Symbolic Techniques for Domain Decomposition Methods

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1 Introduction

Some algorithmic aspects of systems of PDEs based simulations can be better clarified by means of symbolic computation techniques. This is very important since numerical simulations heavily rely on solving systems of PDEs. For the large-scale problems we deal with in today's standard applications, it is necessary to rely on iterative Krylov methods that are scalable (i.e., weakly dependent on the number of degrees on freedom and number of subdomains) and have limited memory requirements. They are preconditioned by domain decomposition methods, incomplete factorizations and multigrid preconditioners. These techniques are well understood and efficient for scalar symmetric equations (e.g., Laplacian, biLaplacian) and to some extent for non-symmetric equations (e.g., convection-diffusion). But they have poor performances and lack robustness when used for symmetric systems of PDEs, and even more so for non-symmetric complex systems (fluid mechanics, porous media…). As a general rule, the study of iterative solvers for systems of PDEs as opposed to scalar PDEs is an underdeveloped subject.

We aim at building new robust and efficient solvers, such as domain decomposition methods and preconditioners for some linear and well-known systems of PDEs. In particular, we shall concentrate on Neumann-Neumann and FETI type algorithms which are very popular for scalar symmetric positive definite second order problems (see, for instance, [9, 11]), and to some extent to different other problems, like the advection-diffusion equations [1], plate and shell problems [16] or the Stokes equations [13]. This work is motivated by the fact that, in some sense, these methods applied to systems of PDEs (such as Stokes, Oseen, linear elasticity) are less optimal than the domain decomposition methods for scalar problems. Indeed, in the

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case of two subdomains consisting of the two half planes, it is well-known that the Neumann-Neumann preconditioner is an exact preconditioner (the preconditioned operator is the identity operator) for the Schur complement equation for scalar equations like the Laplace problem. Unfortunately, this does not hold in the vector case.

In order to achieve this goal, we use algebraic methods developed in constructive algebra, D-modules (differential modules) and symbolic computation such as the so-called Smith or Jacobson normal forms and Gröbner basis techniques for transforming a linear system of PDEs into a set of independent PDEs. These algebraic and symbolic methods provide important intrinsic information (e.g., invariants) about the linear system of PDEs to solve. These build-in properties need to be taken into account in the design of new numerical methods, which can supersede the usual ones based on a direct extension of the classical scalar methods to linear systems of PDEs.

By means of these techniques, it is also possible to transform the linear system of PDEs into a set of decoupled PDEs under certain types of invertible transformations. One of these techniques is the so-called Smith normal form of the matrix of OD operators associated with the linear system. This normal form was introduced by H. J. S. Smith (1826–1883) for matrices with integer entries (see, e.g., [17], Theorem 1.4). The Smith normal form has already been successfully applied to open problems in the design of Perfectly Matched Layers (PML). The theory of PML for scalar equations was well-developed and the usage of the Smith normal form allowed to extend these works to systems of PDEs. In [12], a general approach is proposed and applied to the particular case of the compressible Euler equations that model aero-acoustic phenomena and in [2] for shallow-water equations.

For domain decomposition methods, several results have been obtained on compressible Euler equations [7], Stokes and Oseen systems [8] or in [10] where a new method in the "Smith" spirit has been derived. Previously the computations were performed heuristically, whereas in this work, we aim at finding a systematic way to build optimal algorithms for given PDE systems.

Notations. If R is a ring, then $R^{p\times q}$ is the set of $p\times q$ matrices with entries in R and $\mathrm{GL}_p(R)$ is the group of invertible matrices of $R^{p\times p}$, namely $\mathrm{GL}_p(R) = \{E \in R^{p\times p} \mid \exists\, F \in R^{p\times p} : E\,F = F\,E = I_p\}$. An element of $\mathrm{GL}_p(R)$ is called an *unimodular matrix*. A diagonal matrix with elements d_i's will be denoted by $\mathrm{diag}(d_1,\ldots,d_p)$. If k is a field (e.g., $k=\mathbb{Q}$, $\mathbb{R}$, $\mathbb{C}$), then $k[x_1,\ldots,x_n]$ is the commutative ring of polynomials in $x_1,\ldots,x_n$ with coefficients in k. In what follows, $k(x_1,\ldots,x_n)$ will denote the field of rational functions in $x_1,\ldots,x_n$ with coefficients in k. Finally, if $r,\, r' \in R$, then $r' \mid r$ means that r' divides r, i.e., there exists $r'' \in R$ such that $r = r''\,r'$.

2 Smith Normal Form of Linear Systems of PDEs

We first introduce the concept of *Smith normal form* of a matrix with polynomial entries (see, e.g., [17], Theorem 1.4). The Smith normal form is a mathematical technique which is classically used in module theory, linear algebra, symbolic computation, ordinary differential systems, and control theory. It was first developed to study matrices with integer entries. But, it was proved to exist for any *principal ideal* *domain* (namely, a commutative ring R whose ideals can be generated by an element of R) [15]. Since $R = k[s]$ is a principal ideal domain when k is a field, we have the following theorem only stated for square matrices.

Theorem 1. *Let k be a field, $R = k[s]$, p a positive integer and $A \in R^{p\times p}$. Then, there exist two matrices $E \in \mathrm{GL}_p(R)$ and $F \in \mathrm{GL}_p(R)$ such that*

$$A = E\,S\,F,$$

where $S = \mathrm{diag}(d_1,\dots,d_p)$ and the $d_i \in R$ satisfying $d_1\,|\,d_2\,|\cdots|\,d_p$. In particular, we can take $d_i = m_i/m_{i-1}$, where m_i is the greatest common divisor of all the $i\times i$-minors of A (i.e., the determinants of all $i\times i$-submatrices of A), with the convention that $m_0 = 1$. The matrix $S = \mathrm{diag}(d_1,\dots,d_p) \in R^{p\times p}$ is called a Smith normal form *of A.*

We note that $E \in \mathrm{GL}_p(R)$ is equivalent to $\det(E)$ is an invertible polynomial, i.e., $\det(E) \in k\setminus\{0\}$. Also, in what follows, we shall assume that the d_i's are *monic polynomials*, i.e., their leading coefficients are 1, which will allow us to call the matrix $S = \mathrm{diag}(d_1,\dots,d_p)$ *the* Smith normal form of A. But, the unimodular matrices E and F are not uniquely defined by A. The proof of Theorem 1 is constructive and gives an algorithm for computing matrices E, S and F. The computation of Smith normal forms is available in many computer algebra systems such as `Maple`, `Mathematica`, `Magma`...

Consider now the following model problem in $\mathbb{R}^d$ with $d = 2,3$:

$$\mathscr{L}_d(\mathbf{w}) = \mathbf{g} \quad \text{in } \mathbb{R}^d, \qquad |\mathbf{w}(\mathbf{x})| \to 0 \quad \text{for } |\mathbf{x}| \to \infty. \tag{1}$$

For instance, $\mathscr{L}_d(\mathbf{w})$ can represent the Stokes/Oseen/linear elasticity operators in dimension d. Moreover, if we suppose that the inhomogeneous linear system of PDEs (1) has constant coefficients, then it can be rewritten as

$$A_d\,\mathbf{w} = \mathbf{g}, \tag{2}$$

where $A_d \in R^{p\times p}$, $R = k[\partial_x,\partial_y]$ (resp., $R = k[\partial_x,\partial_y,\partial_z]$) for $d = 2$ (resp., $d = 3$) and k is a field.

In what follows, we shall study the domain decomposition problem in which $\mathbb{R}^d$ is divided into subdomains. We assume that the direction normal to the interface of the subdomains is particularized and denoted by ∂_x. If $R_x = k(\partial_y)[\partial_x]$ for $d = 2$ or $R_x = k(\partial_y,\partial_z)[\partial_x]$ for $d = 3$, then, computing the Smith normal form of the matrix $A_d \in R_x^{p\times p}$, we obtain $A_d = E\,S\,F$, where $S \in R_x^{p\times p}$ is a diagonal matrix, $E \in \mathrm{GL}_p(R_x)$ and $F \in \mathrm{GL}_p(R_x)$. The entries of the matrices E, S, F are polynomials in ∂_x, and E and F are unimodular matrices, i.e., $\det(E), \det(F) \in k(\partial_y)\setminus\{0\}$ if $d = 2$, or $\det(E), \det(F) \in k(\partial_y,\partial_z)\setminus\{0\}$ if $d = 3$. We recall that the matrices E and F are not unique contrary to S. Using the Smith normal form of A_d, we get:

$$A_d\,\mathbf{w} = \mathbf{g} \quad \Leftrightarrow \quad \{\mathbf{w_s} := F\,\mathbf{w},\; S\,\mathbf{w_s} = E^{-1}\,\mathbf{g}\}. \tag{3}$$

In other words, (3) is equivalent to the uncoupled linear system:

$$S\,\mathbf{w_s} = E^{-1}\,\mathbf{g}. \tag{4}$$

Since $E \in \mathrm{GL}_p(R_x)$ and $F \in \mathrm{GL}_p(R_x)$, the entries of their inverses are still polynomial in ∂_x. Thus, applying E^{-1} to the right-hand side $\mathbf{g}$ of $A_d\,\mathbf{w} = \mathbf{g}$ amounts to taking k-linear combinations of derivatives of $\mathbf{g}$ with respect to x. If $\mathbb{R}^d$ is split into two subdomains $\mathbb{R}^- \times \mathbb{R}^{d-1}$ and $\mathbb{R}^+ \times \mathbb{R}^{d-1}$, where $\mathbb{R}^- = \{x \in \mathbb{R} \mid x < 0\}$ and $\mathbb{R}^+ = \{x \in \mathbb{R} \mid x > 0\}$, then the application of E^{-1} and F^{-1} to a vector can be done for each subdomain independently. No communication between the subdomains is necessary.

In conclusion, it is enough to find a domain decomposition algorithm for the uncoupled system (4) and then transform it back to the original one (2) by means of the invertible matrix F over R_x. This technique can be applied to any linear system of PDEs once it is rewritten in a polynomial form. The uncoupled system acts on the new dependent variables $\mathbf{w_s}$, which we shall further call *Smith variables* since they are issued from the Smith normal form.

Remark 1. Since the matrix F is used to transform (4) to (2) (see the first equation of the right-hand side of (3)) and F is not unique, we need to find a matrix F as simple as possible (e.g., F has minimal degree in ∂_x) so that to obtain a final algorithm whose form can be used for practical computations.

Example 1 Consider the two dimensional elasticity operator defined by $\mathscr{E}_2(\mathbf{u}) := -\mu\,\Delta\,\mathbf{u} - (\lambda+\mu)\,\nabla\operatorname{div}\mathbf{u}$. If we consider the commutative polynomial rings $R = \mathbb{Q}(\lambda,\mu)[\partial_x,\partial_y]$, $R_x = \mathbb{Q}(\lambda,\mu)(\partial_y)[\partial_x] = \mathbb{Q}(\lambda,\mu,\partial_y)[\partial_x]$ and

$$A_2 = \begin{pmatrix} (\lambda+2\mu)\,\partial_x^2 + \mu\,\partial_y^2 & (\lambda+\mu)\,\partial_x\,\partial_y \\ (\lambda+\mu)\,\partial_x\,\partial_y & \mu\,\partial_x^2 + (\lambda+2\mu)\,\partial_y^2 \end{pmatrix} \in R^{2\times 2}$$

the matrix of PD operators associated with $\mathscr{E}_2$, i.e., $\mathscr{E}_2(\mathbf{u}) = A_2\,\mathbf{u}$, then the Smith normal form of $A_2 \in R_x^{2\times 2}$ is defined by:

$$S_{A_2} = \begin{pmatrix} 1 & 0 \\ 0 & \Delta^2 \end{pmatrix}. \tag{5}$$

The particular form of S_{A_2} shows that, over R_x, the system of PDEs for the linear elasticity in $\mathbb{R}^2$ is algebraically equivalent to a biharmonic equation.

Example 2 Consider the two dimensional Oseen operator $\mathscr{O}_2(\mathbf{w}) = \mathscr{O}_2(\mathbf{v},q) := (c\,\mathbf{v} - \nu\,\Delta\mathbf{v} + \mathbf{b}\cdot\nabla\mathbf{v} + \nabla q, \nabla\cdot\mathbf{v})$, where $\mathbf{b}$ is the convection velocity. If $\mathbf{b} = 0$, then we obtain the Stokes operator $\mathscr{S}_2(\mathbf{w}) = \mathscr{S}_2(\mathbf{v},q) := (c\,\mathbf{v} - \nu\,\Delta\mathbf{v} + \nabla q, \nabla\cdot\mathbf{v})$. If $R = \mathbb{Q}(b_1,b_2,c,\nu)[\partial_x,\partial_y]$, $R_x = \mathbb{Q}(b_1,b_2,c,\nu)(\partial_y)[\partial_x] = \mathbb{Q}(b_1,b_2,c,\nu,\partial_y)[\partial_x]$ and

$$O_2 = \begin{pmatrix} -\nu\,(\partial_x^2+\partial_y^2) + b_1\,\partial_x + b_2\,\partial_y + c & 0 & \partial_x \\ 0 & -\nu\,(\partial_x^2+\partial_y^2) + b_1\,\partial_x + b_2\,\partial_y + c & \partial_y \\ \partial_x & \partial_y & 0 \end{pmatrix}$$

the matrix of PD operators associated with $\mathscr{O}_2$, i.e., $\mathscr{O}_2(\mathbf{w}) = O_2\,\mathbf{w}$, then the Smith normal form of $O_2 \in R_x^{3\times 3}$ is defined by:

$$S_{O_2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \Delta L_2 \end{pmatrix}, \quad L_2 = c - \nu\,\Delta + \mathbf{b}\cdot\nabla. \tag{6}$$

From the form of S_{O_2} we can deduce that the two-dimensional Oseen equations can be mainly characterized by the scalar fourth order PD operator ΔL_2. This is not surprising since the stream function formulation of the Oseen equations for $d = 2$ gives the same PDE for the stream function.

Remark 2. The above applications of Smith normal forms suggest that one should design an optimal domain decomposition method for the biharmonic operator Δ^2 (resp., $L_2\,\Delta$) in the case of linear elasticity (resp., the Oseen/Stokes equations) for the two-dimensional problems, and then transform it back to the original system.

3 An Optimal Algorithm for the Biharmonic Operator

We give here an example of Neumann-Neumann methods in its iterative version for Laplace and biLaplace equations. For simplicity, consider a decomposition of the domain $\Omega = \mathbb{R}^2$ into two half planes $\Omega_1 = \mathbb{R}^- \times \mathbb{R}$ and $\Omega_2 = \mathbb{R}^+ \times \mathbb{R}$. Let the interface $\{0\} \times \mathbb{R}$ be denoted by Γ and $(\mathbf{n}_i)_{i=1,2}$ be the outward normal of $(\Omega_i)_{i=1,2}$. We consider the following problem:

$$-\Delta u = f \text{ in } \mathbb{R}^2, \quad |u(\mathbf{x})| \to 0 \text{ for } |\mathbf{x}| \to \infty. \tag{7}$$

and the following **Neumann-Neumann algorithm** applied to problem (7):
Let u_Γ^n be the interface solution at iteration n. We obtain u_Γ^{n+1} from u_Γ^n by the following iterative procedure

$$\begin{cases} -\Delta u^{i,n} = f, & in\ \Omega_i, \\ u^{i,n} = u_\Gamma^n, & on\ \Gamma, \end{cases} \qquad \begin{cases} -\Delta \tilde{u}^{i,n} = 0, & in\ \Omega_i, \\ \dfrac{\partial \tilde{u}^{i,n}}{\partial \mathbf{n}_i} = -\dfrac{1}{2}\left(\dfrac{\partial u^{1,n}}{\partial \mathbf{n}_1} + \dfrac{\partial u^{2,n}}{\partial \mathbf{n}_2}\right), & on\ \Gamma, \end{cases} \tag{8}$$

and then $u_\Gamma^{n+1} = u_\Gamma^n + \frac{1}{2}\left(\tilde{u}^{1,n} + \tilde{u}^{2,n}\right)$.
This algorithm is *optimal* in the sense that it converges in two iterations.

Since the biharmonic operator seems to play a key role in the design of a new algorithm for both Stokes and elasticity problem in two dimensions, we need to build an optimal algorithm for it. We consider the following problem:
Find $\phi : \mathbb{R}^2 \to \mathbb{R}$ such that:

$$\Delta^2 \phi = g \text{ in } \mathbb{R}^2, \quad |\phi(\mathbf{x})| \to 0 \text{ for } |\mathbf{x}| \to \infty. \tag{9}$$

and the following **"Neumann-Neumann" type algorithm** applied to (9):
Let $(\phi_\Gamma^n, D\phi_\Gamma^n)$ be the interface solution at iteration n (suppose also that $\phi_\Gamma^0 =$

$\phi^0|_\Gamma, D\phi^0_\Gamma = (\Delta\phi^0)_\Gamma$). *We obtain* $(\phi^{n+1}_\Gamma, D\phi^n_\Gamma)$ *from* $(\phi^n_\Gamma, D\phi^n_\Gamma)$ *by the following iterative procedure*

$$\begin{cases} -\Delta^2\phi^{i,n} = f, & \text{in } \Omega_i, \\ \phi^{i,n} = \phi^n_\Gamma, & \text{on } \Gamma, \\ \Delta\phi^{i,n} = D\phi^n_\Gamma, & \text{on } \Gamma, \end{cases} \quad \begin{cases} -\Delta^2\tilde{\phi}^{i,n} = 0, & \text{in } \Omega_i, \\ \dfrac{\partial\tilde{\phi}^{i,n}}{\partial\mathbf{n}_i} = -\dfrac{1}{2}\left(\dfrac{\partial\phi^{1,n}}{\partial\mathbf{n}_1} + \dfrac{\partial\phi^{2,n}}{\partial\mathbf{n}_2}\right), & \text{on } \Gamma, \\ \dfrac{\partial\Delta\tilde{\phi}^{i,n}}{\partial\mathbf{n}_i} = -\dfrac{1}{2}\left(\dfrac{\partial\Delta\phi^{1,n}}{\partial\mathbf{n}_1} + \dfrac{\partial\Delta\phi^{2,n}}{\partial\mathbf{n}_2}\right), & \text{on } \Gamma, \end{cases} \tag{10}$$

and then $\phi^{n+1}_\Gamma = \phi^n_\Gamma + \frac{1}{2}\left(\tilde{\phi}^{1,n} + \tilde{\phi}^{2,n}\right)$, $D\phi^{n+1}_\Gamma = D\phi^n_\Gamma + \frac{1}{2}\left(\tilde{\Delta}\phi^{1,n} + \tilde{\Delta}\phi^{2,n}\right)$.

This is a generalization of the Neumann-Neumann algorithm for the Δ operator and is also *optimal* (the proof can be found in [8]).

Now, in the case of the two dimensional linear elasticity, ϕ represents the second component of the vector of Smith variables, that is, $\phi = (\mathbf{w}_s)_2 = (F\mathbf{u})_2$, where $\mathbf{u} = (u, v)$ is the displacement field. Hence, we need to replace ϕ with $(F\mathbf{u})_2$ into the algorithm for the biLaplacian, and then simplify it using algebraically admissible operations. Thus, one can obtain an optimal algorithm for the Stokes equations or linear elasticity depending on the form of F. From here comes the necessity of choosing in a proper way the matrix F (which is not unique), used to define the Smith normal form, in order to obtain a "good" algorithm for the systems of PDEs from the optimal one applied to the biharmonic operator. In [7] and [8], the computation of the Smith normal forms for the Euler equations and the Stokes equations was done by hand or using the `Maple` command *Smith*. Surprisingly, the corresponding matrices F have provided good algorithms for the Euler equations and the Stokes equations even if the approach was entirely heuristic.

4 Relevant Smith Variables: A Completion Problem

The efficiency of our algorithms heavily relies on the simplicity of the Smith variables, that is on the entries of the unimodular matrix F used to compute the Smith normal form of the matrix A. In this section, within a constructive *algebraic analysis* approach, we develop a method for constructing many possible Smith variables. Taking into account physical aspects, the user can then choose the simplest one among them. We are going to show that the problem of finding Smith variables can be reduced to a *completion problem*. First of all, we very briefly introduce some notions of module theory [15].

Given a ring R (e.g., $R = k[\partial_1, \ldots, \partial_d]$, where k is a field (e.g., $\mathbb{Q}$, $\mathbb{R}$, $\mathbb{C}$)), the definition of a R*-module* M is similar to the one of a vector space but where the scalars are taken in the ring R and not in a field as for vector spaces. If $A \in R^{p\times p}$, then the kernel of the R-linear map (R*-homomorphism*) $.A : R^{1\times p} \longrightarrow R^{1\times p}$, defined by $(.A)(\mathbf{r}) = \mathbf{r}A$, is the R-module defined by:

$$\ker_R(.A) = \{\mathbf{r} \in R^{1\times p} \mid \mathbf{r}A = 0\}.$$

The image $\mathrm{im}_R(.A)$ of $.A$, simply denoted by $R^{1\times p}A$, is the R-module defined by all the R-linear combinations of the rows of A. The cokernel $\mathrm{coker}_R(.A)$ of $.A$ is the *factor* R-module defined by $\mathrm{coker}_R(.A) = R^{1\times p}/(R^{1\times p}A)$. To simplify the notation, we shall denote this module by M. M is nothing more than the R-module of the row vectors of $R^{1\times p}$ modulo the R-linear combinations of rows of A. Let $R_1 = k(\partial_2,\ldots,\partial_d)[\partial_1]$, $R_i = k(\partial_1,\ldots,\partial_{i-1},\partial_{i+1},\ldots,\partial_d)[\partial_i]$, $i = 2,\ldots,d-1$, and $R_d = k(\partial_1,\ldots,\partial_{d-1})[\partial_d]$ be the polynomial rings in ∂_i with coefficients in the field of rational functions in all other PD operators.

Since the R-module $M = R^{1\times p}/(R^{1\times p}A)$ plays a fundamental role in what follows, let us describe it in terms of generators and relations. Let $\{\mathbf{f_j}\}_{j=1,\ldots,p}$ be the standard basis of $R^{1\times p}$, namely $\mathbf{f_j}$ is the row vector of $R^{1\times p}$ defined by 1 at the jth position and 0 elsewhere, and m_j the residue class of $\mathbf{f_j}$ in M. Then, $\{m_j\}_{j=1,\ldots,p}$ is a family of generators of the R-module M, i.e., for any $m \in M$, then there exists $\mathbf{r} = (r_1,\ldots,r_p) \in R^{1\times p}$ such that $m = \sum_{j=1}^{p} r_j m_j$ [3]. The family of generators $\{m_j\}_{j=1,\ldots,p}$ of M satisfies the relations $\sum_{j=1}^{p} A_{ij} m_j = 0$ for all $i = 1,\ldots,p$ [3]. For more details, see [3, 15].

Let $E, F \in \mathrm{GL}_p(R_i)$ be two unimodular matrices such that $A = ESF$, where $S = \mathrm{diag}(1,\ldots,1,d_{r+1},\ldots,d_q)$ is the Smith normal form of A. Moreover, let us split $F \in \mathrm{GL}_p(R_i)$ into two parts row-wise, i.e., $F = (F_1^T \quad F_2^T)^T$, where $F_1 \in R_i^{r\times p}$, $F_2 \in R_i^{(p-r)\times p}$, and r is the number of ones in S. Then:

$$A = ESF \quad \Leftrightarrow \quad \begin{pmatrix} F_1 \\ S_2 F_2 \end{pmatrix} = E^{-1}A, \quad S_2 = \mathrm{diag}(d_{r+1},\ldots,d_p). \tag{11}$$

Cleaning the denominators of the entries of S_2 (resp., F_2), we can assume without loss of generality that the d_j's (resp., the entries of F_2) belong to R. Then, (11) shows that the jth row of F_2 must be an element of the R_i-module $M_i = R_i^{1\times p}/(R_i^{1\times p}A)$ annihilated by d_j. Consequently, the possible F_2's can be found by computing a family of generators of the R_i-modules $\mathrm{ann}_{M_i}(d_j) = \{m \in M_i \mid d_j m = 0\}$ for $j = r+1,\ldots,p$. These R_i-modules can be computed by means of *Gröbner basis techniques* (see, e.g., [6]). Hence, we get $S_2 F_2 = G_2 A$ for some $G_2 \in R_i^{(p-r)\times p}$. Then, for each choice for F_2, we are reduced to the following *completion problem*:

$$\begin{array}{r} \text{Find } F_1 \in R_i^{r\times p} \text{ such that } F = (F_1^T \quad F_2^T)^T \in \mathrm{GL}_p(R_i) \text{ and } F_1 = G_1 A \\ \text{for some } G_1 \in R_i^{r\times p}. \end{array} \tag{12}$$

Example 3 Let $R = \mathbb{Q}(\lambda,\mu)[\partial_x,\partial_y,\partial_z]$ be the commutative polynomial ring of PD operators in ∂_x, ∂_y and ∂_z with coefficients in the field $\mathbb{Q}(\lambda,\mu)$,

$$A = \begin{pmatrix} -(\lambda+\mu)\,\partial_x^2 - \mu\,\Delta & -(\lambda+\mu)\,\partial_x\,\partial_y & -(\lambda+\mu)\,\partial_x\,\partial_z \\ -(\lambda+\mu)\,\partial_x\,\partial_y & -(\lambda+\mu)\,\partial_y^2 - \mu\,\Delta & -(\lambda+\mu)\,\partial_y\,\partial_z \\ -(\lambda+\mu)\,\partial_x\,\partial_z & -(\lambda+\mu)\,\partial_y\,\partial_z & -(\lambda+\mu)\,\partial_z^2 - \mu\,\Delta \end{pmatrix} \in R^{3\times 3}$$

the matrix of PD operators defining the elastostatic equations in $\mathbb{R}^3$, where $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$, and the associated R-module $M = R^{1\times 3}/(R^{1\times 3}A)$. The Smith normal form of A with respect to x is given by $S=\mathrm{diag}(1,\Delta,\Delta^2)$. With the above notations, we get $r=1$ and $S_2=\mathrm{diag}(\Delta,\Delta^2)\in R^{2\times 2}$. Let $R_x=\mathbb{Q}(\lambda,\mu)(\partial_y,\partial_z)[\partial_x]$, $F_1\in R_x^{1\times 3}$ and $F_2\in R_x^{2\times 3}$. Then, the first (resp. second) row of F_2 must be an element of the R_x-module $M_x=R_x^{1\times 3}/(R_x^{1\times 3}A)$ annihilated by $\Delta\in R$ (resp. $\Delta^2\in R$). Using the OREMODULES package [4], we find that families of generators of $\mathrm{ann}_{M_x}(\Delta)$ and $\mathrm{ann}_{M_x}(\Delta^2)$ are respectively defined by the residue classes of the rows of the following matrices in M_x:

$$A_\Delta=\begin{pmatrix} 0 & -\partial_z & \partial_y \\ \partial_z & 0 & -\partial_x \\ -\partial_y & \partial_x & 0 \\ \partial_x & \partial_y & \partial_z \end{pmatrix}, \quad A_{\Delta^2}=I_3.$$

That simply means that a family of generators of $\mathrm{ann}_{M_x}(\Delta)$ is given by the divergence and the curl of the displacement field and for $\mathrm{ann}_{M_x}(\Delta^2)$ by the components of the displacement fields. Now, the first (resp., second) row of F_2 must be a R_x-linear combination of the rows of A_Δ (resp., A_{Δ^2}). We thus have several choices and for each of them, we are reduced to a completion problem (12). For instance, choosing the first row of A_Δ (resp., the third row of A_{Δ^2}) as first (resp., second) row of F_2, namely

$$F_2=\begin{pmatrix} 0 & -\partial_z & \partial_y \\ 0 & 0 & 1 \end{pmatrix},$$

we then have to find a row vector $F_1\in R_x^{1\times 3}$ such that $F_1=G_1\,A$ for some $G_1\in R_x^{1\times 3}$ and $F=(F_1^T \quad F_2^T)^T\in \mathrm{GL}_3(R_x)$. If such a row vector F_1 exists, then the matrix $F=(F_1^T \quad F_2^T)^T$ provides a good choice of Smith variables.

We first give two necessary conditions for a choice of F_2 to provide a solution of the completion problem (straightforward from the relation $A=E\,S\,F$):

Lemma 1. *With the above notations, given $F_2\in R^{(p-r)\times p}$, necessary conditions for the solvability of the completion problem (12) are:*

1. *F_2 admits a right inverse over R_i, i.e. $\exists\, S_2\in R_i^{p\times(p-r)}:\ F_2\,S_2=I_{p-r}$.*
2. *There exists a matrix $G_2\in R_i^{(p-r)\times p}$ such that $S_2\,F_2=G_2\,A$.*

Since R_i is a *principal ideal domain* (namely, every ideal of R_i can be generated by an element of R_i), Condition 1 of Lemma 1 is equivalent to the condition that the R_i-module $\mathrm{coker}_{R_i}(.F_2)=R_i^{1\times p}/(R_i^{1\times(p-r)}\,F_2)$ is free of rank r, i.e. $\mathrm{coker}_{R_i}(.F_2)$ admits a basis of cardinality r [3, 15]. It is equivalent to the existence of two matrices $Q_2\in R_i^{p\times r}$ and $T_2\in R_i^{r\times p}$ such that $\ker_{R_i}(.Q_2)=R_i^{1\times(p-r)}\,F_2$ and $T_2\,Q_2=I_r$ [3]. Such a matrix Q_2 is called an *injective parametrization* of $\mathrm{coker}_{R_i}(.F_2)$. Matrices Q_2 and T_2 can be computed by Gröbner basis techniques [3]. The corresponding algorithms are implemented in the OREMODULES package [4]. The next theorem characterizes the solvability of the completion problem (12).

Theorem 2. *Let $F_2 \in R^{(p-r)\times p}$ admit a right inverse over R_i and satisfy $S_2 F_2 = G_2 A$ for some $G_2 \in R_i^{(p-r)\times p}$. If Q_2 is an injective parametrization of the free R_i-module* $\operatorname{coker}_{R_i}(.F_2)$ *of rank r, and $T_2 \in R_i^{r\times p}$ a left inverse of Q_2, then a necessary and sufficient condition for the existence of a solution of the completion problem (12) is the existence of two matrices $H \in R_i^{r\times(p-r)}$ and $G_1 \in R_i^{r\times p}$ such that $T_2 = G_1 A - H F_2$. Then, $F_1 = T_2 + H F_2 = G_1 A$ is a solution of the completion problem (12), i.e., $F = ((T_2 + H F_2)^T \quad F_2^T)^T \in \mathrm{GL}_p(R_i)$ is such that $A = E\,S\,F$ for some $E \in \mathrm{GL}_p(R_i)$, where S is the Smith normal form of A.*

From the explanations above, we deduce the following algorithm that, given A, $S_2 = \operatorname{diag}(d_{r+1},\dots,d_p)$, and a choice for F_2 computed from the calculations of $\operatorname{ann}_{M_i}(d_j)$ for $d_j \in R$, find (if it exists) a completion of F_2. The following algorithm

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Input: $A \in R^{p\times p}$, $S_2 \in R^{(p-r)\times(p-r)}$ and $F_2 \in R^{(p-r)\times p}$.
Output: A completion $F = (F_1^T \quad F_2^T)^T$ of F_2 or "No completion exists".

1. Compute a right inverse of F_2 over R_i;
2. **If** no right inverse exists, then RETURN "No completion exists", **Else**
   (a) Factorize $S_2 F_2$ with respect to A over R_i;
   (b) **If** no factorization exists, then RETURN "No completion exists", **Else**
      i. Compute an injective parametrization Q_2 of $\operatorname{coker}_{R_i}(.F_2)$;
      ii. Compute a left inverse T_2 of Q_2 over R_i;
      iii. Factorize T_2 with respect to $(F_2^T \quad A^T)^T$ over R_i;
      iv. **If** no factorization exists, then RETURN "No completion exists", **Else** note $T_2 = (-H \quad G_1)\begin{pmatrix} F_2 \\ A \end{pmatrix}$ and RETURN $F = \begin{pmatrix} T_2 + H F_2 \\ F_2 \end{pmatrix}$.

---

was implemented in `Maple` based on the OREMODULES package.

Example 4 Consider again the elastostatic equations introduced in Example 3. For the choice of F_2 given at the end of Example 3, our implementation succeeds in finding a completion and we get the following completion of F_2:

$$F = \begin{pmatrix} 1 & -\frac{\partial_x \partial_y}{\partial_y^2+\partial_z^2} & -\frac{\partial_x\left((\lambda+2\mu)(\partial_x^2+\partial_y^2)+(2\lambda+3\mu)\partial_z^2\right)}{(\lambda+\mu)\,\partial_z\,(\partial_y^2+\partial_z^2)} \\ 0 & -\partial_z & \partial_y \\ 0 & 0 & 1 \end{pmatrix} \in \mathrm{GL}_3(R_x).$$

For more details and explicit computations, we refer the reader to [5].

5 Reduction of the Interface Conditions

In the algorithms presented in the previous sections, we have equations in the domains Ω_i and interface conditions on Γ obtained heuristically. We need to find an automatic way to reduce the interface conditions with respect to the equations in the domains. In this section, we show how symbolic computations can be used to perform such reductions. The naïve idea consists in gathering all equations and compute a Gröbner basis [6]. However, one has to keep in mind that the independent variables do not play the same role. More precisely, the interface conditions cannot be differentiated with respect to x since the border of the interface is defined by $x = 0$. Consequently, we have developed and implemented an alternative method in `Maple` using the OREMODULES package, which can be sketched as follows:

1. Compute a Gröbner basis of the polynomial equations inside the domain for a relevant monomial order;
2. Compute the normal forms of the interface conditions with respect to the latter Gröbner basis;
3. Write these normal forms in the *jet notations* with respect to the independent variable x, i.e., rewrite the derivatives $\partial_x^i y_k$ of the dependent variables y_k as new indeterminates $y_{k,i}$;
4. Perform linear algebra manipulations to simplify the normal forms.

For more details and explicit computations, we refer the reader to [5].

6 Some Optimal Algorithms

After performing the completion and the reduction of the interface conditions, we can give examples of optimal algorithms (elasticity and Stokes equations).

Example 5 Consider the elasticity operator:

$$\mathscr{E}_d \mathbf{u} = -\operatorname{div} \sigma(\mathbf{u}), \quad \sigma(\mathbf{u}) = \mu\,(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \lambda \operatorname{div} \mathbf{u} I_d.$$

If $d = 2$, then the completion algorithm gives two possible choices for F:

$$F = \begin{pmatrix} -\frac{\partial_x(\mu\,\partial_x^2 - \lambda\,\partial_y^2)}{(\lambda+\mu)\,\partial_y^3} & 1 \\ 1 & 0 \end{pmatrix}, \quad F = \begin{pmatrix} 1 & -\frac{(\lambda+\mu)\partial_x((3\mu+2\lambda)\,\partial_y^2 + (2\mu+\lambda)\,\partial_x^2)}{\partial_y^3} \\ 0 & 1 \end{pmatrix}. \qquad (13)$$

By replacing ϕ into the Neumann-Neumann algorithm for the biLaplacian by $(F\mathbf{u})_2$ and re-writing the interface conditions, using the equations inside the domain like in [8], we get two different algorithms for the elasticity system. Note that, in the first case of (13), $\phi = u$, and, in the second one, $\phi = v$ (where $\mathbf{u} = (u, v)$). Below, we shall write in detail the algorithm in the second case. To simplify the writing, we denote by $u_\tau = \mathbf{u} \cdot \tau$, $u_\mathbf{n} = \mathbf{u} \cdot \mathbf{n}$, $\sigma_{\mathbf{nn}}(\mathbf{u}) = (\sigma(\mathbf{u}) \cdot \mathbf{n}) \cdot \mathbf{n}$, $\sigma_{\mathbf{n}\tau}(\mathbf{u}) = (\sigma(\mathbf{u}) \cdot \mathbf{n}) \cdot \tau$.

Let $(u_\Gamma^n, \sigma_\Gamma^n)$ be the interface solution at iteration n (suppose also that $u_\Gamma^0 = (u_\tau^0)|_\Gamma$, $\sigma_\Gamma^0 = (\sigma_{s\mathbf{nn}}(u^0))|_\Gamma$). We obtain $(u_\Gamma^{n+1}, \sigma_\Gamma^n)$ from $(u_\Gamma^n, \sigma_\Gamma^n)$ by the following iterative procedure

$$\begin{cases} \mathscr{E}_2(\mathbf{u}^{i,n}) &= f, \quad in\ \Omega_i, \\ u^{1,n}_{\tau_\mathbf{i}} &= u^n_\Gamma,\ on\ \Gamma, \\ \sigma_{\mathbf{n_i n_i}}(\mathbf{u}^{i,n}) &= \sigma^n_\Gamma,\ on\ \Gamma, \end{cases} \begin{cases} \mathscr{E}_2(\tilde{\mathbf{u}}^{i,n}) &= 0, & in\ \Omega_i, \\ \tilde{\mathbf{u}}^{i,n}_{\tau_\mathbf{i}} &= -\frac{1}{2}\left(\mathbf{u}^{1,n}_{\mathbf{n_1}} + \mathbf{u}^{2,n}_{\mathbf{n_2}}\right), & on\ \Gamma, \\ \sigma_{\mathbf{n_i}\tau_\mathbf{i}}(\tilde{\mathbf{u}}^{i,n}) &= -\frac{1}{2}\left(\sigma_{\mathbf{n_1}\tau_1}(\mathbf{u}^{1,n}) + \sigma_{\mathbf{n_2}\tau_2}(\mathbf{u}^{2,n})\right), & \\ & & on\ \Gamma, \end{cases} \tag{14}$$

and $u^{n+1}_\Gamma = u^n_\Gamma + \frac{1}{2}\left(\tilde{u}^{1,n}_{\tau_1} + \tilde{u}^{2,n}_{\tau_2}\right)$, $\sigma^{n+1}_\Gamma = \sigma^n_\Gamma + \frac{1}{2}\left(\sigma_{\mathbf{n_1 n_1}}(\tilde{\mathbf{u}}^{1,n}) + \sigma_{\mathbf{n_2 n_2}}(\tilde{\mathbf{u}}^{2,n})\right)$.

Remark 3. We found an algorithm with a mechanical meaning: Find the tangential part of the normal stress and the normal displacement at the interface so that the normal part of the normal stress and the tangential displacement on the interface match. This is very similar to the original Neumann-Neumann algorithm, which means that the implementation effort of the new algorithm from an existing Neumann-Neumann is negligible (the same type of quantities – displacement fields and efforts – are imposed at the interfaces), except that the new algorithm requires the knowledge of some geometric quantities, such as normal and tangential vectors. Note also that, with the adjustment of the definition of tangential quantities for $d = 3$, the algorithm is the same, and is also similar to the results in [8].

7 Conclusion

All algorithms and interface conditions are derived for problems posed on the whole space, since for the time being, this is the only way to treat from the algebraic point of view these problems. The effect of the boundary condition on bounded domains cannot be quantified with the same tools. All the algorithms are designed in the PDE level and it is very important to choose the right discrete framework in order to preserve the optimal properties. For example, in the case of linear elasticity a good candidate would be the TDNNS finite elements that can be found in [14]. The implementation and the impact of the discretizations on the algorithms is an ongoing work.

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