Parallel Implementation of Multilevel BDDC Method

Jakub Šístek

joint work with
J. Mandel, B. Sousedík, P. Burda, M. Čertíková, J. Novotný

Institute of Mathematics of the AS CR, Prague
University of Colorado Denver
University of Southern California, Los Angeles
Czech Technical University in Prague

ENUMATH 2011,
Leicester, September 5th–9th, 2011

Brief overview of BDDC

standard (two-level) BDDC

- Balancing Domain Decomposition based on Constraints
- introduced in [Dohrmann (2003)], convergence theory in [Mandel, Dohrmann (2003)]
- non-overlapping additive DD preconditioner in PCG
- two-level method, additive global coarse correction
- for many subdomains, exact solution of the global coarse problem may become expensive

extension to multiple levels

- **Three-level BDDC** [Tu (2007) – 2D, 3D] – basic theory
- **Multispace and multilevel BDDC** [Mandel, Sousedík, Dohrmann (2008)] - extension to arbitrary number of levels

Brief overview of BDDC

standard (two-level) BDDC

- Balancing Domain Decomposition based on Constraints
- introduced in [Dohrmann (2003)], convergence theory in [Mandel, Dohrmann (2003)]
- non-overlapping additive DD preconditioner in PCG
- two-level method, additive global coarse correction
- for many subdomains, exact solution of the global coarse problem may become expensive

extension to multiple levels

- **Three-level BDDC** [Tu (2007) – 2D, 3D] – basic theory
- **Multispace and multilevel BDDC** [Mandel, Sousedík, Dohrmann (2008)] - extension to arbitrary number of levels

The abstract problem

Variational setting

$$u \in U : a(u, v) = \langle f, v \rangle \quad \forall v \in U$$

- $a(\cdot, \cdot)$ symmetric positive definite form on U
- $\langle \cdot, \cdot \rangle$ is inner product on U
- U is finite dimensional space (typically finite element functions)

Matrix form

$$u \in U : Au = f$$

- A symmetric positive definite matrix on U
- A large, sparse, condition number $\kappa(A) = \frac{\lambda_{\max}}{\lambda_{\min}} = \mathcal{O}(1/h^2)$

Linked together

$$\langle Au, v \rangle = a(u, v) \quad \forall u, v \in U$$

The abstract problem

Variational setting

$$u \in U : a(u, v) = \langle f, v \rangle \quad \forall v \in U$$

- $a(\cdot, \cdot)$ symmetric positive definite form on U
- $\langle \cdot, \cdot \rangle$ is inner product on U
- U is finite dimensional space (typically finite element functions)

Matrix form

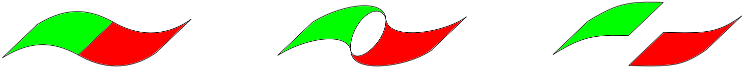
$$u \in U : Au = f$$

- A symmetric positive definite matrix on U
- A large, sparse, condition number $\kappa(A) = \frac{\lambda_{\max}}{\lambda_{\min}} = \mathcal{O}(1/h^2)$

Linked together

$$\langle Au, v \rangle = a(u, v) \quad \forall u, v \in U$$

Function spaces in BDDC

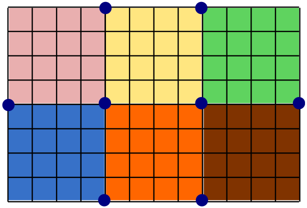


$U \subset \widetilde{W} \subset W$

U		$\widetilde{W}$		W
continuous at all nodes at interface	$\subset$	continuous at selected corners	$\subset$	no continuity at interface

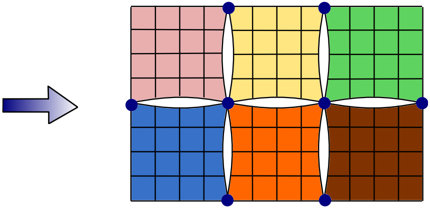
- enough constraints to fix floating subdomains, i.e. rigid body modes eliminated from the space
- continuity at *corners*, and of averages (arithmetic or weighted) over *edges* or *faces* considered
- $a(\cdot,\cdot)$ symmetric positive definite form on $\widetilde{W}$
- corresponding matrix $\widetilde{A}$ symmetric positive definite, almost block diagonal structure, larger dimension than A

Virtual mesh



original mesh of the problem

corresponds to space U



mesh disconnected at interface

corresponds to space $\widetilde{W}$

The abstract BDDC preconditioner

Variational form

$$M_{BDDC} : r \longmapsto u = Ew, \quad w \in \widetilde{W}$$

$$a(w, z) = \langle r, Ez \rangle, \quad \forall z \in \widetilde{W}$$

Matrix form

$$\widetilde{A}w = E^T r$$

$$M_{BDDC} r = Ew$$

Condition number bound [Mandel, Dohrmann (2003)]

$$\kappa = \frac{\lambda_{\max}(M_{BDDC}A)}{\lambda_{\min}(M_{BDDC}A)} \le \omega = \sup_{w \in \widetilde{W}} \frac{\|(I - E)w\|_a^2}{\|w\|_a^2}.$$

The abstract BDDC preconditioner

Variational form

$$M_{BDDC} : r \longmapsto u = Ew, \quad w \in \widetilde{W}$$

$$a(w, z) = \langle r, Ez \rangle, \quad \forall z \in \widetilde{W}$$

Matrix form

$$\widetilde{A} w = E^T r$$

$$M_{BDDC} r = Ew$$

Condition number bound [Mandel, Dohrmann (2003)]

$$\kappa = \frac{\lambda_{\max}(M_{BDDC} A)}{\lambda_{\min}(M_{BDDC} A)} \le \omega = \sup_{w \in \widetilde{W}} \frac{\|(I - E) w\|_a^2}{\|w\|_a^2}.$$

The abstract BDDC preconditioner

Variational form

$$M_{BDDC} : r \longmapsto u = Ew, \quad w \in \widetilde{W}$$

$$a(w, z) = \langle r, Ez \rangle, \quad \forall z \in \widetilde{W}$$

Matrix form

$$\widetilde{A} w = E^T r$$

$$M_{BDDC} r = Ew$$

Condition number bound [Mandel, Dohrmann (2003)]

$$\kappa = \frac{\lambda_{\max}(M_{BDDC} A)}{\lambda_{\min}(M_{BDDC} A)} \le \omega = \sup_{w \in \widetilde{W}} \frac{\|(I - E)w\|_a^2}{\|w\|_a^2}.$$

The coarse space in BDDC

In implementation, space $\widetilde{W}$ is decomposed into $\widetilde{W}_\Delta$ of **independent subdomain spaces** and energy-orthogonal **coarse space** $\widetilde{W}_\Pi$

$$\widetilde{W} = \widetilde{W}_\Delta \oplus \widetilde{W}_\Pi.$$

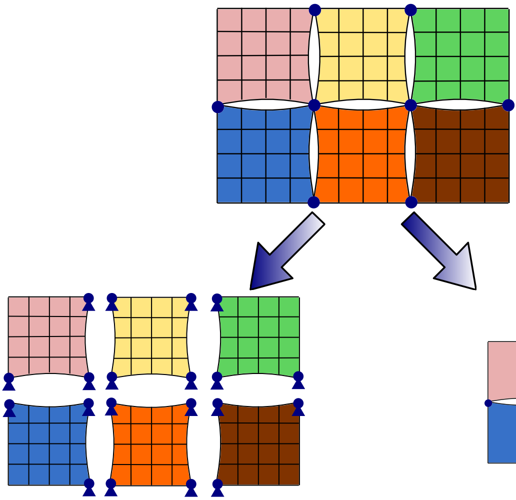
On each subdomain – **coarse degrees of freedom** – basis functions Ψ^i – prescribed values of coarse degrees of freedom, minimal energy elsewhere,

$$\begin{bmatrix} A^i & C^{iT} \\ C^i & 0 \end{bmatrix} \begin{bmatrix} \Psi^i \\ \Lambda^i \end{bmatrix} = \begin{bmatrix} 0 \\ I \end{bmatrix}.$$

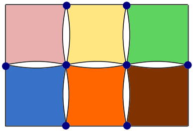
- A^i ... local subdomain stiffness matrix
- C^i ... matrix of constraints – selects unknowns into coarse degrees of freedom

Matrix of **coarse problem** A_C assembled from local matrices $A_{Ci} = \Psi^{iT} A^i \Psi^i = -\Lambda^i$.

The coarse space in BDDC



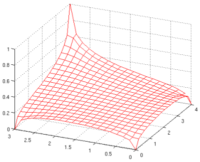
subdomain problems
(independent)



coarse problem
(global)

Multilevel extension

- global coarse problem eventually becomes a bottleneck of parallel processing for very large problems – solve only **approximately** e.g. by
  - several multigrid cycles – [Klawonn, Rheinbach (2010)] (for FETI-DP)
  - by one iteration of BDDC – **Three-level BDDC**
  - recursive application of BDDC – **Multilevel BDDC**
- BDDC is especially suitable for multilevel extension because the coarse problem has the same structure as the original FE problem (unlike in most other DD methods)
- apply BDDC with subdomains playing the role of elements



A basis function from $\widetilde{W}_{\Pi}$ is energy minimal subject to given values of coarse degrees of freedom on the substructure. The function is discontinuous across the interfaces between the substructures but the values of coarse degrees of freedom on the different substructures coincide.

Multilevel BDDC

$$
\begin{array}{ccccccccc}
 & & & U & & & & & \\
 & & & \parallel & & & & & \\
\textit{level } 1 & U_{I1} & \subset & U_1 & \subset & \widetilde{W}_1 & & & \\
 & & & & & \parallel & & & \\
 & & & & \widetilde{W}_{\Pi 1} & \oplus & \widetilde{W}_{\Delta 1} & & \\
 & & & & \parallel & & & & \\
\textit{level } 2 & & U_{I2} & \subset & U_2 & \subset & \widetilde{W}_2 & & \\
 & & & & & & \parallel & & \\
 & & & & & \widetilde{W}_{\Pi 2} & \oplus & \widetilde{W}_{\Delta 2} & \\
 & & & & & \parallel & & & \\
\vdots & & & & & \vdots & & & \\
 & & & & & \parallel & & & \\
\textit{level } L-1 & & & U_{IL-1} & \subset & U_{L-1} & \subset & \widetilde{W}_{L-1} & \\
 & & & & & & & \parallel & \\
 & & & & & & \widetilde{W}_{\Pi L-1} & \oplus & \widetilde{W}_{\Delta L-1}
\end{array}
$$

Local problems and the coarse problem actually solved are in colour.

Condition number bound

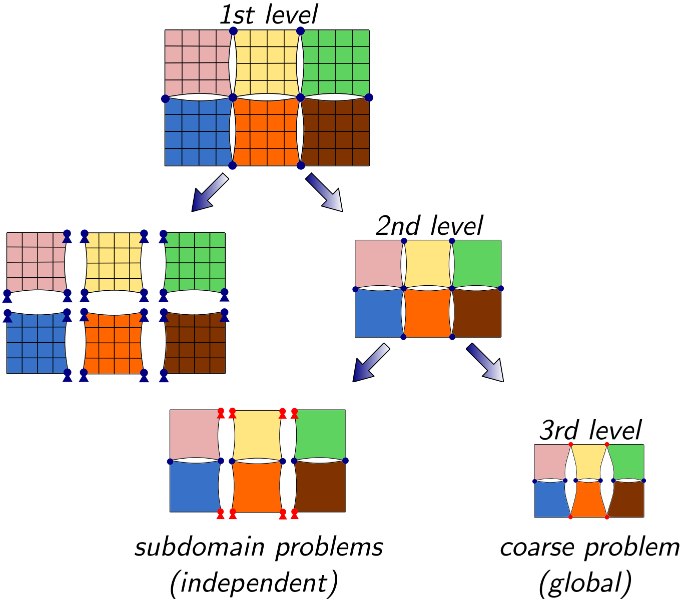
- mathematical efficiency worsens with each additional level

Theorem [Mandel, Sousedík, Dohrmann (2008)]

The condition number bound $\kappa(M_{BDDC}A) \leq \omega$ of Multilevel BDDC is given by

$$\kappa(M_{BDDC}A) \leq \omega = \prod_{\ell=1}^{L-1} \omega_\ell \ , \qquad \omega_\ell = \sup_{w_\ell \in \widetilde{W}_\ell} \frac{\left\| (I - E_\ell)\, w_\ell \right\|_a^2}{\left\| w_\ell \right\|_a^2}.$$

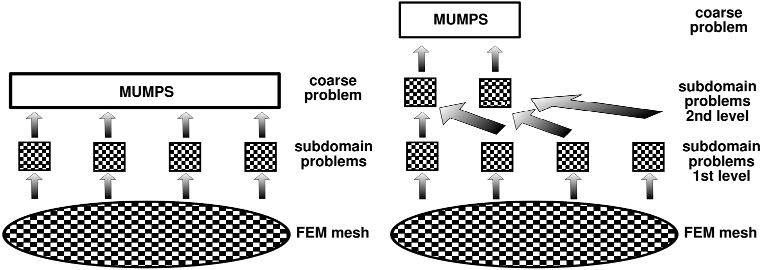
Multilevel BDDC



Parallel implementation

BDDCML solver library

- *http://www.math.cas.cz/∼sistek/software/bddcml.html*
- Fortran 95 + MPI library
- built on top of MUMPS direct solver (both serial and parallel)
- parallel PCG and BICGSTAB (for overlapping vectors)



Two-level BDDC

Three-level BDDC

Numerical results

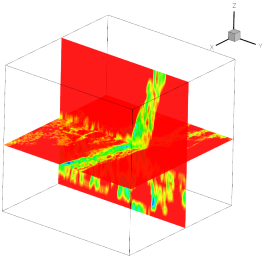
IBM SP6

Location: CINECA, Italy
Architecture: IBM P6-575 Infiniband Cluster
Processor Type: IBM Power6, 4.7 GHz
Computing Cores: 5376
Computing Nodes: 168
RAM: 21 TB (128 GB/node)
access gained through the *HPC Europa 2* project

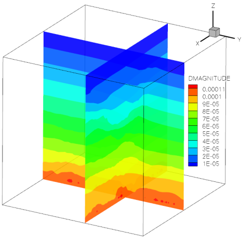
graphics from CINECA website

Elasticity analysis of geocomposite

- problem of geocomposite by Prof. Blaheta and Dr. Starý (Institute of Geonics of AS CR)
- cubic sample, edge 75 mm
- 11.8M linear tetrahedral elements, 6.1M unknowns
- arithmetic averages on edges and faces
- required precision . . . relative residual $= \frac{\|res\|}{\|g\|} < 10^{-6}$



material distribution



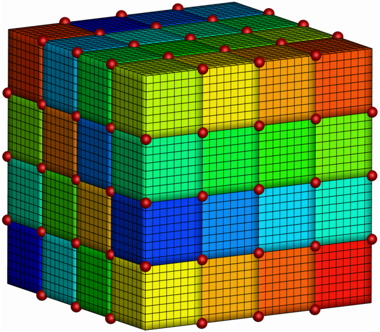
displacement

Strong scaling for geocomposite problem

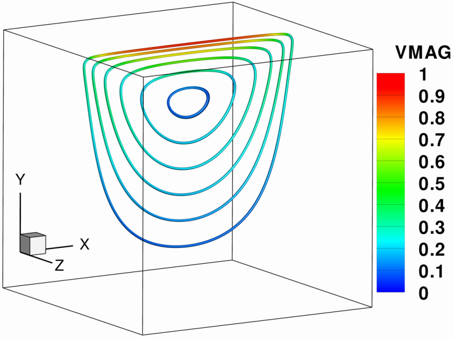
number of procs	64	128	256	512	1024
2 levels (1024/1), **46** PCG its, cond. $\sim$50					
set-up phase (sec)	61.0	37.7	25.7	23.2	39.5
iterations (sec)	22.3	19.9	27.8	44.9	97.5
3 levels (1024/128/1), **56** PCG its, cond. $\sim$79					
set-up phase (sec)	49.5	29.0	18.4	12.6	11.0
iterations (sec)	28.5	22.6	16.7	14.7	13.2
4 levels (1024/128/16/1), **131** PCG its, cond. $\sim$568					
set-up phase (sec)	49.4	28.6	17.8	12.3	9.1
iterations (sec)	60.6	33.2	21.2	15.4	11.8

Stokes flow in 3D cavity

- serendipity Taylor–Hood finite elements
- $32 \times 32 \times 32 = 32.8$k elements, 457k unknowns
- $64 \times 64 \times 64 = 262$k elements, 3.5M unknowns



division into 64 subdomains



streamlines in $z = 0$ plane

Strong scaling for Stokes flow in 3D cavity

- 64×64×64 elements, $H/h = 8$

number of procs	64	128	256	512
2 levels (512/1), **9** BICGSTAB its				
set-up phase (sec)	27.0	14.2	7.9	4.8
iterations (sec)	5.8	4.2	5.3	8.7
3 levels (512/8/1), **11** BICGSTAB its				
set-up phase (sec)	26.9	14.0	7.6	4.2
iterations (sec)	6.0	3.3	1.9	1.2

- 32×32×32 elements, $H/h = 8$

number of procs	64
2 levels (64/1), **9** BICGSTAB its	
set-up phase (sec)	3.7
iterations (sec)	2.5

Conclusions

Implementation of Multilevel BDDC

- mathematical efficiency worsens with each additional level
- computational efficiency may improve for large 3D problems and large numbers of processors
- multiple levels able to reduce cost of collective communication
- good scalability for linear elasticity problems (SPD) as well as Stokes flow (saddle-point)

Future work

- **Adaptive Multilevel BDDC** – may keep the efficiency for multilevel BDDC [Sousedík (2010)] – Matlab tests combination with **Adaptive BDDC** [Mandel, Sousedík 2007], [Mandel, Sousedík, Šístek (accepted)]
- explore ways to extend the solver to flow problems

Conclusions

Implementation of Multilevel BDDC

- mathematical efficiency worsens with each additional level
- computational efficiency may improve for large 3D problems and large numbers of processors
- multiple levels able to reduce cost of collective communication
- good scalability for linear elasticity problems (SPD) as well as Stokes flow (saddle-point)

Future work

- **Adaptive Multilevel BDDC** – may keep the efficiency for multilevel BDDC [Sousedík (2010)] – Matlab tests combination with **Adaptive BDDC** [Mandel, Sousedík 2007], [Mandel, Sousedík, Šístek (accepted)]
- explore ways to extend the solver to flow problems