Karlsruhe Institute of Technology

A Parallel Neutron Transport Solver based on Domain-Decomposition

S. Van Criekingen[1] F. Nataf[2] P. Havé[3]

[1]Karlsruhe Institute for Technology (KIT/INR), Germany

[2]J.-L. Lions Laboratory, Paris VI University, CNRS UMR 7598, France

[3]French Petroleum Institute, Rueil-Malmaison, France

June 15, 2010

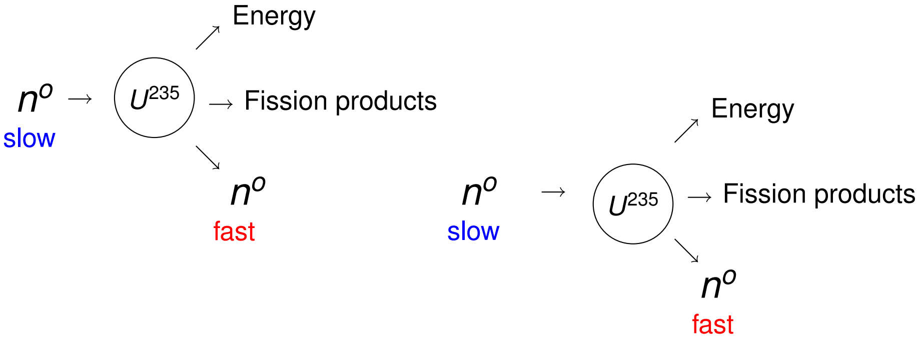
Outline

Nuclear fission chain reaction

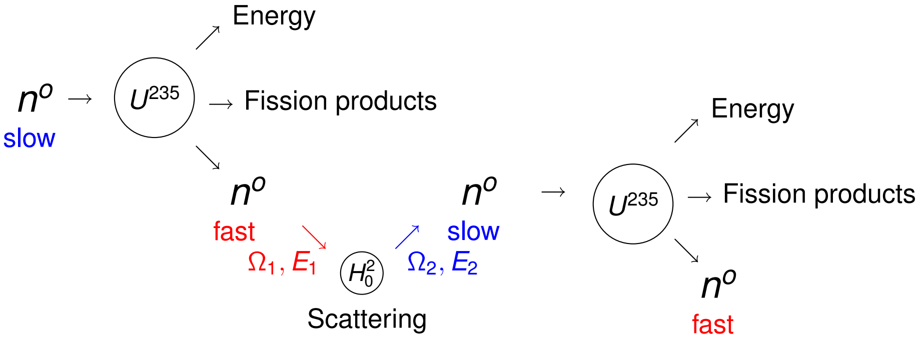
$$n^o \longrightarrow U^{235} \longrightarrow \begin{cases} \nearrow \text{Energy} \\ \longrightarrow \text{Fission products} \\ \searrow n^o \end{cases}$$

Nuclear fission chain reaction

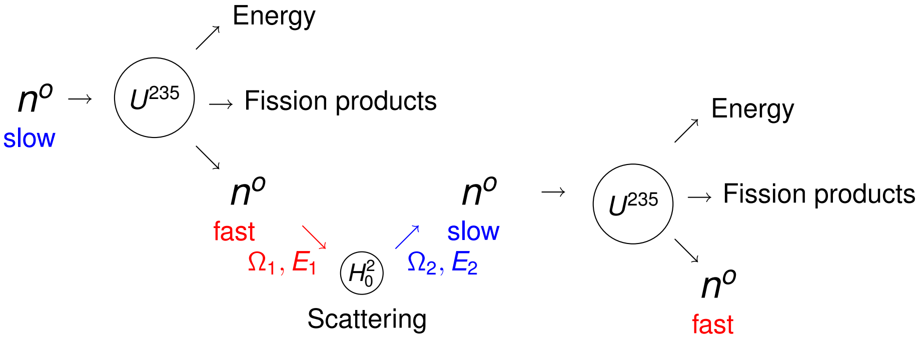
Nuclear fission chain reaction



Nuclear fission chain reaction

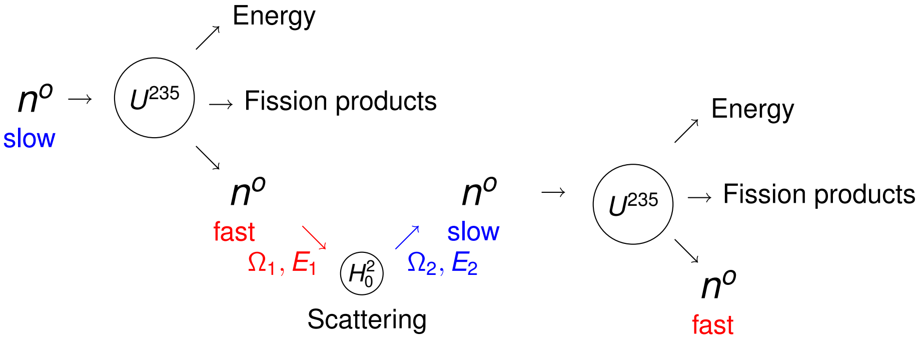


Nuclear fission chain reaction



Chain reaction must be **self-sustainable** in **stationary mode**.

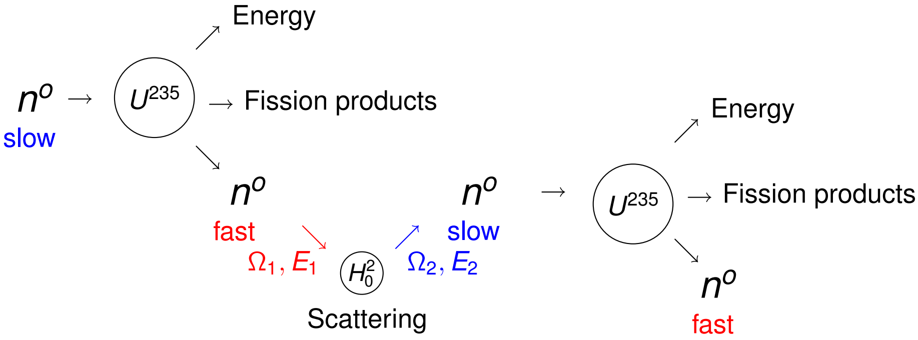
Nuclear fission chain reaction



Chain reaction must be **self-sustainable** in **stationary mode**.

Here 2 energy groups: group 1 $\equiv$ fast, group 2 $\equiv$ slow.

Nuclear fission chain reaction



Chain reaction must be **self-sustainable** in **stationary mode**.

Here 2 energy groups: group 1 $\equiv$ fast, group 2 $\equiv$ slow.

In general: **multigroup** energy discretization, i.e., **piecewise constant**.

Transport equation in stationary mode

- unknown: $\Psi(\mathbf{r}, \Omega, E)$

Transport equation in stationary mode

Karlsruhe Institute of Technology

- unknown: $\Psi(\mathbf{r}, \Omega, E)$
- in each energy group: $\Psi_g(\mathbf{r}, \Omega)$

Transport equation in stationary mode

Karlsruhe Institute of Technology

- unknown: $\Psi(\mathbf{r}, \Omega, E)$
- in each energy group: $\Psi_g(\mathbf{r}, \Omega)$
- balance without external source (self-sustainability):

$$\left[\Omega \cdot \nabla + \sigma_g(\mathbf{r})\right] \Psi_g(\mathbf{r}, \Omega) = \sum_{g'=1}^{G} \int_{S^2} S_{g' \to g}(\mathbf{r}, \Omega' \to \Omega)\, \Psi_{g'}(\mathbf{r}, \Omega')\, d\Omega' + \sum_{g'=1}^{G} \int_{S^2} F_{g' \to g}(\mathbf{r}, \Omega' \to \Omega)\, \Psi_{g'}(\mathbf{r}, \Omega')\, d\Omega'$$

Transport equation in stationary mode

Karlsruhe Institute of Technology

- unknown: $\Psi(\mathbf{r}, \Omega, E)$
- in each energy group: $\Psi_g(\mathbf{r}, \Omega)$
- balance without external source (self-sustainability):

$$\left[\Omega \cdot \nabla \; + \; \sigma_g(\mathbf{r})\right] \Psi_g(\mathbf{r}, \Omega) \; = \; \sum_{g'=1}^{G} \int_{S^2} S_{g' \to g}(\mathbf{r}, \Omega' \to \Omega) \, \Psi_{g'}(\mathbf{r}, \Omega') \, d\Omega'$$

$$+ \frac{1}{k} \sum_{g'=1}^{G} \int_{S^2} F_{g' \to g}(\mathbf{r}, \Omega' \to \Omega) \, \Psi_{g'}(\mathbf{r}, \Omega') \, d\Omega'$$

Transport equation in stationary mode

- unknown: $\Psi(\mathbf{r}, \Omega, E)$
- in each energy group: $\Psi_g(\mathbf{r}, \Omega)$
- balance without external source (self-sustainability):

$$\left[\Omega \cdot \nabla \;+\; \sigma_g(\mathbf{r})\right] \Psi_g(\mathbf{r}, \Omega) \;=\; \sum_{g'=1}^{G} \int_{S^2} S_{g' \to g}(\mathbf{r}, \Omega' \to \Omega)\, \Psi_{g'}(\mathbf{r}, \Omega')\, d\Omega' + \frac{1}{k} \sum_{g'=1}^{G} \int_{S^2} F_{g' \to g}(\mathbf{r}, \Omega' \to \Omega)\, \Psi_{g'}(\mathbf{r}, \Omega')\, d\Omega'$$

Criticality:
- $k > 1$ super-critical
- $k = 1$ critical
- $k < 1$ sub-critical

Transport equation in stationary mode

- unknown: $\Psi(\mathbf{r}, \Omega, E)$
- in each energy group: $\Psi_g(\mathbf{r}, \Omega)$
- balance without external source (self-sustainability):

$$\underbrace{\left[\Omega \cdot \nabla \; + \; \sigma_g(\mathbf{r})\right]}_{A_g(\mathbf{r},\Omega)} \Psi_g(\mathbf{r}, \Omega) \;=\; \sum_{g'=1}^{G} \int_{S^2} S_{g' \to g}(\mathbf{r}, \Omega' \to \Omega)\, \Psi_{g'}(\mathbf{r}, \Omega')\, d\Omega'$$

$$+ \frac{1}{k} \sum_{g'=1}^{G} \int_{S^2} F_{g' \to g}(\mathbf{r}, \Omega' \to \Omega)\, \Psi_{g'}(\mathbf{r}, \Omega')\, d\Omega'$$

Criticality:
- $k > 1$ super-critical
- $k = 1$ critical
- $k < 1$ sub-critical

Criticality problem, if 3 energy groups

$$
\begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = \begin{pmatrix} S_{1\to1} & S_{2\to1} & S_{3\to1} \\ S_{1\to2} & S_{2\to2} & S_{3\to2} \\ S_{1\to3} & S_{2\to3} & S_{3\to3} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} + \frac{1}{k}\begin{pmatrix} F_{1\to1} & F_{2\to1} & F_{3\to1} \\ F_{1\to2} & F_{2\to2} & F_{3\to2} \\ F_{1\to3} & F_{2\to3} & F_{3\to3} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}
$$

Criticality problem, if 3 energy groups

Karlsruhe Institute of Technology

$$\begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = \begin{pmatrix} S_{1\to1} & \simeq 0 & \simeq 0 \\ S_{1\to2} & S_{2\to2} & \simeq 0 \\ S_{1\to3} & S_{2\to3} & S_{3\to3} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} + \frac{1}{k}\begin{pmatrix} F_{1\to1} & F_{2\to1} & F_{3\to1} \\ F_{1\to2} & F_{2\to2} & F_{3\to2} \\ F_{1\to3} & F_{2\to3} & F_{3\to3} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}$$

Criticality problem, if 3 energy groups

Karlsruhe Institute of Technology

$$\begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = \begin{pmatrix} S_{1\to 1} & \simeq 0 & \simeq 0 \\ S_{1\to 2} & S_{2\to 2} & \simeq 0 \\ S_{1\to 3} & S_{2\to 3} & S_{3\to 3} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} + \frac{1}{k}\begin{pmatrix} F_{1\to 1} & F_{2\to 1} & F_{3\to 1} \\ \simeq 0 & \simeq 0 & \simeq 0 \\ \simeq 0 & \simeq 0 & \simeq 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}$$

Criticality problem, if 3 energy groups

$$\begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = \begin{pmatrix} S_{1\to1} & \simeq 0 & \simeq 0 \\ S_{1\to2} & S_{2\to2} & \simeq 0 \\ S_{1\to3} & S_{2\to3} & S_{3\to3} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} + \frac{1}{k}\begin{pmatrix} F_{1\to1} & F_{2\to1} & F_{3\to1} \\ \simeq 0 & \simeq 0 & \simeq 0 \\ \simeq 0 & \simeq 0 & \simeq 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}$$

$$\Rightarrow \overbrace{\begin{pmatrix} H_{1\to1} & \simeq 0 & \simeq 0 \\ H_{1\to2} & H_{2\to2} & \simeq 0 \\ H_{1\to3} & H_{2\to3} & H_{3\to3} \end{pmatrix}}^{H = \text{``}A - S\text{''}}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = \frac{1}{k}\begin{pmatrix} F_{1\to1} & F_{2\to1} & F_{3\to1} \\ \simeq 0 & \simeq 0 & \simeq 0 \\ \simeq 0 & \simeq 0 & \simeq 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}$$

Criticality problem, if 3 energy groups

Karlsruhe Institute of Technology

$$\begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = \begin{pmatrix} S_{1\to1} & \simeq 0 & \simeq 0 \\ S_{1\to2} & S_{2\to2} & \simeq 0 \\ S_{1\to3} & S_{2\to3} & S_{3\to3} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} + \frac{1}{k}\begin{pmatrix} F_{1\to1} & F_{2\to1} & F_{3\to1} \\ \simeq 0 & \simeq 0 & \simeq 0 \\ \simeq 0 & \simeq 0 & \simeq 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}$$

$$\Rightarrow \overbrace{\begin{pmatrix} H_{1\to1} & \simeq 0 & \simeq 0 \\ H_{1\to2} & H_{2\to2} & \simeq 0 \\ H_{1\to3} & H_{2\to3} & H_{3\to3} \end{pmatrix}}^{H = \text{“}A - S\text{”}}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = \frac{1}{k}\begin{pmatrix} F_{1\to1} & F_{2\to1} & F_{3\to1} \\ \simeq 0 & \simeq 0 & \simeq 0 \\ \simeq 0 & \simeq 0 & \simeq 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}$$

$$\Rightarrow \boxed{H\,\Psi = \tfrac{1}{k}\,F\,\Psi}$$ generalized eigenvalue problem

Criticality problem

$$H\,\Psi = \frac{1}{k} F\,\Psi \quad \Rightarrow \quad M\,\Psi = k\,\Psi \qquad \text{with} \quad M = H^{-1}F$$

Criticality problem

$$H\,\Psi = \frac{1}{k} F\,\Psi \quad \Rightarrow \quad M\,\Psi = k\,\Psi \qquad \text{with} \quad M = H^{-1} F$$

Power method (+ Chebyshev) on the standard EV problem

Criticality problem

$$H\,\Psi = \frac{1}{k} F\,\Psi \quad \Rightarrow \quad M\,\Psi = k\,\Psi \qquad \text{with} \quad M = H^{-1} F$$

Power method (+ Chebyshev) on the standard EV problem

Each power iteration ("outer iteration") requires inverting H, with

$$H = \begin{pmatrix} H_{1\to1} & \simeq 0 & \simeq 0 \\ H_{1\to2} & H_{2\to2} & \simeq 0 \\ H_{1\to3} & H_{2\to3} & H_{3\to3} \end{pmatrix}$$

Criticality problem

$$H\,\Psi = \frac{1}{k} F\,\Psi \quad \Rightarrow \quad M\,\Psi = k\,\Psi \qquad \text{with} \quad M = H^{-1} F$$

Power method (+ Chebyshev) on the standard EV problem

Each power iteration ("outer iteration") requires inverting H, with

$$H = \begin{pmatrix} H_{1\to 1} & \simeq 0 & \simeq 0 \\ H_{1\to 2} & H_{2\to 2} & \simeq 0 \\ H_{1\to 3} & H_{2\to 3} & H_{3\to 3} \end{pmatrix}$$

$\Rightarrow$ Gauss-Seidel at the energy level

Criticality problem

$$H\,\Psi = \frac{1}{k} F\,\Psi \quad \Rightarrow \quad M\,\Psi = k\,\Psi \qquad \text{with} \quad M = H^{-1} F$$

Power method (+ Chebyshev) on the standard EV problem

Each power iteration ("outer iteration") requires inverting H, with

$$H = \begin{pmatrix} H_{1\to 1} & \simeq 0 & \simeq 0 \\ H_{1\to 2} & H_{2\to 2} & \simeq 0 \\ H_{1\to 3} & H_{2\to 3} & H_{3\to 3} \end{pmatrix}$$

$\Rightarrow$ Gauss-Seidel at the energy level

$\forall g$, one must invert $H_{g\to g}$ $\equiv$ spatio-angular solve.

Criticality problem

$$H\,\Psi = \frac{1}{k} F\,\Psi \quad \Rightarrow \quad M\,\Psi = k\,\Psi \qquad \text{with} \quad M = H^{-1} F$$

Power method (+ Chebyshev) on the standard EV problem

Each power iteration ("outer iteration") requires inverting H, with

$$H = \begin{pmatrix} H_{1\to1} & \simeq 0 & \simeq 0 \\ H_{1\to2} & H_{2\to2} & \simeq 0 \\ H_{1\to3} & H_{2\to3} & H_{3\to3} \end{pmatrix}$$

$\Rightarrow$ Gauss-Seidel at the energy level

$\forall g$, one must invert $H_{g\to g} \equiv$ spatio-angular solve.

$$H_{g\to g}\Psi_g(\mathbf{r},\Omega) \equiv \left[\,\Omega\cdot\nabla + f_g(\mathbf{r},\Omega)\,\right]\Psi_g(\mathbf{r},\Omega)$$

Spatio-angular solve (i.e., inverting $H_{g\to g}$)

Karlsruhe Institute of Technology

Simplified case: $[\,\Omega\cdot\nabla+\sigma(\mathbf{r})\,]\,\Psi(\mathbf{r},\Omega) \;=\; \text{rhs}(\mathbf{r})$

Spatio-angular solve (i.e., inverting $H_{g\to g}$)

Karlsruhe Institute of Technology

Simplified case: $\left[\,\Omega\cdot\nabla+\sigma(\mathbf{r})\,\right]\Psi(\mathbf{r},\Omega) \;=\; \mathrm{rhs}(\mathbf{r})$

Even-odd (w.r.t. Ω) splitting: $\Psi^{\pm}(\mathbf{r},\Omega)=\frac{1}{2}\left(\Psi(\mathbf{r},\Omega)\pm\Psi(\mathbf{r},-\Omega)\right)$

Spatio-angular solve (i.e., inverting $H_{g \to g}$)

Simplified case: $[\,\Omega \cdot \nabla + \sigma(\mathbf{r})\,]\,\Psi(\mathbf{r},\Omega) \;=\; \text{rhs}(\mathbf{r})$

Even-odd (w.r.t. Ω) splitting: $\Psi^{\pm}(\mathbf{r},\Omega) = \frac{1}{2}\left(\Psi(\mathbf{r},\Omega) \pm \Psi(\mathbf{r},-\Omega)\right)$

$$\Rightarrow \begin{cases} \Omega \cdot \nabla \Psi^{-}(\mathbf{r},\Omega) + \sigma(\mathbf{r})\,\Psi^{+}(\mathbf{r},\Omega) = \text{rhs}(\mathbf{r}) \\ \Omega \cdot \nabla \Psi^{+}(\mathbf{r},\Omega) + \sigma(\mathbf{r})\,\Psi^{-}(\mathbf{r},\Omega) = 0 \end{cases}$$

Spatio-angular solve (i.e., inverting $H_{g\to g}$)

Karlsruhe Institute of Technology

Simplified case: $[\,\Omega\cdot\nabla+\sigma(\mathbf{r})\,]\,\Psi(\mathbf{r},\Omega) \;=\; \mathrm{rhs}(\mathbf{r})$

Even-odd (w.r.t. Ω) splitting: $\Psi^{\pm}(\mathbf{r},\Omega)=\dfrac{1}{2}\left(\Psi(\mathbf{r},\Omega)\pm\Psi(\mathbf{r},-\Omega)\right)$

$$\Rightarrow \begin{cases} \Omega\cdot\nabla\Psi^{-}(\mathbf{r},\Omega)+\sigma(\mathbf{r})\,\Psi^{+}(\mathbf{r},\Omega)=\mathrm{rhs}(\mathbf{r}) \\ \Omega\cdot\nabla\Psi^{+}(\mathbf{r},\Omega)+\sigma(\mathbf{r})\,\Psi^{-}(\mathbf{r},\Omega)=0 \end{cases}$$

Second-order formulation (w.r.t. $\mathbf{r}$):

$$\Omega\cdot\nabla\left[\frac{1}{\sigma(\mathbf{r})}\,\Omega\cdot\nabla\Psi^{+}(\mathbf{r},\Omega)\right]+\sigma(\mathbf{r})\,\Psi^{+}(\mathbf{r},\Omega)=\mathrm{rhs}(\mathbf{r})$$

Spatio-angular solve (i.e., inverting $H_{g\to g}$)

Karlsruhe Institute of Technology

Simplified case: $[\,\Omega\cdot\nabla+\sigma(\mathbf{r})\,]\,\Psi(\mathbf{r},\Omega) \;=\; \mathrm{rhs}(\mathbf{r})$

Even-odd (w.r.t. Ω) splitting: $\Psi^{\pm}(\mathbf{r},\Omega)=\dfrac{1}{2}\left(\Psi(\mathbf{r},\Omega)\pm\Psi(\mathbf{r},-\Omega)\right)$

$$\Rightarrow \begin{cases} \Omega\cdot\nabla\Psi^{-}(\mathbf{r},\Omega)+\sigma(\mathbf{r})\,\Psi^{+}(\mathbf{r},\Omega)=\mathrm{rhs}(\mathbf{r}) \\ \Omega\cdot\nabla\Psi^{+}(\mathbf{r},\Omega)+\sigma(\mathbf{r})\,\Psi^{-}(\mathbf{r},\Omega)=0 \end{cases}$$

Second-order formulation (w.r.t. $\mathbf{r}$): self-adjoint

$$\Omega\cdot\nabla\left[\frac{1}{\sigma(\mathbf{r})}\,\Omega\cdot\nabla\Psi^{+}(\mathbf{r},\Omega)\right]+\sigma(\mathbf{r})\,\Psi^{+}(\mathbf{r},\Omega)=\mathrm{rhs}(\mathbf{r})$$

Spatio-angular discretization

Karlsruhe Institute of Technology

- Space: Finite Elements

Spatio-angular discretization

Karlsruhe Institute of Technology

- Space: Finite Elements
- Angle: Spherical Harmonics Y_{lm}

Spatio-angular discretization

Karlsruhe Institute of Technology

- Space: Finite Elements
- Angle: Spherical Harmonics Y_{lm}
  - A P_N approximation truncates the series at $n = N$ in Y_{nm}.

Spatio-angular discretization

Karlsruhe Institute of Technology

- Space: Finite Elements

- Angle: Spherical Harmonics Y_{lm}
  - A P_N approximation truncates the series at $n = N$ in Y_{nm}.
  - P_1 approximation $\Rightarrow$ second-order formulation $\equiv$ diffusion equation.

$$\Omega \cdot \nabla \left[\frac{1}{\sigma(\mathbf{r})} \Omega \cdot \nabla \Psi^{+}(\mathbf{r}, \Omega) \right] \quad \text{becomes} \quad \nabla \cdot \left[D(\mathbf{r}) \nabla \Psi^{+}(\mathbf{r}) \right]$$

Small wrap-up

We need to invert

$$H = \begin{pmatrix} H_{1\to1} & \simeq 0 & \simeq 0 \\ H_{1\to2} & H_{2\to2} & \simeq 0 \\ H_{1\to3} & H_{2\to3} & H_{3\to3} \end{pmatrix}$$

With the second-order formulation, the $H_{g\to g}$ are symmetric.

Small wrap-up

We need to invert

$$H = \begin{pmatrix} H_{1\to 1} & \simeq 0 & \simeq 0 \\ H_{1\to 2} & H_{2\to 2} & \simeq 0 \\ H_{1\to 3} & H_{2\to 3} & H_{3\to 3} \end{pmatrix}$$

With the second-order formulation, the $H_{g\to g}$ are symmetric.

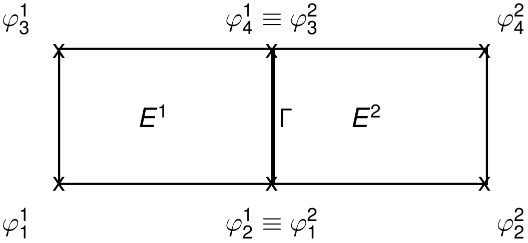
We use algebraic domain decomposition to invert the H_{gg}.

Outline

Karlsruhe Institute of Technology

Two-domain example

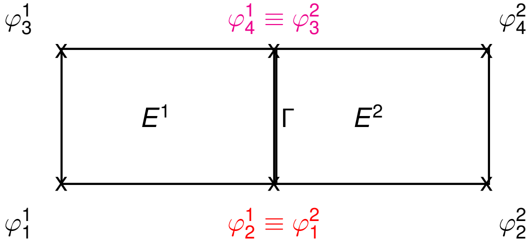
Hyp: each domain is made out of **one** FE.



$$\mathcal{A}\Psi = Q \Rightarrow \begin{pmatrix} a^i_{11} & a^i_{21} & a^i_{31} & a^i_{41} \\ a^i_{21} & a^i_{22} & a^i_{32} & a^i_{42} \\ a^i_{31} & a^i_{32} & a^i_{33} & a^i_{43} \\ a^i_{41} & a^i_{42} & a^i_{43} & a^i_{44} \end{pmatrix} \begin{pmatrix} \varphi^i_1 \\ \varphi^i_2 \\ \varphi^i_3 \\ \varphi^i_4 \end{pmatrix} = \begin{pmatrix} q^i_1 \\ q^i_2 \\ q^i_3 \\ q^i_4 \end{pmatrix}, \qquad i = 1, 2.$$

Two-domain example

Hyp: each domain is made out of **one** FE.



$$\mathcal{A}\Psi = Q \Rightarrow \begin{pmatrix} a_{11}^i & a_{21}^i & a_{31}^i & a_{41}^i \\ a_{21}^i & a_{22}^i & a_{32}^i & a_{42}^i \\ a_{31}^i & a_{32}^i & a_{33}^i & a_{43}^i \\ a_{41}^i & a_{42}^i & a_{43}^i & a_{44}^i \end{pmatrix} \begin{pmatrix} \varphi_1^i \\ \varphi_2^i \\ \varphi_3^i \\ \varphi_4^i \end{pmatrix} = \begin{pmatrix} q_1^i \\ q_2^i \\ q_3^i \\ q_4^i \end{pmatrix}, \qquad i = 1, 2.$$

Coupling : enforcing $\varphi_2^1 = \varphi_1^2$, and $\varphi_4^1 = \varphi_3^2$.

Two-domain example

Karlsruhe Institute of Technology

$$\begin{pmatrix} a^1_{11} & a^1_{21} & a^1_{31} & a^1_{41} & 0 & 0 & 0 & 0 \\ a^1_{21} & a^1_{22} & a^1_{32} & a^1_{42} & 0 & 0 & 0 & 0 \\ a^1_{31} & a^1_{32} & a^1_{33} & a^1_{43} & 0 & 0 & 0 & 0 \\ a^1_{41} & a^1_{42} & a^1_{43} & a^1_{44} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a^2_{11} & a^2_{21} & a^2_{31} & a^2_{41} \\ 0 & 0 & 0 & 0 & a^2_{21} & a^2_{22} & a^2_{32} & a^2_{42} \\ 0 & 0 & 0 & 0 & a^2_{31} & a^2_{32} & a^2_{33} & a^2_{43} \\ 0 & 0 & 0 & 0 & a^2_{41} & a^2_{42} & a^2_{43} & a^2_{44} \end{pmatrix} \begin{pmatrix} \varphi^1_1 \\ \varphi^1_2 \\ \varphi^1_3 \\ \varphi^1_4 \\ \varphi^2_1 \\ \varphi^2_2 \\ \varphi^2_3 \\ \varphi^2_4 \end{pmatrix} = \begin{pmatrix} q^1_1 \\ q^1_2 \\ q^1_3 \\ q^1_4 \\ q^2_1 \\ q^2_2 \\ q^2_3 \\ q^2_4 \end{pmatrix}$$

Two-domain example

with coupling:

$$\begin{pmatrix} a^1_{11} & a^1_{21} & a^1_{31} & a^1_{41} & 0 & 0 & 0 & 0 \\ a^1_{21} & a^1_{22} & a^1_{32} & a^1_{42} & a^2_{11} & a^2_{21} & a^2_{31} & a^2_{41} \\ a^1_{31} & a^1_{32} & a^1_{33} & a^1_{43} & 0 & 0 & 0 & 0 \\ a^1_{41} & a^1_{42} & a^1_{43} & a^1_{44} & a^2_{31} & a^2_{32} & a^2_{33} & a^2_{43} \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a^2_{21} & a^2_{22} & a^2_{32} & a^2_{42} \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & a^2_{41} & a^2_{42} & a^2_{43} & a^2_{44} \end{pmatrix} \begin{pmatrix} \varphi^1_1 \\ \varphi^1_2 \\ \varphi^1_3 \\ \varphi^1_4 \\ \varphi^2_1 \\ \varphi^2_2 \\ \varphi^2_3 \\ \varphi^2_4 \end{pmatrix} = \begin{pmatrix} q^1_1 \\ q^1_2 + q^2_1 \\ q^1_3 \\ q^1_4 + q^2_3 \\ 0 \\ q^2_2 \\ 0 \\ q^2_4 \end{pmatrix}$$

Two-domain example

with coupling:

$$\begin{pmatrix} a^1_{11} & a^1_{21} & a^1_{31} & a^1_{41} & 0 & 0 & 0 & 0 \\ a^1_{21} & a^1_{22} & a^1_{32} & a^1_{42} & a^2_{11} & a^2_{21} & a^2_{31} & a^2_{41} \\ a^1_{31} & a^1_{32} & a^1_{33} & a^1_{43} & 0 & 0 & 0 & 0 \\ a^1_{41} & a^1_{42} & a^1_{43} & a^1_{44} & a^2_{31} & a^2_{32} & a^2_{33} & a^2_{43} \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a^2_{21} & a^2_{22} & a^2_{32} & a^2_{42} \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & a^2_{41} & a^2_{42} & a^2_{43} & a^2_{44} \end{pmatrix} \begin{pmatrix} \varphi^1_1 \\ \varphi^1_2 \\ \varphi^1_3 \\ \varphi^1_4 \\ \varphi^2_1 \\ \varphi^2_2 \\ \varphi^2_3 \\ \varphi^2_4 \end{pmatrix} = \begin{pmatrix} q^1_1 \\ q^1_2 + q^2_1 \\ q^1_3 \\ q^1_4 + q^2_3 \\ 0 \\ q^2_2 \\ 0 \\ q^2_4 \end{pmatrix}$$

± 1 can be replaced by α

Two-domain example

with coupling:

$$\begin{pmatrix} a^1_{11} & a^1_{21} & a^1_{31} & a^1_{41} & 0 & 0 & 0 & 0 \\ a^1_{21} & a^1_{22} & a^1_{32} & a^1_{42} & a^2_{11} & a^2_{21} & a^2_{31} & a^2_{41} \\ a^1_{31} & a^1_{32} & a^1_{33} & a^1_{43} & 0 & 0 & 0 & 0 \\ a^1_{41} & a^1_{42} & a^1_{43} & a^1_{44} & a^2_{31} & a^2_{32} & a^2_{33} & a^2_{43} \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a^2_{21} & a^2_{22} & a^2_{32} & a^2_{42} \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & a^2_{41} & a^2_{42} & a^2_{43} & a^2_{44} \end{pmatrix} \begin{pmatrix} \varphi^1_1 \\ \varphi^1_2 \\ \varphi^1_3 \\ \varphi^1_4 \\ \varphi^2_1 \\ \varphi^2_2 \\ \varphi^2_3 \\ \varphi^2_4 \end{pmatrix} = \begin{pmatrix} q^1_1 \\ q^1_2 + q^2_1 \\ q^1_3 \\ q^1_4 + q^2_3 \\ 0 \\ q^2_2 \\ 0 \\ q^2_4 \end{pmatrix}$$

± 1 can be replaced by α

Interface nodes are duplicated.

Two-domain example

with coupling:

$$\begin{pmatrix} a^1_{11} & a^1_{21} & a^1_{31} & a^1_{41} & 0 & 0 & 0 & 0 \\ a^1_{21} & a^1_{22} & a^1_{32} & a^1_{42} & a^2_{11} & a^2_{21} & a^2_{31} & a^2_{41} \\ a^1_{31} & a^1_{32} & a^1_{33} & a^1_{43} & 0 & 0 & 0 & 0 \\ a^1_{41} & a^1_{42} & a^1_{43} & a^1_{44} & a^2_{31} & a^2_{32} & a^2_{33} & a^2_{43} \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a^2_{21} & a^2_{22} & a^2_{32} & a^2_{42} \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & a^2_{41} & a^2_{42} & a^2_{43} & a^2_{44} \end{pmatrix} \begin{pmatrix} \varphi^1_1 \\ \varphi^1_2 \\ \varphi^1_3 \\ \varphi^1_4 \\ \varphi^2_1 \\ \varphi^2_2 \\ \varphi^2_3 \\ \varphi^2_4 \end{pmatrix} = \begin{pmatrix} q^1_1 \\ q^1_2 + q^2_1 \\ q^1_3 \\ q^1_4 + q^2_3 \\ 0 \\ q^2_2 \\ 0 \\ q^2_4 \end{pmatrix}$$

± 1 can be replaced by α

Interface nodes are duplicated.

Non-overlapping, algebraic DDM (“modified Schwarz method”)

General two-domain formulation

Karlsruhe Institute of Technology

$$\begin{pmatrix} A^{11} & A^{1\,\Gamma} & 0 & 0 \\ A^{\Gamma\,1} & A_1^{\Gamma\,\Gamma} + I^{\alpha} & A^{\Gamma\,2} & A_2^{\Gamma\,\Gamma} - I^{\alpha} \\ 0 & 0 & A^{22} & A^{2\,\Gamma} \\ A^{\Gamma\,1} & A_1^{\Gamma\,\Gamma} - I^{\alpha} & A^{\Gamma\,2} & A_2^{\Gamma\,\Gamma} + I^{\alpha} \end{pmatrix} \begin{pmatrix} \varphi^1 \\ \varphi^{\Gamma,1} \\ \varphi^2 \\ \varphi^{\Gamma,2} \end{pmatrix} = \begin{pmatrix} Q^1 \\ Q_1^{\Gamma\,\Gamma} + Q_2^{\Gamma\,\Gamma} \\ Q^2 \\ Q_1^{\Gamma\,\Gamma} + Q_2^{\Gamma\,\Gamma} \end{pmatrix}$$

with symmetry of the diagonal blocks.

General two-domain formulation

$$\begin{pmatrix} A^{11} & A^{1\Gamma} & 0 & 0 \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} + I^{\alpha} & A^{\Gamma 2} & A_2^{\Gamma\Gamma} - I^{\alpha} \\ 0 & 0 & A^{22} & A^{2\Gamma} \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} - I^{\alpha} & A^{\Gamma 2} & A_2^{\Gamma\Gamma} + I^{\alpha} \end{pmatrix} \begin{pmatrix} \varphi^{1} \\ \varphi^{\Gamma,1} \\ \varphi^{2} \\ \varphi^{\Gamma,2} \end{pmatrix} = \begin{pmatrix} Q^{1} \\ Q_1^{\Gamma\Gamma} + Q_2^{\Gamma\Gamma} \\ Q^{2} \\ Q_1^{\Gamma\Gamma} + Q_2^{\Gamma\Gamma} \end{pmatrix}$$

with symmetry of the diagonal blocks.

Interpretation:

$$\mathcal{A}\Psi = Q \quad \text{within the domains}$$
$$(\mathcal{A}^{\Gamma} + \mathcal{I}^{\alpha})\Psi \quad \text{matching at interfaces}$$

General two-domain formulation

$$\begin{pmatrix} A^{11} & A^{1\Gamma} & 0 & 0 \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} + I^\alpha & A^{\Gamma 2} & A_2^{\Gamma\Gamma} - I^\alpha \\ 0 & 0 & A^{22} & A^{2\Gamma} \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} - I^\alpha & A^{\Gamma 2} & A_2^{\Gamma\Gamma} + I^\alpha \end{pmatrix} \begin{pmatrix} \varphi^1 \\ \varphi^{\Gamma,1} \\ \varphi^2 \\ \varphi^{\Gamma,2} \end{pmatrix} = \begin{pmatrix} Q^1 \\ Q_1^{\Gamma\Gamma} + Q_2^{\Gamma\Gamma} \\ Q^2 \\ Q_1^{\Gamma\Gamma} + Q_2^{\Gamma\Gamma} \end{pmatrix}$$

with symmetry of the diagonal blocks.

Interpretation:

$$\mathcal{A}\Psi = Q \quad \text{within the domains}$$
$$(\mathcal{A}^\Gamma + \mathcal{I}^\alpha)\Psi \quad \text{matching at interfaces}$$

If $\mathcal{A} = \Delta$, $\mathcal{A}^\Gamma = \partial_n$, Robin-type interface continuity condition:

$$\partial_n \Psi + \alpha \Psi$$

cf. P.L. Lions (1991): “On the Schwarz alternating method III: . . . ”

Back to spatio-angular solve

Karlsruhe Institute of Technology

The spatio-angular solve consists in inverting

$$H_{g\to g} = \begin{pmatrix} A^{11} & A^{1\,\Gamma} & 0 & 0 \\ A^{\Gamma\,1} & A_1^{\Gamma\,\Gamma} + I^{\alpha} & A^{\Gamma\,2} & A_2^{\Gamma\,\Gamma} - I^{\alpha} \\ 0 & 0 & A^{22} & A^{2\,\Gamma} \\ A^{\Gamma\,1} & A_1^{\Gamma\,\Gamma} - I^{\alpha} & A^{\Gamma\,2} & A_2^{\Gamma\,\Gamma} + I^{\alpha} \end{pmatrix} \text{ from } \begin{pmatrix} H_{1\to 1} & \simeq 0 & \simeq 0 \\ H_{1\to 2} & H_{2\to 2} & \simeq 0 \\ H_{1\to 3} & H_{2\to 3} & H_{3\to 3} \end{pmatrix}$$

Back to spatio-angular solve

Karlsruhe Institute of Technology

The spatio-angular solve consists in inverting

$$H_{g\to g} = \begin{pmatrix} A^{11} & A^{1\Gamma} & 0 & 0 \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} + I^{\alpha} & A^{\Gamma 2} & A_2^{\Gamma\Gamma} - I^{\alpha} \\ 0 & 0 & A^{22} & A^{2\Gamma} \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} - I^{\alpha} & A^{\Gamma 2} & A_2^{\Gamma\Gamma} + I^{\alpha} \end{pmatrix} \text{ from } \begin{pmatrix} H_{1\to 1} & \simeq 0 & \simeq 0 \\ H_{1\to 2} & H_{2\to 2} & \simeq 0 \\ H_{1\to 3} & H_{2\to 3} & H_{3\to 3} \end{pmatrix}$$

This is done using BiCGStab (“inner iterations”)

with block-diagonal preconditioning.

Back to spatio-angular solve

Karlsruhe Institute of Technology

The spatio-angular solve consists in inverting

$$H_{g\to g} = \begin{pmatrix} A^{11} & A^{1\Gamma} & 0 & 0 \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} + I^{\alpha} & A^{\Gamma 2} & A_2^{\Gamma\Gamma} - I^{\alpha} \\ 0 & 0 & A^{22} & A^{2\Gamma} \\ A^{\Gamma 1} & A_1^{\Gamma\Gamma} - I^{\alpha} & A^{\Gamma 2} & A_2^{\Gamma\Gamma} + I^{\alpha} \end{pmatrix} \text{ from } \begin{pmatrix} H_{1\to 1} & \simeq 0 & \simeq 0 \\ H_{1\to 2} & H_{2\to 2} & \simeq 0 \\ H_{1\to 3} & H_{2\to 3} & H_{3\to 3} \end{pmatrix}$$

This is done using BiCGStab (“inner iterations”)

with block-diagonal preconditioning.

Block inversions (local to one domain, symmetric)

done in parallel with PCG, where P = IC.

Outline

PARAFISH

Karlsruhe Institute of Technology

1. PArallel FInite element Spherical Harmonics code

PARAFISH

Karlsruhe Institute of Technology

1. PArallel FInite element Spherical Harmonics code
2. Started at the French Petroleum Institute with F. Nataf and P. Havé

PARAFISH

1. PArallel FInite element Spherical Harmonics code
2. Started at the French Petroleum Institute with F. Nataf and P. Havé
3. Enables one CPU to handle more than one domain

PARAFISH

Karlsruhe Institute of Technology

1. PArallel FInite element Spherical Harmonics code
2. Started at the French Petroleum Institute with F. Nataf and P. Havé
3. Enables one CPU to handle more than one domain
4. “Adapted” to neutron transport

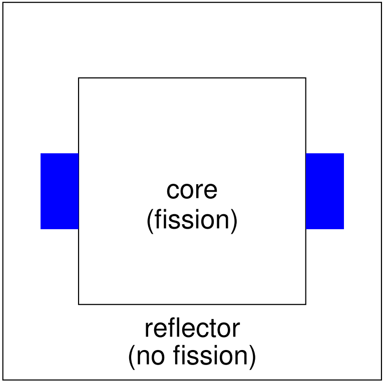
PARAFISH

1. PArallel FInite element Spherical Harmonics code
2. Started at the French Petroleum Institute with F. Nataf and P. Havé
3. Enables one CPU to handle more than one domain
4. “Adapted” to neutron transport
5. Object-oriented C++ with MPI for parallelization.

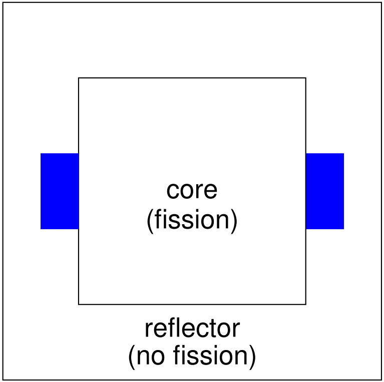
PARAFISH

1. PArallel FInite element Spherical Harmonics code
2. Started at the French Petroleum Institute with F. Nataf and P. Havé
3. Enables one CPU to handle more than one domain
4. “Adapted” to neutron transport
5. Object-oriented C++ with MPI for parallelization.
6. 23,000 lines

2- and 3-D “Takeda 1” Benchmark

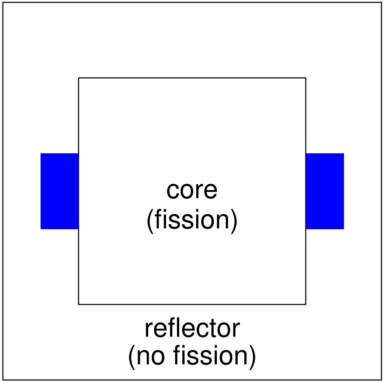


2- and 3-D “Takeda 1” Benchmark



control rod (neutron absorber)

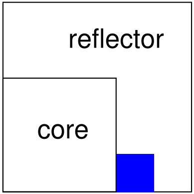
2- and 3-D “Takeda 1” Benchmark



control rod (neutron absorber)

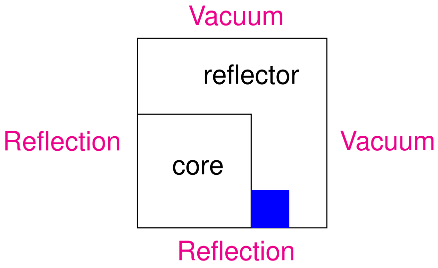
symmetry ⇒ quarter (2-D)
or octant (3-D)

2- and 3-D "Takeda 1" Benchmark



control rod (neutron absorber)

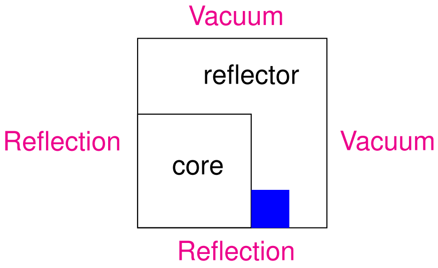
2- and 3-D "Takeda 1" Benchmark



control rod (neutron absorber)

Boundary conditions

2- and 3-D "Takeda 1" Benchmark

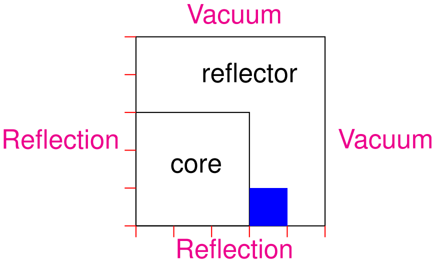


control rod (neutron absorber)

Boundary conditions

FE mesh: 50×50

2- and 3-D “Takeda 1” Benchmark



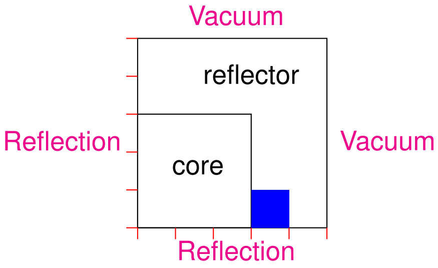
control rod (neutron absorber)

Boundary conditions

FE mesh: 50×50

Domain Decompositions: $3 \times 3,\ 5 \times 5,\ 10 \times 10,\ 25 \times 25$

2- and 3-D “Takeda 1” Benchmark



control rod (neutron absorber)

Boundary conditions

$\alpha = 1$

FE mesh: 50×50

Domain Decompositions: $3 \times 3,\ 5 \times 5,\ 10 \times 10,\ 25 \times 25$

Sequential numerical results in 2-D, P_5

Karlsruhe Institute of Technology

Domains	FE nodes
1	5,100
9 (3×3)	5,300
25 (5×5)	5,500

Sequential numerical results in 2-D, P_5

Domains	FE nodes	Unknowns (2 groups)
1	5,100	91,800
9 (3 $\times$ 3)	5,300	95,400
25 (5 $\times$ 5)	5,500	99,000

Sequential numerical results in 2-D, P_5

Domains	FE nodes	Unknowns (2 groups)	Time (s)
1	5,100	91,800	134
9 (3×3)	5,300	95,400	116
25 (5×5)	5,500	99,000	99

Effective as a sequential method

Sequential numerical results in 2-D, P_5

Karlsruhe Institute of Technology

Domains	FE nodes	Unknowns (2 groups)	Time (s)	Outers (Power)	Inners (BiCGStab)
1	5,100	91,800	134	14	46
9 (3×3)	5,300	95,400	116	59	187
25 (5×5)	5,500	99,000	99	79	234

Effective as a sequential method

Sequential numerical results in 2-D, P_5

Karlsruhe Institute of Technology

Domains	FE nodes	Unknowns (2 groups)	Time (s)	Outers (Power)	Inners (BiCGStab)
1	5,100	91,800	134	14	46
9 (3×3)	5,300	95,400	116	59	187
25 (5×5)	5,500	99,000	99	79	234
100 (10×10)	6,000	108,000	104	145	398

Effective as a sequential method

Acceleration vs. increase of (duplicated) unknowns

Parallel numerical results in 3-D, P_3

Domain decomposition	$5 \times 5 \times 5$	$10 \times 10 \times 10$	$25 \times 25 \times 25$
Number of domains	125	1,000	15,625
FE nodes	412,500	450,000	562,500
Total unknowns	4,950,000	5,400,000	6,750,000
number of CPUs			
25	413	303	1358

Parallel numerical results in 3-D, P_3

Karlsruhe Institute of Technology

Domain decomposition	$5 \times 5 \times 5$	$10 \times 10 \times 10$	$25 \times 25 \times 25$
Number of domains	125	1,000	15,625
FE nodes	412,500	450,000	562,500
Total unknowns	4,950,000	5,400,000	6,750,000
<u>number of CPUs</u>			
25	413	303	1358
125		78 (.78)	728 (.37)
1000		127 (.06)	758 (.04)

increase of communications

Parallel numerical results in 3-D, P_3

Domain decomposition	$5 \times 5 \times 5$	$10 \times 10 \times 10$	$25 \times 25 \times 25$
Number of domains	125	1,000	15,625
FE nodes	412,500	450,000	562,500
Total unknowns	4,950,000	5,400,000	6,750,000
number of CPUs			
25	413	303	1358
125	100 (.83)	78 (.78)	728 (.37)
1000	-	127 (.06)	758 (.04)

No proper speed-up when # CPU $\equiv$ # domain

Outline

Karlsruhe Institute of Technology

Conclusions

Karlsruhe Institute of Technology

1. Algebraic DDM has an inherent acceleration potential, i.e., without increasing the amount of processors (also sequentially)

Conclusions

Karlsruhe Institute of Technology

1. Algebraic DDM has an inherent acceleration potential, i.e., without increasing the amount of processors (also sequentially)
    - limited by the increase in the number of duplicated unknowns

Conclusions

Karlsruhe Institute of Technology

1. Algebraic DDM has an inherent acceleration potential, i.e., without increasing the amount of processors (also sequentially)
   - limited by the increase in the number of duplicated unknowns
   - achievable only if one processor can handle more than one domain

Conclusions

1. Algebraic DDM has an inherent acceleration potential, i.e., without increasing the amount of processors (also sequentially)
   - limited by the increase in the number of duplicated unknowns
   - achievable only if one processor can handle more than one domain

2. Proper speed-up evaluations can be obtained by varying the number of CPUs with a fixed decomposition.

Conclusions

Karlsruhe Institute of Technology

1. Algebraic DDM has an inherent acceleration potential, i.e., without increasing the amount of processors (also sequentially)
   - limited by the increase in the number of duplicated unknowns
   - achievable only if one processor can handle more than one domain
2. Proper speed-up evaluations can be obtained by varying the number of CPUs with a fixed decomposition.
3. There can be an optimum in the amount of processors (increased communications).

Outline

Potential research areas

Karlsruhe Institute of Technology

1. Improvement of numerical acceleration techniques
   - spatio-angular problem (improve block-diagonal and IC preconditioning)

Potential research areas

Karlsruhe Institute of Technology

1. Improvement of numerical acceleration techniques
   - spatio-angular problem (improve block-diagonal and IC preconditioning)
   - criticality (eigenvalue) problem (Arnoldi, J-D, JFNK,...)

Potential research areas

Karlsruhe Institute of Technology

1. Improvement of numerical acceleration techniques
   - spatio-angular problem (improve block-diagonal and IC preconditioning)
   - criticality (eigenvalue) problem (Arnoldi, J-D, JFNK,...)

2. Choice of α

Potential research areas

Karlsruhe Institute of Technology

1. Improvement of numerical acceleration techniques
   - spatio-angular problem (improve block-diagonal and IC preconditioning)
   - criticality (eigenvalue) problem (Arnoldi, J-D, JFNK,...)
2. Choice of α
3. Wavelets instead of Spherical Harmonics

Contact

Serge.Criekingen@kit.edu

http://www.ann.jussieu.fr/∼vancriekingen/