Nonlinear Iterative Solution of the Neutron Transport Equation

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Outline

- motivations and framework
- iterative solution of the multigroup discrete ordinates transport equations
- nonlinear scheme
- coarse equivalent operator
- nonlinear diffusion
- coarse-mesh finite difference method (CMFD)
- test calculations with Apollo2
- stability analysis (1-D case problem)

ongoing works & future works
- domain decomposition (parallel calculation on the 2- levels assembly-core)
- acceleration of the core iterations by CMFD
- free-Jacobian Newton-Krylov methods
- coarse non-equivalent operators
Motivations: 2-Level transport-diffusion scheme

- **fuel pin-cell (transport)**
  - 1D or 2D geometry (infinite lattice)
  - High number of energy groups
  - Self-shielding effects
  - **Output**: effective microscopic cross-sections

- **assembly (transport)**
  - 2D geometry (infinite lattice)
  - High number of energy groups
  - Transport effects (spatial-angular distribution)
  - **Output**: effective few-groups homogenized microscopic cross-sections

- **reactor core (diffusion or SPN)**
  - 3D geometry with homogenized assembly
  - Few number of energy groups
  - Fundamental Mode effects
  - **Output**: Power distribution isotopic concentrations

Construction of a parametric microscopic cross-section library.

**Parameters**: 
- Burn-up
- Control Rod in/out
- Boron concentration
- ...

Error source:
- combined 1D-2D-3D calculations
- lattice homogenization and condensation.
- assembly boundary conditions
- diffusion operator
goals

Why the use of nonlinear iteration scheme for a linear equation?

- to accelerate the transport iterative process.
- to obtain approximated transport solutions.
stationary neutron transport equations

- **Linear transport operator**:
  \[
  (L - H)\psi(x) = \frac{1}{\lambda} F\psi(x) \quad x \in X
  \]
  \[
  \psi(x_-) = \beta\psi(x_-) + s_{in}(x_-) \quad x_- \in X_-
  \]
  \[
  X = (r \in D, \Omega \in S_2, E \in \mathbb{R}^+) \quad X_\pm = (r \in \Gamma_{\pm}(\Omega), \Omega \in S_2, E \in \mathbb{R}^+)
  \]
  \[
  \Gamma_{\pm}(\Omega) = (r \in \partial D, n_+(r) \cdot \Omega \geq 0)
  \]
  \[
  (f, g) = \int_X dx \, fg(x)
  \]
  \[
  \lambda = \frac{(w, F\psi)}{(w, (L - H)\psi)}
  \]

- **Removal operator**:
  \[
  L\psi(x) = \Omega \cdot \nabla \psi(r, \Omega, E) + \Sigma(r, E)\psi(r, \Omega, E)
  \]

- **Scattering operator (hp. isotropic medium)**:
  \[
  H\psi(x) = \int dE' \int d\Omega' \Sigma_s(r, E' \rightarrow E, \Omega \cdot \Omega')\psi(r, \Omega', E')
  \]

- **Fission operator**:
  \[
  F\psi(x) = \chi(E) \int dE' (\nu \Sigma_f)(r, E') \int_{4\pi} d\Omega' \psi(r, \Omega', E')
  \]
multigroup & discrete ordinates framework

- **Multigroup approximation**:
  \[ \mathbb{R}^+ \to E_G \equiv [0, E_{\text{max}}] = \bigcup_{g=1, G} \Delta E_g \]
  \[ \psi_g(r, \Omega) = \int_g dE' \psi(r, \Omega', E') \]
  \[ \Sigma_g(r) = \frac{\int_g dE \Sigma(r, E) \phi(E)}{\int_g dE \phi(E)} \]

- **Angular collocation**:
  \[ S_2 \to S_N \equiv \{ w_d, \Omega_d \}_{d=1, N_D} \]
  \[ \frac{1}{4\pi} \int_{4\pi} d\Omega f(\Omega) \simeq \sum_d w_d f(\Omega_d) ; \sum_d w_d = 1 \]

- **Removal operator**:
  \[ (L\psi)_{g,d}(r) = \Omega_d \cdot \nabla \psi^g(r, \Omega_d) + \Sigma^g(r) \psi^g(r, \Omega_d) \]

- **Scattering operator (Legendre expansion of the scattering kernel)**:
  \[ (H\psi)_{g,d}(r) = \sum_{g'} (H\psi)_{g,g',d}(r) = \sum_h \sum_{g'} \Sigma_{s,h,gg'}(r) A_h(\Omega_d) \phi_{h,g'}(r) \]
  \[ (H\psi)_{gg',d}(r) = \sum_h \Sigma_{s,h,gg'}(r) A_h(\Omega_d) \phi_{h,g'}(r) \]
  \[ \phi_{h,g}(r) = \frac{1}{4\pi} \sum_d w_d A_h(\Omega_d) \int_g dE \psi(r, \Omega_d, E) \]
\[
(F\psi)_g(r) = \chi^g(E)I_f(r)
\]
\[
I_f(r) = \sum_{g'} \Sigma^g_f(r) \phi^g_0(r)
\]
\[
\phi^g_0(r) = \frac{\phi^g(r)}{4\pi} = \frac{1}{4\pi} \sum_d w_d \psi_g(r, \Omega_d)
\]

**iterative solution**

- **Fission operator:**

- **discrete ordinates-multigroup transport equation:**

- **Source iterations for eigenvalue problems:**

\[
(L\psi)_{g,d}(r) = (H\psi)_{g,d}(r) + \frac{1}{\lambda} (F\psi)_g(r)
\]

\[
(L\psi)_{g,d}(r) = (H\psi)_{gg,d}(r) + \sum_{g' < g} (H\psi)_{gg',d}(r) + \sum_{g' > g} (H\psi)_{gg',d}(r) + \frac{1}{\lambda} (F\psi)_g(r)
\]
introduction to non-linear scheme

- **Spatial-angular-energy discretization**: 
  \[ X_N \equiv (r \in \bigcup_n D_n, \Omega \in S_N, E \in \bigcup_{g=1,N_g} \Delta E_g) \]
  
  \( V_N \) is the linear normed space of coefficients equivalent of the space \( \tilde{V}_N \equiv \{ \psi_n(x) \in L^2(X_n) \} \)

- **Transport source iterations**: 
  \[ L_N \psi_N^{(i+1)} = H_N \psi_N^{(i)} + q_N \quad \psi_N, q_N \in V_N \]

  where: 
  \( L_N, H_N : V_N \rightarrow V_N \)

- **Coarsening the phase-space**: 
  \[ K < N \]

  \[ X_K \equiv (r \in \bigcup_k D_k, \Omega \in S_M, E \in \bigcup_{G=1,N_G} \Delta E_G) \equiv \bigcup_k X_k \]

  \[ V_N \equiv \{ \psi_n(x) \in L^2(X_n), n = 1, N \} \Rightarrow V_K \equiv \{ \psi_k(x) \in L^2(X_k), k = 1, K \} \]

- **Nonlinear mapping**: 

  transport operator
  \[ V_N \xrightarrow{(L-H)_N} V_N \]

  prolongation \( P_{NK} \)

  nonlinear operator
  \[ V_K \xleftarrow{A_K(\psi_N)} V_K \]

  projection \( P_{KN} \)
non-liner iterations : generalities

- solve the transport source problem

\[ L_N \psi_N = H_N \psi_N^{(i)} + q_N \]

- construction of the non-linear operator
  
  - the restriction operator (projection) \( P_{KN} \)
  
  \( P_{KN} : V_N \rightarrow V_K \)

  - the prolongation operator \( P_{NK}(\psi_N) \)
  
  \( P_{NK} : V_K \rightarrow V_N \)

  - the coarser operator \( A_K(\psi_N) \)
  
  \( A_K(\psi_N) : V_K \rightarrow V_K \)

- solve the coarser equation

\[ A_K(\psi_N) \psi_K = q_K \]

- correction for the new flux

\[ \psi_N^{(i+1)} = P_{NK}(\psi_N) \psi_K \]
supposing a given converged transport solution \( V_N \):

\[
L_N \psi_N(x) = H_N \psi_N + q_N
\]

it is possible to construct a projective operator \( V_K \):

\[
P_{KN} : V_N \rightarrow V_K
\]

the projected equations serves as statement for neutron conservation on \( V_K \):

\[
P_{KN}(L - H)\psi_N = P_{KN}q_N
\]

the equivalent operator is obtained by imposing:

\[
A_K(\psi_N)P_{KN}\psi_N = P_{KN}(L - H)_N\psi_N
\]

in that way the solution of the equation

\[
A_K(\psi_N)\psi_K = q_K \quad \text{with} \quad q_K = P_{KN}q_N
\]

is

\[
\psi_K = P_{KN}\psi_N
\]

moreover:

\[
\psi_N = P_{NK}(\psi_N)\psi_K \quad \text{only if} \quad P_{NK}(\psi_N)P_{KN} = I_N
\]
the iterative scheme is an explicit discrete dynamical system:

\[ \psi_{N}^{(i+1)} = F(\psi_{N}^{(i)}) \]

\[ F : V_{N} \rightarrow V_{N} \]

if the non-linear coarser operator \( A_{K}(\psi_{N}) \) satisfies the equivalent relation during the iterative process than the transport solution is a fixed point for the mapping.

open investigation field:
- stability of the iterative scheme.

if the non-linear coarser operator does not satisfy the equivalent relation than the open investigation fields are:
- the existence of the solution,
- the quality of the solution (convergence in the phase space),
- the stability of the iterative scheme.
equivalent non-linear diffusion

- point-wise neutron balance equation:
  \[ \nabla \mathbf{J} + \sum_{\alpha} \phi = q \]
  \[ \sum_{\alpha} = \sum - \sum_{s,0} \]

- the transport solution does not satisfy the diffusion closure obtained with the \( P_1 \) approximation (Fick’s law)
  \[ \mathbf{J} \neq -\frac{1}{3\Sigma} \nabla \phi \]

- two ways to correct the diffusion closure:

  **Diagonal Eddington tensor**
  \[ \mathbf{J} = -\frac{\bar{\alpha}}{3\Sigma} \nabla \phi \rightarrow \alpha_i(\psi) = -3\Sigma \frac{J_i}{\partial \phi} \]
  for \( i = x, y, z \)

  **Drift**
  \[ \mathbf{J} = -\frac{1}{3\Sigma} \nabla \phi + \alpha \phi \rightarrow \alpha(\psi) = \frac{(\mathbf{J} + \nabla \phi)}{\phi} \]

 equivalent diffusion operators:

\[ -\nabla \cdot \frac{\bar{\alpha}(\psi)}{3\Sigma} \nabla \phi + \sum_{\alpha} \phi = q \]
\[ -\nabla \cdot \frac{1}{3\Sigma} \nabla \phi + \nabla \cdot \alpha(\psi) \phi + \sum_{\alpha} \phi = q \]
projection on the coarse-mesh: neutron balance

- **defining the scalar products:**
  \[
  (f, g)_k = \frac{1}{4\pi V_k} \int_G dE \int_{4\pi} d\Omega \int_{D_k} dr \ (f)(r) (g)(r, \Omega, E)
  \]
  \[
  \langle f, g \rangle^\pm_k = \frac{1}{\pi S_k} \int_G dE \int_{2\pi^\pm} d\Omega \int_{\partial D_k} d\mathbf{r}_s \ |n_s \cdot \Omega| (f)(r, \Omega, E)
  \]

- **the projection on the coarse-mesh results**
  \[
P_{KN} \left[ \Omega \cdot \nabla \psi(r, \Omega, E) + \Sigma(r, E) \psi(r, \Omega, E) \right] = q(r, \Omega, E)
  \]
  \[
P_{KN} \psi_N = \{(1, \psi_N)_k, k = 1, K\}
  \]

- **the projected equation results in a neutron balance equation on the coarse-mesh**

- **definitions:**

  - **flux weighted cross sections (homogenization):**
    \[
    \Sigma_k = \frac{(1, \Sigma_N \psi_N)_k}{(1, \psi_N)_k}
    \]

  - **prolongation operator:**
    \[
P_{KN}(\psi_N) = \left\{ \frac{\psi_n}{\phi_k} \right\}_{n \in k}
    \]
various types of interface parameter that preserve the transport current:

- Interface Flux Discontinuity Factor:
  \[ J_s = -d_{sk} (\phi_s - \phi_k) \]

- Interface and Average Flux Correction:
  \[ J_s = -d_{sk} (\phi_s - \phi_k) + \alpha_{sk} (\phi_s + \phi_k) \]

- Average Flux Correction:
  \[ J_s = -d_{sk} (\phi_s - \phi_k) + \alpha_{sk} \phi_k \]

Finite-difference diffusion coefficients:
\[ d_{sk} = \frac{2}{3 \tau_{sk}} \]

Transversal optical paths:
\[ \tau_{sk} = \sum_k L_{\perp k} \]

modified methods with quasidiffusion closure:

Eddington factor:
\[ \frac{\theta_s}{\phi_s} = \frac{\int_{4\pi} d\Omega |n_s \cdot \Omega|^2 \psi_s(\Omega)}{\int_{4\pi} d\Omega \psi_s(\Omega)} \]

modified diffusion coefficient:
\[ \hat{d}_{sk} = \frac{\theta_s}{\phi_s \tau_{sk}} \frac{2}{\tau_{sk}} \]
\[ d_{sk} \rightarrow \hat{d}_{sk} \]
MOX assembly 6-group Calculation (Apollo2-IDT)

**IFDF**: Interface Flux Discontinuity Factor (with Eddington Factor)

**AFC**: Average Flux Correction (without Eddington Factor)

**MAFC**: Modified Average Flux Correction (with Eddington Factor)

**IAFC**: Interface and Average Flux correction (with Eddington Factor)

Matrix inversion performed by BiCGStab with ILU(0) preconditioning

**CT**: matrix Construction Time

**ST**: Solution Time, transport (Trn) and acceleration (Acc) percentages

- S8 Level Symmetric angular quadrature formula
- 4-ring Heterogeneous Cartesian Cell with Linear Short Characteristics

<table>
<thead>
<tr>
<th>Method</th>
<th># inn. it.</th>
<th># out. it.</th>
<th>CPU (s)</th>
<th>CT (s)</th>
<th>ST (s)</th>
<th>Trn(%)</th>
<th>Acc(%)</th>
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<td>1.8</td>
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<td>1.2</td>
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</table>
C5G7-MOX benchmark

- **Multi-Cell Mesh**
- **Fast group**
- **Thermal group**
C5G7-MOX benchmark

- S8 Level Symmetric angular quadrature (tracking spacing: 0.01cm)
- 7 pin-cell types
- 7 groups energy mesh
- \( n \): spatial order, \( =0 \) constant, \( =1 \) linear, \( =2 \) bilinear (accelerated by IAFC scheme).
- Running time with free iterations with 1 ring: \( (76 \text{ s}, n=0) \) \( (174 \text{ s}, n=1) \) \( (215 \text{ s}, n=2) \).

<table>
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<tr>
<th>Calculation</th>
<th># reg.</th>
<th>n</th>
<th># it.</th>
<th>CPU(s)</th>
<th>RMS(%)</th>
<th>K-eff</th>
<th>err.(%)</th>
<th>( \Delta \rho )(pcm)</th>
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</table>

- Production \% rel. err. (APOLLO2-IDT vs. MCNP)
Advantages

- efficient and effective technique for the discrete ordinates SI
- reduced computing and storage cost compared to linear synthetic acceleration techniques (excellent candidate for 3D transport calculation!)

Issues

- it is not guaranteed that the non-linear finite difference diffusion matrix is an M-matrix (whose off-diagonal entries are less than or equal to zero and having positive eigenvalues), it might be a problem for iterative matrix inversion methods (ex. Krylov methods)
- the iteration scheme could be unstable! (especially in the presence of strong heterogeneities using detailed multigroup library)
Analytical Stability Analysis

deterministic dynamical system

\[ \phi_N^{(i+1)} = F(\phi_N^{(i)}) \]

- **local stability condition**:
  \[ \left\| DF(\phi_N^{(i)}) \right\|_{\phi_N^{(i)} = \xi_N} < 1 \]
  where \( \xi_N \) is the fixed point

  \[ DF(\phi_N^{(i)}) \bigg|_{\phi_N^{(i)} = \xi_N} = \frac{\partial \phi_N^{(i+1)}}{\partial \phi_N^{(i)}} \bigg|_{\phi_N^{(i)} = \xi_N} \]
  is the Jacobian matrix

- **homogenization and interface parameter effects analyzed separately**:

  \[ \sum_{s \in k} L_s J_s + V_k \sum a_k \phi_k = V_k S_k \quad k = 1, \ldots, K \]

**CASE 1**: the coarse grid is a single homogeneous region \((K=1)\) homogenization effect

**CASE 2**: coarse grid = fine grid \((K=N)\) interface parameter effect
Analytical Stability Analysis

- Problem definition:
  - 1-D 2-region slab problem
  - step characteristics
  - $S_{16}$ Level Symmetric quadrature formula
  - accelerated with MAFC, $J_s = -\delta_{sk}(\phi_s - \phi_k) + j_{sk}\phi_k$
  - specular reflection boundary conditions

- Parametrization:

  \[
  \begin{align*}
  \tau_1 &= \tau \\
  \tau_{s1} &= c\tau \\
  \tau_{a1} &= (1-c)\tau \\
  \tau_2 &= \frac{\tau_{s1}}{\rho} + \tau_{a1}\rho
  \end{align*}
  \]

  $p$ stretching parameter

  \[
  \begin{array}{c}
  \text{region 1} \quad (\tau, c) \\
  \text{region 2} \quad (p)
  \end{array}
  \]

  $\Delta_1 = \Delta_2 = \Delta = 1$

  Flat-flux solution: $\phi_1 = \phi_2 = \frac{S_1}{\Sigma_{a1}} = \frac{S_2}{\Sigma_{a2}} = 1$
**CMFD acceleration for \( S_n \) Source Iterations**

- **2-level angular-spatial multigrid:**
  - **fine grid** \( D_N = \bigcup_{n=1}^{N} D_n \)
  - **coarse grid** \( D_K = \bigcup_{k=1}^{K} D_k \)
  \( K < N \)

1) **source iteration on the discretized transport equation \( (S_n) \):**

\[
\overrightarrow{\phi}_N = A_T\left[\Sigma_{s,N} \overrightarrow{\phi}^{(i)}_N + \overrightarrow{S}_N\right]
\]

2) **construction of the restriction and prolongation operators and finite difference coarse operator :**

\[
\Sigma_{r,K} = P_{KN}(\overrightarrow{\phi}_N)\Sigma_{r,N}, \quad P_{NK}(\overrightarrow{\phi}_N), \quad f_{sk}(\overrightarrow{\phi}_N)
\]

- flux-weighted XS
- shape factors
- interface equivalence parameters

3) **non-linear diffusion system solution:**

\[
A_D(\overrightarrow{\phi}_N) \overrightarrow{\phi}_K = \overrightarrow{V}\overrightarrow{S}_K
\]

4) **correction :**

\[
\overrightarrow{\phi}_N^{(i+1)} = P_{NK}(\overrightarrow{\phi}_N) \overrightarrow{\phi}_K
\]
case 1: homogenization effect (K=1)

The whole domain is homogenized in a single macroscopic region.

- **Jacobian matrix**:
  \[
  \nabla \phi^{(i)}_N \phi^{(i+1)}_N = \alpha(\phi^N) P(\phi^N) A_T \Sigma_{s,N}
  \]

  here \( P(\phi^N) \) is the projector \( P(\phi^N) = I - \frac{\phi^N \otimes V \Sigma_{aN}}{(V \Sigma_{aN} \cdot \phi^N)} \) \( P^2 = P \)

  and \( \alpha(\phi^N) = \frac{(V_N \cdot \bar{S}^N)}{(V \Sigma_{aN} \cdot \phi^N)} \)

- **stability condition**:
  \[
  \| \nabla \phi^{(n)}_N \phi^{(n+1)}_N \| \leq \alpha(\phi^N) \| A_T \Sigma_{s,N} \| \leq \alpha(\phi^N) c
  \]

  where \( c = \max\{\Sigma_{s,n}/\Sigma_n, n = 1, N\} \)

  N.B.: this is a general result valid for infinite lattice problems

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SERMA/ LTSD

22/37
case 1: homogenization effect \((K=1)\)

2-region heterogeneous slab problem

- dominant eigenvalue:

\[
\lambda = (1 - a) \Sigma_{s,1}(A_{11} - A_{21}) + a \Sigma_{s,2}(A_{22} - A_{12})
\]

Here

\[
a = \frac{\tau_{a1}}{\tau_{a1} + \tau_{a2}}
\]

\[
A_T = \{A_{nm}, \ n, m = 1, N\} \text{ is the transport matrix}
\]

by introducing the parametrization:

because of the infinite lattice condition

\[
\alpha(\vec{\phi}_N) = 1
\]

the stability condition is fulfilled.

\[
\lambda(p, c, \tau) = \frac{1}{1 + p c \tau (A_{11} - A_{21}) + \frac{p^2}{1 + p c \tau (A_{22} - A_{12})}
\]
case 1: homogenization effect \((K=1)\)

- **Infinite-absorber material limit**: 
  \[
  \lim_{p \to 0} \lambda = c \left( 1 - 2 \frac{G(\tau)}{\tau} \right)
  \]

- **Infinite-diffusive material limit**: 
  \[
  \lim_{p \to \infty} \lambda = \left( 1 - 2 \frac{G(\tau)}{\tau} \right)
  \]

where 
\[
G(\tau) = \frac{1}{4} \left[ 1 - 2E_3(\tau) \right]
\]
and 
\[
E_n(\tau) = \int_{0}^{1} \mu^{n-2} e^{-\tau/\mu} d\mu
\]
with 
\[
\frac{G(\tau)}{\tau} = \begin{cases} 
\frac{1}{4\tau}, & \tau \to \infty, \\
\frac{1}{2}, & \tau \to 0.
\end{cases}
\]
The coarse mesh is the same as the transport fine mesh.

- **source iteration scheme**:

  \[ \vec{\phi}_N = A_T \left[ \sum_s \vec{\phi}_N^{(i)} + \vec{S}_N \right] \]

  \[ A_D(\vec{\phi}_N^{(i)}) \vec{\phi}_N^{(i+1)} = V \vec{S}_N. \]

- **Jacobian matrix**:

  \[ \nabla \vec{\phi}_N^{(i)} \vec{\phi}_N^{(i+1)} = -A_D^{-1}(\nabla \vec{\phi}_N^{(i)} A_D) \vec{\phi}_N^{(i+1)} \]

  2-region heterogeneous slab problem (K=N=2) with MAFC

\[ A_D(\vec{\phi}_N^{(i)}) = \begin{pmatrix}
\frac{\tau_1 J_x + 2\theta_x}{(\tau_1 + \tau_2)\phi_1} + \tau a_1 & \frac{\tau_2 J_x - 2\theta_x}{(\tau_1 + \tau_2)\phi_2} \\
-\frac{\tau_1 J_x - 2\theta_x}{(\tau_1 + \tau_2)\phi_1} & -\frac{\tau_2 J_x - 2\theta_x}{(\tau_1 + \tau_2)\phi_2} + \tau a_2
\end{pmatrix} \]

\[ J_s = \vec{K}_{T,s} \cdot (\sum_s \vec{\phi}_N^{(i)} + \vec{S}) \]

\[ \theta_s = \vec{L}_{T,s} \cdot (\sum_s \vec{\phi}_N^{(i)} + \vec{S}) \]

- **dominant eigenvalue (flat-flux fixed point)**:

  \[ \lambda = -\frac{1}{\det(A_D)} \left[ (\tau a_2 \Sigma s_1 K_1 + \tau a_1 \Sigma s_2 |K_2|) - \frac{2}{3} \frac{\tau a_2 \Sigma s_1 (A_{11} - A_{21}) + \tau a_1 \Sigma s_2 (A_{22} - A_{12})}{(\tau_1 + \tau_2)} \right] \]

  interface current term

  average flux term

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Paris, 27 April 2010
case2: interface parameter effect (K=N=2)

- **Infinite-diffusive material limit**: 
  \[ \lim_{p \to \infty} \lambda = -\infty \]
  with the leading term \( - (c \tau p)^2 |K_2| \)

- **Infinite-absorber material limit**: 
  \[ \lim_{p \to 0} \lambda = - \frac{c}{2(1 - c)} \frac{G(\tau)}{\tau} \]
  stability condition: 
  \[ c < \frac{2}{2 + \frac{G(\tau)}{\tau}} \bigg|_{\tau=1} = 0.911 \]

- **Numerical bifurcation**: 
  obtained by running the code with 200 iterations without stopping criterion, for each value of \( p \) are plotted the 20 latest iterations
case2: interface parameter effect (K=N=2)

- Scanning the absorber-limit stability condition

Absorber-limit stability condition for $\tau = 10 : c < 0.9996$

Absorber-limit stability condition for $\tau = 0.1 : c < 0.8269$
stabilizing the interface effect

- new finite-difference diffusion coefficient with stability parameter:

\[ \tilde{d}_{sk} = x \frac{\theta_s}{\phi_s} \frac{2}{\tau_{sk}} \]

where \( x \) is the stability parameter

(N:B: \( x \) is surface dependent.)

dominant eigenvalue as a function of the stability parameter:

\[ \lambda(x) = \lambda_\infty \frac{x - x_0}{x - x_\infty} \]

\[ \lambda_\infty = \frac{\tau a_2 \Sigma s_1 (A_{11} - A_{21}) + \tau a_1 \Sigma s_2 (A_{22} - A_{12})}{\tau a_2 + \tau a_1} \]

\[ x_\infty = -\frac{3}{2} \frac{\tau a_2 \tau a_1}{\tau a_2 + \tau a_1} (\tau_2 + \tau_1) \]

\[ x_0 = \frac{3}{2} \frac{(\tau a_2 \Sigma s_1 K_1 + \tau a_1 \Sigma s_2 |K_2|)(\tau_1 + \tau_2)}{\tau a_2 \Sigma s_1 (A_{11} - A_{21}) + \tau a_1 \Sigma s_2 (A_{22} - A_{12})} \]
stabilizing the interface effect

- evaluating the optimal stability parameter:
  \[ \lambda(x_0) = 0 \]

- the optimal stability parameter as a function
  \[ x_0 = x_0(p, c, \tau) \]
  \[ x_0 \propto (\tau_1 + \tau_2) \]
further remarks

- the unstable modes are generated by the interface parameter to establish the equivalence

- the homogenization is a means to stabilize the scheme (…but is problem dependent!)

- heuristic recipe: the ratio between optical paths of 2 neighbor coarse-meshes must be in the interval \([1/5, 5]\)

- the scheme needs a stability parameter to be unconditionally stable

- it is difficult to evaluate the optimal stability parameter for realistic calculations

\[ x_0 = \beta_T (\tau_1 + \tau_2) \]

- alternative strategy to be explored:

\[ J_s = -d_{sk}(\phi_s - \phi_k) + f_{sk}\phi_k + x\phi_s \]
ongoing works: domain decomposition

- for $i = 1, N$
  start loop on assemblies:

  - for $\alpha = 1, A$
    start iterative solution for assembly $\alpha$

    * for $j = 1, M$
      
      $$(L - H)_{\alpha} \psi_{\alpha}^{(i,j+1)}(x) = \frac{1}{\lambda^{(i)}} F_{\alpha} \psi_{\alpha}^{(i,j)}(x) \quad x \in X_{\alpha}$$
      $$
      \psi_{\alpha}^{(i,j+1)}(x) = \psi_{\alpha}^{(i,j)}(x) - x_+ \in X_{\alpha_+}
      $$
      
      with
      
      $$
      \psi_{\alpha\beta}^{(i,j)}(x) = \begin{cases} 
      \psi_{\alpha}^{(i,j)}(x) & \text{for } x_+ \in X_{\alpha_+} \cap X_{\beta_+} \neq 0 \\
      \beta \psi_{\alpha}^{(i,j)}(x) + s_{\alpha}(x) & \text{for } x_+ \in X_{\alpha_+} \cap X \neq 0
      \end{cases}
      $$
    
    * exit if:
    
    $$
    e_F = \left| 1 - \frac{(1, F \psi_{\alpha}^{(i,j+1)})(r)}{(1, F \psi_{\alpha}^{(i,j)})(r)} \right| < \epsilon
    $$
    
    • compute the new $\lambda^{(i+1)}$ with the converged fluxes $\psi_{\alpha}^{(i)}$
    
    $$
    \lambda^{(i+1)} = \sum_{\alpha = 1, A} \left( w, F_{\alpha} \psi_{\alpha}^{(i,j+1)} \right) /
    \sum_{\alpha = 1, A} \left( w, F_{\alpha} \psi_{\alpha}^{(i,j)} \right)
    $$
    current exchange between assemblies:

    $$
    \psi_{\alpha\beta}^{(i+1)}(x) = \psi_{\beta}^{(i+1)}(x) \quad \text{for } x_+ \in X_{\alpha_+} \cap X_{\beta_+} \neq 0
    $$

    • exit if:
    
    $$
    e_\lambda = \left| 1 - \frac{\lambda^{(i+1)}}{\lambda^{(i)}} \right| < \epsilon
    $$

Paris, 27 April 2010
Introducing a non-linear equivalent operator to update the eigenvalue, the interface flux and the volume flux:

\[ (\lambda, \psi_{\alpha\beta}, \psi_{\alpha}) \equiv \text{accelerated quantities} \]

we define the average scalar flux on assembly

\[ \phi_{\alpha} = (1, \psi)_{\alpha} = \sum_{n \in \alpha} (1, \psi_n) \]

at each external iteration we can construct for each assembly:

a volume prolongation operator

\[ p_{\alpha}(x) = \frac{\psi_{\alpha}(x)}{\phi_{\alpha}} \]

a surface prolongation operator

\[ p_{\alpha\beta}(x_{\text{e}}) = \begin{cases} \frac{\psi_{\beta}(x_{\text{e}})}{\phi_{\beta}} & \text{for } x_{\text{e}} \in X_{\alpha-} \cap X_{\beta+} \neq 0 \\ \frac{\beta \psi_{\alpha}(x_{\text{e}}) + s_{in}(x_{\text{e}})}{\phi_{\alpha}} & \text{for } x_{\text{e}} \in X_{\alpha-} \cap X_{\text{e}} \neq 0 \end{cases} \]

the equivalent surface parameters

\[ f_{s\alpha} = \frac{J_{s\alpha} + d_{s\alpha}(\phi_{s\alpha} - \phi_{\alpha})}{\phi_{\alpha}} \]

coarse-mesh finite difference operator

\[ A(\psi_{\alpha}) \equiv \frac{1}{\lambda} F(\psi_{\alpha}) \]

Solve the finite-difference system on the whole core:

\[ A(\psi_{\alpha}) \phi = \frac{1}{\lambda} F(\psi_{\alpha}) \overline{\phi} \]

CMFD solution

\[ \overline{\phi} = \left\{ \phi_{\alpha} \right\}_{\alpha=1,A} \]

at the convergence:

\[ \overline{\phi}_{\alpha} = \phi_{\alpha} \]

\[ \psi_{\alpha}^{(i+1)}(x) = p_{\alpha}(x) \overline{\phi}_{\alpha} \]

\[ \psi_{\alpha\beta}^{(i+1)}(x) = p_{\alpha\beta}(x_{\text{e}}) \overline{\phi}_{\alpha} \]

\[ \lambda^{(i+1)} = \lambda \]
transport non-linear equivalent operator

- Fine transport solution as a statement of linearity

  angular balance equation
  \[ [(\psi_N^+ - \psi_N^-) + \Sigma_N \psi_N](\Omega) = q_N(\Omega) \]

  angular transmission equation
  \[ \psi_N^+(\Omega) = T_N \psi_N^-(\Omega) + E_N q_N(\Omega) \]

- construction of the projection scalar products:
  \[ P_{KN}\psi_N \rightarrow \psi_k(\Delta \Omega_k) = (1, \psi_N)_k = \sum_n (1, \psi_n)_k \]
  \[ (f, g)_k = \frac{1}{4\pi V_k} \int_G dE \int_{\Delta \Omega_k} d\Omega \int_{D_h} dr (fg)(r, \Omega, E) \]
  \[ P_{KN}^{\pm}\psi_N \rightarrow \psi_k^{\pm}(\Delta \Omega_k) = \langle 1, \psi_N \rangle_{sk}^{\pm} = \sum_{n \in k} \langle 1, \psi_n \rangle_{sk}^{\pm} \]
  \[ (f, g)_{sk}^{\pm} = \frac{1}{\pi S_k} \int_G dE \int_{\Delta \Omega_k \in 2\pi} d\Omega \int_{\partial D_h} ds |n_s \cdot \Omega|(fg)(r, \Omega, E) \]

- Angular balance transport equation on the coarser region
  \[ (\psi_K^+ - \psi_K^-) + \Sigma_K \psi_K = q_K \]

  angular dependent homogeneous cross-sections
  \[ q_k(\Delta \Omega_k) = (1, q)_k \]

  implies:
  \[ \Sigma_k(\psi_N, \Delta \Omega_k) = \frac{(1, \Sigma_N \psi_N)_k}{(1, \psi_N)_k} \]

- Angular transmission equation on the coarser grid
  equivalent transmission equation:
  \[ \psi_K^+(\Delta \Omega_k) = P_{KN}^+ [T_N \psi_N^- + E_N q_N](\Delta \Omega_k) \]

  conservation relations for the equivalent transmission equation:
  \[ T_K(\psi_N) P_{KN}^- \psi_N = P_{KN}^+ T_N \psi_N \]
  \[ E_K(q_N) P_{KN} q_N = P_{KN}^+ E_N q_N \]
Jacobian-free Newton-Krylov Method

- Transform the explicit mapping in an implicit mapping
  \[
  \psi = F(\psi) \rightarrow F(\psi) = 0
  \]

- Newton's Method solves a system of nonlinear equations by a sequence of steps including the linear problem. The equation for the error is solved at each iteration
  \[
  J^{(i)} \delta \psi^{(i)} = -F(\psi^{(i)})
  \]
  where the Jacobian is defined by:
  \[
  J^{(i)} = J_{n,m}(\psi^{(i)}) = \left. \frac{\partial F_n}{\partial \psi_m} \right|_{\psi = \psi^{(i)}}, \text{ for } n, m = 1, N
  \]

- Additive correction:
  \[
  \psi^{(i+1)} = \psi^{(i)} + \delta \psi^{(i)}
  \]
  and the iterations continue until
  \[
  \left\| F(\psi^{(i)}) \right\| < \text{tol}_n \left\| F(\psi^{(0)}) \right\|
  \]
  where \( \text{tol}_n \) is a non-linear tolerance

- The Krylov method only needs the action of the Jacobian matrix to construct the j-th iterate of:
  \[
  \delta \psi^{(i,j)} = a_0 r_0 + a_1 J^{(i)} r_0 + a_2 (J^{(i)})^2 r_0 + \ldots + a_N (J^{(i)})^j r_0
  \]
  \[
  r_0 = J^{(i)} \delta \psi^{(i,0)} + F(\psi^{(i)})
  \]

- The matrix-vector product required by the Krylov method can be approximated with a single function evaluation:
  \[
  J^{(i)} r_0 \approx \frac{F(\psi^{(i)} + \epsilon r_0) - F(\psi^{(i)})}{\epsilon}
  \]
non-equivalent operator: 2D-transport / 3D diffusion

Consider the transport equation:

\[ \mathbf{\Omega} \cdot \nabla \psi (\mathbf{r}, \mathbf{\Omega}) + \Sigma (\mathbf{r}) \psi (\mathbf{r}, \mathbf{\Omega}) = q (\mathbf{r}, \mathbf{\Omega}) \]

\[ \psi (\mathbf{r}, \mathbf{\Omega}) = \psi (z, \mathbf{r}_\perp, \mathbf{\Omega}) \quad \rightarrow \quad \mathbf{\Omega} \cdot \nabla \rightarrow \Omega_z \partial_z + \Omega_\perp \cdot \nabla_\perp \]

2D equivalent problem that take into account the 3D axial effects:

\[ \Omega_\perp \cdot \nabla_\perp \psi_k (\mathbf{r}_\perp, \mathbf{\Omega}) + \Sigma_k (\mathbf{r}_\perp) \psi_k (\mathbf{r}_\perp, \mathbf{\Omega}) = q_k (\mathbf{r}_\perp, \mathbf{\Omega}) - \Omega_z [\psi (z^+_k, \mathbf{r}_\perp, \mathbf{\Omega}) - \psi (z^-_k, \mathbf{r}_\perp, \mathbf{\Omega})] \]

where:

\[ \psi_k (\mathbf{r}_\perp, \mathbf{\Omega}) = \int_{z^-_k}^{z^+_k} dz \psi (z, \mathbf{r}_\perp, \mathbf{\Omega}) \]

If the streaming source is known than it is possible to solve the previous equation with the standard 2D transport solver (excepted for a real 3D angular sweeping).

Diffusion approximation of the interface flux on the k-th interface plane:

\[ \psi (z^+_k, \mathbf{r}_\perp, \mathbf{\Omega}) \sim \frac{1}{4\pi} [\phi (z^+_k, \mathbf{r}_\perp) + 3\mathbf{\Omega} \cdot \mathbf{J} (z^+_k, \mathbf{r}_\perp)]_{\text{core}} \]

Such interface scalar fluxes and currents could be provided by a standard 3D diffusion code. The diffusion calculation is alimented by the homogenized transport cross-sections.
Step 1: solve the 2D transport problem for each transversal plane $k$ and each assembly

$$\mathbf{\Omega}_\perp \cdot \nabla_\perp \psi_k(\mathbf{r}_\perp, \mathbf{\Omega}) + \Sigma_k(\mathbf{r}_\perp) \psi_k(\mathbf{r}_\perp, \mathbf{\Omega}) = q_k(\mathbf{r}_\perp, \mathbf{\Omega}) + q_{k,core}(\mathbf{r}_\perp, \mathbf{\Omega})$$

Step 2: assembly homogenization + transverse equivalence

$$\Sigma_{\alpha,k}^{\text{hom}} = \int d\mathbf{r}_\perp \Sigma_k(\mathbf{r}_\perp) \int_{4\pi} d\Omega \psi_k(\mathbf{r}_\perp, \mathbf{\Omega})$$

Step 3: solve the 3D non-linear diffusion problem on the core level with homogenized assemblies

$$\sum_{s \in (\alpha,k)} J_{s,\alpha,k} + \Sigma_{\alpha,k}^{\text{hom}} \phi_{\alpha,k} = q_{\alpha,k}(\mathbf{r}, \mathbf{\Omega})$$

$$J_{s,\alpha,k} = -d_{s,\alpha,k}(\phi_{s,\alpha,k} - \phi_{\alpha,k}) + f_{s,k} \phi_{\alpha,k}$$

Step 4: up-date the streaming source for each plane

$$q_{k,\text{core}}(\mathbf{r}_\perp, \mathbf{\Omega}) \sim -\frac{\Omega}{4\pi} \left[ (\phi_k^+ - \phi_k^-) + 3 \mathbf{\Omega} \cdot (\mathbf{J}_k^+ - \mathbf{J}_k^-) \right]_{\text{core}}(\mathbf{r}_\perp)$$

The approximation could be extended to transversal interface of the assembly (on the 2D plane) to feed each assembly transport calculation with independent boundary conditions. The transversal current and flux are provided by the core code.
open questions

For the non-linear acceleration:

- the stability of the scheme
- the investigation of non-linear operator more rich than finite difference
- a proper way to stabilize the iterations

For non-linear approximated transport solutions

- the existence and the accuracy of the solution.
- the stability of the scheme.