US DOE
Nuclear Criticality
Safety Program

Technical Program
Review

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Automated Acceleration & Convergence Testing for Monte Carlo NCS Calculations

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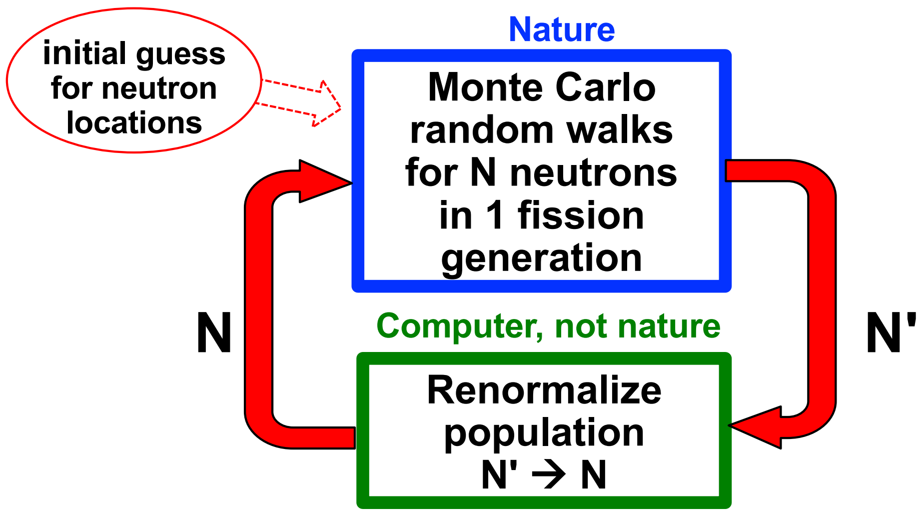
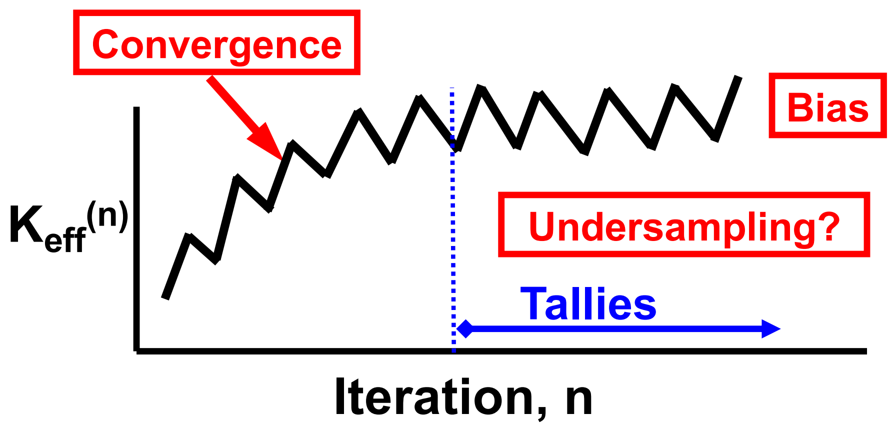
MC Criticality Calculations - Concerns





- **Bias in Keff**
  ~ -1 / (neutrons/cycle)

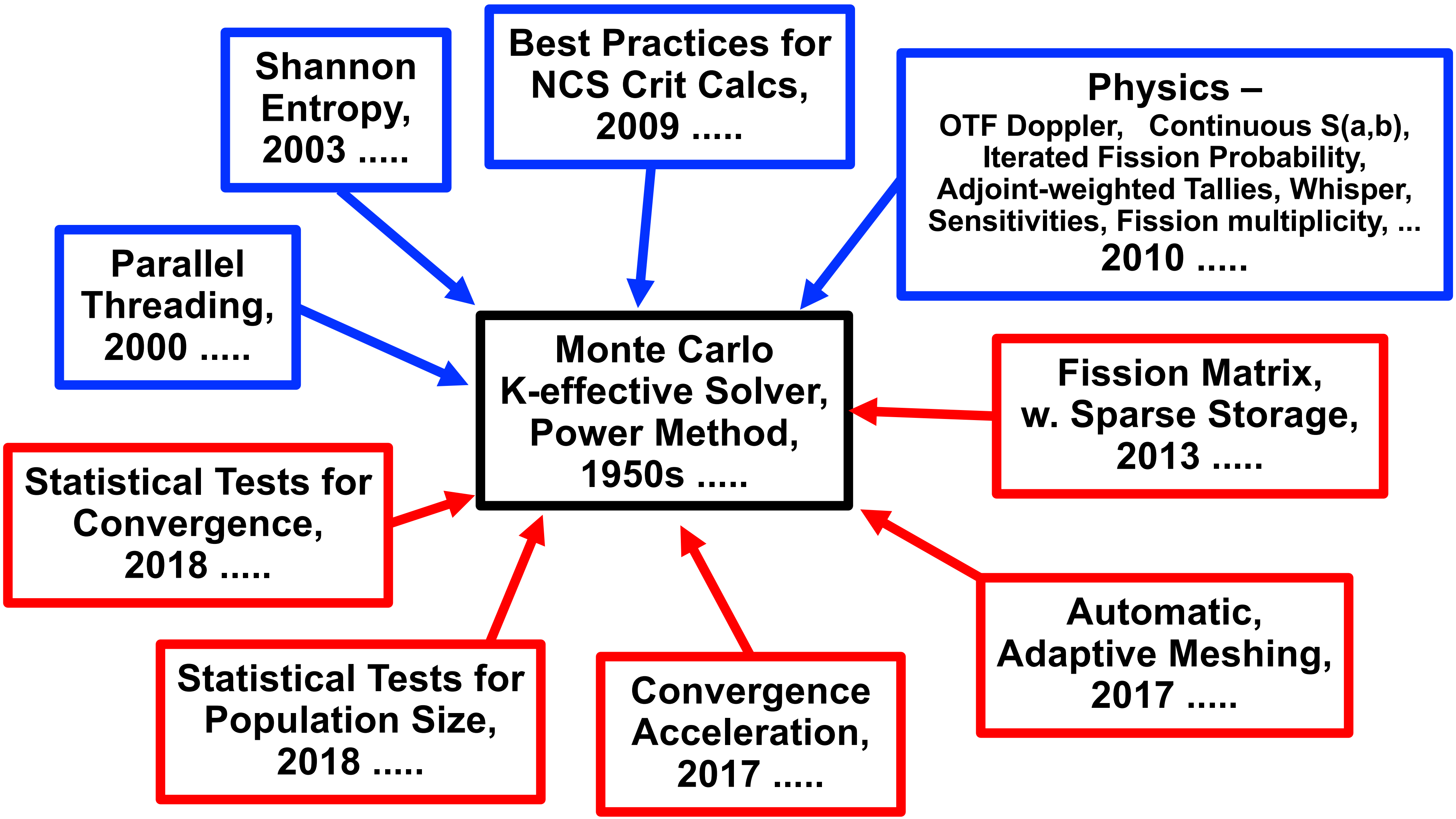
- **Bias in source shape**
  Too low in high-importance regions,
  Too high in low-importance regions

- **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, automate & combine new methods**
  - **Automated, adaptive meshing**
    - Basis for Shannon entropy & fission matrix
  - **Fission-matrix with adaptive sparse storage**
    - Reference solution for fission neutron distribution
  - **Accelerate convergence of neutron distribution**
  - **Statistical tests for convergence**
    - 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 & people time**

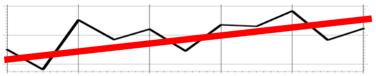
Automated Methods

- **Meshing for convergence tests**
  - **Automatically created & extended if needed, no user input required**
  - **Physics basis = 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)**
  - **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, population size tests**

Statistical tests for convergence

- **Slope test**



  - For a block of cycles (default = 10)
  - For result x from each cycle in block, compute least-squares slope & σ_{slope}

    | slope(x) | < 0.0001 → pass, slope ~ 0

    | slope(x) | < $t_{0.05}\,\sigma_{slope}$ → pass, slope ~ 0 within statistics

- **Metric tests, at end of block for convergence testing**

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

If Test 8 passes, strong evidence of convergence
If Test 8 fails, ignore it – might be low popsize

- **Distribution tests, at end of block for convergence testing**

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

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

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

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

   If Test 11 passes, strong evidence of convergence
   If Test 11 fails, ignore it – might be low popsize

- **If convergence tests all pass, convergence is locked-in**
  - Tests continue for each block
  - Some tests may fail (due to statistics), but convergence not rescinded

Accelerating Source Convergence

- **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**
  - **Pushes neutron distribution toward F-matrix reference**
  - **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 2-20 X**
  - **Further development under consideration:**
    - Investigate using $S_{FM}^{adjoint}$ for source importance sampling
    - Maybe coarsen the fission matrix, to reduce 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. The MESH (adaptive, axis-aligned, cartesian) to be used for computing
comment. Shannon entropy, fission-matrix tallies (if used), and source
comment. convergence checking is initially defined by:
comment.     max mesh spacing for automesh =  1.0052E+01
comment.
comment.     total mesh cells = 3675
comment.
comment.     Xbins=   35   Xmin=-1.6861E+02   Xmax= 1.6856E+02   dx= 9.6334E+00
comment.     Ybins=   35   Ymin=-1.6856E+02   Ymax= 1.6857E+02   dy= 9.6323E+00
comment.     Zbins=    3   Zmin=-9.6460E+00   Zmax= 9.9571E+00   dz= 6.5344E+00
comment.
comment. the mesh will be automatically extended if necessary,
comment. preserving the original mesh cells and 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 & fiss-matrix distributions
comment.     will be used to determine convergence & begin active cycles.
comment.     The 3rd entry on the KCODE card may be ignored.
comment.
comment.     Targets for statistical tests:
comment.       h_slope:   < 0.95 conf level,  or  < 0.0001
comment.       k_slope:   < 0.95 conf level,  or  < 0.0001
comment.       distribs:  < 0.95 conf level,  h_diff:  < 0.01
comment.
comment.
comment.  FMATACCEL option is being used.
comment.    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. -----------------------------------------------------------------------
```

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 (cycles 1–11)

Block of cycles (cycles 12–21)

MCNP6 example

```
fmatrix keff= 1.12400,  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    =  2.06900

  slope of keff (tracklen)       =  2.0E-03,  target:  < 5.3E-04   FAIL
  slope of keff (collide)        =  2.1E-03,  target:  < 5.3E-04   FAIL
  slope of keff (absorb)         =  2.0E-03,  target:  < 5.8E-04   FAIL
  slope of entropy               = -2.6E-03,  target:  < 4.3E-04   FAIL
  slope of entropy X marginal    = -2.1E-03,  target:  < 5.1E-04   FAIL
  slope of entropy Y marginal    = -2.1E-03,  target:  < 4.2E-04   FAIL
  slope of entropy Z marginal    =  8.7E-04,  target:  < 3.3E-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:  < 5.1E+02   FAIL
  rel-h-block,   distrib, stat =  2.5E+00,  target:  < 5.1E-03   n/a

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

MISCELLANEOUS INFO & CHECKS:

  rmse          =     1.16     %
  fmat nnz=          11884,   0.09 %

                                         accelerate: Imin= 0.2, Imax= 4.7
22    1.10782      0.81    0.38309                                          2134
                                         accelerate: Imin= 0.2, Imax= 3.8
23    1.11376      0.85    0.35605                                          1499
                                         accelerate: Imin= 0.2, Imax= 3.2
24    1.11583      0.88    0.35129                                          1233
                                         accelerate: Imin= 0.2, Imax= 5.0
25    1.11726      0.92    0.35104                                          1077
                                         accelerate: Imin= 0.2, Imax= 3.4
```

MCNP6 example

```
 31    1.11257       1.12    0.35069                                      680

      fmatrix keff= 1.11187,  DR= 0.91653,  iters=   138

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

        entropy for fmatrix eigenvector    =  0.35656
        entropy for neutron  last cycle    =  0.35069   dif=   -1.65%
        relative entropy for last cycle    =  0.00972

        slope of keff (tracklen)      =  4.2E-03,  target:  < 5.1E-03   PASS
        slope of keff (collide)       =  4.6E-03,  target:  < 4.9E-03   PASS
        slope of keff (absorb)        =  4.6E-03,  target:  < 4.9E-03   PASS
        slope of entropy              = -1.4E-02,  target:  < 1.6E-02   PASS
        slope of entropy X marginal   = -1.8E-02,  target:  < 1.9E-02   PASS
        slope of entropy Y marginal   = -1.8E-02,  target:  < 1.9E-02   PASS
        slope of entropy Z marginal   =  1.3E-03,  target:  < 1.6E-03   PASS
        entropy dif, neuts vs fmat    = -9.1E-04,  target:  < 1.0E-02   PASS
        Kolmo-Smirnov, distrib, stat =  2.5E-03,  target:  < 9.1E-02   PASS
        Chi-square,    distrib, stat =  9.0E+01,  target:  < 5.1E+02   PASS
        rel-h-block,   distrib, stat =  2.8E-03,  target:  < 5.1E-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 =       32
        Active cycles will end   with cycle =      131
        Total active cycles to be run       =      100
```

Quantitative Evidence For Convergence

Quantitative Evidence For Convergence

MCNP6 example

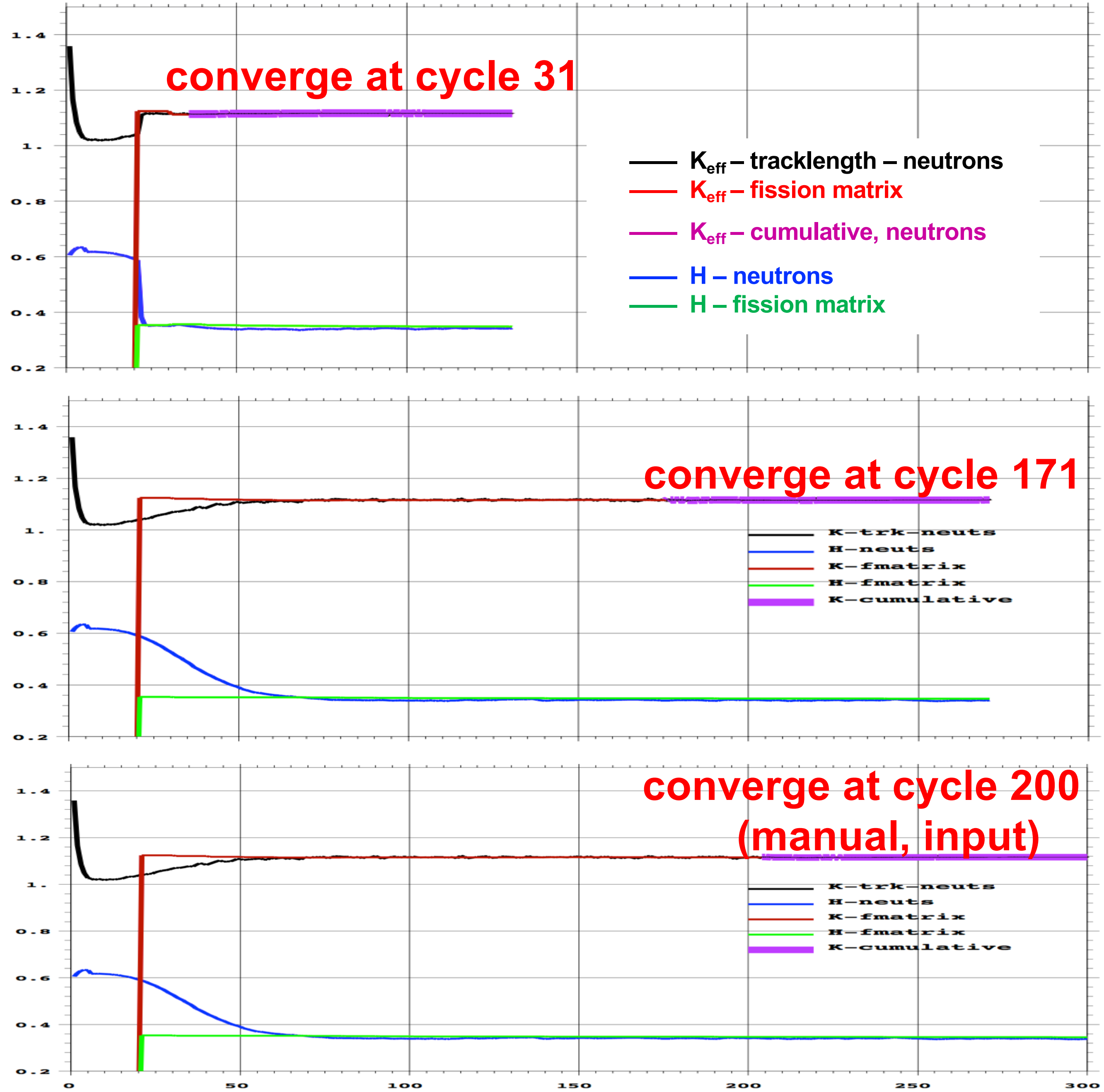
```
    40    1.11130      1.43   3.45E-01         9     1.11344     0.00061           499
    41    1.12440      1.47   3.44E-01        10     1.11454     0.00122           487

          fmatrix keff= 1.11470,  DR= 0.91540,  iters=   126

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

            entropy for fmatrix eigenvector    =  0.35367
            entropy for neutron  last cycle    =  0.34421   dif=   -2.67%
            relative entropy for last cycle    =  0.01140

            slope of keff (tracklen)      = -2.3E-04,  target:  < 3.8E-04   PASS
            slope of keff (collide)       =  9.9E-06,  target:  < 4.6E-04   PASS
            slope of keff (absorb)        = -3.7E-05,  target:  < 4.9E-04   PASS
            slope of entropy              = -9.2E-04,  target:  < 4.7E-04   FAIL
            slope of entropy X marginal   = -1.1E-03,  target:  < 8.0E-04   FAIL
            slope of entropy Y marginal   = -1.4E-03,  target:  < 6.8E-04   FAIL
            slope of entropy Z marginal   =  9.4E-05,  target:  < 3.9E-04   PASS
            entropy dif, neuts vs fmat    = -9.0E-03,  target:  < 1.0E-02   PASS
            Kolmo-Smirnov, distrib, stat =  5.3E-03,  target:  < 9.0E-02   PASS
            Chi-square,     distrib, stat =  8.8E+01,  target:  < 5.1E+02   PASS
            rel-h-block,    distrib, stat =  2.5E-03,  target:  < 5.1E-03   PASS

            convergence checks passed               at cycle =       31
            active cycles based on fmatconvrg begin at cycle =       32

            entropy for fmatrix eigenvector    =  0.35367
            entropy for neutron  active cycles =  0.35111   dif=   -0.72%
            relative entropy for active cycles =  0.00249

          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)

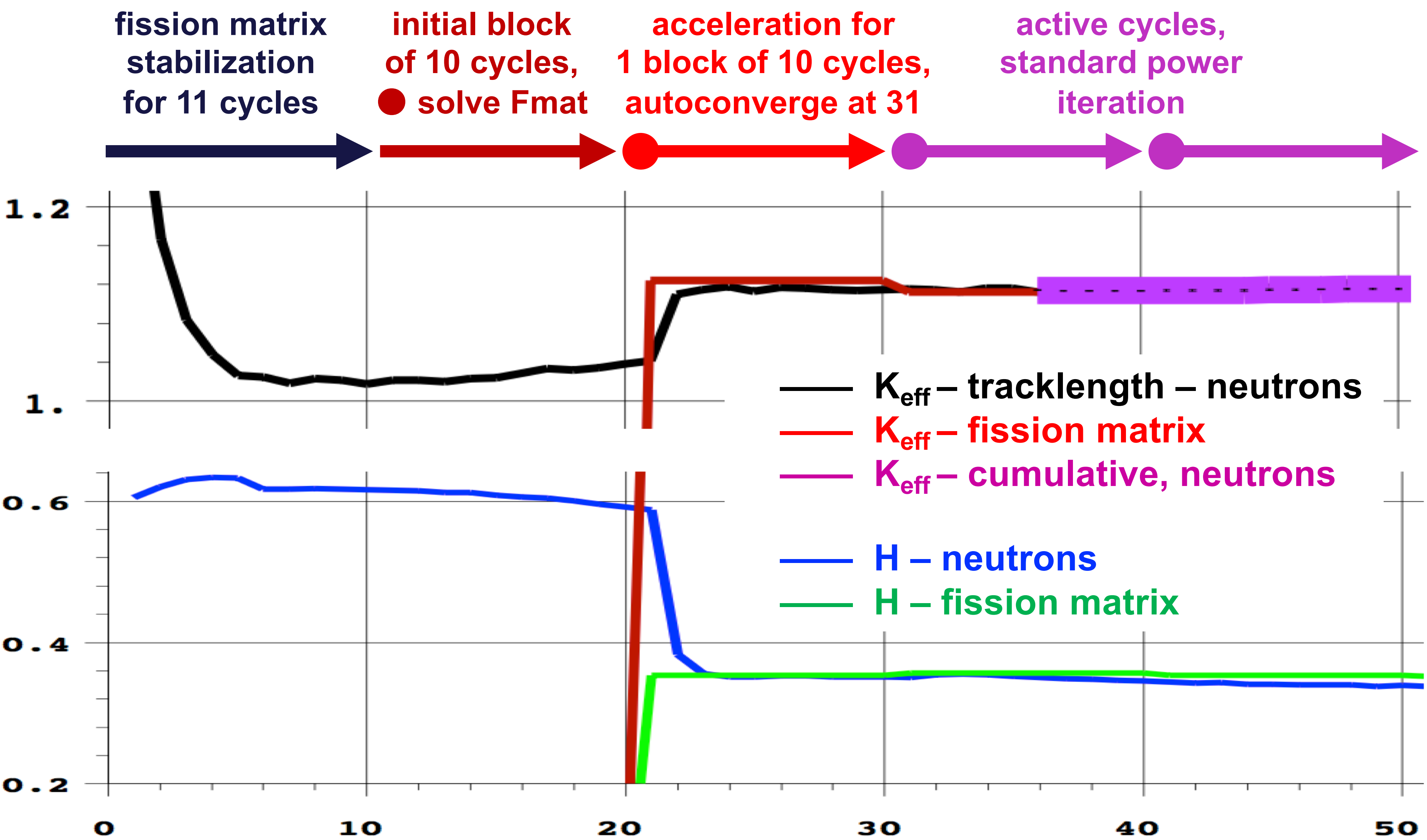
50,000 neuts/cycle
no acceleration
auto-converge
k=1.1161 (2)

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

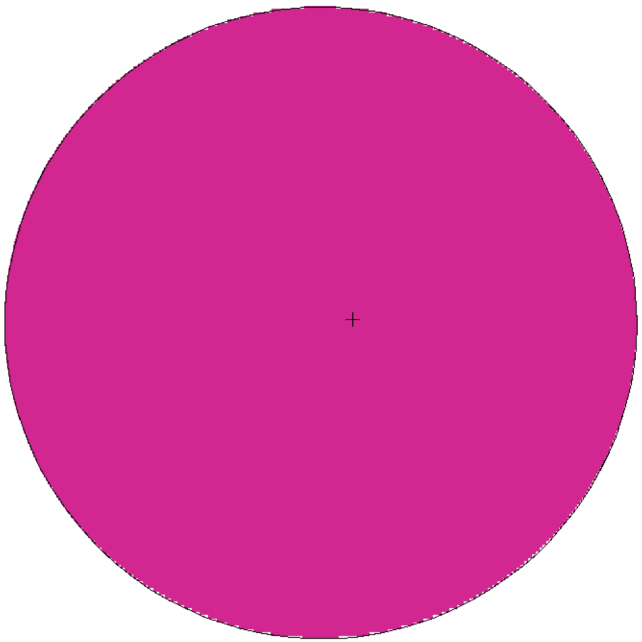
- **Standard MCNP validation suite since 2002 (Mosteller)**
  - 31 ICSBEP Handbook problems, critical experiments
  - Run using ENDF/B-VII.1 nuclear data
  - Timing results include all I/O, input & xsec file processing, Monte Carlo random walks, printing results, etc. for all 31 problems

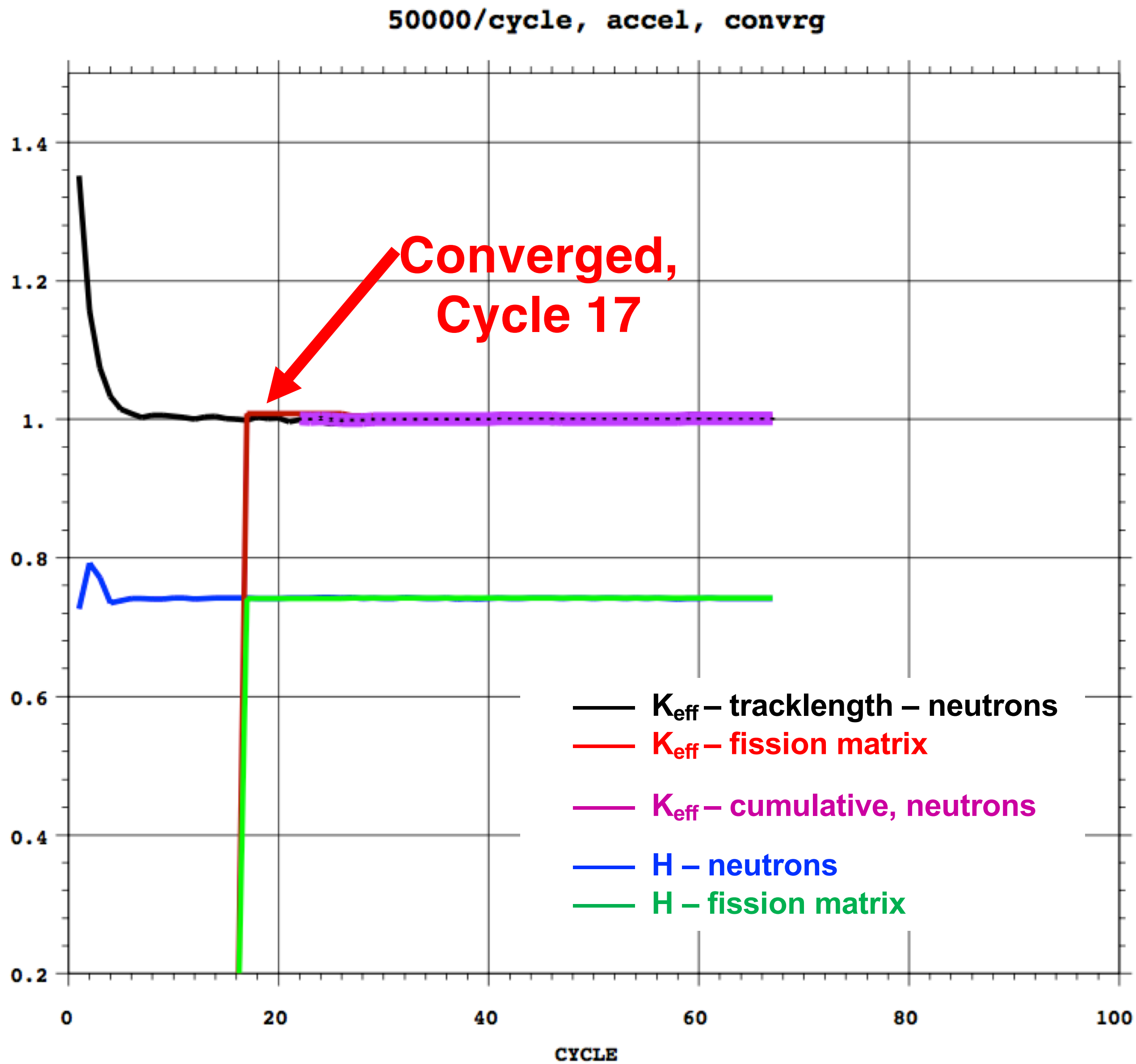
- **Timing tests**
  - 50,000 neutrons/cycle for all runs
  - For standard runs, 100 inactive cycles, 100 active cycles
  - For auto accelerate & converge, 100 active cycles

Standard run:	**106 minutes**
Auto accel & converge:	**70 minutes**

Godiva Problem

Bare HEU sphere

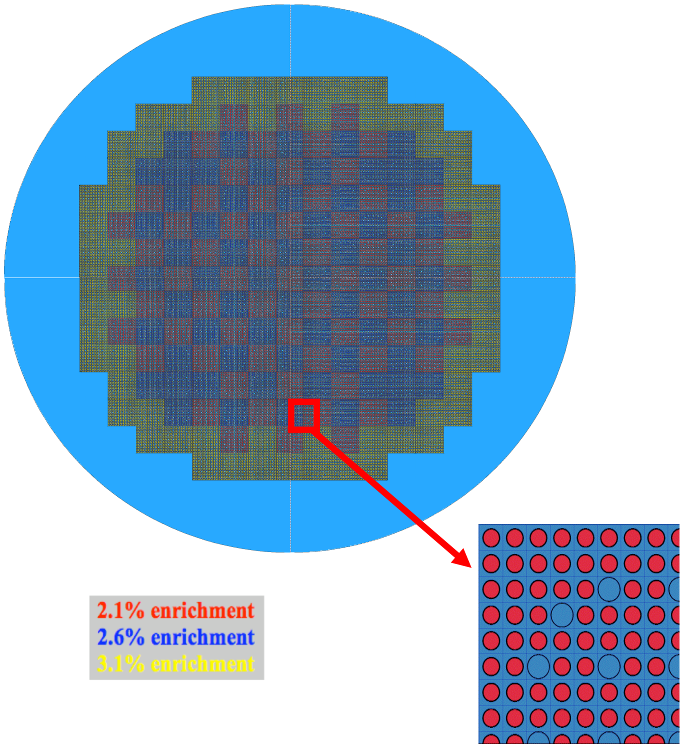


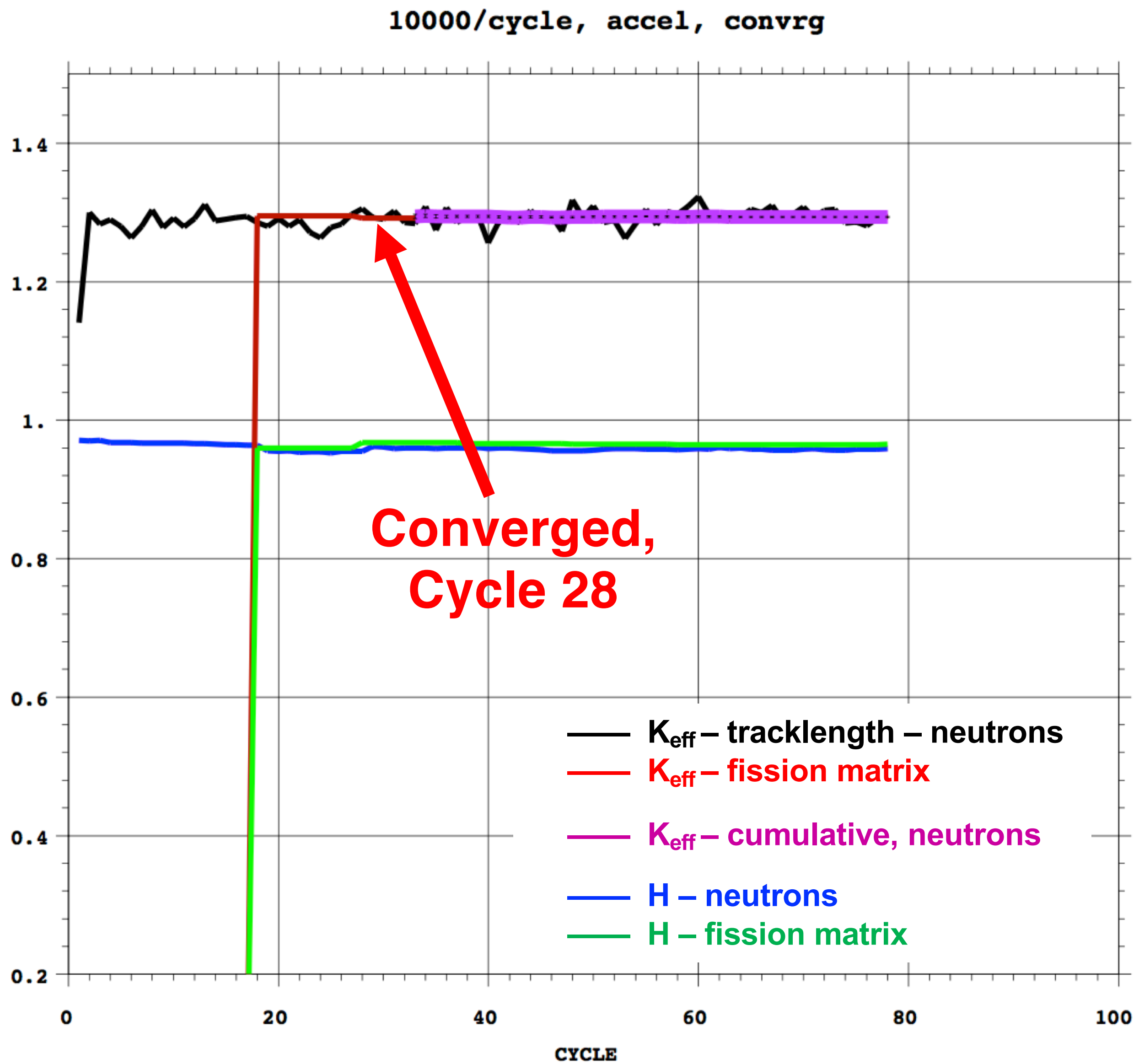


Whole-core 2D PWR Model

2D PWR (Nakagawa & Mori model)

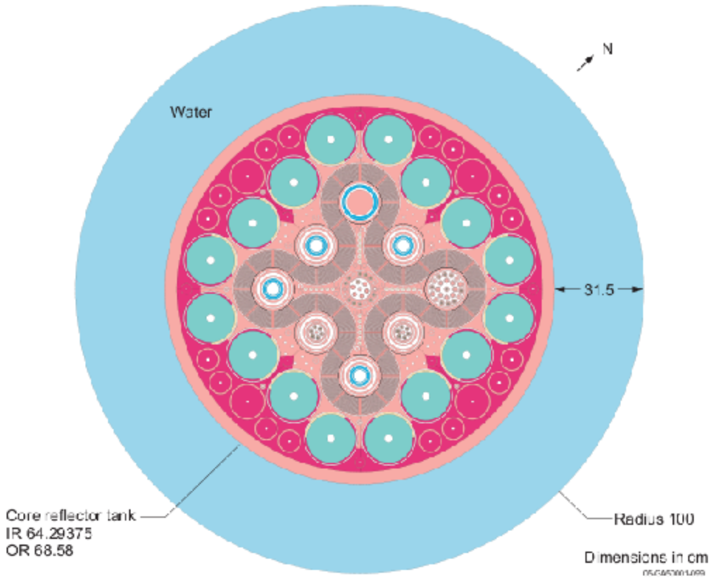
- 193 fuel assemblies:
  - 50,952 fuel pins with cladding
  - 4825 water tubes
- Each assembly:
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- Calculations used whole-core model

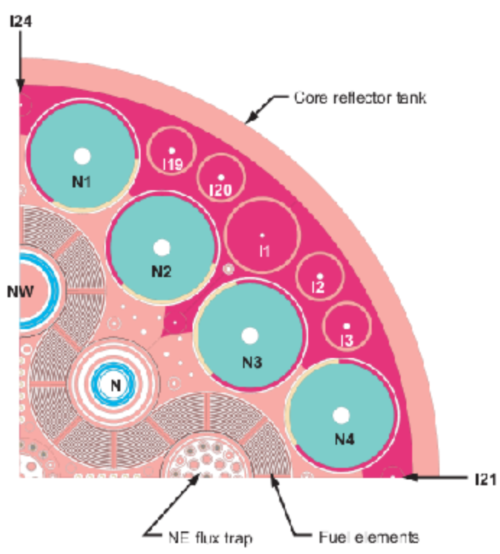


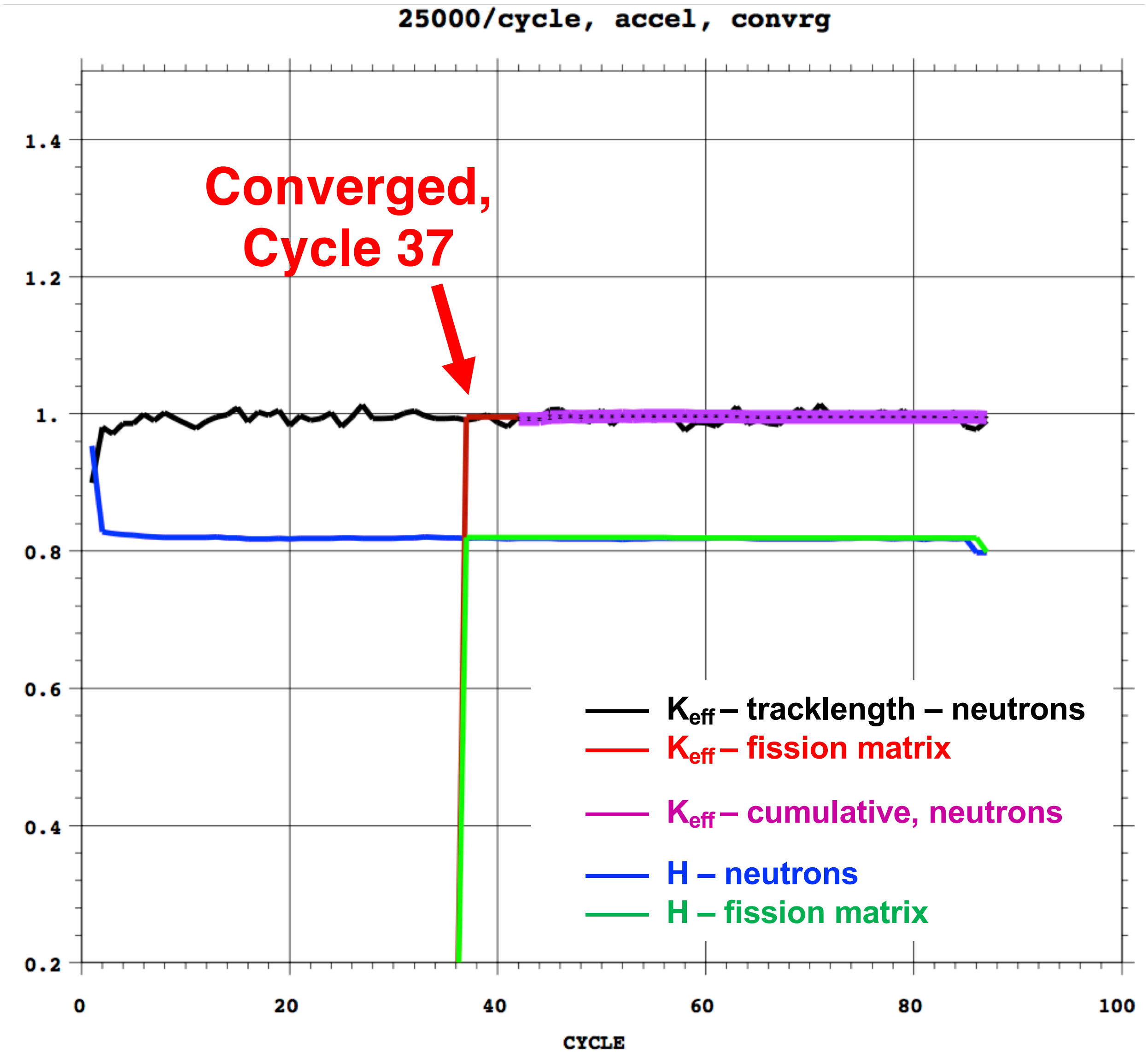


Advanced Test Reactor

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

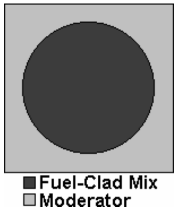






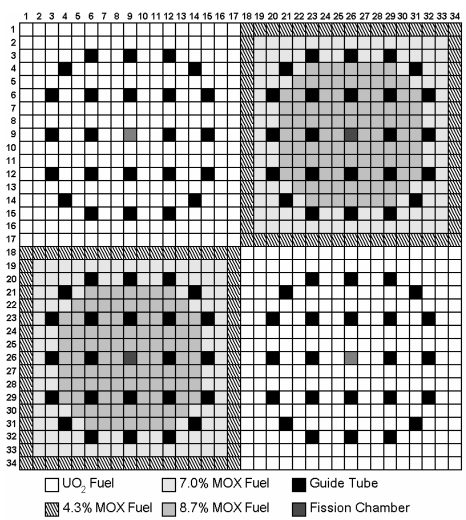
OECD-NEA Benchmark - C5G7

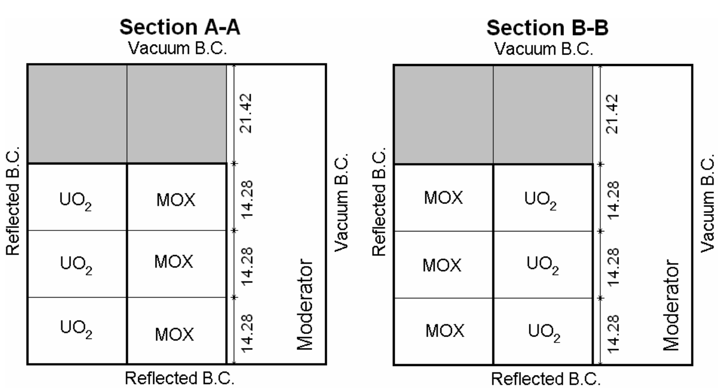
Figure 2. Fuel pin layout

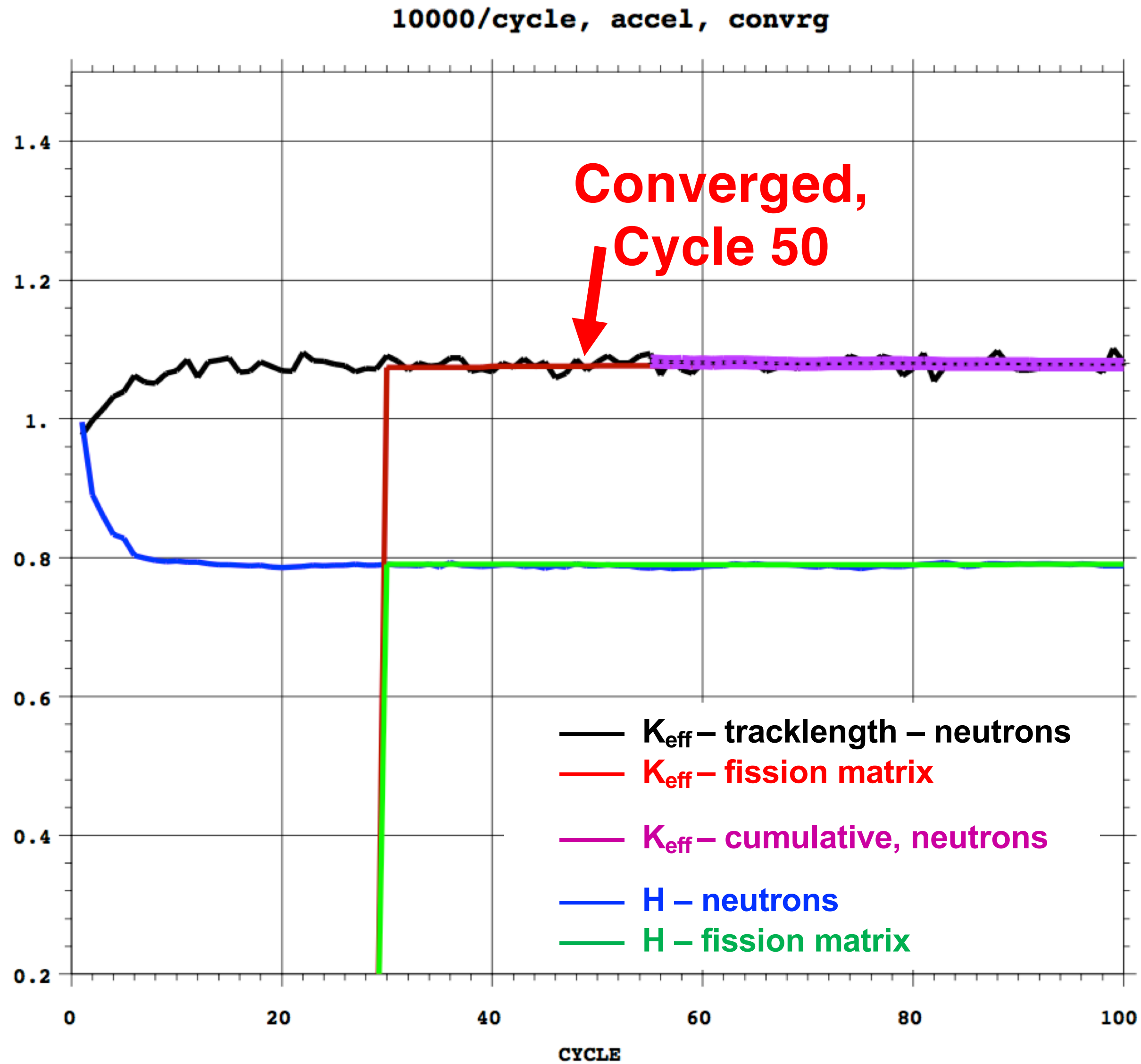


3D model

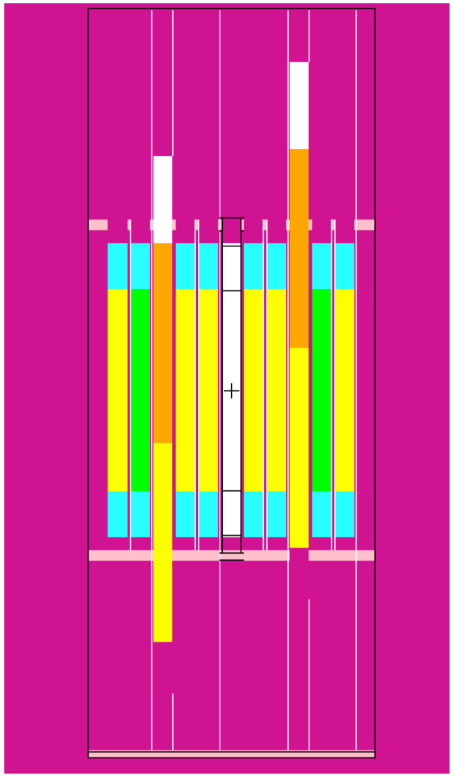
Figure 3. Benchmark fuel pin compositions and numbering scheme

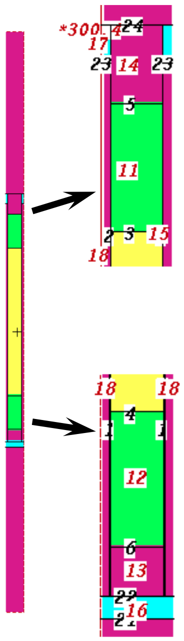


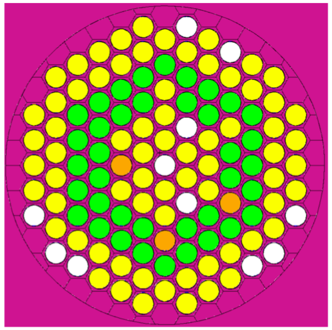


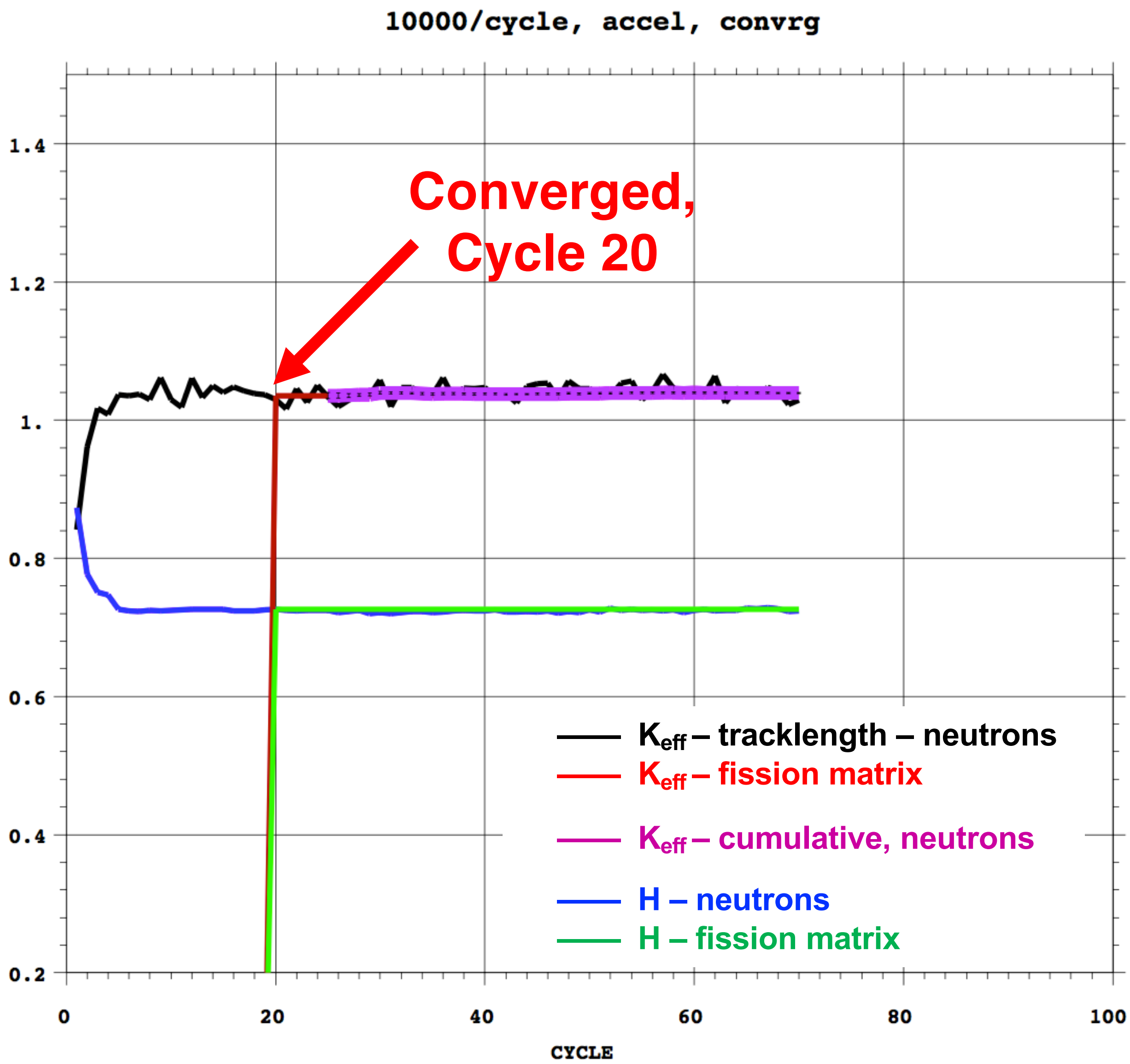


TRIGA Reactor



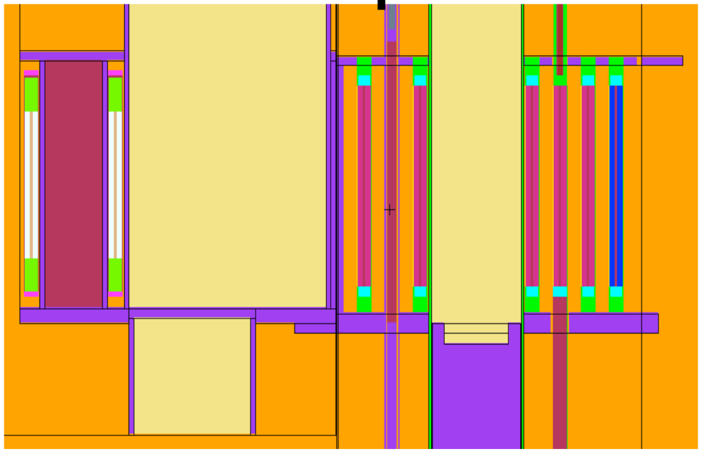




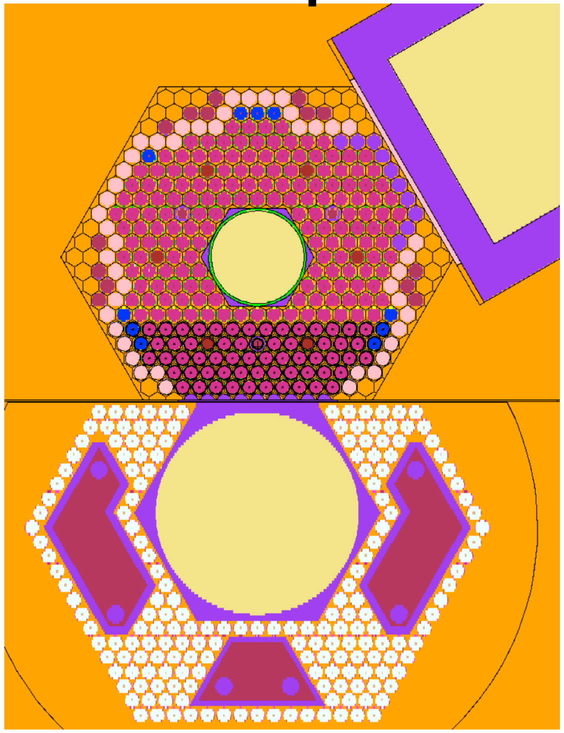


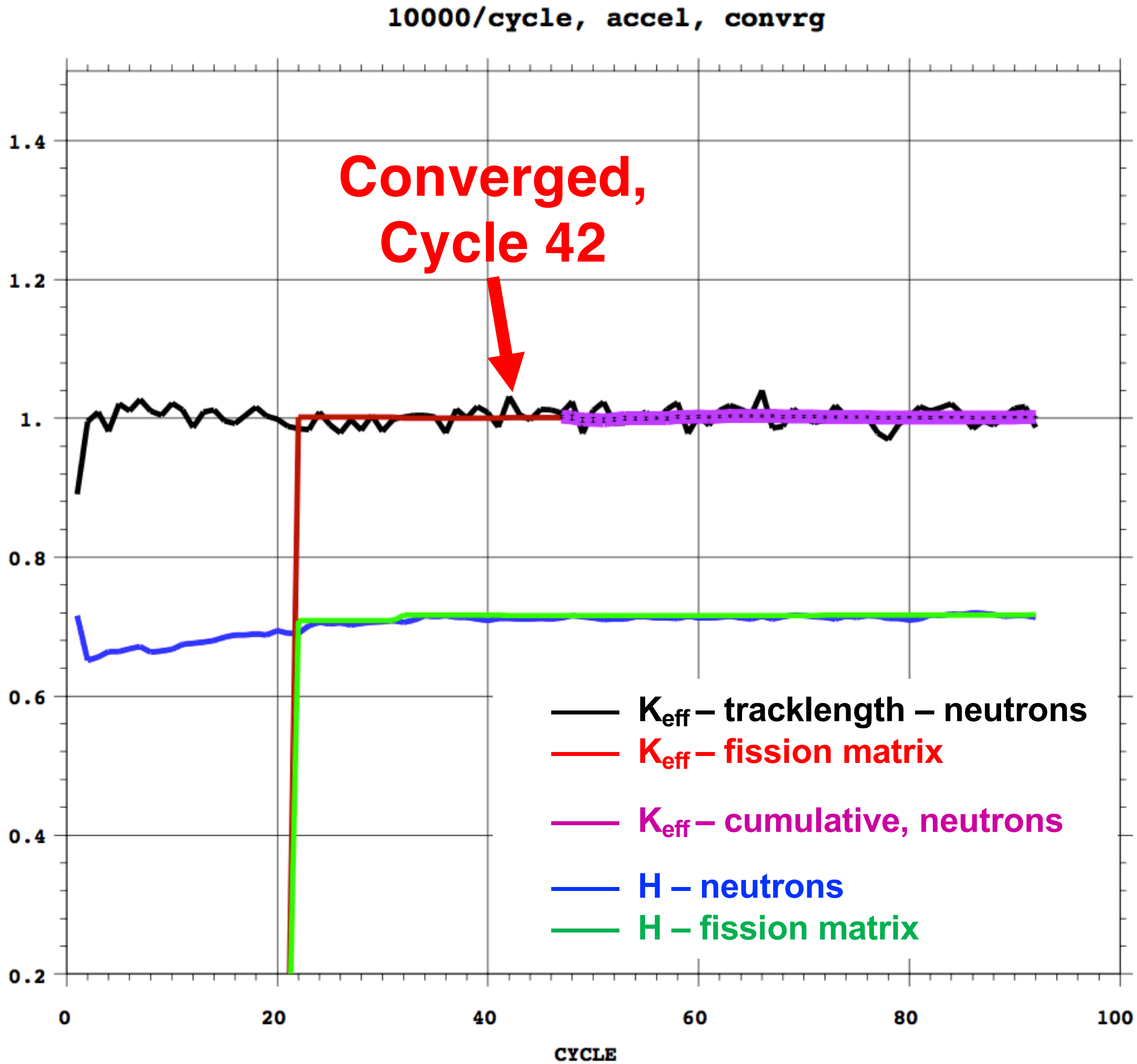
Sandia burst reactor - ACRR, with FREC

Y-Z plot



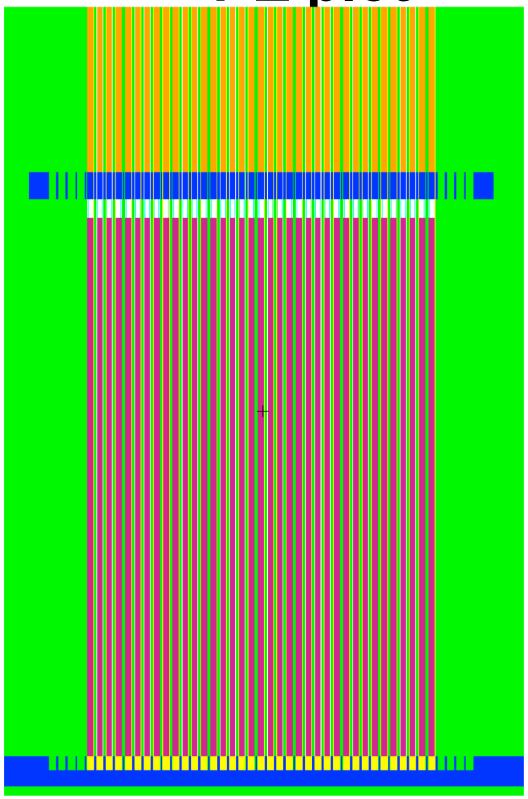
X-Y plot



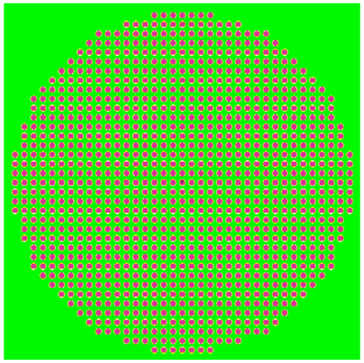


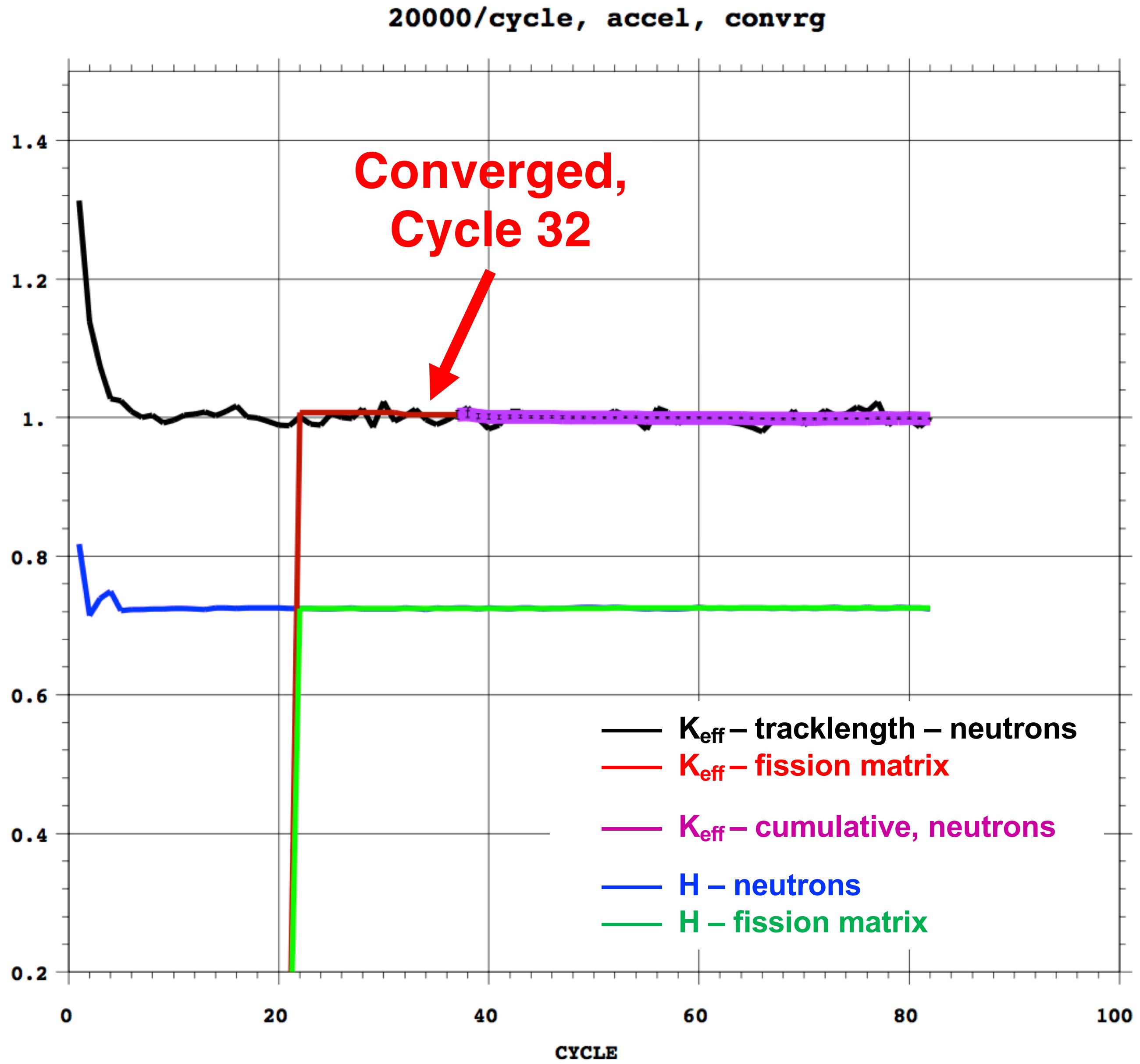
Sandia critical experiment – LCT-078-001, 1,057 rod assembly

Y-Z plot



X-Y plot





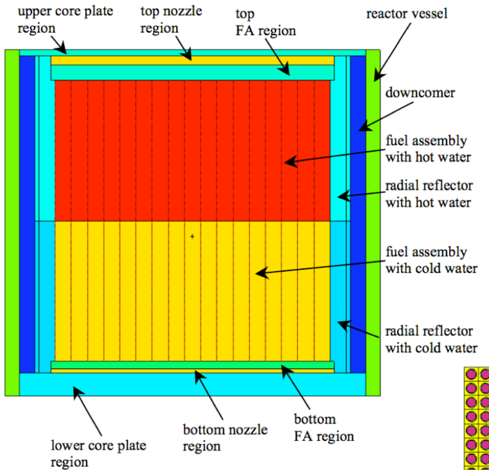
OECD-NEA "Hoogenboom-Martin Performance Benchmark"

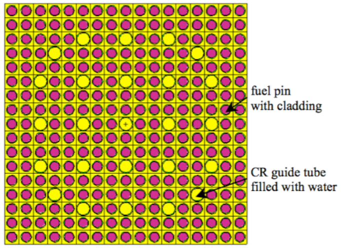
Reactor – full core, 3D

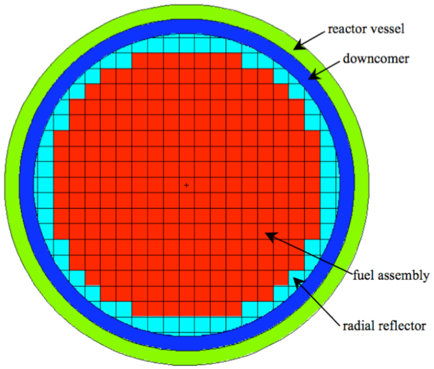
- LWR model: 241 assemblies, 63,624 pins
- Fuel: 17 actinides + 16 FPs; borated water
- Detailed 3D MCNP model

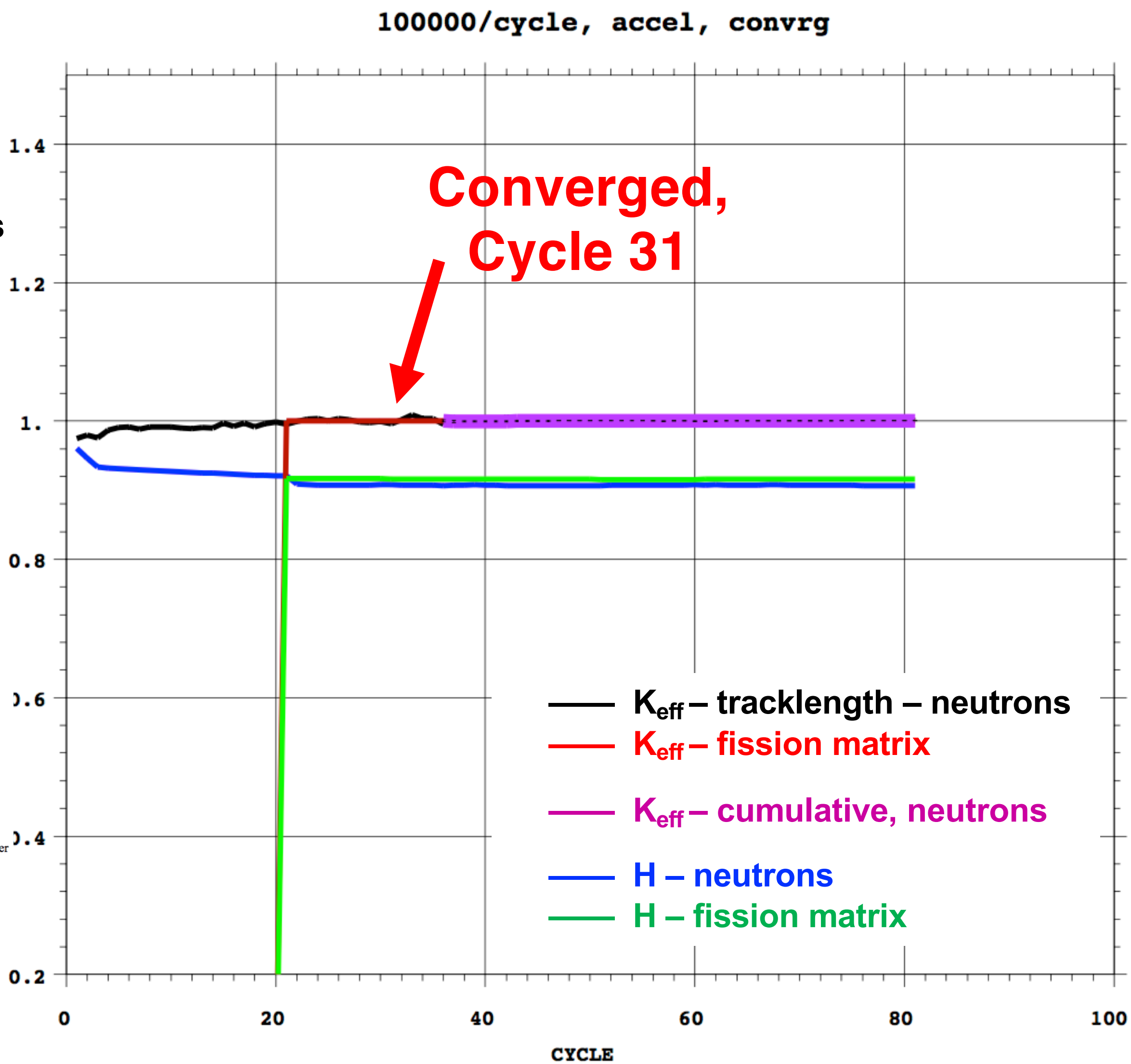
(63,624 pins) x (100 axial) = 6.3M pin powers

Runs easily on deskside computer







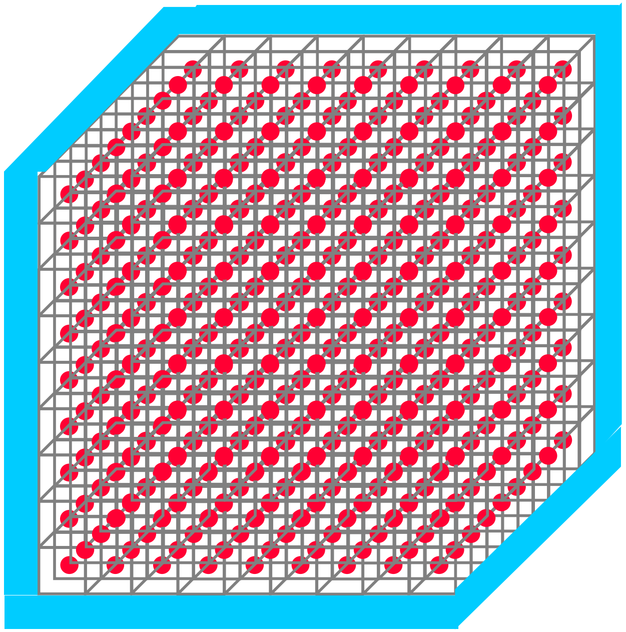


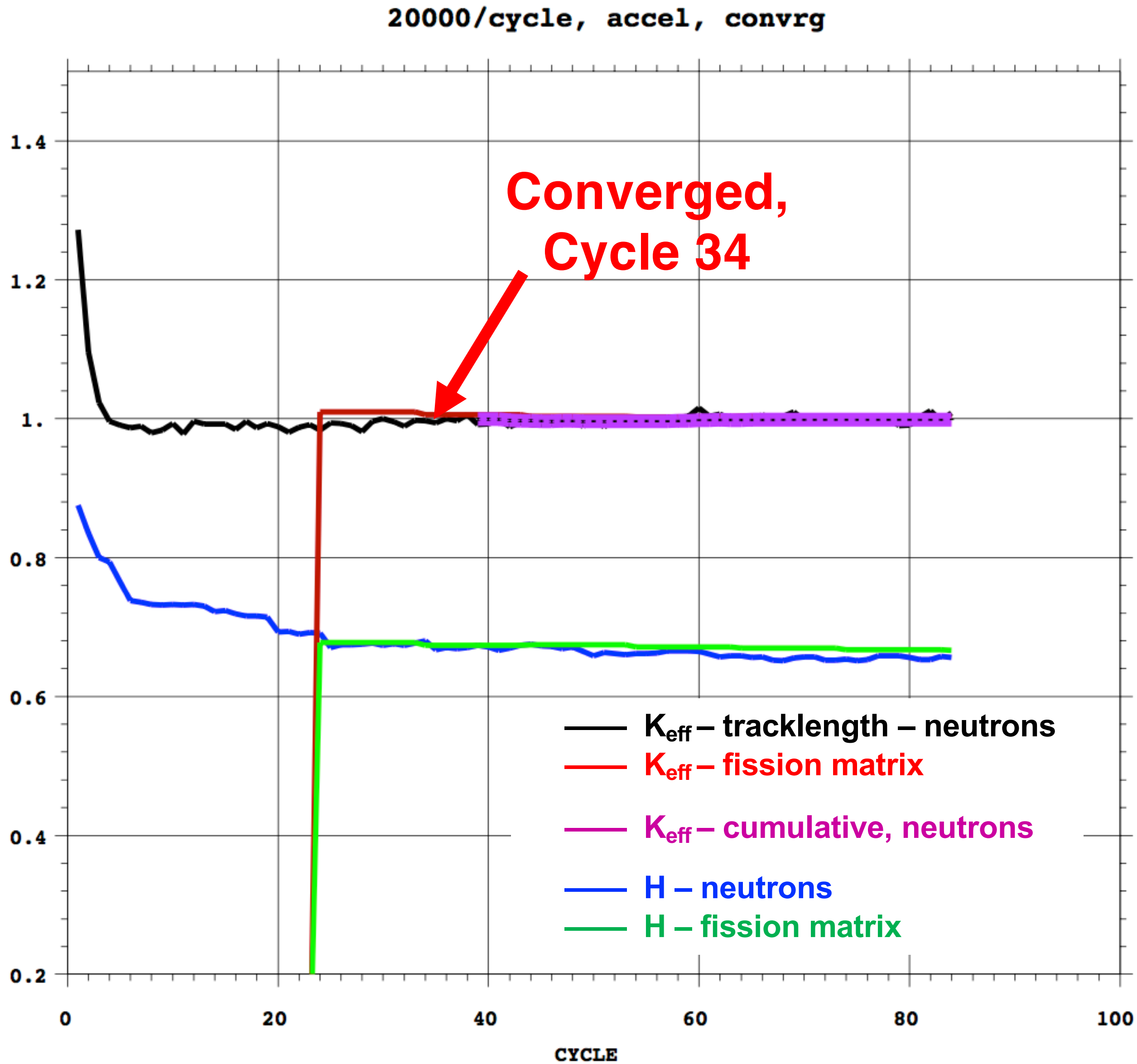
Whitesides' Model Problem – K-eff of the World

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 ?

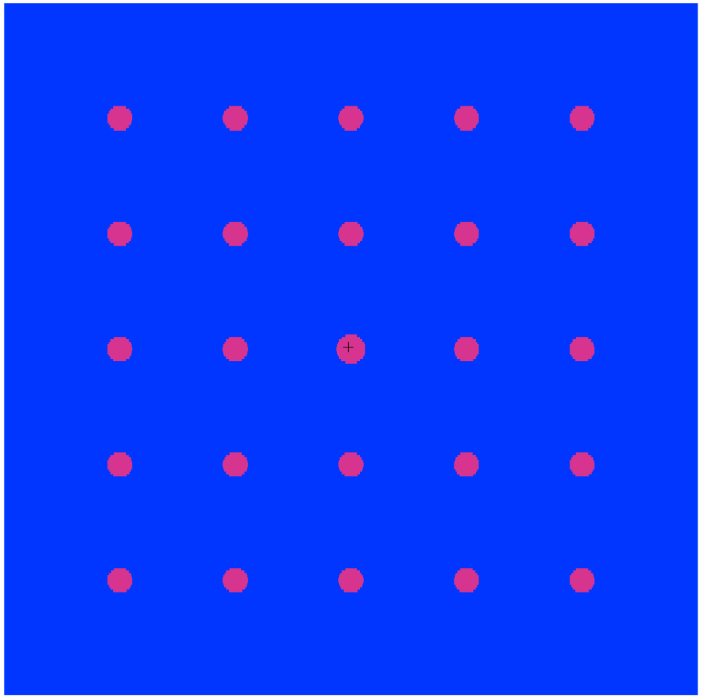


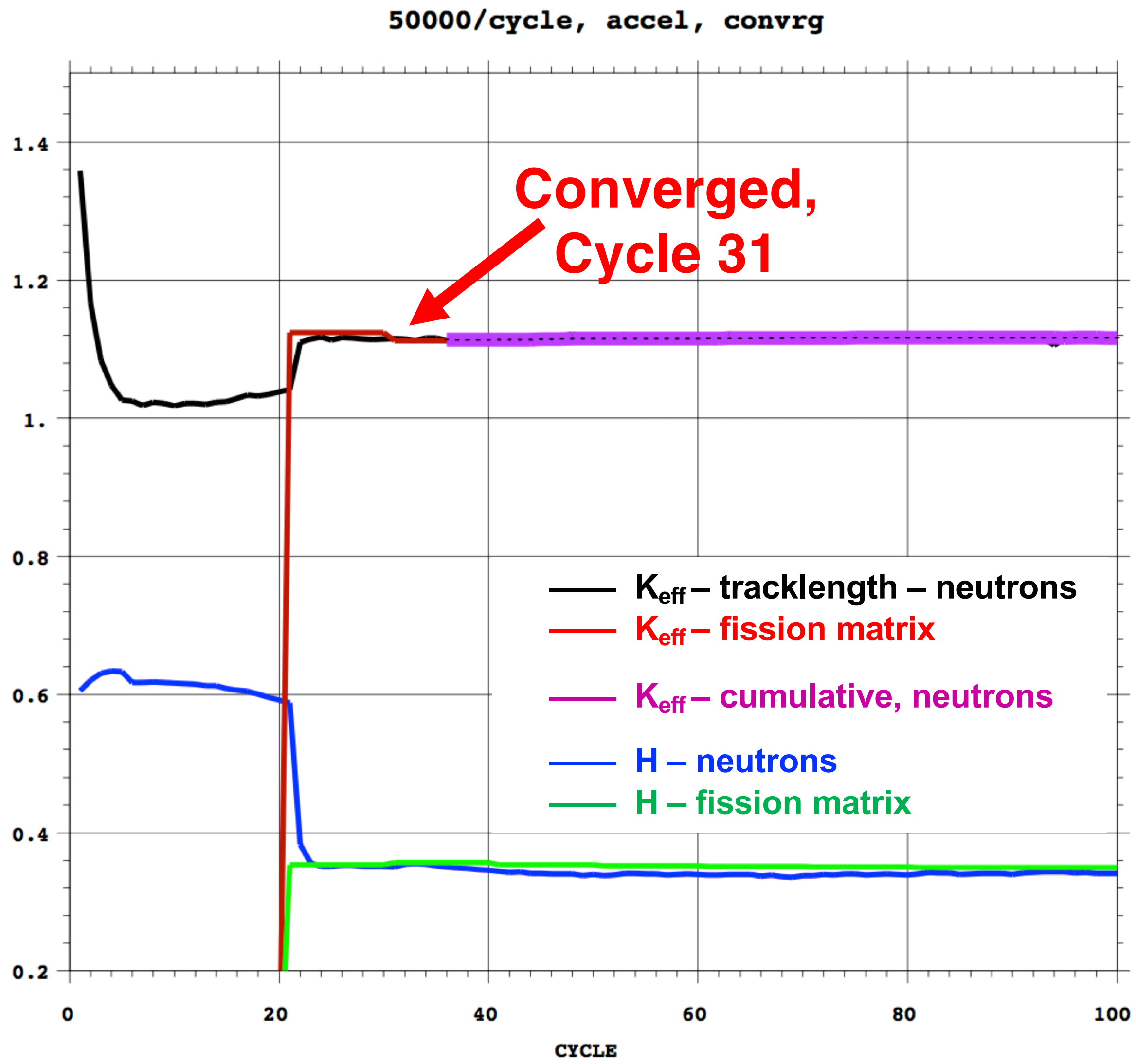


OECD-NEA Source Convergence Problem TEST4S

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

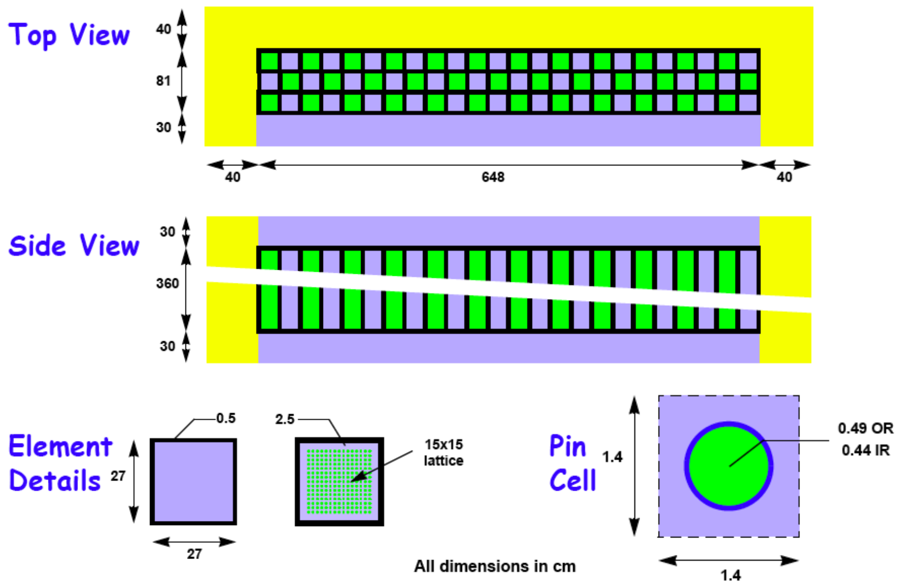




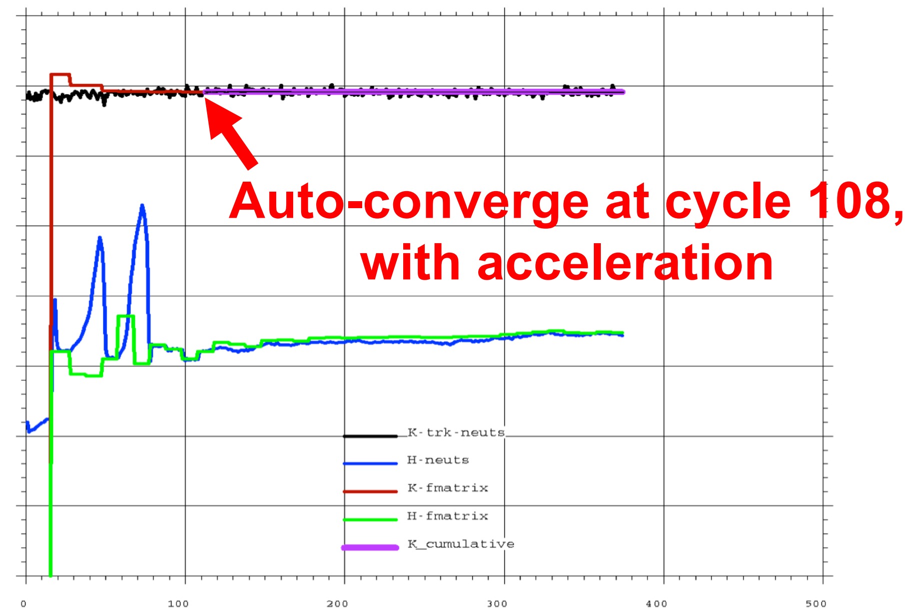
OECD-NEA Fuel Storage Pool

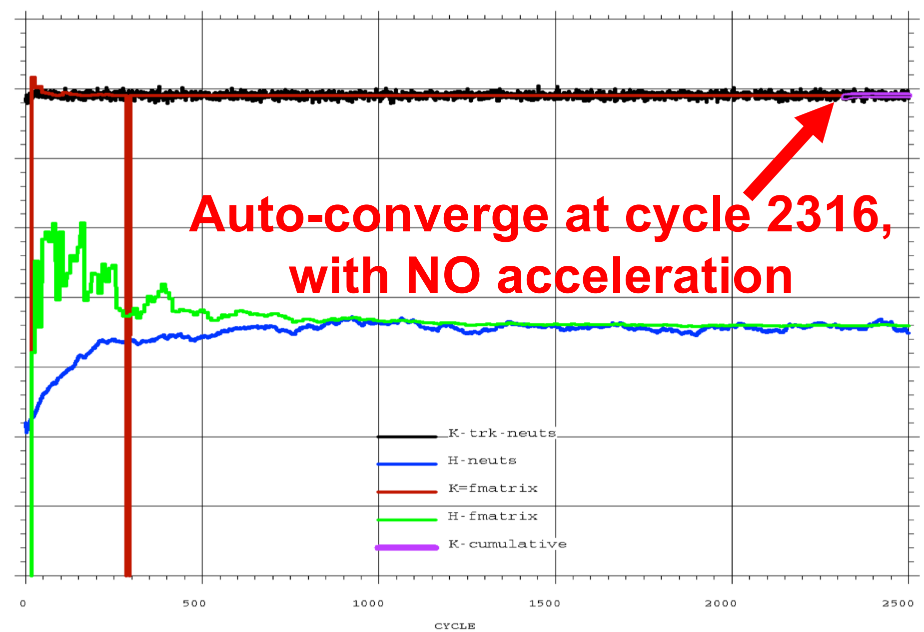
OECD-NEA-WPNCS Expert Group on Source Convergence

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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