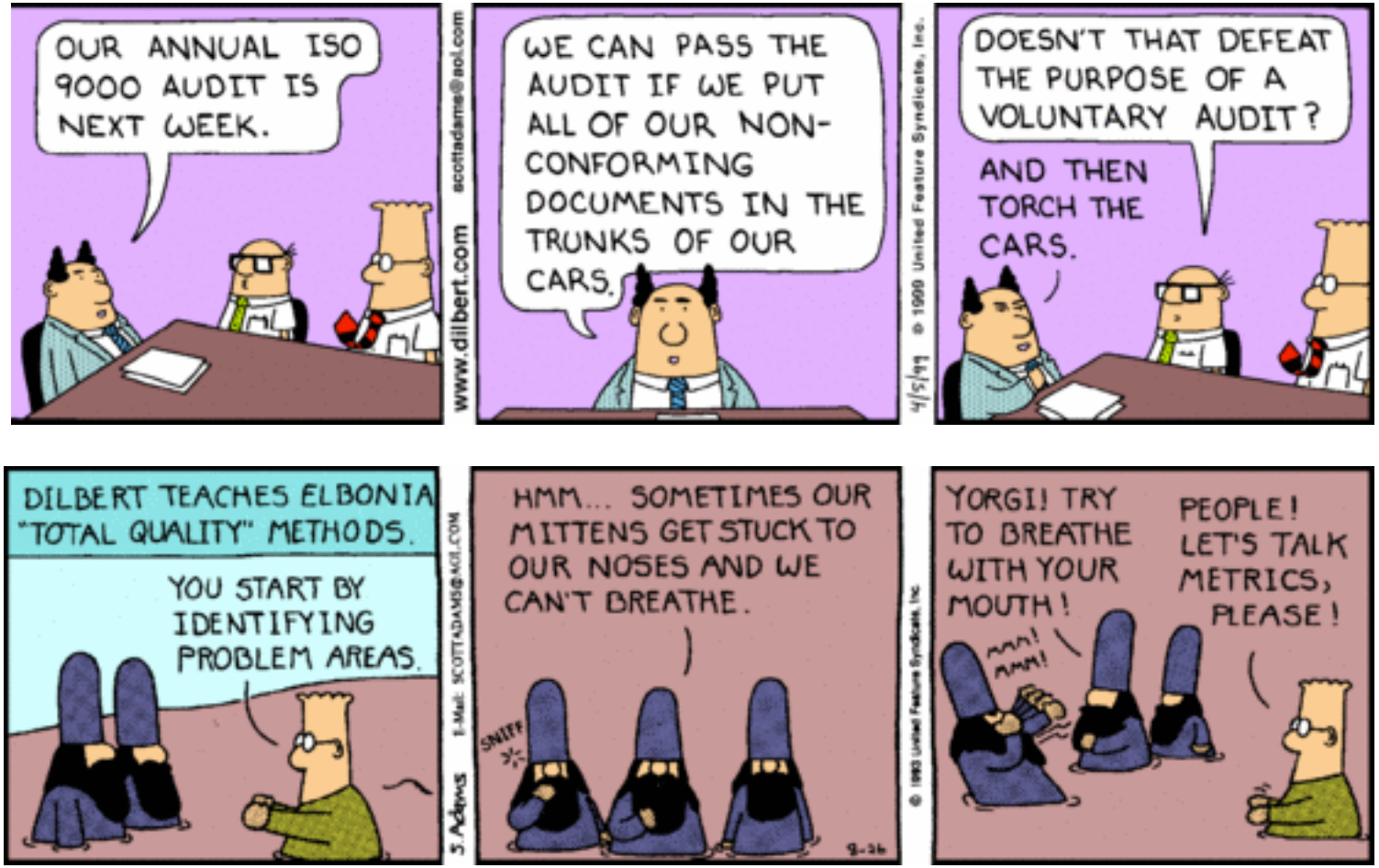
Outline

- Why we have restructured the approach to Simulation Quality (culture and human nature)
- Introduction to PCMM and Objectives
- PCMM Assessment (i.e., interview) process
- Recommendations and Issues generated

Summary for the PCMM Process

Our overall impression is that significant quality measures are implemented in the current analysis and development process. These measures should not be overlooked in the natural CASL emphasis and technical focus. CASL should be careful to not overlook existing quality measures in the development of enhanced capability associated with other aspects of the modeling.

A key issue is culture and basic human behavior toward audits, assessment, quality and metrics



ASC did some things and we can learn from their successes and failures

- What ASC did right.
  - Broad multi-disciplinary program, lots of $$$
  - *Integrated V&V (eventually)*
  - *SQA (eventually)*
- What ASC could have done better.
  - *Originally driven too much by high-end computing. Computer science focus was not application driven enough.*
  - ***Did not get sufficient code user community (i.e. designer/analyst) buy-in to the program's emphasis.***
  - Insufficiently integrated experimental program (with a negative impact on Validation).

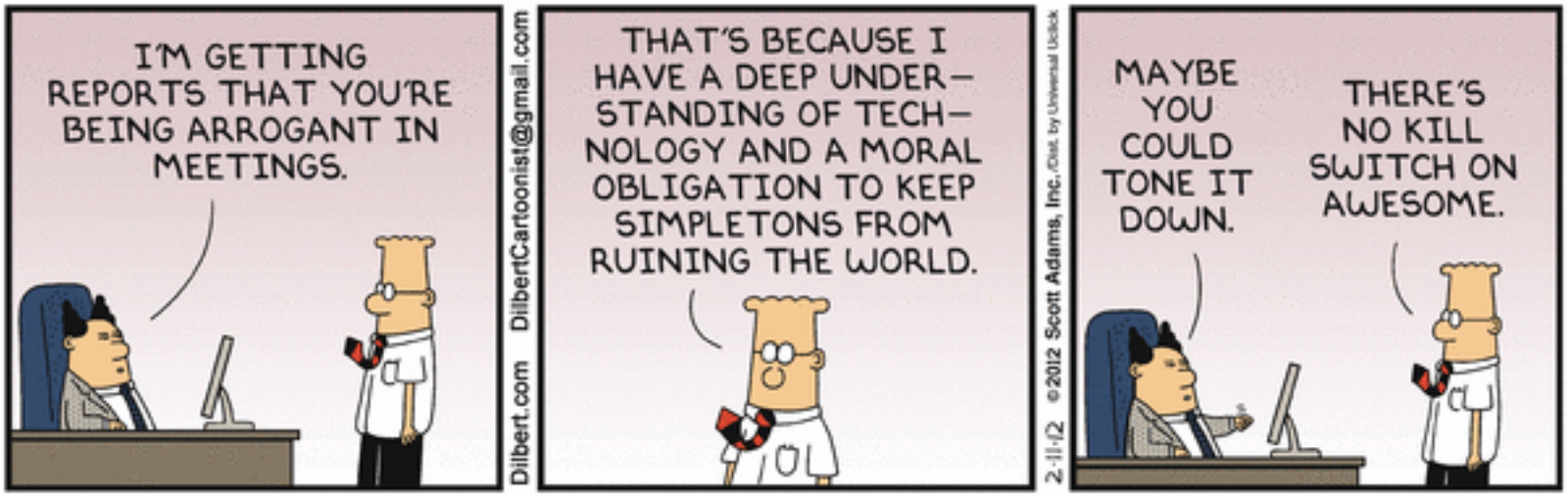
"Begin with the end in mind" - Steven Covey,
7 Principles of Highly Effective People.

There are important lessons on what sort of projects have worked under ASC.

- In one case, the ASC project *"evolved"* from an older code (2-D to 3-D).
  - **The 3-D code was *benchmarked* in by the older 2-D code yielding (complete) substantial continuity.**
  - **This process brought their user community along in its entirety!**
  - The utility of the original code was maintained.
  - The new code did provide access to the enhanced computational resources.
  - The code kept the same name.
- **The code retained a user base throughout.**
- This is arguably the most successful project in ASC.

There are important lessons on what sort of projects have worked under ASC.

- Another successful case is associated with a huge change in the sort of simulation used by a community of users
- **The code involved the direct support and utility by several extremely influential and capable users.**
  - The code demonstrated useful and unique capabilities (solved some old & new problems)
  - The code developers were extremely devoted to V&V feedback and fixed problems promptly.
- The code had a very user-responsive development team along with some intrinsic advantages (and disadvantages) compared with earlier codes.



Dilbert's attitude in the comic strip below is exactly the thing we are trying to avoid. Acting like this would be detrimental to improving quality in CASL. It is exactly how the V&V program was perceived at its onset in the ASC program. It has taken years to fix the damage.

Introduction to PCMM (1/3)

- Developed at SNL for the DOE ASC program as a means of assessing the completeness of the modeling and simulation activities
- It had a focus that was necessarily nuclear weapons and Sandia-Mission focused.
- In broad brushes the basic precepts of PCMM apply to a much broader range of M&S activities.
- **It needs to be extended and removed from an "adversarial" context that naturally arises with an assessment.**

Introduction to PCMM (2/3)

Increasing completeness and rigor →

Decreasing risk

Content ↓

MATURITY / ELEMENT	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and BCs	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built", e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&C) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have an unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown exper-imental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive sensitivity analyses conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

Credit: M. Pilch.

Expectation of Quality is scope dependent

Expectations of the accuracy of scientific simulations vary. Who are you trying to convince?

Code developers

Analysts

The customer

The public

- My house
- My job
- The company
- Your house
- Some money

- I'd bet X on the result; X=
- Uncertainty Quantification
- Error bars on simulation results
- Result converges with refinement
- Mesh refinement
- Eyeball norm
- Trends are reasonable
- Result is plausible
- Result is not ridiculous
- Code returns a result

Courtesy of Greg Weirs (SNL)

Introduction to PCMM (3/3)

- We met with CASL staff and decided to extend the PCMM to include two new subject areas, not found in the original PCMM:
  - Integrated analysis, application in broader terms
  - Regulatory impact
- **We moved PCMM away from "assessment" to something more like a "quality inventory"**
- We have a strong belief that this sort of inventory should have been conducted as part of the early ASCI program.

Roughly speaking, computation moves from science to engineering as time progresses.

The age of computation for understanding is often viewed as a “Golden Age” where standards are
weak, i.e., did the simulation help us understand something?

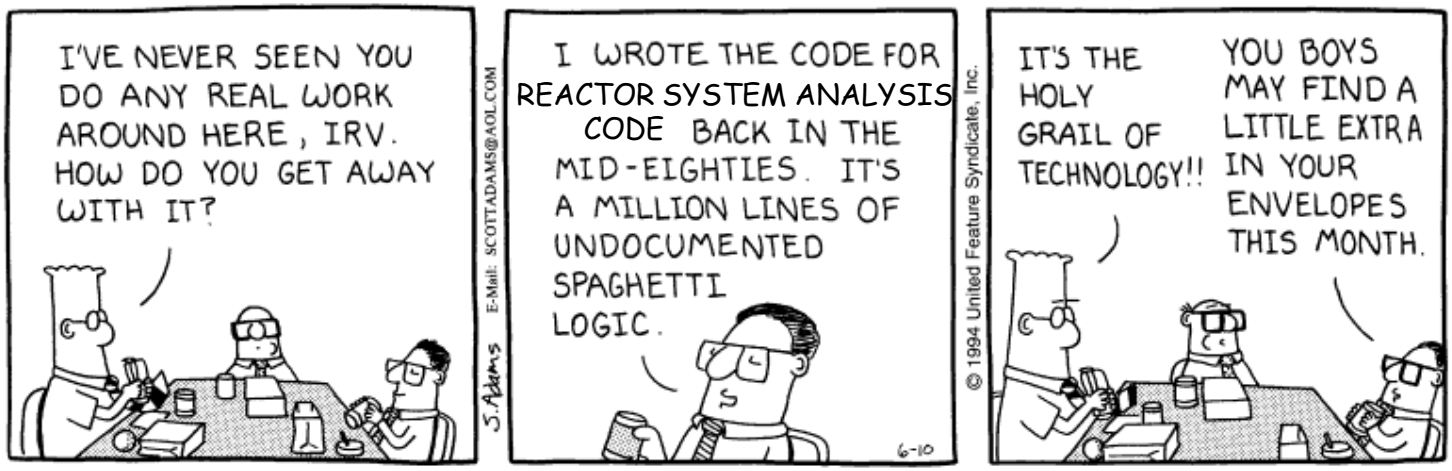
Hence it is an idyllic time that is looked at with fondness.

The age of computation for quantitative value is often viewed as an post-industrial wasteland where standards are strong and consequences are high, i.e., is the simulation right?

Since V&V is key to the question it gets tagged as part of the horror.

Existing technology often defines quality and correct solutions.

Dilbert



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It is essential to understand quality from this perspective if progress is to be made.

A legacy code's solutions and associated practices are the starting definition of "good." We must capture this to make progress.

Maybe Star Wars is more your speed… note who represents V&V!

The PCMM reinterpreted

- Rather than assess the maturity of the M&S in the six areas against some rating of intended use, we **rearticulated the PCMM to an open-ended or guided discussion of solution quality**.
- We interview knowledgeable individuals on the topic being assessed to explore how quality is assured in their current processes.
- The results are collated into recommendations on how we can more completely approach quality in CASL to incorporate existing practices

Diffusion of innovation is useful to understand how ideas advance.

"So easy, even a caveman could do it" - Geico

The Gap!

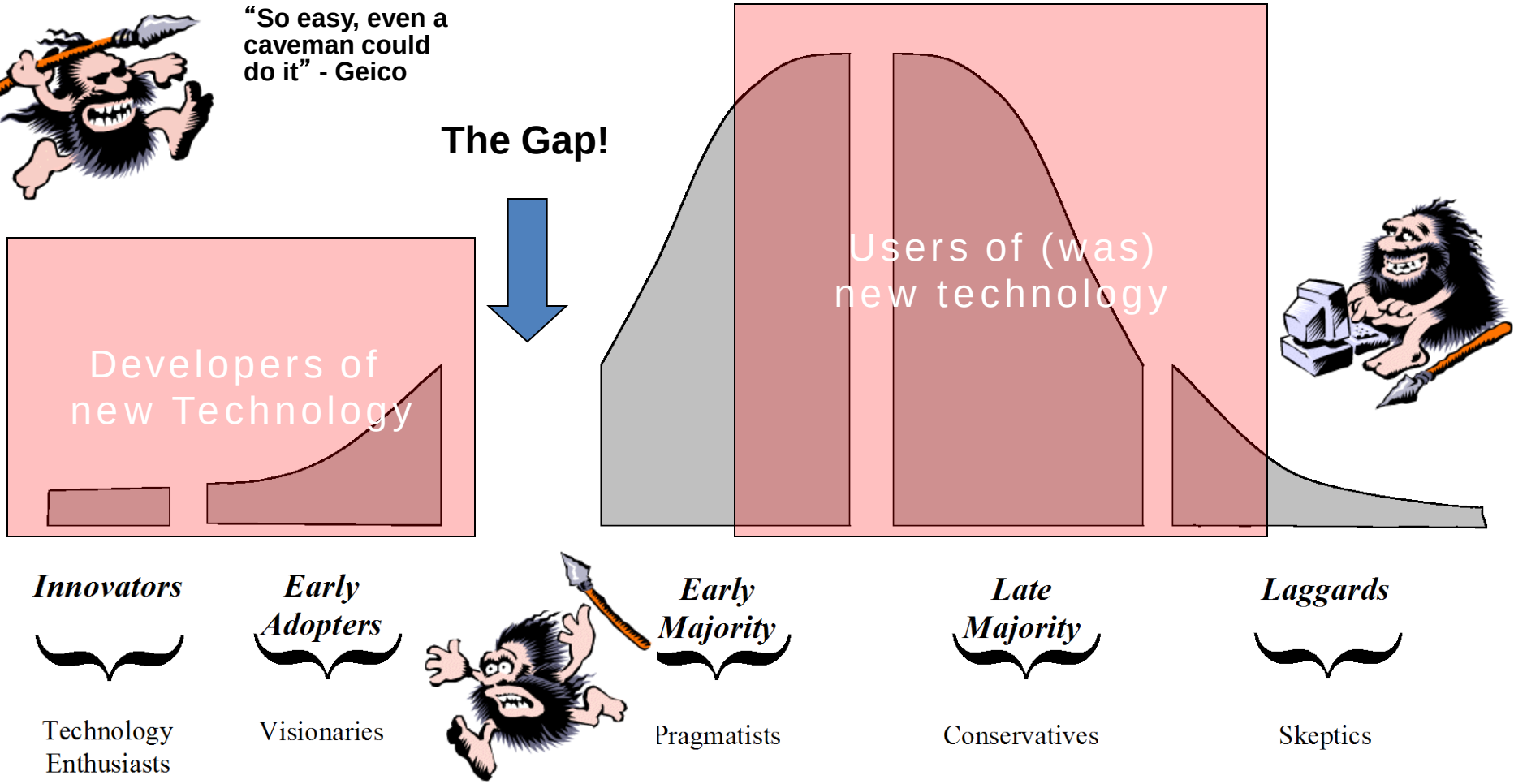


Figure adapted from "After the Goal Rush: Creating a True Profession of Software Engineering" by Steve McConnelll, Microsoft Press 1999

Conducting the Assessment

- The questions are provided in advance to the interviewee
- This is an interview done in person, on the phone or via video link. Each takes between one and a half and three hours.
- We begin with a brief explanation of what we are doing and why. How the questions will be asked, answers scribed, and how it is intended to be used.
- Finally, we pass the responses back to the interviewees after the notes have been cleaned up for corrections, clarifications and approval.

The Interview Process

1. General

1(a) What are the overall objectives of the calculations?

1(b) What sort of information needs to be produced by the calculations and how will these results be used to support decision-making?

1(c) How is the quality of the calculations assessed and justification for their use in the decision-making process specified?

1(d) Is there a well-defined specification of technical requirements for the application that is used guide the development work to address identified issues?

2. Geometric Modeling and Meshing

2(a) How important is the geometry associated with the problem being solved?

2(b) How does the information regarding the detailed geometry of the problem enter into the simulation?

2(c) What measures need to be taken to assure the quality / fidelity of the geometric information associated with the model?

2(d) How should the fidelity of the computational model's representation of the geometry be assessed to ensure it is appropriate for the application?

2(e) How important will geometric errors be in the overall model error or uncertainty?

2(f) What level of technical review of the geometric modeling and meshing effort should be required?

3. Model Fidelity

3(a) How will the physical models needed to address the application of interest be selected?

3(b) What steps are required to select appropriate models for the application?

3(c) Do the models chosen for use in the simulation differ from those used in the in the past (and if so how) and what is the basis for using the new model?

3(d) How important is the model selection within the overall budget of error and uncertainty?

3(e) What level of technical review has been applied to the models selected for use in the simulation?

4. Code Credibility

4(a) How are the codes used for the analysis selected? Do the analysts provide input into the selection?

4(b) How does the software development process and pedigree enter into the selection of the code(s) to be used in the simulation?

4(c) To what extent and how are the testing and results of the code evaluated in selecting it for use?

4(d) To what extent and how are code development and testing specified?

4(e) What role does comparison with (or validation against) other code results play in determining confidence in the code?

4(f) How are technical reviews of the code used for the analysis?

5. Solution Accuracy

5(a) How are the sensitivity of the solutions found (due to mesh resolution, time step size, linear or nonlinear solution stopping criteria, etc.) assessed?

5(b) How are discretization choices assessed for mesh convergence?

5(c) How are applicable acceptance criteria for solution accuracy specified?

5(d) To what extent is the solution accuracy achieved in the simulations subject to a technical review?

6. Validation

6(a) What sources of experimental data are used to validate the modeling?

6(b) What experimental data is needed to evaluate the (sub-) models? What experimental data is needed to evaluate the application simulations?

6(c) What are the uncertainties and/or errors associated with the identified experimental data sources? Where do the uncertainties used for the data come from?

6(d) How do uncertainties in the experimental data become represented in the simulations?

6(e) What (experiments, analyses) need to be accomplished to validate the models for use in the application?

6(f) How are the validation results reviewed?

7. Uncertainty Analysis

7(a) To what extent are the results of the analysis sensitive to the of the modeling choices?

7(b) What steps need to be taken / procedures need to be developed to understand the uncertainty in the simulations that will be performed for the application?

7(c) What uncertainty estimates (and technical details of what is needed – e.g. statistical characterization such as moments, distribution, etc.) are needed to support application decision-making?

7(d) What assumptions are required regarding the nature of the statistics associated with results?

7(e) What technical review requirements are required for the uncertainty (or sensitivity) analysis that need to be performed?

8. Integration

8(a) How are the results from this application coupled with other applications?

8(b) Are the results of this application dependent on the results from another application?

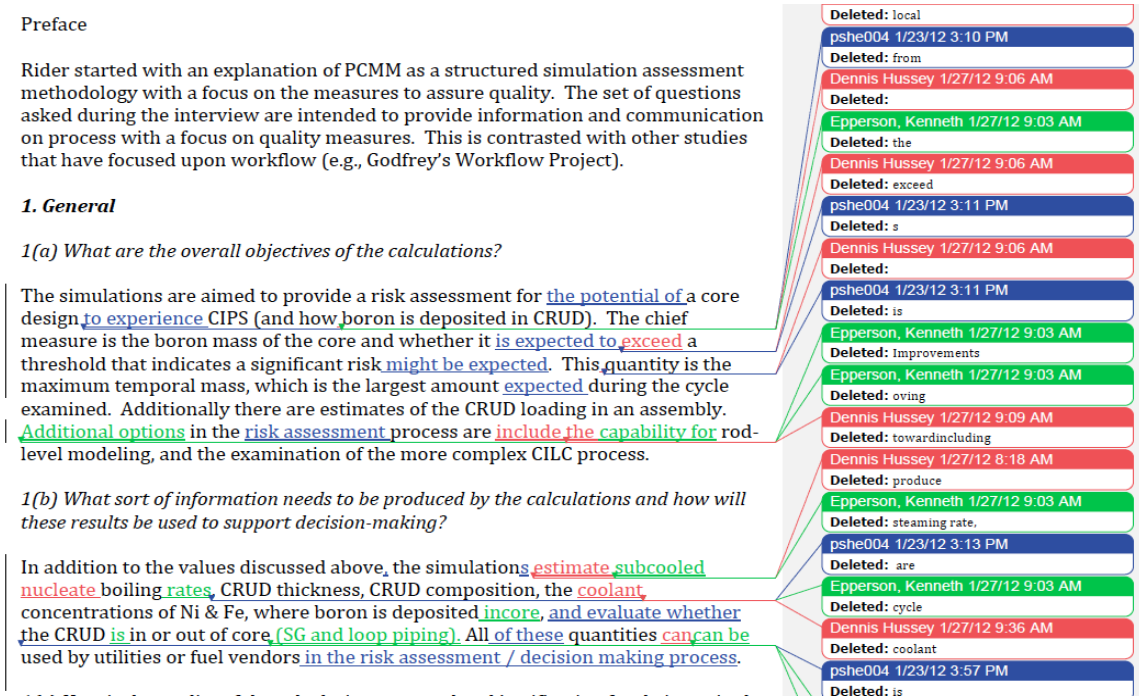
8(c) How is the integration with other application assessed?

9. Regulatory Impact

9(a) Do the results of the simulation for this application have regulator consequences?

9(b) Does the regulatory use of the application produce any changes in the use of the code or development of simulations?

Sample Interview



Preface

Rider started with an explanation of PCMM as a structured simulation assessment methodology with a focus on the measures to assure quality. The set of questions asked during the interview are intended to provide information and communication on process with a focus on quality measures. This is contrasted with other studies that have focused upon workflow (e.g., Godfrey's Workflow Project).

1. General

1(a) What are the overall objectives of the calculations?

The simulations are aimed to provide a risk assessment for the potential of a core design to experience CIPS (and how boron is deposited in CRUD). The chief measure is the boron mass of the core and whether it is expected to exceed a threshold that indicates a significant risk might be expected. This quantity is the maximum temporal mass, which is the largest amount expected during the cycle examined. Additionally there are estimates of the CRUD loading in an assembly. Additional options in the risk assessment process are include the capability for rod-level modeling, and the examination of the more complex CILC process.

1(b) What sort of information needs to be produced by the calculations and how will these results be used to support decision-making?

In addition to the values discussed above, the simulations estimate subcooled nucleate boiling rates, CRUD thickness, CRUD composition, the coolant concentrations of Ni & Fe, where boron is deposited incore, and evaluate whether the CRUD is in or out of core (SG and loop piping). All of these quantities cancan be used by utilities or fuel vendors in the risk assessment / decision making process.

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- Dennis Hussey, Steve Hess at EPRI Palo Alto
- Kenny Epperson (EPRI), by Phone
- John Westacott (CSA), by phone
- Brian Adams in person at SNL
- Jeff Secker (WEC) by phone

Recommendations

- Any development of tools should both support and assist the current quality processes. No effort should be undertaken that undermines current practices. The current practices are strong with regard to the applied analyses.
- Efforts to formalize existing sensitivity studies would be useful
- The built-in quality checks should be retained and strengthened.
- Any automation of the documentation and analysis that assists the peer review of the overall analysis of CIPS and CILC would be highly beneficial.
- For any application of regulatory significance, a substantial expansion and slightly different focus will need to be pursued in the evaluation.
- A great deal of effort should be spent in supporting and improving the analysis of validation data.
- CASL should provide built-in seamless uncertainty quantification and sensitivity analysis capability without undue user intervention.
- CASL should make certain that over-emphasis is not placed on CASL strengths such as code and solution verification or uncertainty analysis in comparison to the needs of existing validation-centric QA. The support for a broad analysis QA must be maintained.

Summary

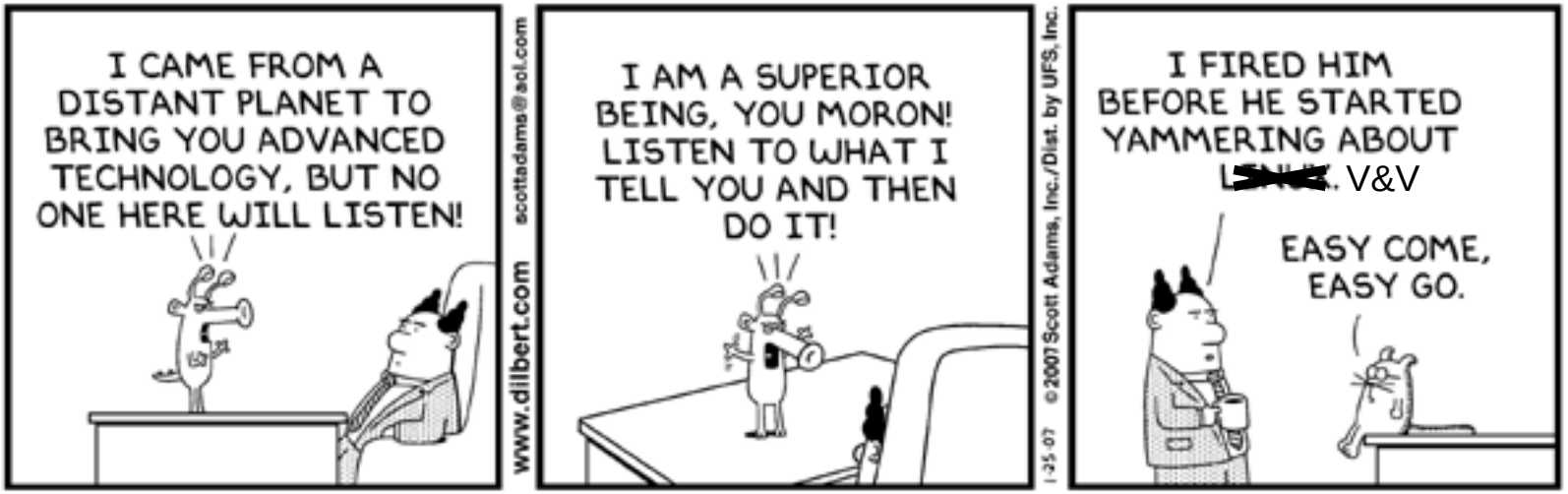
- **The overall impression is that significant quality measures are implemented in the current analysis and development process** that should not be overlooked in the natural CASL emphasis.
- CASL should be careful to not overlook existing quality measures in the development of enhanced capability associated with other aspects of the modeling.
- Interviews are useful if they are held in an open-ended and open-minded format ("a judgment-free zone")
  - **I believe the applications "people" need to be heard and welcome the opportunity to communicate their understanding on these matters.**

In M&S, you don't know how good (or bad) you are if you don't ask.

- "Due diligence" means asking all the questions, even if you don't think you'll like the answers.

Credit: M. Pilch.

“Dilbert isn’t a comic strip, it’s a documentary” – Paul Dubois



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