TRITON/Shift Depletion Validation and other Enhancements

2018 SCALE Users' Group

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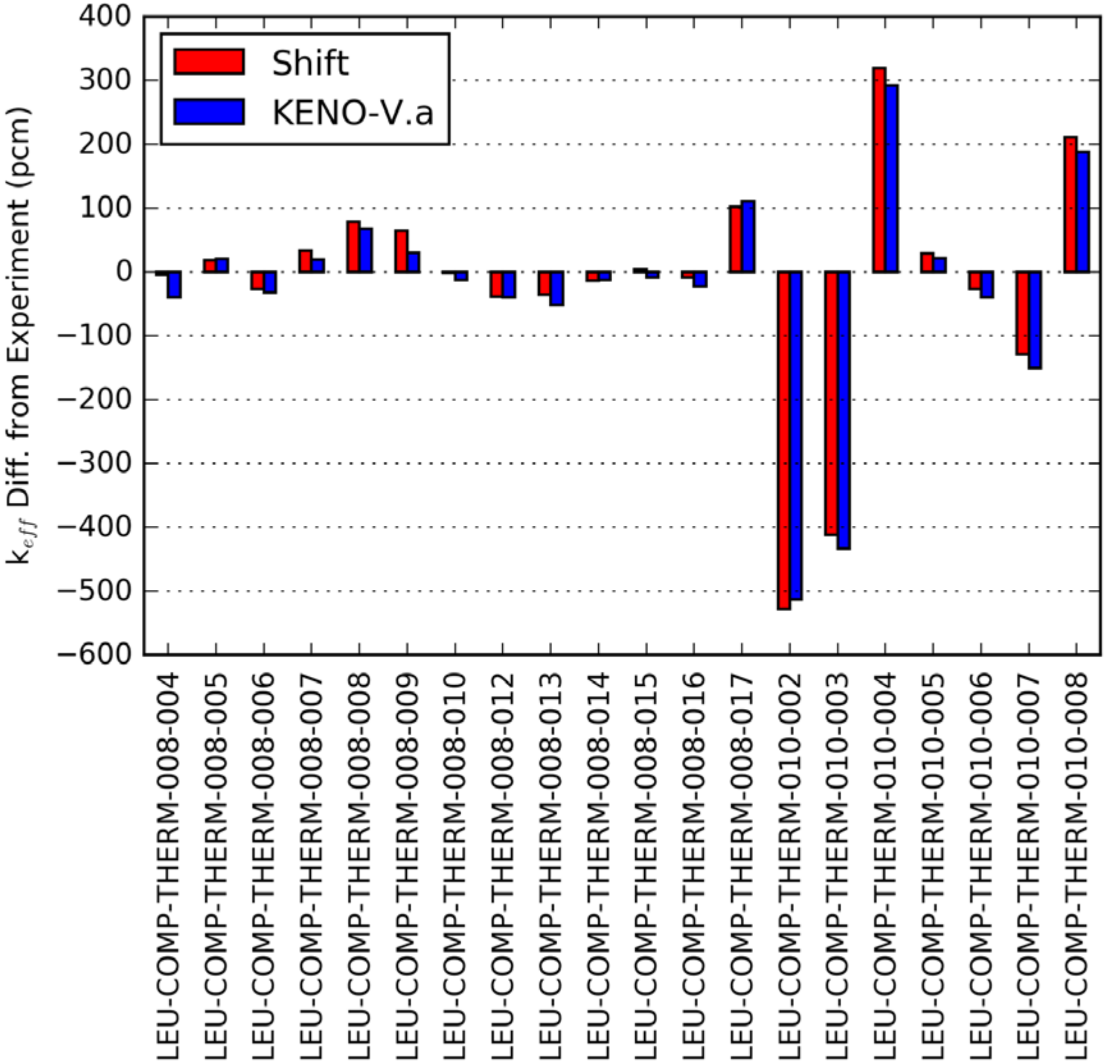
Project Goals

- Integrate Shift as a Monte Carlo transport method in 3D TRITON
- Enable ***fast and accurate*** Monte Carlo depletion solutions using high-performance modern parallelization
- Nodal data generation capabilities (covered in separate presentation)
- Motivations
  - Before this work
    - TRITON had general 3D transport (KENO) + depletion (ORIGEN), but required significant CPU time and yielded poor parallelization
    - No isotopic validation for TRITON/Shift
    - No ability to generate nodal data (T16) along with depletion
  - After this work: reference depletion solutions and preliminary validation basis

Verification Testing: VALID Test Suite

- Shift implemented into CSAS as well as TRITON, enabling criticality safety and depletion methods
- VALID is a suite of criticality safety benchmarks
- New VALID results correspond well with KENO-V.a and KENO-VI, as well as previously generated results using legacy CSAS/Shift
- VALID calculations were run on a single processor, so computational time comparison between KENO and Shift is similar



Experiment type	Number of cases	Difference from KENO[a] (pcm)	Standard deviation[b] (pcm)
LEU-COMP-THERM	128	21	31
IEU-MET-FAST	11	16	160
PU-MET-FAST	10	-23	27
MIX-SOL-THERM	3	23	21
MIX-COMP-FAST	2	506	19
MIX-COMP-THERM	20	18	17
HEU-MET-FAST	22	-14	18
PU-SOL-THERM	81	6	20

[a] Computed as the average over all KENO and Shift simulations for an experiment set.
[b] Computed as the standard deviation of the difference in k_{eff} between Shift and KENO.

Depletion Validation Engine

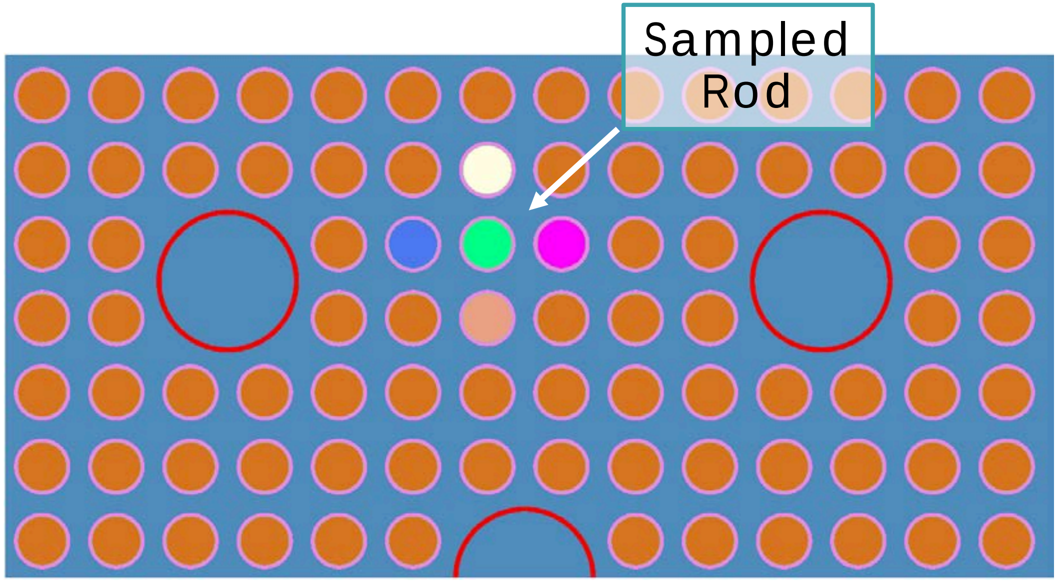
- Automatically searches a directory for KENO- or NEWT-based geometry, and then sets up new cases with modified high-level options specified by the users
  - **First-level options**: cross section library, *addnux* set, major XS processing options
  - **Second-level options**: transport solver options (CMFD, convergence criteria, angular quadrature, numbers of particles/cycles, etc.)
  - **Third-level options** (not yet available): NEWT grid spacing, multigroup XS processing options, material modifications

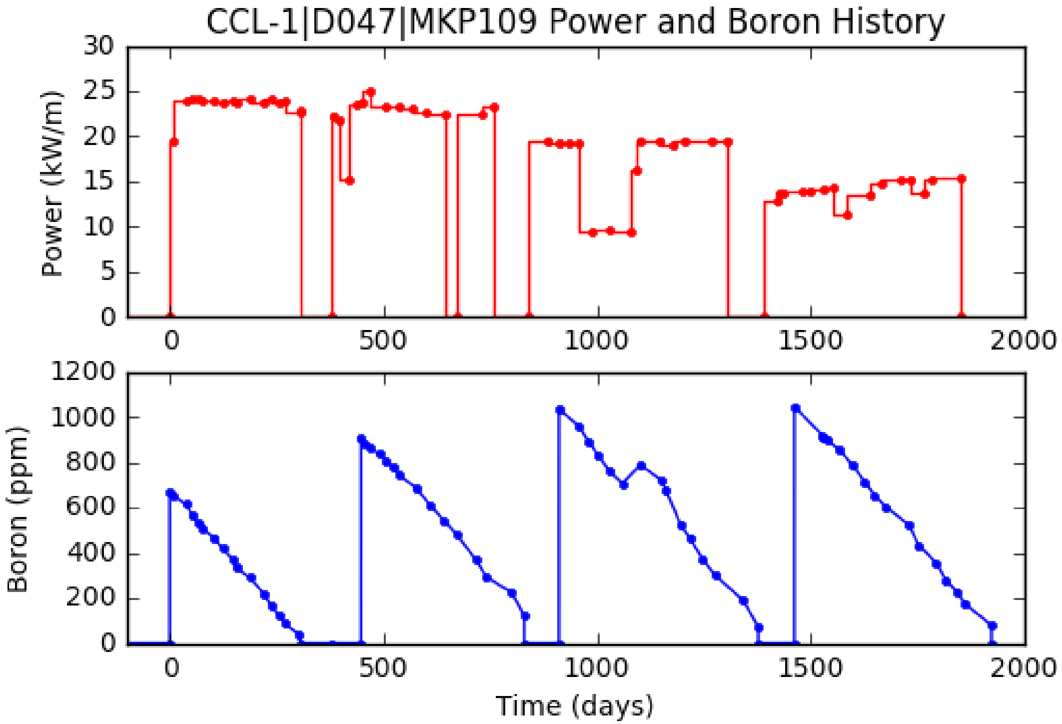
```
from pyvalid import *

validdir = '/path/to/VALID/inputs/'
rundir = './validtest_s63b1'

s63b1 = pyvaliddepl()
s63b1.readvalid(validloc=validdir)

s63b1.makeNew(rundir, simtype= ('crit','keno5'),
                      seqlibs=[('shift5','v7-252'),
                               ('shift5','ce_v7.1')
                               ('keno5', 'v7-252')
                               ('keno5', 'ce_v7.1')],
                    gparmopts=['centrm'],
                     parmopts=['npg=10000', 'gen=1100', 'nsk=100'])

s63b1.runFiles(runtype='all')
```

- Post-processing capabilities read *ft71f001* file, performs decay, and compares directory to SFCOMPO data (http://www.oecd-nea.org/sfcompo/)

Depletion Validation Cases: Calvert Cliffs Unit 1

- CE 14x14 assembly design
- Enrichment: 3.038 wt % ^{235}U
- Axial location
  Sample P: 270.3 mm
  Sample CC: 1637.1 mm
- Sample Burnup
  Sample P: 37.12 GWd/MTHM
  Sample CC: 44.34 GWd/MTHM

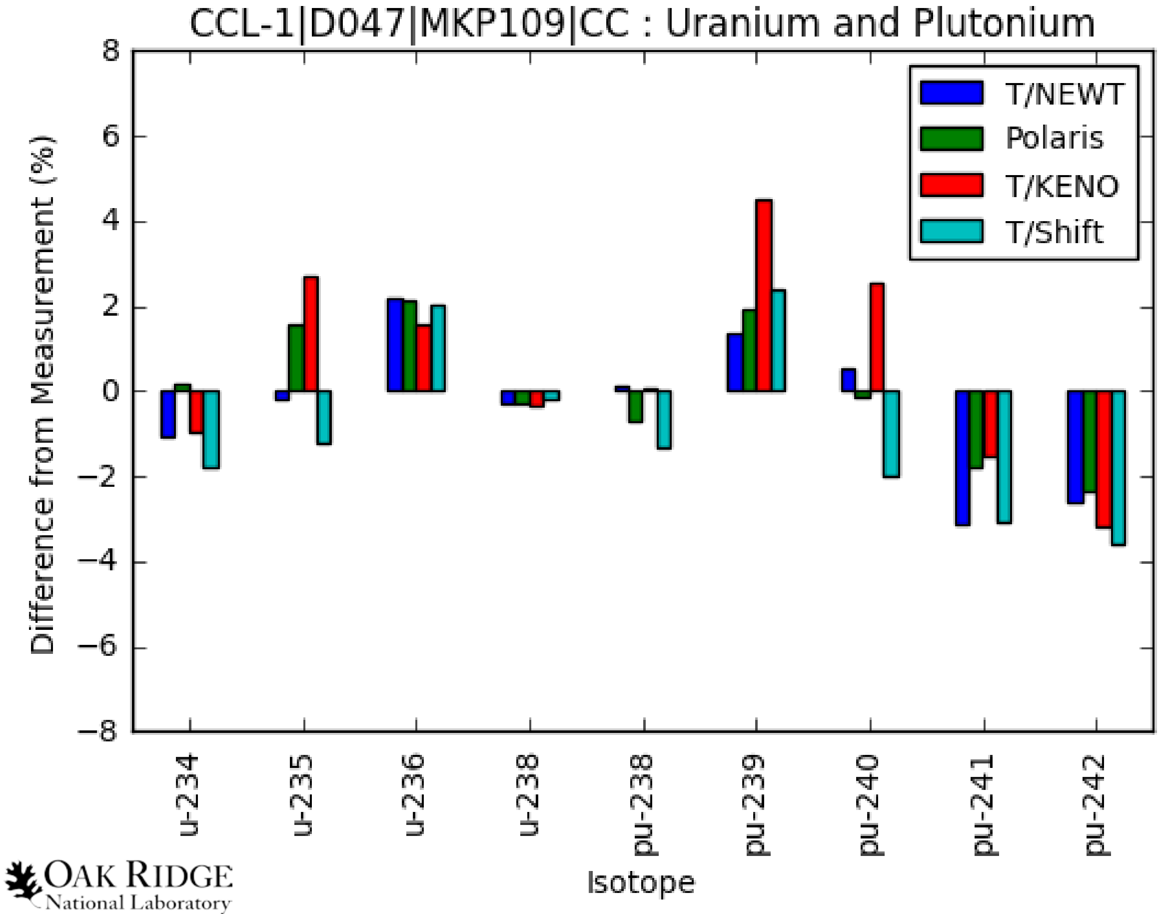


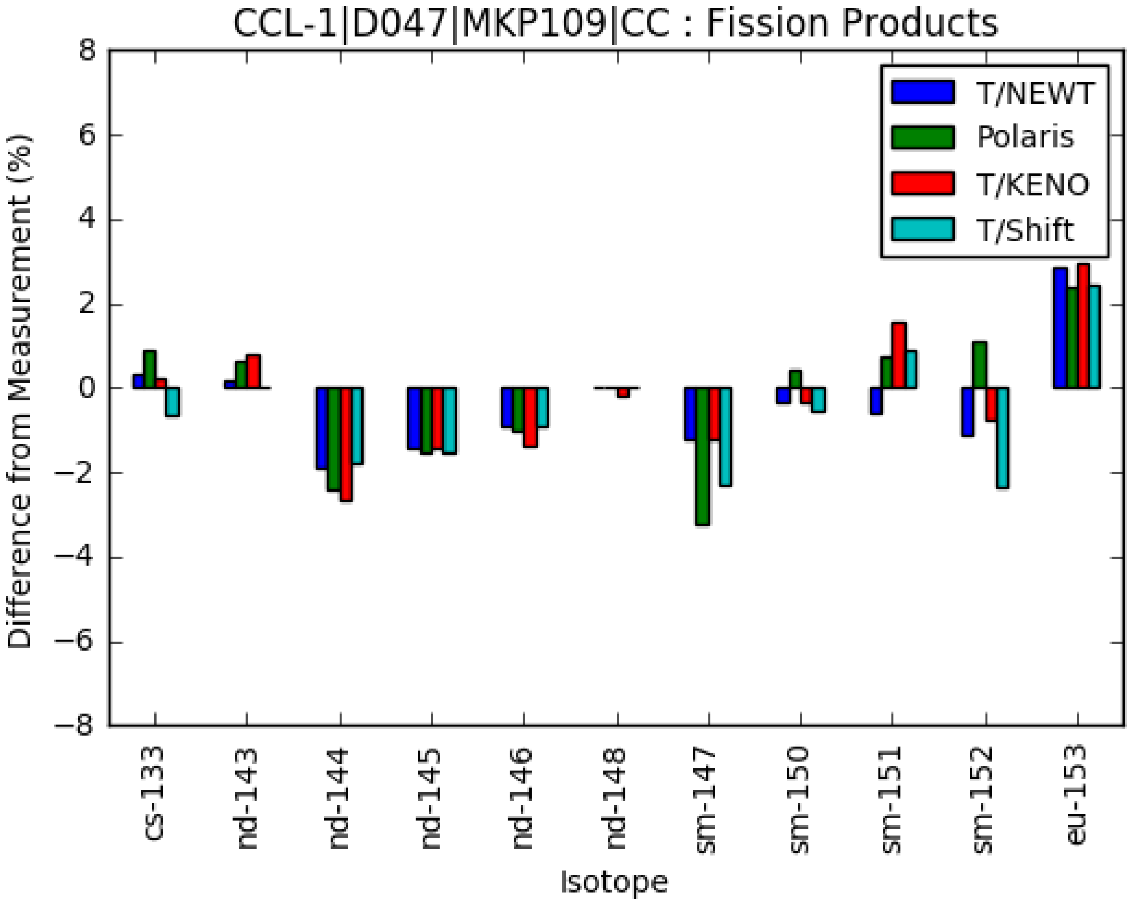


OAK RIDGE National Laboratory

Depletion Validation Cases: Calvert Cliffs Unit 1 (PWR)

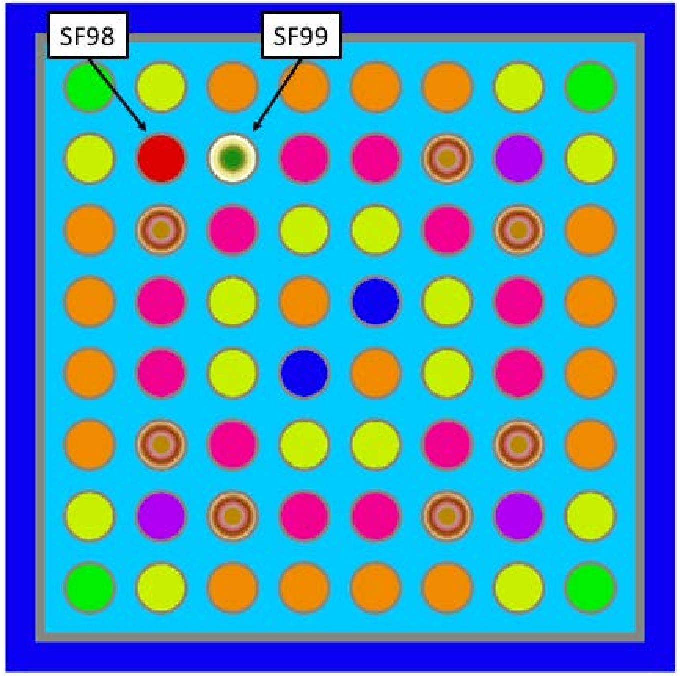
	RMSE (%)		
Code	Uranium	Plutonium	Fission Prod.
T/NEWT	1.2	1.9	15.8
Polaris	1.3	1.6	15.4
T/KENO	1.7	2.8	15.5
T/Shift	1.5	2.6	16.6

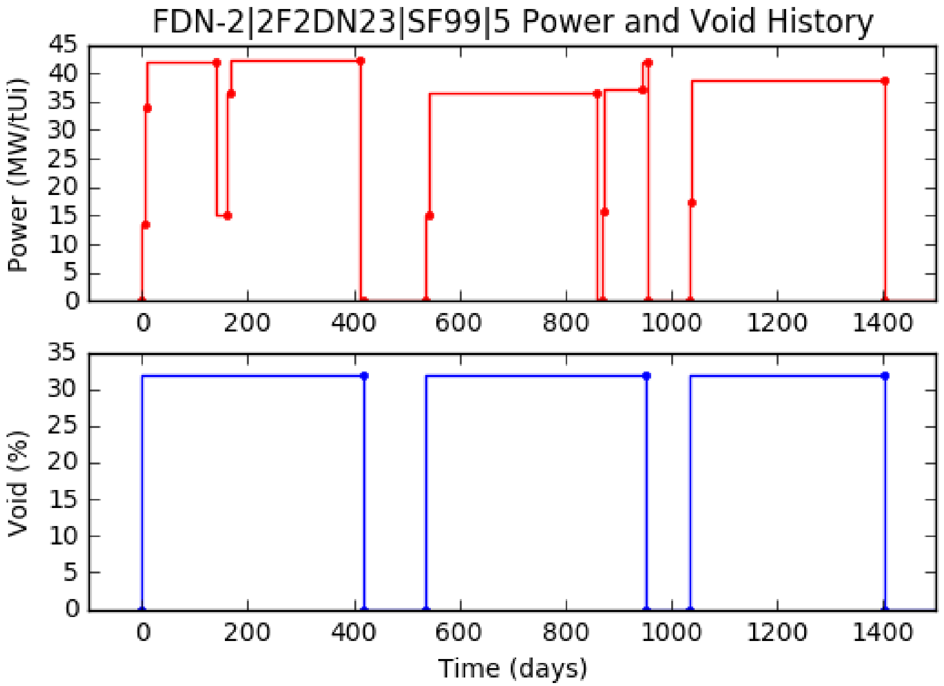




Depletion Validation Cases: Fukushima Daini Unit 2

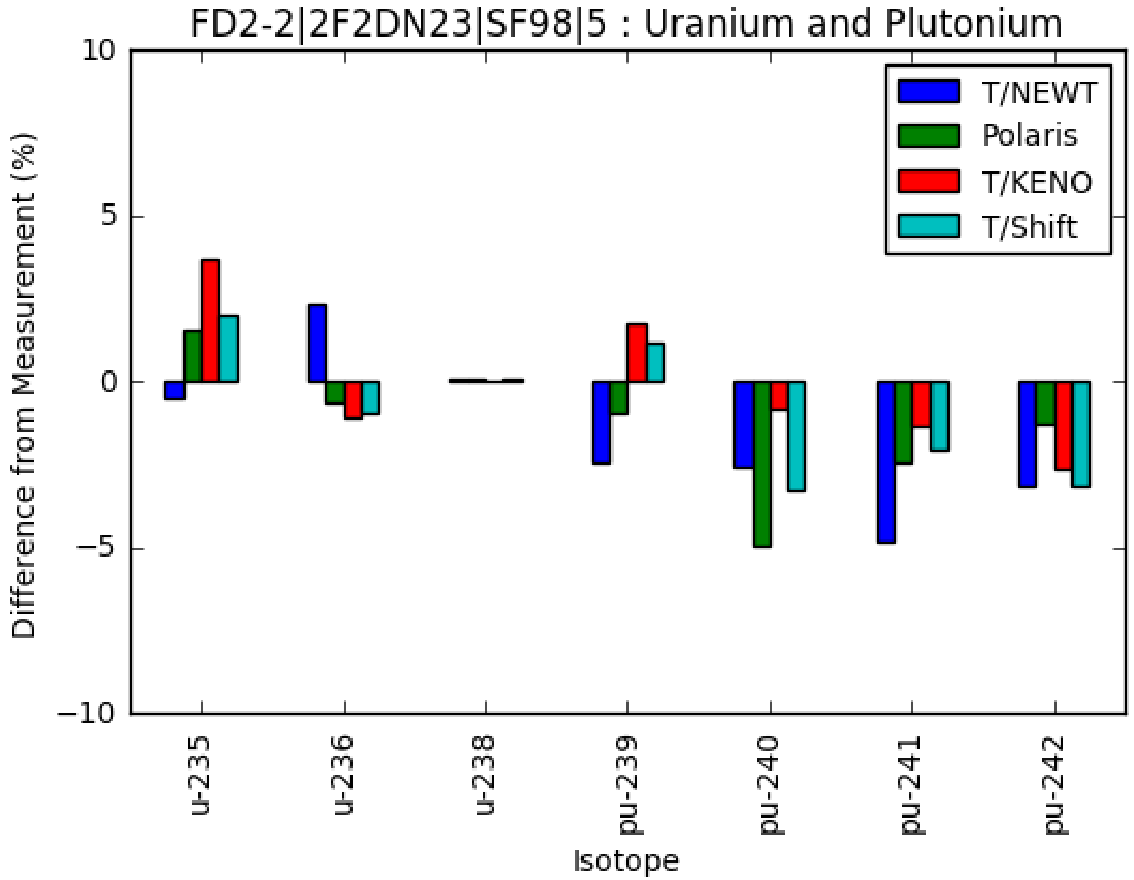
- GE 8×8-2 assembly (two small central water rods)
- Enrichment: 3.91 wt % ^{235}U in measured pin, but variable through the assembly
- Axial location
  Sample SF98-5: 1214 mm
  Sample SF98-6: 2050 mm
- Sample Burnup
  Sample SF98-5: 43.99 GWd/MTU
  Sample SF98-5: 39.92 GWd/MTU

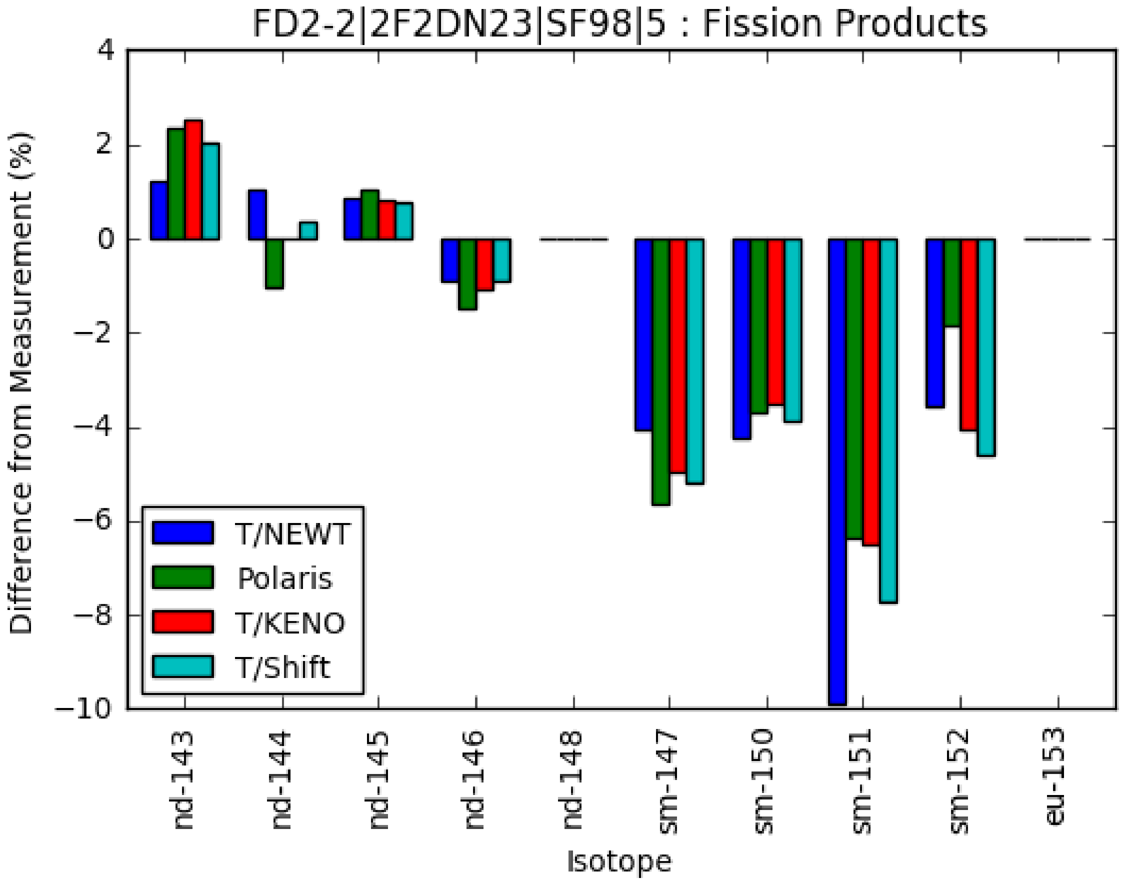




Depletion Validation Cases: Fukushima Daini Unit 2

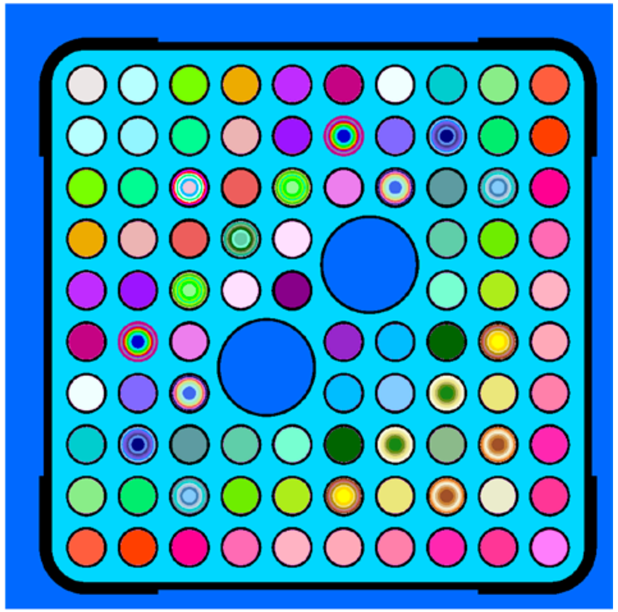
	RMSE (%)		
Code	**Uranium**	**Plutonium**	**Fission Prod.**
T/NEWT	1.4	5.5	6.8
Polaris	1.0	4.8	5.7
T/KENO	2.2	5.3	6.2
T/Shift	1.3	5.8	6.5

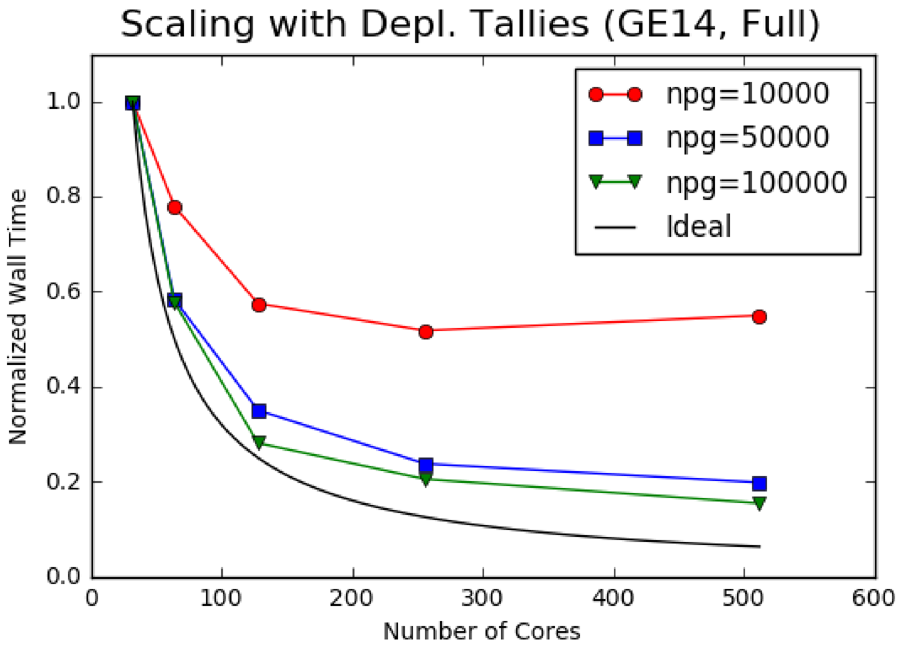


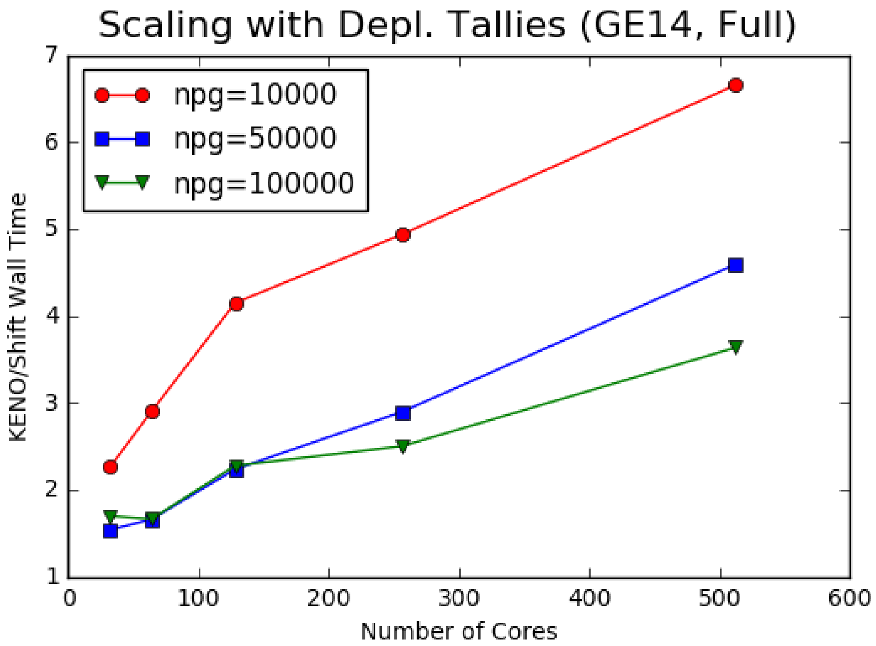


Shift Depletion Scaling

- **Test Case:** GE14 fuel assembly with depletion tallies
  - A number of identical simulations were run and the average time over the set simulations was used to estimate CPU time
- Shift scales close to ideally up to hundreds of processors when using O(50k) particles per generation
- Shift is only slightly faster than KENO on a single node (1.5x – 2x), but much faster on many nodes (3x - 7x)

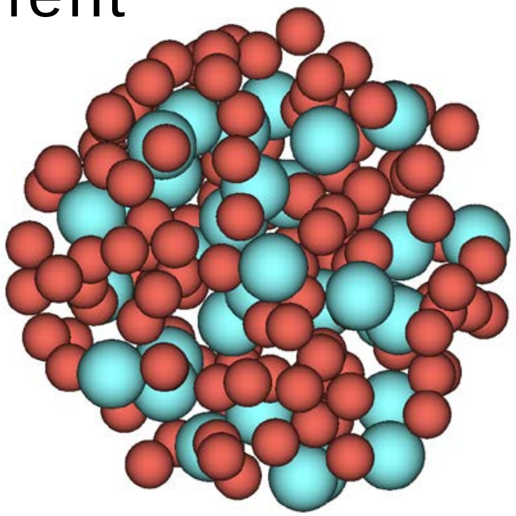






Stochastic Geometry

- **Goal:** Enable more straightforward generation of reference solutions for stochastic geometry (TRISO, pebble bed, FCM, etc.)
- Current capabilities
  - Multiple particle types and sizes (spherical only)
  - Sphere, cylinder, and cuboid boundaries
  - Random or regular array placement
  - Visualization of geometry enabled in Fulcrum
- Implemented only in Shift-based sequences



Pebble Input Example

```
=csas-shift
...
unit 1
    sphere 1    2.500000e-02
    sphere 2    3.400000e-02
    sphere 3    3.800000e-02
    sphere 4    4.150000e-02
    sphere 5    4.550000e-02
    media  100 1    1
    media  101 1    2  -1
    media  102 1    3  -2
    media  103 1    4  -3
    media  104 1    5  -4
    boundary 5
unit 10
    com='pebble'
    sphere 1    2.500000e+00
    sphere 2    3.000000e+00
    media  101 1    1  randommix='trisos'
    media  106 1    2  -1
    boundary 2
...
end geometry
...
read randomg eom
  randommix = 'trisos'
    type=    random
    units=    1  end
    pfs=    0.10 end
    clip=    no
    seed=    1000
  end randommix
end randomgeom
...
end
```

Questions?

"Before I came here I was confused about this subject. Having listened to your lecture I am still confused. But on a higher level."

—Enrico Fermi