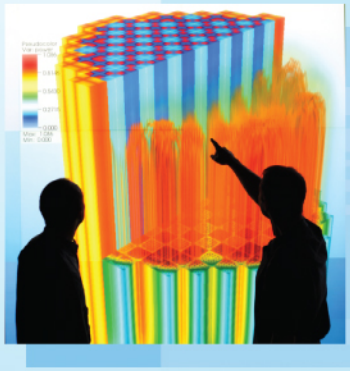
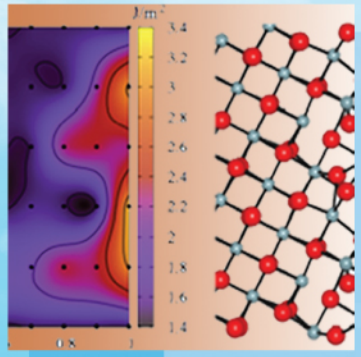
CASL-U-2012-0245-000

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

L3:RTM.PTR.P4.03

Demonstrate Initial Deterministic Transport Capability through VERA-CS

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U.S. DEPARTMENT OF ENERGY | Nuclear Energy

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Sample Python Input (Problem 2)

```
## PWR Parameterized Assembly -> Single fuel lattice

passembly = Ppwr_assembly(17,17,10)

pfuel  = Pcyl_pin([0.4096, 0.418, 0.475], 1.26, 1.0, 12)
pgt    = Pcyl_pin([        0.561, 0.602], 1.26, 1.0, 13)
ppyrex = Pcyl_pin([ 0.214, 0.230, 0.241, 0.427, 0.437, 0.484, 0.5 ...

# Pin compositions
vac   = Mat_String(0, [""], 0)
fuel  = Mat_String(1, ["uo2   $ID den=10.36     1.0    600 92234 0.0179 92235 3.1 ...
gap   = Mat_String(2, ["he    $ID den=0.0001786 1.0    600 end"], 0)
clad  = Mat_String(3, ["zirc4 $ID den=6.56      1.0    600 end"], 1)
mod   = Mat_String(4, ["h2o   $ID den=0.743     0.9987 600 end",
                       "boron $ID den=0.743     0.0013 600 end"], 0)
pyrex = Mat_String(3, ["pyrex $ID den=2.25      1.0    600 end"], 1)
ss304 = Mat_String(3, ["ss304 $ID den=8.00      1.0    600 end"], 1)

# Pins
t0 = RTK_Tag("fuel")
t0.add_int("id", 0)
t0.add_int("mesh", 30)
t0.add_str("type", "fuel")

t1 = RTK_Tag("guide tube")
t1.add_int("id", 1)
t1.add_int("mesh", 10)
t1.add_str("type", "guide")

t2 = RTK_Tag("guide tube with pyrex")
t2.add_int("id", 2)
t2.add_int("mesh", 10)
t2.add_str("type", "guide")

# pin compositions
fuel_pin = Mat_Strings()
fuel_pin.add(fuel)
fuel_pin.add(gap)
fuel_pin.add(clad)
fuel_pin.add(mod)
t0.add_mat_strings("compositions", fuel_pin)

# guide tube compositions
gt_pin = Mat_Strings()
gt_pin.add(mod)
gt_pin.add(clad)
gt_pin.add(mod)
t1.add_mat_strings("compositions", gt_pin)
```

Pin Radii

SCALE Strings

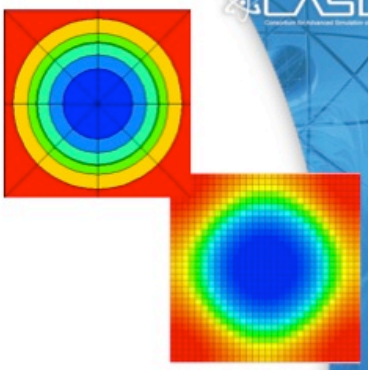
```
# guide tube with pyrex compositions
gt_bp = Mat_Strings()
gt_bp.add(gap)
gt_bp.add(ss304)
gt_bp.add(gap)
gt_bp.add(pyrex)
gt_bp.add(gap)
gt_bp.add(ss304)
gt_bp.add(mod)
gt_bp.add(clad)
gt_bp.add(mod)
t2.add_mat_strings("compositions", gt_bp)

# assembly gap compositions
agap = Mat_Strings()
agap.add(mod)

# make the pin
p0 = Cyl_Pin(pfuel, t0)
p1 = Cyl_Pin(pgt  , t1)
p2 = Cyl_Pin(ppyrex, t2)

# assign pins
passembly.assign_pin(p0)
passembly.assign_pin(p1)
passembly.assign_pin(p2)

# assembly map
mapper = Assembly()
s = [[ 1, 0, 0, 2, 0, 0, 2, 0, 0],
     [    0, 0, 0, 0, 0, 0, 0, 0],
     [       0, 0, 0, 0, 0, 0, 0],
     [          2, 0, 0, 2, 0, 0],
     [             0, 0, 0, 0, 0],
     [                2, 0, 0, 0],
     [                   0, 0, 0],
     [                      0, 0],
     [                         0]]

a = mapper.eighth_symmetry(s, 1)

passembly.assign_pin_map(a)

# assemble
passembly.assemble(0.04, 0.04)
```

Assign Materials

Lattice Layout

Problem 1 Status

- Four Pin Cells with varying fuel temperatures and moderator densities
- Very good agreement between CE KENO and MCNP
- Very good performance by DeCART
- Good agreement between stand alone BONAMI-IR / DENOVO and VERA-CS (DENOVO/XSPROC)



Eigenvalue Differences from CE KENO (pcm)

Code	Energy Groups	1A 565K	1B 600K	1C 900K	1D 1200K
KENO-VI*	CE	1.18699	1.18221	1.17163	1.16226
MCNP-V*	CE	18	18	34	127
KENO-VI	999g	-210	-210	-211	-198
	238g	-520	-521	-605	-604
	60g	-203	-206	-244	-243
NEWT	238g	-581	-597	-664	-676
DeCART	47g	37	19	-53	-56
VERA-CS	238g 10x10	-590	-605	-744	-876
	238g 30x30	**-297**	**-292**	**-393**	**-484**

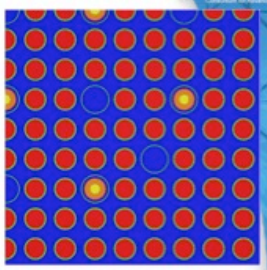
* CE KENO Uncertainty <= 11 pcm

* CE MCNP Uncertainty <= 7 pcm

- -200 pcm CE-MG bias
- -300 pcm 238g bias
- +200 pcm IR bias (BONAMI)
- 30x30 DENOVO mesh required for 238g
- 238g required for IR

Problem 2 Status

- Ten 2D lattices from Watts Bar 1 Cycle 1
  - Four with same temperature variations as Problem 1
  - Six with various guide tube poisons and instrumentation
- Good agreement between CE KENO and MCNP
- Good performance by DeCART except for controlled cases
- Consistent performance compared to Problem 1



Eigenvalue Differences from CE KENO (pcm)

Pattern	Description	Eigenvalue	CE MCNP	MG KENO	NEWT	DeCART	VERA-CS
2A	565K @ 0.743 g/cc	1.18239 +/- 0.00012	40	-451	-564	116	**-338**
2B	600K @ 0.661 g/cc	1.18386 +/- 0.00012	50	-480	-605	65	**-353**
2C	900K @ 0.661 g/cc	1.17403 +/- 0.00011	129	-542	-650	13	**-432**
2D	1200K @ 0.661 g/cc	1.16601 +/- 0.00012	116	-610	-717	-14	**-575**
2E	12 Pyrex Poison Rods	1.07251 +/- 0.00013		-347	-444	-5	**-335**
2F	24 Pyrex Poison Rods	0.98047 +/- 0.00013		-244	-335	-70	**-284**
2G	24 AIC Control Rods	0.84695 +/- 0.00012	216	164	54	806	**-613**
2H	24 B4C Control Rods	0.78746 +/- 0.00013	215	104	32	712	**-849**
2I	Instrument Thimble	1.18061 +/- 0.00012		-485	-583	91	**-395**
2J	Instrument Thimble + 24 Pyrex	0.97941 +/- 0.00012		-214	-306	-62	**-254**
Maximum			**216**	**164**	**54**	**806**	**-254**

- All controlled cases indicate +bias, except for VERA-CS, which is negative (?)
- AIC control rods require self-shielding in SCALE (worth 800 pcm and 0.5% peaking)
- Controlled cases need more evaluation.

Problem 2 Fission Distributions

- Pin fission rate distributions calculated and compared to CE KENO-VI

Pattern	Description	Pin Fission Sigma	RMS Difference (%)					Maximum Absolute Difference (%)				
			CE MCNP	MG KENO	NEWT	DeCART	VERA-CS	CE MCNP	MG KENO	NEWT	DeCART	VERA-CS
2A	565K @ 0.743 g/cc	0.09%	0.16	0.16	0.23	0.15	0.21	0.33	0.30	0.47	0.35	0.44
2B	600K @ 0.661 g/cc	0.09%	0.11	0.10	0.17	0.11	0.14	0.23	0.28	0.39	0.27	0.33
2C	900K @ 0.661 g/cc	0.09%	0.13	0.12	0.20	0.10	0.15	0.29	0.26	0.41	0.20	0.36
2D	1200K @ 0.661 g/cc	0.09%	0.11	0.11	0.18	0.10	0.14	0.26	0.32	0.58	0.28	0.40
2E	12 Pyrex Poison Rods	0.09%		0.12	0.21	0.17	0.15		0.47	0.49	0.41	0.35
2F	24 Pyrex Poison Rods	0.10%		0.13	0.22	0.21	0.15		0.25	0.74	0.41	0.31
2G	24 AIC Control Rods	0.10%	0.12	0.22	0.41	0.24	0.23	0.31	0.59	1.14	0.54	0.48
2H	24 B4C Control Rods	0.11%	0.16	0.27	0.50	0.28	0.37	0.49	0.61	1.21	0.72	0.82
2I	Instrument Thimble	0.09%		0.13	0.18	0.11	0.17		0.33	0.37	0.32	0.37
2J	Instrument + 24 Pyrex	0.10%		0.13	0.22	0.19	0.15		0.28	0.72	0.40	0.33
Maximum		**0.11%**	**0.16**	**0.27**	**0.50**	**0.28**	**0.37**	**0.49**	**0.61**	**1.21**	**0.72**	**0.82**

- KENO results are nu*fission – bug in /scale_dev prevents calculation of fission rates
- 2A CE KENO and MCNP are at 600K, while MG codes are at 565K
- DeCART results are ENDF/B-VI compared to CE KENO ENDF/B-VII
- NEWT results are kappa*fission
- Controlled cases need more evaluation, especially NEWT. May require 2D xs treatment (ESSM)
- Dancoff factors not used because of complexity and insignificant effect on fission distribution

Problem 2 Runtimes

- VERA-CS using 900 cells per pin, and 238 energy groups, full lattice, on ORTHANC
- DeCART using MOC mesh with 47 groups, full lattice, on FROST (OLCF)
- NEWT using ESC mesh with 238 groups, quarter lattice, on CPILE2

Runtimes for Single Lattice Problems (CPU-hours)

Problem	NEWT	DeCART	VERA-CS
2a	0.92	0.12	12.4
2b	1.00	0.12	12.5
2c	1.07	0.12	12.5
2d	0.58	0.12	12.9
2e	1.32	0.13	13.2
2f	1.50	0.13	18.1
2g	2.00	0.23	17.9
2h	1.50	0.15	21.9
2i	1.57	0.13	12.8
2j	1.57	0.13	18.4

- Feedback from DENOVO team indicates 40% speedup of VERA-CS is possible (2a = **7.2 CPU-hours**).
- DeCART and NEWT using CMFD acceleration
- NEWT performance can be sporatic on CPILE2