Parallel Implementation of BDDC for Mixed-Hybrid Formulation of Flow in Porous Media

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joint work with Jan Březina² and Bedřich Sousedík³

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Geoengineering simulations

- numerous examples of flow in porous media oil and gas reservoirs, pollutant transport, nuclear waste deposits, ...
- in the Czech Republic, plans to build the long-term nuclear waste deposit by 2065 currently seven *candidate sites*
- massive granite rock with cracks





Source: www.surao.cz



Subsurface flow simulations

- 20+ years of development of simulation tools at TUL
- mixed-hybrid finite element method combined meshes of 3D, 2D and 1D elements
- need for robust scalable parallel solvers to handle finer models

Governing equations



Darcy law

$$\mathbb{k}^{-1}\mathbf{u} + \nabla p = -\nabla z \quad \text{in } \Omega \nabla \cdot \mathbf{u} = f \quad \text{in } \Omega p = p_N \quad \text{on } \partial\Omega_N \mathbf{u} \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega_E$$

•
$$\Omega \subset \mathbb{R}^3$$
, $\partial \Omega = \overline{\partial \Omega}_N \cup \overline{\partial \Omega}_E$

- $\partial \Omega_N$, $\partial \Omega_E$... natural (Dirichlet) and essential (Neumann) b. c.
- \blacksquare **u** ... velocity of the fluid
- p . . . pressure head
- \Bbbk ... tensor of the hydraulic conductivity (sym. pos. def.)
- z ... third spatial coordinate
- $p_h = p + z \dots$ piezometric head for which $\mathbf{u} = -\mathbf{k} \nabla p_h$



Raviart-Thomas (*RT*₀**) finite elements**

$$\begin{split} \mathbf{V} \subset \mathbf{H}(\Omega; \operatorname{div}) &= \left\{ \mathbf{v} \in L^2(\Omega); \ \nabla \cdot \mathbf{v} \in L^2(\Omega) \text{ and } \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \partial \Omega_E \right\} \\ Q \subset L^2(\Omega) \end{split}$$

Mixed formulation

Find a pair $\{\mathbf{u}, p\} \in \mathbf{V} \times Q$ that satisfies

$$\int_{\Omega} \mathbb{k}^{-1} \mathbf{u} \cdot \mathbf{v} \, dx - \int_{\Omega} p \nabla \cdot \mathbf{v} \, dx = -\int_{\partial \Omega_N} p_N \mathbf{v} \cdot \mathbf{n} \, ds - \int_{\Omega} v_z dx, \quad \forall \mathbf{v} \in \mathbf{V} \\ -\int_{\Omega} q \nabla \cdot \mathbf{u} dx = -\int_{\Omega} fq \, dx, \qquad \forall q \in Q$$



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Space of Lagrange multipliers

$$\begin{split} \mathbf{V}^{i} &= \left\{ \mathbf{v} \in \mathbf{H}(T^{i}; \operatorname{div}) : \mathbf{v} \in RT_{0}(T^{i}) \right\} \\ \mathbf{V}^{-1} &= \mathbf{V}^{1} \times \cdots \times \mathbf{V}^{N_{\mathcal{E}}} \\ \Lambda &= \left\{ \lambda \in L^{2}\left(\mathcal{F}\right) : \lambda = \mathbf{v} \cdot \mathbf{n}|_{\mathcal{F}}, \ \mathbf{v} \in \mathbf{V} \right\} \end{split}$$

$\blacksquare \ \mathcal{F} \ \ldots$ set of all *faces* of the elements in triangulation \mathcal{T}

Mixed-hybrid formulation

Find a triple $\{\mathbf{u}, p, \lambda\} \in \mathbf{V}^{-1} \times Q \times \Lambda$ that satisfies

$$\begin{split} \sum_{i=1}^{N_E} \left[\int_{T^i} \mathbb{k}_i^{-1} \mathbf{u} \cdot \mathbf{v} \, dx - \int_{T^i} p \nabla \cdot \mathbf{v} \, dx + \int_{\partial T^i \setminus \partial \Omega} \lambda(\mathbf{v} \cdot \mathbf{n}) |_{\partial T_i} \, ds \right] = \\ - \int_{\partial \Omega_N} p_N \mathbf{v} \cdot \mathbf{n} \, ds - \sum_{i=1}^{N_E} \int_{T^i} v_z \, dx, \quad \forall \mathbf{v} \in \mathbf{V} \\ - \sum_{i=1}^{N_E} \left[\int_{T^i} q \nabla \cdot \mathbf{u} \, dx \right] &= - \int_{\Omega} fq \, dx, \quad \forall q \in Q \\ \sum_{i=1}^{N_E} \left[\int_{\partial T^i \setminus \partial \Omega} \mu(\mathbf{u} \cdot \mathbf{n}) |_{\partial T_i} \, ds \right] &= 0, \qquad \forall \mu \in \Lambda \end{split}$$



Space of Lagrange multipliers

$$\begin{split} \mathbf{V}^{i} &= \left\{ \mathbf{v} \in \mathbf{H}(\mathcal{T}^{i}; \operatorname{div}) : \mathbf{v} \in R\mathcal{T}_{0}(\mathcal{T}^{i}) \right\} \\ \mathbf{V}^{-1} &= \mathbf{V}^{1} \times \cdots \times \mathbf{V}^{N_{\mathcal{E}}} \\ \Lambda &= \left\{ \lambda \in L^{2}\left(\mathcal{F}\right) : \lambda = \mathbf{v} \cdot \mathbf{n}|_{\mathcal{F}}, \ \mathbf{v} \in \mathbf{V} \right\} \end{split}$$

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$$-\sum_{i=1}^{N_{E}} \left[\int_{T^{i}} q \nabla \cdot \mathbf{u} \, dx \right] = -\int_{\Omega} fq \, dx, \quad \forall q \in Q$$
$$\sum_{i=1}^{N_{E}} \left[\int_{\partial T^{i} \setminus \partial \Omega} \mu(\mathbf{u} \cdot \mathbf{n}) |_{\partial T_{i}} \, ds \right] = 0, \qquad \forall \mu \in \Lambda$$



Saddle-point system

$$\begin{bmatrix} A & B^{T} & B_{\mathcal{F}}^{T} \\ B & 0 & 0 \\ B_{\mathcal{F}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \\ \lambda \end{bmatrix} = \begin{bmatrix} g \\ \overline{f} \\ 0 \end{bmatrix}$$
(1)

■ A ... symmetric positive definite (s.p.d.), block-diagonal matrix with respect to *elements*

•
$$\mathcal{B} = \begin{bmatrix} B \\ B_{\mathcal{F}} \end{bmatrix} \dots$$
 full row rank if $\partial \Omega_N \neq \emptyset$

- analysis e.g. in [Brezzi, Fortin (1991)], [Maryška, Rozložník, Tůma (2000)], [Tu (2007)], ...
- problem (1) has a **unique solution**



Combined meshes

$$\mathcal{T}_{123} = \mathcal{T}_1 \cup \mathcal{T}_2 \cup \mathcal{T}_3$$
 $\mathcal{T}_{d-1}^i \subset \mathcal{F}_d$

•
$$d = 2, 3 \dots$$
 spatial dimension

System with fluxes

$$\mathbb{k}_d^{-1} \frac{u_d}{\delta_d} + \nabla p_d = -\nabla z$$

• $u_d \ldots$ flux — volume per second per unit

■ δ_d ... conversion to velocity in dimension d ($\delta_3 = 1$, δ_2 is thickness of a fracture, δ_1 cross-section of a channel)



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System with fluxes

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- $u_d \dots$ flux volume per second per unit
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Coupling of mesh dimensions



Introduce Robin (a.k.a. Newton) boundary conditions

3D-2D

$$f_{2} = \delta_{2}\tilde{f}_{2} + \mathbf{u}_{3}^{+} \cdot \mathbf{n}^{+} + \mathbf{u}_{3}^{-} \cdot \mathbf{n}^{-}$$
$$\mathbf{u}_{3}^{+} \cdot \mathbf{n}^{+} = \sigma_{3}^{+}(p_{3}^{+} - p_{2})$$
$$\mathbf{u}_{3}^{-} \cdot \mathbf{n}^{-} = \sigma_{3}^{-}(p_{3}^{-} - p_{2})$$

• $\sigma_3^{+/-} > 0$... transition coefficients on sides of a 2D element

Ũ

$$f_1 = \delta_1 \tilde{f}_1 + \sum_k \mathbf{u}_2^k \cdot \mathbf{n}^k$$
 $\mathbf{u}_2^k \cdot \mathbf{n}^k = \sigma_2^k (p_2^k - p_1)$

• $\sigma_2^k > 0$... transition coefficient from k-th 2D element to 1D channel

Coupling of mesh dimensions



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$$\mathbf{u}_{3}^{-} \cdot \mathbf{n}^{-} = \sigma_{3}^{-}(p_{3}^{-} - p_{2})$$

• $\sigma_3^{+/-} > 0$. . . transition coefficients on sides of a 2D element

2D-1D

$$f_1 = \delta_1 \tilde{f}_1 + \sum_k \mathbf{u}_2^k \cdot \mathbf{n}^k$$
$$\mathbf{u}_2^k \cdot \mathbf{n}^k = \sigma_2^k (p_2^k - p_1)$$

• $\sigma_2^k > 0 \dots$ transition coefficient from k-th 2D element to 1D channel



Saddle-point system with couplings

$$\begin{bmatrix} A & B^{T} & B_{\mathcal{F}}^{T} \\ B & -\overline{C} & -C_{\mathcal{F}}^{T} \\ B_{\mathcal{F}} & -C_{\mathcal{F}} & -\widetilde{C} \end{bmatrix} \begin{bmatrix} u \\ p \\ \lambda \end{bmatrix} = \begin{bmatrix} g \\ \overline{f} \\ 0 \end{bmatrix}$$
(2)

■ A ... symmetric positive definite (s.p.d.), block-diagonal matrix with respect to *elements*

• $C = \begin{bmatrix} \overline{C} & C_{\mathcal{F}}^T \\ C_{\mathcal{F}} & \widetilde{C} \end{bmatrix} \dots$ symmetric positive semi-definite • $\mathcal{B} = \begin{bmatrix} B \\ B_{\mathcal{F}} \end{bmatrix} \dots$ generally **no longer full row rank**





Theorem (Solvability of the saddle-point system)

Let natural boundary conditions be prescribed at a certain part of the boundary, i.e. $\partial \Omega_{N,d} \neq \emptyset$ for at least one $d \in \{1,2,3\}$. Then the discrete mixed-hybrid problem (2) has a unique solution.

■ details in [Šístek, Březina, Sousedík (2015)]

Iterative substructuring



- \mathcal{T}_{123} divided into N_S substructures $\Omega^i, i = 1, \dots, N_S$
- Γ ... interface among substructures shared degrees of freedom

Local problem on Ω

$$\begin{bmatrix} A^{i} & B^{iT} & B^{iT}_{\mathcal{F},l} & B^{iT}_{\mathcal{F},\Gamma} \\ B^{i} & -\overline{C}^{i} & -C^{iT}_{\mathcal{F},\Gamma} & -C^{iT}_{\mathcal{F},\Gamma} \\ B^{i}_{\mathcal{F},l} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{iI}_{ll} & -\widetilde{C}^{iT}_{\Gamma} \\ B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{i}_{\Gamma} & -\widetilde{C}^{i}_{\Gamma} \end{bmatrix} \begin{bmatrix} u^{i} \\ p^{i} \\ \lambda^{i}_{l} \\ \lambda^{i}_{\Gamma} \end{bmatrix} = \begin{bmatrix} g^{i} \\ \overline{f}^{i} \\ 0 \\ 0 \end{bmatrix}$$

- λ_{Γ}^{i} ... Lagrange multipliers on $\Omega^{i} \cap \Gamma$
- λ_I^i ... Lagrange multipliers interior to Ω^i
- **u**^{*i*}, p^{i} , λ_{I}^{i} ... interior unknowns from substructuring view-point
- $\blacksquare \ \Lambda_{\Gamma} = \Lambda_{\Gamma}^{1} \times \cdots \times \Lambda_{\Gamma}^{N_{S}}$
- $\widehat{\Lambda}_{\Gamma} \subset \Lambda_{\Gamma}$... subspace of Lagrange multipliers coinciding on Γ

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- $\blacksquare\ \Gamma\ \dots\ interface\ {\sf among\ substructures}\ --\ {\sf shared\ degrees\ of\ freedom}$

Local problem on Ω^i

$$\begin{bmatrix} A^{i} & B^{iT} & B^{iT}_{\mathcal{F},I} & B^{iT}_{\mathcal{F},\Gamma} \\ B^{i} & -\overline{C}^{i} & -C^{iT}_{\mathcal{F},I} & -C^{iT}_{\mathcal{F},\Gamma} \\ B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},I} & -\widetilde{C}^{i}_{II} & -\widetilde{C}^{iT}_{\Gamma\Gamma} \\ B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{i}_{\Gamma} & -\widetilde{C}^{i}_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} u^{i} \\ p^{i} \\ \lambda^{i}_{I} \\ \lambda^{i}_{\Gamma} \end{bmatrix} = \begin{bmatrix} g^{i} \\ \overline{f}^{i} \\ 0 \\ 0 \end{bmatrix}$$

- λ_{Γ}^{i} ... Lagrange multipliers on $\Omega^{i} \cap \Gamma$
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- u^i , p^i , λ_I^i ... interior unknowns from substructuring view-point

$$\bullet \ \Lambda_{\Gamma} = \Lambda_{\Gamma}^{1} \times \cdots \times \Lambda_{\Gamma}^{N_{S}}$$

 \blacksquare $\widehat{\Lambda}_{\Gamma} \subset \Lambda_{\Gamma}$... subspace of Lagrange multipliers coinciding on Γ

Substructure Schur complements

$$S^i: \Lambda^i_{\Gamma} \mapsto \Lambda^i_{\Gamma}, \quad i = 1, \dots, N_S$$

Action of S^i on a given λ^i_{Γ} defined by

$$\begin{bmatrix} A^{i} & B^{iT} & B^{iT}_{\mathcal{F},I} & B^{iT}_{\mathcal{F},\Gamma} \\ B^{i} & -\overline{C}^{i} & -C^{iT}_{\mathcal{F},I} & -C^{iT}_{\mathcal{F},\Gamma} \\ B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},I} & -\widetilde{C}^{i}_{II} & -\widetilde{C}^{iT}_{\Gamma I} \\ B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{i}_{\Gamma I} & -\widetilde{C}^{i}_{\Gamma \Gamma} \end{bmatrix} \begin{bmatrix} w^{i} \\ q^{i} \\ \mu^{i}_{I} \\ \lambda^{i}_{\Gamma} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -S^{i}\lambda^{i}_{\Gamma} \end{bmatrix}$$

Global Schur complement $\widehat{S} : \lambda_{\Gamma} \in \widehat{\Lambda}_{\Gamma} \to \widehat{S}\lambda_{\Gamma} \in \widehat{\Lambda}_{\Gamma}$

Formally assembled as

$$\widehat{S} = \sum_{i=1}^{N_S} R^{iT} S^i R^i$$

R^{*i*} ... 0-1 mapping matrix, $\lambda_{\Gamma}^{i} = R^{i}\lambda_{\Gamma}, \lambda_{\Gamma}^{i} \in \Lambda_{\Gamma}^{i}, \lambda_{\Gamma} \in \widehat{\Lambda}_{\Gamma}$



Substructure Schur complements

$$S^i : \Lambda^i_{\Gamma} \mapsto \Lambda^i_{\Gamma}, \quad i = 1, \dots, N_S$$

Action of S^i on a given λ^i_{Γ} defined by

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Formally assembled as

$$\widehat{S} = \sum_{i=1}^{N_S} R^{iT} S^i R^i$$

• $R^i \dots 0-1$ mapping matrix, $\lambda_{\Gamma}^i = R^i \lambda_{\Gamma}$, $\lambda_{\Gamma}^i \in \Lambda_{\Gamma}^i$, $\lambda_{\Gamma} \in \widehat{\Lambda}_{\Gamma}$





Interface problem

$$\widehat{S}\lambda_{\Gamma} = \widehat{b}$$
 (3)

reduced right-hand side

$$\begin{split} \widehat{b} &= \sum_{i=1}^{N_{\mathcal{S}}} R^{iT} b^{i} \\ b^{i} &= \begin{bmatrix} B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{i}_{\Gamma I} \end{bmatrix} \begin{bmatrix} A^{i} & B^{iT} & B^{iT}_{\mathcal{F},I} \\ B^{i} & -\overline{C}^{i} & -C^{iT}_{\mathcal{F},I} \\ B^{i}_{\mathcal{F},I} & -C^{i}_{\mathcal{F},I} & -\widetilde{C}^{i}_{II} \end{bmatrix}^{-1} \begin{bmatrix} g^{i} \\ \overline{f}^{i} \\ 0 \end{bmatrix} \end{split}$$



Interface problem

$$\widehat{S}\lambda_{\Gamma} = \widehat{b}$$
 (3)

reduced right-hand side

$$\widehat{b} = \sum_{i=1}^{N_{S}} R^{iT} b^{i}$$
$$b^{i} = \begin{bmatrix} B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{i}_{\Gamma I} \end{bmatrix} \begin{bmatrix} A^{i} & B^{iT} & B^{iT}_{\mathcal{F},I} \\ B^{i} & -\overline{C}^{i} & -C^{iT}_{\mathcal{F},I} \\ B^{i}_{\mathcal{F},I} & -C^{i}_{\mathcal{F},I} & -\widetilde{C}^{iT}_{II} \end{bmatrix}^{-1} \begin{bmatrix} g^{i} \\ \overline{f}^{i} \\ 0 \end{bmatrix}$$



Theorem (Solvability of the interface problem)

Let natural boundary conditions be prescribed at a certain part of the boundary, i.e. $\partial \Omega_{N,d} \neq \emptyset$ for at least one $d \in \{1,2,3\}$. Then the matrix \hat{S} in (3) is symmetric and positive definite.

- using the Preconditioned Conjugate Gradient (PCG) method for solving (3)
- only applications of \hat{S} needed performed by parallel solution of discrete Dirichlet problems on each substructure
- BDDC used as the preconditioner
- details in [Šístek, Březina, Sousedík (2015)]

BDDC preconditioner



BDDC method for Darcy flow

- Balancing Domain Decomposition by Constraints [Dohrmann (2003)] — elasticity
- mixed FEM [Tu (2005)], multilevel [Tu (2011)], [Sousedík (2013)]
- mixed-hybrid FEM [Tu (2007)], without cracks, Lagrange multipliers introduced only on Γ — different local problems
- define constraints enforcing continuity of functions from Λ_Γ at coarse degrees of freedom among substructures

■ space Â_Γ

$$\widehat{\Lambda}_{\Gamma}\subset \widetilde{\Lambda}_{\Gamma}\subset \Lambda_{\Gamma}$$

- substructure faces arithmetic averages basic constraints
- *edges* may appear at intersections of 2D elements
- corners pointwise continuity not needed for RT0 elements but improve convergence for numerically difficult problems, selected by the *face-based algorithm* from [Šístek et al. (2012)]



Algebraic coarse basis functions on Ω^i

Solve for multiple right-hand sides



- D^i ... matrix of coarse degree of freedom
- I ... identity matrix
- Φ^i_{Γ} ... coarse basis functions
- X^i , Z^i , Φ^i_I ... auxiliary matrices not used further
- local coarse matrix $S_{CC}^{i} = \Phi_{\Gamma}^{iT} S^{i} \Phi_{\Gamma}^{iT} = -L^{i}$ [Pultarová (2012)]
- **global coarse matrix** $S_{CC} = \sum_{i=1}^{N_S} R_C^{iT} S_{CC}^i R_C^i$
- R_C^i ... 0-1 matrix relating local-to-global coarse degrees of freedom

BDDC action



Algorithm (BDDC preconditioner M_{BDDC} : $r_{\Gamma} \in \widehat{\Lambda}_{\Gamma} \rightarrow \lambda_{\Gamma} \in \widehat{\Lambda}_{\Gamma}$)

1 Solve the global coarse problem

$$S_{CC} \eta_C = \sum_{i=1}^{N_S} R_C^{iT} \Phi_{\Gamma}^{iT} W^i R^i r_{\Gamma}$$

2 Solve local Neumann problems

$$\begin{bmatrix} A^{i} & B^{iT} & B^{iT}_{\mathcal{F},I} & B^{iT}_{\mathcal{F},\Gamma} & 0\\ B^{i} & -\overline{C}^{i} & -C^{iT}_{\mathcal{F},I} & -C^{iT}_{\mathcal{F},\Gamma} & 0\\ B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{i}_{II} & -\widetilde{C}^{iT}_{\Gamma I} & 0\\ B^{i}_{\mathcal{F},\Gamma} & -C^{i}_{\mathcal{F},\Gamma} & -\widetilde{C}^{i}_{\Gamma I} & -\widetilde{C}^{i}_{\Gamma I} & D^{iT}\\ 0 & 0 & 0 & D^{i} & 0 \end{bmatrix} \begin{bmatrix} x^{i} \\ z^{i} \\ \eta^{i}_{I\Delta} \\ \eta^{i}_{\Gamma\Delta} \\ l^{i} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ W^{i}R^{i}r_{\Gamma} \\ 0 \end{bmatrix}$$

3 Combine and average the corrections

$$\lambda_{\Gamma} = -\sum_{i=1}^{N_{S}} R^{iT} W^{i} \left(\eta_{\Gamma\Delta}^{i} + \Phi_{\Gamma}^{i} R_{C}^{i} \eta_{C} \right)$$



 studied e.g. in [Klawonn, Rheinbach, Widlund (2008)], [Čertíková, Šístek, Burda (2013)], [Oh, Widlund, Dohrmann (TR2013)], ...

Generalized scaling by diagonal stiffness

Diagonal entry given by

$$W^i_{jj} = \widetilde{C}^i_{\Gamma\Gamma,jj} + rac{1}{A^i_{kk}}$$

■ k(j) ... the row in block A^i of the element face to which the Lagrange multiplier $\lambda_{\Gamma,j}^i$ belongs



Flow123d

- simulation of subsurface flow and pollution transport
- mixed-hybrid FEM
- open-source (GPL license)
- developed at TUL
- current version 1.8.2 (15/3/'15)
- \blacksquare object-oriented C++ code
- 10+ years of development
- ~5 active developers lead developer J. Březina

http://flow123d.github.io

BDDCML equation solver

- Adaptive-Multilevel BDDC [Sousedík, Šístek, Mandel (2013)]
- open-source (LGPL license)
- developed at IM AS CR
- current version 2.5 (8/6/'15)
- Fortran 95 + MPI library
- 5+ years of development
- relies on MUMPS both serial and parallel

http://www.math.cas.cz/~sistek/software/ bddcml.html



Fox

Location: CTU Supercomputing Centre, Prague Architecture: SGI Altix UV Processor Type: Intel Xeon 2.67GHz Computing Cores: 72 RAM: 576 GB (8 GB/core)



HECToR

Location: EPCC, Edinburgh Architecture: Cray XE6 Processor Type: 16 core AMD Opteron 2.3GHz Interlagos Computing Cores: 90,112 Computing Nodes: 2816 RAM: 90 Tb TB (32 GB/node) access through *PRACE-DECI*



graphics from www.hector.ac.uk

Benchmark problems: Weak scaling on a square



- unit square domain, only 2D elements
- 2–64 cores of SGI Altix UV
- PCG tolerance $||r^{(k)}||/||\widehat{b}|| < 10^{-7}$



pressure head with mesh

velocity vectors

velocity mag.

13.12612

2.629e-5

•		n/N		n _f	ne	:+-	اممم	time (sec)		
	п		П		n _c	ILS.	cond.	set-up	PCG	solve
2	207k	103k	155	1	2	7	1.37	8.3	1.6	9.9
4	440k	110k	491	5	10	8	1.60	12.2	2.2	14.4
8	822k	103k	1.2k	13	26	9	1.78	11.0	2.5	13.5
16	1.8M	111k	2.8k	33	66	8	1.79	14.3	2.7	17.0
32	3.3M	104k	5.9k	74	148	9	1.79	12.1	3.3	15.4
64	7.2M	113k	13.0k	166	332	9	1.85	14.8	4.4	19.2

Benchmark problems: Weak scaling on a cube



- unit cube domain, only 3D elements
- 2–64 cores of SGI Altix UV
- PCG tolerance $||r^{(k)}||/||\widehat{b}|| < 10^{-7}$





pressure head with mesh

velocity vectors

N		n/N	n		n.,	ite	cond	time (sec)			
	11		11	n_{f}	II _C	ILS.	conu.	set-up	PCG	solve	
2	217k	108k	884	1	3	11	2.88	11.7	2.3	14.0	
4	437k	109k	2.3k	6	18	12	3.04	11.7	2.5	14.2	
8	945k	118k	5.7k	21	63	15	12.00	15.4	4.0	19.3	
16	1.6M	103k	12.8k	56	168	16	6.58	12.9	4.0	17.0	
32	3.4M	106k	29.8k	132	401	18	10.10	15.4	5.2	20.6	
64	6.1M	95k	59.6k	307	931	19	16.58	13.7	6.3	20.0	

Benchmark problems: Strong scaling test on a cube



- unit cube domain, 1D, 2D and 3D elements ($k = \nu I$, $\nu = 10$, 1, 0.1)
- 2.1 million elements, 14.6 million degrees of freedom
- 16–512 cores of HECToR
- PCG tolerance $||r^{(k)}||/||\widehat{b}|| < 10^{-7}$





pressure head with mesh

velocity vectors

N	m / N/			n _c	:+-	أممم	time (sec)			
	n/n	n _E	Πf		ILS.	cond.	set-up	PCG	solve	
16	912k	47k	53	159	26	59.3	171.6	84.5	256.2	
32	456k	65k	126	380	48	2091.0	90.1	109.8	200.0	
64	228k	86k	301	914	81	1436.1	36.8	77.1	114.0	
128	114k	116k	689	2076	109	2635.8	14.3	43.1	57.4	
256	57k	151k	1436	4365	164	1700.5	6.7	31.2	38.0	
512	28k	196k	3021	9244	254	42614.5	4.0	26.9	30.9	





Speed-up on *np* processors computed as

$$s_{np} = \frac{16 \ t_{16}}{t_{np}}$$

Geoengineering problem: Bedřichov tunnel



- experimental measurement site
- 2.1 km long tunnel with water pipes for the city of Liberec
- fractured granite rock
- data by courtesy of Dalibor Frydrych (TUL)
- $\blacksquare \ 3D \ elements + 2D \ elements \ for \ cracks$
- 1.1 million elements, 7.8 million degrees of freedom
- hydraulic conductivity $k = \nu I$, $\nu = 10^{-10} 10^{-7} \text{ ms}^{-1}$
- transition coefficient $\sigma_3 = 1 \text{ s}^{-1}$, thickness of cracks $\delta_2 = 1.1 \text{ m}$
- 32–1024 cores of HECToR
- PCG tolerance $||r^{(k)}||/||\widehat{b}|| < 10^{-7}$



Bedřichov tunnel — strong scaling test





system of cracks



division into 64 substructures



detail of tunnel geometry



enforced refinement at cracks



N/	m / N/				:+-	اممم	t	ime (sec))
	n/n		Πf	Π _C	its.	.s. cond.	set-up	PCG	solve
32	245k	20k	106	322	112	1514.1	110.3	144.0	254.3
64	123k	28k	192	597	63	117.7	42.2	36.0	78.3
128	61k	45k	413	1293	75	194.4	13.4	16.8	30.3
256	31k	72k	902	2791	119	526.7	4.2	10.9	15.1
512	15k	110k	2009	6347	137	1143.4	1.8	7.1	9.0
1024	8k	155k	4575	14725	173	897.0	1.6	8.0	9.7





Comparison of different weighting options

Ν		<i>n</i> -	arithmetic avg.		mo	d. ρ -scal.	diagonal scal.	
11	//F	Π _C	its.	cond.	its.	cond.	its.	cond.
32	20k	322	637	9811.7	110	1467.8	112	1514.1
64	28k	597	618	10254.1	62	115.1	63	117.7
128	45k	1293	2834	$1.0e{+}11$	206	401641.4	75	194.4
256	72k	2791	799	11172.9	117	512.9	119	526.7
512	110k	6347	883	15449.6	136	1160.1	137	1143.4
1024	155k	14725	n/a	2.5e+10	504	99023.6	173	897.0

Effect of using corners

Ν									
	time (sec)				time (sec)				
				112					
64		40.4							
				75	13.4				
		12.5		119	4.2		15.1		
	1.4		11.4	137	1.8	7.1			
1024	1.0	14.5		173	1.6				



Comparison of different weighting options

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Effect of using corners

		without	t corners		with corners				
N	ite	time (sec)			ite	time (sec)			
	Its.	set-up	PCG	solve	its.	set-up	PCG	solve	
32	131	107.5	175.0	282.5	112	110.3	144.0	254.3	
64	70	40.3	40.4	80.7	63	42.2	36.0	78.3	
128	96	10.9	21.6	32.6	75	13.4	16.8	30.3	
256	139	3.7	12.5	16.2	119	4.2	10.9	15.1	
512	197	1.4	10.0	11.4	137	1.8	7.1	9.0	
1024	312	1.0	14.5	15.6	173	1.6	8.0	9.7	

Conclusions



Parallel BDDC solver for flows in porous media

- BDDC for Darcy flow with combined mesh dimensions
- connection of two existing codes *Flow123d* + *BDDCML*
- good scalability for single mesh dimension and 3D–2D couplings
- geoengineering problems challenging highly refined meshes, large hydraulic conductivities in cracks, ...
- generalized averaging by diagonal stiffness on interface
- positive effect of using corners

Future work

- analysis for 1D–2D–3D couplings
- application of Adaptive-Multilevel BDDC



Šístek, J., Březina, J., Sousedík, B.: BDDC for mixed-hybrid formulation of flow in porous media with combined mesh dimensions. *Numer. Linear Algebra Appl., 2015, available online.*

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Parallel BDDC solver for flows in porous media

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Thank you for your attention.



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BDDCML library webpage

http://users.math.cas.cz/~sistek/software/bddcml.html