DE LA RECHERCHE À L'INDUSTRIE

On the Ronen Method in simple 1D geometries

Derivation of accurate expressions for the current in the slab and in the curvilinear reference frames

Daniele Tomatis
CEA SERMA, France (daniele.tomatis@cea.fr),

Roy Gross and Erez Gilad
Ben-Gurion University of the Negev

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Outline

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- Diffusion Theory
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- The Ronen Method
  - Principles & Implementation
  - Expressions for the current in simple 1D geometries
- Conclusion

Introduction and Motivation

- The use of diffusion theory is very practical in ordinary full core calculations in terms of *computational time* and *numerical schemes*

  $\rightarrow$ fast calculations, parabolic/elliptic equations, diagonal dominance

- Cross section preparation by homogenization and equivalence theory form a consistent frame-work with nodal expansion or finite-element solving methods

  $\rightarrow$ current standard approach in nuclear industry

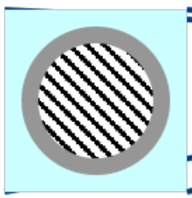
- Diffusion cannot reproduce strong transport effects with sufficient accuracy

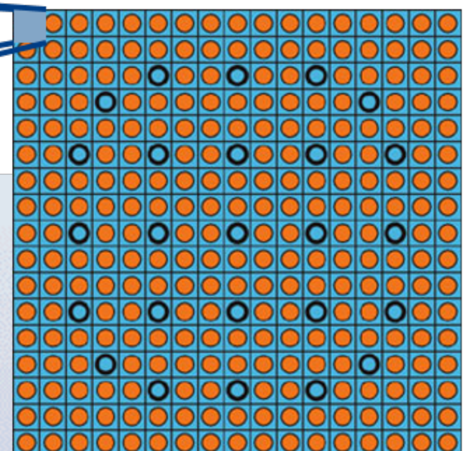
  $\rightarrow$ fails with strong absorption and flux gradients, rather miss anisotropy

- What's the *best definition* of the diffusion coefficient? Is there any?
- Influence of the geometry frame on the *flux convergence* by Ronen iterations

Two-step core calculations

Few group cross section homogenization

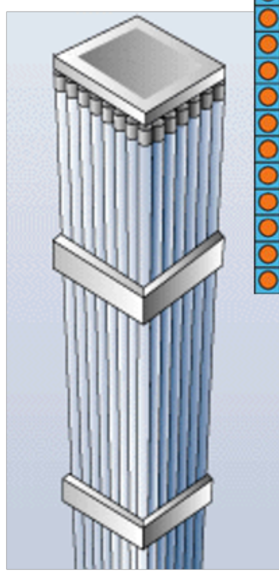




Detailed lattice transport codes

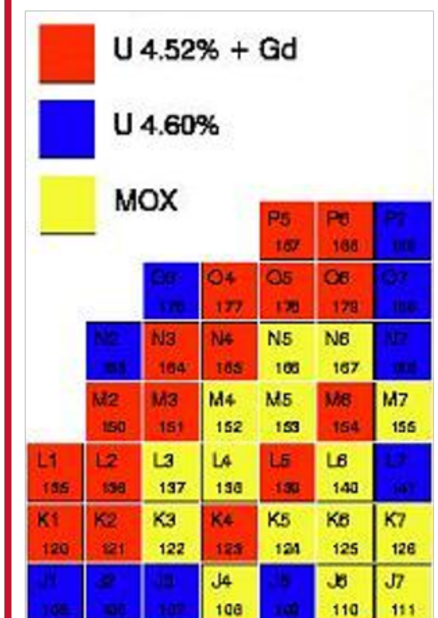
+

Infinite critical medium approx



multi-group xs library

Nodal core calculations in diffusion



Transport effects in core calculations

General issues for safety and design calculations

- High absorption and low scattering: presence of black materials to neutrons (mechanical and chemical shim), weak moderation, spectrum hardening
- scattering anisotropy: e.g. forward-peaked moderation in water
- potential occurrence of void under operation or in accidental transients (LWR/FR)
- angle-dependent boundary conditions: free-surfaces-vacuum, anisotropic albedos
- steep flux gradients: proximity to the reflector in thermal reactor, strong localized absorption
- material heterogeneity: heterogeneous core loading with material discontinuities at the interfaces between fuel elements (MOX/UO2 mixed cores, with both radial and axial discontinuities)
- *memory-effects* due to temporary and localized short reactivity insertion (incore instrumentation, rapid geometry and material changes, presence of noise)

Continuity equation with approximated transport law

Integro-differential Neutron Transport Equation (NTE)

[Duderstadt and Martin(1979)]

$$\left[\frac{1}{v}\frac{\partial}{\partial t} + \mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\varphi(\mathbf{r},E,\mathbf{\Omega},t) = \frac{\chi(E)}{4\pi}\int_0^\infty dE'\nu\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',t) + s_{\text{ext}}(\mathbf{r},E,\mathbf{\Omega},t) +$$
$$\int_{4\pi} d\Omega' \int_0^\infty dE'\Sigma_s(\mathbf{r},E'\to E,\Omega'\to\mathbf{\Omega})\varphi(\mathbf{r},E',\Omega',t) = q(\mathbf{r},E,\mathbf{\Omega},t).$$

Let us introduce the scalar flux and the current, respectively:

$$\phi = \int_{4\pi} d\Omega\varphi(\mathbf{r},\Omega[,*]) \quad \text{and} \quad \mathbf{J} = \int_{4\pi} d\Omega\Omega\varphi(\mathbf{r},\Omega[,*]),$$

and integrate the NTE to get the continuity equation:

$$\frac{1}{v}\frac{\partial\phi}{\partial t} + \nabla\cdot\mathbf{J} + \Sigma_t\phi = \int_{4\pi} d\Omega\, q(\mathbf{r},\Omega[,*]).$$

Use Fick's law as closure $\mathbf{J} = -\mathcal{D}\nabla\phi$, with the vacuum bnd. conds. $-\partial_{\hat{n}}\phi = \phi/\zeta$ and the extrapolated length $\zeta = 2\mathcal{D}$ ($\approx 2.13\mathcal{D}$ in computer codes).

N.B. A unique family of fissiles is represented here; precursors of delayed neutrons are also necessary for kinetics with fission; $\Sigma_t(\Omega[,*])$ if no rotational symmetry in scattering events.

The P_1 branding of the diffusion coefficient

P_N: flux expansion on sph. harmonics and projections over 4π of the NTE on $1, \mathbf{\Omega}, \ldots$

If we limit the expansion to the first moment:

$$\begin{cases} \dfrac{1}{v}\dfrac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{J} + \Sigma_t \phi = \displaystyle\int_0^\infty dE' \Sigma_{s,\ell=0}(E' \to E)\, \phi(\mathbf{r}, E', t) \; + S_{\mathrm{ext},\ell=0}, & (1) \\ \dfrac{1}{v}\dfrac{\partial \mathbf{J}}{\partial t} + \nabla \cdot \mathbf{\Pi} + \Sigma_t \mathbf{J} = \displaystyle\int_0^\infty dE' \Sigma_{s,\ell=1}(E' \to E)\, \mathbf{J}(\mathbf{r}, E', t) + \mathbf{S}_{\mathrm{ext},\ell=1}, & (2) \end{cases}$$

with $\mathbf{\Pi} = \int_{4\pi} d\Omega (\mathbf{\Omega}\mathbf{\Omega}) \varphi(\mathbf{r}, \mathbf{\Omega}[, *])$, or $\mathbf{\Pi} = \phi/3$ if $\varphi = (\phi + 3\mathbf{J} \cdot \mathbf{\Omega})/4\pi$, i.e. the P_1 approximation.

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Use then the multi-group energy formalism in Eq. 2, assume stationarity and an isotropic external source to write:

$$\frac{1}{3}\nabla \phi_g + \Sigma_{t,g} \mathbf{J}_g = \sum_{g'=1}^{G} \Sigma_{s,1,g' \to g} \mathbf{J}_{g'}$$

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In presence of dominant scattering and at *thermal equilibrium* $\sum_{g'} \Sigma_{s,1,g'\to g}\mathbf{J}_{g'} \approx \mathbf{J}_g \sum_{g'} \Sigma_{s,1,g\to g'}$, thus yielding a specific diffusion coefficient:

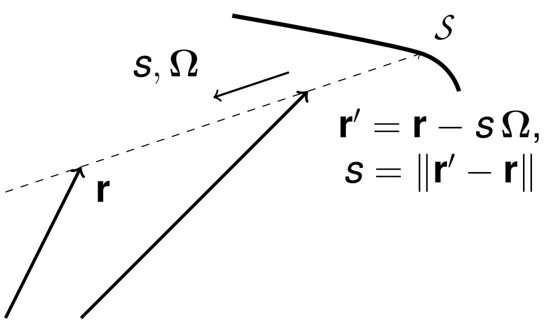
$$\mathbf{J}_g = -D_g \nabla\phi_g \implies D_g(\mathbf{r}) = \frac{1}{3\Sigma_{tr,g}} \quad \text{with} \quad \Sigma_{tr,g} = \Sigma_{t,g} - \Sigma_{s,1,g},\ \forall g.$$

Drift, diffusion tensors, and more. . .

Integral Neutron Transport Equation

$$\varphi(\mathbf{r}, E, \boldsymbol{\Omega}) = \int_0^{\mathcal{S}(\mathbf{r},\boldsymbol{\Omega})} ds\, q(\mathbf{r} - s\,\boldsymbol{\Omega}, E, \boldsymbol{\Omega}) \exp\left[-\mathscr{L}_{op}(\mathbf{r}, s, E, \boldsymbol{\Omega})\right] \text{ with } \mathscr{L}_{op} = \int_0^{s} ds'\, \Sigma_t(\mathbf{r} - s'\,\boldsymbol{\Omega}, E),$$

$$q(\mathbf{r}', E, \boldsymbol{\Omega}) = \sum_{\ell m} Y_{\ell m}(\boldsymbol{\Omega}) \int_0^{\infty} dE'\, \left(\Sigma_{s,\ell}(\mathbf{r}', E' \to E) + \chi(E)\nu\Sigma_f(\mathbf{r}', E')\delta_{\ell 0}\delta_{m0}\right) \phi_\ell^m(\mathbf{r}', E') + \text{b.c.}$$



Assume isotropic sources (with pure scattering and one group for simplicity), expand the flux by Taylor around **r** and integrate to obtain the current:

$$\mathbf{J}(\mathbf{r}) = \int d\mathbf{r}' \frac{\mathbf{r}' - \mathbf{r}}{4\pi\|\mathbf{r}' - \mathbf{r}\|^3} \Sigma_{s,0}(*) e^{-\mathscr{L}_{op}}.$$
$$\left(\phi(\mathbf{r}) - s\,\boldsymbol{\Omega} \cdot \nabla\phi + s^2\, \boldsymbol{\Omega}\mathbf{H}\boldsymbol{\Omega} + O(s^3)\right)$$

$$\Rightarrow \mathbf{J}(\mathbf{r}, E) = \underbrace{\vec{d}(\mathbf{r}, E)\phi(\mathbf{r}, E)}_{\text{advection / drift}} - \underbrace{\mathbf{D}(\mathbf{r}, E)\nabla\phi(\mathbf{r}, E)}_{\text{term w. diffusion tensor}} + \ldots$$

Under the following conditions:

i. smooth flux gradient and small higher derivatives
ii. weakly absorbing and highly scattering media
iii. constant cross sections in space

$$\Rightarrow \mathbf{J} = -D\nabla\phi \quad \text{with} \quad D = \frac{\Sigma_s}{3\Sigma_t^2}$$

Principles & Implementation

[Ronen(2004), Tomatis and Dall'Osso(2011)]

- The best diffusion coefficient would be the one satisfying exactly Fick's law with the same flux and current computed by transport (with the current containing all contributions from higher order moments!)

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- Such agreement is sought numerically by non-linear iterations
- Alternative implementation by a CMFD-like scheme [Smith(1983)], with currents at cell interfaces as:

$$J^{(k,+)} \approx \underbrace{-2D_{\text{DIFF}}\frac{\phi^{(k+1,+)}-\phi^{(k,+)}}{\Delta_{k+1}+\Delta_k}}_{\text{Diffusive current}} \underbrace{-2\left(\delta D\right)\frac{\phi^{(k+1,+)}+\phi^{(k,+)}}{\Delta_{k+1}+\Delta_k}}_{\text{Transport correction}},$$

where $\delta D \propto (J_{\text{TRANSP}} - J_{\text{DIFF}})$.

Boundary conditions (bc.)

A known issue...

bc. apply on the angular flux in transport and we solve only for the scalar flux in diffusion.

Generalized form for finite difference equations:

$$J = -\frac{D\phi_{bc}}{\Delta_{bc}/2+\zeta} \text{ with } \begin{cases} \zeta \propto \lambda_t & \text{extrapolated length for vacuum,} \\ \zeta = 0 & \text{zero flux,} \\ \zeta \to 0^+ & \text{reflection by vanishing current;} \end{cases} \qquad \delta J_{bc} = \delta D\phi_{bc}.$$

The problem of reflection and periodic translation

We expand the angular flux on spherical harmonics to get expressions based on moments. Now consider a bare homogeneous slab ($\varphi \approx \phi/2 + 3/2J\mu$) with specular reflection at one side. $J^+ + J^- \neq 0$ at the refl. boundary for $\varphi \approx \phi/2$. $\longrightarrow$ Fix $J = 0$ by corrections from higher moments as:

$$J^+(x) = \frac{\phi_0(a)}{2}E_3(\tau(a,x)) + \frac{5}{4}\tilde{\phi}_2(a)\left[3E_5(\tau(a,x)) - E_3(\tau(a,x))\right],$$

$$\text{with } \tilde{\phi}_2(a) = -\frac{16}{5}\left(\frac{1}{4}\phi_0(a) + J^-\right) \text{ and } \phi(a,\mu) = \frac{1}{2}\phi_0 + \frac{3}{2}\mu\phi_1 + \frac{5}{4}\left(3\mu^2-1\right)\tilde{\phi}_2.$$

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Expressions for the current in simple 1D geometries

Derivation of the equation for the current in mono-dimensional problems (*bare bodies*) by escape probabilities. The current of particles crossing the surface S at r is

$$J(r)S(r) = \sum_j q_j V_j e_j(r), \text{ where}$$

- q_j is the (isotropic) source in the region j of volume V_j and
- $e_j(r)$ is the probability for a particle isotropically emitted in region j to cross S(r) uncollided.

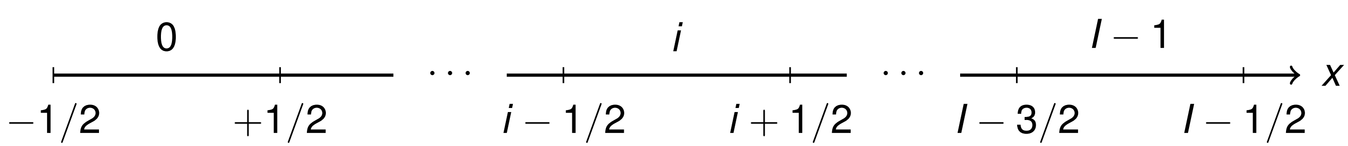

Figure: Mesh notation for the 1d problems.

In **1D slab**, integration on the polar angle is resolved *analytically* by exponential integral functions E_n:

$$J_{i+1/2} = \int_0^1 d\mu\, \mu\varphi(a,\mu)e^{-\tau(a,x_{i+1/2})/\mu} - \int_0^{-1} d\mu\, \mu\varphi(b,\mu)e^{-\tau(b,x_{i+1/2})/\mu}$$
$$+ \sum_{j=0}^{I-1} \text{sign}(x_{i+1/2} - x_{j+1/2}) \frac{q_{0,j}}{2} \int_{x_{j-1/2}}^{x_{j+1/2}} dx' E_2\left(|\tau(x', x_{i+1/2})|\right).$$

An example in the bare homogeneous slab I

[Tomatis and Dall'Osso(2011)]

APPROX: 2G problem with isotropic scattering, extrapolated length $\zeta = 2.13\mathcal{D}$
b.c.: reflection at left, vacuum or zero flux at right.

Table: Cross section data of the homogenized FA ($k_\infty = 1.07838$); scattering cross section comes from sum on columns.

Group g	$\Sigma_{t,g}$	$\Sigma_{s,0,g' \to g}$		χ_g	$\nu\Sigma_f$
1	5.31150E-01	5.04664E-01	2.03884E-03	1	7.15848E-03
2	1.30058E+00	1.62955E-02	1.19134E+00	0	1.41284E-01

Table: 17×17 PWR UO2 FA data (3.5% enr. w/o ^{235}U).

Slab width	21.5 cm
Fuel temp.	900 K
Water temp.	600 K
Water density	0.66 g/cm^3
Boron conc.	500 ppm

Table: Results on the multiplication factor k

Left b.c.:	vacuum		zero flux
	k	Δk (pcm)	Δk (pcm)
Ref. S16	0.745675	0	-
$D = 1/(3\Sigma_t)$	0.741377	-429.8	-5800.1
$D = \Sigma_s/(3\Sigma_t^2)$	0.746360	68.5	-5150.1
Ronen corr.	0.743860	-181.5	164.4

An example in the bare homogeneous slab II

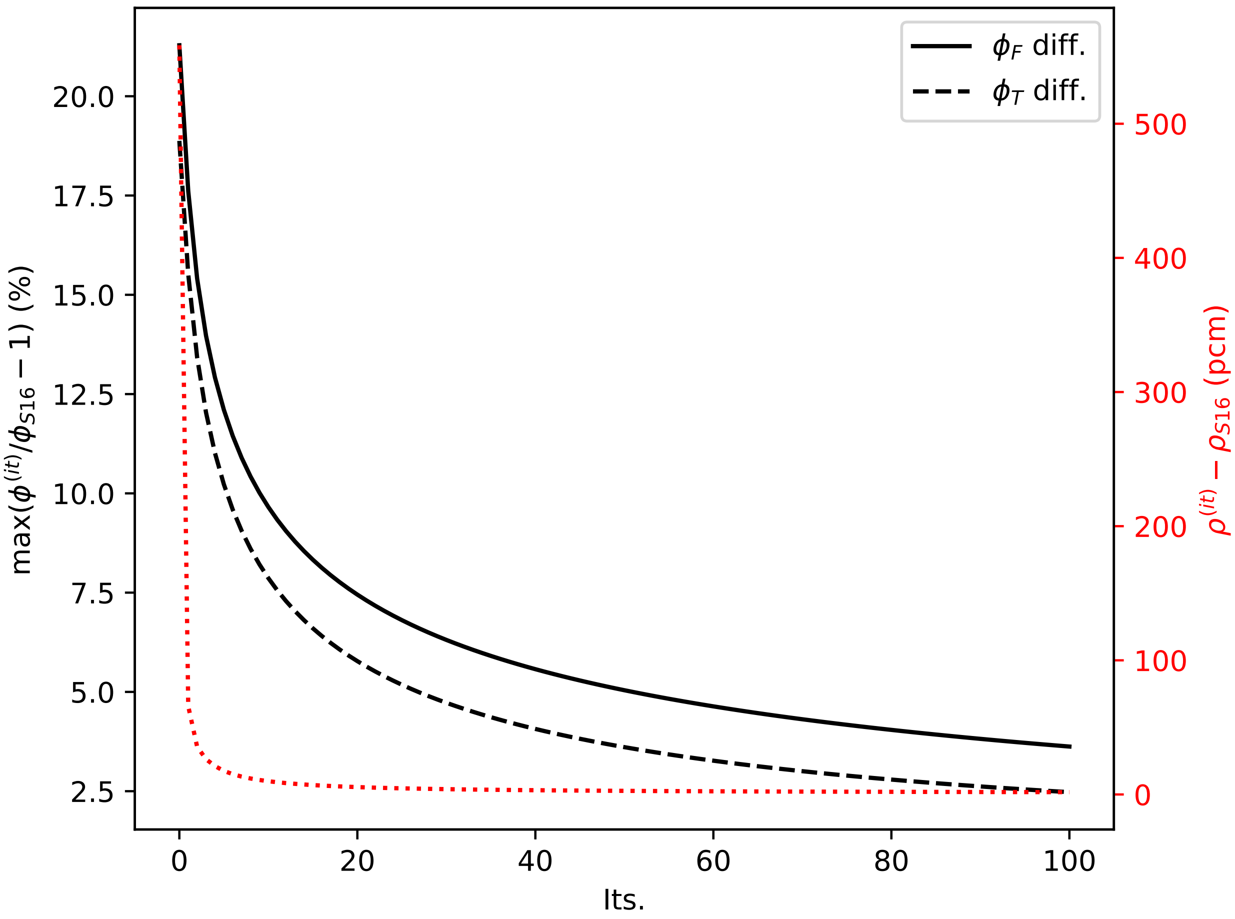

Figure: Convergence trend.

An example in the bare homogeneous slab III

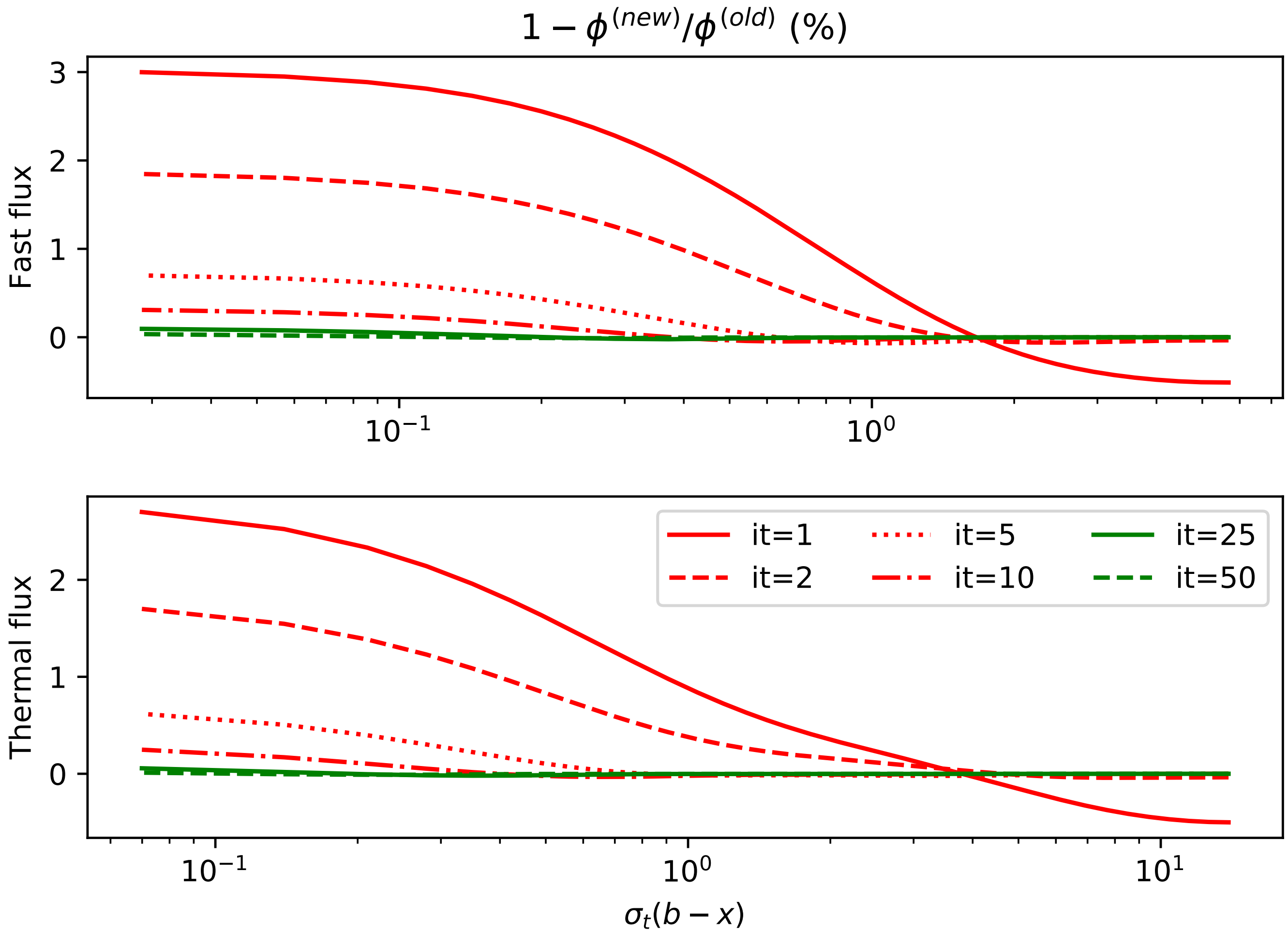

Figure: Relative flux error in optical lengths from the boundary through iterations.

An example in the bare homogeneous slab IV

Discussion

- The Ronen method drives the diffusion solution towards a transport-like solution even with unphysical b.c.
- The error concentrates at the boundary interface, and asks for many iterations
- $D = 1/(3\Sigma_t)$ is the P_1 diffusion coefficient here
- Although $D = \Sigma_s/(3\Sigma_t^2)$ results in a smaller Δk, $\Delta\phi$ is 20% off near the left boundary

Same issues and remarks for multi-dimensional *n*-D cases

- Can we prove convergence?
- Can we compute all components of the diffusion tensor in a coarse mesh?
- What are the special functions in n-D?
- Are there regions (like *void* for instance) where the method cannot be applied?

Derivation of the current in 1D curvilinear geometries

Escape probability in **1D cylindrical geometry**:

$$e_j(r) = \frac{2}{rV_j} \int_0^r dh\, y \int_{L_j} d\ell\, \mathrm{Ki}_2\left[\tau(y, y-\ell)\right],$$

with $y(r,h) = \sqrt{r^2 - h^2}$ and $L_j(h) = [-Y, y] \cap V_j$ $(Y = y(R,h))$.

Escape probability in **1D spherical geometry**:

$$e_j(r) = \frac{2\pi}{r^2 V_j} \int_0^r dh\, hy \int_{L_j} d\ell\, \exp\left[-\tau(y, y-\ell)\right].$$

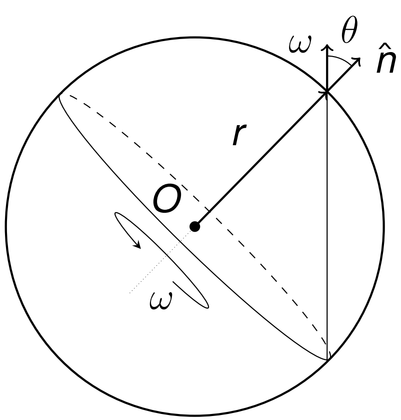

Figure: Spherical symmetry.

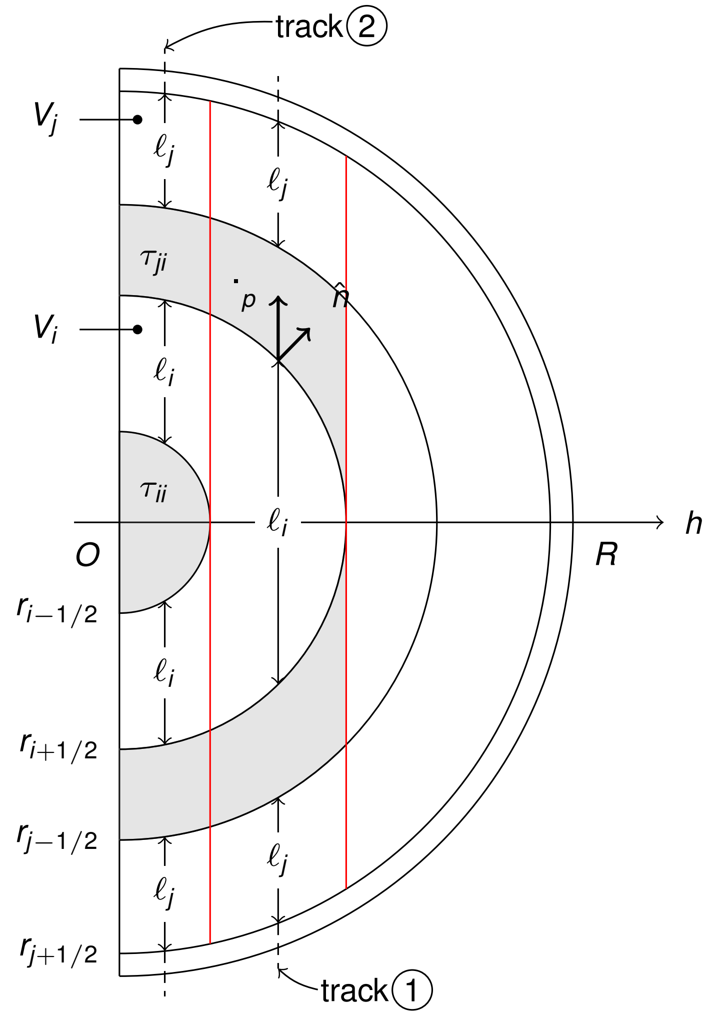

Figure: Tracking integration [Hébert(2009)].

Conclusion

Summary

- Diffusion theory is practical for (fast) core calculations
- Possible improvements by second-order transport approximations (SP_N, A_N, . . .)
- The use of equivalence theory compensates the lack of physical information in the diffusive model
- Introduction of the Ronen Method: principles & implementation options
- Similarities with collision probability methods (see the escape probabilities), without solving CPM, i.e. no matrix inversion
- The Ronen Method could provide an online equivalence between diffusion and integral transport on coarse meshes

Future development

(i) Convergence and stability analysis (using the CMFD scheme)

(ii) Formal and numerical investigation of the Ronen Method as a mean for an online equivalence

(iii) 3D implementation of the Ronen method in nodal codes

(iv) Extension to time-dependent problem

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Thanks for your attention!

Commissariat à l’énergie atomique et aux énergies alternatives
Centre de Saclay | 91191 Gif-sur-Yvette Cedex, France
T. +33 (0)1 XX XX XX XX

Etablissement public à caractère industriel et commercial | R.C.S Paris B 775 685 019

Direction de l’Énergie Nucléaire
Département de Modélisation des Systèmes et Structures
Service d’études des réacteurs et de mathématiques appliquées (SERMA)

Thanks for your attention!

Bòja brigant

Ciao Piero!

Commissariat à l'énergie atomique et aux énergies alternatives
Centre de Saclay | 91191 Gif-sur-Yvette Cedex, France
T. +33 (0)1 XX XX XX XX

Etablissement public à caractère industriel et commercial | R.C.S Paris B 775 685 019

Direction de l'Énergie Nucléaire
Département de Modélisation des Systèmes et Structures
Service d'études des réacteurs et de mathématiques appliquées (SERMA)

The B_N leakage model

Objective

Get a critical flux by adjusting the leakage in each group, and obtain a consistent definition of the diffusion coefficient [Benoist(1964), Hébert(2009)].

Assumptions

- Closed system by *reflective* or *periodic* bnd. conds. in a finite lattice of cells or assemblies.
- Flux factorization with a *macroscopic* quantity ϕ and a *homogeneous* or *periodic* fundamental flux ψ,

$$\varphi(\mathbf{r}[,*]) = \phi(\mathbf{r})\,\psi(\mathbf{r}[,*]),$$

  where ϕ fulfills the Helmholtz eqn. $\nabla^2\phi + B^2\phi = 0$ with the (critical) buckling $B^2 \in \mathbb{R}$. It follows that $\phi \propto \exp(i\mathbf{B}\cdot\mathbf{r})$ $(B^2 = \mathbf{B}\cdot\mathbf{B})$.
- homogeneous or heterogeneous variants (acc. to the dependence of ψ on $\mathbf{r}$)

Homogeneous B_1 Equations

After a flux-volume homogenization of the NTE, substitute $\varphi = \psi(E,\Omega)\exp(i\mathbf{B}\cdot\mathbf{r})$ and integrate on angle to obtain the system of eqs. (with γ as polynomial function of $(B/\Sigma_t)^2$):

$$\begin{cases} (\Sigma_t(E) + D(B,E)B^2)\psi(E) = \displaystyle\int_0^\infty dE'\,(\Sigma_{s,0}(E' \to E) + \chi(E)\nu\Sigma_f(E'))\,\psi(E') \\ D(B,E) = \dfrac{1}{3\gamma(B,\Sigma_t)\Sigma_t}\left[1 + 3\displaystyle\int_0^\infty dE'\Sigma_{s,1}(E' \to E)D(B,E')\frac{\psi(E')}{\psi(E)}\right] \end{cases}$$

Other diffusive-like approximations from radiative transfer problems

Flux-limited diffusion

The angular flux is factored in a term slowly varying in space and a normalized angular component [Levermore and Pomraning(1981)]:

$$\varphi \approx \phi(\mathbf{r}, E)\psi(\mathbf{r}, \Omega) \quad \text{with} \quad \int_{4\pi} d\Omega\psi = 1, \qquad \Longrightarrow \mathbf{J}_g = \mathbf{f}(\mathbf{r})\,\phi_g \;\wedge\; \frac{\|\mathbf{J}_g\|}{\phi_g} = \text{const},\; \forall g.$$

The diffusion coefficient (“the flux-limiting parameter”) come from the solution of a *transcendental equation*. In the limit of weak gradients, the diffusion coefficient is obtained as (for all groups):

$$D_g(\mathbf{r}) = \frac{1}{3}\left[\Sigma_{t,g} - \sum_{g'} \Sigma_{s,1,g'\to g} \frac{\phi_{g'}}{\phi_g}\right]^{-1}$$

Variable Eddington factor

Postulate a factorization of the second moment by another factor (or *tensor*) slowly varying in space [Pomraning(1982)]:

$$\varphi \approx E(\mathbf{r}[,*])\phi(\mathbf{r}[,*]),\ \text{and}\ \partial_{\mathbf{r}} E \approx 0 \implies D_{i,g}(\mathbf{r}) = E_g(\mathbf{r})\left[\Sigma_{t,g} - \sum_{g'} \Sigma_{s,1,g'\to g} \frac{J_{i,g'}}{J_{i,g}}\right]^{-1}, i \in (\hat{e}_x, \hat{e}_y, \hat{e}_z).$$

Homogenization and Equivalence Theory

What for? Prepare *in advance* all reactor data for later core calculations in low-order transport (diffusion, SP_N and others).

Main rational of Homogenization

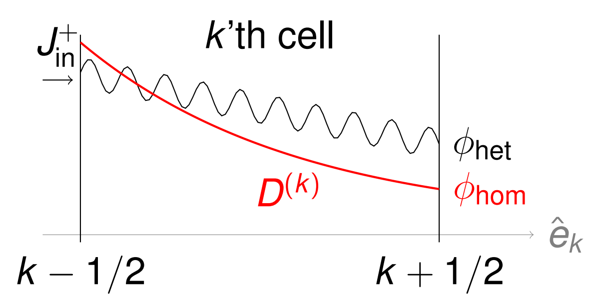
Conservation of reaction rates in the volume $\mathcal{V}$ of *spatial homogenization* and in the g-th group of *energy condensation* with $E \in [E_g, E_{g+1}]$, $g = 1, \ldots, G$.

$$\Sigma_g = \frac{\int_{\mathcal{V}} d\mathbf{r} \int_{E_{g+1}}^{E_g} dE\, \Sigma(\mathbf{r}, E)\, \phi(\mathbf{r}, E)}{\int_{\mathcal{V}} d\mathbf{r} \int_{E_{g+1}}^{E_g} dE\, \phi(\mathbf{r}, E)} \quad \text{with} \quad \chi_g = \int_{E_{g+1}}^{E_g} dE\, \chi(E).$$

Equivalence

Why? …Diffusion $\neq$ transport, conservation of reaction rates does not imply to reproduce the *same currents* at the boundaries of $\mathcal{V}$. Available techniques:

- (A)DF$= \phi_{\text{het}}/\phi_{\text{hom}}$ (discontinuity factors), *two per direction*
- SPH (SuPer-Homogenization) factors, *one per group and homog. region*: $(\Sigma_g^{(k)}/s)(s\phi_g^{(k)})$



Special functions

Integral exponential function E_n:

$$\mathrm{E}_n(\tau) = \int_1^\infty du\, \frac{e^{-|tau|\,u}}{u^n} = \int_0^1 d\mu\, \mu^{n-2} e^{-|\tau|/\mu}.$$

Useful properties: $d_\tau \mathrm{E}_n = -\mathrm{E}_{n-1}(\tau)$ and $\mathrm{E}_n(0) = frac1n+1$. Bickley-Naylor functions Ki_n:

$$\mathrm{Ki}_n(\tau) = \int_0^{\pi/2} d\theta \sin^{n-1}\theta \exp\left(-\frac{\tau}{\sin\theta}\right).$$

Useful properties: $d_\tau \mathrm{Ki}_n = -\mathrm{Ki}_{n-1}(\tau)$.