Direct solution of elliptic problems under coefficient updates

Xiao Liu[1]

Jianlin Xia[2]   Maarten V. de Hoop[1]

[1]Computational and Applied Mathematics, Rice University

[2]Department of Mathematics, Purdue University

Conference on Fast Direct Solvers, Purdue University

November 10, 2018

Outline

- Coefficient update problem
- Factorization of interior and exterior sub-problems
- Solution update
- Performance tests

Coefficient update problem

Given the direct factorization of a reference elliptic problem

$$Lu = f, \quad L = \nabla \cdot p_2(x)\nabla + p_1(x) \cdot \nabla + p_0(x)$$

Goal: solve the coefficient update problem

$$\tilde{L}\tilde{u} = f, \quad \tilde{L} = \nabla \cdot \tilde{p}_2(x)\nabla + \tilde{p}_1(x) \cdot \nabla + \tilde{p}_0(x)$$

Applications: inverse problems, computational biology

Types of update:

- small magnitude, L as a preconditioner
- low-rank update, SMW formula
- ► local support, factorization update

Existing methods

Matrix computation

- Bennett's method [Bennett; Chan, Brandwajn et al.]
- CHOLMOD [Chen, Davis et al.]

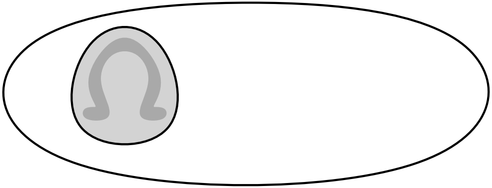
Geophysics

- volume integral equation [Jakobsen, Ursin et al.]
- boundary integral equation [Willemsen, Malcolm et al.]

Typical restrictions

- small problem/update size
- prior knowledge about the location
- selected blocks of the inverse

Updates in a fixed subdomain



Ω – interior subdomain where $L \neq \tilde{L}$

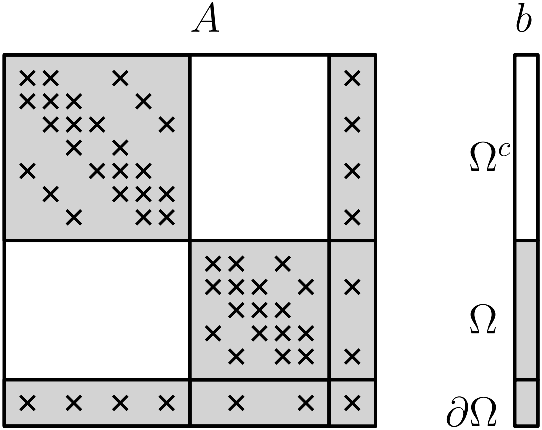
Ω^c – exterior subdomain where $L = \tilde{L}$

$$\tilde{L}\tilde{u} - \tilde{L}u = Lu - \tilde{L}u$$

$$\tilde{L} \underbrace{(\tilde{u} - u)}_{\text{solution update}} = \underbrace{(L - \tilde{L})}_{\text{operator update}} u$$

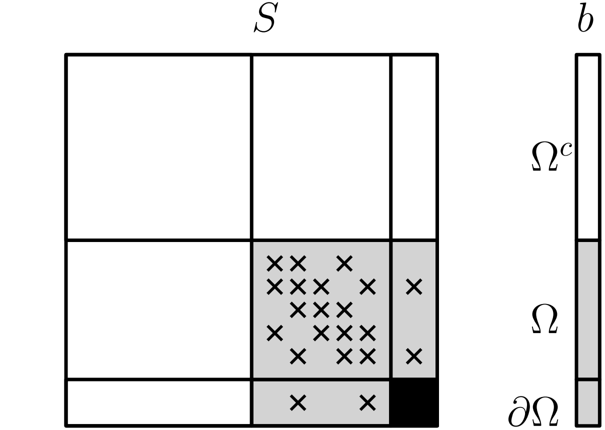
No update and zero right hand side in Ω^c

Separation of interior and exterior unknowns



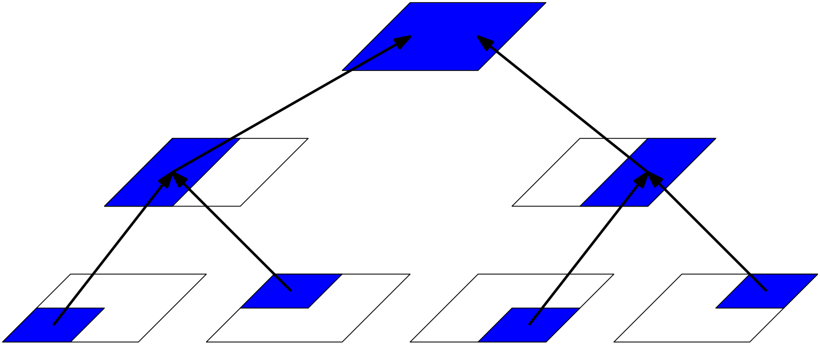
$$\begin{pmatrix} A_{11} & & A_{13} \\ & \tilde{A}_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ b_2 \\ b_3 \end{pmatrix}$$

Separation of interior and exterior unknowns



$$\begin{pmatrix} A_{11} & & A_{13} \\ & \tilde{A}_{22} & A_{23} \\ 0 & A_{32} & A_{33} - A_{31}A_{11}^{-1}A_{13} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ b_2 \\ b_3 \end{pmatrix}$$

Nested domain partitioning

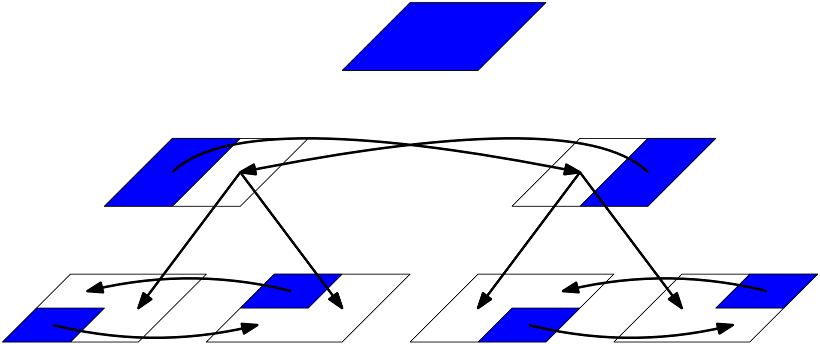


Binary tree of interior subdomains

- each node depends on its children
- updates propagate to ancestors

updating the root $\sim$ factorizing the new problem

Nested domain partitioning



Exterior subdomains

- each node depends on its parent and sibling
- isolated updates because of exterior factors

Factorization

For each node i with children c_1 and c_2

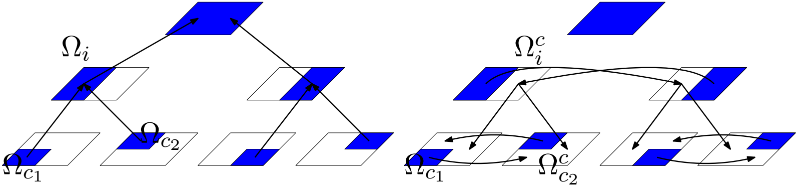
- interior factors

$$\mathcal{I}_i \Leftarrow \mathcal{I}_{c_1}, \mathcal{I}_{c_2} \quad \text{because} \quad \Omega_i \Leftarrow \Omega_{c_1}, \Omega_{c_2}$$

- exterior factors

$$\mathcal{E}_{c_1} \Leftarrow \mathcal{E}_i, \mathcal{I}_{c_2} \quad \text{because} \quad \Omega_{c_1}^c \Leftarrow \Omega_i^c, \Omega_{c_2}$$

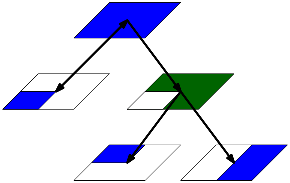
$$\mathcal{E}_{c_2} \Leftarrow \mathcal{E}_i, \mathcal{I}_{c_1} \quad \text{because} \quad \Omega_{c_2}^c \Leftarrow \Omega_i^c, \Omega_{c_1}$$



Solution update with localized right-hand side

For coefficient update in Ω_i

- re-factorize and forward sweep in Ω_i
- backward sweep in Ω_i and Ω_i^c



Partitioning of Ω_i unchanged

Partitioning of Ω_i^c extracted from the data dependency graph

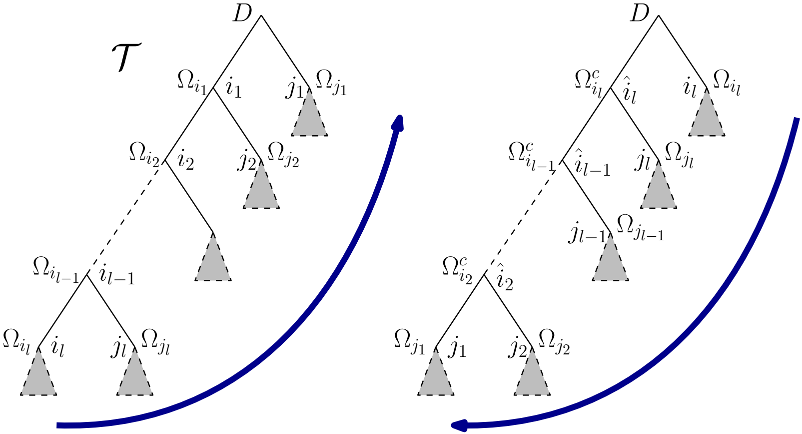
Efficiency: minimum update cost, almost half the solution cost

Flexibility: change of support

Modified domain partitioning

Theorem (L., Xia, and de Hoop, 2018)

For a level-l subdomain, the domain partitioning $\mathcal{T}$ can be modified with $O(l)$ operations to exclude its supersets



Non-overlapping Schur-complement domain decomposition [Hackbusch; Martinsson et al.]

Dirchlet-to-Neumann maps for two siblings

$$F \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \begin{pmatrix} \partial_n u_0 \\ \partial_n u_1 \end{pmatrix}, \quad G \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} = \begin{pmatrix} -\partial_n u_0 \\ \partial_n u_2 \end{pmatrix}$$

u_0 on the shared interface

For their parent

$$\left(\begin{array}{c|cc} F_{00} + G_{00} & F_{01} & G_{02} \\ \hline F_{10} & F_{11} & \\ G_{20} & & G_{22} \end{array}\right) \begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ \partial_n u_1 \\ \partial_n u_2 \end{pmatrix}$$

Benefits

- no permutation or index matching issue
- fewer fill-ins for high-order discretization

Complexity

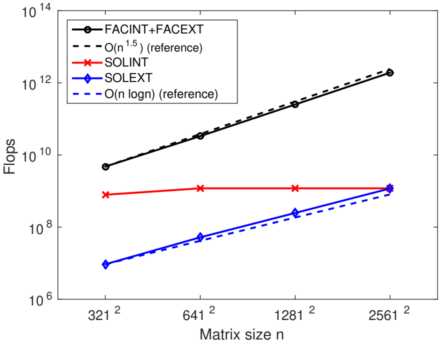
the problem size $n \gg$ the update size m

	2D		3D	
	time	space	time	space
Factorization	$O(n^{1.5})$	$O(n \log n)$	$O(n^2)$	$O(n^{4/3})$
New update	$O(m^{1.5})$	$O(m \log m)$	$O(m^2)$	$O(m^{4/3})$
Partial LU	$O(n^{1.5})$	$O(n)$	$O(n^2)$	$O(n^{4/3})$

assuming balanced domain partitioning

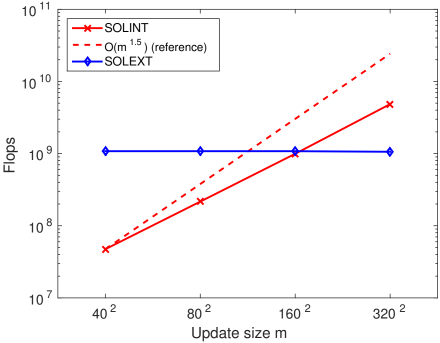
Performance test: $m = 160^2$, n increases

Helmholtz equation, FEM with 4th-order basis



n	321^2	641^2	1281^2	2561^2
FACINT	1.8s	7.7s	33.1s	156.3s
FACEXT	0.5s	3.8s	25.0s	170.3s
SOLINT	0.46s	0.56s	0.58s	0.67s
SOLEXT	0.03s	0.14s	0.63s	2.89s

Performance test: $n = 2561^2$, m increases



m	40^2	80^2	160^2	320^2
SOLINT	0.12s	0.14s	0.47s	1.86s
SOLEXT	2.93s	2.52s	2.50s	2.47s

Reuse of existing factorization as a preconditioner:
32, 180, 717, 2585 GMRES iterations for 10^{-5} residual

Conclusions

Direct solution algorithm for localized coefficient update

- top-down factorization of exterior problems
- fast solution update with localized right-hand side
- flexibility w.r.t. locations
  efficiency w.r.t. size and magnitude

Future work: approximate update, purely-algebraic version

References

- L., Xia, and de Hoop, *Fast factorization update for general elliptic problems under many coefficient updates*, submitted
- L., Xia, and de Hoop, *Interconnected hierarchical rank-structured methods for directly solving and preconditioning the Helmholtz equation*, submitted
  - Xia, Xi et al., *Fast sparse selected inversion*, SIMAX, 2015

Thank you!