A Fast Finite Difference Method for Elliptic PDEs in Domains with Non-Grid Aligned Boundaries with Application to 3D Linear Elasticity

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Summary. The Explicit Jump Immersed Interface Method reduces the irregular domain problem with non-grid aligned boundaries to solving a sequence of problems in a rectangular parallelepiped on a Cartesian grid using standard central finite differences. Each subproblem is solved using a Fast Fourier Transform based fast solver.

The resulting method is second order convergent for the displacements in the maximum norm as the grid is refined. It makes the method attractive for applications where information about the local displacements, stresses and strains is needed, like optimal shape design and others.

Key words: Elliptic PDE, linear elasticity, irregular domain, finite differences, fast solvers.

1 Model Equations

We consider the equations of isotrope linear elasticity (Navier or Lamé equations) in the domain $\Omega \in \Re^3$:

$$\mu\Delta\mathbf{u} + (\lambda+\mu)\nabla\nabla\cdot\mathbf{u} = \mathbf{f}(\lambda+\mu)\ . \tag{1}$$

$\mathbf{f} : \Omega \to \Re^3$ is the body force and $\mathbf{u} = (u, v, w)^T$ is the displacement vector. μ and λ are shear and Lamé modulus. The stress tensor is

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix} := \mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) + \lambda \begin{pmatrix} \partial_x & 0 & 0 \\ 0 & \partial_y & 0 \\ 0 & 0 & \partial_z \end{pmatrix} \mathbf{u}\ .$$

Boundary conditions are given as prescribed displacements $\mathbf{u} = \mathbf{u}_\Gamma$ on $\partial\Omega_D$ or by an acting force $\boldsymbol{\sigma}\mathbf{n} = \mathbf{g}$ on $\partial\Omega_T$, $\mathbf{n}$ is the outer normal to Ω (tractions). Require $\partial\Omega_D \cup \partial\Omega_T = \partial\Omega$, $\partial\Omega_D \cap \partial\Omega_T = \emptyset$ and $\text{area}(\partial\Omega_D) \geq \delta > 0$.

2 Numerical Method

The building blocks of the method are 1) *EJIIM discretization*, 2) *Conjugated Gradient method* together with *FFT based fast elastostatic solver* for inverse in a *Schur Complement.*

2.1 EJIIM

As one of the extensions of the original Immersed Interface Method ([LL94]), the EJIIM was developed in [Wie98]. In [SW00] EJIIM and the Level Set Method were used for optimal shape design of 2D elasticity.

The first step of the EJIIM is to extend the original domain to a rectangular parallelepiped Ω^*. The solution is extended to the complement $\Omega^c = \Omega^* \setminus \text{closure}(\Omega)$ by zero. This extension satisfies the homogeneous Lamé equations in Ω^c. *Under this extension, the original boundary becomes an interface, where the solution and the right hand side are discontinuous. The boundary conditions turn into jump conditions.*

A regular grid is imposed on Ω^*. The discrete Lamé operator Λ_h is the discretization of (1) with standard central finite differences with meshwidth h. We use capital letters to denote the discrete scalar functions, e.g., $U_{i,j,k} \approx u(x_i, y_j, z_k) =: u_{i,j,k}$, $V_{i,j,k} \approx v(x_i, y_j, z_k) =: v_{i,j,k}$ and $W_{i,j,k} \approx v(x_i, y_j, z_k) =: w_{i,j,k}$. The calligraphic font is used for discrete vectors, like $\mathcal{U}_{i,j,k} \approx \mathbf{u}(x_i, y_j, z_k)$ and $\mathcal{F}_{i,j,k} \approx \mathbf{f}(x_i, y_j, z_k)$. (x_i, y_j, z_k) are the grid points.

We call points where the 27 point stencil of Λ_h is not cut by the interface, *regular points*, all others *irregular points*. At regular points we can use the standard discrete Lamé operator Λ_h. At irregular points, solution dependent *correction terms* that reduce the truncation error to first order (which turns out to be enough to keep the second order convergence of the solution) are added:

$$\Lambda_h \mathcal{U} + \text{correction} = \mathcal{F} \ . \tag{2}$$

Suppose that the interface intersects the stencil at the position (x_α, y_j, z_k) with $x_i \le x_\alpha < x_{i+1}$. Then,

$$\partial_{xx} u_{i,j,k} = \frac{1}{h^2}(u_{i+1,j,k} - 2u_{i,j,k} + u_{i-1,j,k}) - \frac{1}{h^2}\sum_{m=0}^{2}\frac{(h^+)^m}{m!}[\partial_x^m u]_\alpha + \mathcal{O}(h)$$

with $h^+ = x_{i+1} - x_\alpha$. $[g]_\alpha$ denotes the jump in the function g at position α. The ∂_{yy} and ∂_{zz} operators are not influenced by this interface point. For mixed derivatives,

$$\begin{aligned}\partial_{xy} u_{i,j,k} = &\frac{1}{4h^2}(u_{i+1,j+1,k} - u_{i-1,j+1,k} - u_{i+1,j-1,k} + u_{i-1,j-1,k}) \\ &- \frac{1}{2h}\sum_{m=0}^{1}\frac{(h^+)^m}{m!}[\partial_x^m(\partial_y u)]_\alpha + \mathcal{O}(h) \ .\end{aligned}$$

The same interface point affects also discretizations at points $(x_i, y_{j\pm1}, z_k)$ and $(x_i, y_j, z_{k\pm1})$. E.g., at the point (x_i, y_{j+1}, z_k) we have

$$\partial_{xy} u_{i,j+1,k} = \frac{1}{4h^2}(u_{i+1,j+1,k} - u_{i-1,j+1,k} - u_{i+1,j-1,k} + u_{i-1,j-1,k}) - \frac{1}{4h^2}\sum_{m=0}^{2}\frac{(h^+)^m}{m!}[\partial_x^m u]_\alpha + \mathcal{O}(h) \ .$$

The other set of points is analogous, with the x-coordinate x_{i+1}. Similar approximations hold for other derivatives and several interface points affecting the stencil, see [Wie98, SW00] for the proofs and more details.

In short, the correction terms can be always written in a form

$$\text{correction} = \sum_s \sum_{m=0}^{2} \psi_{m,s}[\partial^m u]_{\alpha_s} \tag{3}$$

with α_s denoting the intersections of the interface with the grid lines.

The essential distinction between the EJIIM and other methods is to *explicitly introduce the jumps as additional variables* in the system. The additional equations can be gotten by the boundary condition and some extrapolation, thus relating the function values at the grid points and the jumps

$$[\partial^m u]_{\alpha_s} = \tilde{F}_s^u - \sum_{(i,j,k)\in \text{grid}} d^u_{s,(i,j,k)} U_{i,j,k} \ , \tag{4}$$

where $\tilde{F}^u$ denotes some constant vector, containing, e.g., given boundary values. In our computations second order polynomials are used for the extrapolation.

The complete discretization can be written as

$$\begin{pmatrix} \mathbf{A} & \boldsymbol{\Psi} \\ \mathbf{D} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathcal{U} \\ \mathcal{J} \end{pmatrix} = \begin{pmatrix} \mathcal{F} \\ \tilde{\mathcal{F}} \end{pmatrix} \ , \tag{5}$$

where $\mathbf{A}$ is the standard finite difference matrix, $\mathcal{F}$ is the extended discrete right hand side function, $\boldsymbol{\Psi}$ is the correction matrix (see (2) and (3)), $\mathcal{J}$ is the vector of the additional jump variables, $\mathbf{I}$ is the identity, $\mathbf{D}$ with components d^u, d^v, d^w and $\tilde{\mathcal{F}} := (\tilde{F}^u, \tilde{F}^v, \tilde{F}^w)^T$ are coming from extrapolation (4).

2.2 Fast Solver

The key points for accelerating the computations are 1) *Schur complement for jumps*, 2) *iterative solver as a basis*, 3) *Fast Fourier Transform.*

In three dimensions, interface is a two-dimensional manifold. Thus, if we denote by N the number of grid points in one direction, we have $\mathcal{U} \in \Re^{3N^3}$. The first order truncation error at the interface points requires correction terms up to those involving the second order jumps. Thus, each intersection point enters the system with $3 \cdot 10$ new additional variables. The amount of intersection points is of order N^2 and $\mathcal{J} \in \Re^{c30N^2}$.

Schur complement for the jumps.

First, we reduce the dimensionality of the discrete problem (5) using the Schur complement for the jump variable $\mathcal{J}$. $\mathbf{M}\mathcal{J} = \tilde{\mathcal{F}} - \mathbf{D}\mathbf{A}^{-1}\mathcal{F}$ with $\mathbf{M} := \mathbf{I} - \mathbf{D}\mathbf{A}^{-1}\boldsymbol{\Psi}$. The displacements are found by $\mathcal{U} = \mathbf{A}^{-1}\left(F - \boldsymbol{\Psi}\mathcal{J}\right)$.

Iterative solver and Fast Fourier Transform

The benefit of an iterative method (e.g. BiCGSTAB, [Kel95]) for solving $\mathbf{M}\mathcal{J} = \mathcal{G}$, is that only the matrix vector product $\mathbf{M}\mathcal{J}^K$ is needed at iteration k. This product $\mathcal{Y} = (\mathbf{I} - \mathbf{D}\mathbf{A}^{-1}\boldsymbol{\Psi})\mathcal{J}^k$ is found in stages: 1) $\mathcal{X}^1 = \boldsymbol{\Psi}\mathcal{J}^k$, 2) $\mathcal{X}^2 = \mathbf{A}^{-1}\mathcal{X}^1$, 3) $\mathcal{Y} = \mathcal{J}^k - \mathbf{D}\mathcal{X}^2$. Storing $\mathbf{M}$ explicitely would be impossible for large problems, as it is dense.

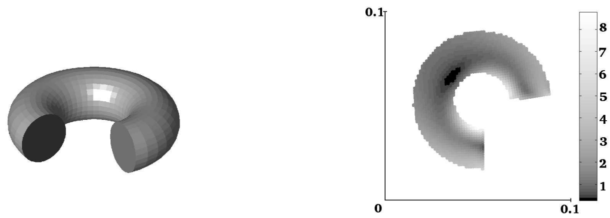
Each application of $\mathbf{M}$ requires application of $\mathbf{A}^{-1}$ to a vector. This is done in $N^3 \log(N^3)$ time using FFT. For more details we refer to [Wie99].

The approach above also avoids the explicit construction of the EJIIM matrix in (5).

2.3 Example

Let Ω be a part of a torus, with surface parametrized by $x = (r\cos\theta + a)\cos\phi + x_c$, $y = (r\cos\theta + a)\sin\phi + y_c$, $z = r\sin\theta + z_c$ with $\theta \in [-\pi, \pi)$ and $\phi \in [-\pi, \pi - \alpha]$. Add the closing planes at $\phi = -\pi$ and $\phi = \pi - \alpha$, see Fig. 1.

We keep the plane at $\phi = -\pi$ (the darker one in Fig. 1) fixed, and rotate the plane at $\phi = \pi - \alpha$ by $\pi/20$ thus compressing the material. On the rest of the surface, we set zero traction b.c., also there are no body forces.



Original — von Mises stress in deformed state (MPa)

Fig. 1. Original and deformed geometries

The necessary geometry information (normals and tangentials and intersections of the interface with grid lines) in this case are computed analytically, for more general geometries it can be found by e.g., the Level Set method.

As output we get displacements and jumps in the function values and its derivatives. The knowledge of jumps allows accurate differentiation according to formulas given in [Wie98]. As the displacements are second order accurate, the stresses and strains are first order accurate in maximum norm under the grid refinement. In Fig. 1, right, we have plotted the stresses of von Mises, calculated as $S_m = \sqrt{S_1^2 - 3S_2}$, where S_1 and S_2 are first and second stress invariants, respectively. We have shown the cut of the deformed geometry along the plane $z = z_c$.

3 Conclusions

We have presented a fast solver for linear elasticity problems, which is based on the Explicit Jump Immersed Interface Method (EJIIM) together with an FFT and Conjugated Gradient based fast solver. The EJIIM is a finite difference method, where the standard central differences are corrected by jump-dependent correction terms. Jumps are introduced as additional variables, that result from embedding or discontinuities in coefficients. Embedding in a box allows the use of the FFT and an iterative solution of the Schur complement formulation for the jumps.

As an input the method needs the geometry information to be provided, which includes intersections of the surface with grid lines, normal and tangential fields. This can be found e.g., by the Level Set method [Set96].

From standard central difference methods, second order convergence of the displacements in the maximum norm under grid refinement is preserved. This guarantees the local convergence of the displacements, stresses and strains.

References

[Kel95] Kelley, C. T.: Iterative Methods for Linear and Nonlinear Equations. Society for Industrial and Applied Mathematics, Philadelphia (1995).

[Mus63] Muskhelishvili, N. I.: Some basic problems of the mathematical theory of elasticity. P. Noordhoff Ltd (1963)

[Set96] Sethian, J. A.: Level Set Methods: Evolving Interfaces in Geometry, Fluid Mechanics, Computer Vision, and Materials Science. Cambridge Univ. Press, 1996.

[LL94] LeVeque, R. J. and Li, Z.: The Immersed Interface Method for Elliptic Equations with Discontinuous Coefficients and Singular Sources. SIAM J. Numer. Anal., **31**, 1019—1044 (1994)

[SW00] Sethian, J. A. and Wiegmann, A.: Structural Boundary Design via Level Set and Explicit Jump Immersed Interface Methods. J. Comp. Phys., **163**(2), 489—528 (2000)

[Wie99] Wiegmann, A.: Fast Poisson, fast Helmholtz and fast linear elastostatic solvers on rectangular parallelepipeds. Lawrence Berkeley National Laboratory, MS 50A-1148, One Cyclotron Rd, Berkeley CA 94720 LBNL-43565, June 1999.

[Wie98] Wiegmann, A.: The Explicit–Jump Immersed Interface Method and Interface Problems for Differential Equations. PhD Thesis, Univ. of Washington (1998)