Paralelní implementace metody BDDC a její aplikace na analýzy napjatosti v tělesech

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na práci se podílejí
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Brief overview of BDDC method

- **B**alancing **D**omain **D**ecomposition based on **C**onstraints
- 2003 C. Dohrmann, theory with J. Mandel
- nonoverlapping primary domain decomposition method
- additive Schwarz method of Neumann-Neumann type
- iterative substructuring – preconditioner in PCG
- equivalent with FETI-DP [Mandel, Dohrmann, Tezaur 2005]

The 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

Matrix form

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

- A symmetric positive definite matrix on U

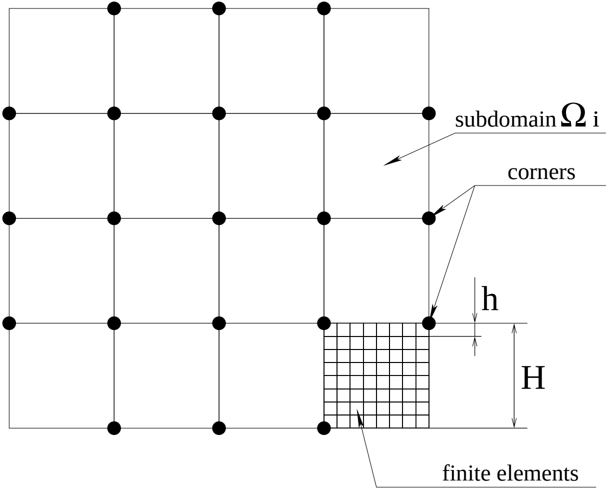
Linked together

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

Applying PCG, a preconditioner $M \approx A^{-1}$ needed!

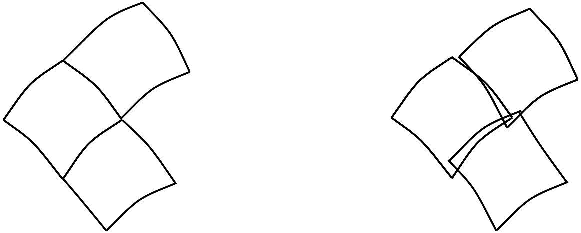
BDDC set-up

- division into subdomains
- selection of corners



Inflating spaces in domain decomposition

Natural to define $W = W_1 \times \cdots \times W_N$ (spaces on substructures)



$U \quad \subset \quad W$

continuous functions — discontinuous along interface

- space of block vectors, one block per substructure
- $a(\cdot, \cdot)$ defined on the bigger space W, but only **semidefinite**
- corresponding matrix A^W symmetric positive **semidefinite**, block diagonal structure, larger dimension
- no communication on interface $\longrightarrow$ floating subdomains

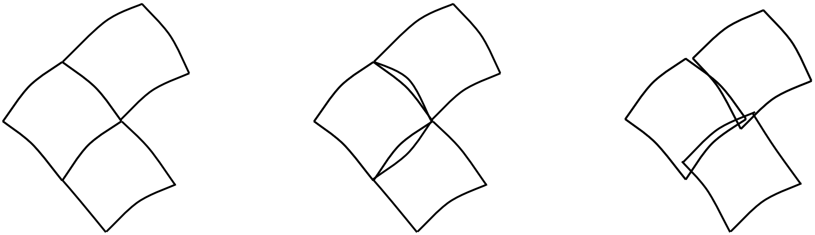
Connection of U and W

Operator of projection

$$\begin{aligned} E: &\quad W \longrightarrow U, \quad Range(E) = U \\ E^T: &\quad U' \longrightarrow W' \end{aligned}$$

Example: averaging across interfaces (arithmetic, weighted)

The first intermediate space in BDDC



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

continuous — continuous at corners — no continuity

- enough corners to fix floating subdomains – rigid body modes captured
- $a(\cdot, \cdot)$ symmetric positive definite form on $\widetilde{W}^c$
- corresponding matrix $\widetilde{A}^c$ symmetric positive definite, almost block diagonal structure, larger dimension
- minimal communication on interface

The BDDC preconditioner with corners

Define $M_{BDDC} : r \in U' \longrightarrow u \in U$

variational form

$$M_{BDDC} : r \longmapsto u = Ew, \quad w \in \widetilde{W}^c : a\,(w, z) = \langle r, Ez \rangle\,, \forall z \in \widetilde{W}^c$$

matrix form

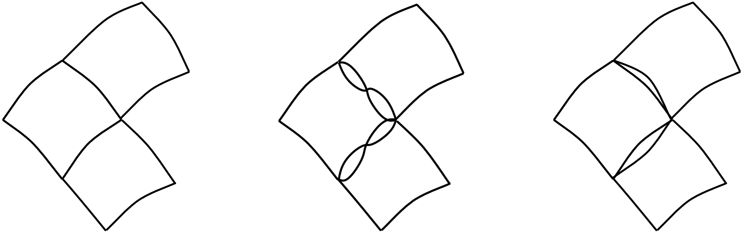
$$\widetilde{A}^c w = E^T r$$
$$M_{BDDC} r = Ew$$

equivalently

$$M_{BDDC} = E(\widetilde{A}^c)^{-1} E^T$$

The second intermediate space in BDDC

Only corners do not suffice for optimal preconditioning
$\Rightarrow$ **additional constraints** on functions from $\widetilde{W}^c$ necessary
[Farhat, et al. 2000], [Klawonn, et al. 2002] for FETI-DP



$U \quad \subset \quad \widetilde{W}^{avg} \quad \subset \quad \widetilde{W}^c$

continuous — add constraints — only corners

Examples: equivalent averages on subsets of interface (*edges*, *faces*) across interface, additional pointwise continuity constraints

Enforcing additional constraints

introduce matrix G with constraints

- each row of G corresponds to a continuity constraint between two subdomains
- introduces new coupling between subdomains

Example: for arithmetic averages on an edge between subdomains i and j, a row of G is

$$g_k = [0 \dots 0 \quad \underbrace{1\ 1\ 1\ 1}_{\text{edge dof on } \Omega_i} \quad 0 \dots 0 \underbrace{-1 - 1 - 1 - 1}_{\text{edge dof on } \Omega_j} 0 \dots 0]$$

define intermediate space as

$$\widetilde{W}^{avg} = \left\{ w \in \widetilde{W}^c : \quad Gw = 0 \right\}$$

The BDDC preconditioner with averages

Define $M_{BDDC} : r \in U' \longrightarrow u \in U$

variational form

$$M_{BDDC} : r \longmapsto u = Ew, \quad w \in \widetilde{W}^{avg} : a(w, z) = \langle r, Ez \rangle, \forall z \in \widetilde{W}^{avg}$$

matrix form

$$\begin{array}{rcl} \widetilde{A}^c w + G^T \lambda & = & E^T r \\ Gw & = & 0 \end{array}$$

$$M_{BDDC} r = Ew$$

Using Lagrange multiplier

Compute $M_{BDDC} r = Ew$, where w is the solution to the system

$$\begin{array}{rcccl} \widetilde{A}^c w & + & G^T \lambda & = & E^T r \\ Gw & & & = & 0 \end{array} .$$

Substituting $w = (\widetilde{A}^c)^{-1}(E^T r - G^T \lambda)$ from the first equation to the second one, solved as

1. $$G(\widetilde{A}^c)^{-1} G^T \lambda = G(\widetilde{A}^c)^{-1} E^T r$$

2. $$\widetilde{A}^c w = E^T r - G^T \lambda$$

Drawback: Dense global problem for Lagrange multiplier λ.

Projected BDDC

Project the system onto $null(G)$ by projection operator

$$P = I - G^T(GG^T)^{-1}G$$

construct $\widetilde{A}^{avg}$ explicitely as

$$\widetilde{A}^{avg} = P\widetilde{A}^c P + t(I - P)$$

with $t > 0$ scaling constant.

Compute $M_{BDDC}r = Ew$, where w is the solution to the system

$$\widetilde{A}^{avg}w = PE^T r$$

Drawback: Off-diagonal blocks in $\widetilde{A}^{avg}$.

Change of variables

Change of variables on each subdomain, such that averages appear as single node constraints.

$$\overline{w} = Tw, \quad w = B\overline{w}, \quad B = T^{-1}$$

Matrix T invertible, contains weights of averages.

Compute $M_{BDDC}r = EB\overline{w}$, where $\overline{w}$ is the solution to

$$\begin{array}{lcrcc} B^T\widetilde{A}^c B\overline{w} & + & B^T G^T \lambda & = & B^T E^T r \\ GB\overline{w} & & & = & 0 \end{array}.$$

Transformed averages may be handled as corners and further assembled [Li, Widlund 2006].
Drawback: The distinction between $\widetilde{W}^c$ and $\widetilde{W}^{avg}$ lost.

Projected change of variables

Combination of projected BDDC and change of variables.
Define matrix $\overline{G} = GB$ – reduces to one 1 and one -1 in each row.
Projection onto $null(\overline{G})$

$$\overline{P} = I - \overline{G}^T(\overline{G}\,\overline{G}^T)^{-1}\overline{G}$$

Construct matrix

$$\widetilde{A}^{avg} = \overline{P}B^T\widetilde{A}^c B\overline{P} + t(I - \overline{P})$$

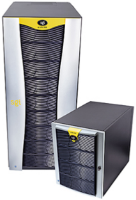
BDDC preconditioner as

$$\widetilde{A}^{avg}\overline{w} = \overline{P}B^T E^T r$$

$$M_{BDDC}r = EB\overline{w}$$

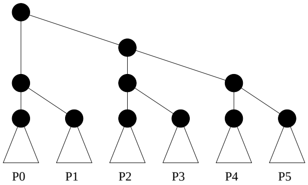
Parallel implementation

- built on multifrontal solver MUMPS
- based on $\widetilde{W}^c$
- Fortran 90 programming language, MPI library
- succesfully ported to
  - SGI Altix 4700, CTU, Prague, CR
    72 processors Intel Itanium 2, OS Linux
  - IBM Blue Gene/L, NCAR+UCB+UCD, Boulder, CO
    2048 processors PowerPC-440 / 700 MHz, OS AIX



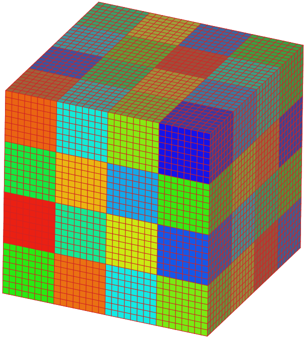
MUMPS

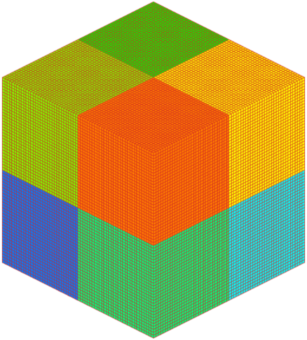
- **MU**ltifrontal **M**assively **P**arallel sparse direct **S**olver
- Patrick Amestoy, Iain Duff, Abdou Guermouche, Jacko Koster, Jean-Yves L'Excellent, and Stephane Pralet
- *http://graal.ens-lyon.fr/MUMPS/*
- open source package in Fortran 90
- built on BLAS, BLACS, ScaLAPACK, METIS, MPI
- SPD, general symmetric and unsymmetric matrices
- multifrontal method (I. S. Duff, J. K. Reid, 1983)



Cube

- 64 subs, $32^3 = 32,769$ elements, $H/h = 8$, $107,811$ dof
- 8 subs, $64^3 = 262,144$ elements, $H/h = 32$, $823,875$ dof





Comparison of enforcing averages

- 64 sub, $H/h = 8$, *SGI Altix*, 64 processors
- averages on all edges and faces – number of rows in G is 1,404
- 23 PCG iterations, condition number $\sim$11.7

approach	LM	PB	PCV
matrix transformation	-	-	6.5
projection	-	13.6	5.9
analysis (sec)	2.9	42.2	12.2
factorization (sec)	0.2	41.3	0.6
dual factorization (sec)	1,698.2	-	-
PCG iter (sec)	316.6	8.4	7.1
total (sec)	2,034.9	106.3	33.2

- LM – Lagrange multiplier
- PB – projected BDDC
- PCV – projected change of variables

Variable $\widetilde{W}^{avg}$ on cube

64 sub, $H/h = 8$, *IBM Blue Gene/L*, 64 processors, *Edges*, *Faces*

coarse problem	$\widetilde{W}^c$	$\widetilde{W}^c+E$	$\widetilde{W}^c+F$	$\widetilde{W}^c+E+F$	MUMPS
PCG iterations	103	49	41	24	-
cond. number est.	292.8	76.4	60.5	11.7	-
analysis (sec)	7.5	9.7	26.5	30.9	9.8
factorization (sec)	1.1	1.7	3.2	5.0	25.6
PCG iter (sec)	50.0	23.9	20.7	12.2	-
total (sec)	62.6	47.4	69.8	75.6	39.4

8 sub, $H/h = 32$, *SGI Altix*, 8 processors

coarse problem	$\widetilde{W}^c$	$\widetilde{W}^c+E$	$\widetilde{W}^c+F$	$\widetilde{W}^c+E+F$	MUMPS
PCG iterations	131	75	n/a	n/a	-
cond. number est.	5941.0	903.1	n/a	n/a	-
analysis (sec)	25.6	23.5	n/a	n/a	27.1
factorization (sec)	1097.4	1426.4	n/a	n/a	12998.0
PCG iter (sec)	743.4	356.2	n/a	n/a	-
total (sec)	1885.1	1890.3	n/a	n/a	13060.6

Conclusion

Formulation of BDDC

- distinguish between $\widetilde{W}^c$ and $\widetilde{W}^{avg}$
- matrix G of global constraints
- define $\widetilde{W}^{avg}$ using this matrix
- generalized change of variables

Implementation

- various approaches to applying constraints tested
- implementation based on multifrontal solver is simple
- promising results
- faces might be too expensive for certain type of problems
- more sophisticated (adaptive) way for selection of constraints - ongoing research
- advance in MUMPS package desired