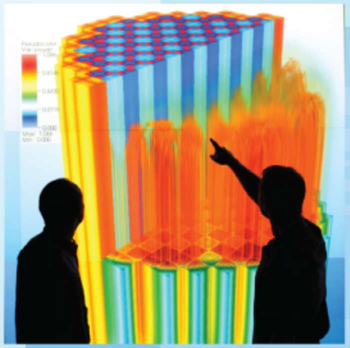
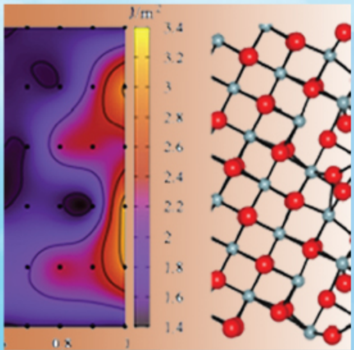
CASL-U-2013-0274-000-a

Power uprates
and plant life extension



Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

Materials Performance Optimation (MPO) with an Emphasis on MAMBA

Chris Stanek and Brian Kendrick

Los Alamos National Laboratory

Brian Wirth

University of Tennessee

PWROG Meeting

Westinghouse Electric Co., LLC

Cranberry, PA

December 3, 2013

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Materials Performance Optimization (MPO), with an Emphasis on MAMBA

Chris Stanek and Brian Kendrick
Los Alamos National Laboratory

Brian Wirth
University of Tennessee

On behalf of the MPO team

PWROG meeting
Westinghouse, Cranberry PA
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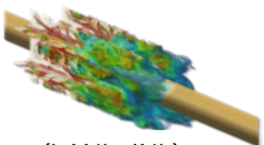
Overview

- CASL Thermal-Hydraulics Focus Area Overview
- Hydra-TH Status and Plans
- Closure Modeling Status and Plans
- Meshing Challenges and Plans
- Future Directions

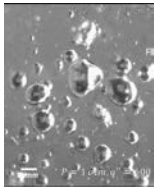
The Thermal-Hydraulics Focus Area is Using a Combined Experimental/Theoretical/Computational Approach

- Objective: Deliver next-generation Thermal-Hydraulics simulation tools to VERA, interfaced with the latest VUQ technologies, and accommodating tight coupling with other physics

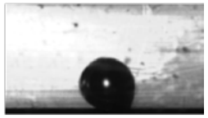
NVIDIA



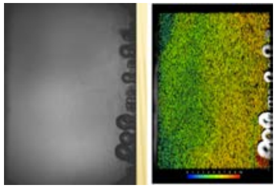
(LANL, INL)



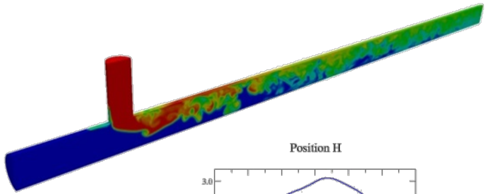
(MIT)

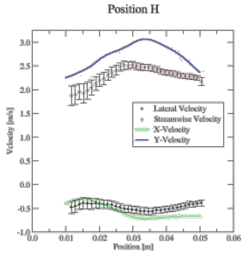


(CCNY)



(TAMU
)



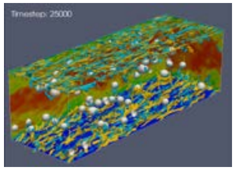


(LANL, SNL,U. Michigan)

Experiments
- Fundamental Understanding
- Code Validation
- Multiphase Closure Models

Algorithms & Architectures
- Advanced CFD Algorithms
- Multiphase Solution Methods
- Advanced Architectures – NVIDIA nvAMG Library

V&V, Uncertainty Quantification
- Intrusive VUQ Algorithms
- Multiphase Model Sensitivities
- CFD Verification



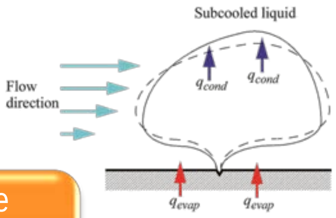
(NCSU)

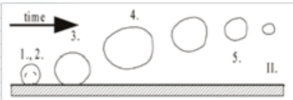
VERA -CFD (Hydra-TH)

DNS - Interface Tracking
- Fundamental Understanding
- Multiphase Closure Models
- Code Validation

(Notre Dame)

Multiphase Closure Models
- Mechanistic Subcooled Boiling
- Refined momentum closures
- Integrated lift/drag forces

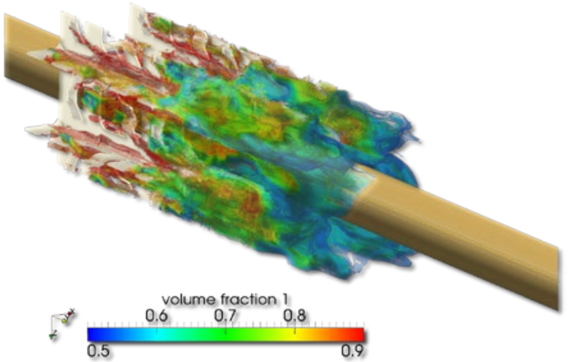


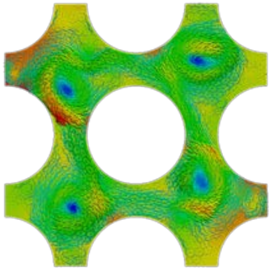


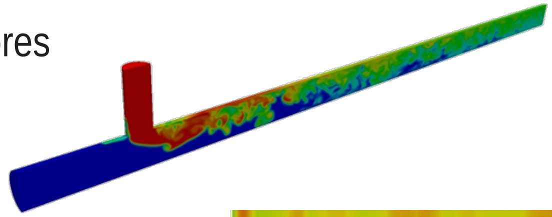
(MIT, RPI, U. Michigan)

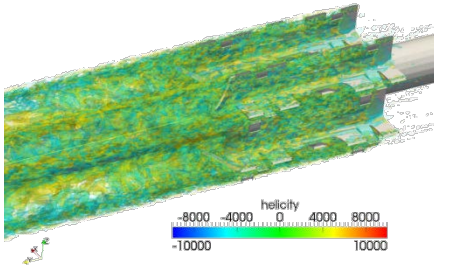
Hydra-TH for Thermal-Hydraulics

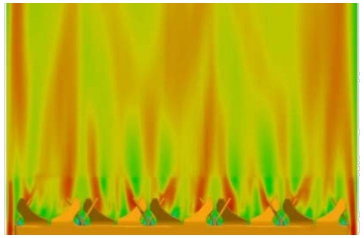
- Single-phase flow w. multiple turbulence models
  - Projection for transients, fully-implicit for slow transients
  - ILES, WALE, DES, RNG k-ε, Spalart-Allmaras
- Multi-phase (N-field) code base in place
  - Fully-implicit under development
  - Beginning to integrate closure terms
  - Scaled to 192M 3x3 rod bundle on 36,000 cores
- Advanced Closure Models
  - Mechanistic multiphase boiling models
  - Integrated drag/lift forces
- Experimentally Supported Closure Models
  - Closure model development and validation
  - Single and multiphase validation experiments
- ITM/DNS
  - Single/multi-bubble databases used for momentum closure models
  - Assessment of multiphase turbulence closure
- Meshing: Hexpress/Hybrid, GridGen, ICEM, Cubit, TrueGrid, …
- Visualization: ParaView, Ensight, VisIt, …
- GUI: Kitware SimBuilder – Hydra-TH specific GUI

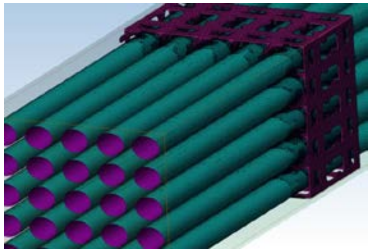


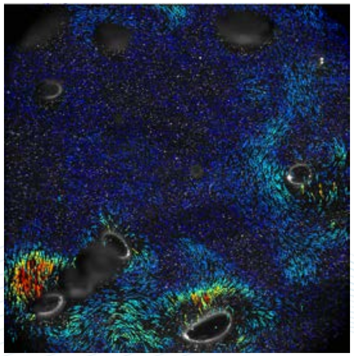












Y. Hassan, TAMU

The Hydra-TH Development Path

FY2011 - 2012

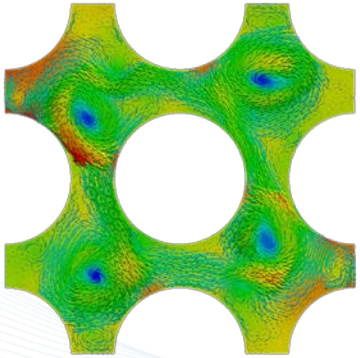
- Hybrid Parallel Meshing of V5H. 3x3 and 5x5 V5H meshes up to 192M cells
- Development of a priori mesh assessment based on y+
- Runtime turbulence statistics
- Parallel Visualization (ParaView)
- L1 Milestone: Determine sensitivity of structural response to GTRF RMS forces
- Investigate sensitivity of GTRF forces to URANS and LES models
- Validation LES calculations with 5x5 V5H TAMU Data
- Direct integration of Hydra-TH forces using WEC VITRAN code. Less than 1.7% difference compared to STAR-CCM+ “gold standard”
- Development of Hydra-TH Multiphase development roadmap

FY2013

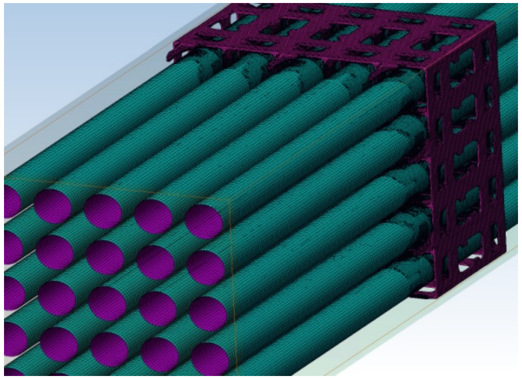
- Hydra-TH Assessment on THM Benchmark Problems
- Development of Hydra-TH V&V/Benchmark Problems and Documents
- General-purpose Steam Property Library (IAPWS-95/97)
- Fully-implicit single-phase
- Initial (anelastic) multiphase flow demonstration
- Integration of asymmetry preserving drag model
- Enthalpy and Internal Energy form of Energy Equation
- Enhanced surface/statistics output
- Direct nightly code integration into VERA
- Addition of ~ 60-70 licensed users

FY2014

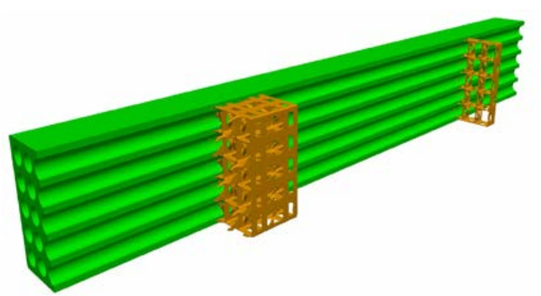
- Expose Native CHT Capabilities
- Release porous drag for simplified meshing
- Single-phase validation for fuel applications
- Improved parallel linear algebra
- Enhanced turbulence single/multiphase turbulence models
- Fully-implicit multiphase
- Boiling closure models
- Single/multiphase V&V
- Hydra-Mamba direct coupling
- Expanded “open” Hydra development model



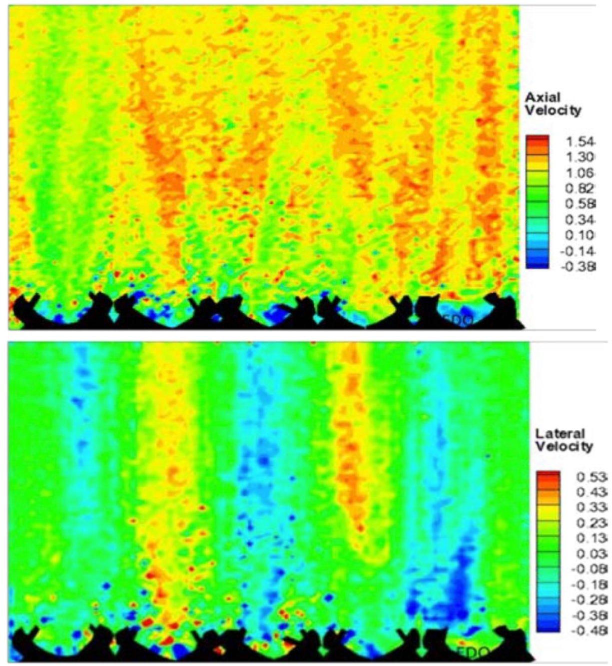
5x5 V5H study shows good agreement with experimental data



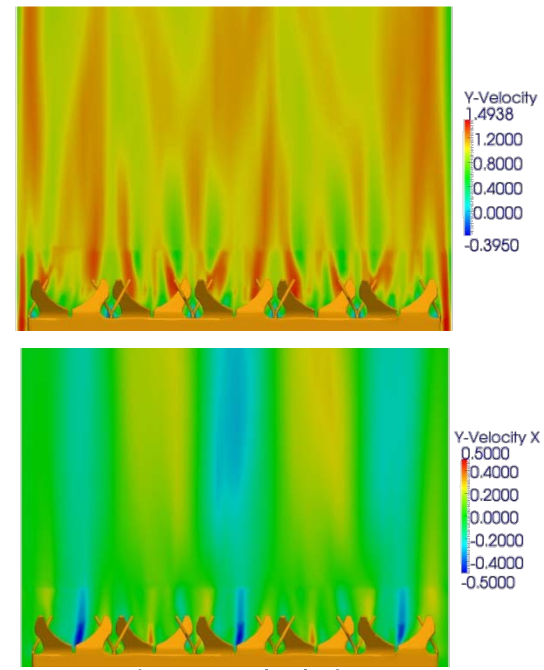
- Predicted mean peak velocities within 5% of experiments



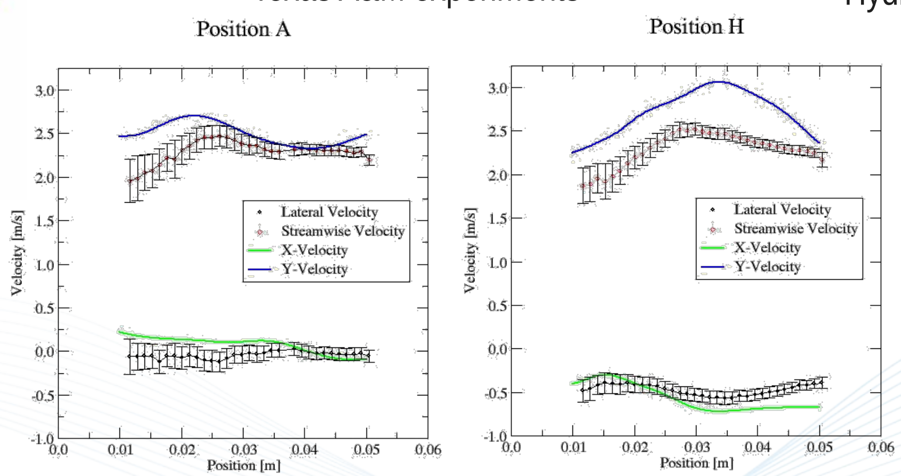
- Time-averaged velocity profiles downstream of mixing vanes (96M mesh)

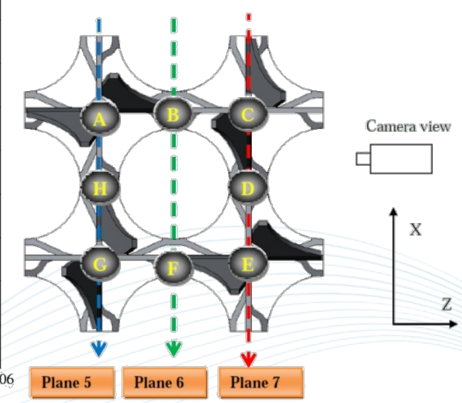


Texas A&M experiments



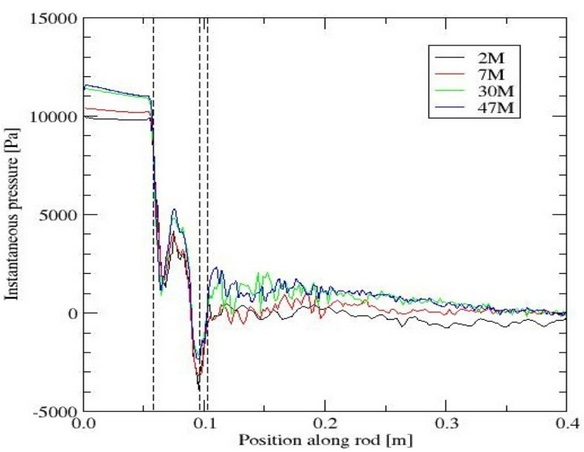
Hydra-TH calculations

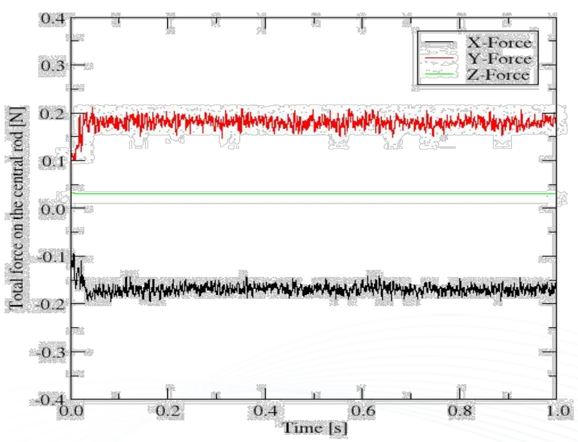


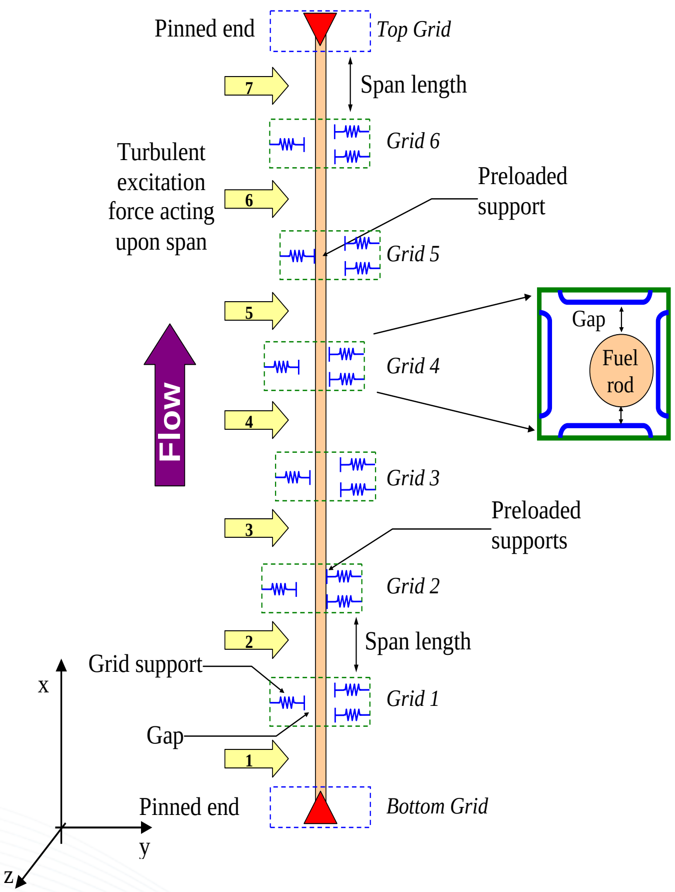


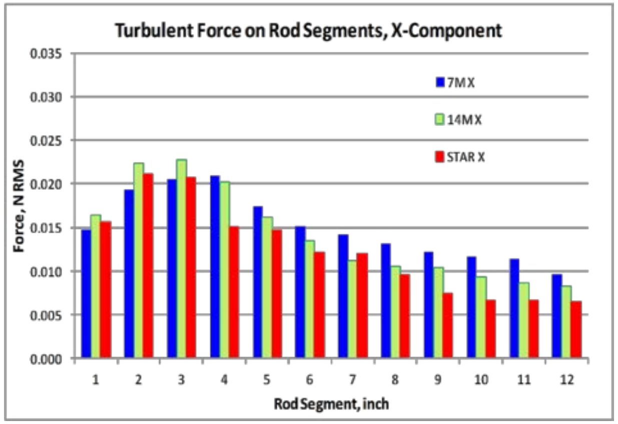
Large-Eddy Simulations Used to Drive Modal Dynamics and Wear Work Rate Calculations using VITRAN

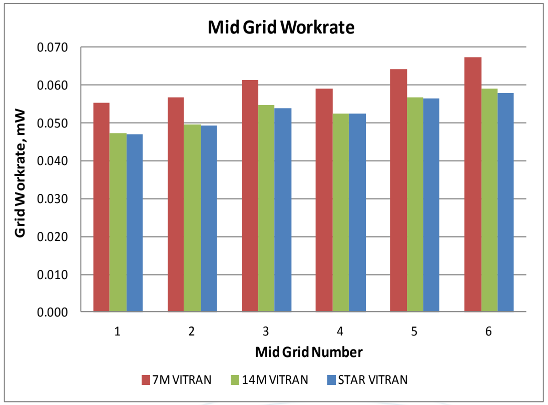
- Pressure Profiles and Rod Forces are extracted from Hydra-TH for the 3x3 Rod Bundle
- The data are used as input to VITRAN to compute rod acceleration/displacement
- 7 to 14M meshes required for reasonable fidelity in design analysis ~ 8 – 24 hour calculations









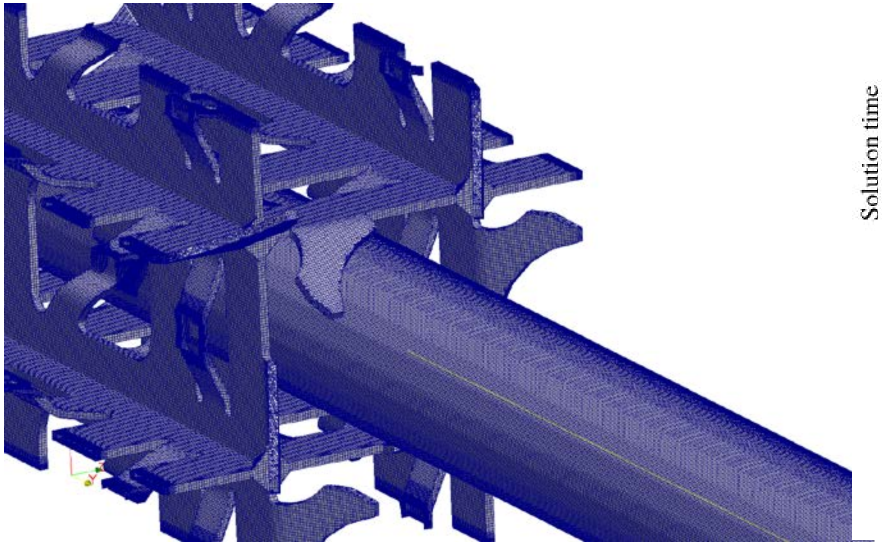


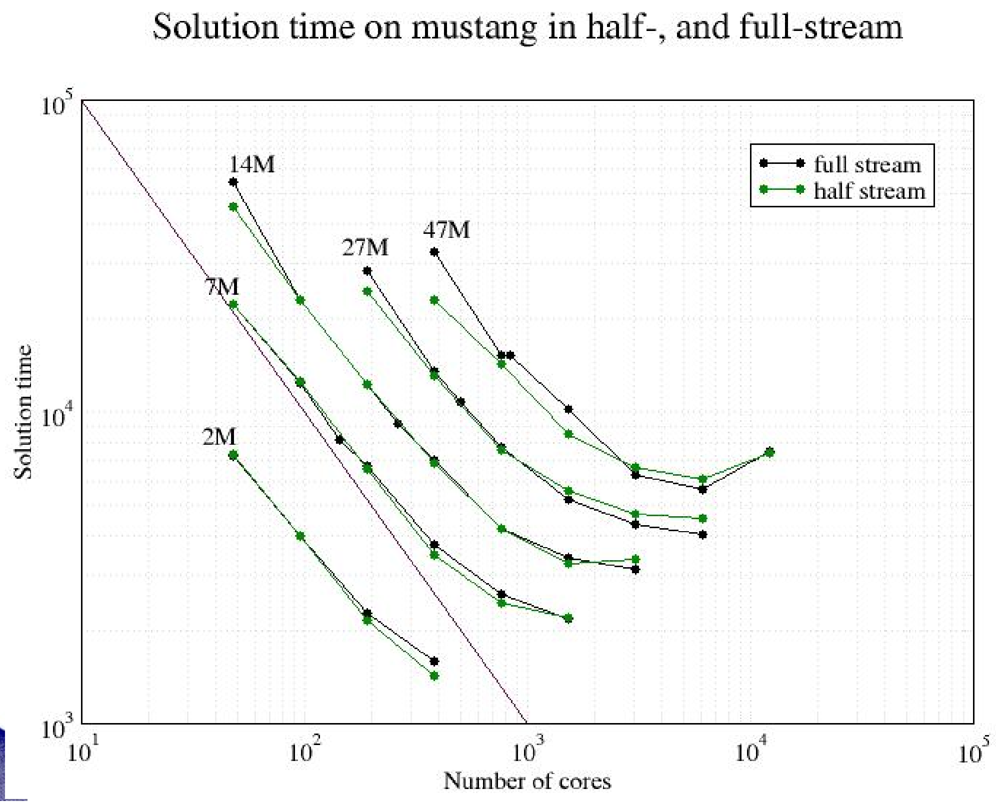
2% difference between CCM+ and Hydra-TH wear work-rates

Force time history data is used for subsequent rod dynamic analysis, e.g., with VITRAN

Some performance numbers using the V5H 3x3 rod bundle

- Mustang – AMD 6176 Opteron
  24 cores per node





Titan early profiling studies

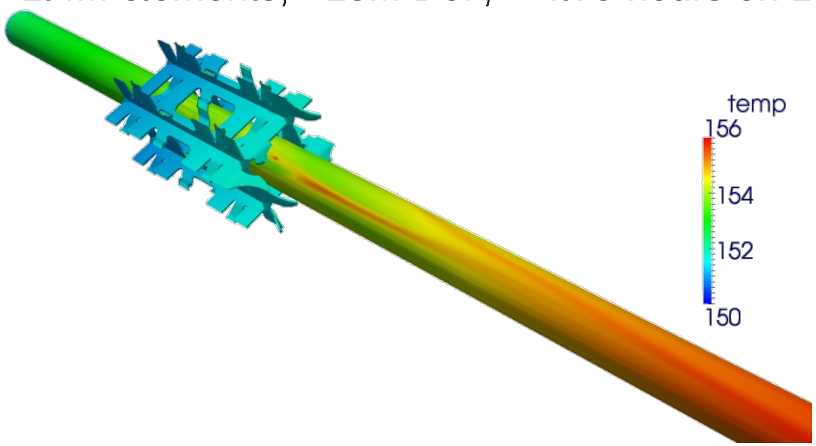
- 1024 nodes, 8 FP cores ea.
- 1.8 – 3.2% of peak FLOPs rate for AMD’s

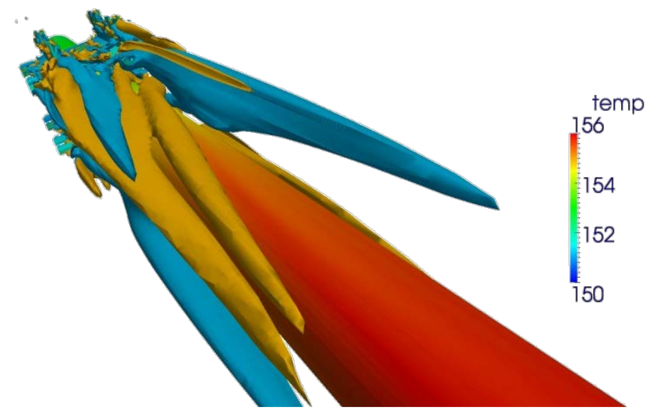
CASL L3 Milestone: Computational Performance Assessment of Hydra-TH

- *NVIDIA Tesla K20s delivered to LANL & ORNL*
- *Beginning to work with NVAMG library*

Some Sample Calculations for FY2013/14 Milestones

- Fully-implicit projection, RNG k-e model, Re ~ 4.0 x 10^5, $q_w = 10^6$ W/m^2
  - 2.4M elements, ~18M DoF, ~ 4.75 hours on 16-core Intel Xeon desktop

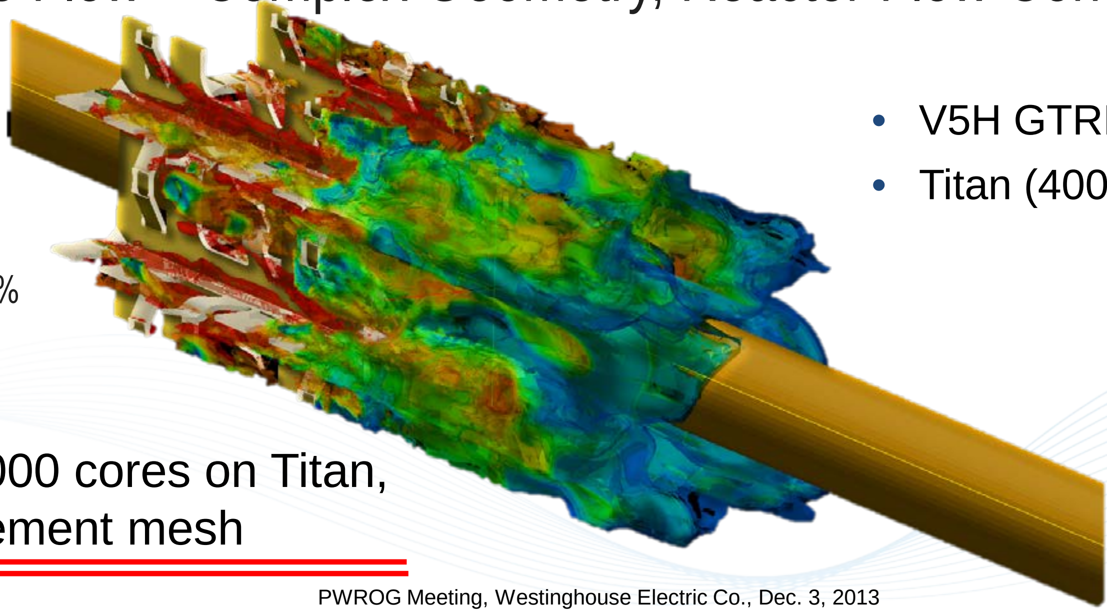




- MultiPhase Flow – Complex Geometry, Reactor Flow Conditions

VF1 = 90%

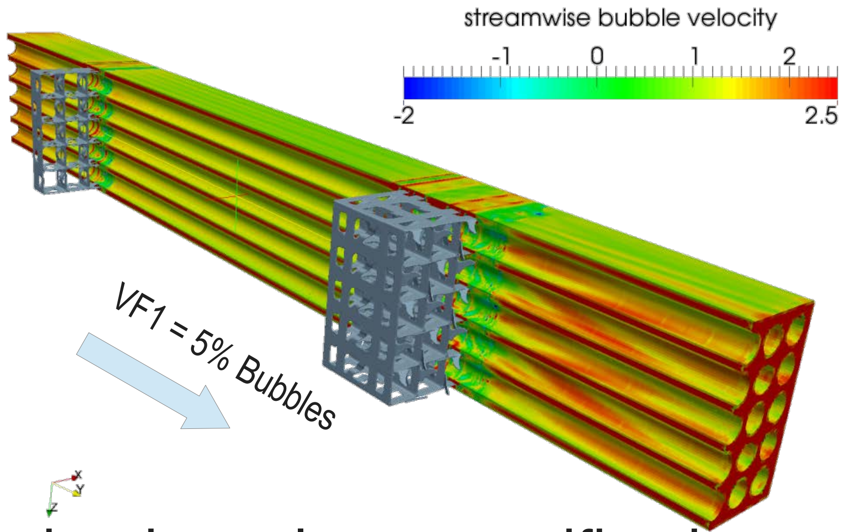
IC: VF1, VF2 = 50%



- V5H GTRF 3x3 2M cells
- Titan (400 CPU cores)

Scaled to 36,000 cores on Titan,
192 Million element mesh

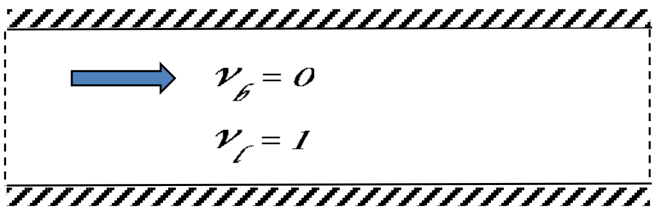
MultiPhase Flow in 5x5 Rod-Bundle



- "Option-1" Calculation w. Drag
- V5H 5x5 Spacer – 14M Cells
- Re=28,000 (TAMU Exp. Cond.)
- 100:1 water/air density ratio

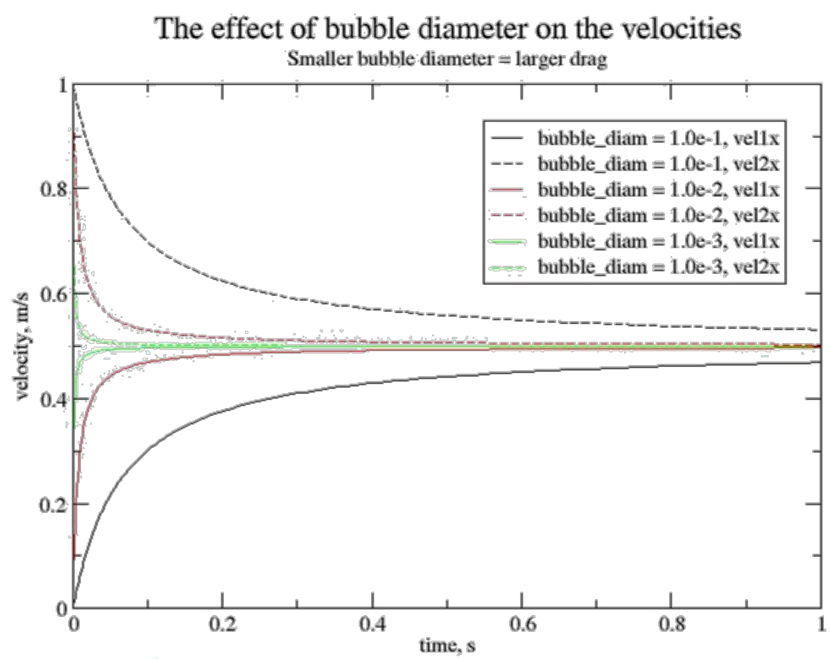
Verifies force anti-symmetry and momentum conservation!!

- In-situ drag closure verification



$$\mathcal{F}_D = -\frac{3}{4}\frac{C_D}{D_b}\alpha_l \rho_l \left\| v_b - v_l \right\| \left(v_b - v_l \right)$$

$$C_D = \begin{cases} \frac{24}{Re_b}\left[1 + 0.15 Re_b^{0.687}\right] & 0 < Re_b \le 1000 \\ 0.44 & Re_b > 1000 \end{cases}$$



Closure Modeling Status and Plans

FY2011 - 2012

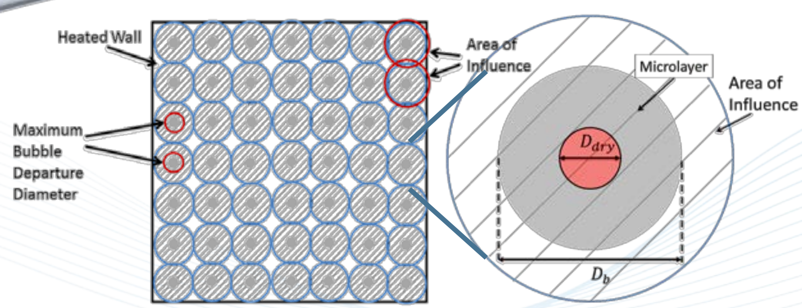
- Initial experiments intended to validate ITM/DNS studies
- ITM/DNS studies probing a number of areas but not focused on closure models
- VUQ studies initiated to study boiling model sensitivities
- Investigation of 7-equation model for multiphase flows
- Demonstration of "upscaling" processes for multiphase
- Initial work on refined mechanistic heat flux partitioning
- ITM/DNS simulations of nucleate boiling

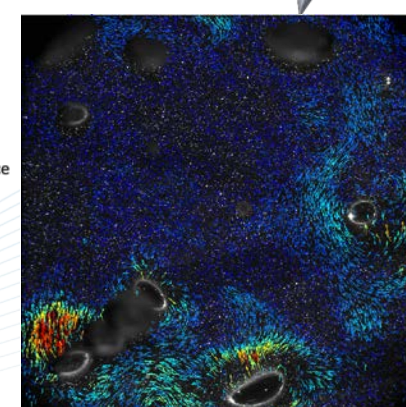
FY2013

- Mechanistic model for subcooled boiling in PWR assemblies
- ITM/DNS database for drag, lift and wall effects
- Shake-down of a single baseline set of closures for multiphase using NPHASE and Star-CCM+
- Analytic study of near-wall lift effects for an integrated drag/lift model
- Microlayer model for heat transfer during nucleate boiling
- Experimental database(s) for subcooled boiling
- Growth and detachment of vapor bubbles during subcooled boiling
- Development of a hardened M-CFD boiling model

FY2014

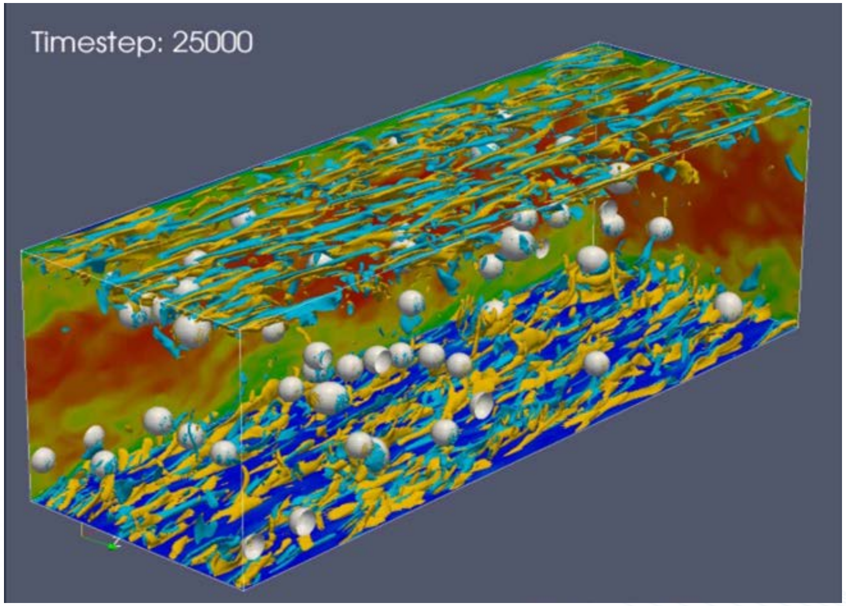
- ITM/DNS studies in realistic subchannel geometries
- Transient evolution of bubbles with new lift/drag models
- Experimental study of (synthetic) crud effects on subcooled boiling
- Advanced momentum closure models for use in Hydra-TH
- Further work on mechanistic subooled boiling models
- Adiabatic bubbly flow validation data
- Advanced boiling closure models



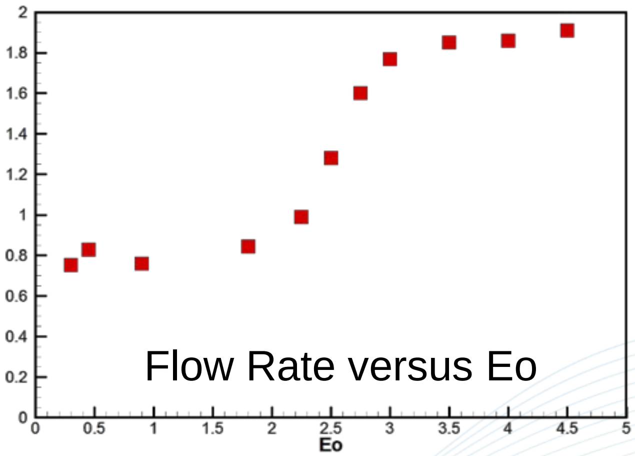


ITM/DNS Data Changes Closure Model Development in a Fundamental Way

- Permits direct computation of modeled terms at given points in space/time and to assess their mean and fluctuation components
- Approach in single-phase flows has led to significant advances in understanding and developing closure models
- Provides the foundations for more complete multiphase CFD turbulence modeling
- Developing a DNS lift/drag database for integral momentum closure model



Bubble Deformability Effects



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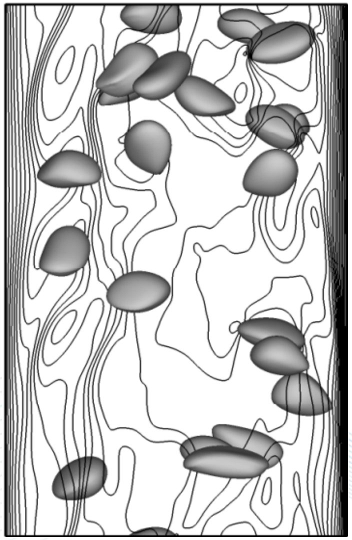


Meshing Strategies and Challenges

Meshing Requirements

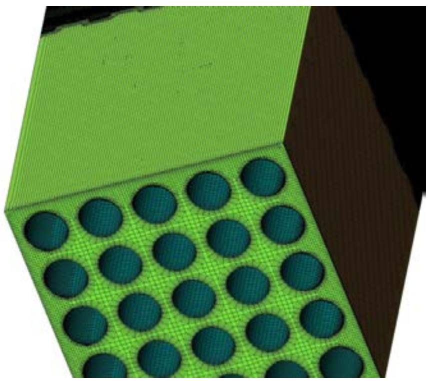
- Direct CAD – to – Mesh methodology
- Treatment of complex geometry for rod bundles and assemblies
- Hybrid meshes may be used to close complex geometries, but not required by the physics
- Conversion from polyhedral meshes may not be possible at reasonable development cost
- Scaling from desktop to O(1) billion cell meshes
- Ability to setup set-based node-centered and face-centered boundary conditions
- Common file format for input to CFD and Mechanics calculations, and for visualization is highly desirable
  - ✓ The Exodus-II/HDF format current fits this need with multiple meshers and visualization tools

Meshing Challenges, Status and Plans

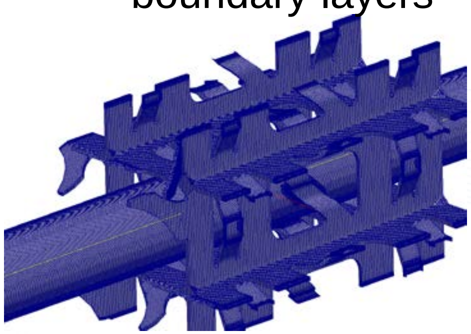
Status: meshing capabilities

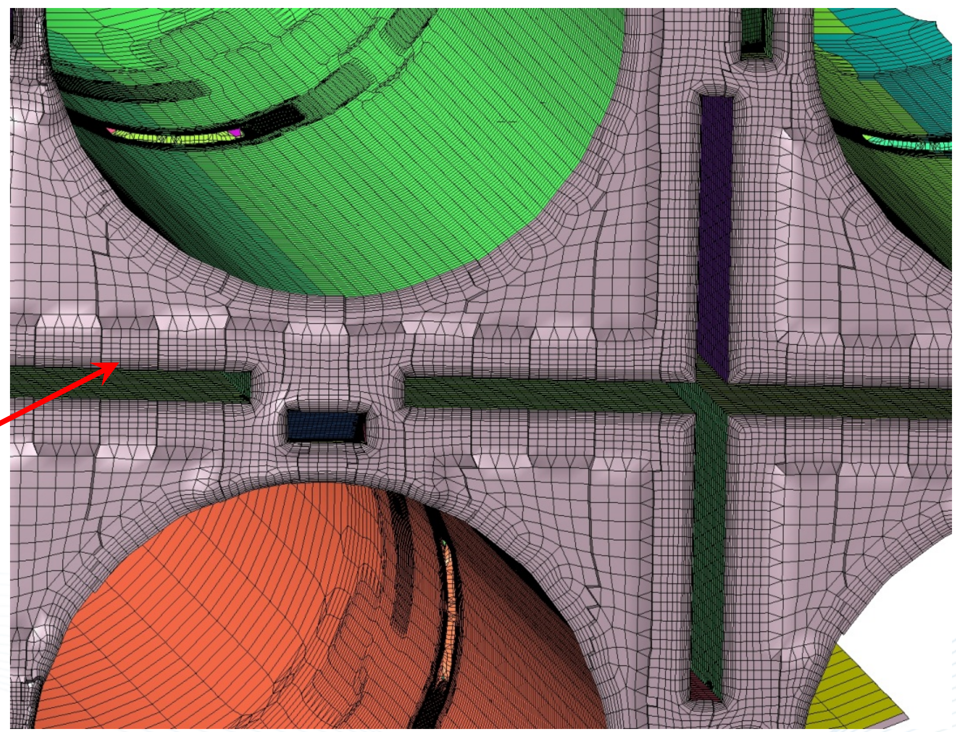
- In collaboration with E. Popov (ORNL), F. Kickinger (CAE Solutions), NUMECA using HEXPRESS/Hybrid (aka Spider)
  - From STL geometry to 90 Million element mesh in ~ 45 minutes
  - 1 Billion element mesh using 80-core PGV Super Server, 250 Gbytes of memory

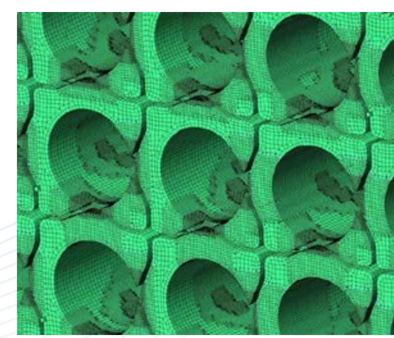
→ Exceptional Efficiency



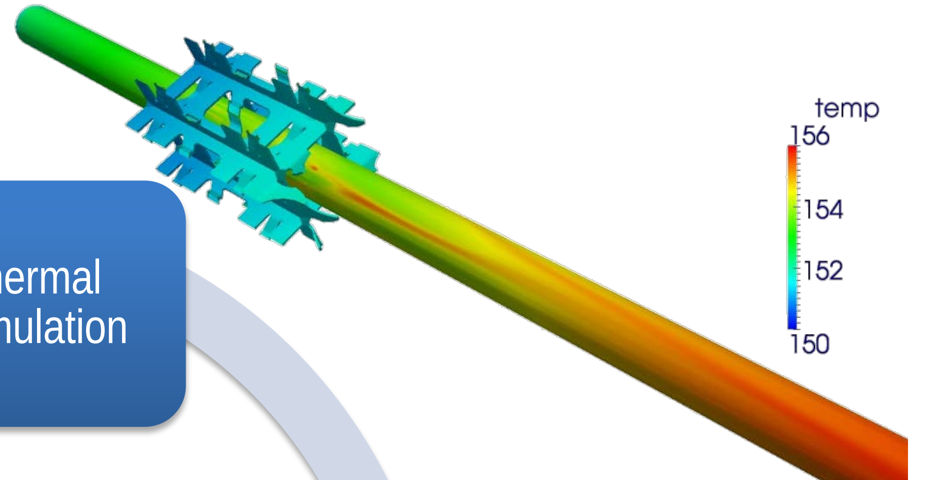
Hex-dominant boundary layers

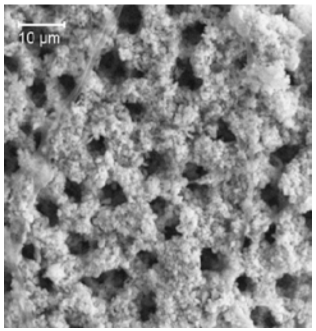






Hydra-TH <-> Mamba Coupling for CRUD Deposition

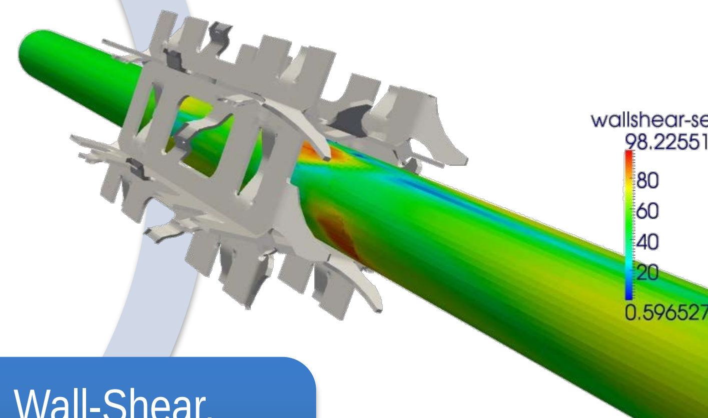




- Local CRUD Chemistry
- Boiling, chimney formation
- CRUD deposition
- Thermal resistance

Hydra-TH Thermal Hydraulics Simulation

- **CRUD Induced Power Shift**
- **CRUD Induced Localized Corrosion**



MAMBA Sub-Grid Scale Model

Wall-Shear, Temperature, Heat Flux

THM FY2014 Hydra-TH Development Milestones

- Demonstration of multiphase boiling flow with Hydra-TH in realistic subchannels with mixing vanes using “vetted” THM closure models
- Expose porous drag capabilities for DNB single-phase “mixing” calculations
  - Currently exercising 250M element model on INL fission machine
- Expose native CHT in Hydra-TH for stand-alone rod-bundle calculations
- Multiphase CFD assessment, verification and validation
- Investigation of FSI coupling approximations for GTRF (is sequential analysis good enough?)
- Single/multiphase CFD assessment, verification and validation
- Advanced turbulence models for multiphase flow (BHR, cascade, etc.)
- ITM/DNS simulations in support of turbulence closures, model development for momentum/boiling closures
  - Simulations of bubbly flow in realistic subchannels and its statistical analysis
- Hydra-Mamba Coupling, i.e., Mamba as a sub-grid scale model
- Extreme-scale computing with Hydra-TH using GPUs on TITAN
- Enhanced fully-implicit projection algorithms using nonlinear Krylov acceleration for both single and multiphase flows