J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system

Resolution

On-going work

Flow simulations in 3D Discrete Fracture Networks

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J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system

Resolution

On-going work

Problem description

- Geometry
- Flow equations
- Derivation of the linear system
 MHFFM
 - MHMFEM

3 Resolution

- Schur complement matrix
- Preconditioned Conjugate gradient
- Results

On-going work

Stochastic Generation of DFN

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Geometry Flow equation

Derivation o the linear system

Resolution

On-going work

Following a Discrete Fracture Network approach, fractures are planes with the following statistical properties :

Parameter	Random distribution
length	power law
shape	disks / ellipses
position	uniform
orientation	uniform
Conductivity	homogeneous
	/ correlated log-normal



Example of DFN with 217 fractures

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Geometry

Flow equations

Derivation on the linear system

Resolution

On-going work

Stochastic Generation of DFN

The broad natural fracture length distribution is modeled by a power law distribution (Bour et al, 2002) :

$$p(l)dl = rac{1}{a-1} rac{l^{-a}}{l_{min}^{-a+1}} dl$$

where p(I)dI is the probability of observing a fracture with a length in the interval [I, I + dI], I_{min} is the smallest fracture length, and *a* is a characteristic exponent.



Flow model

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Geometry

Flow equations

Derivation on the linear system

. . .

Current assumptions :

- The rock matrix is impervious : flow is only simulated in the fractures,
- Study of steady state flow,
- There is no longitudinal flux in the intersections of fractures.

Flow equations within each fracture Ω_f :

$ abla \cdot \mathbf{u}(\mathbf{x}) = \mathbf{f}(\mathbf{x}),$	for $\mathbf{x} \in \Omega_f$,
$\mathbf{u}(\mathbf{x}) = -\mathcal{T}(\mathbf{x}) \nabla p(\mathbf{x}),$	for $\mathbf{x} \in \Omega_f$,
$p(\mathbf{x}) = p^D(\mathbf{x}),$	on $\Gamma_D \cap \Gamma_f$,
$\mathbf{u}(\mathbf{x}).\mathbf{\nu} = q^N(\mathbf{x}),$	on $\Gamma_N \cap \Gamma_f$,
$\mathbf{u}(\mathbf{x}).\mathbf{\mu} = 0,$	on $\Gamma_f \setminus \{ (\Gamma_f \cap \Gamma_D) \cup (\Gamma_f \cap \Gamma_N) \},\$

• u (resp. μ) outward normal unit vectors

• T(x) a given transmissivity field (unit $[m^2.s^{-1}]$), $f(x) \in L^2(\Omega_f)$ sources/sinks.

Continuity conditions in each intersection :

$$p_{k,f} = p_k, \qquad \text{on } \Sigma_k, \forall f \in F_k,$$
$$\sum_{f \in F_k} \mathbf{u}_{k,f}.\mathbf{n}_{k,f} = 0, \qquad \text{on } \Sigma_k,$$

with F_k the set of fractures with Σ_k (the k-th intersections) on the boundary,

Mixed-Hybrid Finite Element Method

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system

MHFEM MHMFEM

Resolution

On-going work

Mixed-Hybrid Finite Element Method (MHFEM) for DFNs Réf. J. Erhel et al., SIAM SISC, Vol. 31, No. 4, pp. 2688-2705, 2009

• Makes it easy to deal with complex geometry;

• Conforming mesh at the fracture intersections;

• A linear system with only trace of pressure unknowns :

 $\mathbf{A}\mathbf{\Lambda}=\mathbf{b},$

with A a symmetric positive definite matrix, the flux at the edges and the mean pressure are then easily derived locally on each triangle.

Specific mesh generation :

- A first discretization of boundaries and intersections is done in 3D by using elementary cubes
- **2** The discretization of the boundaries and intersections within the fracture f is obtained by a projection of the previous voxel discretization within the fracture plane.
- Some local corrections to ensure some topological properties.
- Once the borders and intersections are discretized, a 2D mesh of each fracture, using triangular elements.



Mixed-Hybrid Mortar Finite Element Method

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Resolution

On-going work

In DFN, flow is highly channelled = an opportunity to reduce the number of unknowns and the computational cost, by using a non conforming mesh at intersections.



J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Resolution

On-going work

Mixed-Hybrid Mortar Finite Element Method (MHMFEM) for DFNs Réf. G. Pichot et al., Applicable Analysis, In print, 2010

A method to mesh the fractures independently and to refine the chosen fractures using a posteriori estimators.

- Same advantages as MHFEM
- A simple mesh generation
- A reduced number of unknowns while keeping a solution of good quality
- a complex numerical method with Mortar conditions

Mixed-Hybrid Mortar Finite Element Method

A new specific mesh generation : For each fracture f,



choose a mesh step and perform :

- A first discretization of boundaries and intersections in 2D by using elementary squares, it leads to a stair-case like discretizations;
- Some local corrections to ensure some topological properties.
- Once the borders and intersections are discretized, a 2D mesh of each fracture, using triangular elements.

Meshing procedure : Example

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Resolution



The discretization of intersections is non matching \Rightarrow Mortar conditions are required to ensure the continuity of heads and fluxes.

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Mortar principle

Mortar method principle :

It consists in choosing arbitrarily for each intersection a master fracture (m) and a slave fracture (s).



- Particular case : each edge is either master or slave
- General case : some edges have several master or slave properties Réf. *G. Pichot et al., in preparation, 2010*

Definitions

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plar

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Resolution

On-going work

Unknowns	Local (fracture f)	Global (network)
Cell mean	P _f	$P = (P_{f})_{f}$
hydraulic head		
Traces of hydraulic head	$ \begin{split} \mathbf{\Lambda}_{\mathbf{f}} &= \begin{pmatrix} \mathbf{\Lambda}_{\mathbf{f}, \mathbf{in}} \\ \mathbf{\Lambda}_{\mathbf{f}, \mathbf{\Sigma}} \end{pmatrix} \\ \mathbf{\Lambda}_{\mathbf{f}, \mathbf{in}} &= (\lambda_E)_{\mathrm{E} \text{ inter edge}} \\ \mathbf{\Lambda}_{\mathbf{f}, \mathbf{\Sigma}} &= (\lambda_E)_{\mathrm{E} \text{ intersection edge}}, \\ \mathbf{\Lambda}_{\mathbf{f}, \mathbf{m}} &= (\lambda_E)_{\mathrm{E} \text{ master edge}} \\ \mathbf{\Lambda}_{\mathbf{f}, \mathbf{s}} &= (\lambda_E)_{\mathrm{E} \text{ slave edge}} \end{split} $	$ \begin{split} \Lambda_{in} &= (\Lambda_{f,in})_f \\ \Lambda_{\Sigma} &= (\Lambda_{f,\Sigma})_f \\ \Lambda_m &= (\Lambda_{f,m})_f \\ \Lambda_s &= (\Lambda_{f,s})_f \end{split} $
Jump of flux	$Q_{f,in} = (Q_{E,f})_{\mathrm{E \ inner \ edge}}$	
through the edges	$Q_{f,\Sigma} = (Q_{E,f})_{\text{E intersection edge}}$	$Q_{\Sigma} = (Q_{\mathbf{f},\Sigma})_f$
	$Q_{f,m} = (Q_{E,f})_{\mathrm{E} ext{ master edge}}$	$\mathbf{Q}_{\mathbf{m}} = (\mathbf{Q}_{\mathbf{f},\mathbf{m}})_f$
	$Q_{f,s} = (Q_{E,f})_{\mathrm{E \ slave \ edge}}$	$\mathbf{Q}_{s} = (\mathbf{Q}_{f,s})_{f}$

Notations : $N_{f,m}$ (resp. $N_{f,s}$) number of master (resp. slave) edges within the fracture f, and $N_{f,\Sigma}$, number of intersection edges. Global numbers are : $N_m = \sum_{f=1}^{N_f} N_{f,m}, N_s = \sum_{f=1}^{N_f} N_{f,s}$ and $N_{\Sigma} = \sum_{f=1}^{N_f} N_{f,\Sigma}$.

Mortar global conditions

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Trace of hydraulic head	Jump of flux
$\Lambda_s = C \Lambda_m$	$\mathbf{Q}_{\mathbf{m}} + \mathbf{C}^{T} \mathbf{Q}_{\mathbf{s}} = 0$
$\Lambda_{\Sigma}=A_m\Lambda_m+A_s\Lambda_s$	$ \begin{array}{l} \mathbf{A_m}^T \mathbf{Q_{\Sigma}} = \mathbf{Q_m} \\ \mathbf{A_s}^T \mathbf{Q_{\Sigma}} = \mathbf{Q_s} \end{array} $

with **C** a block matrix of dimension $N_s \times N_m$, with blocks (**C**_k) of dimension $N_{k,s} \times N_{k,m}$ for which each block represents the L^2 -projection from the master side to the slave side with coefficients C_{ln} , $l \in \{1, ..., N_{k,s}\}$, $n \in \{1, ..., N_{k,m}\}$:

$$C_{ln} = \left(\frac{|E_n^m \cap E_l^s|}{|E_l^s|} \right),$$

where the notation |E| stands for the length of the edge E.

 A_s and A_m are ponderation matrices that gives Λ_Σ as the mean of Λ_m and $\Lambda_s.$

Linear system

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem descriptio

Derivation of the linear system MHFEM MHMFEM

Resolution

On-going work

$$\begin{split} D \, P \, - \left(\begin{array}{cc} R_{in} & R_{\Sigma}(A_m + A_s C) \end{array} \right) \left(\begin{array}{c} \Lambda_{in} \\ \Lambda_m \end{array} \right) = f, \\ \left(\begin{array}{cc} M_{in} & M_{\Sigma}(A_m + A_s C) \\ (A_m^{\ T} + C^{\ T} A_s^{\ T}) M_{\Sigma}^{\ T} & (A_m^{\ T} + C^{\ T} A_s^{\ T}) B_{\Sigma}(A_s C + A_m) \end{array} \right) \left(\begin{array}{c} \Lambda_{in} \\ \Lambda_m \end{array} \right) \\ - \left(\begin{array}{c} R_{in}^T \\ (A_m^{\ T} + C^{\ T} A_s^{\ T}) R_{\Sigma}^{\ T} \end{array} \right) P - v = 0. \end{split}$$

obtained by inverting locally Poiseuille's law on each triangle and by expressing the fluxes in term of traces of hydraulic head and mean heads in the following equations :

- First set of equations : mass conservation
- Second set of equations : continuity of flux through inner edges
- Third set of equations : continuity of flux through intersection edges

Linear system

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Resolution

We get a linear system of the form

$$\begin{pmatrix} \mathbf{D} & -\mathbf{R} \\ -\mathbf{R}^{\mathsf{T}} & \mathbf{M} \end{pmatrix} \begin{pmatrix} \mathbf{P} \\ \mathbf{\Lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{v} \end{pmatrix}$$

Then the system reduces to :

$$\begin{split} \mathbf{A} \mathbf{\Lambda} &= \mathbf{b}, \\ \text{with } \mathbf{A} \,=\, \mathbf{M} \,-\, \mathbf{R}^{\, T} \, \mathbf{D}^{-1} \, \mathbf{R}, \, \mathbf{\Lambda} &= \left(\begin{array}{c} \Lambda_{\text{in}} \\ \Lambda_{\text{m}} \end{array}\right) \, \text{and} \, \, \mathbf{b} = \mathbf{v} + \mathbf{R}^{\, T} \mathbf{D}^{-1} \mathbf{f}. \end{split}$$

Assuming the transmissivity is locally symmetric positive definite, the matrix

$$\mathcal{J} = \left(\begin{array}{cc} \mathbf{D} & -\mathbf{R} \\ \\ -\mathbf{R}^{\mathsf{T}} & \mathbf{M} \end{array} \right)$$

is symmetric and, with the presence of Dirichlet boundary conditions within at least one fracture, it is positive definite.

Then A is also symmetric positive definite.

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system MHFEM MHMFEM

Resolution

On-going work

Consistency of the results

Criteria checked for all simulations :

- Null sum of the fluxes over all the system
- Null sum of the fluxes over all intersections between fractures
- Boundary conditions satisfied
- Continuity of the flux on inner edges (that is egdes that are not intersection).



Convergence criterium

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Resolution

On-going work

Numerical convergence is estimated via a discrete relative L^2 error :

- \blacksquare A computation is performed on a fine mesh \mathcal{T}_η that gives a reference mean pressure p_η
- 2 Simulations are performed on coarsened grids T_h of mesh step $h > \eta$.

The mean head obtained on coarse meshes, p_h , are then compared with p_η [Martin et al. 2005] :

$$||\boldsymbol{p}_{h}-\boldsymbol{p}_{\eta}||_{L^{2}(\Omega)}^{2}=\frac{\sum_{T_{\eta}\in\mathcal{T}_{\eta}}(\Pi_{\eta}\boldsymbol{p}_{h}-\boldsymbol{p}_{\eta})^{2}|T_{\eta}|}{\sum_{T_{\eta}\in\mathcal{T}_{\eta}}(\boldsymbol{p}_{\eta})^{2}|T_{\eta}|},$$

- $|\mathcal{T}_{\eta}|$ the area of the triangle $\mathcal{T}_{\eta}\in\mathcal{T}_{\eta}$
- $\Pi_{\eta} p_h$ the projection of p_h onto the fine mesh \mathcal{T}_{η} .

Convergence analysis

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system MHFEM MHMFEM

Resolution

On-going work

• On 25 Monte-Carlo simulations :

Parameter	Random distribution
length	power law
shape	disks
position	uniform
orientation	uniform

Parameter	Value
а	3.5
L/I _{min}	2
N _{MC}	25
Mesh step	from 0.05 to 0.09
Density	2



Log10 of the Convergence criterium vs mesh scale

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system

Resolution

Schur complement matrix

Preconditioned Conjugate gradient Results

On-going work

Linear system

Linear system to solve :

In the previous section, we have seen that using MHFEM or MHFEM with Mortar leads to a linear system in term of trace of hydraulic head unknowns :

 $A\Lambda = b.$

with A a symmetric positive definite matrix.

Possible solvers :

- Direct solver (using Cholesky factorization) : ok but is memory and CPU expensive for large DFNs
- Iterative solver : multigrid method
- Iterative solver : Preconditioned Conjugate Gradient (PCG) method
- Semi-iterative solver : Domain Decomposition method

Remark :

On the next slides, the PCG approach is applied to the matrix obtained via a conforming Mixed-Hybrid FEM. But there should be not difficulty to use it on the matrix obtained using a non-conforming mesh (with Mortar). It is part of our forthcoming work.

Schur complement matrix construction

Flow A specific matrix shape : simulations in 3D Discrete

Networks J-R. de Dreuzv . J. Erhel . G. Pichot. B. Poirriez

Fracture

Schur complement matrix

The network : $\Omega_s = \bigcup_i \Omega_i$, $i = 1, ..., N_f$, N_f total number of fractures. $\mathbf{A}_{1,1}$... $\mathbf{A}_{1,N_{f}+1}$ ۰. 0 $\mathbf{A}_{i,i}$ \mathbf{A}_{i,N_f+1}

- One block for each fracture
- Same memory complexity as a 2D problem

Schur complement matrix :

$$\mathbf{S} = \mathbf{A}_{N_f+1, N_f+1} - \sum_{i=1}^{N_f} \mathbf{A}_{i, N_f+1}^T \mathbf{A}_{i, i}^{-1} \mathbf{A}_{i, N_f+1}$$

Equivalent system : $S\Lambda_{\Sigma} = \tilde{b}$, with $\tilde{b} = b_{N_f+1} - \sum A_{i,N_f+1}^{T} A_{i,i}^{-1} b_i$

With Λ_{Σ} the trace of hydraulic head unknowns at the intersection edges.

 \Rightarrow Solving with PCG : no need to compute S : only matrix-vector products involving subdomain solutions

Schur complement and fractures

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system

Resolution

Schur complement matrix

Preconditione Conjugate gradient Results

On-going work

 $\mathbf{A}_{i}^{\#} = \begin{bmatrix} \mathbf{0} & \dots & \dots & \dots \\ \vdots & \mathbf{A}_{i,i} & \mathbf{A}_{i,N_{f}+1} \\ \vdots & \ddots & \vdots \\ \vdots & \mathbf{A}_{i,N_{f}+1}^{T} & \dots & \mathbf{A}_{N_{f}+1,N_{f}+1}^{(i)} \end{bmatrix}, \ \mathbf{A} = \sum_{i=1}^{N_{f}} \mathbf{A}_{i}^{\#}$

Local system construction : For a fracture numbered (*i*)

- Network geometry is relevant for a Schur complement approach
- With too many fractures, one subdomain contains several fractures

Creation of connected fractures set

- Software Scotch : decomposes the network in N_k connected fractures sets F_k , $k = 1, ..., N_k$, $F_k = \cup_i \Omega_i$, $i \in I_k$, with I_k the set of indices generated by Scotch
- Constructs the k-th block-matrix $\mathbf{B}_{k}^{\#} = \mathbf{P}^{T}(\sum_{i \in I_{k}} \mathbf{A}_{i}^{\#})\mathbf{P}$, $k = 1, ...N_{k}$, and \mathbf{P} a permutation matrix.

Schur complement and fractures

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system

Resolution

Schur complement matrix

Precondition Conjugate gradient Results

On-going work

Local block matrix : For a block k, $k = 1, ... N_k$:



Initial matrix :

$$\mathbf{B} = \sum_{k=1}^{N_k} \mathbf{B}_k^{\#} = \mathbf{P}^T \mathbf{A} \mathbf{P}$$

Schur Complement for the matrix B :

$$\mathbf{S}_{\mathbf{B}} = \mathbf{B}_{N_k+1,N_k+1} - \sum_{k=1}^{N_k} \mathbf{B}_{k,N_k+1}^{\mathsf{T}} \mathbf{B}_{k,k}^{-1} \mathbf{B}_{k,N_k+1}$$

Equivalent system : $S_B \Lambda_{\Sigma} = \tilde{b}_B$, with $\tilde{b}_B = b_{N_k+1} - \sum_k B_{k,N_k+1}^T B_{k,k}^{-1} b_k$

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J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation of the linear system

Resolution

Schur complement matrix

Preconditioned Conjugate gradient

Results

On-going work

Conjugate gradient

Initialisation :

- Choose $\Lambda_{\Sigma,0}$
- $\mathbf{r}_0 = \tilde{\mathbf{b}}_B \mathbf{S}_{\mathbf{B}} \mathbf{\Lambda}_{\Sigma,0}$
- $\mathbf{p}_0 = r_0$

Iterations : Do

• $\mathbf{q}_j = \mathbf{S}_{\mathbf{B}} \mathbf{p}_j \leftarrow \text{Computation of matrix/vector product}$

$$\boldsymbol{\alpha}_j = \frac{\mathbf{r}_j^T \mathbf{r}_j}{\mathbf{p}_j^T \mathbf{q}_j}$$

•
$$\Lambda_{\Sigma,j+1} = \Lambda_{\Sigma,j} + \alpha_j \mathbf{p}_j$$

$$\mathbf{r}_{j+1} = \mathbf{r}_j - \alpha_j \mathbf{q}_j$$

$$\beta_j = \frac{\mathbf{r}_{j+1}\mathbf{r}_{j+1}}{\mathbf{r}_j^T\mathbf{r}_j}$$

•
$$\mathbf{p}_{j+1} = \mathbf{r}_{j+1} + \beta_j \mathbf{p}_j$$

•
$$j = j + 1$$

Until convergence.

Computation of matrix/vector product :

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system

Resolution

Schur complement matrix

Preconditioned Conjugate gradient

Results

On-going work

$$\begin{split} i &= \sum_{\substack{k=1\\N_k}}^{N_k} \mathbf{S}_k \mathbf{p}_j \\ &= \sum_{\substack{k=1\\N_k}}^{N_k} \left(\mathbf{B}_{N_k+1,N_k+1}^{(k)} \mathbf{p}_j - \mathbf{B}_{k,N_k+1}^T \mathbf{B}_{k,k}^{-1} \mathbf{B}_{k,N_k+1} \mathbf{p}_j \right) \\ &= \sum_{k=1}^{N_k} \left(\mathbf{B}_{N_k+1,N_k+1}^{(k)} \mathbf{p}_j - \mathbf{B}_{k,N_k+1}^T \mathbf{B}_{k,k}^{-1} \mathbf{v}_{k,j} \right) \end{split}$$

Cholesky factorization :

S_Bp

$$\mathbf{B}_{k,k} = \mathbf{L}_{k,k} \mathbf{L}_{k,k}^{\mathsf{T}}$$
$$\mathbf{B}_{k,k}^{-1} \mathbf{v}_{k,j} = \mathbf{L}_{k,k}^{-\mathsf{T}} \mathbf{L}_{k,k}^{-1} \mathbf{v}_{k,j}$$

PCG with Neumann-Neumann Preconditioning

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system

Resolution

Schur complement matrix

Preconditioned Conjugate gradient

Result

On-going work

Initialisation :

- Choose $\Lambda_{\Sigma,0}$
- $\mathbf{r}_0 = \tilde{\mathbf{b}}_B \mathbf{S}_B \, \mathbf{\Lambda}_{\Sigma,0}$ • $\mathbf{z}_0 = \mathbf{M}^{-1} \mathbf{r}_0$ • $\mathbf{p}_0 = \mathbf{z}_0$

Iterations : Do

•
$$\mathbf{q}_j = \mathbf{S}_{\mathbf{B}}\mathbf{p}_j$$

• $\alpha_j = \frac{\mathbf{r}_j^T \mathbf{z}_j}{\mathbf{p}_j^T \mathbf{q}_j}$

$$\mathbf{A}_{\mathbf{\Sigma},j+1} = \mathbf{A}_{\mathbf{\Sigma},j} + \alpha_j \mathbf{p}_j$$

•
$$\mathbf{r}_{j+1} = \mathbf{r}_j - \alpha_j \mathbf{q}_j$$

• $\mathbf{z}_{j+1} = \mathbf{M}^{-1} \mathbf{r}_{j+1}$
• $\beta_j = \frac{\mathbf{r}_{j+1}^T \mathbf{z}_{j+1}}{\mathbf{r}_i^T \mathbf{z}_j}$

•
$$\mathbf{p}_{j+1} = \mathbf{z}_{j+1} + \beta_j \mathbf{p}_j$$

• $j = j + 1$

Until convergence.

- $\textbf{Preconditioner}: \textbf{M}^{-1} = \frac{1}{N_k} \sum_{k=1}^{N_k} \tilde{S}_k^{-1}$
 - If floating subdomain = subdomain with no Dirichlet boundary condition : S_k singular ⇒ Non singular approximation S̃_k
 - Otherwise $\tilde{\mathbf{S}}_k = \mathbf{S}_k$

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Computation of $\mathbf{z}_{j+1} = \mathbf{M}^{-1}\mathbf{r}_{j+1}$

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem description

Derivation o the linear system

Resolution

Schur complement matrix

Preconditioned Conjugate gradient

Results

On-going work

M⁻¹ not given explicitly

• Solving $\mathbf{z}_{k,j} = \mathbf{\tilde{S}}_k^{-1} \mathbf{r}_j$ can be done by solving

$$\mathbf{B}_{k} \begin{pmatrix} \mathbf{x}_{k} \\ \mathbf{z}_{k,j} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{r} \end{pmatrix} \text{ with } \mathbf{B}_{k} = \begin{pmatrix} \mathbf{B}_{k,k} & \mathbf{B}_{k,N_{k}+1} \\ \mathbf{B}_{k,N_{k}+1}^{T} & \mathbf{B}_{N_{k}+1,N_{k}+1}^{(k)} \end{pmatrix}$$
$$\mathbf{z}_{j} = \sum_{k=1}^{N_{k}} \mathbf{z}_{k,j}$$

Cholesky factorization :

0

$$\mathbf{B}_{k} = \mathbf{L}_{k} \mathbf{L}_{k}^{T} \text{ with } \mathbf{L}_{k} = \begin{pmatrix} \mathbf{L}_{k,k} & \mathbf{0} \\ \mathbf{L}_{k,N_{k}+1} & \mathbf{L}_{N_{k}+1,N_{k}+1}^{(k)} \end{pmatrix}$$

This factorization is used within CG to compute $\mathbf{B}_{k,k}^{-1}\mathbf{v}_{k,j}$.

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Results

Flow simulations in 3D Discrete Fracture Networks

J-R. de Dreuzy , J. Erhel , G. Pichot, B. Poirriez

Plan

Introduction

Problem descriptio

Derivation o the linear system

Resolution

Schur complement matrix

Preconditione Conjugate gradient

Results

On-going work

number of	Number of iterations and execution time		
subdomains	Without NN	With NN	
2	153 it / 10.8 s	37 it / 4.4 s	
4	164 it / 12.5 s	75 it / 9.3 s	
8	166 it / 13.7 s	96 it / 12.4 s	
16	165 it / 14.4 s	149 it / 20.2 s	

 $\ensuremath{\mathrm{TABLE}}$: Iteration number and execution time for a network with 128 fractures for a varying number of subdomains

- PCG with Neumann-Neumann is efficient with a few subdomains
- Parallel computation can improve significantly the results (in terms of memory and CPU requirements)
- When the number of subdomains is too large, global preconditioning can improve convergence.

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Plan

Introduction

Problem description

Derivation of the linear system

Resolution

On-going work

On-going work

Non conforming mesh and Mortar method

- Build a posteriori estimators to optimize mesh generation
- Perform more large scale Monte-Carlo simulations to check convergence
- Run large scale DFNs simulations to derive upscaling rules

Solving the linear system

- compare subdomain decompositions with other methods
- Apply PCG to the matrix obtained with a non conforming mesh
- Parallelize PCG with Neumann-Neumann to reduce memory requirements and improve execution time
- Use global preconditioning (Coarse Grid, Deflation, Balancing) to optimize PCG with Neumann-Neumann