Hybrid Monte-Carlo Deterministic Algorithms for Neutron Transport

C. T. Kelley, Jeff Willert, Dana Knoll,
NC State University
tim_kelley@ncsu.edu

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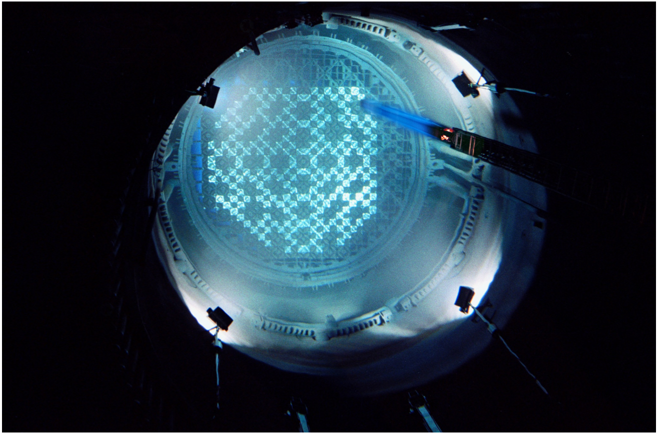
Outline

Region of Interest: Heterogeneous



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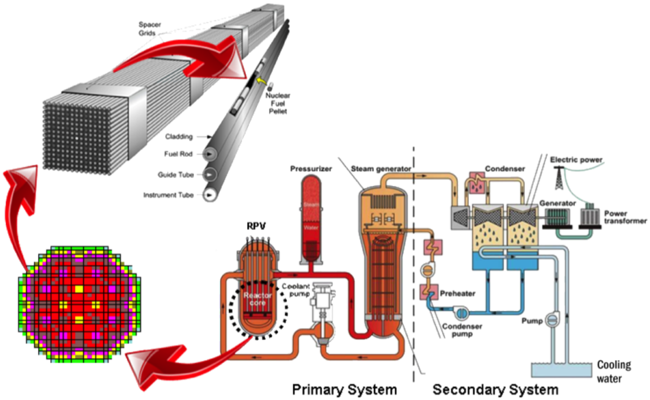
Region of Interest II



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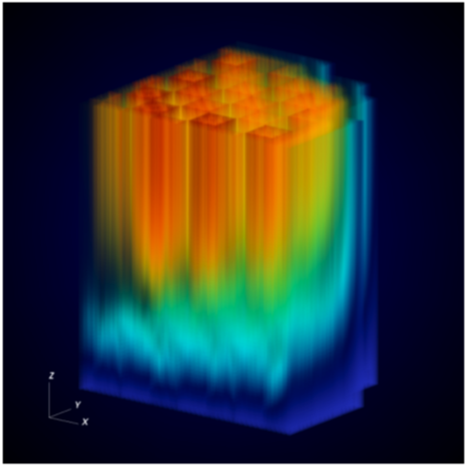
Quarter Core



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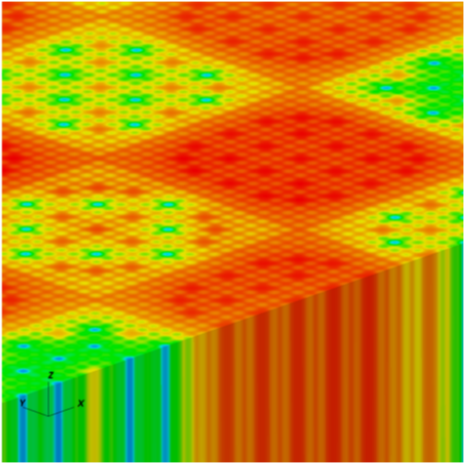
Fuel Assembly



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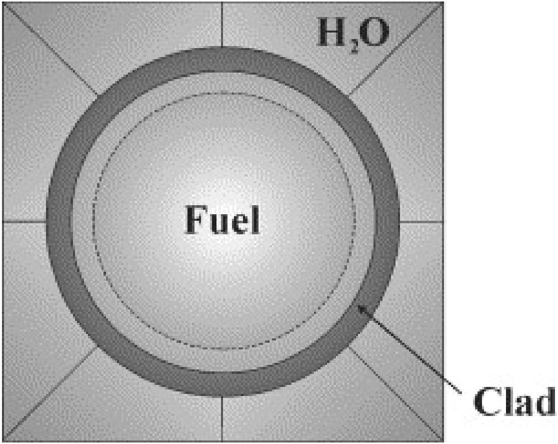
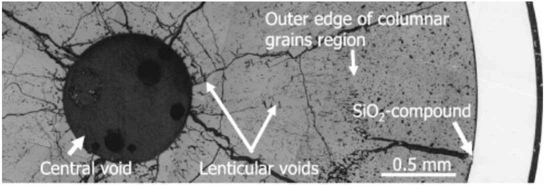
Fuel Pin Cross Section (New)

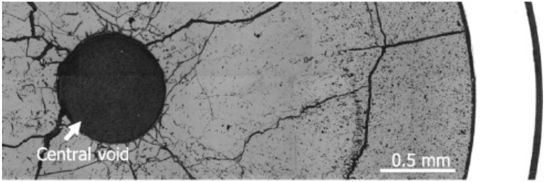


From Maeda et al (2009)

Fuel Pin Cross Section (OLD)



(a) $(Am,Pu,Np,U)O_{2-x}$ (z/L=0.50)



(b) MOX (z/L=0.74)

From Núñez-Carrera et al (2004)

Neutron Transport Equation: Ia

Notation:

- $D \subset R^3$, $r = (x, y, z)^T \in D$
- $\hat{\Omega} \in S^2$
- $\psi(r, E, \hat{\Omega})$ angular flux of Neutrons at r in direction $\hat{\Omega}$ with energy $E \geq 0$.

Boundary conditions on incoming flux.

Neutron Transport Equation: Ib

This is a high-dimensional problem:

- One space dimension is 3D (space+direction+energy)
- Two space dimensions is 4D (space+$\times$ direction+energy)
- Three space dimensions is 6D (space+2 $\times$ direction+energy)

Why does one space dimension lead to a continuum of directions? Stay tuned.

Neutron Transport Equation: II

Simplifications: round 1

- No time dependence.
  Solve time-independent problems to integrate in time.
- Neglect fission sources.
  Methods don't change much if we put them in.

Neutron Transport Equation: III

$$\hat{\Omega} \cdot \nabla \psi(r, E, \hat{\Omega}) + \Sigma_t(r, E)\psi(r, E, \hat{\Omega})$$

$$= \frac{1}{4\pi} \int_{S^2} d\hat{\Omega}' \int_0^\infty dE' \Sigma_s(r, E' \to E, \hat{\Omega}' \to \hat{\Omega})\psi(r, E', \hat{\Omega}')$$

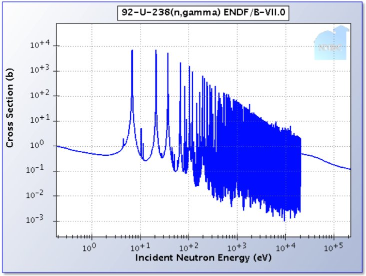
$$+q(r, E, \hat{\Omega})/4\pi,$$

Quantity of interest: scalar flux

$$\phi(r, E) = \frac{1}{4\pi} \int_{S^2} \psi(r, E, \hat{\Omega}')d\hat{\Omega}'$$

Neutron Transport Equation: III

Σ_t and Σ_s are transmission and scattering cross sections.
They are ugly!



From CASL Image Gallery

Solution Methods: two of many

- S^N: Faster and easier to analyze
  - quadrature in angle,
  - differences/elements/volumes in space,
  - piecewise constant in Energy (multi-group approximation).
  - Solve with standard linear (or nonlinear!!) solvers.
- Monte-Carlo (MC): Slower with better results
  - Let many neutrons randomly scatter via scattering/energy cross sections
  - Accumulate fluxes (and other angular moments) at the end.

More Simplification

This is too much, so we simplify again to

- Monoenergetic (no E)
- Isotropic (no $\hat{\Omega}' \rightarrow \hat{\Omega}$)
- One space dimension

You can learn a lot from even this simple case.

1-D Model Problem: version 1

$$\mu \frac{\partial \psi}{\partial r}(r, \mu) + \Sigma_t \psi(r, \mu) = \frac{\Sigma_s}{2} \int_{-1}^{1} \psi(r, \mu')\, d\mu' + q(r)/2$$

Change variables:

$$c(x) = \Sigma_s(r)/\Sigma_t(r) \text{ and } r = \int_0^x \Sigma_t(\xi)^{-1} d\xi$$

and you get

1-D Model Problem: version 2

$$\mu \frac{\partial \psi}{\partial x}(x,\mu) + \psi(x,\mu) = \frac{c(x)}{2} \int_{-1}^{1} \psi(x,\mu')\, d\mu' + q(x)/2,$$

Boundary Conditions:

$$\psi(0,\mu) = \psi_l(\mu), \mu > 0; \psi(\tau,\mu) = \psi_r(\mu), \mu < 0.$$

Quantity of interest: $\phi(x) = \int_{-1}^{1} \psi(x,\mu')\, d\mu'$

Nonlinear Diffusion Acceleration (NDA): Step 1

Nonlinear compact fixed point problem for ϕ.
Transport sweep: Given input ϕ^{LO}, solve the high-order problem

$$\mu \frac{\partial \psi}{\partial x}(x, \mu) + \psi(x, \mu) = \frac{c(x)}{2} \phi^{LO}(x) + q(x)/2$$

Then compute the high-order flux

$$\phi^{HO}(x) = \int_{-1}^{1} \psi(x, \mu') \, d\mu'$$

and current

$$J^{HO}(x) = \int_{-1}^{1} \mu' \psi(x, \mu') \, d\mu'$$

Nonlinear Diffusion Acceleration (NDA): Step 2

Define

$$\hat{D} = \frac{J^{HO} + \frac{1}{3}\frac{d\phi^{HO}}{dx}}{\phi^{HO}}.$$

The low-order nonlinear equation for ϕ^{LO} is $\mathcal{F}(\phi^{LO}) = 0$, where

$$\mathcal{F}(\phi) = \frac{d}{dx}\left[\frac{-1}{3}\frac{d\phi}{dx}\right] + (1-c)\,\phi + \frac{d}{dx}\left[\hat{D}(\phi^{HO}, J^{HO})\phi\right]$$

with boundary conditions $\phi^{LO} = \phi^{HO}$.
Equivalent to original formulation!

Preconditioner

Preconditioner inverts

$$Lw = \frac{d}{dx}\left[\frac{-1}{3}\frac{dw}{dx}\right] + (1-c)\,w + \hat{D}(\phi^{HO}, J^{HO})\frac{dw}{dx}$$

with correct boundary conditions to obtain

$$F(\phi) = \mathcal{F}(L^{-1}\phi) = 0.$$

This is a compact fixed point problem.

Compactness

$I - F'$ is compact, and so

- F' is well conditioned for all spatial grids.
- Krylov methods like GMRES perform well when solving

$$F'(\phi)s = -F(\phi)$$

- Computation is mathematically scalable, ie Krylovs/Newton is independent of mesh width.

NDA Hybrid Method

- Solve the high-order problem with Monte Carlo for ϕ and J
  - better results + higher cost
  - BUT we are asking MC to solve a scattering-free problem
- Solve the low-order problem in a standard way
- Resolve a few details

Abstract Formulation

We seek to solve a nonlinear equation

$$F(\phi) = 0$$

where F has the decomposition

$$F(\phi) = G(A\phi + Q)$$

where A is linear and Q is known.
Motivation: ϕ^{HO} and J^{HO} are affine functions of ϕ^{LO}

Facts of Interest

- A and Q may come from a Monte Carlo simulation
- The MC simulation of $A\phi$ requires $\phi \geq 0$ componentwise.
- Matrix-vector product with A is the expensive part.
- The action of G' on a vector is cheap.
- F' (in exact arithmetic) is very well conditioned.

Newton-GMRES solver

Solve linear equation for Newton step with GMRES. All we need is a Jacobian-vector proeuct:
Deterministic Mat-Vec for A:

$$F'(\phi)v = G'(A\phi + Q)Av$$

MC Mat-Vec: As above but define Av if v is not nonnegative by

$$Av \equiv A(\|v\|_\infty \mathbf{1} + v) - A(\|v\|_\infty \mathbf{1})$$

where $\mathbf{1} = (1, 1, \ldots, 1)^T$.
A finite-difference Jacobian is a very poor idea in this case.

Newton-Iterative Algorithm

knl(x, F, τ_a, τ_r)

evaluate $F(x)$; $\tau \leftarrow \tau_r|F(x)| + \tau_a$.
while $\|F(x)\| > \tau$ **do**
Find d such that $\|F'(x)d + F(x)\| \leq \eta\|F(x)\|$
If no such d can be found, terminate with failure.
$\lambda = 1$
while $\|F(x + \lambda d)\| > (1 - \alpha\lambda)\|F(x)\|$ **do**
$\lambda \leftarrow \sigma\lambda$ where $\sigma \in [1/10, 1/2]$ is computed by minimizing a polynomial model of $\|F(x_n + \lambda d)\|^2$.
end while
$x \leftarrow x + \lambda d$
end while

Modifications for Hybrid Method

The inexact Newton condition (INC)

$$\|F'(x)d + F(x)\| \leq \eta \|F(x)\|$$

and the sufficient decrease condition (SDC)

$$\|F(x + \lambda d)\| \leq (1 - \alpha\lambda)\|F(x)\|$$

may fail.
Such failures signal that the MC error is dominating the function/Jacobian evaluations.

Quantifying MC Error

Approximate F by

$$F(\phi, N_{MC}) \approx F(\phi)$$

where N_{MC} is the number of trials within the MC.
If INC or SDC fail, either accept the results or increase N_{MC}.

Hybrid Solver

Evaluate $R_{MC} = F(u, N_{MC})$; $\tau \leftarrow \tau_r \|R_{MC}\| + \tau_a$.
while $\|R_{MC}\| > \tau$ **do**
  Use GMRES with a limit of I_{max} iterations to get INC
  if INC fails **then**
    $N_{MC} \leftarrow 100 * N_{MC}$; Evaluate $R_{MC} = F(u, N_{MC})$
  else
    $\lambda = 1$; Evaluate $R_{Trial} = F(u + \lambda d, N_{MC})$
    while $\|R_{Trial}\| > (1 - \alpha\lambda)\|R_{MC}\|$ and $\lambda \geq \lambda_{min}$ **do**
      Reduce λ and evaluate $R_{Trial} = F(u + \lambda d, N_{MC})$
    end while
    if $\lambda \geq \lambda_{min}$ **then**
      $u \leftarrow u + \lambda d$; $R_{MC} = R_{Trial}$
    else
      $N_{MC} \leftarrow 100 * N_{MC}$; Evaluate $R_{MC} = F(u, N_{MC})$
    end if
  end if
end while

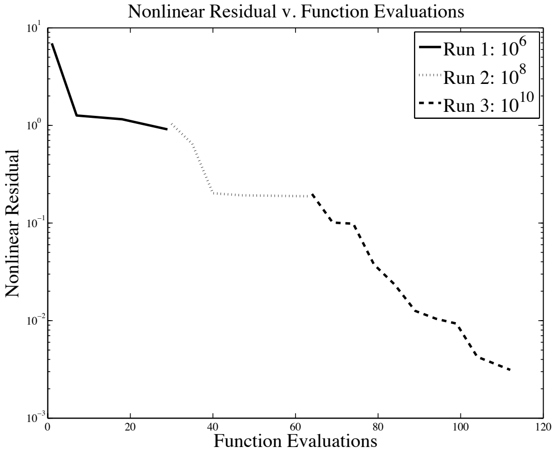
Sample Problem I

Phyiscal parameters:

$$c = .99; \tau = 10; q = .5;$$

$$N_{MC} = 10^6, 10^8, 10^{10}$$

Iteration History



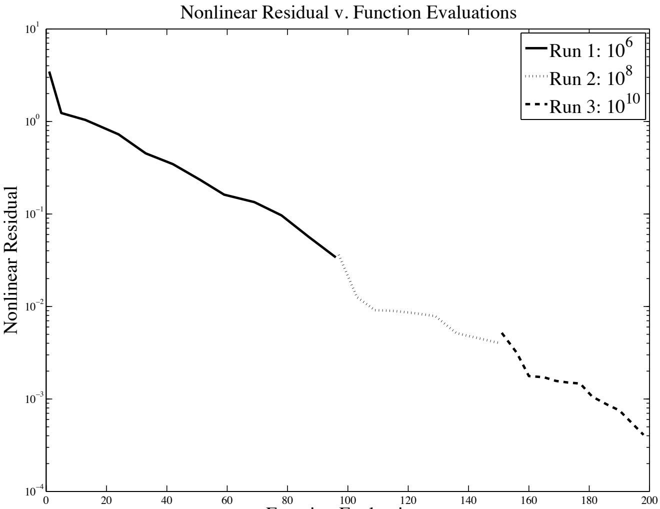
Sample Problem II: Slower convergence

Phyiscal parameters:

$$c = .99; \tau = 100; q = .5;$$

$$N_{MC} = 10^6, 10^8, 10^{10}$$

Iteration History



Conclusions

- Noisy nonlinear equations.
- Application: neutron transport
- Deterministic/MC Hybrid.