LA-UR-19-20984
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Title: Automated Acceleration & Convergence Testing for Monte Carlo Criticality Calculations

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Intended for: DOE NCSP Technical Program Review, 2019-03-26/2019-03-27 (Amarillo, Texas, United States)

Issued: 2019-02-06

US DOE
Nuclear Criticality
Safety Program

Technical Program
Review

Pantex, Amarillo TX

26-27 March, 2019

Automated Acceleration & Convergence Testing for Monte Carlo Criticality Calculations

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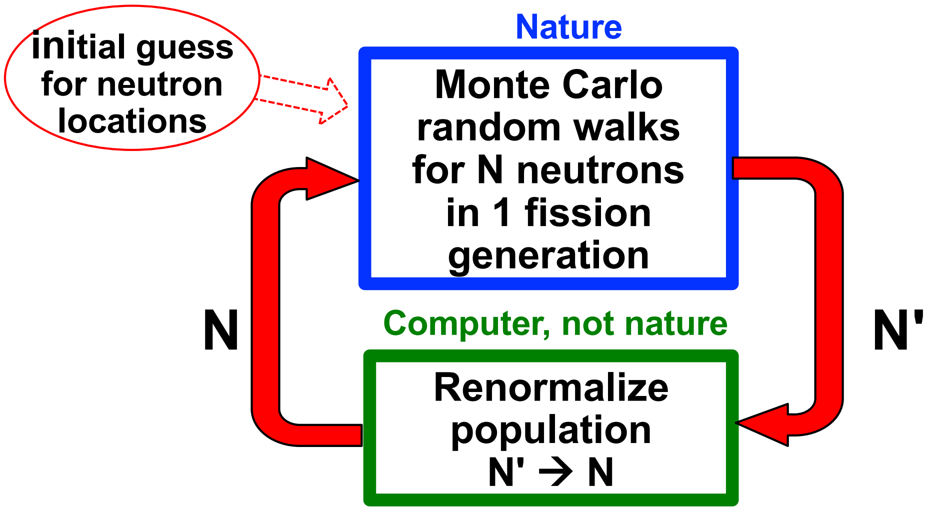
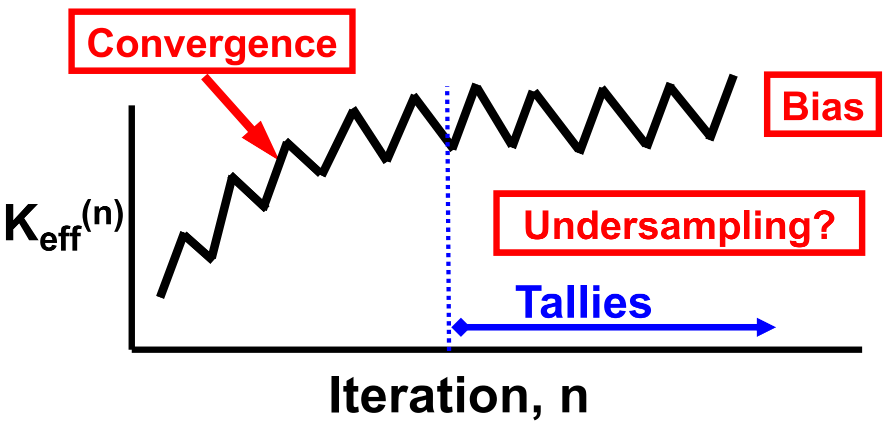
NUCLEAR ENGINEERING

Los Alamos NATIONAL LABORATORY EST. 1943

MC Criticality Calculations - Concerns





- **Bias in Keff**

  ~ -1 / (neutrons/cycle)

- **Bias in source shape**

  Too low in high-importance regions,
  Too high in low-importance regions

- **Undersampling/clustering**

  Not enough neutrons/cycle to cover space

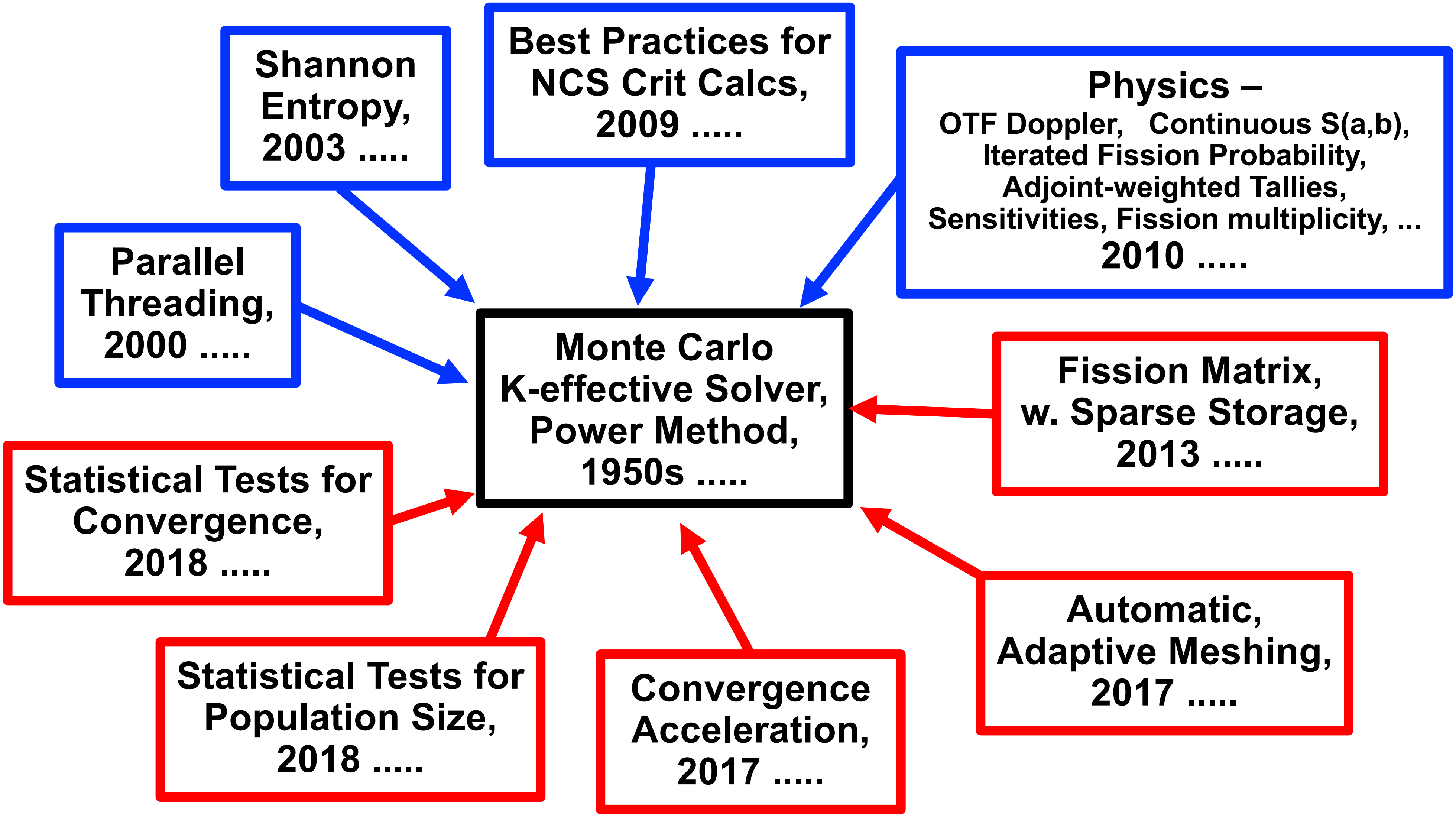
- **Convergence**

  source shape takes longer than keff

- **Best Practices**

  Source in all fissile regions.
  Examine H_{src} plot for convergence.
  >10k neuts/cycle (>100k big probs).
  A few 100 cycles.

LANL R&D for MC Criticality Calculations



This work: Combine & automate the red boxes

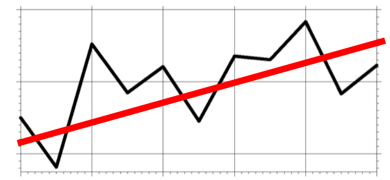
Automated acceleration & convergence testing for MC criticality

- **Enabling technology advancements, combined new methods**
  - **Fission-matrix with adaptive sparse storage**
    - Reference solution for fission neutron distribution
    - Used to accelerate convergence of neutron distribution
    - Used in statistical tests for convergence & population size
  - **Statistical tests for convergence of neutron distribution**
    - 8 tests on metrics, 3 tests on distributions
    - Automatically begin active cycles & tallies
  - **Population size tests**
- **Eliminates the need to run trial calculations, examine Shannon entropy plots, set parameters on KCODE card, & then rerun**
  - **Provides quantitative evidence of convergence**
  - **Enables parameter studies & coupled TH feedback**
  - **Saves significant computer time**

Automated Methods

- **Meshing for convergence tests**
  - Automatically created & extended if needed, no user input required
  - Uniform mesh spacing in x,y,z = L_{fiss} = RMS-distance-to-fission
  - Used for sources, entropy, fission matrix: S_{neut}, H_{src}, $F(I \leftarrow J)$, S_{FM}
- **Cycle 1**
  - Estimate L_{fiss} & set initial mesh
- **Initial cycles**
  - Iterate until S_{neut} & F tallies stabilize
  - Automated, test that (Δ nonzero tallies) < 2%, 5%
- **For blocks of cycles (default = 10)**
  - At end, solve F matrix equations for S_{FM}
  - Convergence tests
    - **9 statistical tests must all pass for convergence** (also 2 other tests)
  - If not converged, accelerate source convergence by importance sampling, weights: $S_{FM}(m) / S_{neut}(m)$, m = bin
  - If converged, set active cycles to begin with next cycle, perform tests on population size

Statistical tests for convergence – Metric Tests



- **Slope test**
  - For a block of cycles (default = 10)
  - For some MC result *x* from each cycle in block, compute least-squares slope & σ_{slope}
  - If abs(slope(x)) < 0.0001 → pass test, slope ~ 0
  - If abs(slope(x)) < 2 σ_{slope} → pass test, slope ~ 0 within statistics

Metric tests, at end of block for convergence testing

1. Slope test for $K_{tracklen}$
2. Slope test for $K_{collide}$
3. Slope test for K_{absorb}
4. Slope test for H, Shannon entropy of source distribution
5. Slope test for H_X, Shannon entropy of X marginal source distribution
6. Slope test for H_Y, Shannon entropy of Y marginal source distribution
7. Slope test for H_Z, Shannon entropy of Z marginal source distribution
8. H_{block} within 1% of H_{FM}

Note: If Test 8 passes, provides more evidence of convergence
If Test 8 fails, ignore it – might be due to low popsize

Statistical tests for convergence – Distribution Tests

Distribution tests, at end of block for convergence testing

9. **Kolmogorov-Smirnov test passed at 95% level,**
   S_{block} & S_{FM} have same distribution

   For multi-D distributions, KS statistic depends on ordering.
   Take worst case KS statistic for many random permutations.

10. **Chi-square 2-point test passed at 95% level,**
    S_{block} & S_{FM} have same distribution

11. **Relative entropy (Kullback-Liebler discrepancy) test passed at 95% level for S_{block} & S_{FM}**

    Note: If Test 11 passes, provides more evidence of convergence
    If Test 11 fails, ignore it – might be due to low popsize

Statistical tests for convergence

- Convergence tests at end of a block of cycles:
  – Perform Metric tests 1-8
  – Perform Distribution tests 9-11

  – If metric tests 1-7 and distribution tests 9-10 all pass, declare convergence
  – If metric test 8 passes, additional evidence. If not, ignore it.
  – If distribution test 11 passes, additional evidence. If not, ignore it.

- If convergence tests all pass, convergence is locked-in for the remainder of the calculation
  – Tests continue for each block
  – Some tests may occasionally fail (due to statistics, it happens), but convergence is not rescinded

Accelerating Source Convergence

fmataccel option

- **At the end of each cycle**
  - S_{FM} is available – source from fission matrix at end-of-block
  - S_{neuts} is available – actual neutron source at end-of-cycle
- **During inactive cycles, can optionally use (S_{FM} / S_{neuts}) for importance sampling of the fission source**
  - Recomputed each cycle using S_{FM} from previous end-of-block, and S_{neuts} for current end-of-cycle
  - Works – typically reduces inactive cycles by 2-10 X
  - Effectiveness depends on:
    - Large neuts/cycle &/or not-too-fine mesh for fission matrix
    - Not effective if (S_{FM} / S_{neuts}) has too much statistical noise
  - Further development under consideration:
    - Investigate using $S_{FM}^{adjoint}$ for source importance sampling
    - Maybe coarsen the fission matrix, to get less statistical noise

Statistical tests for Population Size

Performed after convergence, at end of each block of cycles

1. Relative entropy < 0.05 for S_{block} vs S_{FM}
2. $< H_{cycle} >$ within 1% of H_{FM}

If both tests pass, population size is adequate

If either test fails, it is likely that larger neutrons/cycle should be used. A warning message is printed.

For future work, if the popsize tests fail, neutrons/cycle could be automatically increased. That could create resource issues – memory size, run time, etc.

MCNP6 example

```
comment.
comment. ---------------------------------------------------------------------
comment. entropy of the fission source distribution will be computed
comment.
comment. the mesh for source entropy is based on the site coordinates
comment.   using  3675  mesh cells with spacing approx  1.00*rms-fiss-dist
comment.
comment.     Xbins=   35      Xmin= -1.6861E+02     Xmax=  1.6856E+02
comment.     Ybins=   35      Ymin= -1.6856E+02     Ymax=  1.6857E+02
comment.     Zbins=    3      Zmin= -9.6460E+00     Zmax=  9.9571E+00
comment.
comment. the mesh will be automatically extended if necessary to encompass the
comment.   entire fission distribution, preserving the original mesh spacing.
comment. ---------------------------------------------------------------------
comment.

comment.
comment. ---------------------------------------------------------------------
comment.  FISSION MATRIX WILL BE COMPUTED to estimate dominance ratio,
comment.      based on fission sites only - not flights or collisions
comment.
comment.  The mesh for the fission matrix is the same as the entropy mesh,
comment.      using  3675  mesh bins for tallying fission neutrons
comment.
comment.      Fission matrix mesh will be extended if
comment.         any fission sites are found outside this mesh.
comment.
comment.      Fission matrix tallies will be reset after cycle   1
comment.      Fission matrix eigenfunction will be found every  10 cycles.
comment.
comment.      Fission matrix dimensions:  3675 x 3675
comment.
comment.      Compressed-row-storage is used for the fission matrix.
comment.         max number of nonzero entries:  13505625
comment.
comment.
comment.  FMATCONVRG option is being used.
comment.     Statistical tests on the neutron and fission-matrix distributions
comment.     will be used to determine convergence and begin active cycles.
comment.     The 3rd entry on the KCODE card may be ignored.
comment.
comment.     Targets for statistical tests:
comment.       h_slope: < 0.0001 or <2.0 sig,     h_diff:   0.01
comment.       k_slope: < 0.0001 or <2.0 sig,     distribs: 0.95 conf level
comment.
comment.
comment.  FMATACCEL option is being used.
comment.    The fission matrix will be used to ACCELERATE source convergence
comment.    of the neutron distribution during inactive cycles.
comment.    Importance-factor-limits:   min= 0.20,   max= 5.00
comment.
comment. ---------------------------------------------------------------------
comment.
```

MCNP6 example

```
cycle       k(col)        ctm    entropy    active      k(col)     std dev      chains
    1      1.35733        0.04    0.60521                                        35416
                                              extend H-mesh to:    36 x 35 x 4
    2      1.16857        0.10    0.62080                                        22433
                                              extend H-mesh to:    37 x 35 x 4
    3      1.08223        0.13    0.63109                                        17100
                                              dS=  3%, dF= 34%, shift window
                                              extend H-mesh to:    37 x 36 x 4
    4      1.05100        0.17    0.63410                                        13800
                                              dS=  2%, dF= 19%, shift window
                                              extend H-mesh to:    37 x 37 x 4
    5      1.02827        0.21    0.63348                                        11529
                                              dS=  1%, dF= 14%, shift window
                                              extend H-mesh to:    37 x 37 x 5
    6      1.02118        0.25    0.61732                                         9997
                                              dS=  0%, dF= 10%, shift window
    7      1.02018        0.29    0.61762                                         8746
                                              dS=  1%, dF=  9%, shift window
    8      1.02413        0.32    0.61845                                         7790
                                              dS=  0%, dF=  7%, shift window
    9      1.01974        0.37    0.61766                                         6974
                                              dS=  0%, dF=  7%, shift window
   10      1.01709        0.43    0.61656                                         6313
                                              dS=  1%, dF=  5%, shift window
   11      1.02129        0.48    0.61606                                         5815
                                              dS=  1%, dF=  5%, shift window
   12      1.01705        0.53    0.61452                                         5351
   13      1.02459        0.58    0.61263                                         4975
   14      1.02193        0.65    0.61214                                         4640
   15      1.02741        0.70    0.60894                                         4372
   16      1.03005        0.73    0.60600                                         4091
   17      1.03266        0.78    0.60435                                         3852
   18      1.03369        0.83    0.60065                                         3628
   19      1.03485        0.87    0.59622                                         3426
   20      1.03631        0.91    0.59177                                         3245
   21      1.04159        0.96    0.58774                                         3074

        fmatrix keff= 1.12401,   DR= 0.91098,   iters=    199
```

Source, fission matrix, & mesh stabilization

Block of cycles

MCNP6 example

```
20    1.03631      0.67    0.59177                                          3245
21    1.04159      0.71    0.58774                                          3074

      fmatrix keff= 1.12401,  DR= 0.91098,  iters=   199

      CONVERGENCE INFO & CHECKS:         (based on last  10 cycles)

        entropy for fmatrix eigenvector    =  0.35378

        entropy for neutron  last cycle    =  0.58774   dif=   66.13%
        relative entropy for last cycle    =  2.06901

        slope of keff (tracklen)     =  2.0E-03,  target:  < 4.7E-04   FAIL
        slope of keff (collide)      =  2.1E-03,  target:  < 4.8E-04   FAIL
        slope of keff (absorb)       =  2.0E-03,  target:  < 5.2E-04   FAIL
        slope of entropy             = -2.6E-03,  target:  < 3.9E-04   FAIL
        slope of entropy X marginal  = -2.1E-03,  target:  < 4.5E-04   FAIL
        slope of entropy Y marginal  = -2.1E-03,  target:  < 3.7E-04   FAIL
        slope of entropy Z marginal  =  8.7E-04,  target:  < 3.0E-04   FAIL
        entropy dif, neuts vs fmat   =  7.1E-01,  target:  < 1.0E-02   n/a
        Kolmo-Smirnov, distrib, stat =  6.8E-01,  target:  < 9.1E-02   FAIL
        Chi-square,    distrib, stat =  5.0E+04,  target:  < 5.0E+02   FAIL
        rel-h-block,   distrib, stat =  2.5E+00,  target:  < 5.0E-03   n/a

        ***** convergence tests were NOT passed *****

      MISCELLANEOUS INFO & CHECKS:

        rmse          =    1.16    %
        fmat nnz=         11882,  0.09 %

                                         accelerate: Imin= 0.2, Imax= 4.7
22    1.10895      0.75    0.38293                                          2130
                                         accelerate: Imin= 0.2, Imax= 2.5
23    1.11427      0.78    0.35428                                          1477
                                         accelerate: Imin= 0.2, Imax= 5.0
24    1.11602      0.81    0.35248                                          1258
                                         accelerate: Imin= 0.2, Imax= 5.0
25    1.12045      0.84    0.35200                                          1108
```

MCNP6 example

```
fmatrix keff= 1.11538,  DR= 0.91466,  iters=   127

CONVERGENCE INFO & CHECKS:          (based on last  10 cycles)

  entropy for fmatrix eigenvector    =  0.35254

  entropy for neutron  last cycle    =  0.35212   dif=   -0.12%
  relative entropy for last cycle    =  0.00744

  slope of keff (tracklen)      = -5.3E-05,  target:  < 6.5E-04   PASS
  slope of keff (collide)       =  7.1E-05,  target:  < 5.0E-04   PASS
  slope of keff (absorb)        = -6.8E-06,  target:  < 5.0E-04   PASS
  slope of entropy              = -2.2E-05,  target:  < 2.9E-04   PASS
  slope of entropy X marginal   =  5.8E-05,  target:  < 5.4E-04   PASS
  slope of entropy Y marginal   = -1.5E-04,  target:  < 4.1E-04   PASS
  slope of entropy Z marginal   = -5.8E-05,  target:  < 2.7E-04   PASS
  entropy dif, neuts vs fmat    =  2.6E-03,  target:  < 1.0E-02   PASS
  Kolmo-Smirnov, distrib, stat  =  2.4E-03,  target:  < 9.1E-02   PASS
  Chi-square,    distrib, stat  =  3.4E+01,  target:  < 5.0E+02   PASS
  rel-h-block,   distrib, stat  =  9.7E-04,  target:  < 5.0E-03   PASS

  ******************************************************************
  ******************************************************************
  ** FISSION SOURCE HAS CONVERGED, based on last     10   cycles  **
  **   Metrics:                                                   **
  **     slope of keff (tracklen)           is 0   (within uncert) **
  **     slope of keff (collide)            is 0   (within uncert) **
  **     slope of keff (absorb)             is 0   (within uncert) **
  **     slope of entropy                   is 0   (within uncert) **
  **     slope of entropy X marginal        is 0   (within uncert) **
  **     slope of entropy Y marginal        is 0   (within uncert) **
  **     slope of entropy Z marginal        is 0   (within uncert) **
  **     entropy dif, neuts vs fmat         is 0   (within uncert) **
  **   Distribution checks:                                       **
  **     Kolmo-Smirnov, distrib, stat, neut vs fmat (within conf) **
  **     Chi-square,    distrib, stat, neut vs fmat (within conf) **
  **     rel-h-block,   distrib, stat, neut vs fmat (within conf) **
  ******************************************************************
  ******************************************************************
  Convergence is locked-in, even if some tests fail in future cycles

  Active cycles will begin with cycle =       42
  Active cycles will end   with cycle =      241
  Total active cycles to be run       =      200
```

Quantitative Evidence For Convergence

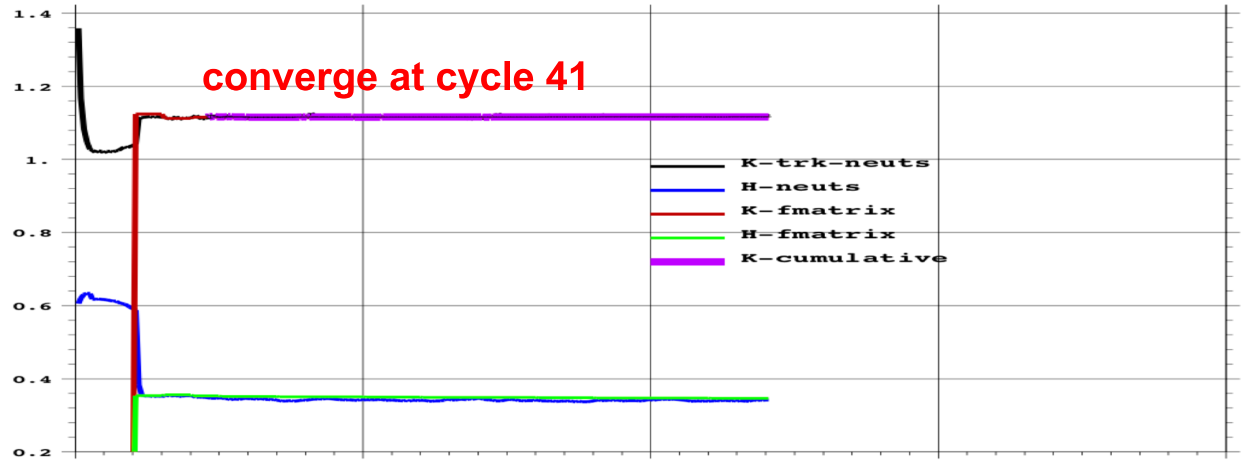
Quantitative Evidence For Convergence

MCNP6 example

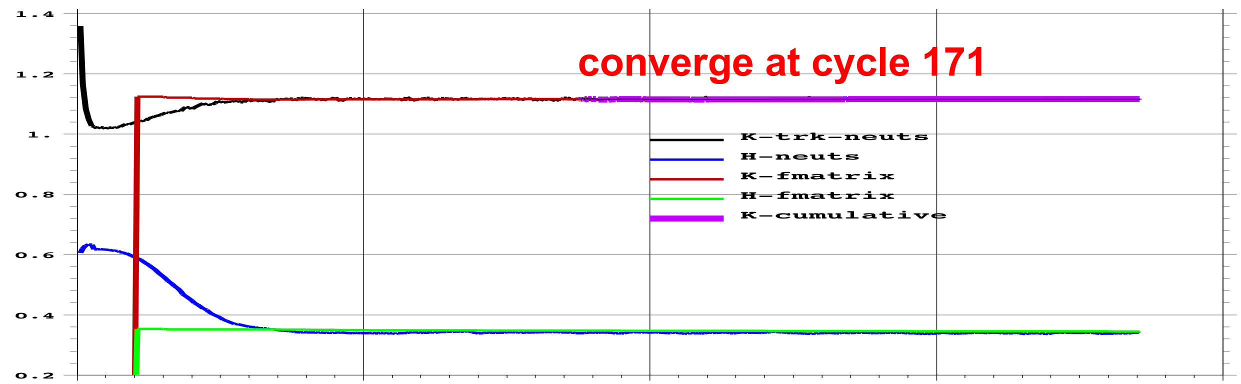
```
    50   1.12150       2.29   0.34704         9    1.11528    0.00178         401
    51   1.10686       2.33   0.34698        10    1.11444    0.00180         395

         fmatrix keff= 1.11491,  DR= 0.91140,  iters=   114

         CONVERGENCE INFO & CHECKS:          (based on last  10 cycles)

           entropy for fmatrix eigenvector    =  0.35151

           entropy for neutron  last cycle    =  0.34698   dif=   -1.29%
           relative entropy for last cycle    =  0.01079

           slope of keff (tracklen)      =  3.9E-04,  target:  < 8.8E-04   PASS
           slope of keff (collide)       =  5.1E-04,  target:  < 1.1E-03   PASS
           slope of keff (absorb)        =  4.2E-04,  target:  < 1.1E-03   PASS
           slope of entropy              = -5.8E-04,  target:  < 2.1E-04   FAIL
           slope of entropy X marginal   = -6.2E-04,  target:  < 3.6E-04   FAIL
           slope of entropy Y marginal   = -7.9E-04,  target:  < 4.4E-04   FAIL
           slope of entropy Z marginal   =  7.1E-07,  target:  < 2.2E-04   PASS
           entropy dif, neuts vs fmat    = -9.6E-03,  target:  < 1.0E-02   PASS
           Kolmo-Smirnov, distrib, stat =  5.6E-03,  target:  < 9.1E-02   PASS
           Chi-square,    distrib, stat =  9.9E+01,  target:  < 5.0E+02   PASS
           rel-h-block,   distrib, stat =  2.8E-03,  target:  < 5.0E-03   PASS

           convergence checks passed              at cycle =       41
           active cycles based on fmatconvrg begin at cycle =       42

           entropy for fmatrix eigenvector    =  0.35151
           entropy for neutron  active cycles =  0.34819   dif=   -0.94%
           relative entropy for active cycles =  0.00298

         POPULATION SIZE INFO & CHECKS:      (based on last  10 cycles)

           population check using relative entropy                           PASS

           warning: The average entropy for the last      cycles
                    differs from the entropy for the fission matrix
                    fundamental mode by  -1.1%.  This indicates
                    undersampling or possible clustering.
                    CONSIDER USING MORE NEUTRONS/CYCLE.
```

OECD-NEA Source Convergence Problem TEST4S

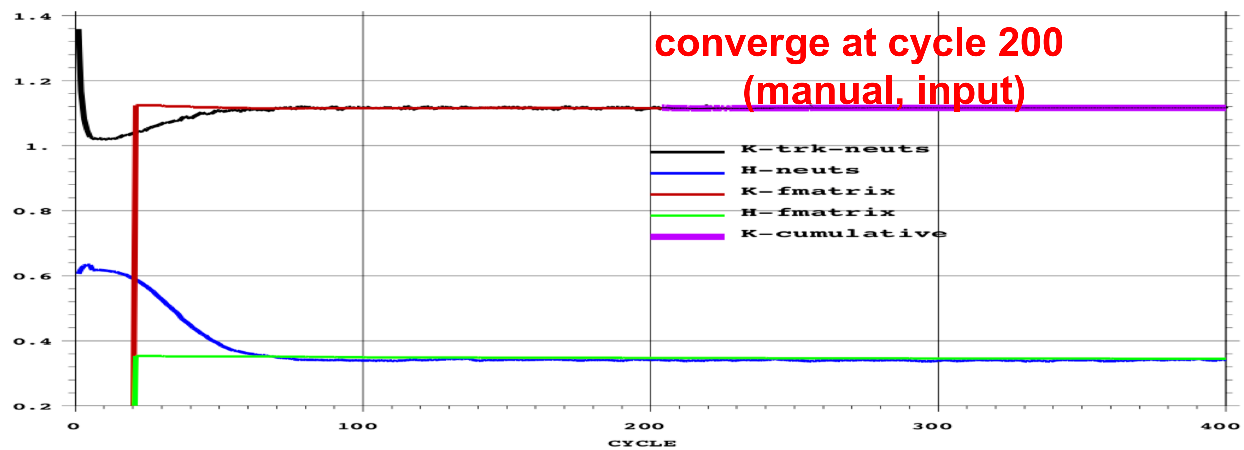
50,000 neuts/cycle
acceleration
auto-converge
k = 1.1165 (2)



50,000 neuts/cycle
no acceleration
auto-converge
k=1.1161 (2)

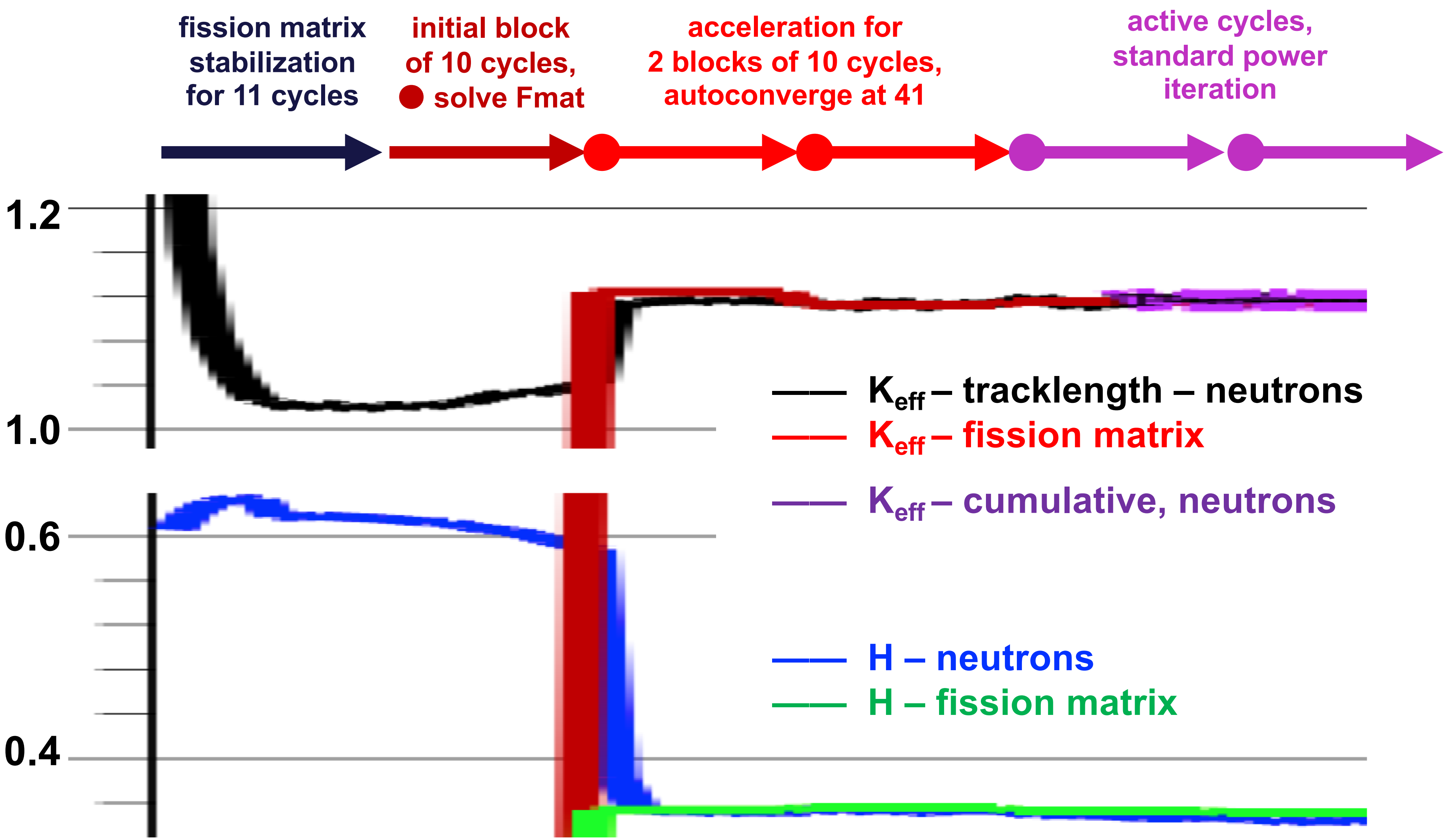


50,000 neuts/cycle
no acceleration
no auto-converge
k = 1.1164 (2)



OECD-NEA Source Convergence Problem TEST4S

50,000 neuts/cycle, acceleration, auto-converge, k = 1.1165 (2)



MCNP6 Test Problems for Fission Matrix Based Automated Convergence & Acceleration of K-eigenvalue Problems

- VALIDATION_CRITICALITY benchmark suite
- Godiva – bare HEU sphere
- PWR2d – commercial PWR
- ATR – advanced test reactor
- C5G7 3D U-Mox benchmark, OECD-NEA
- Triga reactor
- ACRR burst reactor, with FREC
- LCT-078-001 - Sandia critical experiment
- 3D PWR – Hoogenboom-Martin benchmark, OECD-NEA
- Whitesides problem – K-effective of the world model
- TEST4S – simplified Whitesides, OECD-NEA
- FPOOL – OECD-NEA source convergence benchmark 1

VALIDATION_CRITICALITY benchmark suite

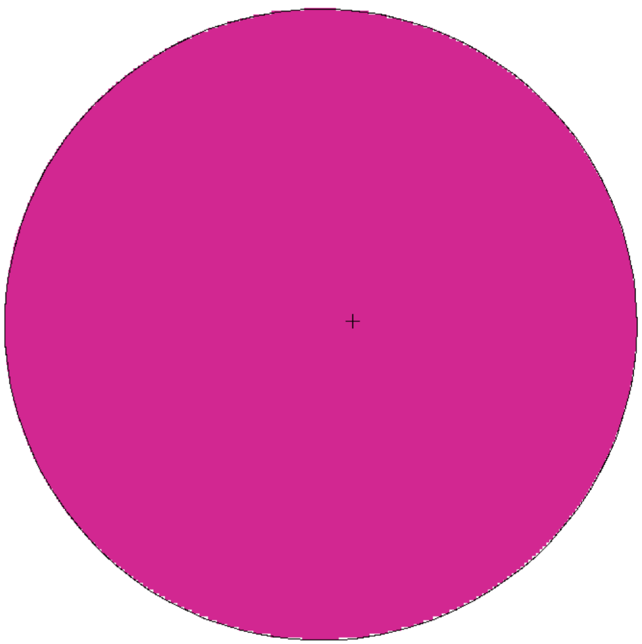
- **Standard MCNP validation suite since 2002 (Mosteller)**
  - 31 ICSBEP Handbook problems, critical experiments
  - Run using ENDF/B-VII.1 nuclear data
  - Timing results include all I/O, input & xsec file processing, Monte Carlo random walks, printing results, etc. for all 31 problems

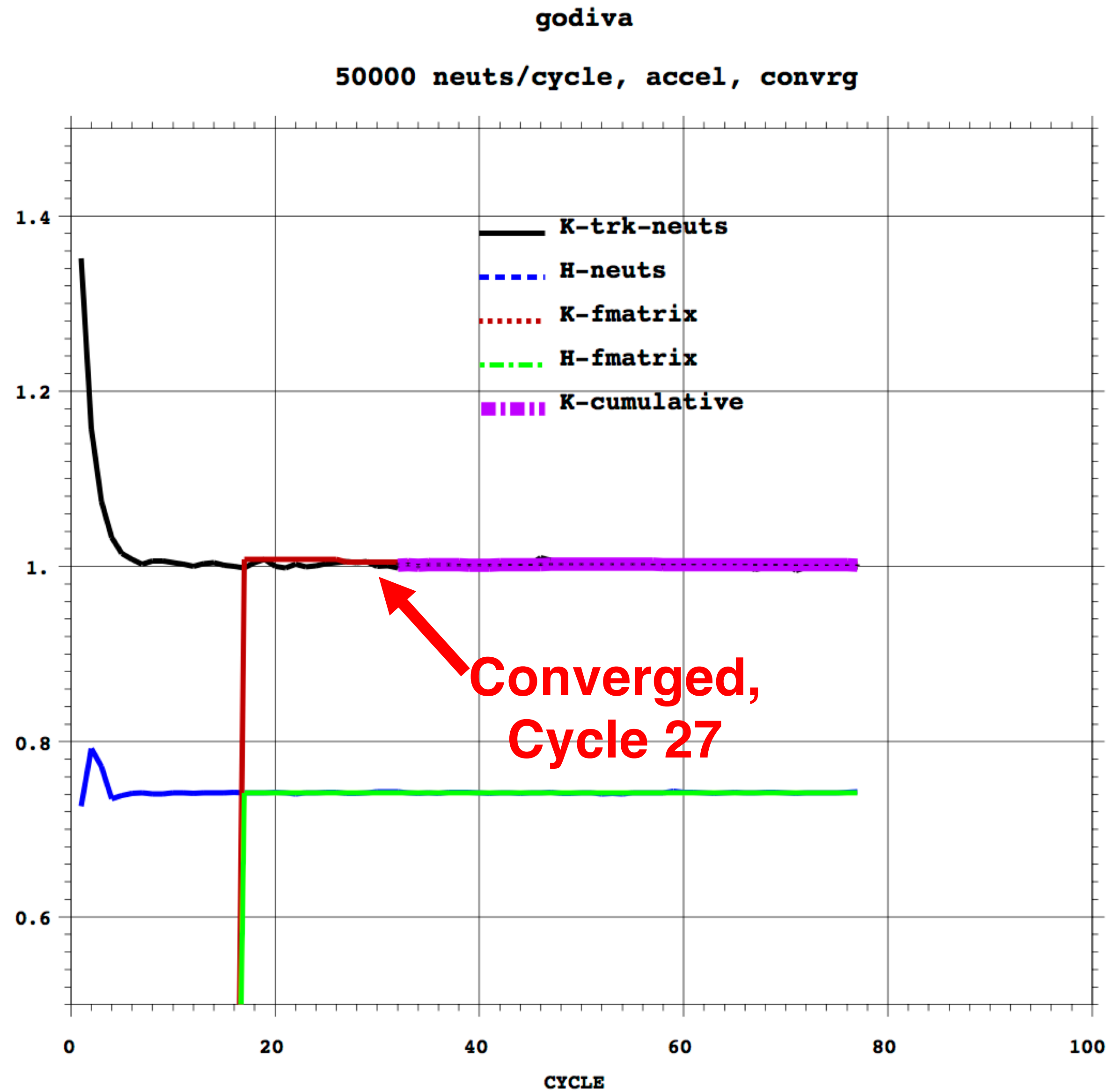
- **Timing tests**
  - 50 M neutrons/cycle for all runs
  - For standard runs, 100 inactive cycles, 100 active cycles
  - For auto accelerate & converge, 100 active cycles

Standard run:	**106 minutes**
Auto accel & converge:	**80 minutes**

Godiva Problem

Bare HEU sphere

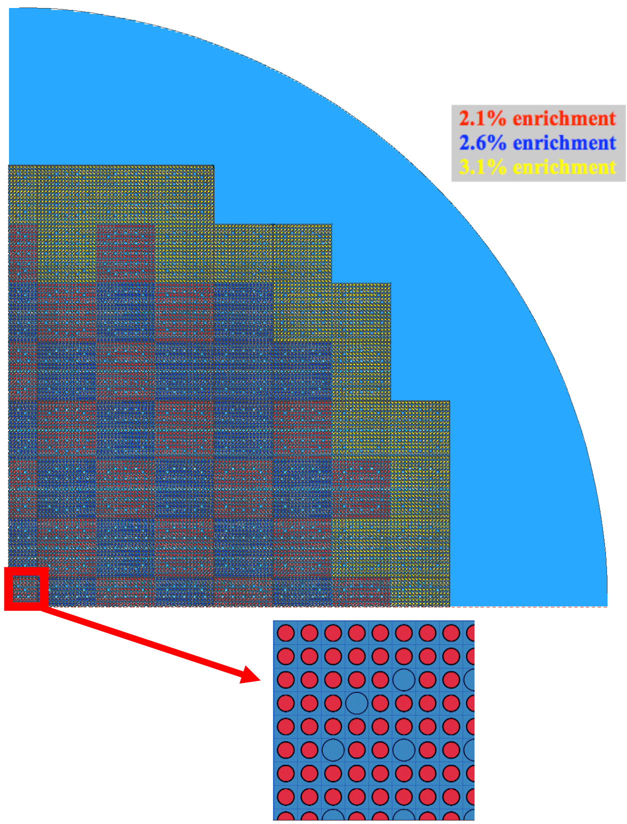


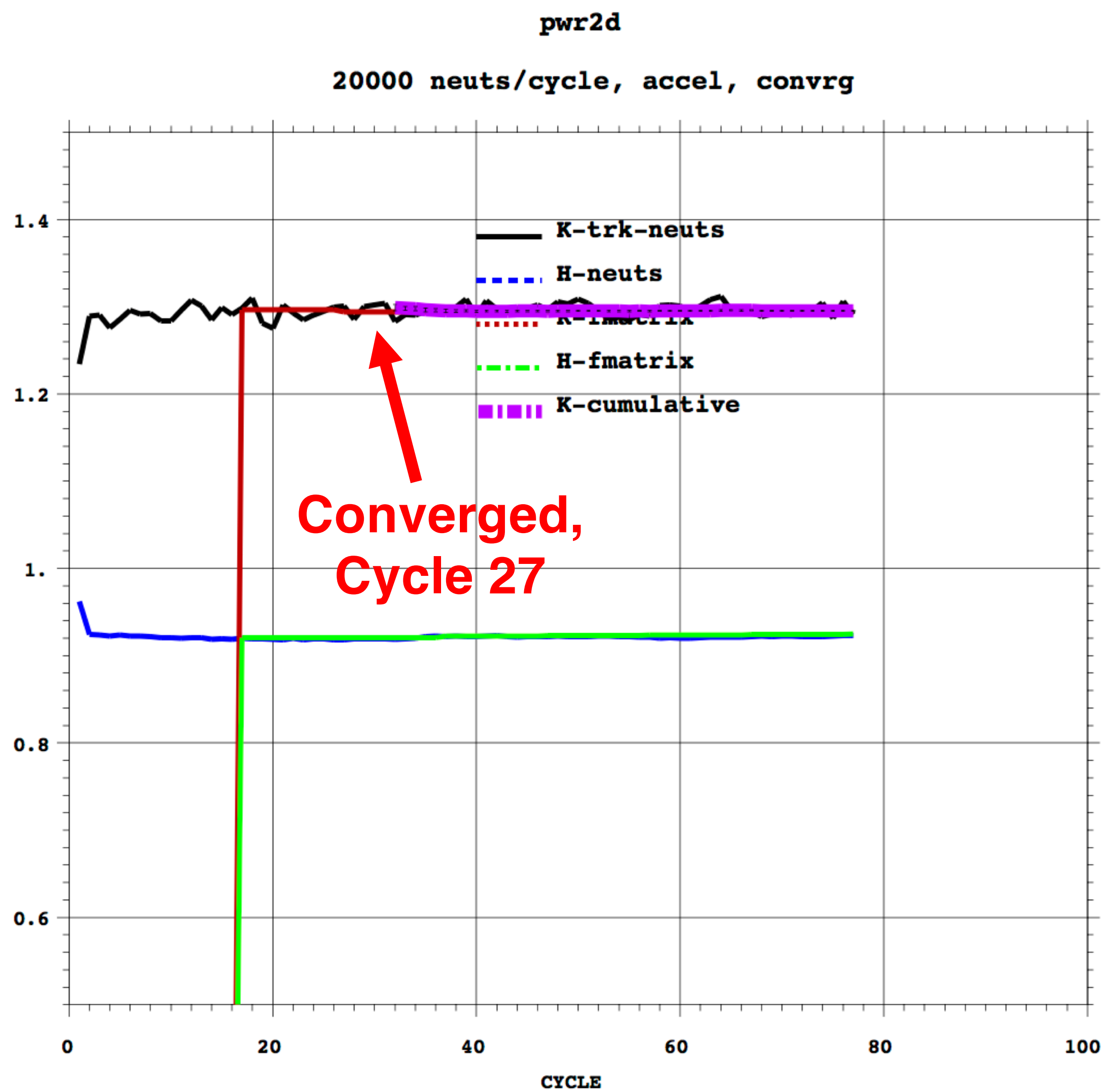


Whole-core 2D PWR Model

2D PWR (Nakagawa & Mori model)

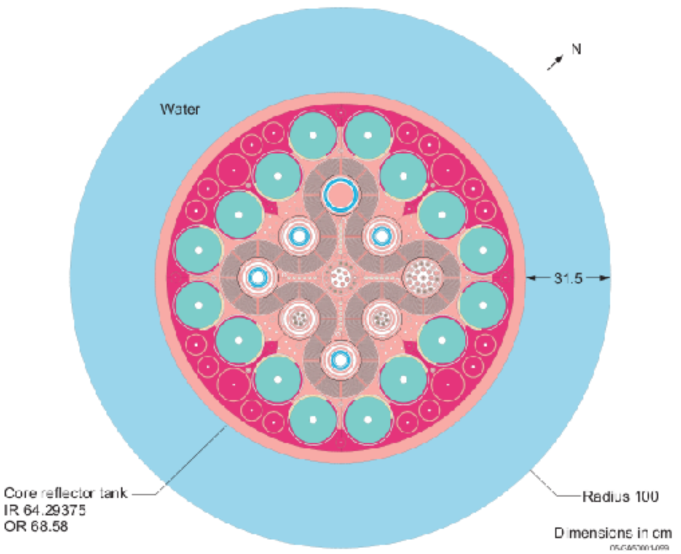
- 48 1/4 fuel assemblies:
  - 12,738 fuel pins with cladding
  - 1206 1/4 water tubes
- Each assembly:
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- Calculations used whole-core model, symmetric quarter-core shown below

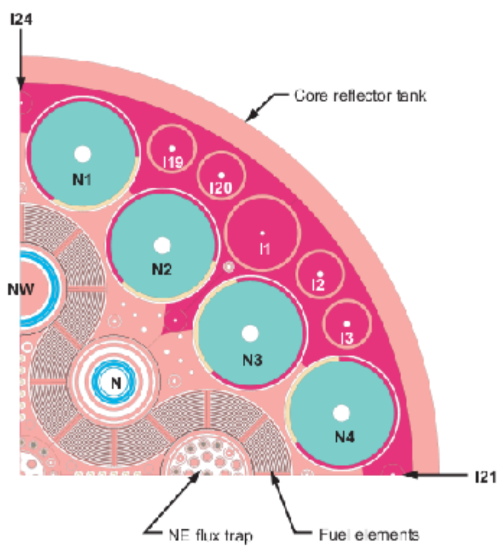


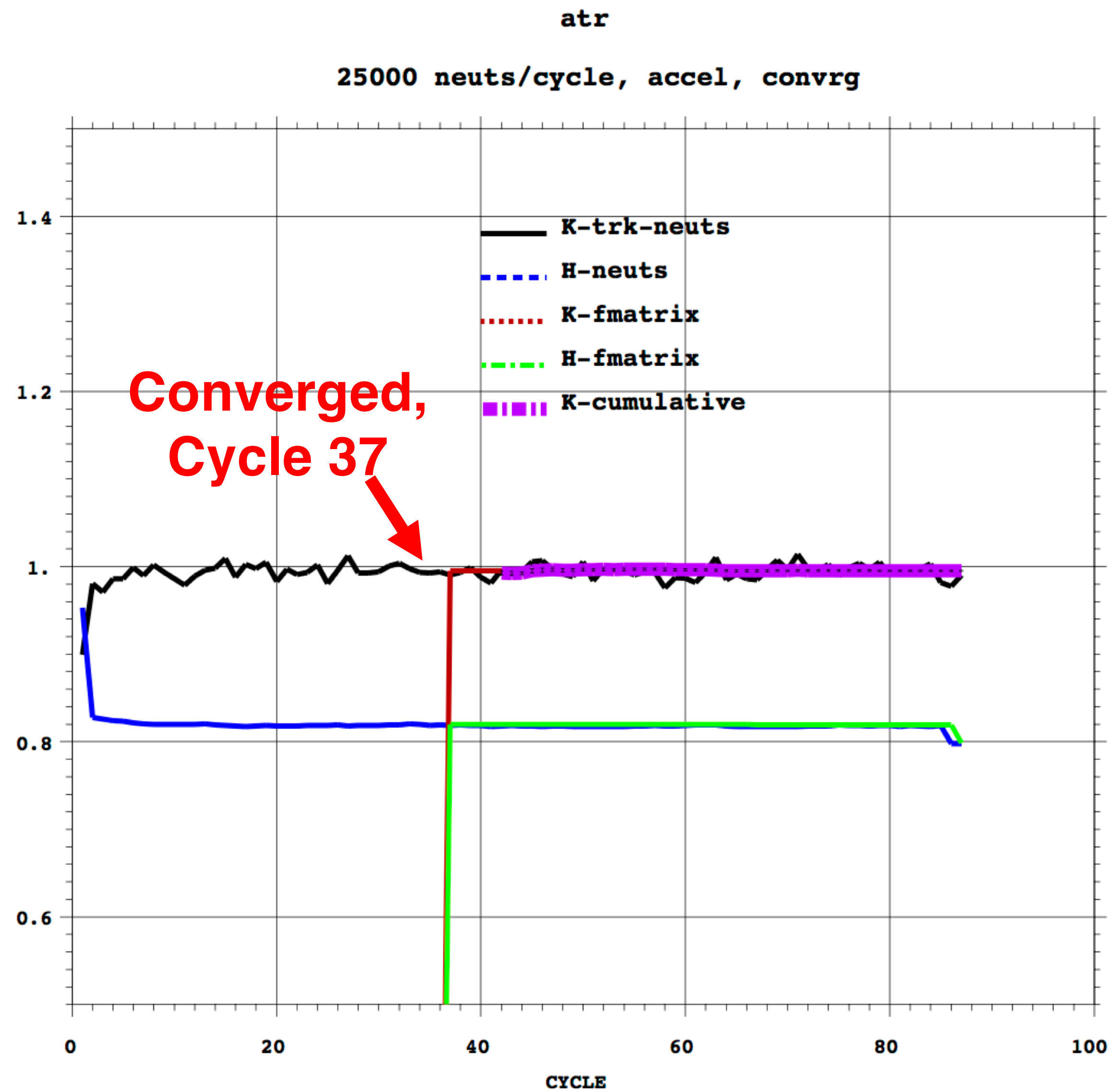


Advanced Test Reactor

"Serpentine Arrangement of Highly Enrichment Water-Moderated Uranium-Aluminide Fuel Plates Reflected by Beryllium"







OECD-NEA Benchmark - C5G7

Figure 2. Fuel pin layout

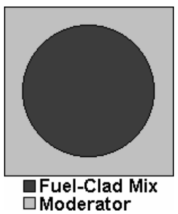
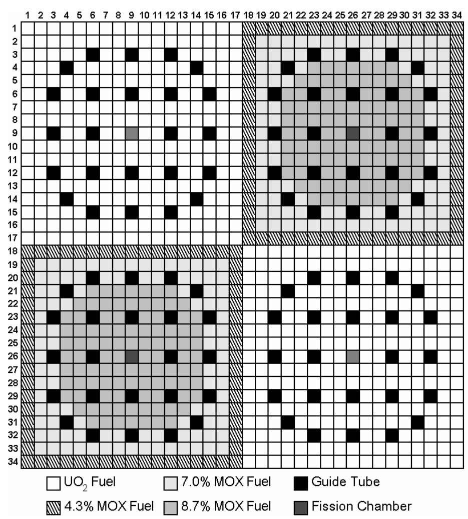
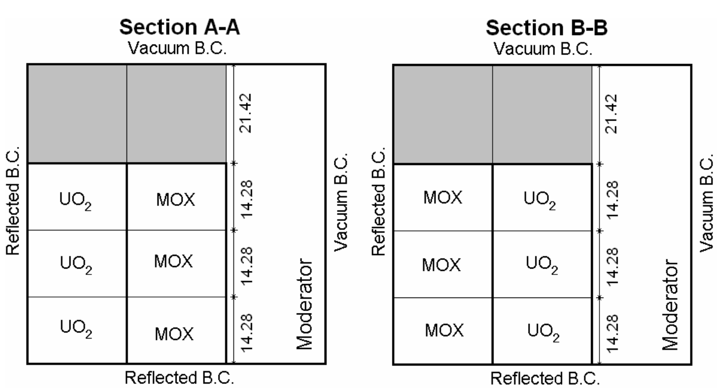
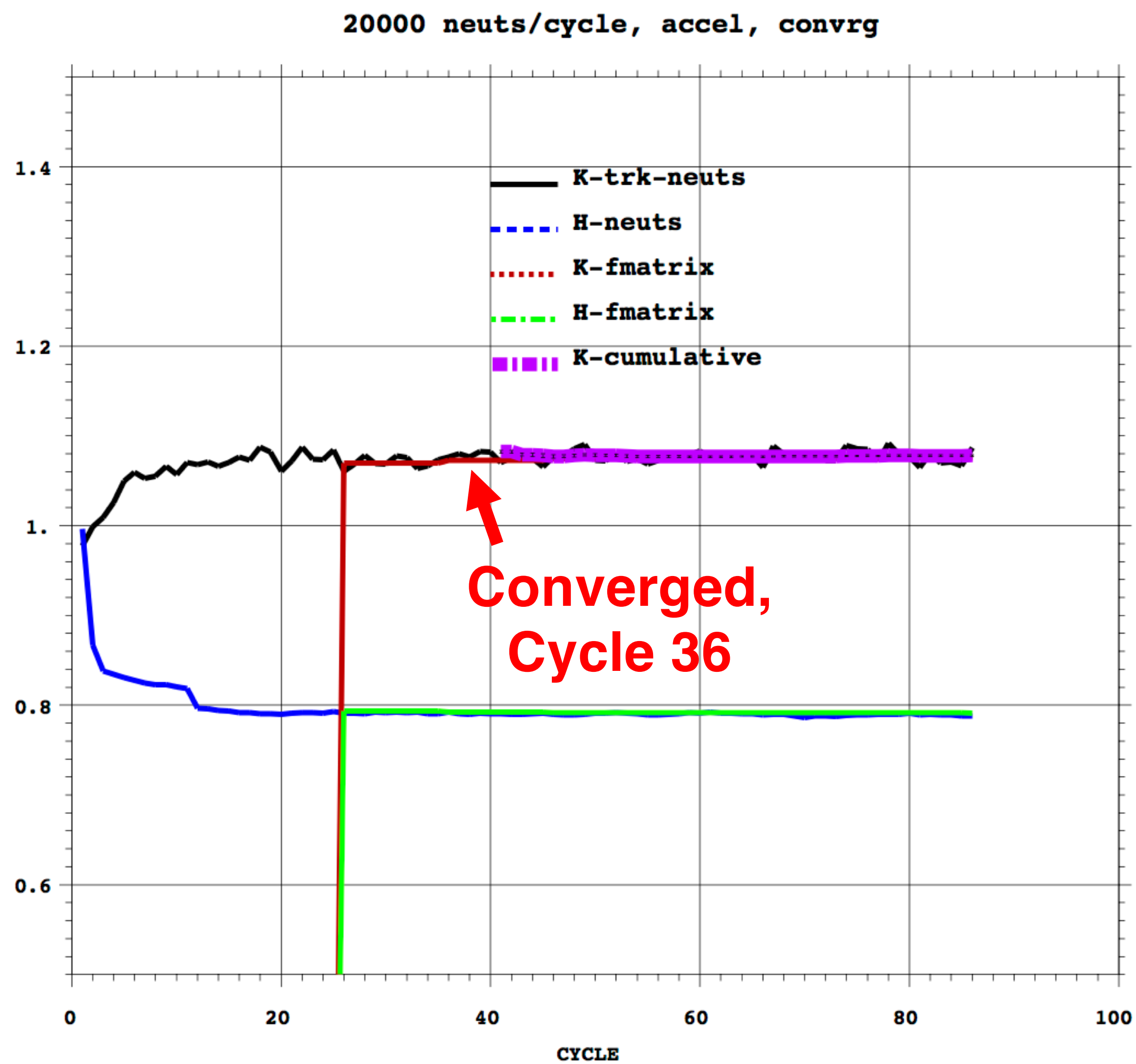


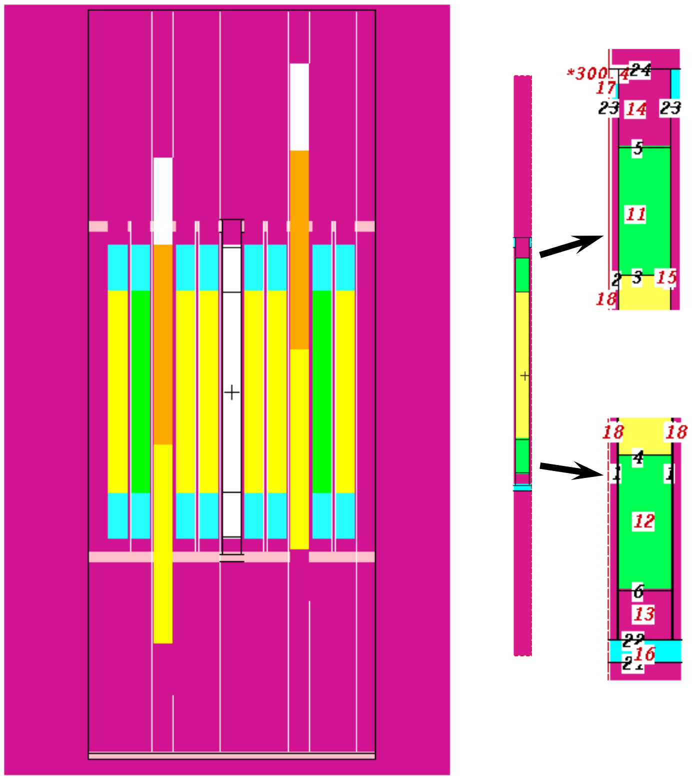
Figure 3. Benchmark fuel pin compositions and numbering scheme

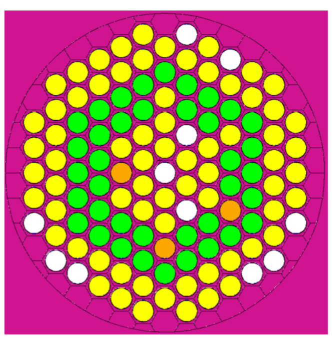


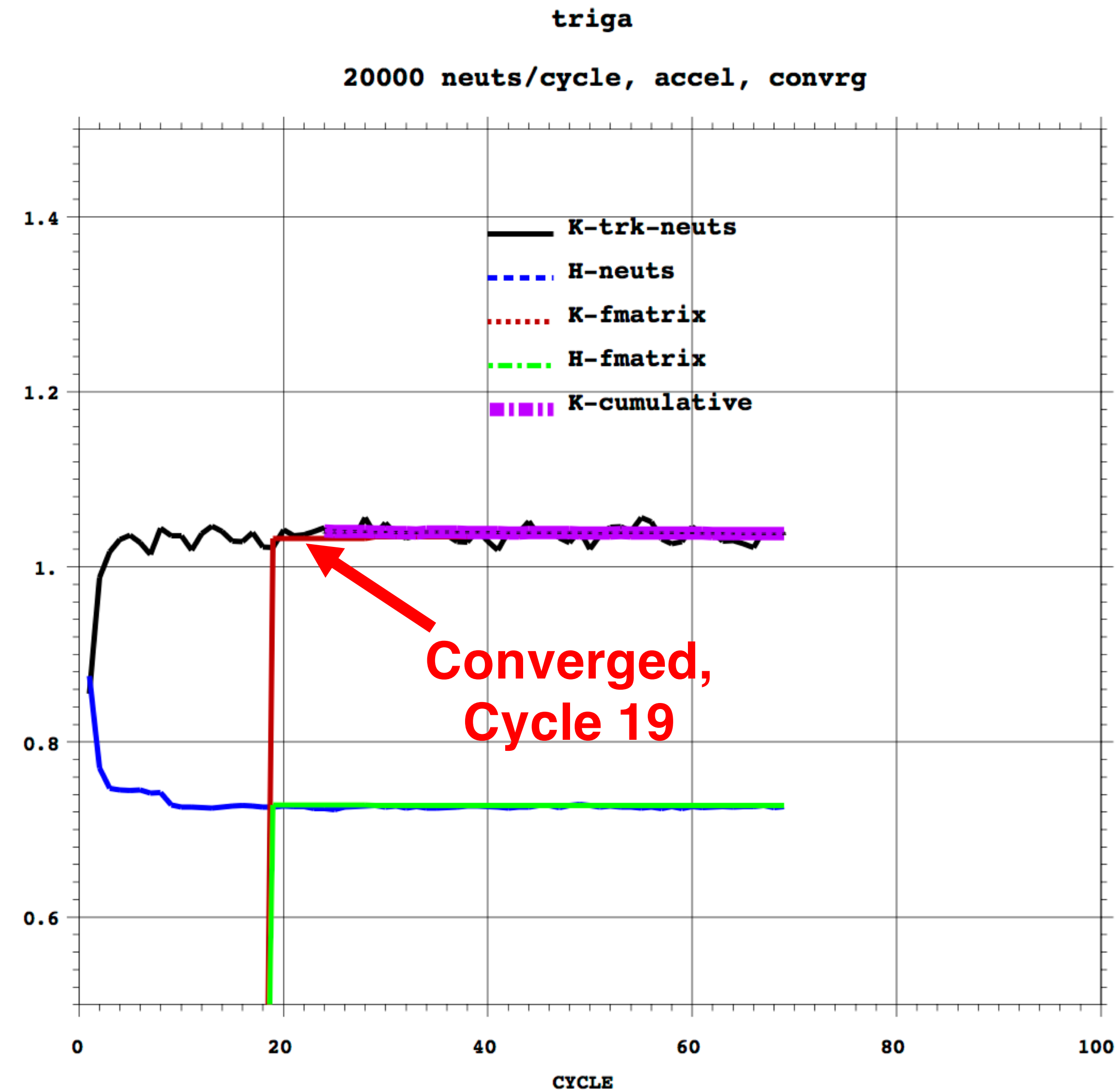




TRIGA Reactor

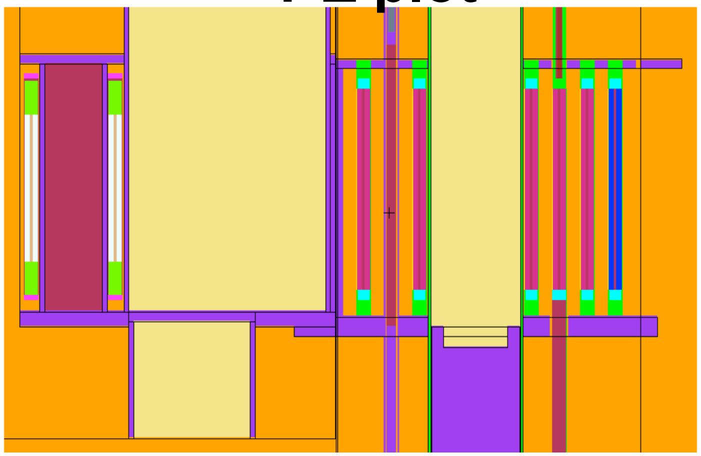




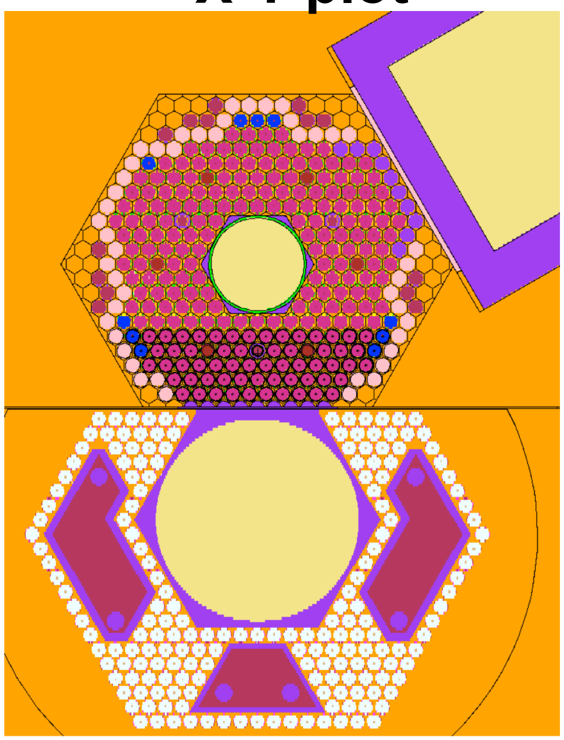


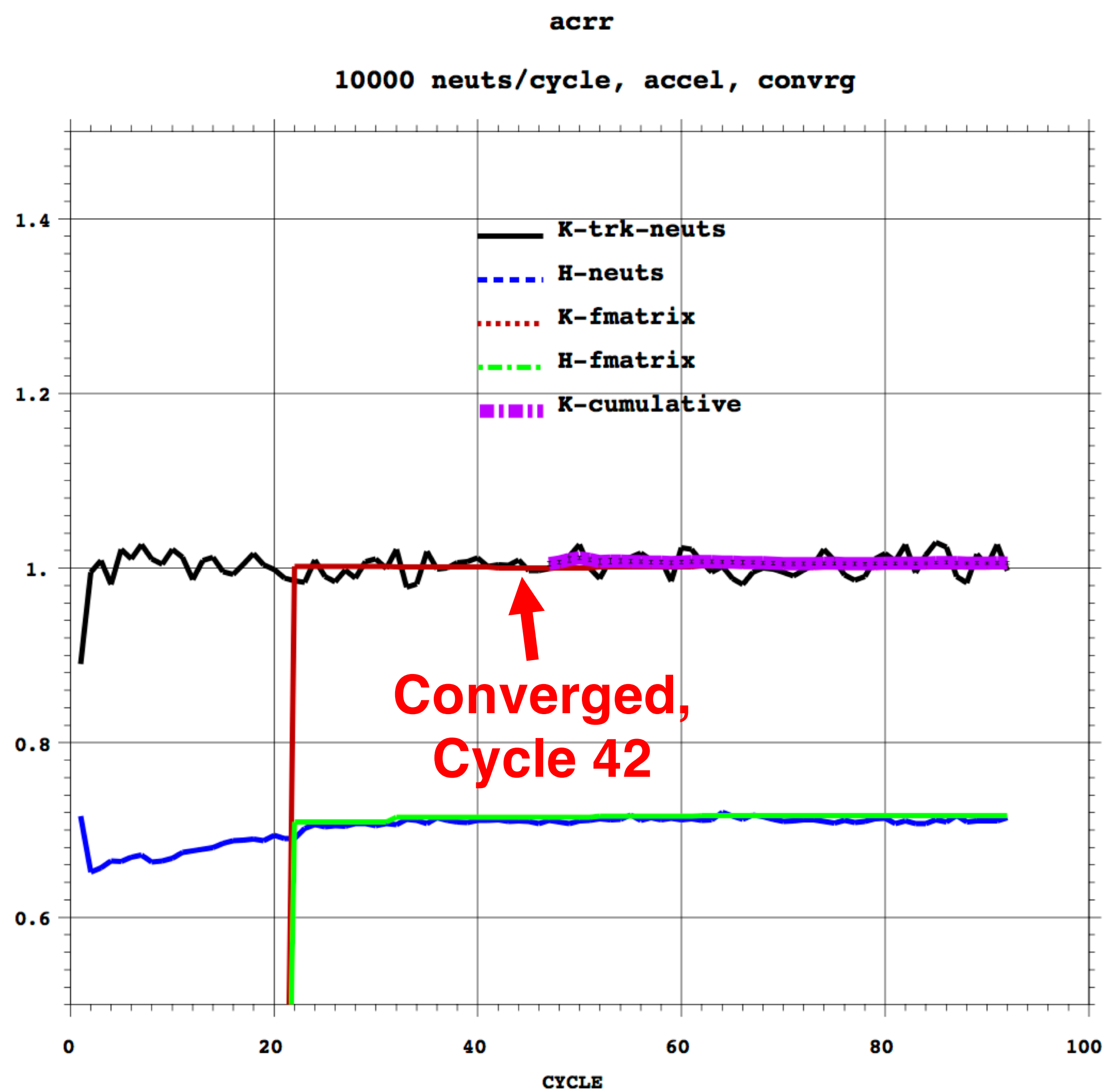
Sandia burst reactor - ACRR, with FREC

Y-Z plot



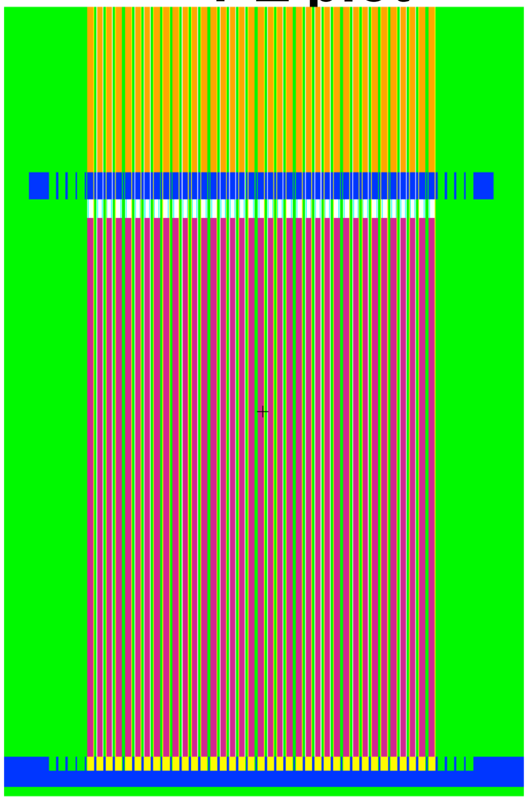
X-Y plot



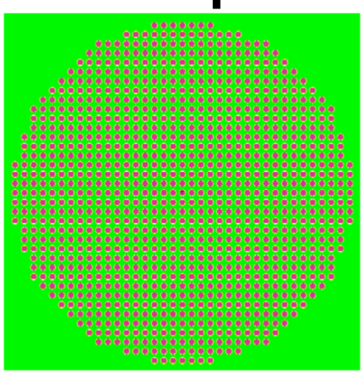


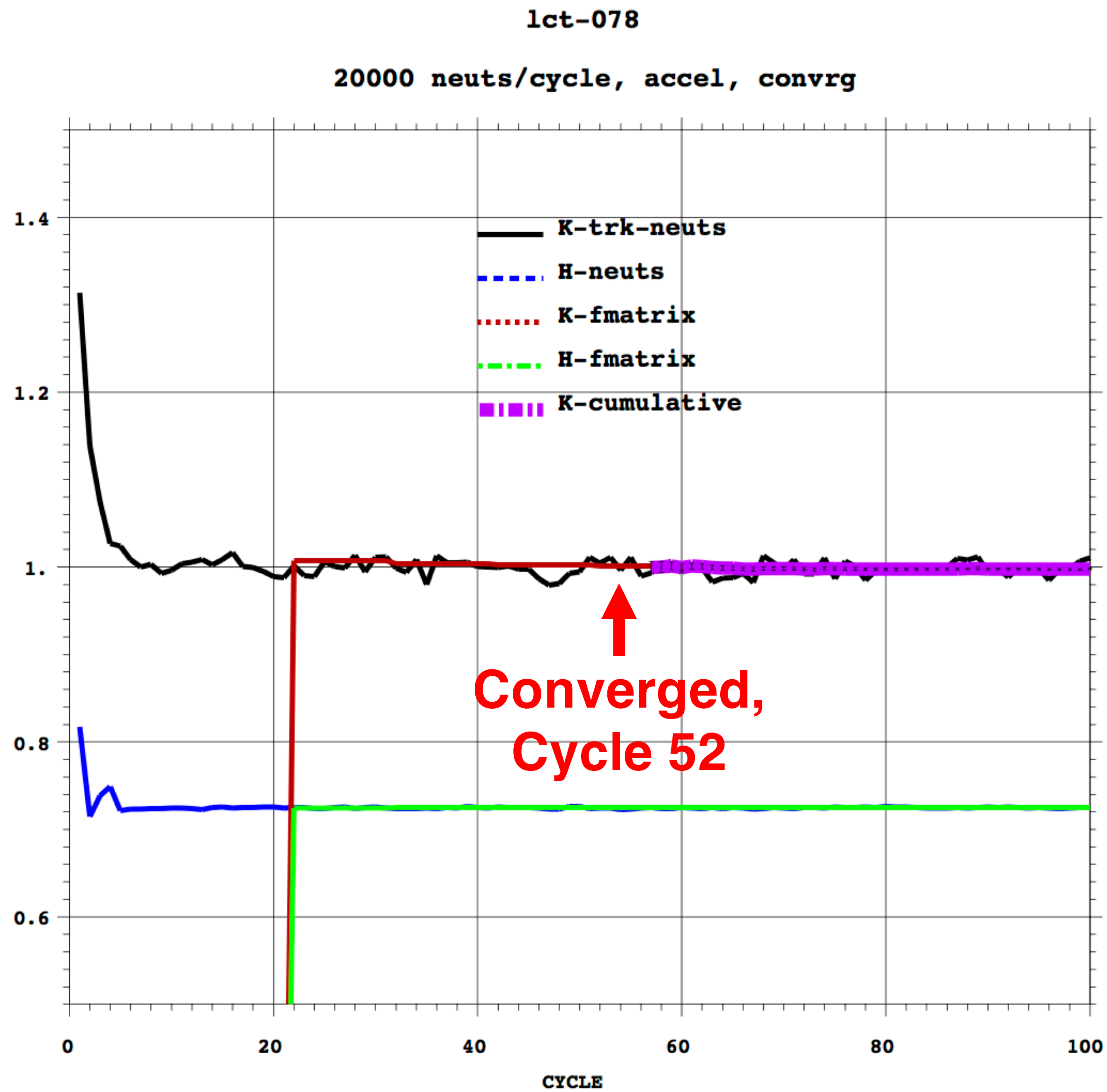
Sandia critical experiment – LCT-078-001, 1,057 rod assembly

Y-Z plot



X-Y plot





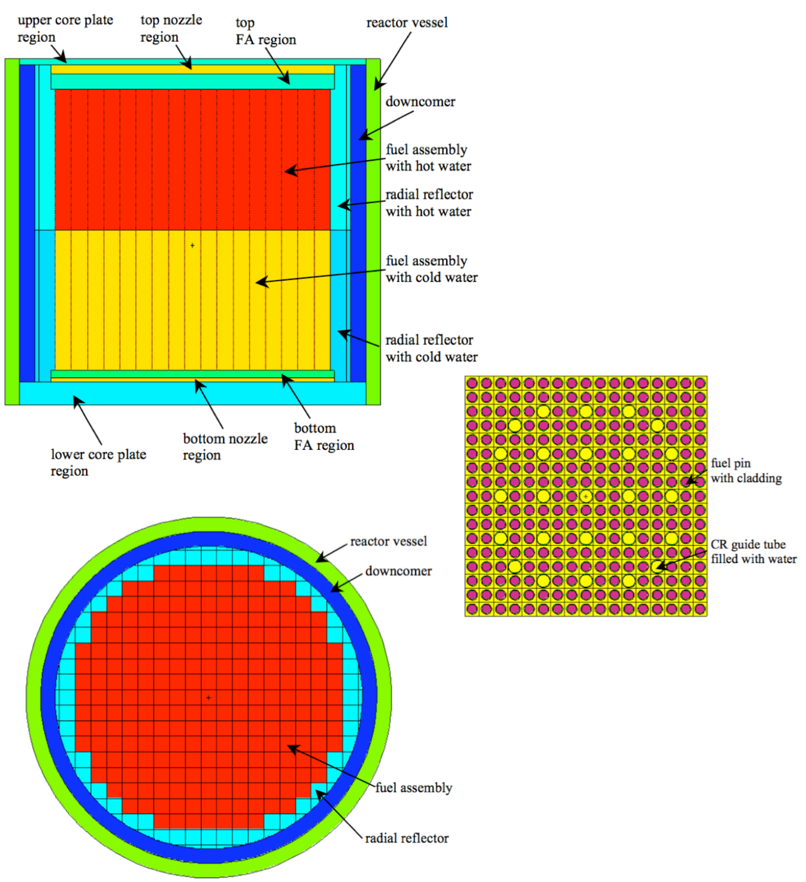
OECD-NEA "Hoogenboom-Martin Performance Benchmark"

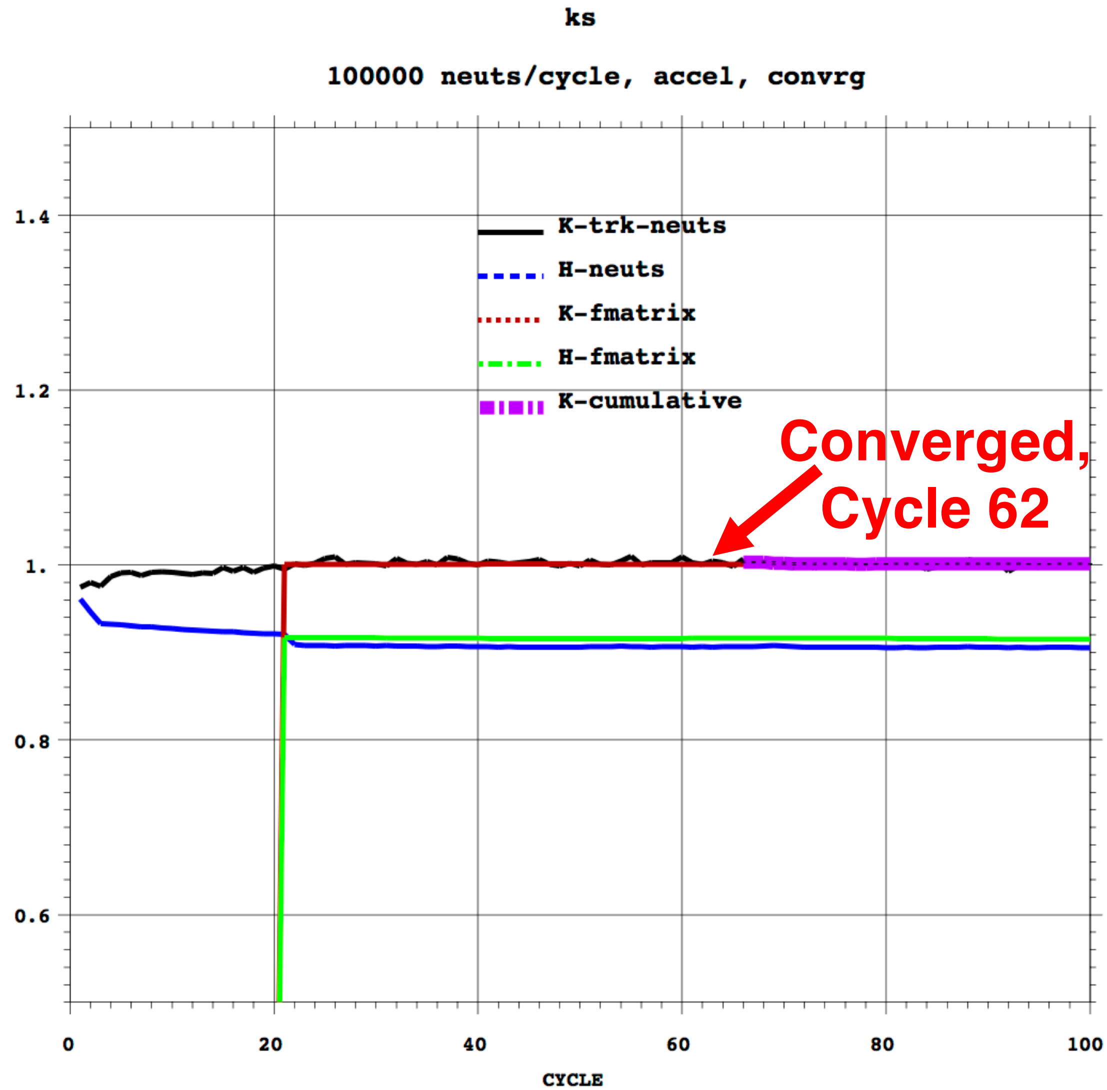
Reactor – full core, 3D

- **LWR model: 241 assemblies, 264 pins/assy**
- **Fuel: 17 actinides + 16 FPs; borated water**
- **Detailed 3D MCNP model**

  (63,624 pins) x (100 axial) = 6.3M pin powers

  Runs easily on deskside computer





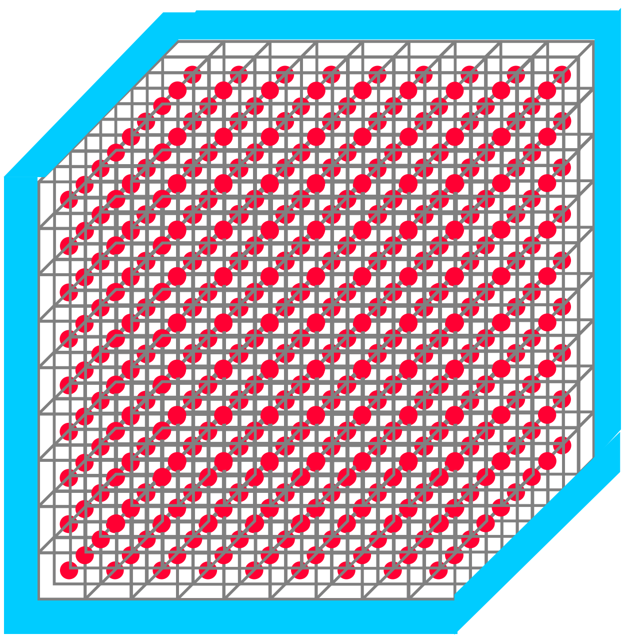
Whitesides' Model Problem – K-eff of the World

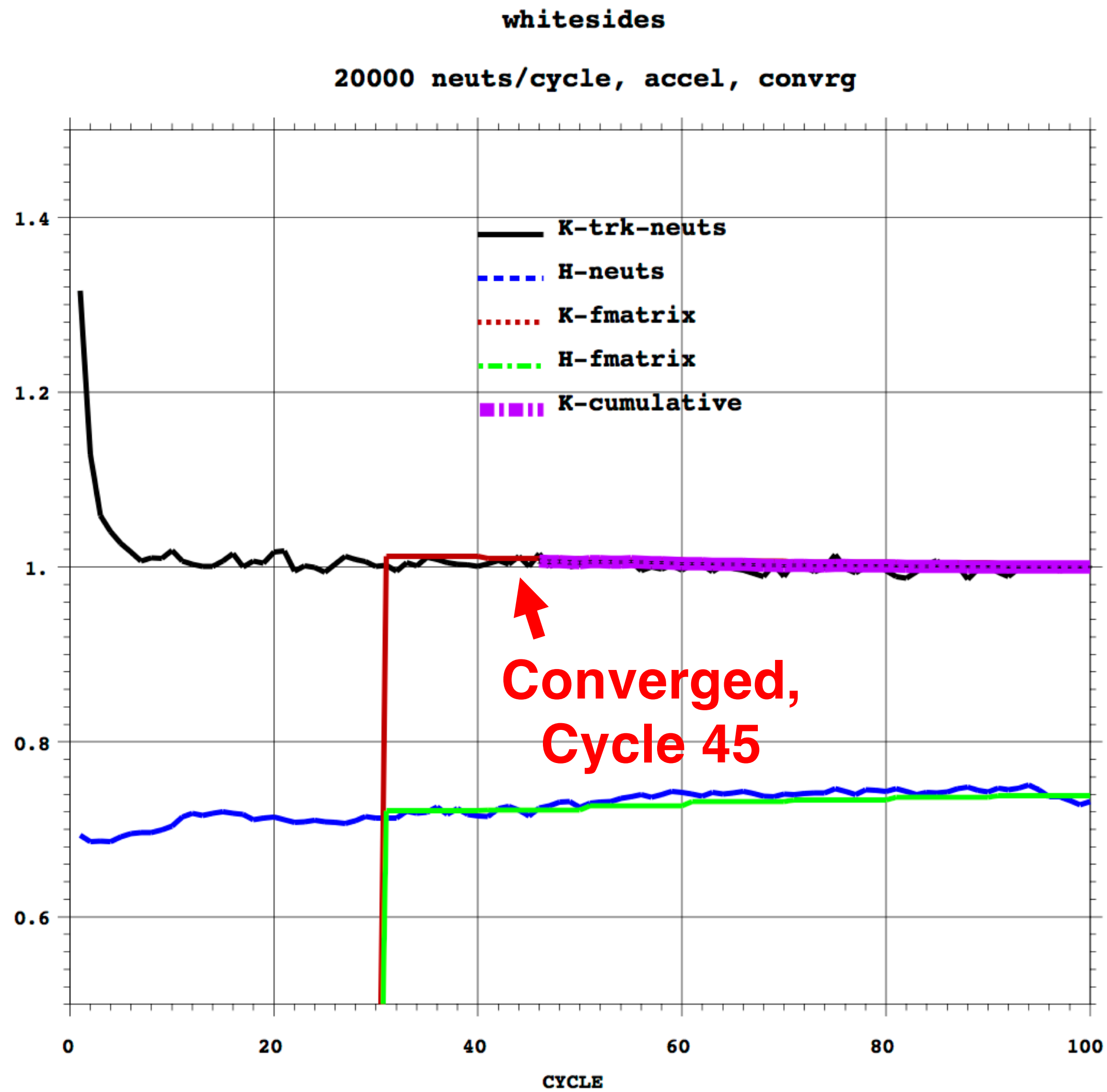
9 x 9 x 9 array of Pu-239 spheres

- 729 spheres
- Void between spheres
- Surrounded by 30 cm water
- Sphere radii ~ 4 cm
- Pitch = 60 cm
- Keff ~ 0.93

Replace center sphere of array by larger (critical) sphere

Should be supercritical - is it ?

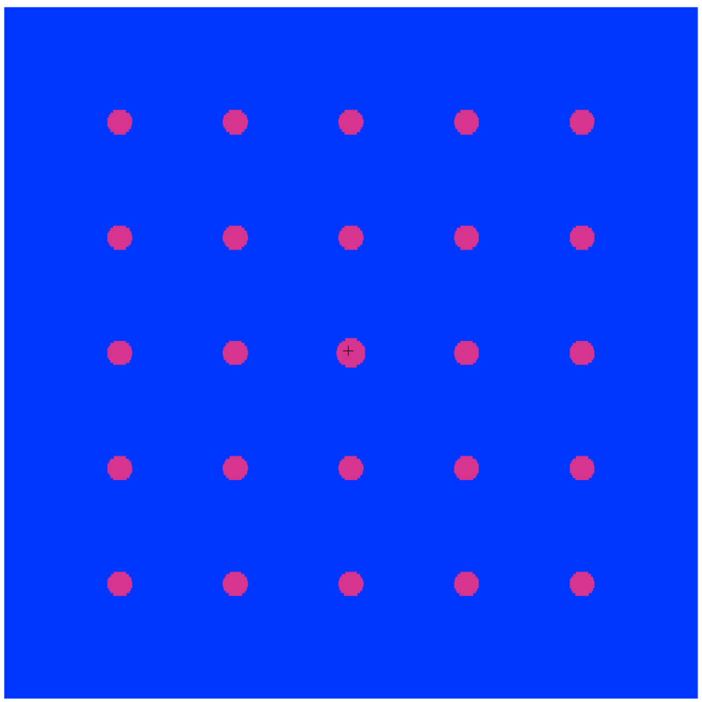


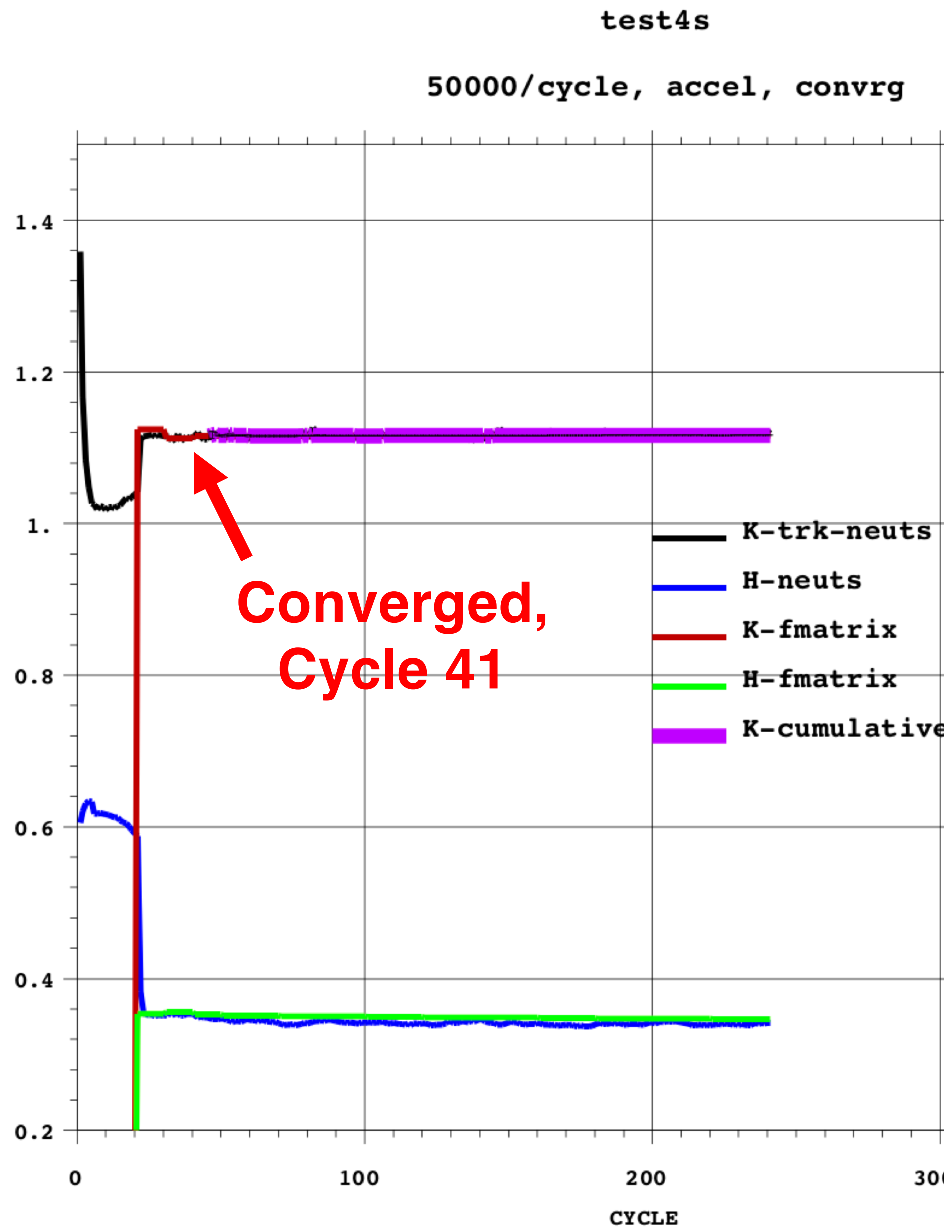


OECD-NEA Source Convergence Problem TEST4S

OECD-NEA source convergence benchmark

- Simplified version of Whitesides problem
- 5 x 5 array of HEU spheres
  - center sphere, R = 10 cm
  - others, R = 8.71 cm
  - pitch = 80 cm
  - air in between spheres
  - vacuum boundary conditions

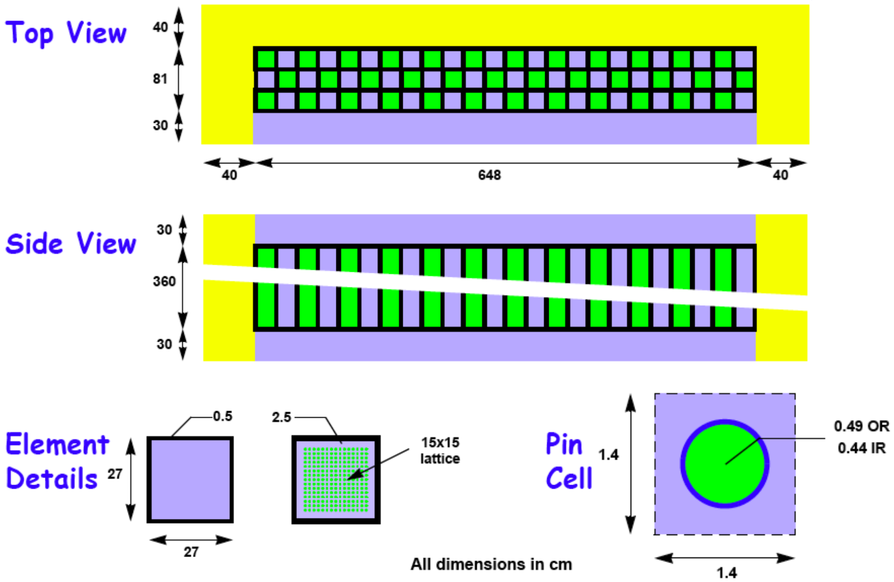




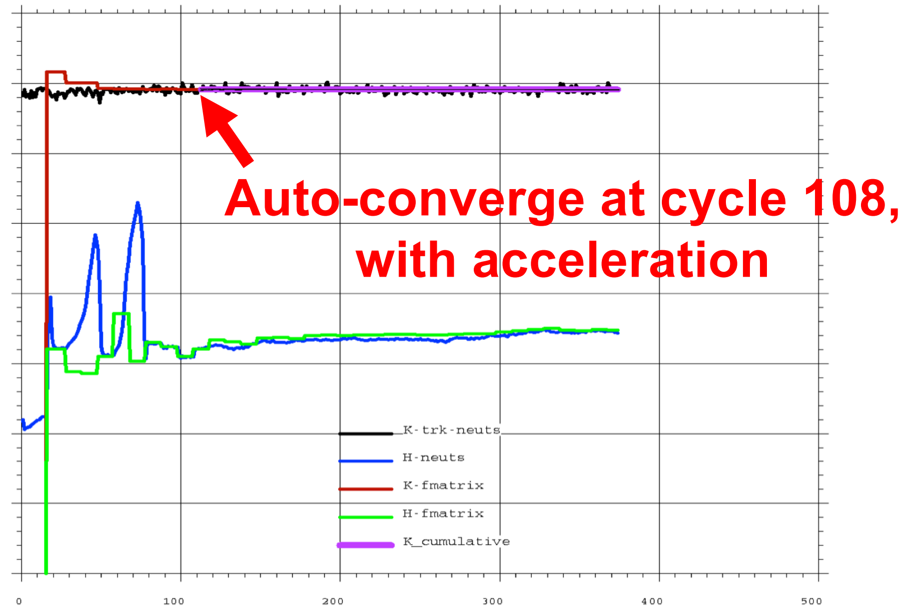
OECD-NEA Fuel Storage Pool

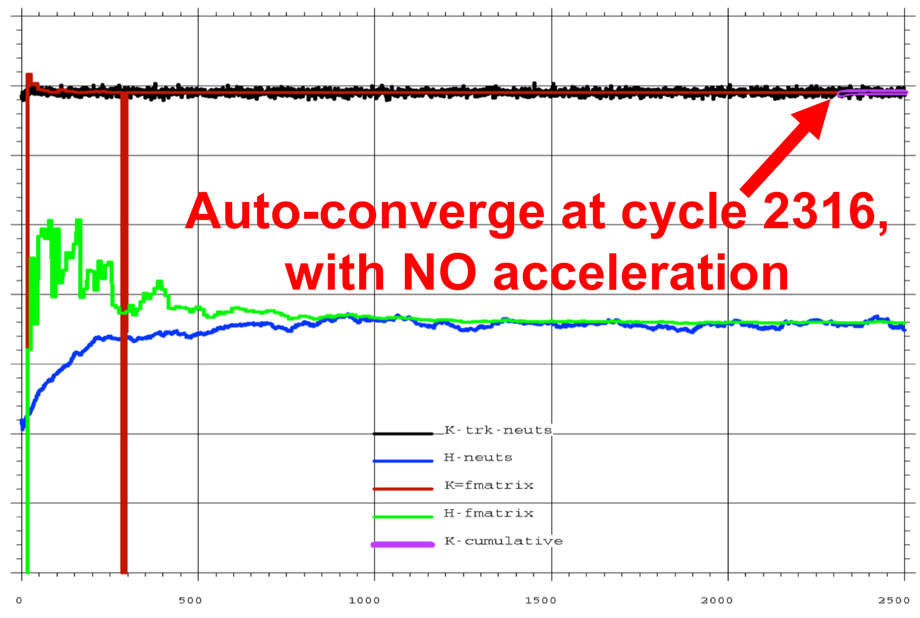
OECD-NEA-WPNCS Expert Group on Source Convergence

Benchmark 1



100k neuts/cycle





Current Work

- **Summer 2019**
  - **Limited release to NCS early adopters, more testing & feedback**

- **Near-term R&D Work**
  - **Source guess**
    - Handle a list of axis-oriented bounding boxes (AABB)
    - For 1 large bounding box, handle source overruns
    - Should be possible to completely automate
  - **Fission matrix**
    - Better eigensolver ?
    - Investigate matrix size vs neutrons/cycle
      - Statistical noise on matrix elements – effect on solution & stability
      - Kord-Smith problem, fuel storage pool problem
  - **Convergence tests**
    - Add more ?
    - Determine precise confidence level for passing all tests
  - **Acceleration**
    - Possibly find more robust, stable method
  - **Population size tests**
    - Scheme for predicting adequate size
  - **More examples & tests**

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