Inria Project Lab C2S@Exa

Parallelizing the Traces software

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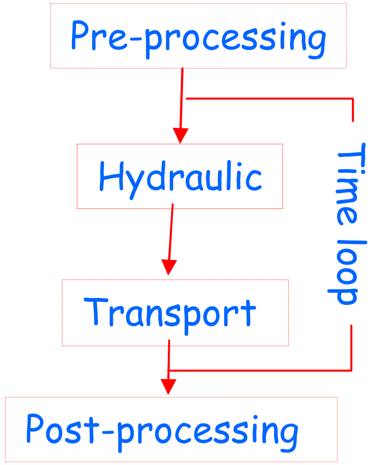
Context & Motivation

Traces: numerical simulation of radio-active waste storage in profound geological layers

Two sorts of problem can be treated:

- Hydraulic: single-phase flow in porous media
- Transport: migration of radioactive waste in porous media



Large-scale problems in both points of view: spatial and temporal

- Long-term performance and safety assessment
- Large-size domains have to be dealt with

Parallelizing the Traces software

- To make more realistic and reliable studies
- To take advantage from computing capabilities

Outline

1. Hydraulic problem
2. Mesh partitioning
3. Parallel assembling and resolving
4. Numerical results
5. Conclusion

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Hydraulic: Mathematical Model

$$\begin{cases} s\dfrac{\partial u}{\partial t} = -div(q) - s\lambda u + f & \text{Mass balance equation} \\ q = D.\nabla u & \text{Darcy's law} \end{cases}$$

Unknowns

u hydraulic charge

q filtration velocity

Parameters

D hydraulic conductivity

s storage coefficient

f source/sink term

λ a kinetic term

- Temporal discretization: implicit
- Spatial discretization: Mixed Hybrid Finite Element Method

→ Algebraic linear system whose unknowns are associated to the mesh faces

→ Parallel assembling and resolving of the resulting linear algebraic system is the most challenging part of the hydraulic problem

Parallelization strategy

Parallelization for coarse grain MIMD architectures with distributed memory

- Mesh partitioning
- Message passing programming trough MPI standard

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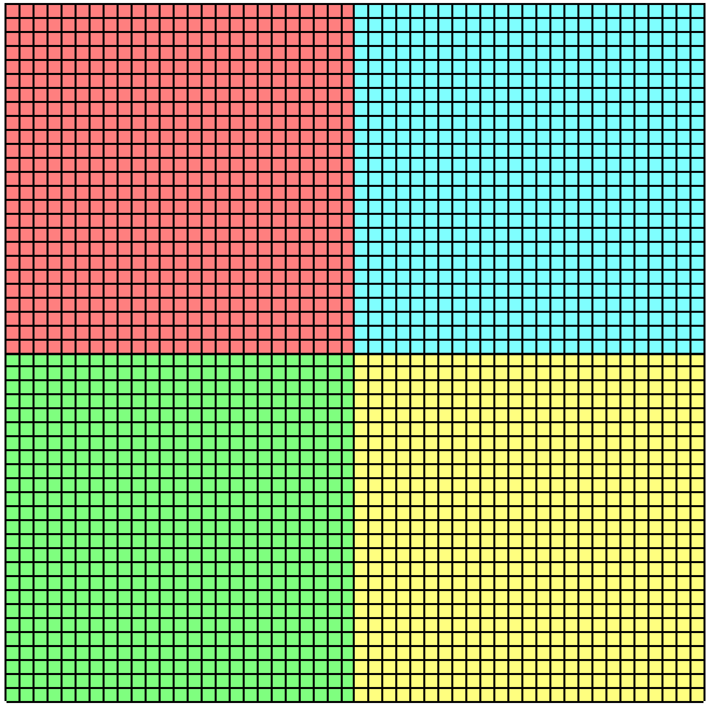
Unstructured mesh partitioning

Static, non-overlapping and homogeneous partitioning

Partitioning software: Metis, Scotch

Mapping of the mesh elements: divide mesh elements into groups of elements



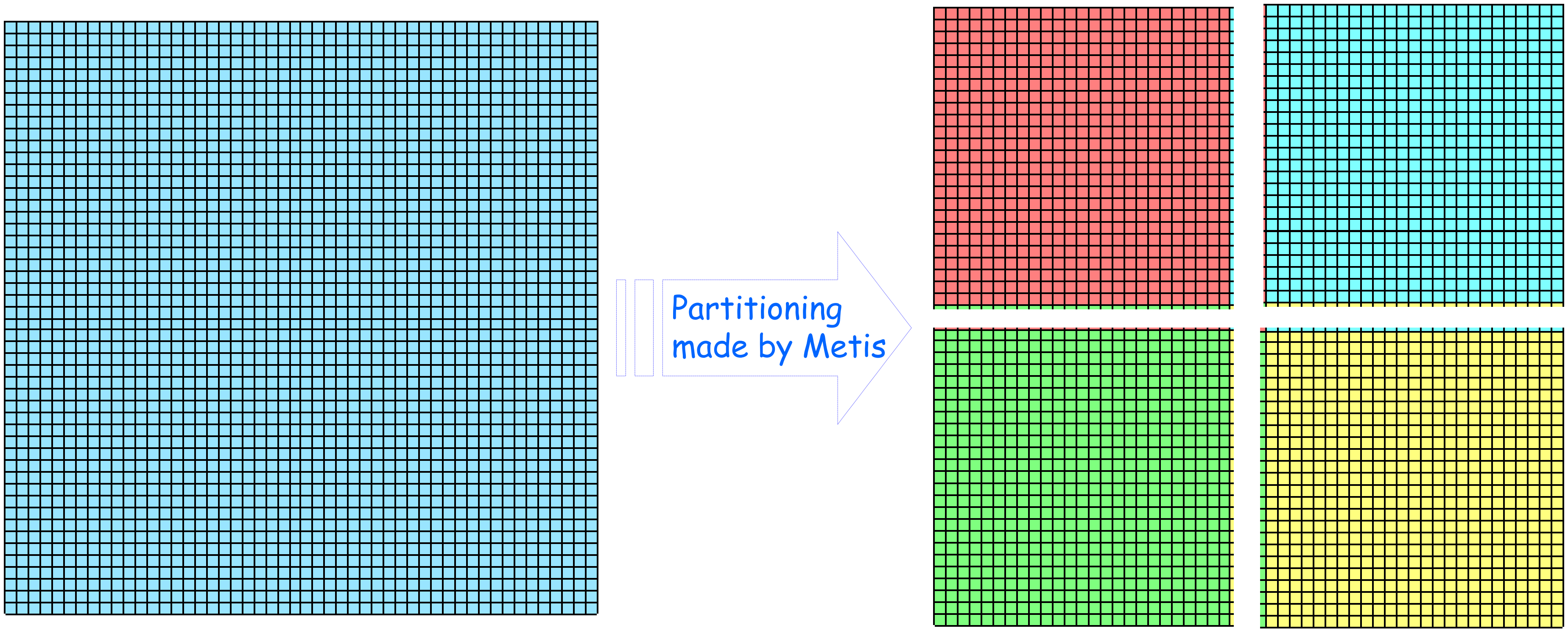
- Partitioning of mesh nodes
- Partitioning of mesh faces (edges in 2D)
- Neighboring relations between processors

→ New input file

→ Distributed data

Mesh partitioning

Non-overlapping homogeneous mesh partitioning



Communication lists

Communication list: list of the local numbers of the common faces in each couple of neighbors

[neighbor1, neighbor2] → [(neighbor1,list1) , (neighbor2,list2)]

Matched lists

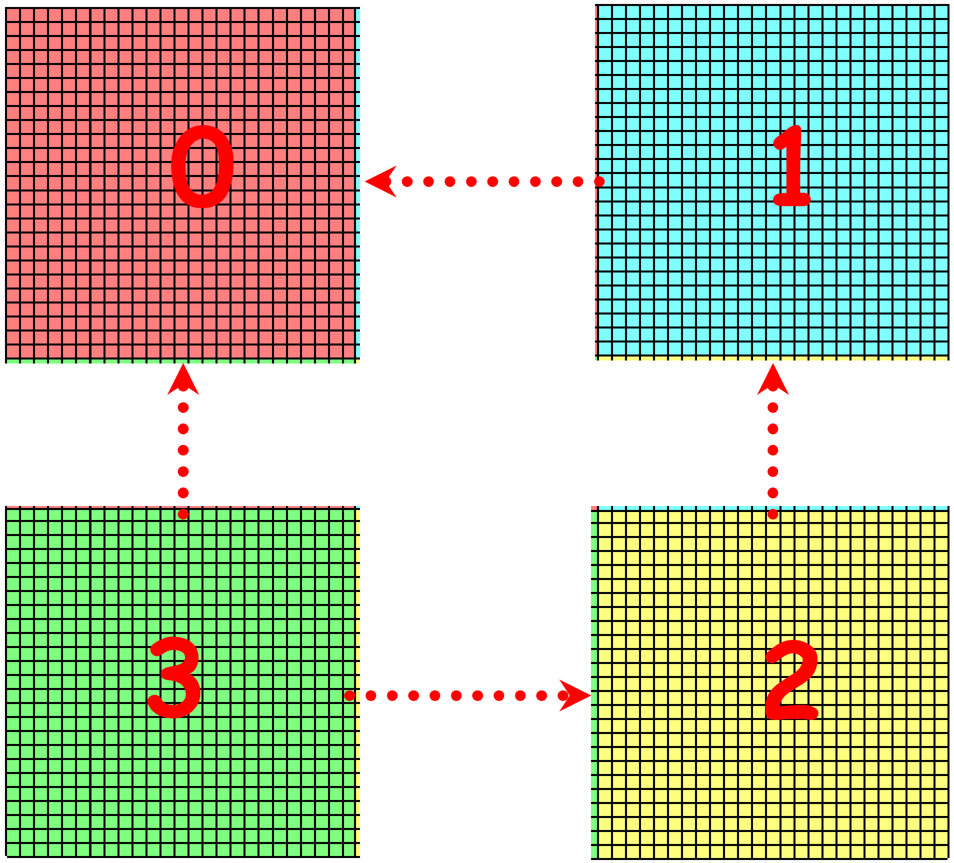
❖ Each processor builds communication lists with its neighbors

❖ Matching up: the order in the lists is imposed by the highly ranked processor of each couple of neighbors

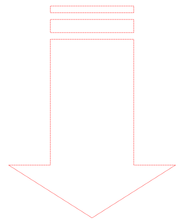
❖ Communication cost: each processor sends the common lists to its neighbors that have a lower rank than him.

Communication lists

Communication cost: each processor sends the common lists to its neighbors that have a lower rank than him



4 couple of neighbors



4 messages transferred

Transferring only 4 messages of integers to build matched communication lists

→ There are as many messages as the number of couples of neighbors

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The Hypre librairy

What is Hypre?

Software library of high performance preconditioners and solvers for the solution of **large, sparse linear systems** on massively parallel computers

Krylov space solvers

- Symmetric system: Conjugate Gradient
- Asymmetric system: GMRES, Bi-Conjugate Gradient stabilized …

Preconditioners

Algebraic Multigrid, ILU(k), Block Jacobi ILU(k), Diagonal …

How to use Hypre

Linear-Algebraic System interface (IJ)

Hypre-Traces interfacing

Distributed data form

Matrices are assumed to be distributed across the processors by contiguous blocks of rows

$$A = \begin{pmatrix} A_0 \\ A_1 \\ . \\ . \\ A_{p-1} \end{pmatrix}$$

Hypre defines a new numbering of the DOF

The DOF 1 to n_0 reside in processor 0

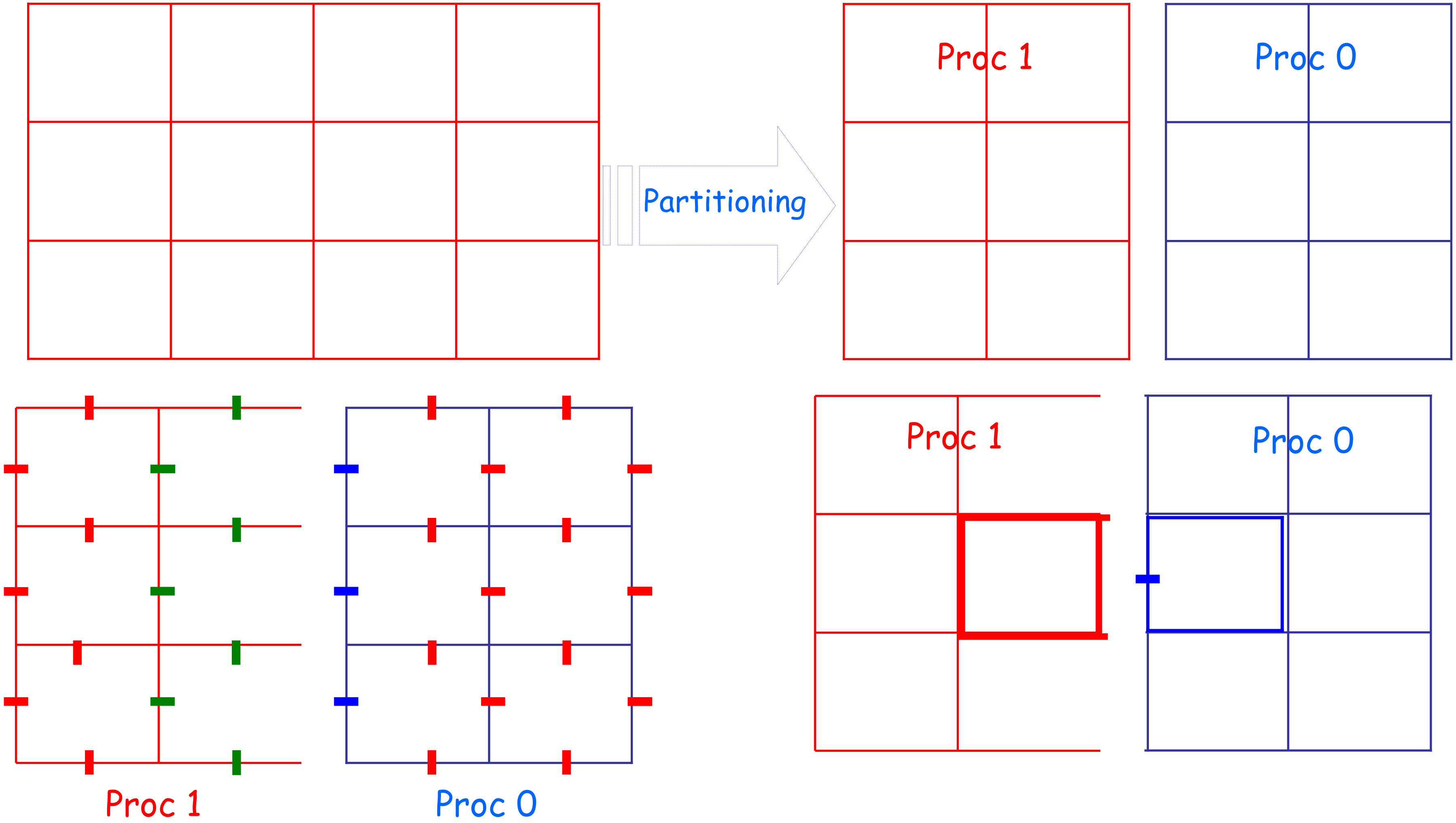
The DOF n_0+1 to n_1 reside in processor 1

The DOF $n_{k-1}+1$ to n_k reside in processor k

Main points

- Hypre defines its own numbering of the DOF
- Hypre requires a mapping of the DOF on the processors
- Processors define actual blocks of the system for Hypre independently

Matrix parallel assembling



For each DOF in common

- From processor 1 to processor 0: 4 Coefficients + 4 indices

→ Two messages are transferred

Matrix parallel assembling

Each processor computes its own FE matrix then transmits it for Hypre

$$\begin{pmatrix} \\ \beta_1 \;.\; \beta_2 \;.\; \beta_3 \;.\;.\; \beta \\ \\ \end{pmatrix}$$

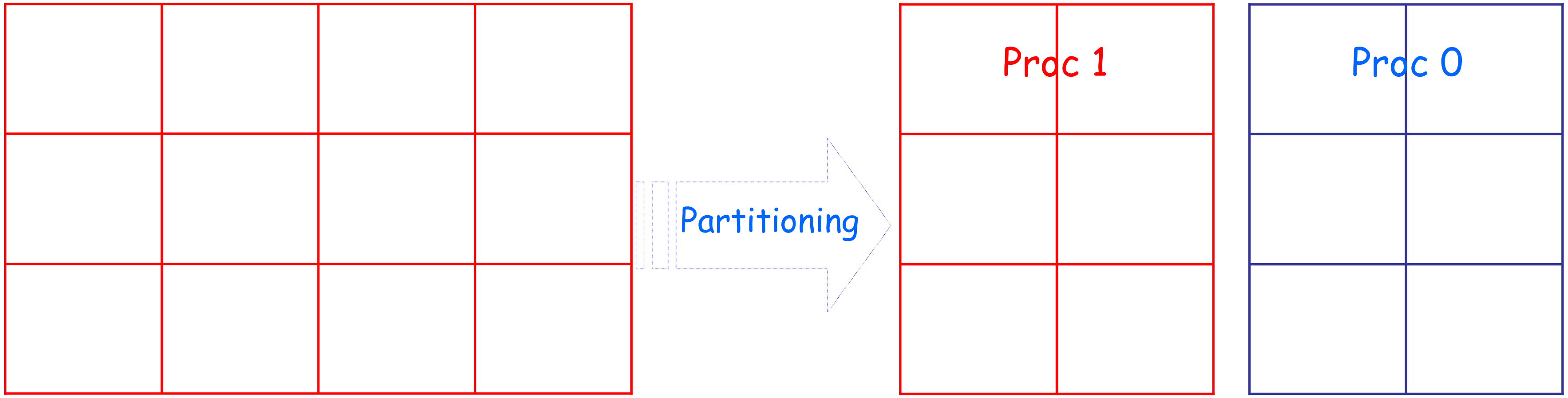
DOF
in common

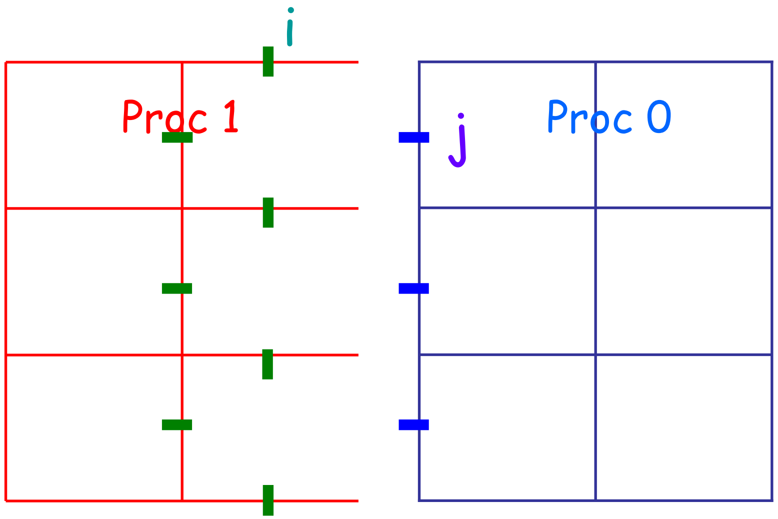
$$\begin{pmatrix} \\ \alpha_1 \;.\; \alpha_2 \;.\; \alpha_3 \;.\;.\; \alpha \\ \\ \end{pmatrix}$$

$$\begin{pmatrix} \\ \beta_1 \;.\; \beta_2 \;.\; \beta_3 \;.\;.\; \beta \\ \\ \end{pmatrix}$$

$$\begin{pmatrix} \\ \alpha_1 \;.\; \alpha_2 \;.\; \alpha_3 \;.\;.\; \alpha+\beta \;.\;.\; \beta_1 \;.\; \beta_2 \;.\; \beta_3 \\ \\ \end{pmatrix}$$

Matrix parallel assembling





Processor 1 needs the column number j from the processor 0 to put correctly the coefficient a_{ij} in the Hypre matrix

Processor 0 sends the Hypre numbering of the DOF in common to processor 1

→ One message of integers from processor 0 to processor 1

Hypre: solving

Parallel assembling and transmitting the RHS to Hypre

Define an initial guess of the solution …

Choice a solver and its parameters, preconditioner…

Get the solution from Hypre and adapt it to the Traces numbering

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Performance: PCG/DS

Mesh: hexahedral, 1 685 600 elements, 5 114 900 faces

Solver: Preconditioned Conjugate gradient PCG, Convergence tolerance 1e-10

PCG / DS			
Number of processors	CPU Time(s) Solve+Setup	Speed-up	Number of iterations
1	4322		8305
2	2143	2,02	8305
4	1066	4,05	8305
8	539	8,02	8305
16	272	15,88	8305
20	218	19,85	8305

Validation of parallel interfacing of Traces-Hypre

Setup

- ❖ Parallel passing of the linear system to Hypre
- ❖ Hypre's setup

Performance: PCG/ILU(1)

Mesh: hexahedral, 1 685 600 elements, 5 114 900 faces

Solver: Preconditioned Conjugate gradient PCG, Convergence tolerance 1e-10

PCG/ILU(1)			
Number of processors	CPU Time(s) Solve+Setup	Speed-up	Number of iterations
1	2510		1668
2	1213	2,07	1677
4	622	4,03	1677
8	321	7,82	1682
16	190	13,2	1688
20	149	16,8	1689

Performance: PCG/AMG

Mesh: hexahedral, 1 685 600 elements, 5 114 900 faces

Solver: Preconditioned Conjugate gradient PCG, Convergence tolerance 1e-10

PCG / AMG			
Number of processors	CPU Time(s) Solve+Setup	Speed-up	Number of iterations
1	235		2
2	130	1,81	2
4	69,6	3,38	2
8	38,2	6,16	2
16	25,5	9,22	2
20	22,7	10,37	2

Performance: comparison

Mesh: hexahedral, 1 685 600 elements, 5 114 900 faces

Solver: Preconditioned Conjugate gradient PCG, Convergence tolerance 1e-10

	PCG / DS		PCG / ILU(1)		PCG / AMG	
Number of processors	CPU Time(s) Solve+Setup	Speed-up	CPU Time(s) Solve+Setup	Speed-up	CPU Time(s) Solve+Setup	Speed-up
1	4322		2510		235	
2	2143	2,02	1213	2,07	130	1,81
4	1066	4,05	622	4,03	70	3,38
8	539	8,02	321	7,82	38	6,16
16	272	15,88	190	13,19	26	9,22
20	218	19,85	149	16,83	23	10,37

PCG/AMG is less scalable than PCG/DS and PCG/ILU(1)

However

It is more efficient in bringing down the CPU Time Than the others

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Conclusion

- Hydraulic problem has been parallelized using MPI and Hypre librairies

- Scotch and Metis were used to perform mesh partitioning

- Distributed data form

- Other Parallel solvers of linear systems can be easily interfaced with Traces software