Prise en compte des discontinuités des coefficients dans les méthodes de décomposition de domaine

Frédéric Nataf
nataf@ann.jussieu.fr, www.ann.jussieu.fr/~nataf
Laboratoire J.L. Lions, CNRS UMR7598.
Université Pierre et Marie Curie, France

Joint work with E. Flauraud
Institut Français du Pétrole

Plan

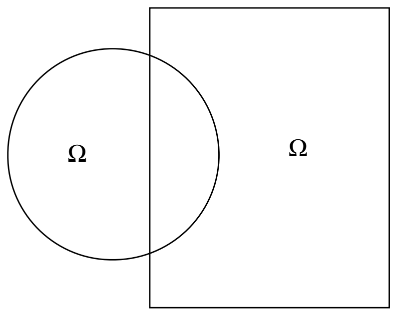
1. Short introduction to domain decomposition methods
2. Optimal Interface Conditions
3. Optimized Interface Conditions
4. Optimized IC Discontinuous coefficients equations
5. Conclusion

The First Domain Decomposition Method

The original Schwarz Method

(H.A. Schwarz, 1870)

$$-\Delta(u) = f \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega.$$



Multiplicative Schwarz Method : $(u_1^n, u_2^n) \to (u_1^{n+1}, u_2^{n+1})$ with

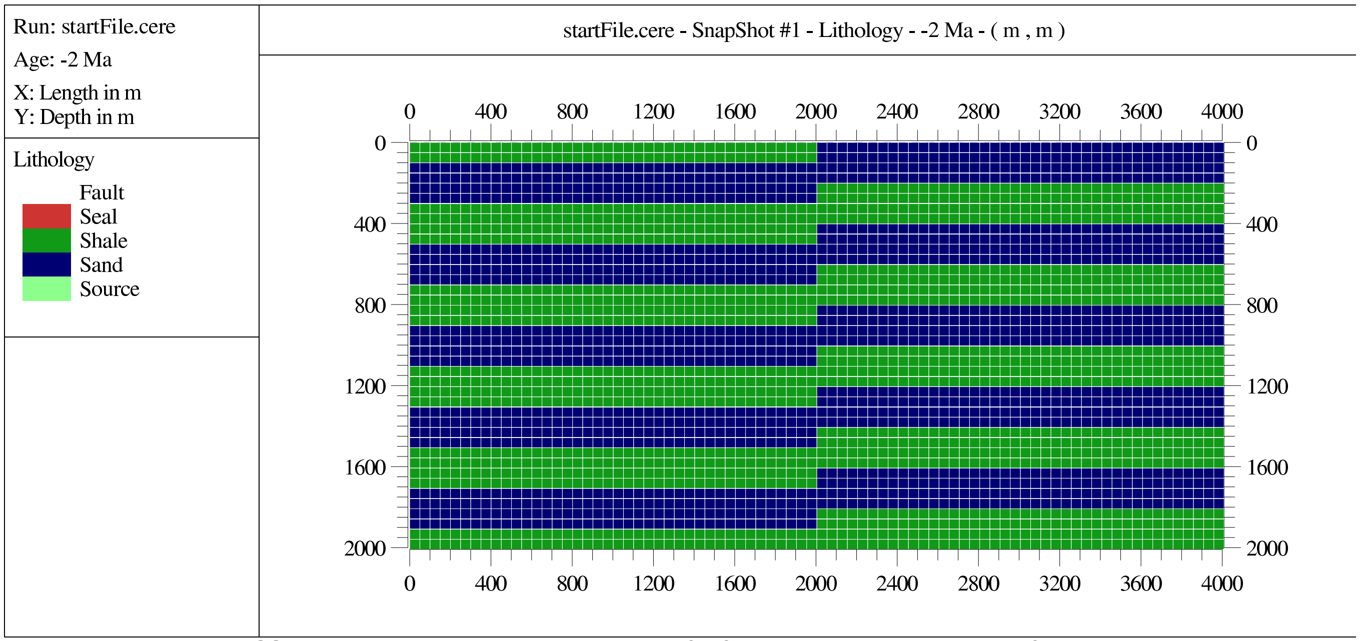
$$\begin{aligned} -\Delta(u_1^{n+1}) &= f \quad \text{in } \Omega_1 \\ u_1^{n+1} &= 0 \text{ on } \partial\Omega_1 \cap \partial\Omega \\ u_1^{n+1} &= u_2^n \quad \text{on } \partial\Omega_1 \cap \overline{\Omega_2}. \end{aligned} \qquad \begin{aligned} -\Delta(u_2^{n+1}) &= f \quad \text{in } \Omega_2 \\ u_2^{n+1} &= 0 \text{ on } \partial\Omega_2 \cap \partial\Omega \\ u_2^{n+1} &= u_1^{n+1} \quad \text{on } \partial\Omega_2 \cap \overline{\Omega_1}. \end{aligned}$$

Easily parallelized algorithm, converges

but very slowly, overlapping subdomains only.

Goal: Domain decompostion methods for such problems

$$\eta u - div(\kappa \nabla u) = f$$



Jumps in the coefficients η and κ of four orders of magnitude.

Anisotropic tensor κ: $10^{-4} \leq \kappa_x/\kappa_y \leq 10^4$.

Discontinuous coefficients both across and along the interface.

$\Rightarrow$ Plateau in the convergence of Krylov methods even with "good" preconditioners. Except for recent multigrid methods but poor parallel efficiency.

One possible Improvement: other interface conditions

(P.L. Lions, 1988)

$$
\begin{aligned}
&-\Delta(u_1^{n+1}) = f \quad \text{ in } \Omega_1,\\
&u_1^{n+1} = 0 \quad \text{ on } \partial\Omega_1 \cap \partial\Omega,\\
&(\frac{\partial}{\partial n_1} + \alpha)(u_1^{n+1}) = (-\frac{\partial}{\partial n_2} + \alpha)(u_2^n) \quad \text{ on } \partial\Omega_1 \cap \overline{\Omega_2},
\end{aligned}
$$

(n_1 and n_2 are the outward normals to the subdomains' boundaries)

$$
\begin{aligned}
&-\Delta(u_2^{n+1}) = f \quad \text{ in } \Omega_2,\\
&u_2^{n+1} = 0 \quad \text{ on } \partial\Omega_2 \cap \partial\Omega\\
&(\frac{\partial}{\partial n_2} + \alpha)(u_2^{n+1}) = (-\frac{\partial}{\partial n_1} + \alpha)(u_1^n) \quad \text{ on } \partial\Omega_2 \cap \overline{\Omega_1}.
\end{aligned}
$$

with $\alpha > 0$. Overlap is not necessary for convergence.

Extended to the Helmholtz equation (B. Desprès, 1991)

a.k.a Two-Lagrange Multiplier FETI Method, Farhat 1998.

How to choose the interface conditions?

Questions and Answers in the smooth case

- Optimal α? $\alpha_{opt} = Ct/\sqrt{h}$ Optimized of order 0 IC
- More general interface conditions

  $$(\frac{\partial}{\partial n_2}+\alpha-\frac{\partial}{\partial \tau}\gamma\frac{\partial}{\partial \tau})(u_2^{n+1}) = (-\frac{\partial}{\partial n_1}+\alpha-\frac{\partial}{\partial \tau}\gamma\frac{\partial}{\partial \tau})(u_1^{n}) \quad \text{on } \partial\Omega_2\cap\overline{\Omega_1}.$$

  Formulas for $(\alpha_{opt}, \gamma_{opt})$ are available. Optimized of order 2 IC
- Works for many other PDEs: Convection-diffusion, Helmholtz, Maxwell, heterogeneous problems, ...

How to handle the discontinuous coefficient case?

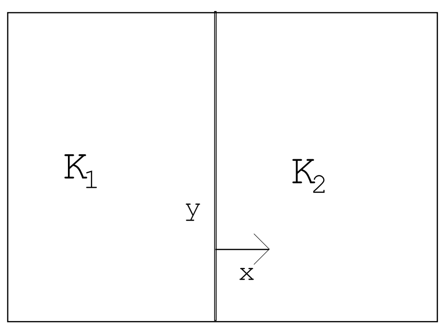
Optimal Interface Conditions for Heterogeneous Domain Decomposition

Let us consider the problem

$$
\begin{aligned}
&\mathcal{L}_i(P_i) = f \quad \text{in } \Omega_i, \quad i = 1,2\\
&P_1 = P_2 \quad \text{on } \Gamma_{12},\\
&\kappa_1 \frac{\partial P_1}{\partial n_1} + \kappa_2 \frac{\partial P_2}{\partial n_2} = 0 \quad \text{on } \Gamma_{12}.
\end{aligned}
$$

where

$$\mathcal{L}_i = \eta_i - div(\kappa_i \nabla \dot{)}$$



Optimal Interface Conditions for Heterogeneous Domain Decomposition

Let

$$u_i = \kappa_i \nabla P_i$$

Let us consider a Schwarz method:

$$\begin{array}{ll}
\mathcal{L}_1(P_1^{n+1}) = f \quad \text{in } \Omega_1 & \mathcal{L}_2(P_2^{n+1}) = f \quad \text{in } \Omega_2 \\
P_1^{n+1} = 0 \text{ on } \partial\Omega_1 \cap \partial\Omega & P_2^{n+1} = 0 \text{ on } \partial\Omega_2 \cap \partial\Omega \\
u_1^{n+1}.\vec{n}_1 + \mathcal{B}_1(P_1^{n+1}) & u_2^{n+1}.\vec{n}_2 + \mathcal{B}_2(P_2^{n+1}) \\
= -u_2^n.\vec{n}_2 + \mathcal{B}_1(P_2^n) \quad \text{on } \Gamma_1 & = -u_1^n.\vec{n}_1 + \mathcal{B}_2(P_1^n) \quad \text{on } \Gamma_2
\end{array}$$

We take

$$\mathcal{B}_1 = DtN_2.$$

and have convergence in two iterations.

ICs for discontinuous coefficients at the continuous level

$$\mathcal{L}_i(P) = \eta_i P - \frac{\partial}{\partial x}(C_i \frac{\partial}{\partial x} P) - \frac{\partial}{\partial y}(\kappa_{i,y} \frac{\partial}{\partial y} P), \qquad i = 1, 2$$

with η_i, C_i and $\kappa_{i,y}$ independant of the x variable.
Let $\Omega_1 = \mathbb{R}^- \times]0, L[$, $\Omega_2 = \mathbb{R}^+ \times]0, L[$ and $\Gamma = \{0\} \times]0, L[$. Consider a Schwarz type method:

$$\begin{array}{ll}
\mathcal{L}_1(P_1^{n+1}) = f \quad \text{in } \Omega_1 & \mathcal{L}_2(P_2^{n+1}) = f \quad \text{in } \Omega_2 \\
P_1^{n+1} = 0 \text{ on } \partial\Omega_1 \backslash \Gamma & P_2^{n+1} = 0 \text{ on } \partial\Omega_2 \backslash \Gamma \\
(C_1 \partial_x + \Lambda_{ap,2})(P_1^{n+1}) & (C_2 \partial_x + \Lambda_{ap,1})(P_2^{n+1}) \\
= (-C_2 \partial_x + \Lambda_{ap,2})(P_2^n) \quad \text{on } \Gamma & = (-C_1 \partial_x + \Lambda_{ap,1})(P_1^n) \quad \text{on } \Gamma
\end{array}$$

We seek a partial differential approximation to the DtN_i map:

$$\Lambda_{ap,i} \simeq C_i^{1/2} \sqrt{C_i^{-1/2}(\eta_i - \frac{\partial}{\partial y}(\kappa_{i,y} \frac{\partial}{\partial y}))C_i^{-1/2}} C_i^{1/2} \ (:= \Lambda_i)$$

How to approximate DtN_i by a partial differential operator?

$$DtN_i := C_i^{1/2}\sqrt{C_i^{-1/2}(\eta_i - \frac{\partial}{\partial y}(\kappa_{i,y}\frac{\partial}{\partial y}))C_i^{-1/2}}C_i^{1/2}$$

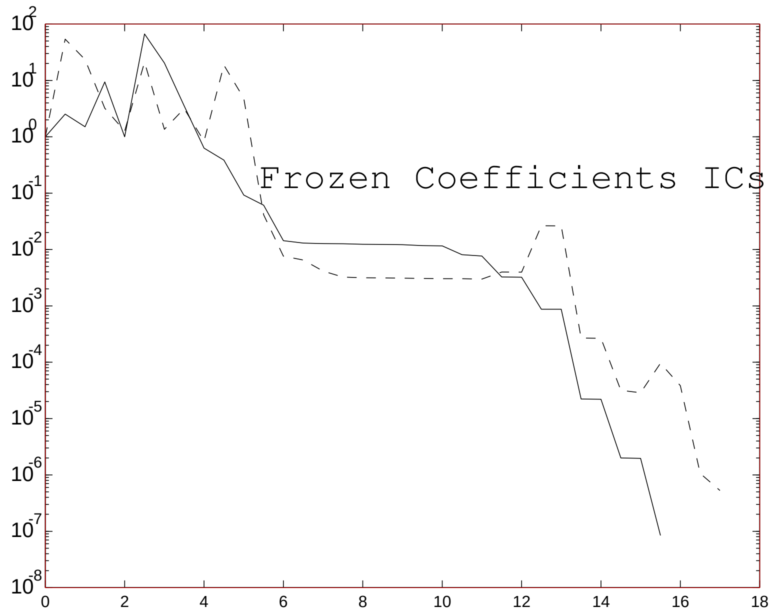
Previous works were based on Fourier transform.

But jumps in the coefficients η and κ of four orders of magnitude.

Anisotropic tensor κ: $10^{-4} \leq \kappa_x/\kappa_y \leq 10^4$.

Fourier transform or other analytic tools give poor results

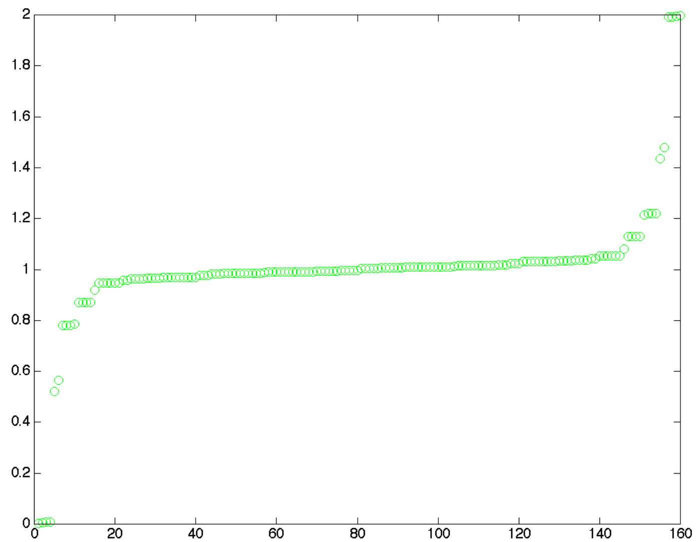
“Frozen” coefficients ICs



residual vs. iteration counts for various interface conditions (IC)

- Willien, Faille, Nataf, Schneider. Domain decomposition methods for fluid flow in porous medium.(1998)
- Roux, Magoulès, Series, Boubendir. Approximation of optimal interface b.c. for two-lagrange multiplier feti method. (2004)
- Genseberger, Sleijpen, van der Vorst. Using domain decomposition in the Jacobi-Davidson method (2002)

“Frozen” coefficients ICs



Eigenvalues of the interface problem (Genseberger, Sleijpen, van der Vorst, 2002)

The few very low eigenvalues are responsible for the plateau in the convergence of the Krylov method.

Two possible solutions: deflation techniques or more efficient ICs.

Deflation or Coarse Grid $\Rightarrow$ All the corresponding eigenvectors are needed (Morgan, Segal, Meijerink, Frank, Vuik, Saad, Erhel, Nabben, van der Vorst, Graham and Hagger. ...)

ICs for discontinuous coefficients at the continuous level

$$\mathcal{L}_i(P) = \eta_i P - \frac{\partial}{\partial x}(C_i \frac{\partial}{\partial x} P) - \frac{\partial}{\partial y}(\kappa_{i,y} \frac{\partial}{\partial y} P), \qquad i = 1, 2$$

with η_i, C_i and $\kappa_{i,y}$ independant of the x variable.
Let $\Omega_1 = \mathbb{R}^- \times]0, L[$, $\Omega_2 = \mathbb{R}^+ \times]0, L[$ and $\Gamma = \{0\} \times]0, L[$. Consider a Schwarz type method:

$$\begin{array}{ll}
\mathcal{L}_1(P_1^{n+1}) = f \quad \text{in } \Omega_1 & \mathcal{L}_2(P_2^{n+1}) = f \quad \text{in } \Omega_2 \\
P_1^{n+1} = 0 \text{ on } \partial\Omega_1 \backslash \Gamma & P_2^{n+1} = 0 \text{ on } \partial\Omega_2 \backslash \Gamma \\
(C_1 \partial_x + \Lambda_{ap,2})(P_1^{n+1}) & (C_2 \partial_x + \Lambda_{ap,1})(P_2^{n+1}) \\
= (-C_2 \partial_x + \Lambda_{ap,2})(P_2^n) \quad \text{on } \Gamma & = (-C_1 \partial_x + \Lambda_{ap,1})(P_1^n) \quad \text{on } \Gamma
\end{array}$$

We seek a partial differential approximation to the DtN_i map:

$$\Lambda_{ap,i} \simeq C_i^{1/2} \sqrt{C_i^{-1/2}(\eta_i - \frac{\partial}{\partial y}(\kappa_{i,y} \frac{\partial}{\partial y}))C_i^{-1/2}} C_i^{1/2} \; (:= \Lambda_i)$$

Optimized ICs for discontinuous coefficients at the semi discrete level

After a discretization in y, the operator $\mathcal{L}_i$ reads

$$\mathcal{L}_{i,h} := -\frac{\partial}{\partial x} C_i \frac{\partial}{\partial x} + B_i$$

where B_i is the finite volume discretization of

$$\eta_i(y) - \frac{\partial}{\partial y} \kappa_{i,y}(y) \frac{\partial}{\partial y}$$

These matrices are symmetric positive and definite.
The discrete Steklov-Poincaré (Dirichlet to Neumann) operator Λ_i, of subdomain Ω_i is

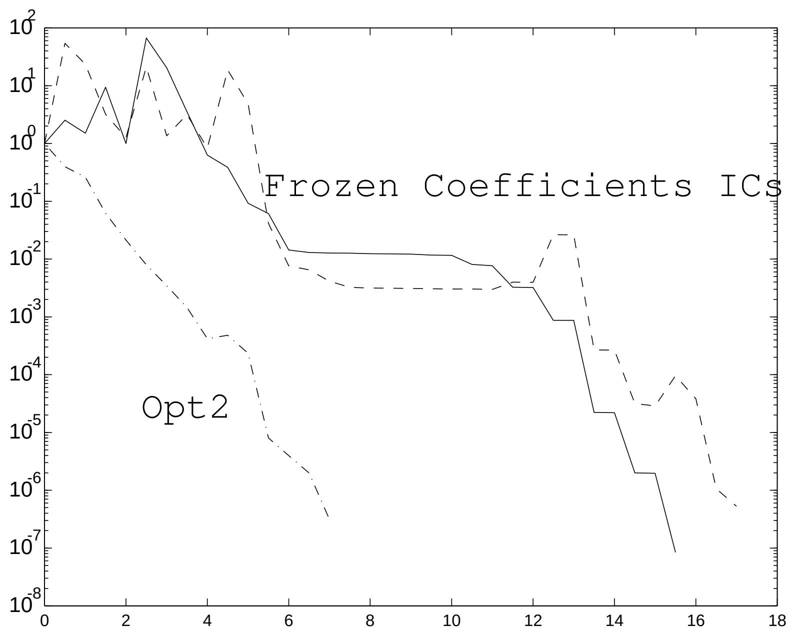
$$\Lambda_i = C_i^{1/2} (C_i^{-1/2} B_i C_i^{-1/2})^{1/2} C_i^{1/2}$$

We seek sparse approximations to Λ_i: $\Lambda_{ap,i}$.
An approximation by a diagonal matrix corresponds to a condition of order 0. An approximation by a tridiagonal matrix corresponds to a condition of order 2.

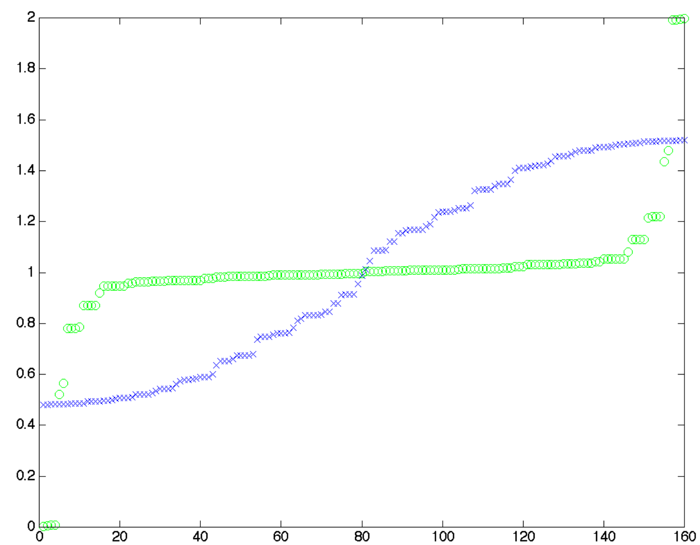
The approximation of a full matrix by a sparse matrix is reminiscent and indeed equivalent up to an optimal multiplicative constant to a preconditioner problem.

It can be "solved" by using some linear algebra tools

see L. Gerardo-Giorda, F. Nataf, JNM (2005) and E. Flauraud, F. Nataf, J. Comput. Appl. Math (2006)



Convergence curve



Eigenvalues of the interface problem

Optimized ICs for discontinuous coefficients

Lemma 1 *Let* Λ_{ap} *be a SPD matrix and* λ_M *(resp.* λ_m*) be the largest (resp. smallest) eigenvalue of* $\Lambda_{ap}^{-1/2}\Lambda\Lambda_{ap}^{-1/2}$*.*
Then,

$$\min_{\beta\in\mathbb{R}^+}\rho_{Sc}(\beta\Lambda_{ap}) = \rho_{Sc}(\beta_{opt}\Lambda_{ap})) = \frac{\sqrt{\frac{\lambda_M}{\lambda_m}}-1}{\sqrt{\frac{\lambda_M}{\lambda_m}}+1}$$

where

$$\beta_{opt} = \sqrt{\lambda_M\lambda_m}$$

We have to find sparse matrices D that minimize the condition number of $D^{-1/2}\Lambda D^{-1/2}$ and then take $\Lambda_{ap} = \beta_{opt}D$.

Optimized zeroth order ICs for discontinuous coefficients

In order to use the previous Lemma, we have to find the best diagonal matrix D that minimizes the condition number of $D^{-1/2}\Lambda D^{-1/2}$.

Theorem 1 (van der Sluis, 1969) *If F is SPD matrix, then*

$$\begin{aligned}\min_{D\in\mathcal{D}}\kappa(D^{-1/2}FD^{-1/2}) \leq \;& \kappa(diag(F)^{-1/2}Fdiag(F)^{-1/2}) \\ & \leq m\,.\min_{D\in\mathcal{D}}\kappa(D^{-1/2}FD^{-1/2})\end{aligned}$$

where $\mathcal{D} = \{positive\ definite\ diagonal\ matrices\}$ and m is the maximum number of nonzeros in any row of F.

We are led to take

$$D := diag(\Lambda) = diag(C^{1/2}\,(C^{-1/2}BC^{-1/2})^{1/2}\,C^{1/2}),$$

$$\beta_{opt} = \sqrt{\lambda_M(D^{-1/2}\Lambda D^{-1/2})\lambda_m(D^{-1/2}\Lambda D^{-1/2})}$$

and
$$\Lambda_{ap} = \beta_{opt} D$$

Optimized ICs of order two

Combination of two zeroth order ICs thanks to Higdon's trick (Math. of Comp., 1986)

$$\mathcal{Q} := (C\frac{\partial}{\partial x} + \beta_1 \tilde{D})(C\frac{\partial}{\partial x} + \beta_2 \tilde{D})$$

for some positive parameters β_1, β_2.
This product yields a second order derivative w.r.t x the normal direction to the interface:

$$\mathcal{Q} := C\frac{\partial}{\partial x}(C\frac{\partial}{\partial x}) + (\beta_1 + \beta_2)\tilde{D}C\frac{\partial}{\partial x} + \beta_1\beta_2\tilde{D}^2$$

By using the operator $\mathcal{L}_h = -\partial_x C \partial_x + B$ this second order derivative can be replaced by

$$CB$$

so that condition $\mathcal{Q}$ is equivalent to

$$\mathcal{Q} := CB + (\beta_1 + \beta_2)\tilde{D}C\frac{\partial}{\partial x} + \beta_1\beta_2\tilde{D}^2.$$

Optimized second order ICs

We still have to write this condition in the form

$$C\frac{\partial}{\partial x} + \Lambda_{ap,2}$$

for some operator $\Lambda_{ap,2}$. Since interface conditions are equivalent up to the left composition with any invertible operator acting along the interface, we obtain an equivalent condition $\mathcal{R}$ by left multiplying $\mathcal{Q}$ by the inverse of $(\beta_1 + \beta_2)\tilde{D}$:

$$\mathcal{R} := C\frac{\partial}{\partial x} + C^{1/2}\frac{\tilde{D}^{-1}A + \beta_1\beta_2\tilde{D}}{\beta_1 + \beta_2}C^{1/2} \tag{1}$$

In other words, we choose to approximate Λ by

$$\Lambda_{ap,\beta_1,\beta_2} := C^{1/2}\frac{\tilde{D}^{-1}A + \beta_1\beta_2\tilde{D}}{\beta_1 + \beta_2}C^{1/2} \tag{2}$$

with $\beta_1, \beta_2 > 0$.

Optimized second order ICs: best β_1, β_2

Based on Wachspress optimization of ADI methods, we have

Theorem 2 *Suppose matrices $\tilde{D}$ and $A^{1/2}$ commute. Let $\lambda_m := \lambda_{min}(\tilde{D}^{-1}A^{1/2})$ and $\lambda_M := \lambda_{max}(\tilde{D}^{-1}A^{1/2})$. The choice*

$$\beta_{1,opt}\beta_{2,opt} = \lambda_m \, \lambda_M \tag{3}$$

$$\beta_{1,opt} + \beta_{2,opt} = \left(\min_{\lambda \in Sp(\tilde{D}^{-1}A^{1/2})} (\lambda + \frac{\lambda_m \lambda_M}{\lambda}) \, (\lambda_m + \lambda_M) \right)^{1/2} \tag{4}$$

is optimal in the sense that:

$$\min_{\beta_1 \in \mathbb{R}^+, \beta_2 \in \mathbb{R}^+} \kappa(Sub(\Lambda_{ap,\beta_1,\beta_2})) = \kappa(Sub(\Lambda_{ap,\beta_{1,opt},\beta_{2,opt}}))$$

We have a bound on the condition number

$$\kappa(Sub(\Lambda_{ap,\beta_{1,opt},\beta_{2,opt}})) \leq \frac{1}{\sqrt{2}} \left(\sqrt{\frac{\lambda_M}{\lambda_m}} + \sqrt{\frac{\lambda_m}{\lambda_M}} \right)^{1/2}$$

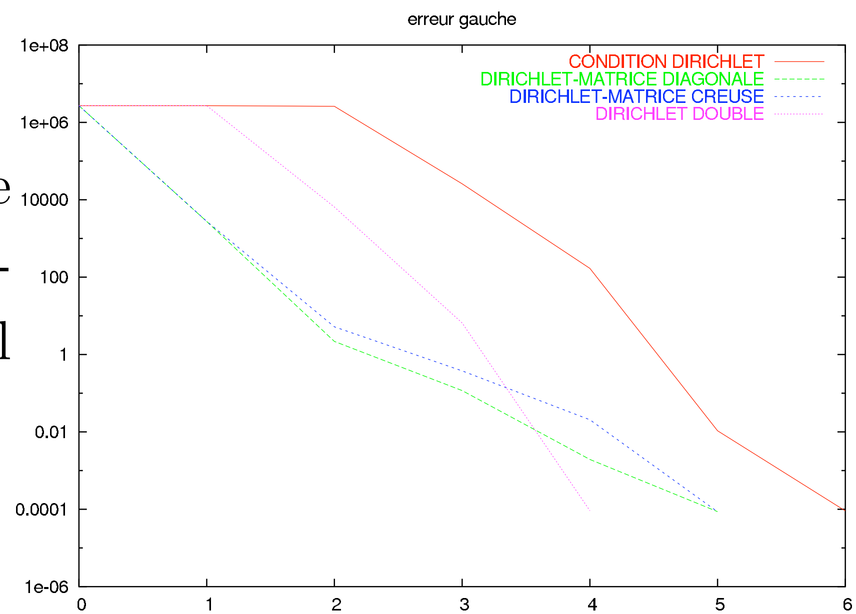
In practice, $\lambda_{m,M} \simeq \lambda_{m,M}(D^{-2}A)^{1/2}$.

Conclusion

We proposed an algebraic approach for the semi continuous problem.

Prospects

• Generalizing the method to the purely algebraic level. First numerical results on 3D but small problems.

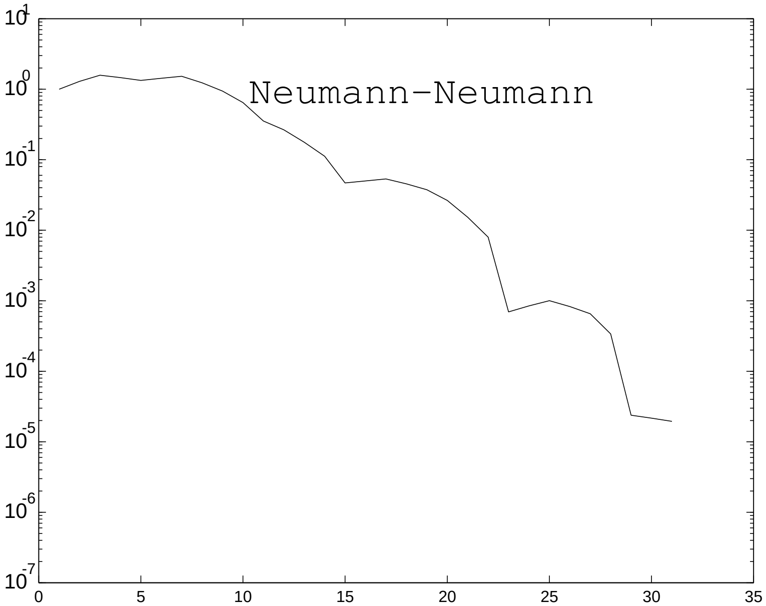


• Work in progress: a general code at the algebraic level in order to perform realistic test cases with an automatic mesh partitioner.

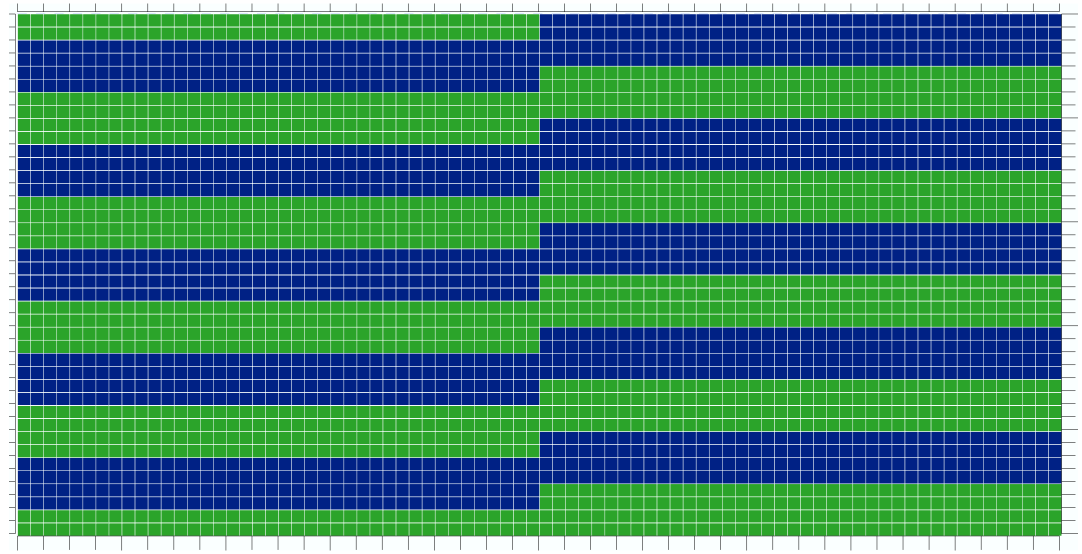
• Coarse grid solver in collaboration with R. Scheichl (Bath University)

Thanks !

Generalized Neumann-Neumann/ FETI



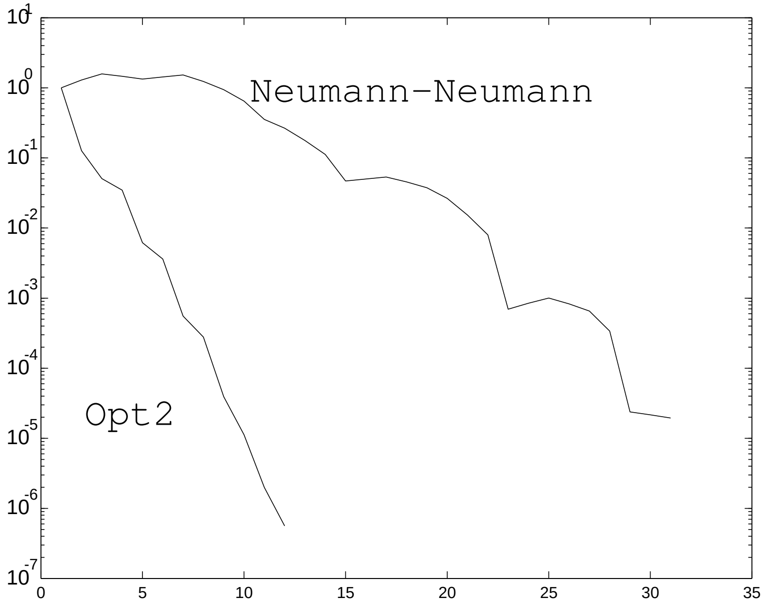
residual vs. subdomain solve counts

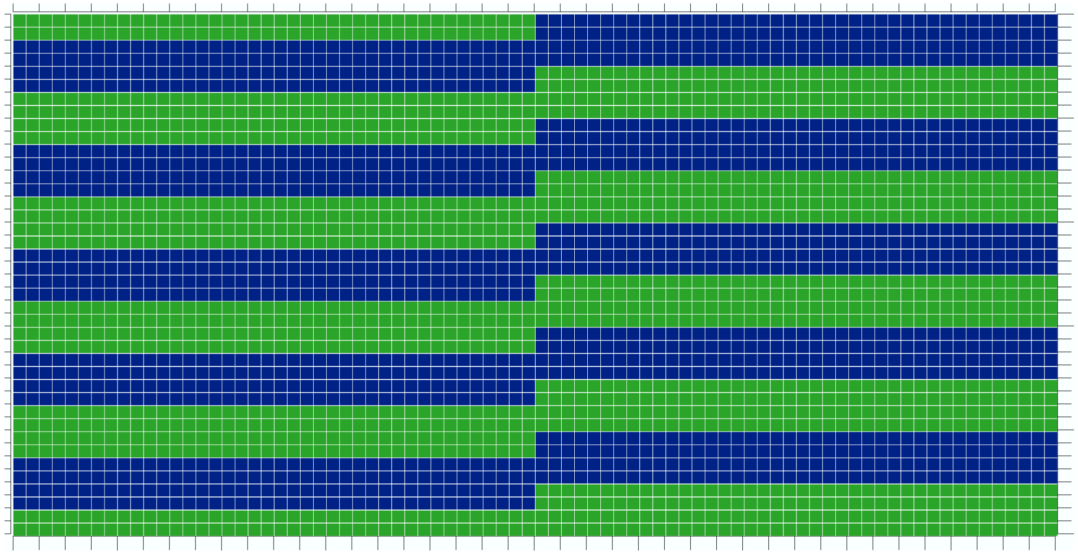


Lythology

- Klawonn, Widlund, Dryja, Dual-Primal FETI methods for three-dimensional elliptic problems with heterogeneous coefficients (2002)
- Le Tallec. M. Vidrascu, Generalized Neumann-Neumann preconditioners for iterative substructuring (1996)
- Cowsar, J. Mandel, M.F. Wheeler, Balancing domain decomposition for mixed Finite elements (1995)

Generalized Neumann-Neumann/ FETI





residual vs. subdomain solve counts

Lythology

- Klawonn, Widlund, Dryja, Dual-Primal FETI methods for three-dimensional elliptic problems with heterogeneous coefficients (2002)
- Le Tallec. M. Vidrascu, Generalized Neumann-Neumann preconditioners for iterative substructuring (1996)
- Cowsar, J. Mandel, M.F. Wheeler, Balancing domain decomposition for mixed Finite elements (1995)