Preconditionning Techniques for Systems of PDEs using Algebraic Tools

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http://www-math.unice.fr/~dolean/saddles/

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Outline of the talk

1. Motivation and goal of the project
2. Smith normal form and domain decomposition algorithms
3. Relevant Smith variables
4. Reduction of interface conditions
5. Conclusion / Perspectives

I

Motivation and goal of the project

Motivation : Solving systems of PDEs

$\diamond$ Many numerical simulations rely on solving linear or non-linear systems of PDEs

$\diamond$ Non-linear : fixed-point or Newton-types methods $\rightsquigarrow$ linear

$\diamond$ Direct numerical methods only when small numbers of unknowns (important memory requirement and computational cost)

$\Rightarrow$ For large scale problems: iterative (Krylov) methods

$\diamond$ They use preconditioners: domain decomposition methods

Motivation : Solving systems of PDEs

$\diamond$ Methods well-understood and efficient for scalar symmetric equations (Laplacian, biLaplacian)

$\diamond$ To some extend for scalar non-symmetric equations (convection-diffusion)

$\diamond$ But poor performances and lack robustness for symmetric and non-symmetric systems (fluid mechanics,...)

$\Rightarrow$ The study of iterative solvers for systems of PDEs is an under developed subject

Goal of the SADDLES project

⋄ Aim: building new robust and efficient solvers (domain decomposition methods and preconditioners) for some well-known linear systems of PDEs (elasticity, Stokes, Oseen,...)

⋄ Tool: algebraic methods developed in constructive algebra, D-modules and symbolic computation

⇝ General principle:

- Uncouple the equations (Smith normal form) to get a set of independent scalar PDEs
- Use the known efficient numerical techniques dedicated to scalar PDEs

II

Smith normal form and domain decomposition algorithms

Methodology

◇ Linear systems of PDEs in the whole plane $\mathbb{R}^d$ with $d = 2, 3$:

$$\mathcal{L}_d(\vec{w}) = \vec{g} \quad \text{in } \mathbb{R}^d, \quad |\vec{w}(\vec{x})| \to 0 \quad \text{for } |\vec{x}| \to \infty,$$

with right hand-side $\vec{g}$ and $\mathcal{L}_d$ represents for example the linear elasticity, Stokes or Oseen operator in dimension d.

◇ Write it as

$$A_d \hat{w} = \hat{G}$$

where $A_d \in D^{q \times q}$ with D a ring of partial differential operators

Example: linear elasticity problem in $\mathbb{R}^d$

◇ Linear elasticity system of PDEs given by $\mathcal{E}_d(\vec{u}) = \vec{g}$ where

$$\mathcal{E}_d = -\mu\,\Delta - (\lambda + \mu)\,\nabla\,\mathrm{div}$$

⇝ for $d = 2$, the system can be written $A_2\,\hat{w} = \hat{G}$ with

$$A_2 = \begin{bmatrix} -\mu\,\Delta - (\lambda+\mu)\,dx^2 & -(\lambda+\mu)\,dx\,dy \\ -(\lambda+\mu)\;dx\,dy & -\mu\,\Delta - (\lambda+\mu)\,dy^2 \end{bmatrix} \in D^{2\times 2},$$

with $D = \mathbb{R}(\lambda, \mu)[dx, dy]$.

Example: Oseen and Stokes problems in $\mathbb{R}^d$

◇ Oseen system of PDEs given by $\mathcal{O}_d(\vec{w}) = \mathcal{O}_d(\vec{v}, q) = \vec{g}$ with

$$\mathcal{O}_d(\vec{v}, q) = (-\nu\Delta\vec{v} + c\vec{v} + \vec{b}\cdot\nabla\vec{v} + \nabla q, \nabla\cdot\vec{v})$$

where $\vec{b} = (b_j)_{1\leq j\leq d}$ is the convection velocity.

◇ $\vec{b} = 0 \rightsquigarrow$ Stokes problem given by $\mathcal{S}_d(\vec{w}) = \mathcal{S}_d(\vec{v}, q) = \vec{g}$ with

$$\mathcal{S}_d(\vec{v}, q) = (-\nu\Delta\vec{v} + c\vec{v} + \nabla q, \nabla\cdot\vec{v}).$$

$\rightsquigarrow$ for $d = 2$, the Stokes system can be written $A_2\hat{w} = \hat{G}$ with

$$A_2 = \begin{bmatrix} -\nu\,\Delta + c & 0 & dx \\ 0 & -\nu\,\Delta + c & dy \\ dx & dy & 0 \end{bmatrix} \in D^{3\times 3},$$

with $D = \mathbb{R}(\nu, c)[dx, dy]$.

Smith normal form

$\diamond$ $D = k[s]$, k field (e.g., $\mathbb{Q}$, $\mathbb{R}$, $\mathbb{C}$) : euclidian ring.

Theorem. $\forall\, A \in D^{q \times p}$, $\exists\, E \in \mathrm{GL}_q(D)$, $F \in \mathrm{GL}_p(D)$:

$$A = E\,S\,F, \text{ with } S = \begin{pmatrix} \alpha_1 & 0 & \dots & \dots & 0 & \dots & 0 \\ 0 & \alpha_2 & \ddots & & \vdots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots & & \vdots \\ 0 & \dots & 0 & \alpha_r & 0 & \dots & 0 \\ 0 & \dots & \dots & \dots & 0 & \dots & 0 \\ \vdots & & & & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & \dots & 0 & \dots & 0 \end{pmatrix} \in D^{q \times p},$$

where $\alpha_1 \,|\, \alpha_2 \,|\, \dots \,|\, \alpha_r \neq 0$ et $\alpha_i \in D$, $i = 1, \dots, r$.

$\diamond$ The matrices E and F are not unique!

Examples: linear elasticity and Stokes 2D

◇ Linear elasticity problem in 2D:

$$A_2 = \begin{bmatrix} -\mu\,\Delta - (\lambda+\mu)\,dx^2 & -(\lambda+\mu)\,dx\,dy \\ -(\lambda+\mu)\,dx\,dy & -\mu\,\Delta - (\lambda+\mu)\,dy^2 \end{bmatrix}$$

$\rightsquigarrow$ Smith normal form w.r.t. dx: $\begin{bmatrix} 1 & 0 \\ 0 & \Delta^2 \end{bmatrix}$

◇ Stokes problem in 2D:

$$A_2 = \begin{bmatrix} -\nu\,\Delta + c & 0 & dx \\ 0 & -\nu\,\Delta + c & dy \\ dx & dy & 0 \end{bmatrix}$$

$\rightsquigarrow$ Smith normal form w.r.t. dx: $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \Delta\,L_2 \end{bmatrix}, L_2 = -\nu\,\Delta + c.$

Uncoupling the equations

$\diamond$ Consider a linear system of PDEs written as $A_d \vec{w} = \vec{G}$ with $A_d \in D^{q \times q}$ with D a ring of partial differential operators

$\diamond$ Smith normal form of A_d w.r.t. 1 direction: $E_d, F_d \in \mathrm{GL}_q(D)$:

$$A_d = E_d\, S_d\, F_d \Rightarrow A_d \vec{w} = \vec{G} \Leftrightarrow S_d\,(F_d\, \vec{w}) = E_d^{-1}\, \vec{G}.$$

$\diamond$ S_d diagonal $\Rightarrow$ scalar equations in the Smith variables $F_d\, \vec{w}$

$\Rightarrow$ We have uncoupled the equations to get a set of independent scalar PDEs

Domain decomposition method for the Δ^2 operator

◇ Problem: find $\phi : \mathbb{R}^2 \to \mathbb{R}$ such that

$$\begin{cases} \Delta^2 \phi = g \text{ in } \mathbb{R}^2, \\ |\phi(\vec{x})| \to 0 \text{ for } |\vec{x}| \to \infty \end{cases}$$

where g is a given right hand side.

◇ Domain $\Omega = \mathbb{R}^2$ decomposed into $\Omega_1 = \mathbb{R}^- \times \mathbb{R}$, $\Omega_2 = \mathbb{R}^+ \times \mathbb{R}$

◇ Interface $\Gamma = \{0\} \times \mathbb{R}$, $(\vec{n}_i)_{i=1,2}$ the outward normal of $(\Omega_i)_{i=1,2}$.

◇ Choose initial values ϕ_1^0 and ϕ_2^0 such that:

$$\phi_1^0 = \phi_2^0, \quad \Delta\phi_1^0 = \Delta\phi_2^0, \text{ on } \Gamma$$

Algorithm (optimal) for the Δ^2 operator

$\diamond$ Correction step: compute the corrections $(\tilde{\phi}_i^{n+1})_{i=1,2}$

$$\left\{\begin{array}{l} \Delta^2 \tilde{\phi}_1^{n+1} = 0 \text{ in } \Omega_1 \\ \lim_{|\vec{x}|\to\infty} |\tilde{\phi}_1^{n+1}| = 0 \\ \frac{\partial \tilde{\phi}_1^{n+1}}{\partial \vec{n}_1} = \gamma_1^n \text{ on } \Gamma \\ \frac{\partial \Delta \tilde{\phi}_1^{n+1}}{\partial \vec{n}_1} = \gamma_2^n \text{ on } \Gamma \end{array}\right. \qquad \left\{\begin{array}{l} \Delta^2 \tilde{\phi}_2^{n+1} = 0 \text{ in } \Omega_2 \\ \lim_{|\vec{x}|\to\infty} |\tilde{\phi}_2^{n+1}| = 0 \\ \frac{\partial \tilde{\phi}_2^{n+1}}{\partial \vec{n}_2} = \gamma_1^n \text{ on } \Gamma \\ \frac{\partial \Delta \tilde{\phi}_2^{n+1}}{\partial \vec{n}_2} = \gamma_2^n \text{ on } \Gamma \end{array}\right.$$

where $\gamma_1^n = -\frac{1}{2}\left(\frac{\partial \phi_1^n}{\partial \vec{n}_1} + \frac{\partial \phi_2^n}{\partial \vec{n}_2}\right)$ and $\gamma_2^n = -\frac{1}{2}\left(\frac{\partial \Delta \phi_1^n}{\partial \vec{n}_1} + \frac{\partial \Delta \phi_2^n}{\partial \vec{n}_2}\right)$.

$\diamond$ Updating step: update $(\phi_i^{n+1})_{i=1,2}$ by solving the local problems

$$\left\{\begin{array}{l} \Delta^2 \phi_1^{n+1} = g \text{ in } \Omega_1 \\ \lim_{|\vec{x}|\to\infty} |\phi_1^{n+1}| = 0 \\ \phi_1^{n+1} = \phi_1^n + \delta_1^{n+1} \text{ on } \Gamma \\ \Delta \phi_1^{n+1} = \Delta \phi_1^n + \delta_2^{n+1} \text{ on } \Gamma \end{array}\right. \qquad \left\{\begin{array}{l} \Delta^2 \phi_2^{n+1} = g \text{ in } \Omega_2 \\ \lim_{|\vec{x}|\to\infty} |\phi_2^{n+1}| = 0 \\ \phi_2^{n+1} = \phi_2^n + \delta_1^{n+1} \text{ on } \Gamma \\ \Delta \phi_2^{n+1} = \Delta \phi_2^n + \delta_2^{n+1} \text{ on } \Gamma \end{array}\right.$$

where $\delta_1^{n+1} = \frac{1}{2}(\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})$ and $\delta_2^{n+1} = \frac{1}{2}(\Delta\tilde{\phi}_1^{n+1} + \Delta\tilde{\phi}_2^{n+1})$.

Role of algebraic computations

◇ Observations on existing algorithms:

- They use the Smith variables provided by the F given by the computer algebra system $\rightsquigarrow$ not necessarily the simpler one
- The interface conditions are reduced by hand calculations

◇ Ameliorations using algebraic tools:

- Find Smith variables as simple as possible
- Use eliminations techniques to reduce automatically the interface conditions

$\Rightarrow$ Final algorithm that can be used for practical computations

III

Relevant Smith variables

Statement of the general problem

◇ Let $R \in D^{q \times q}$ where D is a ring of partial differential operators

◇ Smith normal form of R w.r.t. one direction: $E, F \in \mathrm{GL}_q(D)$ s.t.

$$R = E\, S\, F, \quad S = \begin{pmatrix} I_r & 0 \\ 0 & S_2 \end{pmatrix}, \quad S_2 = \mathrm{diag}(d_{r+1}, \ldots, d_q).$$

◇ E, F not unique! We want to find a F as simple as possible

A completion problem

$\diamond$ Let $M = D^{1\times q}/(D^{1\times q}\, R)$ be the left D-module associated to R

$\diamond$ Let $F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}$ so that $R = E\, S\, F \Leftrightarrow \begin{pmatrix} F_1 \\ S_2\, F_2 \end{pmatrix} = E^{-1}\, R$.

$\diamond$ $S_2 = \mathrm{diag}(d_{r+1}, \ldots, d_q) \Rightarrow$ The rows of F_2 must be elements of M annihilated by a partial differential operators d_i.

$\rightsquigarrow$ The possible F_2's can be found by computing a family of generators of the $\mathrm{Ann}_M(d_i)$, $i = r+1, \ldots, q$.

$\Rightarrow$ For each choice for F_2, we are reduced to the completion problem of finding (if it exists) F_1 such that:

$$F_1 = \Lambda\, R, \quad F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} \text{ unimodular.}$$

A solution to the completion problem

◇ Necessary conditions:

- The rows of F_2 must be linearly independent
- There must exists E_2 such that $S_2\, F_2 = E_2\, R$.

◇ Theorem: let Q_2 be a minimal parametrization of F_2.
If $\mathrm{coker}_D(.F_2)$ is a free left D-module, then Q_2 admits a left inverse T. If there exists Z and Λ such that $T = \begin{pmatrix} -Z & \Lambda \end{pmatrix} \begin{pmatrix} F_2 \\ R \end{pmatrix}$,
then $F_1 = T + Z\, F_2$ is a solution to the completion problem.

◇ All the computations can be done using OreModules
$\rightsquigarrow$ We provide an implementation

Example: elasticity 3D

◇ Consider the elastostatic equations (Navier-Stokes in $\mathbb{R}^3$):

$$R = \begin{bmatrix} -(\lambda+\mu)\,dx^2 - \mu\,\Delta & -dx\,dy\,(\lambda+\mu) & -dx\,dz\,(\lambda+\mu) \\ -dx\,dy\,(\lambda+\mu) & -(\lambda+\mu)\,dy^2 - \mu\,\Delta & -dy\,dz\,(\lambda+\mu) \\ -dx\,dz\,(\lambda+\mu) & -dy\,dz\,(\lambda+\mu) & -(\lambda+\mu)\,dz^2 - \mu\,\Delta \end{bmatrix}$$

with $\Delta = dx^2 + dy^2 + dz^2$

◇ Let $D = \mathbb{Q}(\lambda, \mu)[dx, dy, dz]$ and $M = D^{1\times 3}/(D^{1\times 3}\,R)$

◇ Its Smith normal form w.r.t. dx is $S = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \Delta & 0 \\ 0 & 0 & \Delta^2 \end{pmatrix}$.

Example: elasticity 3D

$\diamond$ The 2nd (resp. 3rd) row of $F \in \mathrm{GL}_3(D)$ satisfying $R = E\,S\,F$ with $E \in \mathrm{GL}_3(D)$ must belong to $\mathrm{Ann}_M(\Delta)$ (resp. $\mathrm{Ann}_M(\Delta^2)$).

$\diamond$ Families of generators of $\mathrm{Ann}_M(\Delta)$ and $\mathrm{Ann}_M(\Delta^2)$ are given by the rows of the following matrices F_2 and F_3

$$F_2 = \begin{bmatrix} -dz\,\mu & 0 & dx\,\mu \\ -dy\,\mu & dx\,\mu & 0 \\ 2\,dx\,\mu + dx\,\lambda & dy\,\lambda + 2\,dy\,\mu & dz\,\lambda + 2\,dz\,\mu \\ 0 & -dz\,\mu & dy\,\mu \end{bmatrix}$$

$$F_3 = \begin{bmatrix} 2\,\mu^2 + \lambda\,\mu & 0 & 0 \\ 0 & 2\,\mu^2 + \lambda\,\mu & 0 \\ 0 & 0 & 2\,\mu^2 + \lambda\,\mu \end{bmatrix}$$

Example: elasticity 3D

⋄ Choosing the 4th row of F_2 (resp.the 3rd row of F_3) as 2nd (resp. 3rd) row of F

⋄ Completion problem: find $F_1 \in D^{1\times 3}$ such that $F_1 = \Lambda\, R$ for some $\Lambda \in D^{1\times 3}$ and $F = \begin{pmatrix} F_1 \\ F_{23} \end{pmatrix}$ is unimodular where

$$F_{23} = \begin{bmatrix} 0 & -dz\,\mu & dy\,\mu \\ 0 & 0 & 1 \end{bmatrix}.$$

⋄ Our Maple implementation succeeds: we get

$$F = \begin{bmatrix} 1 & -\frac{dy\,dx}{dy^2+dz^2} & -\frac{dx\left(dy^2\lambda+2\,dz^2\lambda+dx^2\lambda+3\,dz^2\mu+2\,dy^2\mu+2\,dx^2\mu\right)}{(\lambda+\mu)\left(dy^2+dz^2\right)dz} \\ 0 & -dz\,\mu & dy\,\mu \\ 0 & 0 & 1 \end{bmatrix}.$$

Example: elasticity 3D

◇ Choosing the 3rd row of F_2 (resp.the 1st row of F_3) as 2nd (resp. 3rd) row of F

◇ Completion problem: find $F_1 \in D^{1\times 3}$ such that $F_1 = \Lambda\, R$ for some $\Lambda \in D^{1\times 3}$ and $F = \begin{pmatrix} F_1 \\ F_{23} \end{pmatrix}$ is unimodular where

$$F_{23} := \begin{bmatrix} 2\, dx\, \mu + dx\, \lambda & dy\, \lambda + 2\, dy\, \mu & dz\, \lambda + 2\, dz\, \mu \\ 1 & 0 & 0 \end{bmatrix}$$

◇ Our Maple implementation fails.

◇ The choice made for F_{23} is not a good one.

IV

Reduction of interface conditions

Algorithm (optimal) for the Δ^2 operator

◇ Correction step: compute the corrections $(\tilde{\phi}_i^{n+1})_{i=1,2}$

$$\begin{cases} \Delta^2 \tilde{\phi}_1^{n+1} = 0 \text{ in } \Omega_1 \\ \lim_{|\vec{x}|\to\infty} |\tilde{\phi}_1^{n+1}| = 0 \\ \frac{\partial \tilde{\phi}_1^{n+1}}{\partial \vec{n}_1} = \gamma_1^n \text{ on } \Gamma \\ \frac{\partial \Delta \tilde{\phi}_1^{n+1}}{\partial \vec{n}_1} = \gamma_2^n \text{ on } \Gamma \end{cases} \qquad \begin{cases} \Delta^2 \tilde{\phi}_2^{n+1} = 0 \text{ in } \Omega_2 \\ \lim_{|\vec{x}|\to\infty} |\tilde{\phi}_2^{n+1}| = 0 \\ \frac{\partial \tilde{\phi}_2^{n+1}}{\partial \vec{n}_2} = \gamma_1^n \text{ on } \Gamma \\ \frac{\partial \Delta \tilde{\phi}_2^{n+1}}{\partial \vec{n}_2} = \gamma_2^n \text{ on } \Gamma \end{cases}$$

where $\gamma_1^n = -\frac{1}{2}\left(\frac{\partial \phi_1^n}{\partial \vec{n}_1} + \frac{\partial \phi_2^n}{\partial \vec{n}_2}\right)$ and $\gamma_2^n = -\frac{1}{2}\left(\frac{\partial \Delta \phi_1^n}{\partial \vec{n}_1} + \frac{\partial \Delta \phi_2^n}{\partial \vec{n}_2}\right)$.

◇ Updating step: update $(\phi_i^{n+1})_{i=1,2}$ by solving the local problems

$$\begin{cases} \Delta^2 \phi_1^{n+1} = g \text{ in } \Omega_1 \\ \lim_{|\vec{x}|\to\infty} |\phi_1^{n+1}| = 0 \\ \phi_1^{n+1} = \phi_1^n + \delta_1^{n+1} \text{ on } \Gamma \\ \Delta \phi_1^{n+1} = \Delta \phi_1^n + \delta_2^{n+1} \text{ on } \Gamma \end{cases} \qquad \begin{cases} \Delta^2 \phi_2^{n+1} = g \text{ in } \Omega_2 \\ \lim_{|\vec{x}|\to\infty} |\phi_2^{n+1}| = 0 \\ \phi_2^{n+1} = \phi_2^n + \delta_1^{n+1} \text{ on } \Gamma \\ \Delta \phi_2^{n+1} = \Delta \phi_2^n + \delta_2^{n+1} \text{ on } \Gamma \end{cases}$$

where $\delta_1^{n+1} = \frac{1}{2}(\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})$ and $\delta_2^{n+1} = \frac{1}{2}(\Delta \tilde{\phi}_1^{n+1} + \Delta \tilde{\phi}_2^{n+1})$.

Problem

◇ In the algorithm: we have

- Equations in the domain Ω_i
- Interface conditions on Γ

◇ First idea to reduce the interface conditions: gather all the equations and compute a Gröbner basis

◇ Problem: the independent variables do not play the same role since the border of the interface is defined by $x = 0$
$\rightsquigarrow$ The interface conditions cannot be differentiated w.r.t. x

Our method

◇ Algorithm to reduce the interface conditions:

1. Compute a Gröbner basis of the equations inside the domain for a relevant monomial order;
2. Compute the normal forms of the interface conditions w.r.t. the latter Gröbner basis;
3. Write this normal forms in a jet space in the variable x;
4. Perform linear algebra manipulations to simplify the normal forms.

◇ All the computations can be done using OreModules

$\rightsquigarrow$ We provide an implementation

V

Conclusion / Perspectives

Conclusions / Perspectives

Conclusion

◇ Algebraic computations can help in designing practical algorithms for solving linear systems of PDEs

◇ Calculations obtained using our implementations can be found at

http://www-math.unice.fr/~dolean/saddles/

Perspectives

◇ Implement the whole numerical algorithm using our algebraic preconditionners for the elasticity, Stokes and Oseen systems

◇ Formulation of the domain decomposition method with an algebraic analysis point of view

◇ Study of the discrete case