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Automated Acceleration & Convergence Testing for Monte Carlo Criticality Calculations

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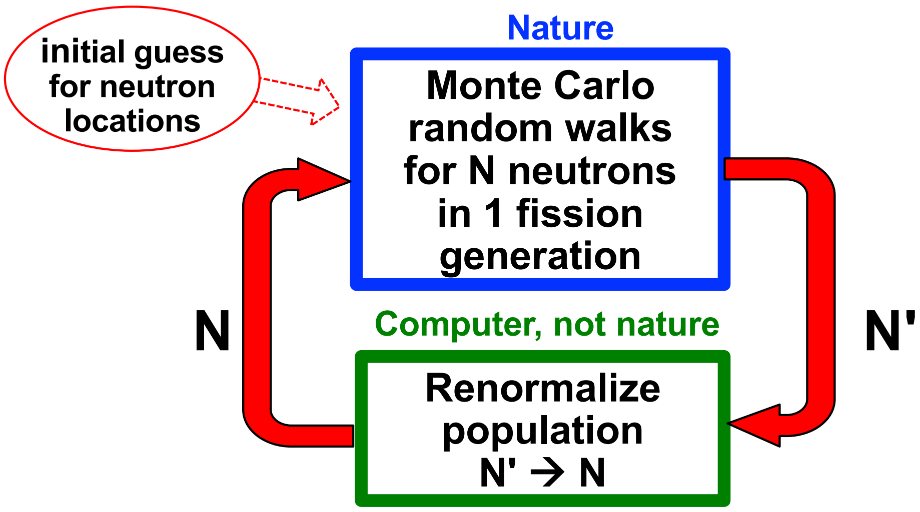
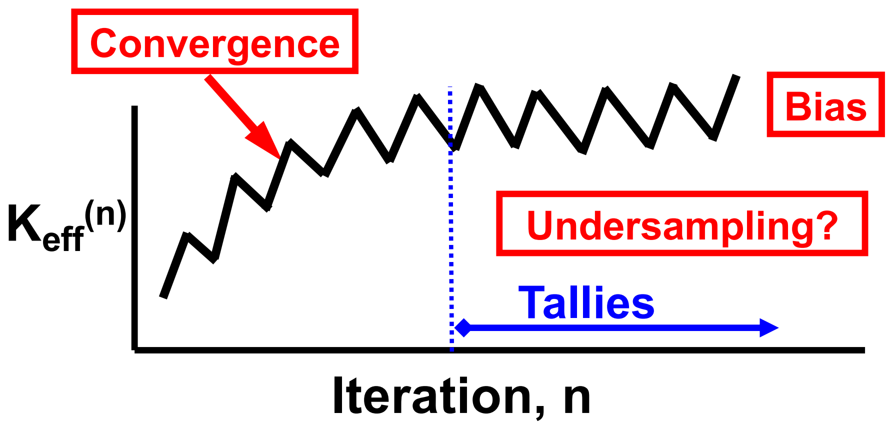
MC Criticality Calculations - Concerns

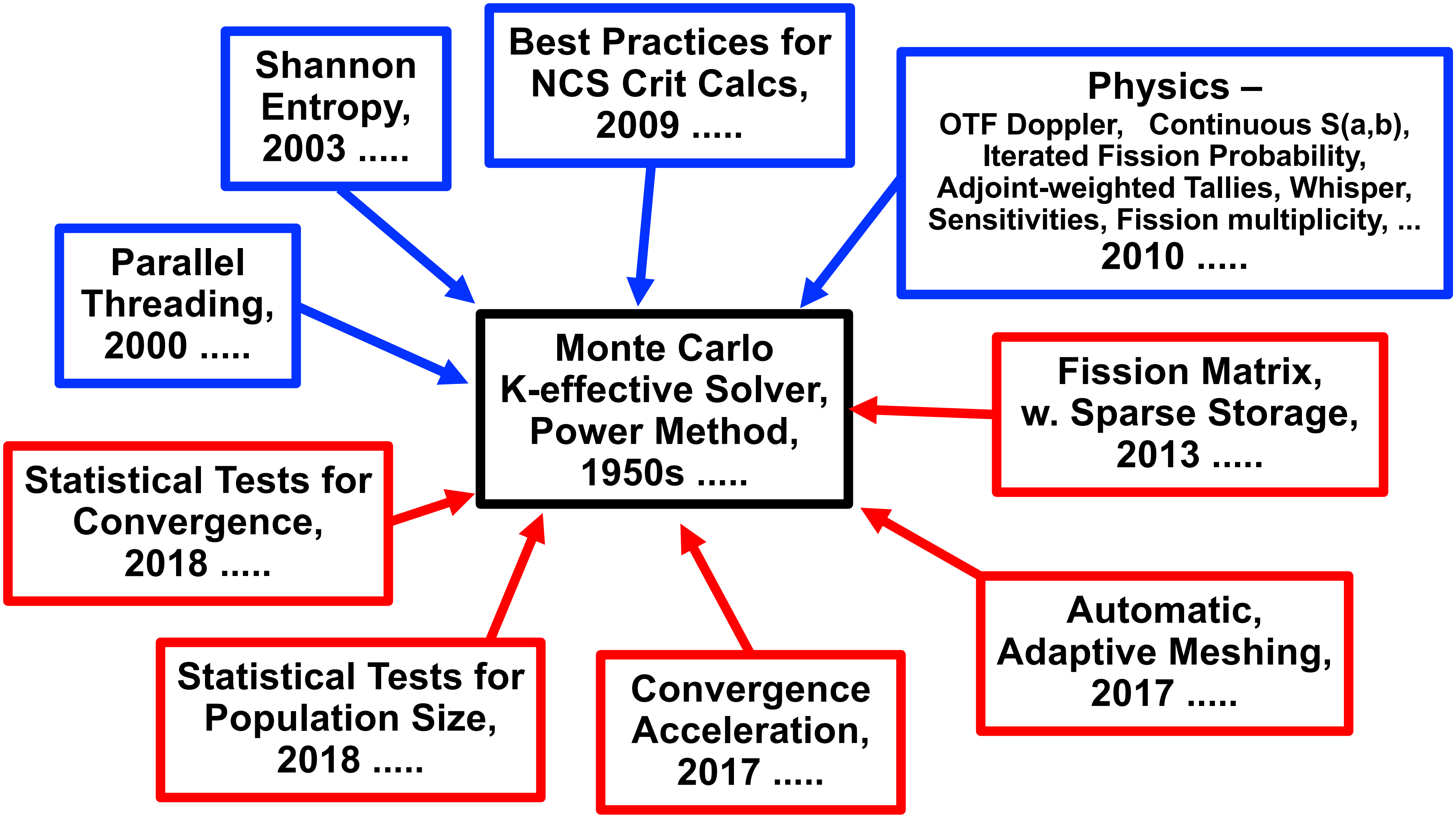




- **Bias in Keff**
  Nonconservative, ∝ -1 / (neutrons/cycle)
- **Bias in source shape**
  Too low in high-importance regions,
  Too high in low-importance regions
- **Undersampling/clustering**
  Not enough neutrons/cycle to cover space
- **Convergence**
  Source shape takes longer than keff
- **Underestimate statistics**
  Typically by 3-5x for local tallies

- **Best Practices**
  Source in all fissile regions.
  Examine H_{src} plot for convergence.
  >10k neuts/cycle (>100k big probs).
  A few 100 active cycles, or more

LANL R&D for MC Criticality Calculations



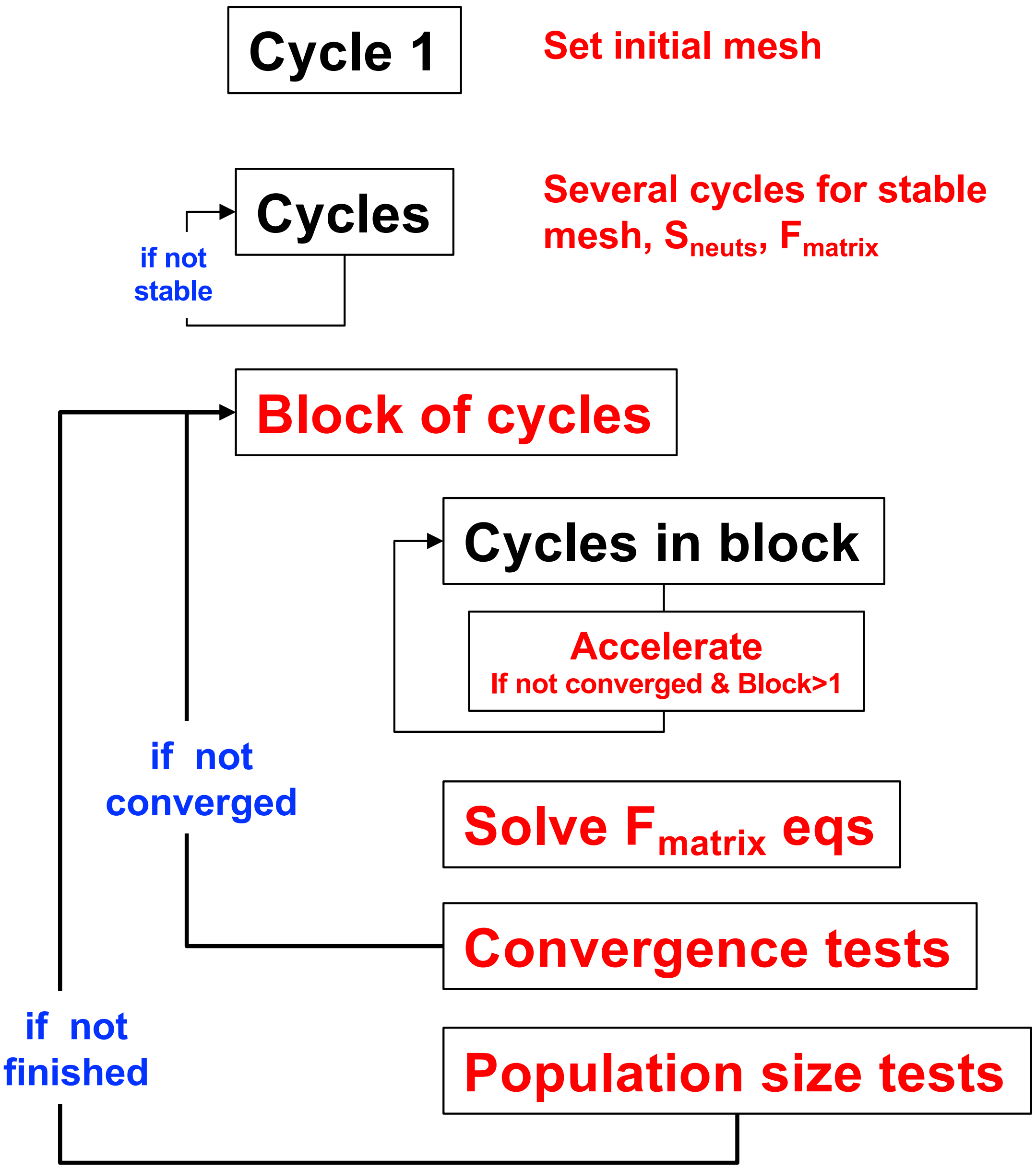
This work: Combine & automate the red boxes

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 global fission 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



Black = conventional
Red = new

Each Cycle:

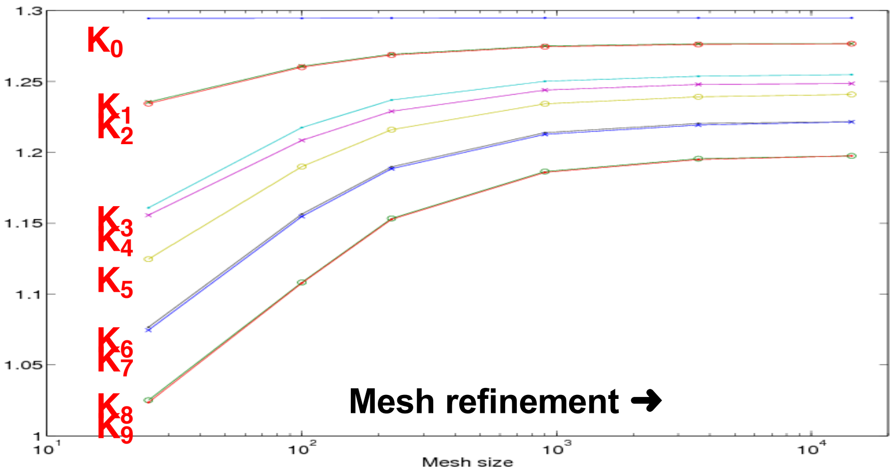
- Retrieve neutrons from fission bank
- Run neutron histories, 1 generation
- Compute Shannon entropy
- Next-gen neutrons to fission bank

- Extend mesh if needed
- Tallies on mesh for S_{neuts} & F_{matrix}

- Renormalize fission bank

Meshing for Shannon Entropy, Fission Matrix, & Convergence (1)

- **From MCD 2013, Sun Valley:**
  - Sparse-storage fission matrix introduced
  - Mesh was refined until higher-mode eigenvalue spectrum appeared converged
  - Fine resolution needed for detailed analysis of higher eigenmodes



- **Present work:**
  - Detailed solution not needed
  - Global solution for fundamental mode is needed for convergence checking & acceleration
  - Uniform meshing in each direction, with separate n_X, n_Y, n_Z
  - Need simple, physical metric to automatically choose mesh resolution

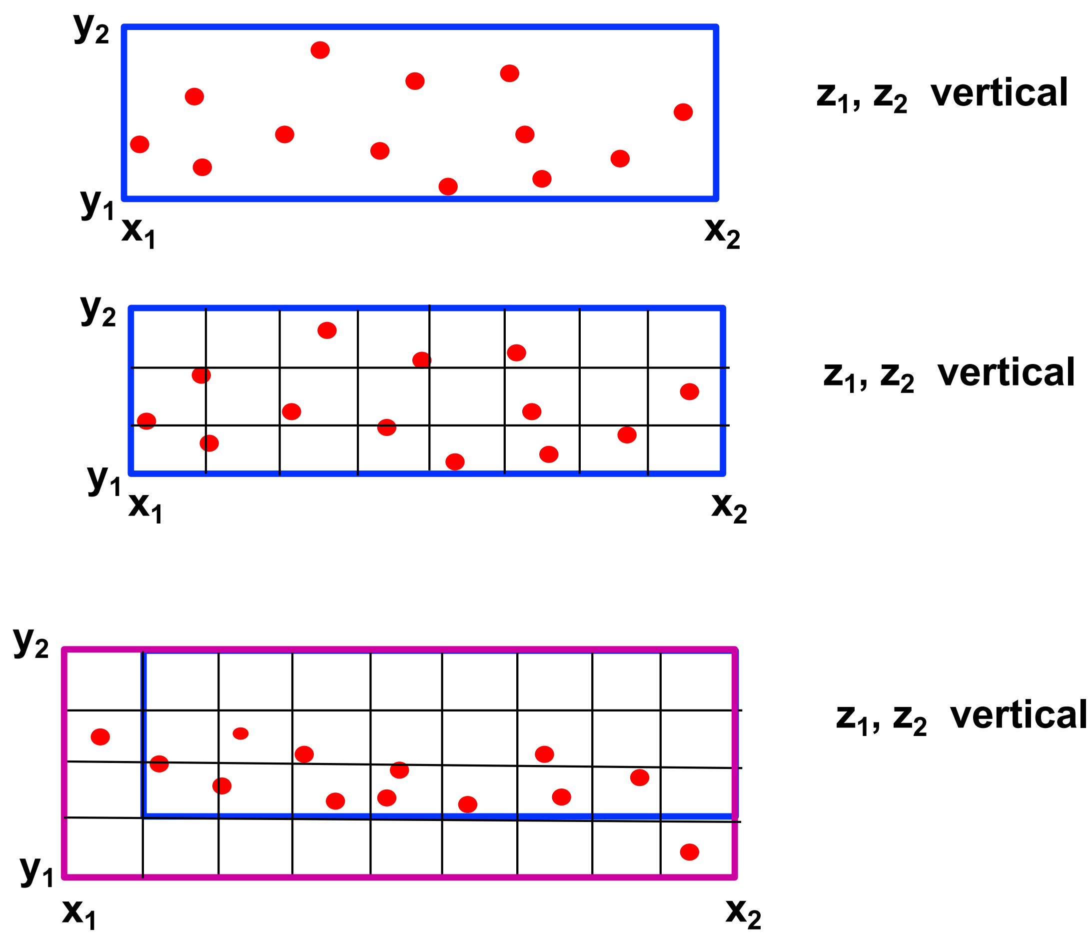
L_{Fiss} = RMS distance from birth to next-generation fission

- **Mesh resolution**
  - For previous detailed analysis, $\Delta\{x,y,z\} \sim .1 \cdot L_{Fiss}$ works best
  - For current work, $\Delta\{x,y,z\} \sim L_{Fiss}$ works best
  - Mesh is extended as needed in {x,y,z} directions, preserving all previous mesh tallies for sources & fission matrix

Meshing for Shannon Entropy, Fission Matrix, & Convergence (2)

- **Cycle 1 – set initial mesh**
  - Compute L_{Fiss}
  - Bounding-box
  - Set n_X, n_Y, n_Z for mesh spacing of $\sim L_{fiss}$
- **Later cycles**
  - Extend mesh if needed
  - Never shrink the mesh
  - Add same-size cells
  - New x_1, x_2, y_1, y_2, z_1, z_2
  - New n_x, n_y, n_z
  - Reallocate/reindex s.t.

    $i \in [1,n_x]$, $j \in [1,n_y]$, $k \in [1,n_z]$



Initial meshing & later extension are automated – no user input required

Mesh is used for tallying S_{neut}, H, F_{IJ}, S_{FM}

Shannon Entropy & Marginal Entropy

- To permit consistent comparisons of *H* if the mesh is extended, use normalized variant of Shannon entropy:
  - (Shannon entropy) / (maximum Shannon entropy)
  - For S_n = (fraction of fission neutrons in mesh cell n)

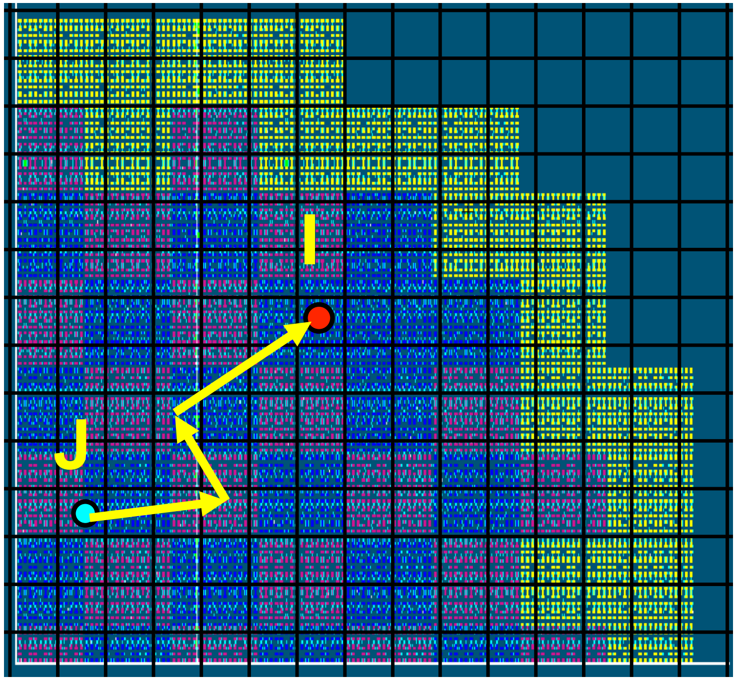
$$H = \frac{\sum_{i=1}^{n_x} \sum_{j=1}^{n_y} \sum_{k=1}^{n_z} S_{i,j,k} \cdot \ln S_{i,j,k}}{\ln(n_x n_y n_z)}, \qquad 0 \leq H \leq 1$$

- Marginal entropy
  - Collapse in *j,k* to get 1D distribution in *X*

$$H_X = \frac{\sum_{i=1}^{n_x} \left\{ \left(\sum_{j=1}^{n_y} \sum_{k=1}^{n_z} S_{i,j,k} \right) \ln\left(\sum_{j=1}^{n_y} \sum_{k=1}^{n_z} S_{i,j,k} \right) \right\}}{\ln(n_x)}, \quad 0 \leq H_X \leq 1$$

  - Similar for H_Y & H_Z
  - H_X, H_Y, H_Z can be useful for detecting side-to-side shifts or oscillations

Fission Matrix - Introduction



- For global shape analysis of fission source convergence, choose mesh spacing of $\sim L_{Fiss}$ (This work)
- For detailed analysis of higher-mode eigenvalues & eigenfunctions, choose mesh spacing of $\sim .1 \cdot L_{Fiss}$ or less
- Mesh does not have to be aligned with material or geometric boundaries

- **From neutron simulation in a cycle, tally $F(I \leftarrow J)$**
  - Neutrons produced in region I due to source in region J
  - Accumulate over all cycles (even inactive)
  - Estimate of point-to-point Green's functions

- **For n_x x n_y x n_z mesh**
  - $N = n_x \cdot n_y \cdot n_z$ mesh cells
  - F matrix is N • N
  - Example: 100 x 100 x 100 mesh
    F is $10^6 \times 10^6$, nonsymmetric
    10^{12} tallies for Green's function

- **Fission matrix equation for fission neutron source:**

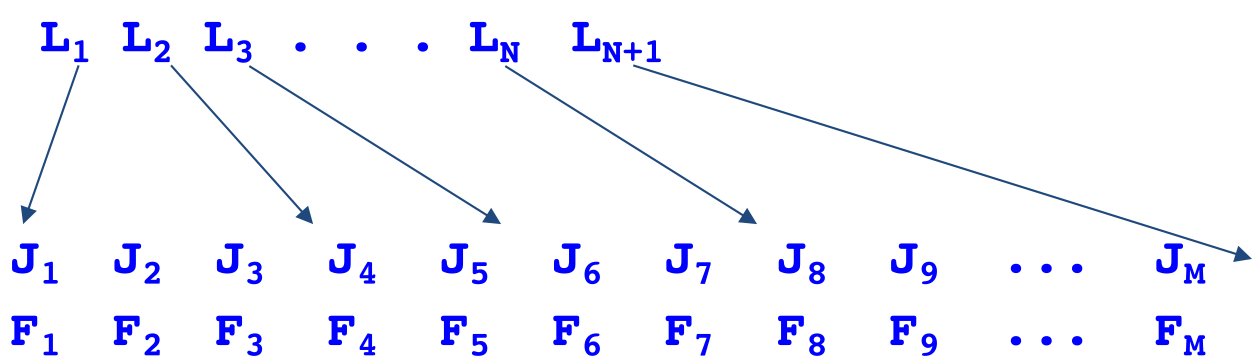
$$S = 1/k \; F \cdot S$$

Given F, can solve for k & S

Fission Matrix – Sparse Storage

- **Compressed Row Storage Scheme (CRS)**
  - **General sparsity, no approximations or assumptions**
  - $N = n_x\, n_y\, n_z$ **mesh cells**
  - $(i_S, j_S, k_S) \rightarrow (i_T, j_T, k_T)$ ➜ $J \rightarrow I$ $\quad J = i_S + (j_S\text{-}1)n_x + (k_S\text{-}1)n_x n_y$

    $I = i_T + (j_T\text{-}1)n_x + (k_T\text{-}1)n_x n_y$
  - **Only the nonzero *F(I,J)* entries are stored.**
  - **MC tallies: If element exists – add to it; if not – insert it**
  - ***L(I)* array entries point to the start of a list of *J* indices and corresponding nonzero *F(I,J)* tallies**



  - **Highly optimized tally coding, typically requires less than 1 second at the end of each cycle in the Monte Carlo simulation.**

Fission Matrix – Solver

- Power iteration to determine fundamental mode eigenvalue & eigenvector only

$$S_n = 1/k_{n-1} \cdot F \cdot S_{n-1}$$

- Normalize f_{IJ} tallies

$F_{ij} = f_{ij} / S_j$ for all i,j

- Power iteration

```
Initialize  k0, s0, res0
Do  n = 1, …
      sn   = f·sn-1
      kn   = sn·sn  /  sn·sn-1

      khi  = max( sn/sn-1 )
      klow = min( sn/sn-1 )

      resn = (sn/kn-1 – sn-1)^2
      DR   = (resn/resn-1)^1/2

      sn   = sn / sum(sn)
      if( khi-klow <  eps )  exit
```

Sparse-matrix * vector multiply →

Rayleigh quotient →

Max & min bounds for k_{eff} →

Dominance Ratio from residual decay →

Test absolute bounds for convergence →

Automated Methods

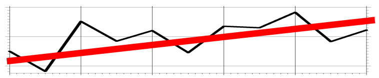
- Cycle 1
  - Estimate L_{Fiss} & set initial mesh
- Initial cycles
  - Iterate until mesh and S_{neut} & F tallies are stable
    - Automated, test that (Δ nonzero tallies) $<$ 2%, 5%
  - When S_{neut} & F tallies are stable, begin a block of cycles

- At the end of a block of cycles (default = 10)
  - Solve F matrix equations for S_{FM}, fundamental mode eigenfunction
  - Convergence tests
    - 11 statistical tests must all pass for convergence
    - If converged, set active cycles to begin with next cycle, start population size tests after next block
    - If not converged, accelerate source convergence for each cycle by importance sampling with weights:

$$S_{FM}(m) / S_{neut}(m), \quad m = \text{bin}$$

Statistical tests for convergence (1)

- **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) | < $t_{0.025}\ \sigma_{slope}$ → 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 later fail (due to statistics), but convergence not rescinded

Statistical tests for convergence (2)

- **Relative entropy & statistical testing**
  - **Kullback-Liebler discrepancy, relative entropy between distributions:**

    $$D_{KL}(o|e) = \sum_i o_i \, ln({}^{o_i}/_{e_i}), \qquad o_i = observed, \quad e_i = expected$$

  - **G-test of goodness-of-fit**
    - Also known as likelihood ratio test or log-likelihood ratio test
    - Chi-square test of goodness-of-fit is an approximation of G-test
    - G statistic has approximately a chi-squared distribution

      $$G(O|E) = 2 \cdot \sum_i O_i \, ln\left({}^{O_i}/_{E_i}\right) = 2N \cdot \sum_i o_i \, ln({}^{o_i}/_{e_i}) = 2N \cdot D_{KL}$$

    - ***G* = *2N* · *D*$_{KL}$ has chi-squared distribution with *N-1* degrees of freedom**
    - **For hypothesis testing of observed & expected distribution, can test**

      $$D_{KL}(o|e) \quad <_? \quad \chi^2_{N-1,\,0.025} \;/\; 2N$$

    - **For current work,**

      o$_i$ **= observed neutron distribution on mesh**

      e$_i$ **= expected distribution on mesh = FM fundamental mode**

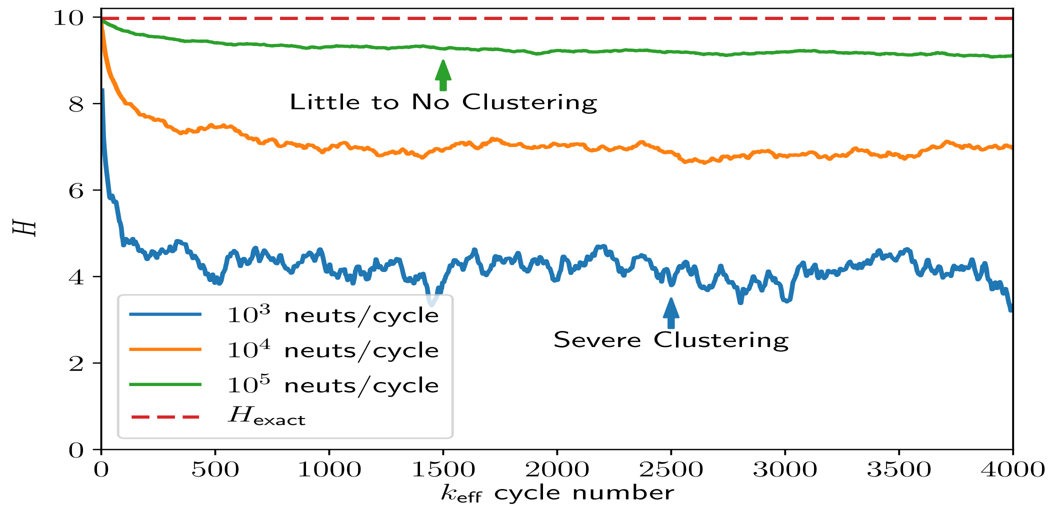
Accelerating Source Convergence

- **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 (1)

- **From LA-UR-18-27656, Source renormalization leads to:**
  - **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



- **At the end of a block of cycles**
  - **S_{FM} is available – source from fission matrix fundamental at end-of-block**
  - **S_{block} is available – neutron source accumulated in mesh during block**
  - **S_{FM} can be considered a <u>reference solution</u>**

- **If population size is large enough such that source renormalization bias is negligible,**
  - **$S_{block} \sim S_{FM}$,** **compare distributions using relative entropy**
  - **$< H(S_{cycle}) >_{block} \sim H(S_{FM})$,** **compare FM entropy to neutron entropy averaged over cycles in block**

Statistical tests for Population Size (2)

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

Extra MCNP input to activate new features:

```
kopts    fmat=        yes
         fmatconvrg=  yes
         fmataccel=   yes
```

MCNP6 example

```
comment. -----------------------------------------------------------------------
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.  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. -----------------------------------------------------------------------
```

← L_{Fiss}

Bounding Box

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

← from F-matrix solution

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

OECD-NEA Source Convergence Problem TEST4S

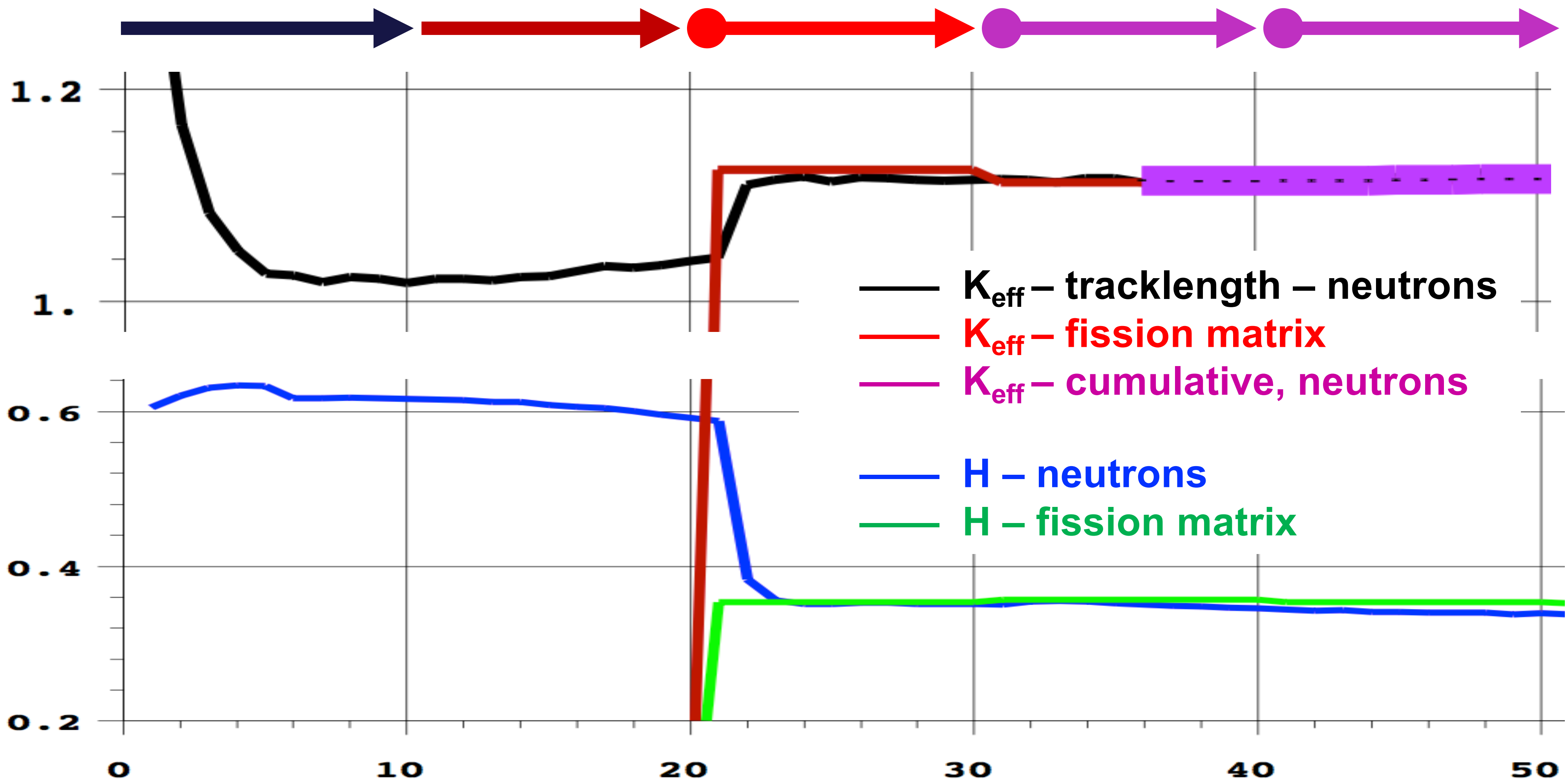
50,000 neuts/cycle, acceleration, auto-converge, k = 1.1165 (2)

fission matrix stabilization for 11 cycles

initial block of 10 cycles, ● solve Fmat

acceleration for 1 block of 10 cycles, autoconverge at 31

active cycles, standard power iteration

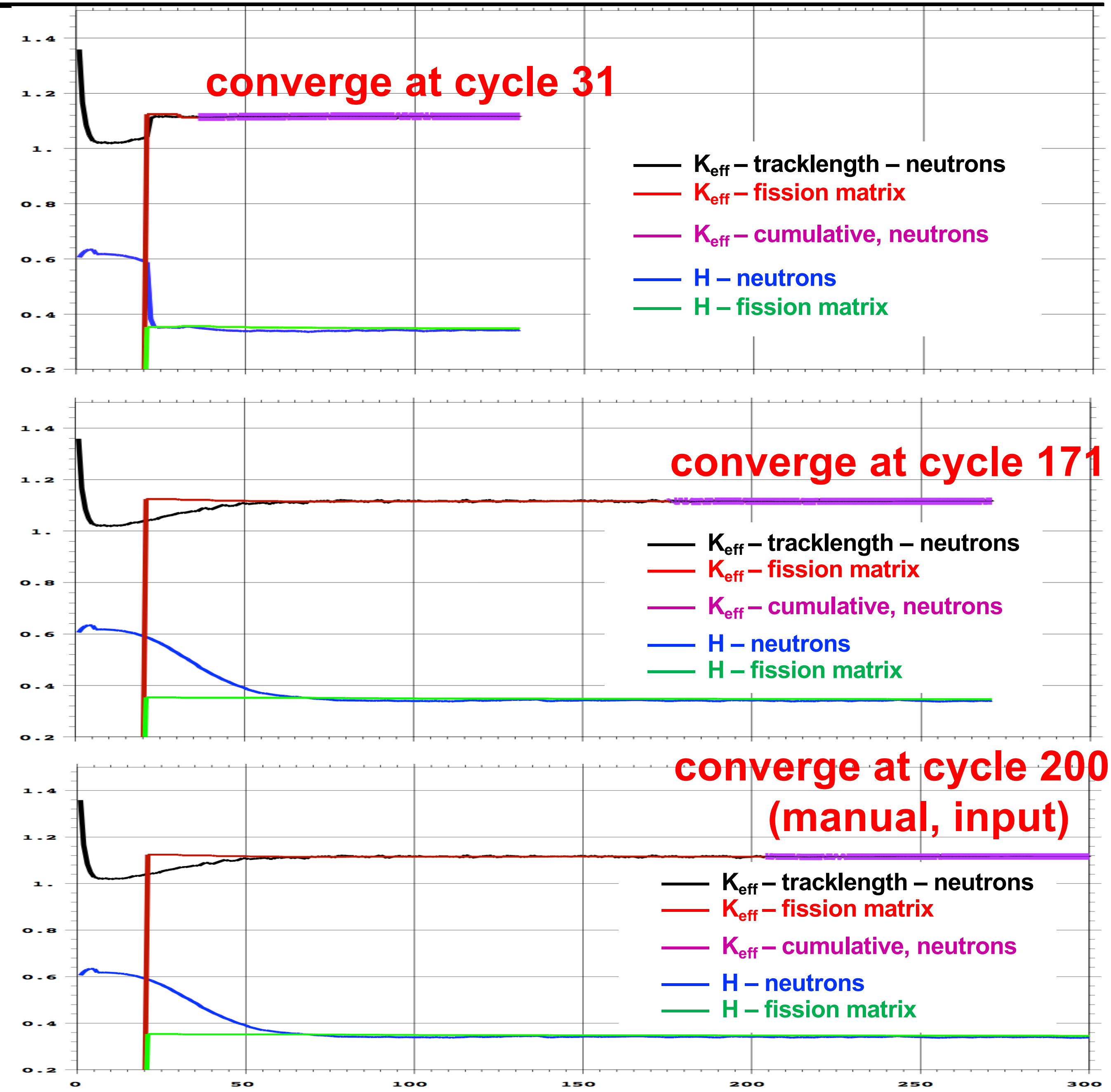


MCNP6 example

```
 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)

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 – INL advanced test reactor
- AGN-201m – UNM research reactor
- C5G7 - 3D U-Mox benchmark, OECD-NEA
- Triga reactor
- ACRR – Sandia 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

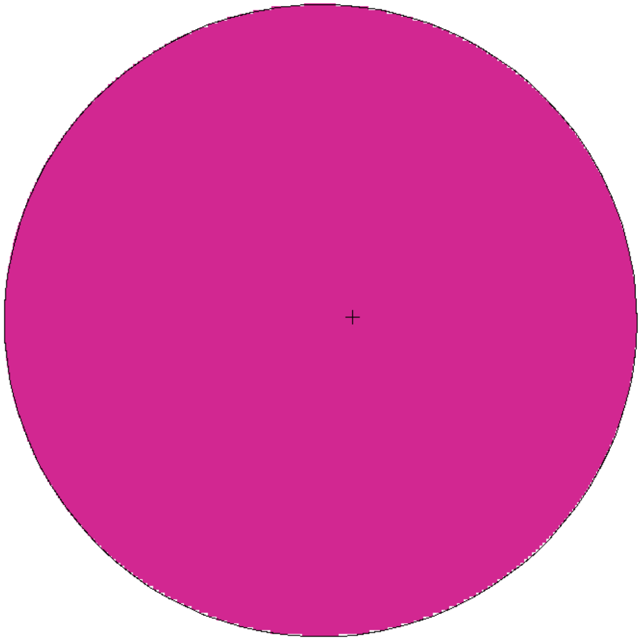
- **Timing tests**
  - 50,000 neutrons/cycle for all runs
  - For standard runs, 100 inactive cycles, 100 active cycles
  - For auto accelerate & converge, 100 active cycles

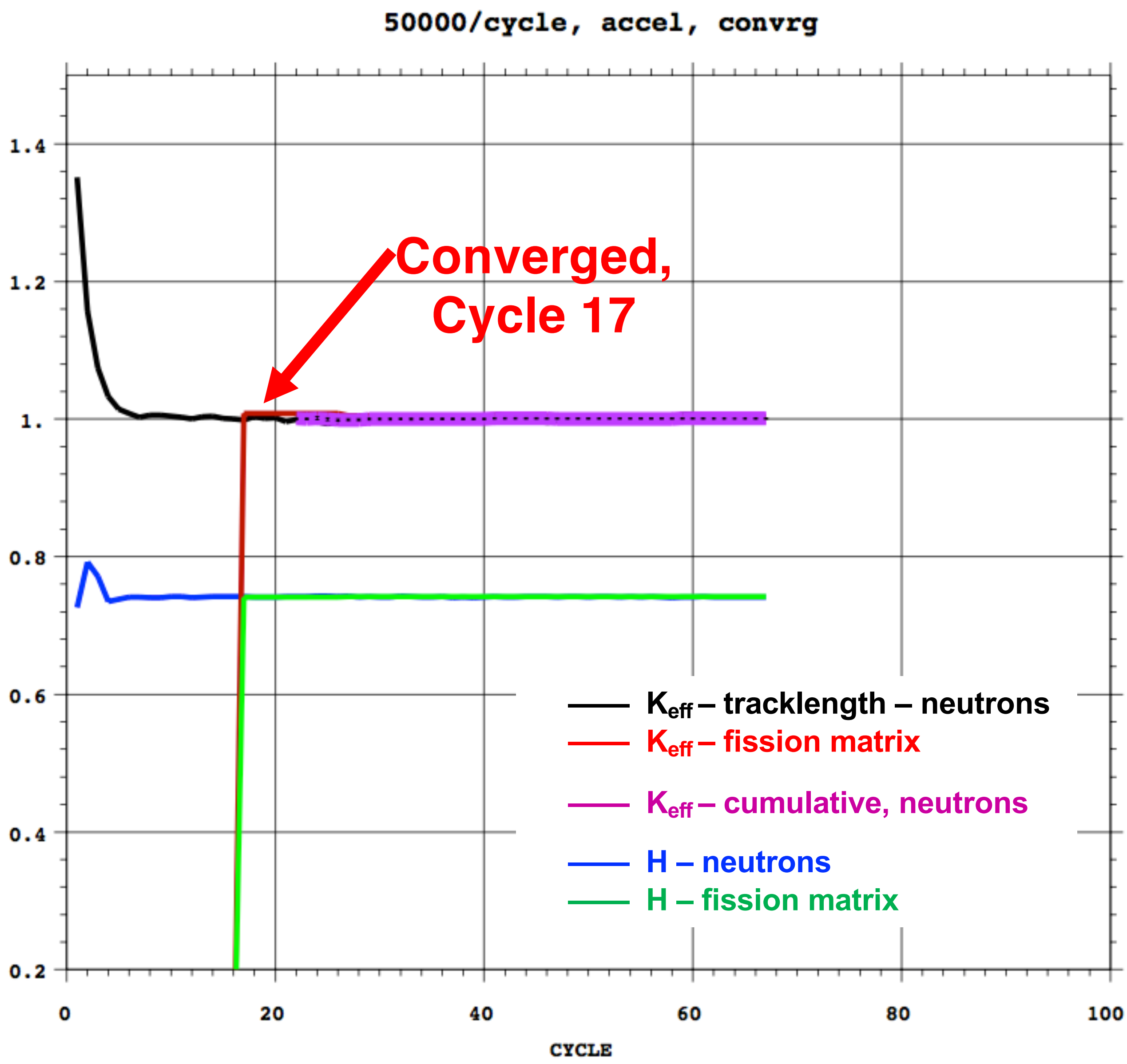
Standard run: 106 minutes

Auto accel & converge: 70 minutes

Godiva Problem

Bare HEU sphere

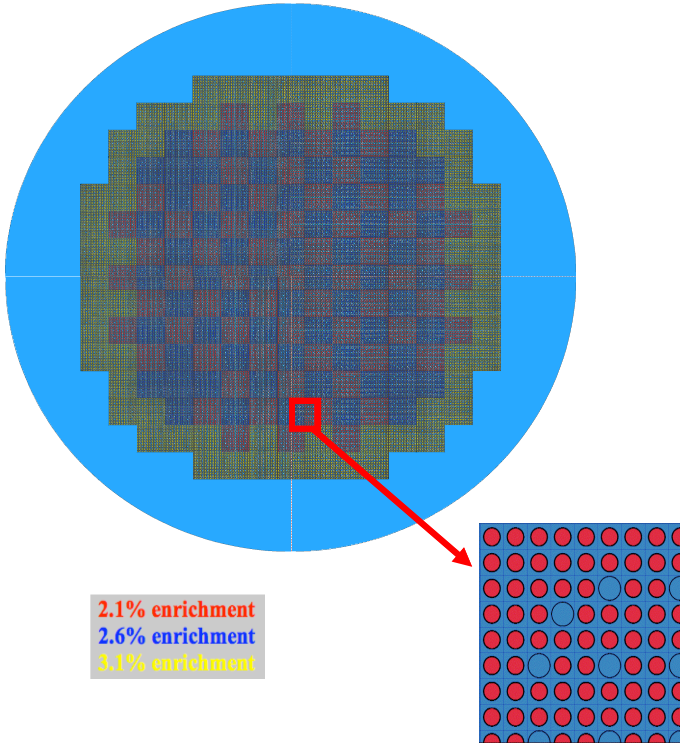


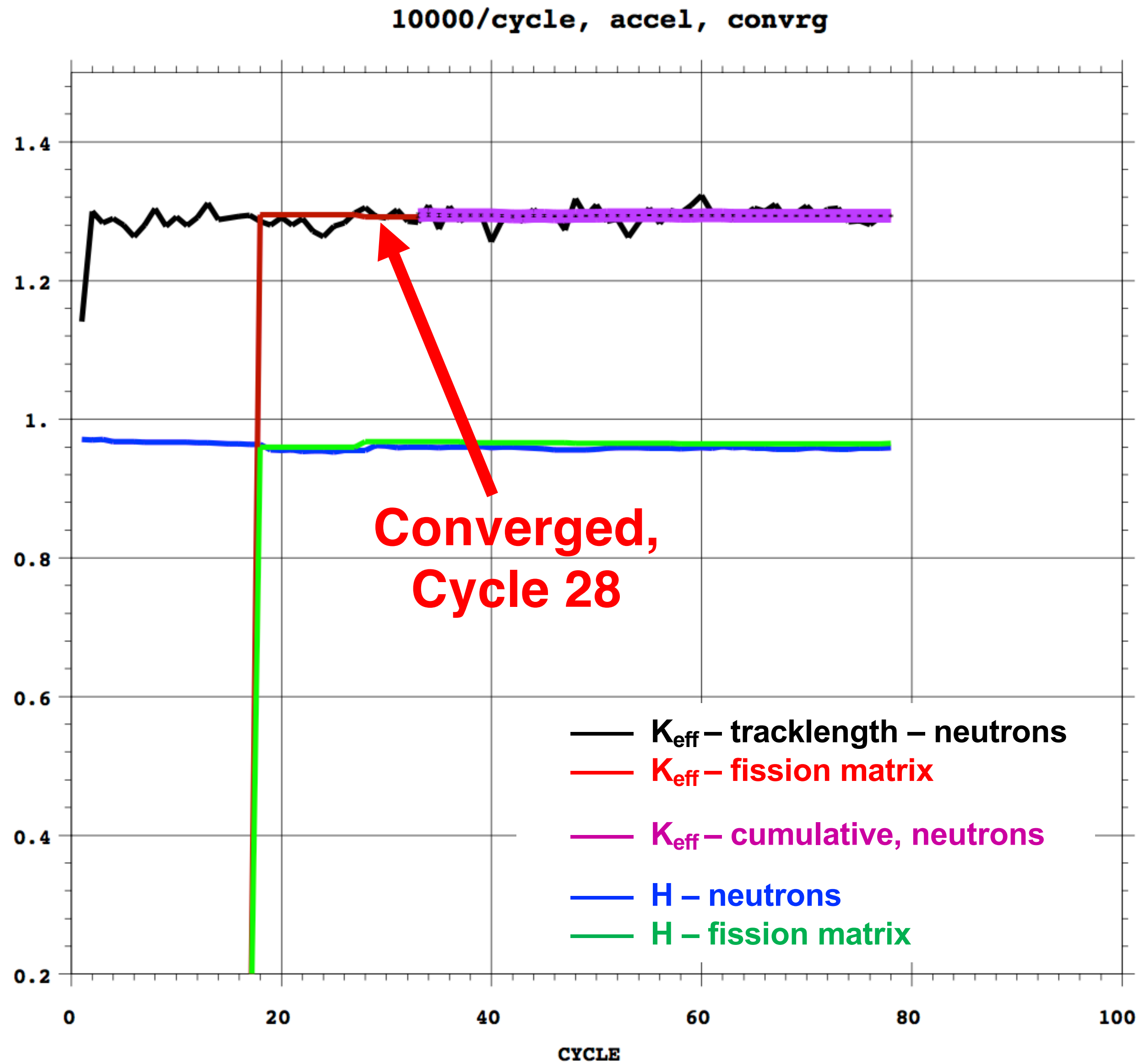


Whole-core 2D PWR Model

2D PWR (Nakagawa & Mori model)

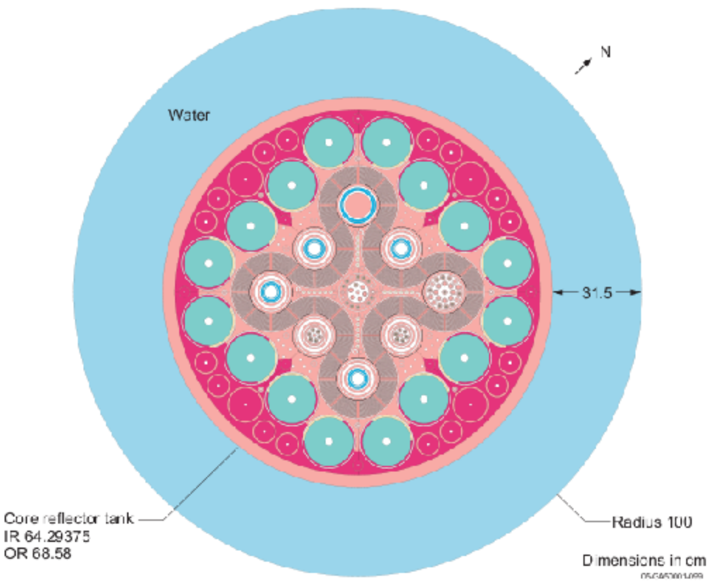
- 193 fuel assemblies:
  - 50,952 fuel pins with cladding
  - 4825 water tubes
- Each assembly:
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- Calculations used whole-core model

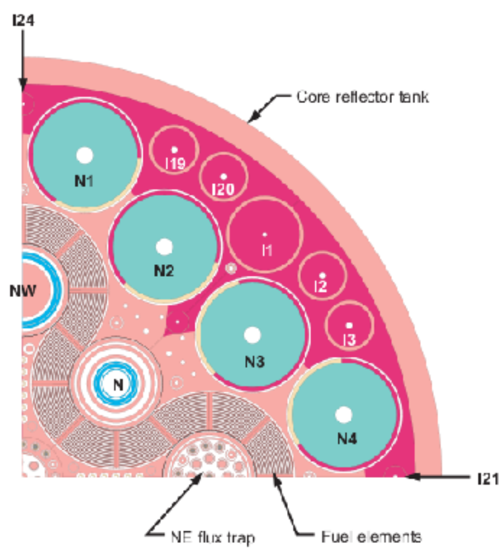


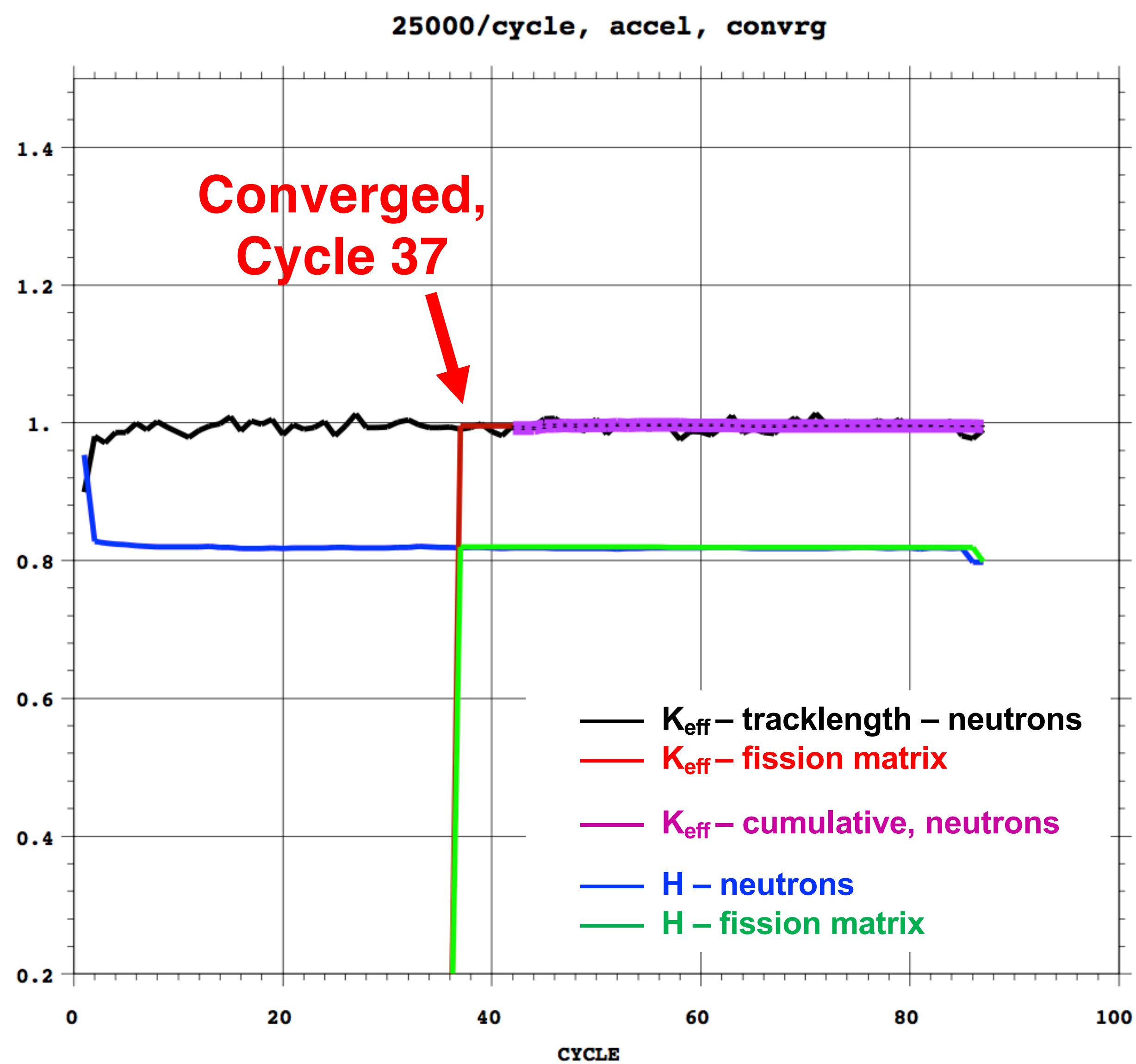


Advanced Test Reactor

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



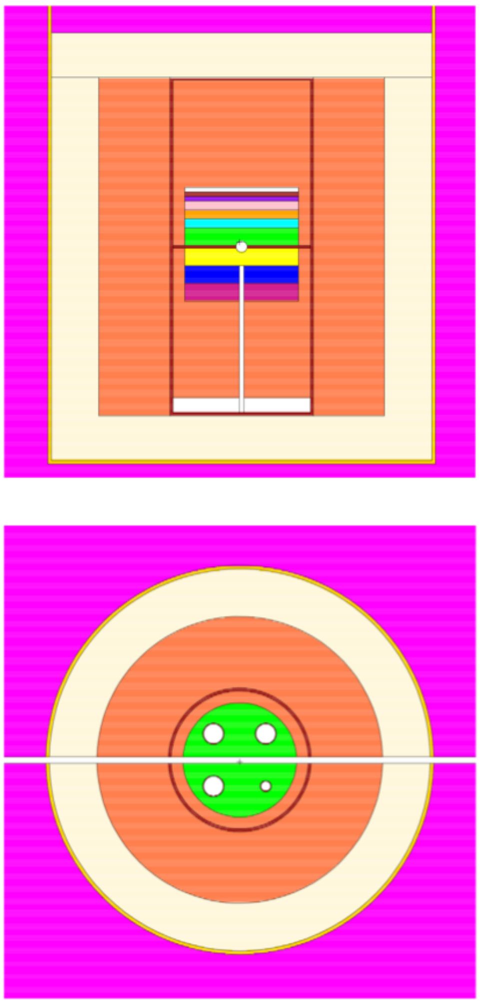


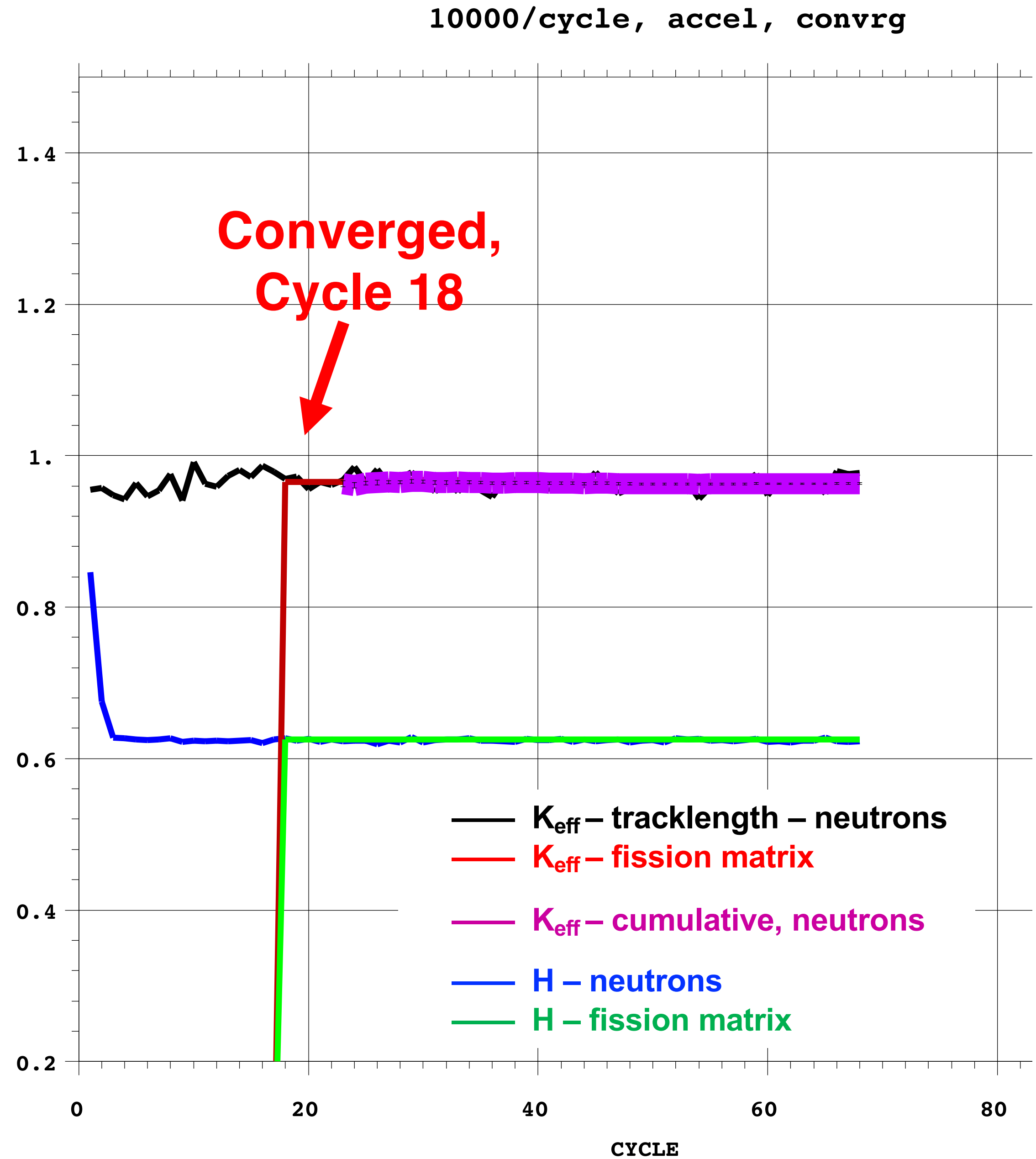


AGN-201 - Univ. New Mexico Research Reactor

AGN

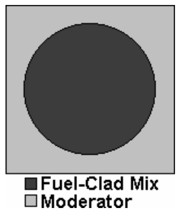
UNM Research Reactor





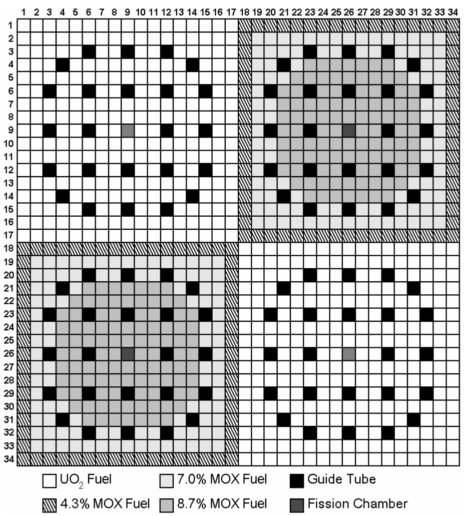
OECD-NEA Benchmark - C5G7

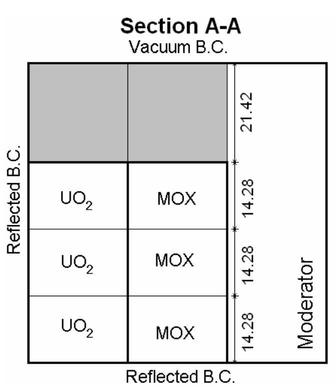
Figure 2. Fuel pin layout

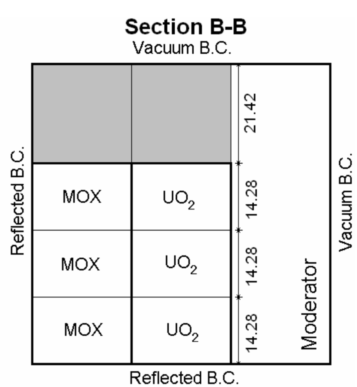


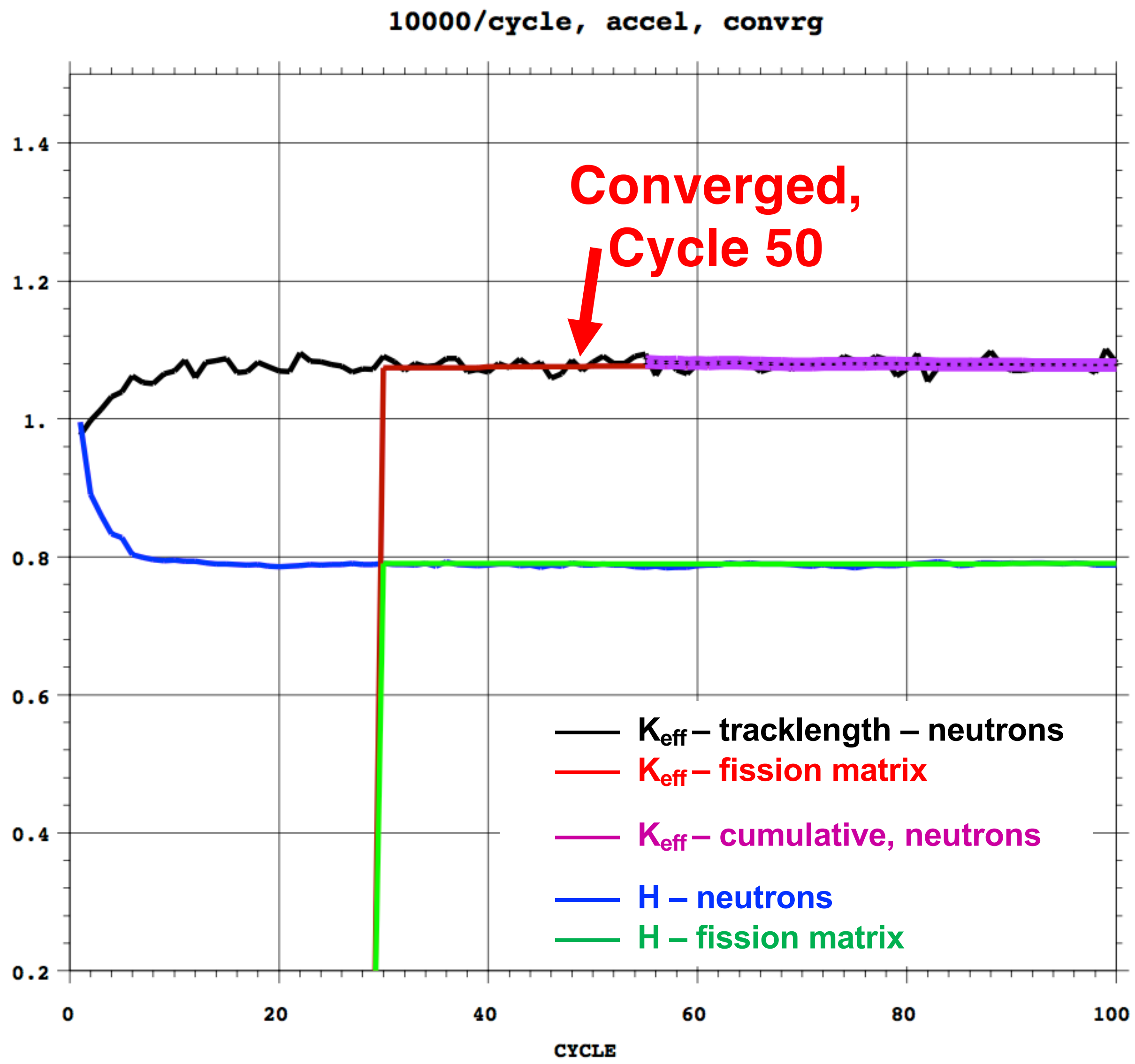
3D model

Figure 3. Benchmark fuel pin compositions and numbering scheme

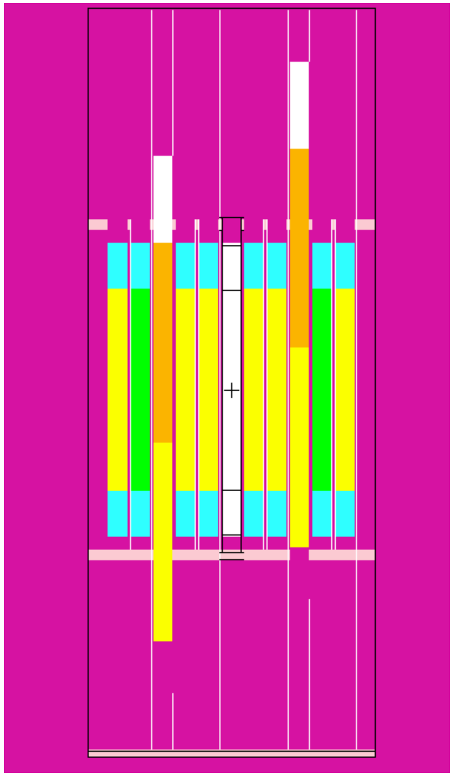


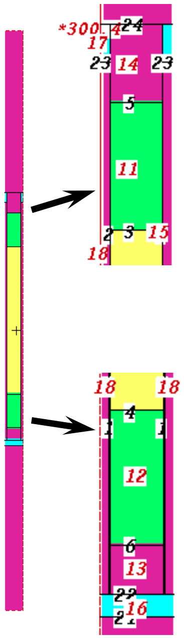


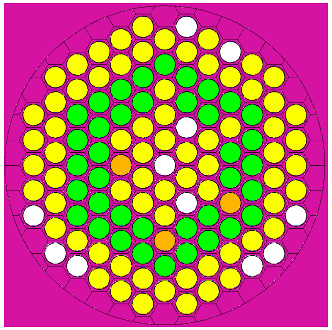


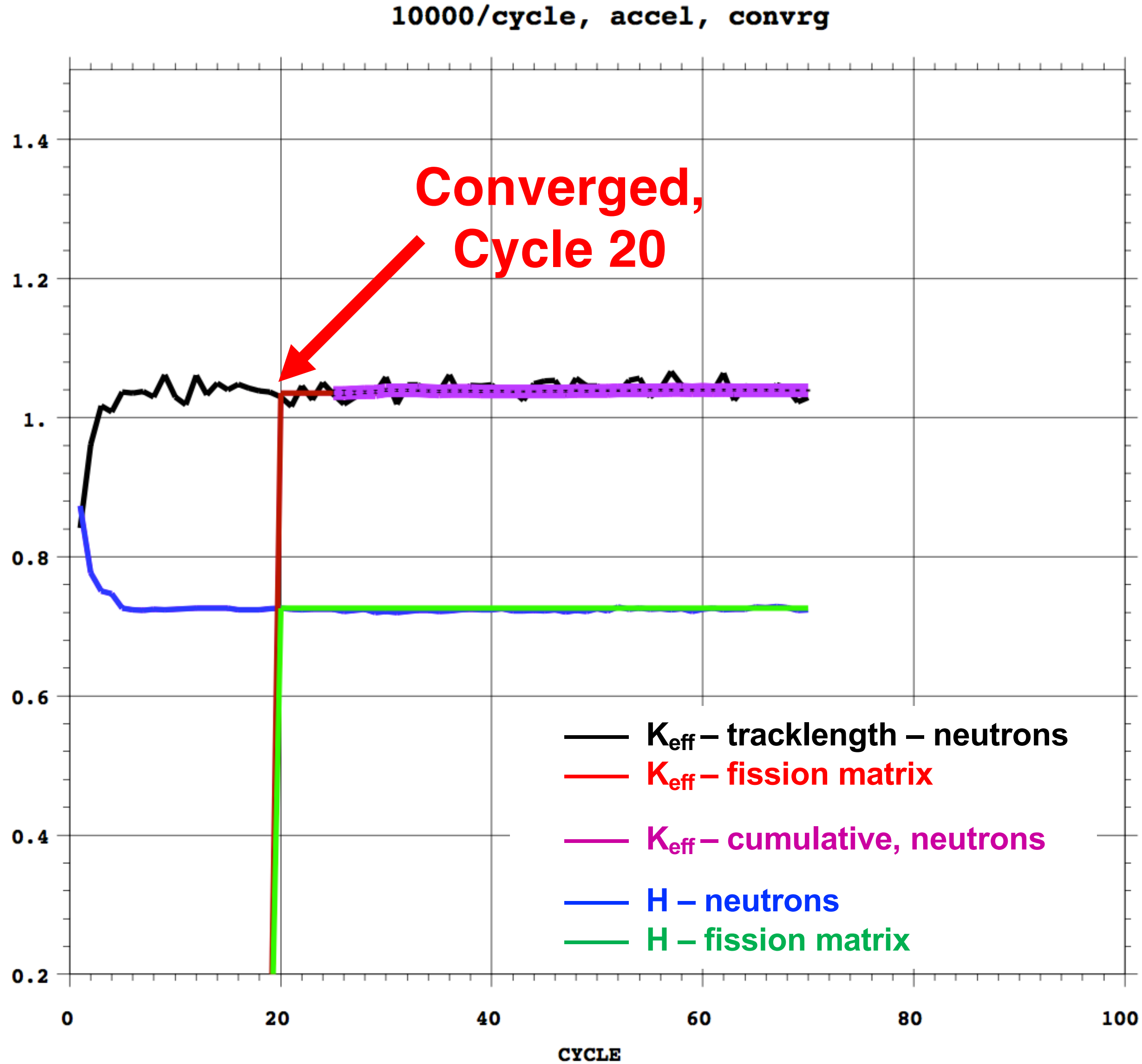


TRIGA Reactor



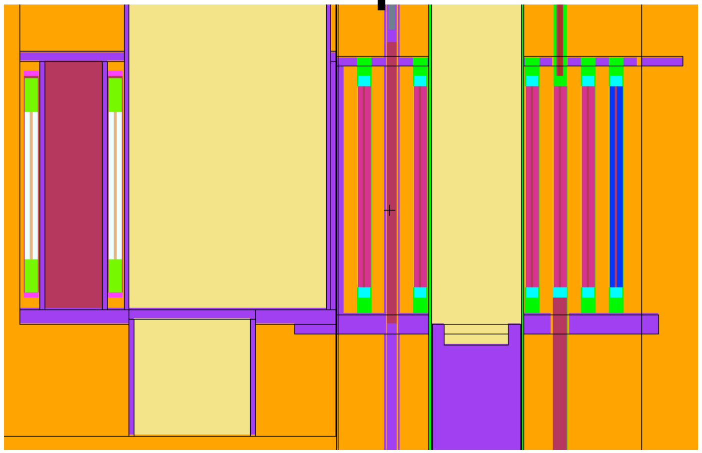




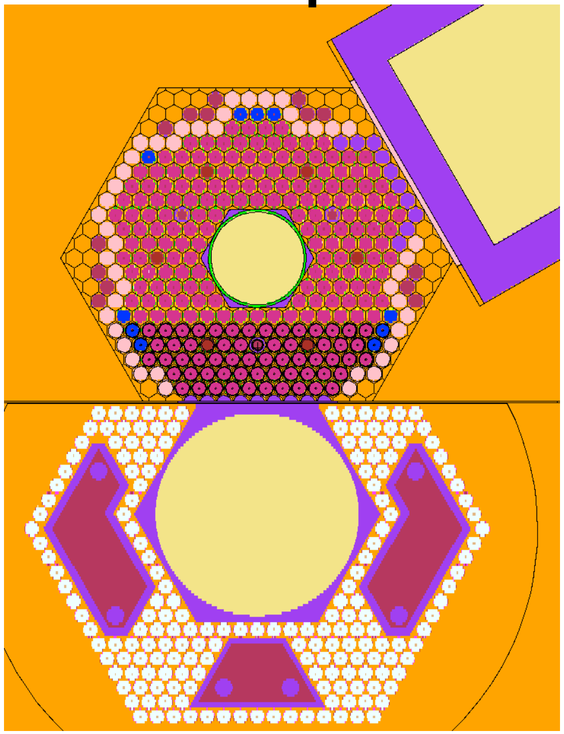


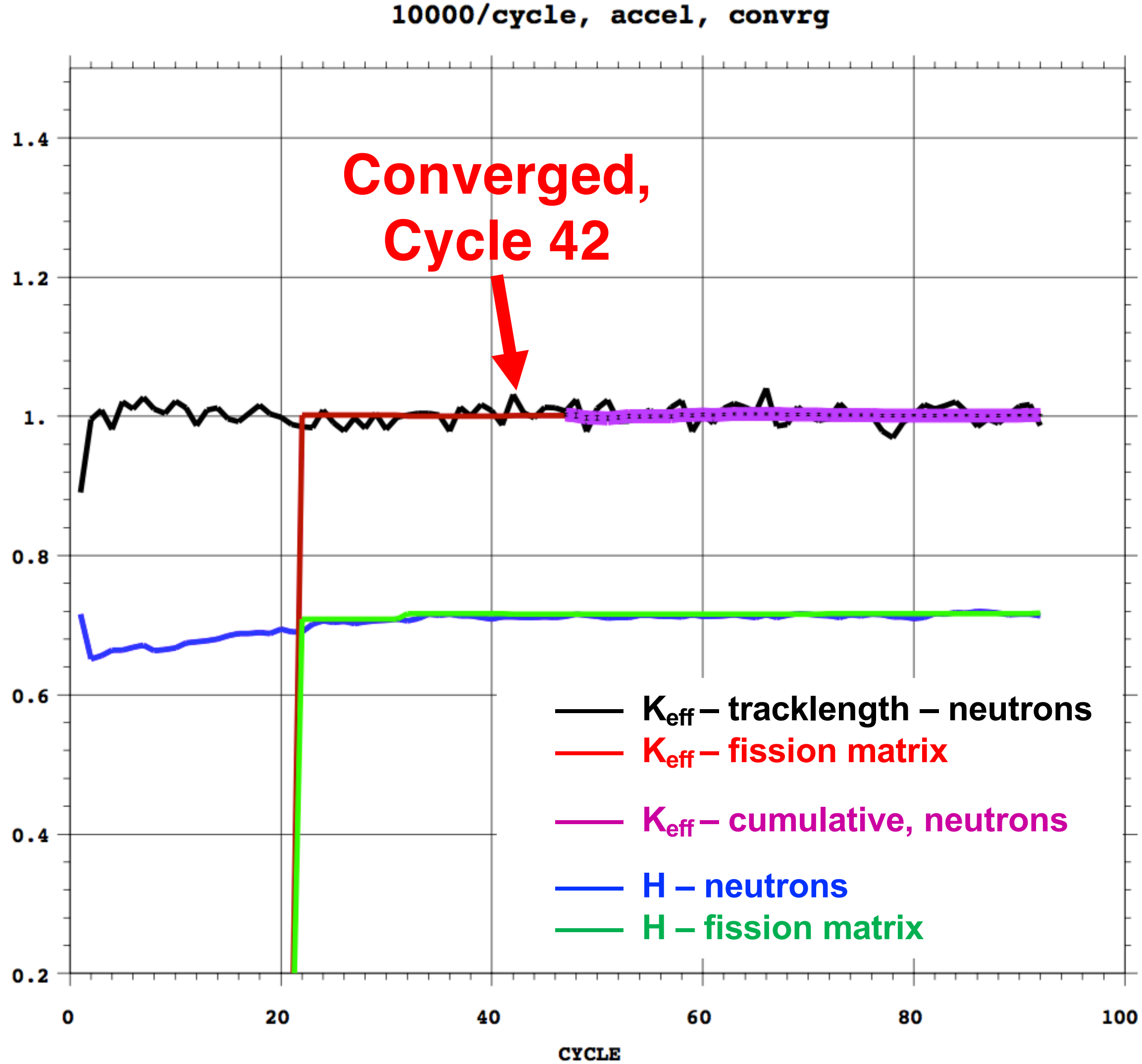
Sandia burst reactor - ACRR, with FREC

Y-Z plot



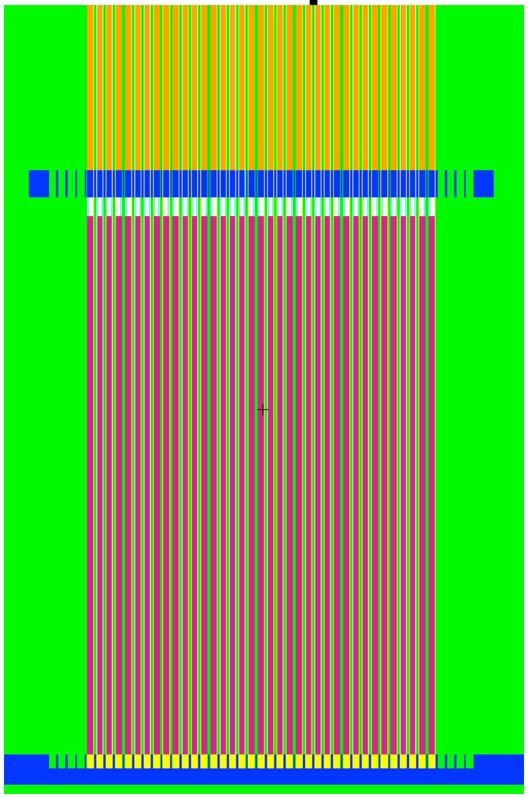
X-Y plot



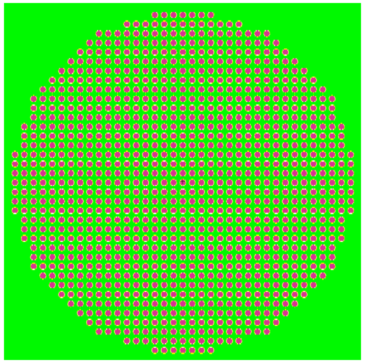


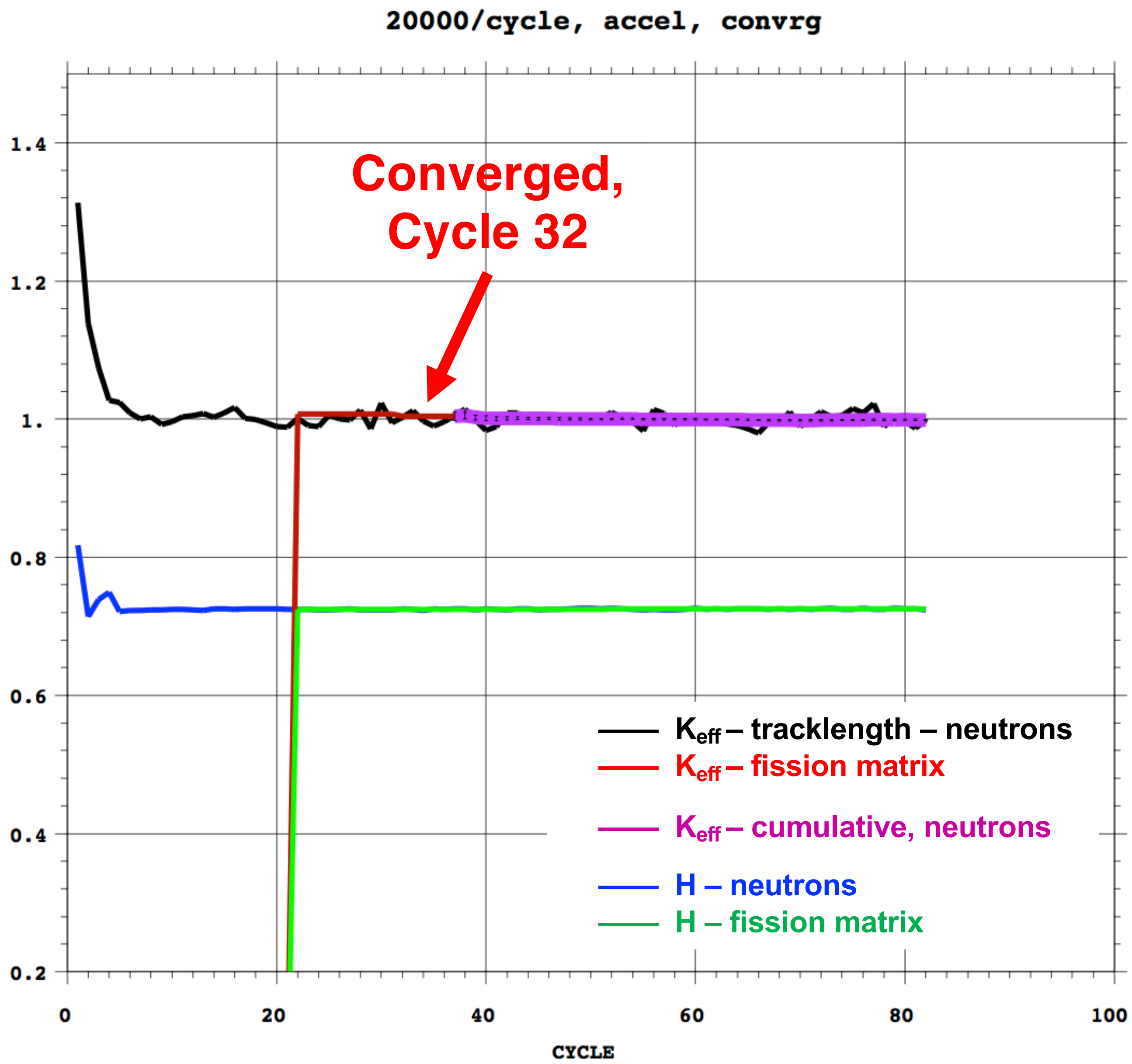
Sandia critical experiment – LCT-078-001, 1,057 rod assembly

Y-Z plot



X-Y plot





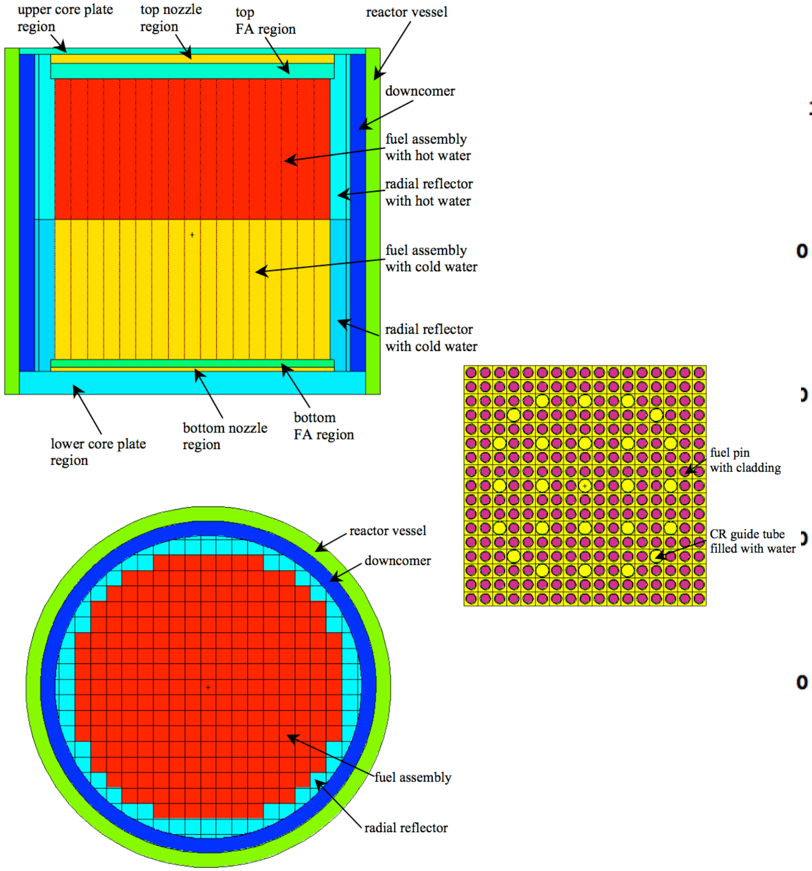
OECD-NEA "Hoogenboom-Martin Performance Benchmark"

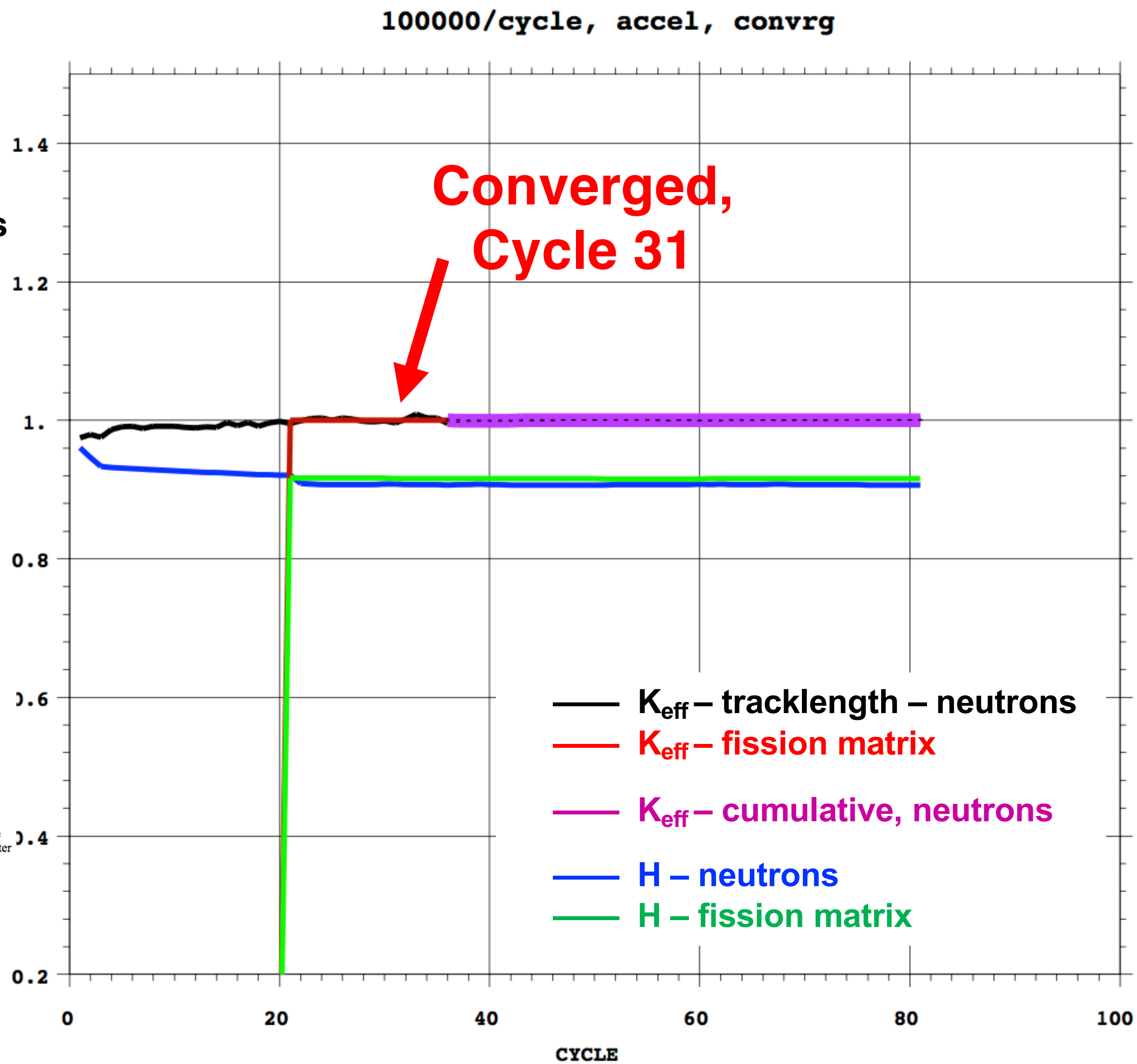
Reactor – full core, 3D

- **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



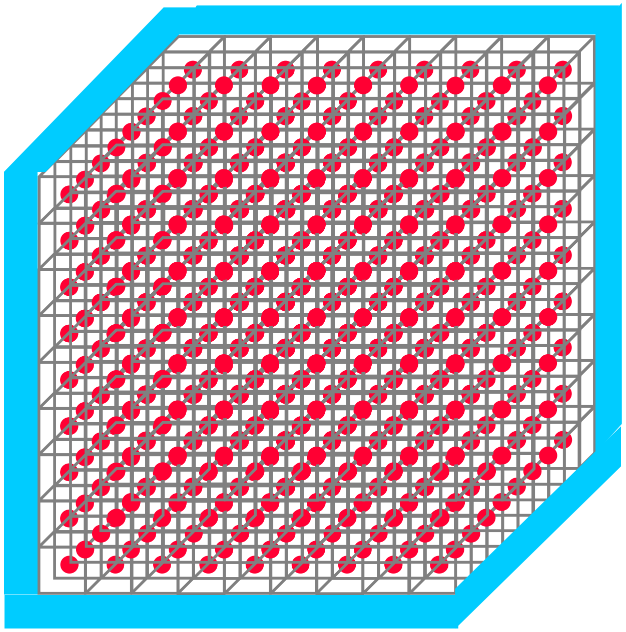


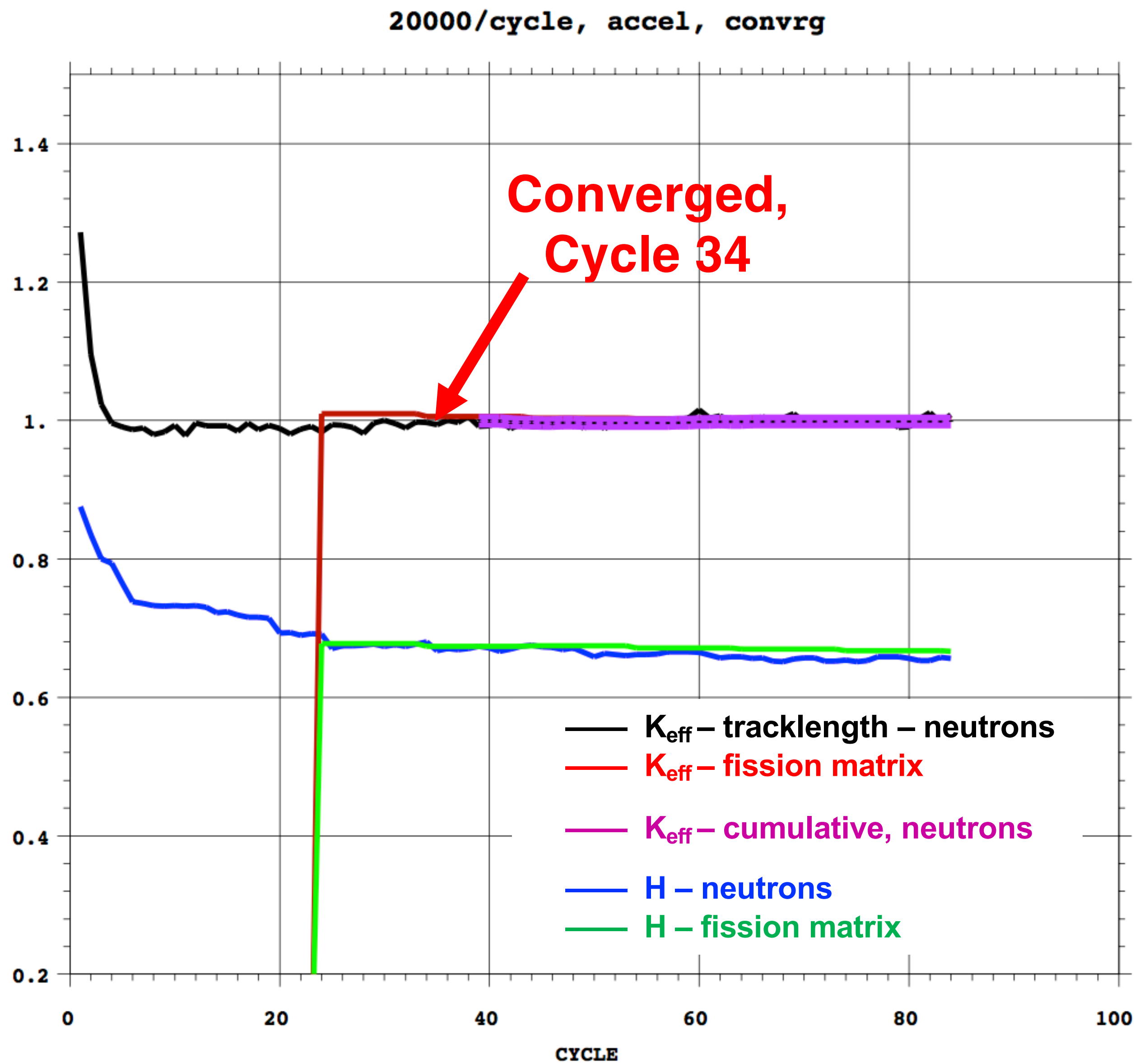
Whitesides' Model Problem – K-eff of the World

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 ?

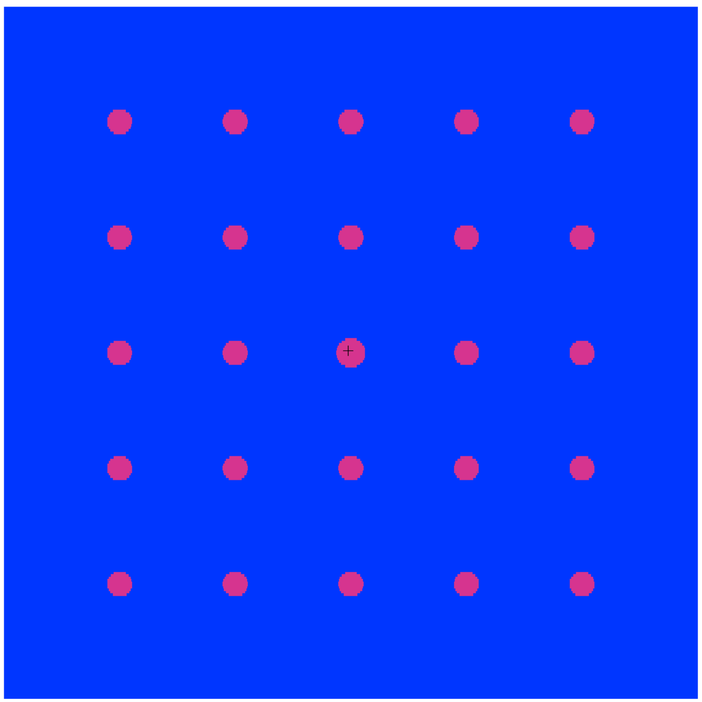


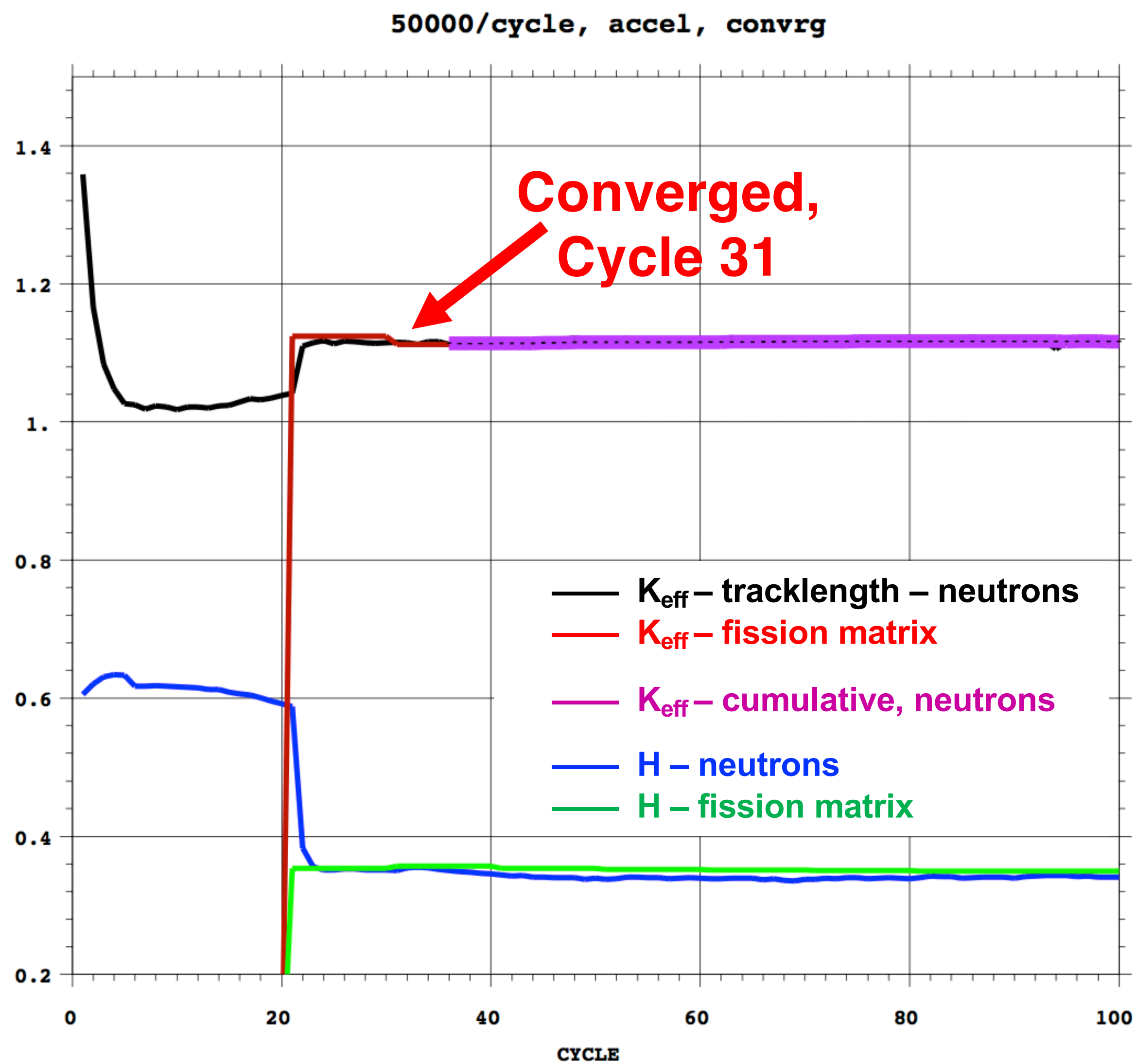


OECD-NEA Source Convergence Problem TEST4S

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

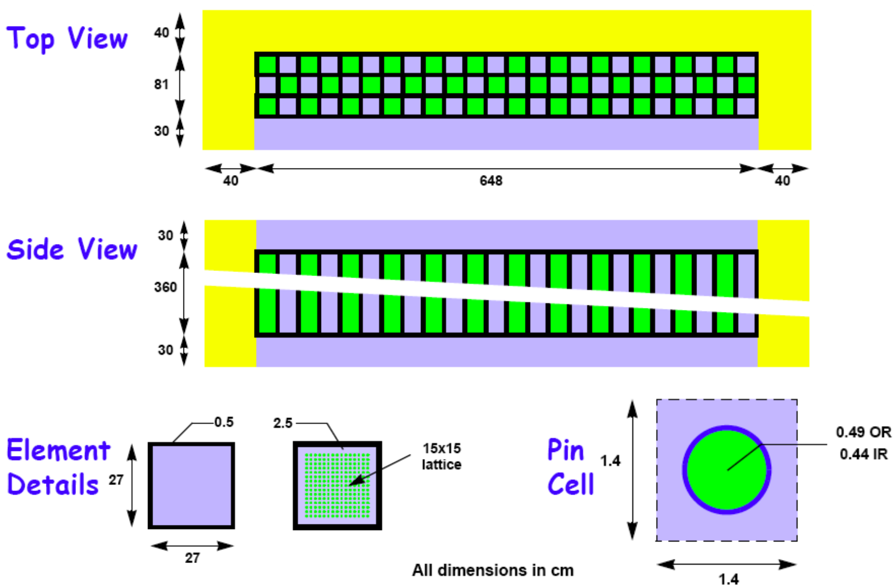




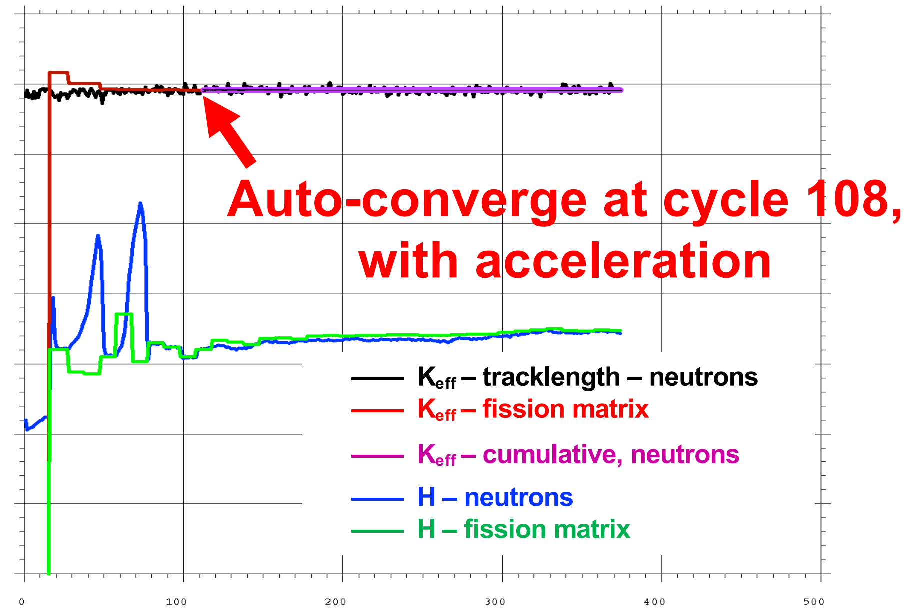
OECD-NEA Fuel Storage Pool

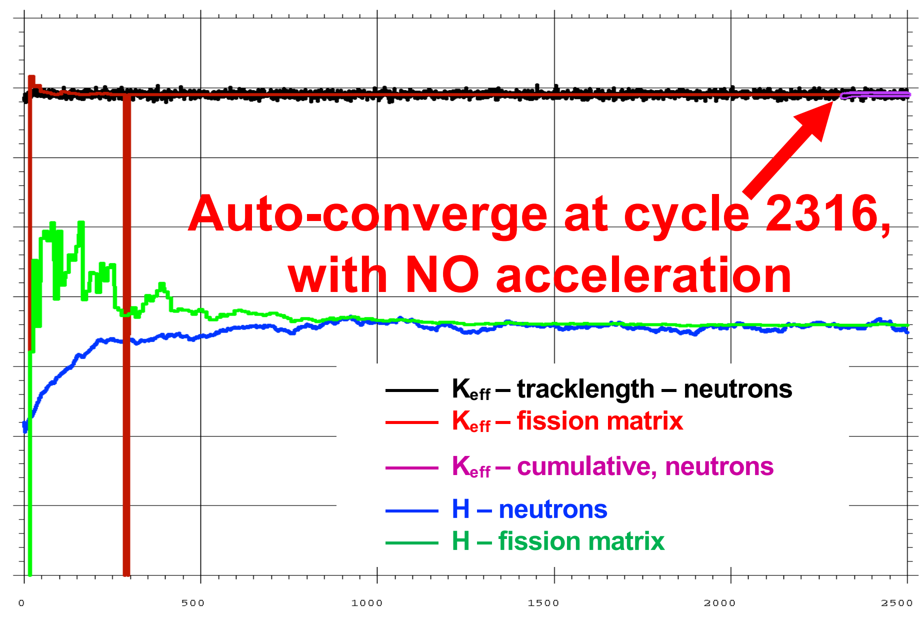
OECD-NEA-WPNCS Expert Group on Source Convergence

Benchmark 1



100k neuts/cycle





Current Work

- **2019**
  - **Limited release to NCS early adopters at DOE labs, more testing & feedback**
  - **General release with next MCNP6 distribution through RSICC, 202?**

- **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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