On the Accuracy of the Differential Operator Monte Carlo Perturbation Method for Eigenvalue Problems

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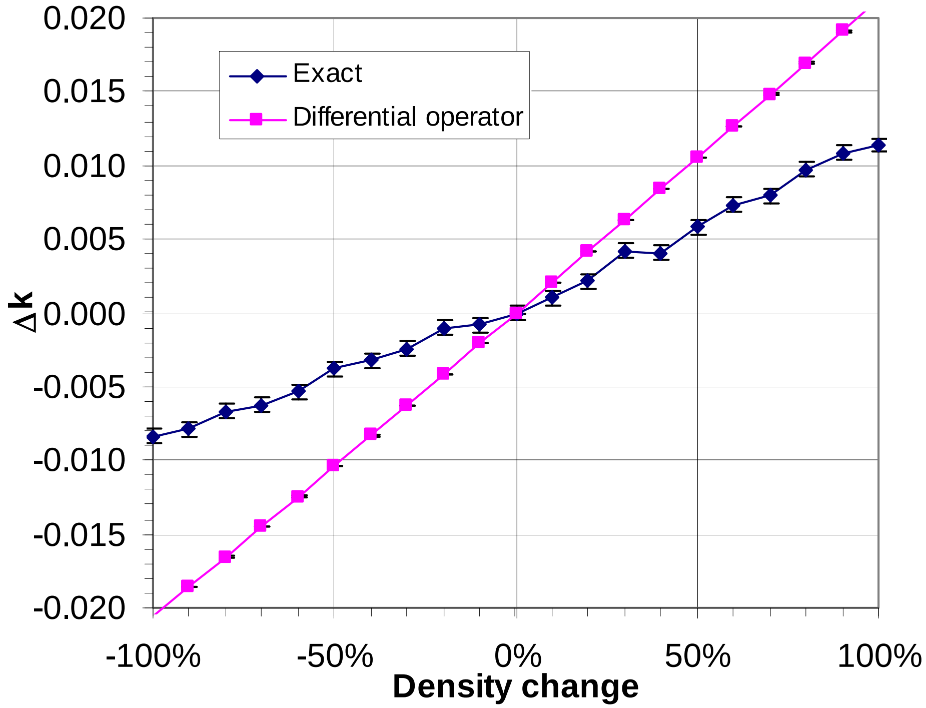
Introduction

- Many studies have pointed out the inaccuracy of the differential operator Monte Carlo perturbation method for k_{eff} eigenvalue problems.

Example: Density change in outer 0.1-cm shell of 8.741-cm radius HEU sphere:



- The standard implementation of the differential operator method (as in MCNP) assumes that the fission source distribution is unperturbed.

  + This talk discusses the mathematical implications of that assumption.
  + This problem is unrelated to the number of Taylor terms retained in the expansion.

- Recently, it has been observed that k_{eff} sensitivities were more accurate for capture and fission cross sections than for scattering.

  + Conclusion: Perturbations to the scattering cross section affect the fission source distribution more than perturbations to the capture cross section do.

The k_{eff} Eigenvalue Equation

- The one-group k_{eff} eigenvalue equation, isotropic scattering:

$$\hat{\mathbf{\Omega}} \cdot \vec{\nabla}\, \psi(r,\hat{\mathbf{\Omega}}) + \Sigma_t(r)\psi(r,\hat{\mathbf{\Omega}}) - \Sigma_s(r)\phi(r) = \frac{1}{k_{eff}} \nu\Sigma_f(r)\phi(r).$$

Scalar flux: $\phi(r) \equiv \int_{4\pi} d\hat{\mathbf{\Omega}}\, \psi(r,\hat{\mathbf{\Omega}})$

Total cross section: $\Sigma_t(r) = \Sigma_c(r) + \Sigma_f(r) + \Sigma_s(r).$

- Define $S(r) \equiv \nu\Sigma_f(r)\phi(r).$

- Let the flux be normalized to $\int dV\, \nu\Sigma_f(r)\phi(r) = k_{eff}.$

- The inhomogeneous equation

$$\hat{\mathbf{\Omega}} \cdot \vec{\nabla}\, \psi(r,\hat{\mathbf{\Omega}}) + \Sigma_t(r)\psi(r,\hat{\mathbf{\Omega}}) - \Sigma_s(r)\phi(r) = S(r)$$

has the same solution as the homogeneous equation, and this solution satisfies the normalization.

- These concepts are not specific to any code or solution method.

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$$L\,\psi(r,\hat{\mathbf{\Omega}}) = \frac{1}{k_{eff}}\nu\Sigma_f(r)\phi(r)$$

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Notation for Perturbation Theory

- The initial, unperturbed configuration is denoted with a subscript 0:

$$L_0\psi_0(r,\hat{\mathbf{\Omega}}) = \frac{1}{k_{eff,0}}\nu\Sigma_{f,0}(r)\phi_0(r), \text{ or}$$

$$L_0\psi_0(r,\hat{\mathbf{\Omega}}) = S_0(r),$$

with

$$k_{eff,0} = \int dV\, \nu\Sigma_{f,0}(r)\phi_0(r).$$

- The perturbed configuration is denoted with a prime:

$$L'\psi'(r,\hat{\mathbf{\Omega}}) = \frac{1}{k_{eff}}\nu\Sigma'_f(r)\phi'(r), \text{ or}$$

$$L'\psi'(r,\hat{\mathbf{\Omega}}) = S'(r),$$

with

$$k'_{eff} = \int dV\, \nu\Sigma'_f(r)\phi'(r).$$

- The perturbation in k_{eff} is

$$\Delta k_{eff} = k'_{eff} - k_{eff,0} = \int dV\, \nu\Sigma'_f(r)\phi'(r) - \int dV\, \nu\Sigma_{f,0}(r)\phi_0(r).$$

The Power Series Solution Method

- The standard power series method of solving the eigenvalue problem with Monte Carlo:
  - Start with a guess for the fission source distribution $S(r)$.
  - Simulate the transport process, saving new fission source points and scoring k_{eff} for information.
  - Use the new collection of fission source points as $S(r)$ in the next iteration.
  - Repeat until the fission source converges.
  - (+ Aside: How do you know if the fission source converges? Until recently, you guess, using cycle-by-cycle k_{eff}.)
  - Once the fission source converges, continue as before, but collect k_{eff} and tallies for real.

- This process essentially solves $L\psi(r,\hat{\boldsymbol{\Omega}}) = S(r)$, a fixed-source problem, in each cycle.

- The differential operator method attempts to estimate the effect of the perturbed transport operator on k_{eff} and tallies in active cycles.

Putting It All Together

- **warning: fundamental eigenfunction (fission distribution) approximated as unperturbed.**

- The differential operator method uses the unperturbed source but the perturbed transport operator, estimating the solution to

$$L'\tilde{\psi}(r,\hat{\mathbf{\Omega}}) = S_0(r)$$

and using it in

$$\Delta k_{eff,DO} = \int dV\, \nu\Sigma'_f(r)\tilde{\phi}(r) - \int dV\, \nu\Sigma_{f,0}(r)\phi_0(r).$$

- The accuracy of the differential operator method is affected not only by whether $S_0(r)$ is a good approximation of $S'(r)$, but also by whether $\tilde{\phi}(r)$ is a good approximation of $\phi'(r)$.

Relating to Deterministic Perturbation Methods

- In deterministic perturbation theory, “ignoring the effect of the perturbation on the flux distribution” leads from the exact expression for the eigenvalue difference

$$\Delta\lambda = \frac{1}{k'_{eff}} - \frac{1}{k_{eff,0}} = \frac{\left\langle \psi_0^*, \left(\Delta L - \frac{1}{k_0}\Delta F \right)\psi' \right\rangle}{\left\langle \psi_0^*, F'\psi' \right\rangle}$$

to the approximation

$$\Delta\lambda_{1\mathrm{st}} = \frac{\left\langle \psi_0^*, \left(\Delta L - \frac{1}{k_0}\Delta F \right)\psi_0 \right\rangle}{\left\langle \psi_0^*, F'\psi_0 \right\rangle}.$$

- In the differential operator method, “ignoring the effect of the perturbation on the fission source distribution” leads from

$$\Delta k_{eff} = k'_{eff} - k_{eff,0} = \int dV\, \nu\Sigma'_f \phi' - \int dV\, \nu\Sigma_{f,0}\phi_0$$

to the approximation

$$\Delta k_{eff,DO} = \int dV\, \nu\Sigma'_f \tilde{\phi} - \int dV\, \nu\Sigma_{f,0}\phi_0.$$

Test Problem

- One group, spherical, two regions, fuel (radius 6.12745 cm) surrounded by reflector (thickness 3.063725 cm). Analytic $k_{eff,0} = 1$. PARTISN S_{64} $k_{eff,0} = 1.0000128$.

- Results for fuel capture and fuel scattering cross-section perturbations (independent):

Exact Δk_{eff} → ($k'_{eff} - k_{eff,0}$)

	Σ_c Pert. (–20%)	Σ_s Pert. (+5%)	Calc. Type
k'_{eff}	1.0130141	1.0069433	Deterministic
$\widetilde{k}$	1.0132118	1.0060818	Deterministic
$k'_{eff} - k_{eff,0}$	0.0130013	0.0069305	Deterministic
$\widetilde{k} - k_{eff,0}$	0.0131990	0.0060690	Deterministic
Error	1.52%	–12.43%	N/A
$\Delta k_{eff,DO}$	0.0131810 ± 0.01%	0.0060493 ± 0.12%	Stochastic
Error	1.38%	–12.71%	N/A

- k_{eff} is much more sensitive to the fuel scattering cross section than to the fuel capture cross section, since a 5% change in the former has about half the effect of a –20% change in the latter.

- Although the Σ_s perturbation is smaller than the Σ_c perturbation and has a smaller effect on k_{eff}, the differential operator method is much less accurate at predicting the effect.

- In both cases, the differential operator method very accurately estimates $\widetilde{k} - k_{eff,0}$.

Test Problem Fluxes

- Deterministic fluxes (differences are plotted; the maximum unperturbed flux is 9.745×10^{-3} cm^{-2}s^{-1}):

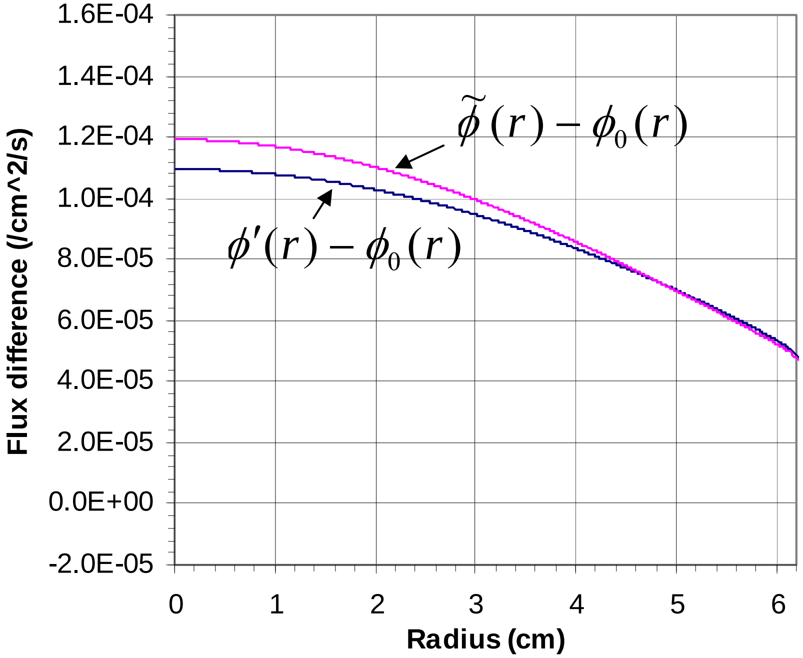

Fig. 1. Fluxes for the capture cross section perturbation.

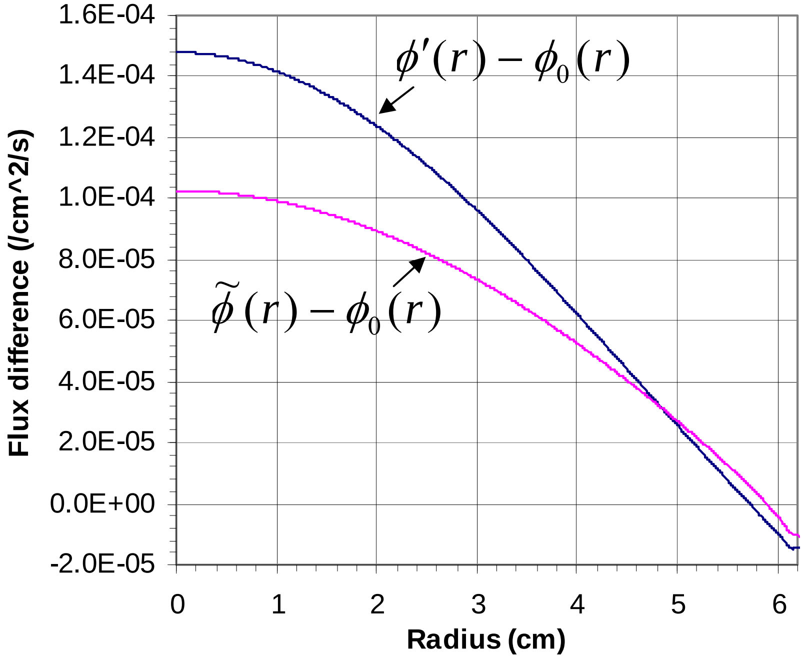

Fig. 2. Fluxes for the scattering cross section perturbation.

- ϕ_0 more closely matches ϕ' (therefore S_0 more closely matches S') for the capture cross section perturbation than for the scattering cross section perturbation (the difference is flatter).
- $\tilde{\phi}$ more closely matches ϕ' for the capture cross section perturbation than for the scattering cross section perturbation.

Summary and Conclusions

- The differential operator method essentially solves the inhomogeneous transport equation with a perturbed transport operator and an unperturbed fission source and uses the resulting flux $\tilde{\phi}(r)$ to estimate Δk_{eff}.

- This conclusion is *suggested* by the consistency between the argument and the numerical results, but it is not *proven*.

- MCNP5 has more trouble estimating Δk_{eff} due to scattering cross section perturbations than capture cross section perturbations because $\tilde{\phi}(r)$ differs more significantly from $\phi'(r)$ when the scattering cross section is perturbed, even when the effect on Δk_{eff} is smaller.
  + However, in one test problem, the k_{eff} sensitivity to $S(\alpha,\beta)$ matched the TSUNAMI-3D result.

- It would be more accurate to use the usual "deterministic" first-order perturbation formula, as does TSUNAMI-3D:
  + $$\Delta\lambda_{1st} = \frac{\left\langle \psi_0^*, \left(\Delta L - \frac{1}{k_0}\Delta F \right)\psi_0 \right\rangle}{\left\langle \psi_0^*, F'\psi_0 \right\rangle}.$$

See Brian Kiedrowski, "Estimating Reactivity Changes from Material Substitutions with Continuous-Energy Monte Carlo," Wednesday morning.

Results: One-Group k_{eff} Test Problem

- A homogeneous spherical fuel region (radius 6.12745 cm) surrounded by a spherical reflector shell (thickness 3.063725 cm).

- "Exact" derivatives were calculated with direct k_{eff} calculations using data libraries with perturbed cross sections (±10% and ±20%), and fitting the results with a line.

- Results:

		Direct	PERT Estimate	Difference Rel. to Direct
Fuel	S_{k_{eff},σ_t}	0.75801 ± 0.040%	0.73178 ± 0.088%	–3.460%
	S_{k_{eff},σ_f}	0.68296 ± 0.044%	0.67463 ± 0.024%	–1.219%
	S_{k_{eff},σ_c}	–0.06416 ± 0.461%	–0.06507 ± 0.063%	1.417%
	S_{k_{eff},σ_s}	0.13917 ± 0.213%	0.12222 ± 0.516%	–12.178%
	S_{k_{eff},σ_t}, sum	0.75797 ± 0.068%	0.73178 ± 0.089%	–3.455%
Refl.	S_{k_{eff},σ_t}	0.10891 ± 0.275%	0.12381 ± 0.165%	13.676%
	S_{k_{eff},σ_c}	–0.01825 ± 1.641%	–0.02137 ± 0.155%	17.076%
	S_{k_{eff},σ_s}	0.12742 ± 0.229%	0.14517 ± 0.150%	13.931%
	S_{k_{eff},σ_t}, sum	0.10917 ± 0.383%	0.12381 ± 0.178%	13.405%

- The PERT estimate is accurate in the fuel, except for scattering, but not accurate in the reflector.

Results: One-Group *k* Test Problem

- Same geometry and materials; fixed source is the fission distribution; fission is treated as capture; quantity of interest is $k = \int dV\, \nu\Sigma_f(r)\phi(r)$.

- Results:

		Direct	PERT Estimate	Difference Rel. to Direct
Fuel	S_{k,σ_t}	0.73216 ± 0.124%	0.73162 ± 0.213%	–0.381%
	S_{k,σ_f}	0.67584 ± 0.134%	0.67561 ± 0.100%	–0.318%
	S_{k,σ_c}	–0.06498 ± 1.387%	–0.06518 ± 0.161%	0.312%
	S_{k,σ_s}	0.12117 ± 0.744%	0.12119 ± 1.128%	–0.002%
	S_{k,σ_t}, sum	0.73203 ± 0.213%	0.73162 ± 0.209%	–0.321%
Refl.	S_{k,σ_t}	0.12433 ± 0.723%	0.12330 ± 0.412%	–0.866%
	S_{k,σ_c}	–0.02133 ± 4.439%	–0.02128 ± 0.354%	5.029%
	S_{k,σ_s}	0.14524 ± 0.619%	0.14458 ± 0.379%	–0.467%
	S_{k,σ_t}, sum	0.12391 ± 1.018%	0.12330 ± 0.448%	–1.358%

- Conclusion: The inability to account for the perturbed fission source distribution leads to inaccurate perturbation estimates of the sensitivity.