LA-UR-11-04820

Approved for public release;
distribution is unlimited.

Title: Coarse Mesh Finite Difference in MCNP

Author(s): Mitchell T. Young
Forrest B. Brown
Brian C. Kiedrowski
William R. Martin

Intended for: MCNP Documentation

Coarse Mesh Finite Difference in MCNP

Mitchell T.H. Young   Forrest Brown   Brian Kiedrowski
William Martin

August 15, 2011

Lee, et. al.[2] [3] have demonstrated the feasibility of applying a Coarse Mesh Finite Difference (CMFD) acceleration technique to accelerate fission source distribution (FSD) convergence in monte carlo criticality calculations. Most of this work has been done in 1- and 2-D with multigroup monte carlo. In this work, a CMFD solver has been implemented in MCNP to facilitate FSD acceleration in 3-D with continuous-energy cross sections for more general applications. Promising results have been obtained for full-core reactor simulations.

CMFD is based upon diffusion theory, represented (1-D) by the equation

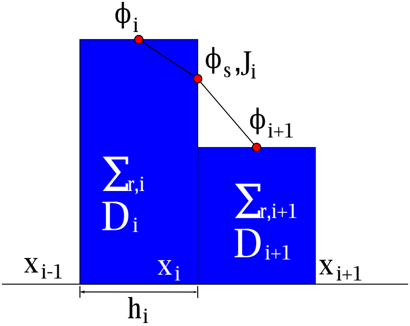
$$-D\nabla\phi(x) + \Sigma_a(x)\phi(x) = \frac{1}{k}\nu\Sigma_f(x)\phi(x). \tag{1}$$

Fick's law is used to represent neutron current,

$$J = -D\frac{d\phi}{dx}. \tag{2}$$

Spatial discretization of the diffusion equation results in the Finite Difference Method (FDM).

"Box scheme" used for discretization



Solving for J_s from both sides:

$$J_{s,l} = \frac{-D_i(\phi_s - \phi_i)}{h_i/2}, \text{ and} \quad (3)$$

$$J_{s,r} = \frac{-D_{i+1}(\phi_{i+1} - \phi_s)}{h_{i+1}/2}. \quad (4)$$

$$\frac{-D_i(\phi_s - \phi_i)}{h_i/2} = \frac{-D_{i+1}(\phi_{i+1} - \phi_s)}{h_{i+1}/2} \quad (5)$$

Solving for ϕ_s [1]:

$$\phi_s = \frac{\frac{D_i}{h_i}\phi_i + \frac{D_{i+1}}{h_{i+1}}\phi_{i+1}}{\frac{D_i}{h_i} + \frac{D_{i+1}}{h_{i+1}}}. \quad (6)$$

Defining *relative diffusivity*, $\beta_i = \frac{D_i}{h_i}$,

$$\phi_s = \frac{\beta_i \phi_i + \beta_{i+1}\phi_{i+1}}{\beta_i + \beta_{i+1}}. \tag{7}$$

Plug back into the current equation, (5) and after some goofy algebra,

$$J_i = -\frac{2\beta_i \beta_{i+1}}{\beta_i + \beta_{i+1}}(\phi_{i+1} - \phi_i). \tag{8}$$

Coupling Coefficient

$$\tilde{D}_i = \frac{2\beta_i \beta_{i+1}}{\beta_i + \beta_{i+1}} \tag{9}$$

Our current equation for surface i is now

$$J_i = -\tilde{D}_i(\phi_{i+1} - \phi_i) \tag{10}$$

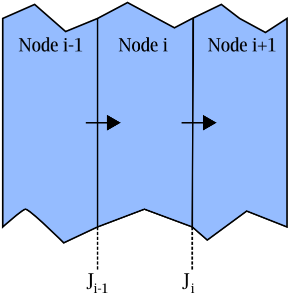
The interface current from a higher-order solution is now preserved by applying following correction

$$J_i = -\tilde{D}_i(\phi_{i+1} - \phi_i) + \hat{D}_i(\phi_i + \phi_{i+1}). \quad (11)$$

Given the higher-order solution for ϕ and J, $\hat{D}$ can be obtained easily,

$$\hat{D}_i = \frac{J_i + \tilde{D}_i(\phi_{i+1} - \phi_i)}{\phi_{i+1} + \phi_i}. \quad (12)$$

Multigroup neutron balance equation in 1D



Fission source:

$$F_g^i = h_i \chi_g^i \frac{1}{k} \sum_{g \in G} \nu \Sigma_{fg}^i \phi_g^i \qquad (13)$$

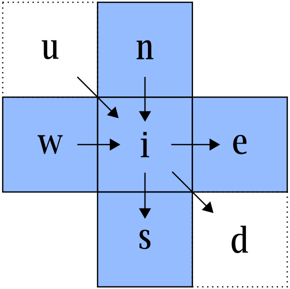
Scattering source:

$$S_g^i = h_i \sum_{g' \neq g} \Sigma_{sg'g}^i \phi_{g'}^i \qquad (14)$$

$$J_g^i + \Sigma_{rg}^i \phi_g^i = J_g^{i-1} + F_g^i + S_g^i \qquad (15)$$

$$\phi_g^{i-1}(-\tilde{D}_g^{i-1} - \hat{D}_g^{i-1}) + \phi_g^i(h_i \Sigma_{r,g}^i + \tilde{D}_g^{i-1} + \tilde{D}_g^i + \hat{D}_g^i - \hat{D}_g^{i-1}) + \phi_g^{i+1}(-\tilde{D}_g^i + \hat{D}_g^i) = S_g^i + F_g^i \qquad (16)$$

Extending balance equation to 3D



Current direction conventions:

- west→ east
- north→ south
- top→ bottom

Most terms remain the same except:

- Use volume for source terms,
- four more current-based coupling terms, and
- interface area must be included in node coupling.

3D Balance Equation for node i, group g

$$\phi_g^w A_x(-\tilde{D}_g^w - \hat{D}_g^w) + \phi_g^e A_x(-\tilde{D}_g^e + \hat{D}_g^e) + \phi_g^i A_x(\tilde{D}_g^w + \tilde{D}_g^e + \hat{D}_g^e - \hat{D}_g^w) +$$
$$\phi_g^n A_y(-\tilde{D}_g^n - \hat{D}_g^n) + \phi_g^s A_y(-\tilde{D}_g^s + \hat{D}_g^s) + \phi_g^i A_y(\tilde{D}_g^n + \tilde{D}_g^s + \hat{D}_g^s - \hat{D}_g^n) +$$
$$\phi_g^u A_z(-\tilde{D}_g^u - \hat{D}_g^u) + \phi_g^d A_z(-\tilde{D}_g^d + \hat{D}_g^d) + \phi_g^i A_z(\tilde{D}_g^u + \tilde{D}_g^d + \hat{D}_g^d - \hat{D}_g^u) +$$
$$V_i \phi_g^i \Sigma_{r,g}^i = S_g^i + F_g^i \quad (17)$$

$$F_g^i = V_i \chi_g^i \frac{1}{k} \sum_{g \in G} \nu \Sigma_{fg}^i \phi_g^i \quad (18)$$

$$S_g^i = V_i \sum_{g' \neq g} \Sigma_{sg'g}^i \phi_{g'}^i \quad (19)$$

- The previous balance equation is formed for each mesh region, forming a large system of linear equations.
- Power method is applied directly to the system

$$\mathbf{M}\phi = (\lambda\mathbf{F} + \mathbf{S})\,\phi \tag{20}$$

to find the eigenvalue, $\lambda = 1/k$.
- The **F** and **S** matrices contain the fission and scattering sources.
- The *migration matrix*, **M** contains the LHS of Eq. (17).
- ϕ is a vector caintaining the flux in each node/group.

- To solve the CMFD equations we need
  - fluxes ϕ,
  - partial currents J,
  - diffusion coefficients D,
  - removal cross sections Σ_r,
  - scattering cross sections $\Sigma_{sg'g}$,
  - fission neutron production cross section $\nu\Sigma_f$.
- Scalar flux is obtained with a normal FMESH tally.
- Partial currents are tallied using a modified FMESH.
- Basic cross sections are obtained using tally multipliers for the interation(s) of interest and forming the ratio

$$\Sigma = \frac{\text{reaction tally}}{\text{flux tally}}. \tag{21}$$

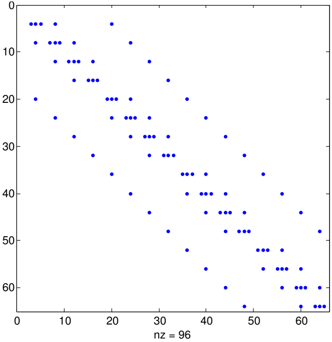
- Diffusion coefficients are calculated as $1/3\Sigma_t$.

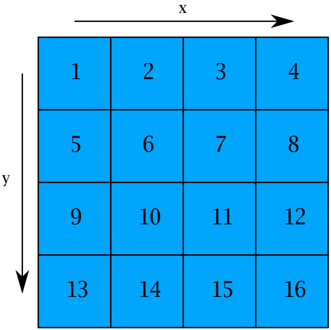
- For general multigroup calculations, a full scattering matrix $\Sigma_S[g', g]$ would be needed.
- A two-group calculation is used instead, such that Σ_{s12} can be calculated from the group 2 balance equation,

$$\Sigma_{s12}\phi_1 = \Sigma_{a2}\phi_2 + J^{+}_{net,2} - J^{-}_{net,2}. \tag{22}$$

- Typically, $\Sigma_{rg} \equiv \Sigma_t g - \Sigma_{sgg}$. In the absence of Σ_{sgg}
  - $\Sigma_r 1 = \Sigma_{a1} + \Sigma_{s12}$ and
  - $\Sigma_r 2 = \Sigma_{a2}$.

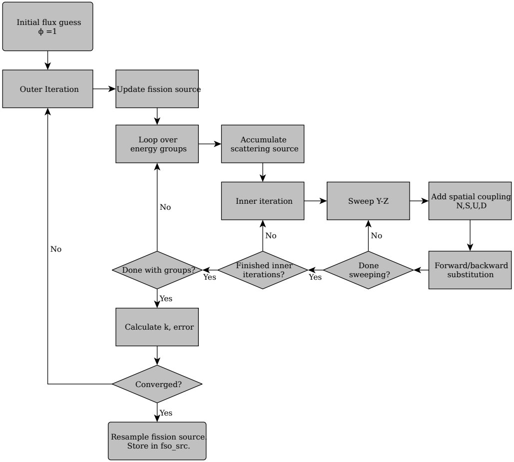
- Nodes arranged in a "natural ordering" scheme. The Migration matrix assumes the form below.
- Matrices and flux vector sorted with group-major scheme.
    - Energy group is major sort index.
    - Nodes sorted within each energy group.





$$\phi = \begin{bmatrix} \vdots \\ \begin{bmatrix} \vdots \\ \phi^{i-1} \\ \phi^{i} \\ \phi^{i+1} \\ \vdots \end{bmatrix}_{g-1} \\ \begin{bmatrix} \vdots \\ \phi^{i-1} \\ \phi^{i} \\ \phi^{i+1} \\ \vdots \end{bmatrix}_{g} \\ \begin{bmatrix} \vdots \\ \phi^{i-1} \\ \phi^{i} \\ \phi^{i+1} \\ \vdots \end{bmatrix}_{g+1} \\ \vdots \end{bmatrix}$$

- Outer iterations are used to update fission and scattering sources.
- Gauss-Seidel method is used to solve fixed-source, single-group system.
  - Four outer bands (n,s,u,d coupling) of **M** subtracted to LHS.
  - Previous estimate of flux is used for these couplings.
  - Several *inner iterations* are required to achieve convergence within outer iterations.
  - The remaining RHS (tridiagonal matrix) represents a series of strips along x-axis.
  - Each strip is solved directly using LU decomposition and forward-backward substitution.


Initial flux guess
ϕ =1
Outer Iteration
Update fission source
Loop over
energy groups
Accumulate
scattering source
Inner iteration
Sweep Y-Z
Add spatial coupling
N,S,U,D
Forward/backward
substitution
Done
sweeping?
Finished inner
iterations?
Done with groups?
No
No
No
No
Yes
Yes
Yes
Calculate k, error
Converged?
Yes
Resample fission source.
Store in fso_src.

- New fission source distribution (FSD) must now be given to MCNP for the next cycle.
- Existing fission bank points are used.
- Based on the FSD obtained from CMFD, points in some regions are drawn more preferentially than others.
- The resultant fission bank is made up of points from the old fission bank, but with the corrected FSD.

- FMESH tallies must be added for the following:
  - Flux (no multiplier)
  - Total cross section
  - Absorption cross section (capture + fission)
  - Fission production ($\nu\Sigma_f$)
  - Partial current
- All meshes must have the same geometric properties.
- Mechanics of the current tally require a “halo” of ghost cells to obtain incoming current at the domain boundary.
- The meshes must be uniform in each direction.

Example FMESH definition:

```
C nu-Sigma_f
FMESH24:n GEOM=xyz
      ORIGIN=-203.49 -203.49 -211.8
      IMESH=203.49  IINTS=19 $ 17 active mesh regions $
      JMESH=203.49  JINTS=19 $ 17 active mesh regions $
      KMESH=201.800 KINTS=22 $ 20 active mesh regions $
      EMESH=1.e-6 20.0 EINTS=1 1 $ 2-group structure $
FM24  -1.0 0 -6 -7
```

Table: Magic numbers and FM cards for each FMESH tally. Interaction numbers assume continuous energy.

Interaction	FMESH Number	FM Card[4]
Partial current	1[a]	None
Flux	4	None
Total	14	FM -1.0 0 -1
Absorption	34	FM -1.0 0 -2:-6
Fission	24	FM -1.0 0 -6 -7

[a] Any number ending in a 1 will result in a partial current tally.

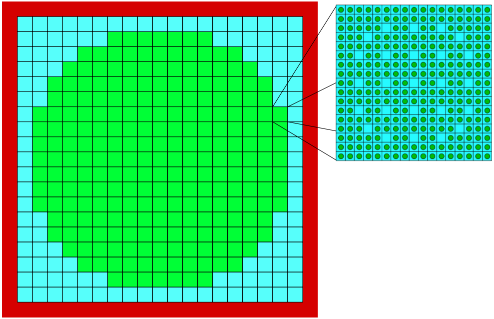
IDUM Array

The MCNP IDUM array is used to provide several inputs to the CMFD module:

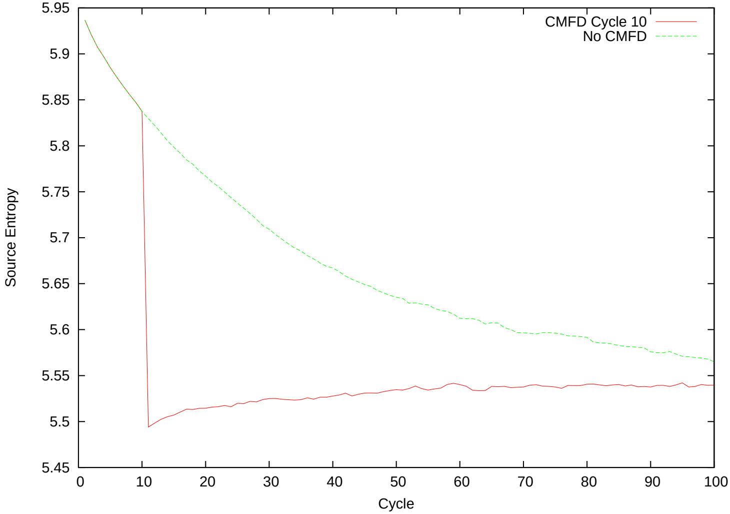
1. KCODE cycle at which to implement CMFD,
2. number of inner iterations per outer iteration, and
3. the maximum number of outer iterations allowed.

```
IDUM [cycle] [inner] [outer]
```

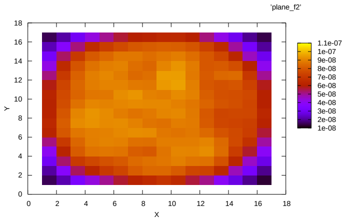
Problem



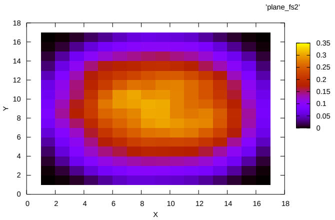
- Blue = Water
- Green = Core/Fuel
- Red = Reactor vessel


CMFD Cycle 10
No CMFD
Source Entropy
Cycle
5.95
5.9
5.85
5.8
5.75
5.7
5.65
5.6
5.55
5.5
5.45
0
10
20
30
40
50
60
70
80
90
100

Before CMFD



After CMFD



- Pure FDM shown to greatly accelerate convergence of FSD, though not perfectly accurate.
- Still some issues with CMFD correction.
- FDM solution tends to be close enough to significantly aid convergence.
- Discrete FSD sampling method results in over-concentrated FSD.

Future Work

- Investigate other FSD re-sampling methods to more accurately reproduce CMFD solution.
- Debug CMFD correction.
- Improve solver stability and error-handling capabilities.
- Thoroughly examine applicability of method to other problems types.

References

H. G. Joo.
Solution of one-dimensional, one-group neutron diffusion equation.
NERS 561 Lecture Notes. University of Michigan., 2011.

Min-Jae Lee, Han Gyu Joo, Deokjung Lee, and Kord Smith.
Investigation of cmfd accelerated monte carlo eigenvalue calculationi with simplified low dimensional multigroup formulation.
PHYSOR, 2010.

Min-Jae Lee, Han Gyu Joo, Deokjung Lee, and Kord Smith.
Multigroup monte carlo reactor calculation with coarse mesh finite difference formulation for real variance reduction.
Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo, 2010.

X-5 Monte Carlo Team.
MCNP A General Monte Carlo N-Particle Transport Code, Version 5 Volume II: Users Guide.
Los Alamos National Laboratory, LA-CP-03-0245, February 2008.

Questions?