A User Friendly Toolbox for Parallel PDE-Solvers

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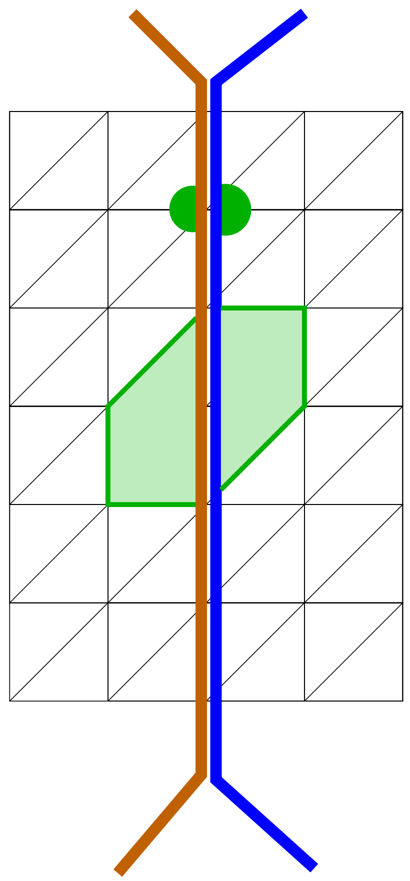
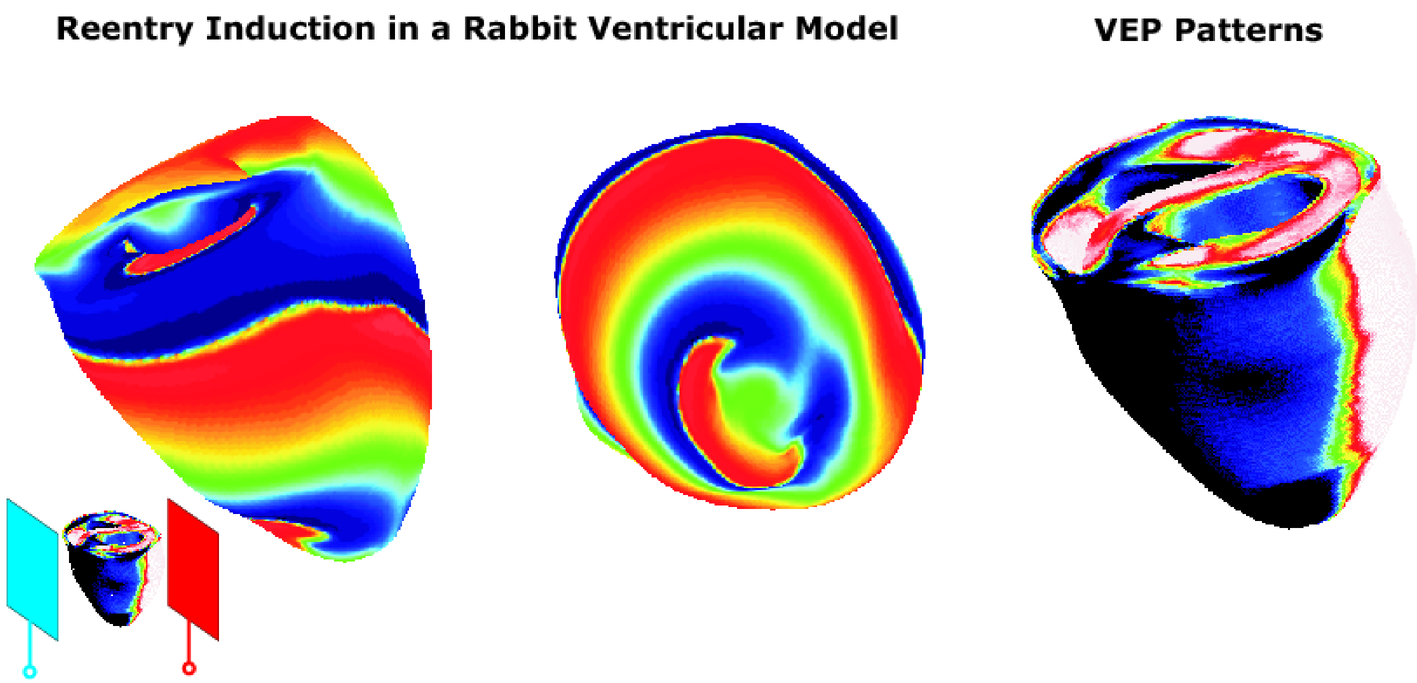
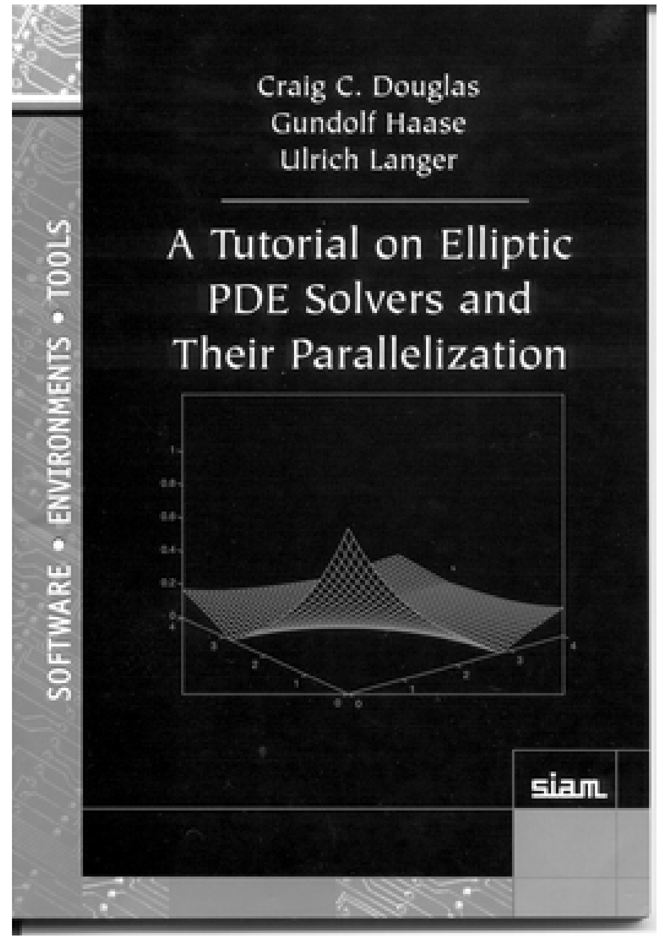




Contents

Motivation



- We have developed parallel codes for 15 years, incl. Multigrid, Multilevel, AMG, Krylov methods, ...
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- Approx. 25 licences for the parallel code PEBBLES.
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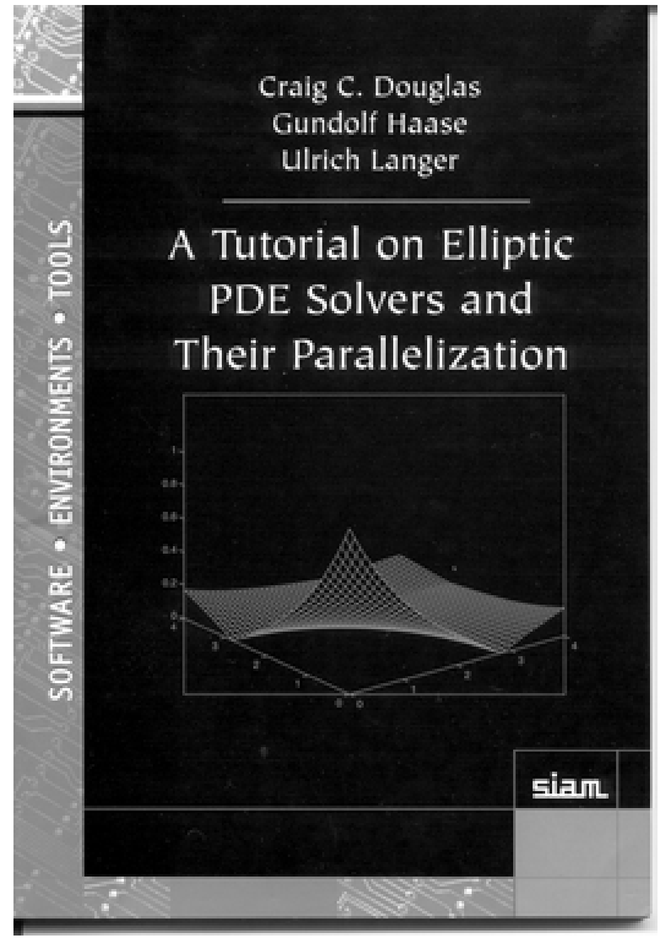

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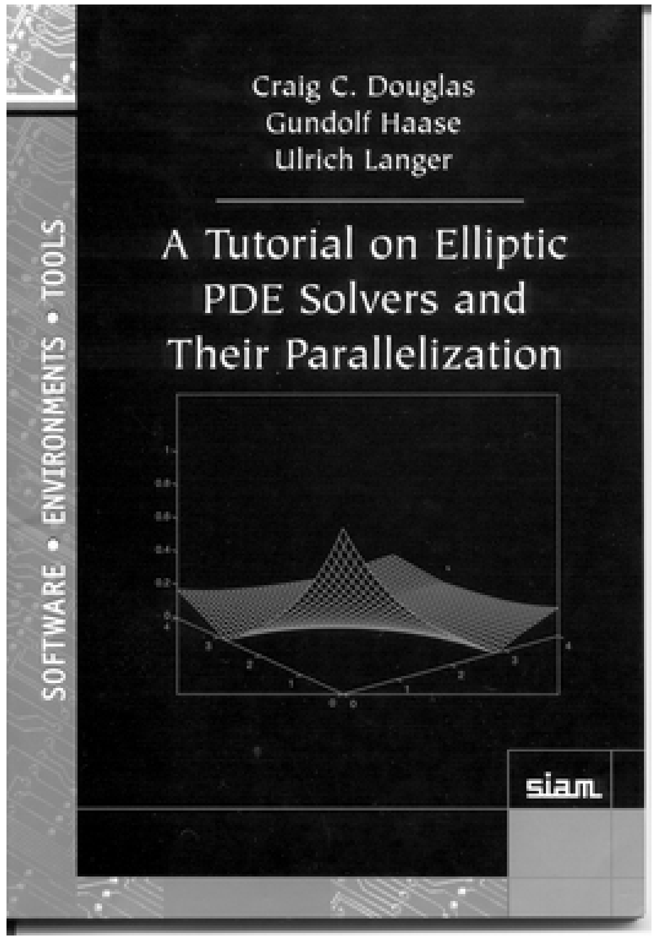

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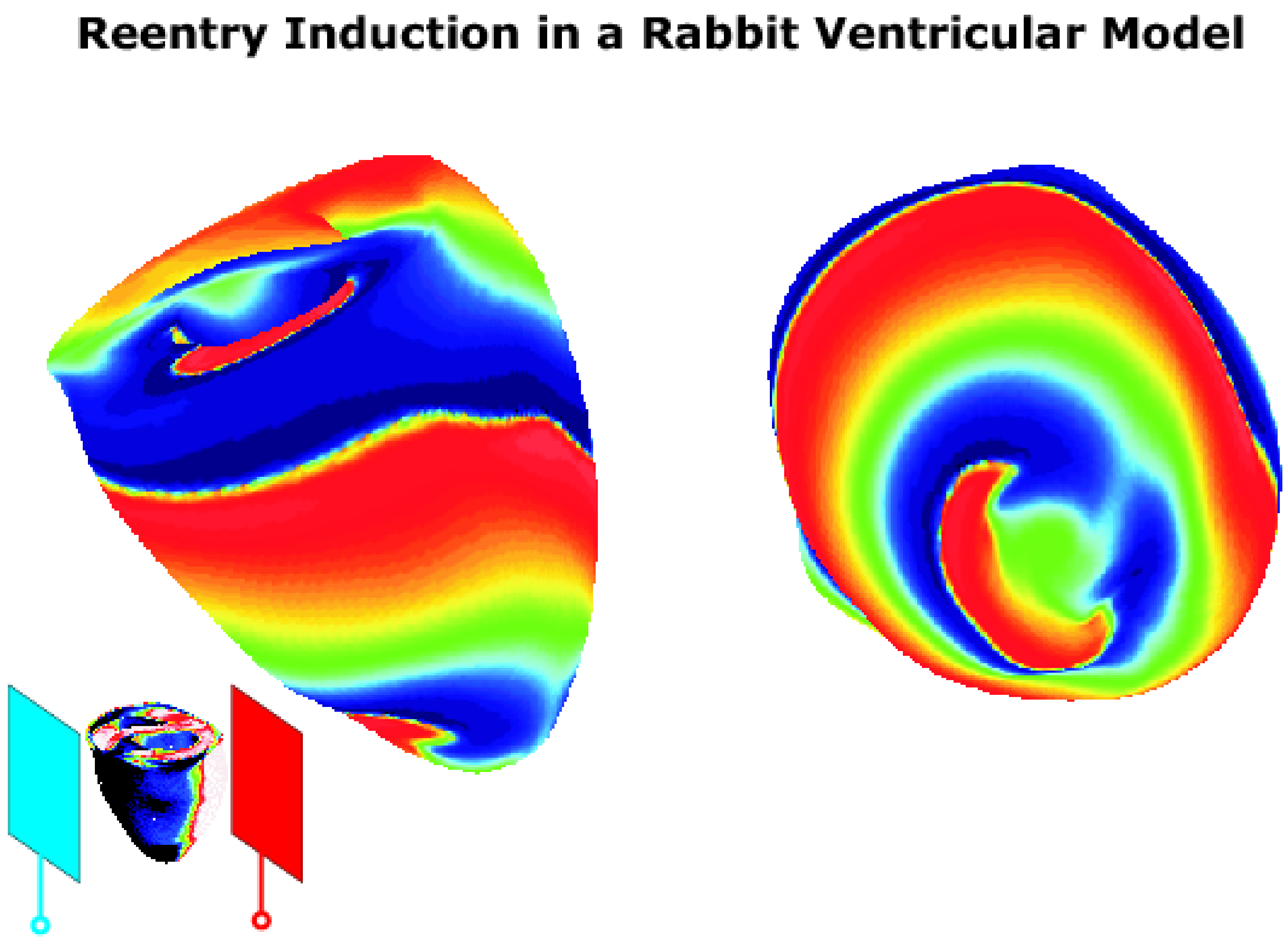
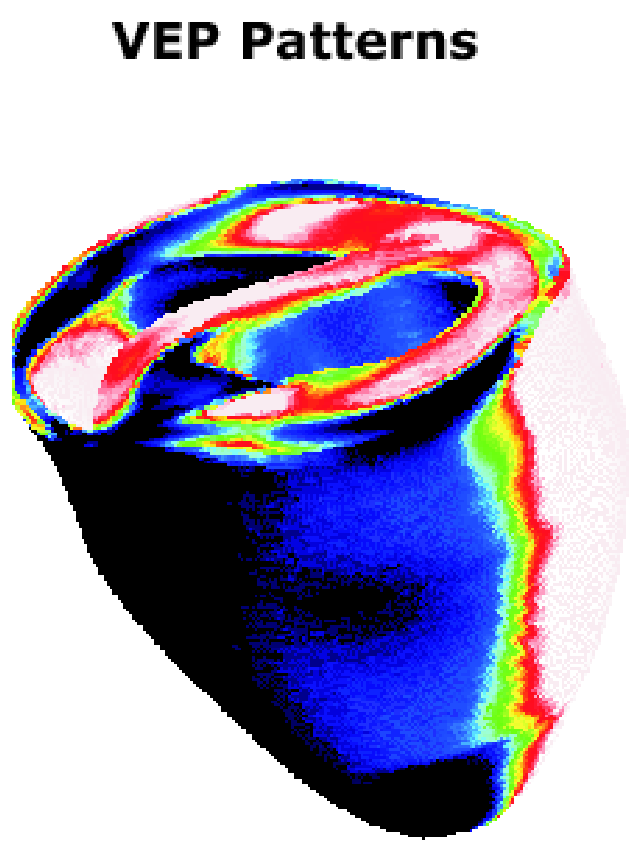
$\Longrightarrow$ Let's have a look at an example.

Rabbit Heart [G. Planck, M. Liebmann, G. Haase]





- time-dependent electrical potential, anisotropic coefficients
- 5.082.272 tetrahedrons with 862.525 FEM-nodes
- Goal: 150 Mill. tetrahedrons using parallel mesh generator Spider by F. Kickinger

PEBBLES as AMG–preconditioner in the heart problem ($\varepsilon = 10^6$)

- sequentially, 111.589 nodes, Pentium4 3GHz :

solver	solution [sec.]	Iterations
ILU/CG	12.0	211
Hypre	1.9	5
SuperLU	1.2	(but 70 sec. in setup)
PEBBLES/CG	0.8	10

- parallel, 862.515 nodes, Opteron nodes, PEBBLES:

processors	1	2	4	8
solver iterations	13	12	12	14
coarse grid	3059	4008	4850	3070
solver in sec.	10.3	9.0	5.0	3.2
	[0.3]	[0.6]	[0.7]	[0.4]
setup in sec.	37.1	22.4	17.9	11.3
	[3.7]	[7.0]	[9.7]	[5.4]

- Some obscurities wrt. *re*construction of PEBBLES.
- Our parallel data structures didn't fit into global code.
- Conclusion: It's worth to continue the development of the code. But we have to re–write the code.

Motivation for a new code

- PETSc [B. Smith] is used by cooperation partners but we need more/other information for an efficient parallel AMG.

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- The professional code cannot be used in education (too much overhead from data setup)
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$\Rightarrow$ Redesign of interfaces, data structures and funtionality.

Goal: Toolbox provides all needed **basic** routines for **parallel** funtionality.

Goal: Write your own parallel code by **re-using sequential** code.

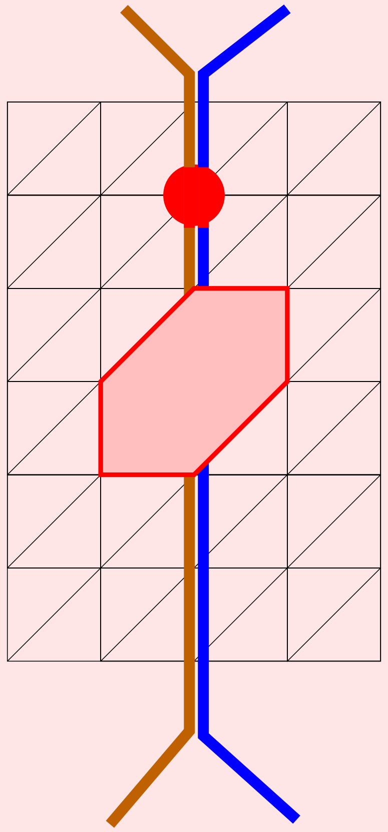
Menu

Parallel Algebra

- Concept for Parallelization
- Extended Parallelization Concept
- Parallel Multigrid
- Parallel factorization
- Parallelization of Algebraic Multigrid
- Contents

Non-overlapping Data Decomposition

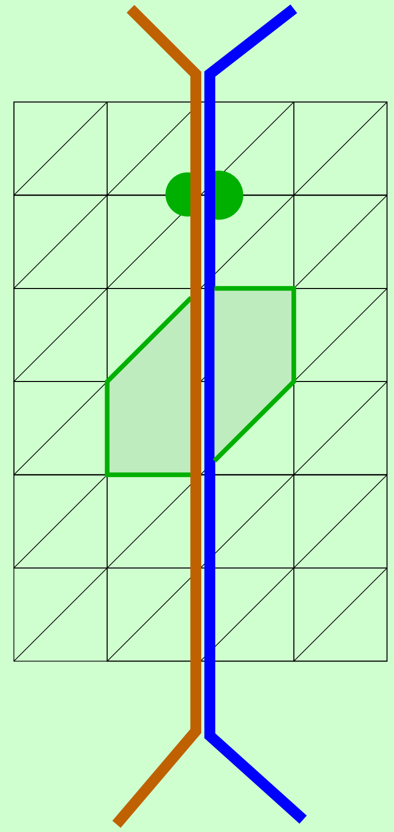
accumulated



$$\underline{\mathfrak{u}}_s = A_s \underline{\mathfrak{u}}$$

$$\mathfrak{M}_s = A_s \mathfrak{M} A_s^T$$

distributed



$$\underline{\mathsf{r}} = \sum_{s=1}^{P} A_s^T \underline{\mathsf{r}}_s$$

$$\mathsf{K} = \sum_{s=1}^{P} A_s^T \mathsf{K}_s^{\mathsf{FEM}} A_s$$

Overlapping Domain Decomposition

accumulated

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BUT, how to choose K_s ?

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BUT, how to choose K_s ?

$$\mathsf{K}_s := \sum_{\delta^{(r)} \subseteq \Omega_s} \frac{1}{W^{(r)}} \cdot K^{\mathsf{FEM},r}$$

$W^{(r)} := \# \, \Omega_s$ an element $\delta^{(r)}$ associated with..

Basic Operations

<u>without communication</u>

$$\underline{\mathsf{v}} \leftarrow \mathsf{K} \cdot \underline{\mathfrak{s}}$$

$$\underline{\mathsf{r}} \leftarrow \underline{\mathsf{f}} + \alpha \cdot \underline{\mathsf{v}}$$

$$\underline{\mathfrak{w}} \leftarrow \underline{\mathfrak{u}} + \alpha \cdot \underline{\mathfrak{s}}$$

$$\underline{\mathsf{r}} \leftarrow R^{-1} \cdot \underline{\mathfrak{w}}$$

<u>global reduce</u>

$$\alpha \Leftarrow \langle \mathfrak{w}, \mathsf{r} \rangle = \sum_{s=1}^{P} \langle \mathfrak{w}_s, \mathsf{r}_s \rangle$$

<u>next neighbor comm.</u>

$$\underline{\mathfrak{w}} \leftarrow \underline{\mathsf{r}} = \sum_{s=1}^{P} A_s^T \underline{\mathsf{r}}_s$$

with $R = \text{diag}\{R_{ii}\}_{i=1}^{N} = \text{diag}\{\#\text{ subdomains } x_i \text{ is associated with}\} = \sum_{s=1}^{P} A_s^T \cdot A_s$

and $\mathsf{R}^{-1} = \sum_{s=1}^{P} A_s^T \cdot \mathbf{I}_s \cdot A_s$ (partition of unity)

Parallel CG : PCG(K, $\underline{\mathfrak{u}}$, $\underline{\mathsf{f}}$)

repeat

$$
\begin{aligned}
\underline{\mathsf{v}} &\leftarrow \mathsf{K} \cdot \underline{\mathfrak{s}} \\
\alpha &\Leftarrow \sigma / \langle \underline{\mathfrak{s}}, \underline{\mathsf{v}} \rangle \\
\underline{\mathfrak{u}} &\leftarrow \underline{\mathfrak{u}} + \alpha \underline{\mathfrak{s}} \\
\underline{\mathsf{r}} &\leftarrow \underline{\mathsf{r}} - \alpha \underline{\mathsf{v}} \\
\underline{\mathfrak{w}} &\Leftarrow C^{-1} \cdot \underline{\mathsf{r}} \\
\sigma &\Leftarrow \langle \underline{\mathfrak{w}}, \underline{\mathsf{r}} \rangle \\
\beta &\leftarrow \sigma / \sigma_{\text{old}} \quad , \quad \sigma_{\text{old}} \leftarrow \sigma \\
\underline{\mathfrak{s}} &\leftarrow \underline{\mathfrak{w}} + \beta \underline{\mathfrak{s}}
\end{aligned}
$$

until termination

Menü

Basic Operations (revisited)

without communication

$$\underline{\mathsf{v}} \leftarrow \mathsf{K} \cdot \underline{\mathfrak{s}}$$

$$\underline{\mathsf{r}} \leftarrow \underline{\mathsf{f}} + \alpha \cdot \underline{\mathsf{v}}$$

$$\underline{\mathfrak{w}} \leftarrow \underline{\mathfrak{u}} + \alpha \cdot \underline{\mathfrak{s}}$$

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global reduce

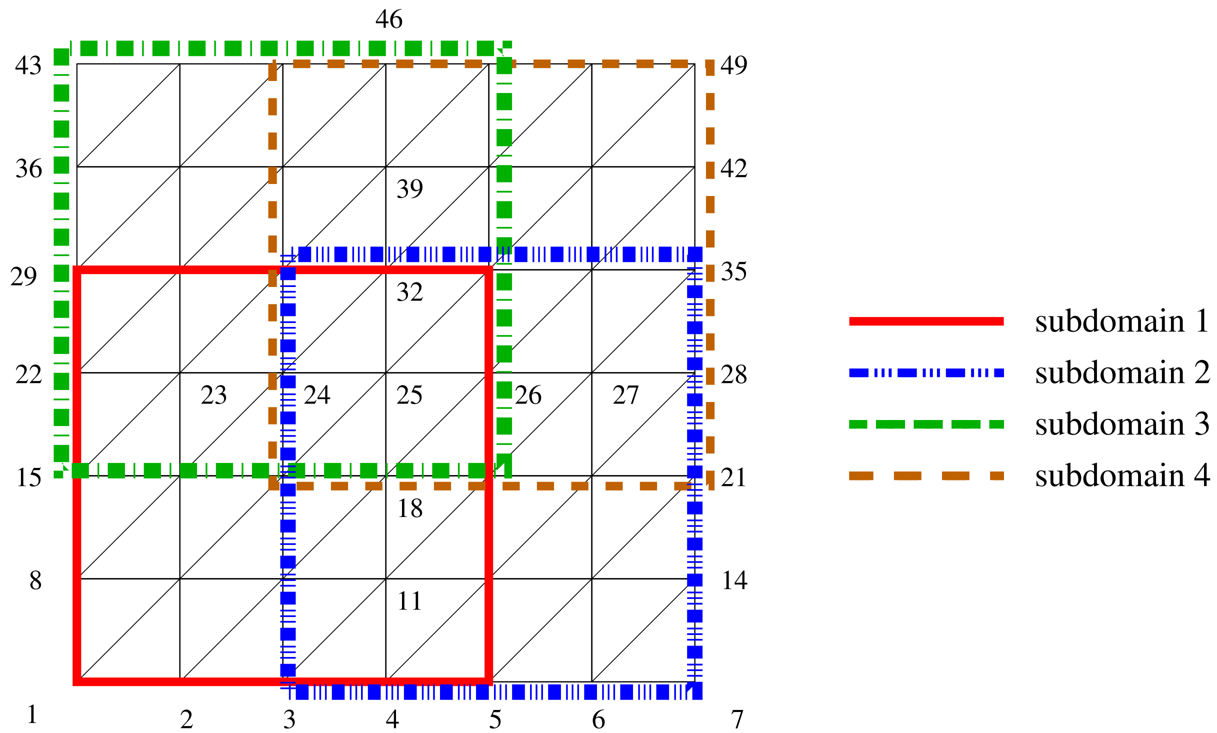
$$\alpha \Leftarrow \langle \mathfrak{w}, \mathsf{r} \rangle = \sum_{s=1}^{P} \langle \mathfrak{w}_s, \mathsf{r}_s \rangle$$

next neighbor comm.

$$\underline{\mathfrak{w}} \leftarrow \underline{\mathsf{r}} = \sum_{s=1}^{P} A_s^T \underline{\mathsf{r}}_s$$

What can be done with $\mathfrak{M} \cdot \underline{v}$?

Some Definitions



Set of subdomains :

$$\sigma^{[i]} = \{ s : x^{[i]} \in \overline{\Omega}_s \}$$

Set of indices/nodes :

$$\omega(\sigma) := \{ i \in \omega : \sigma^{[i]} = \sigma \}$$

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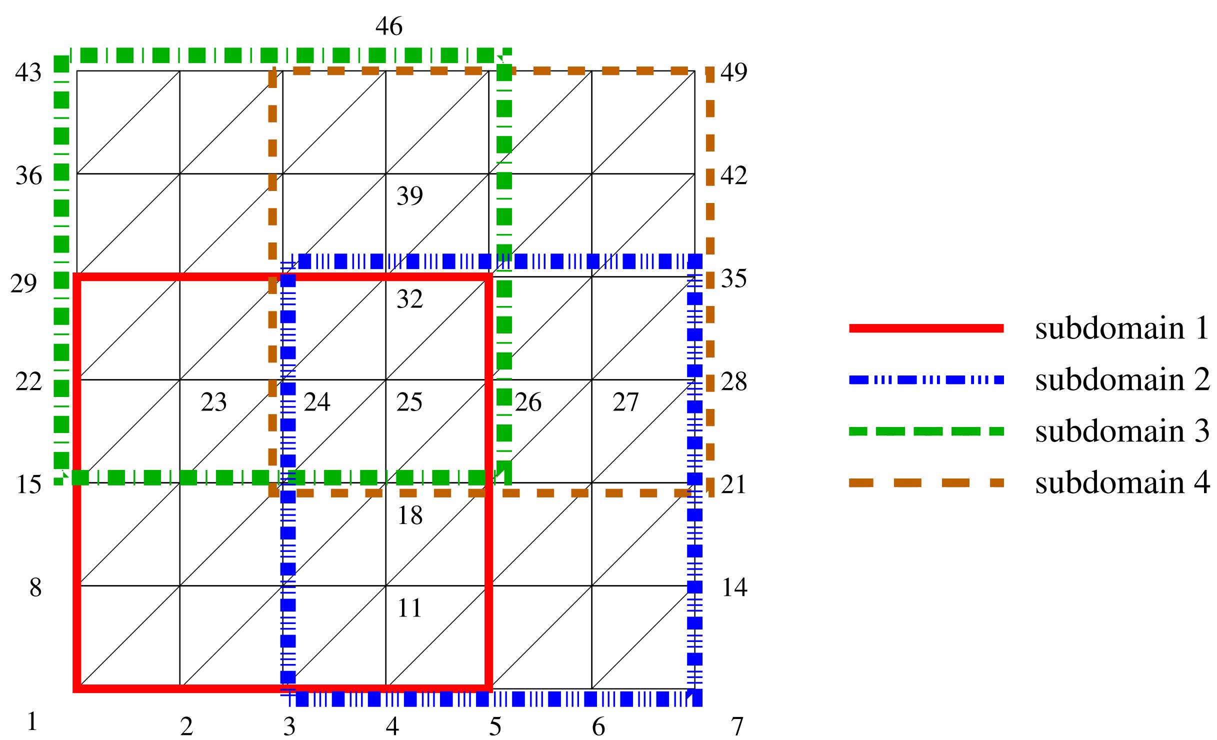

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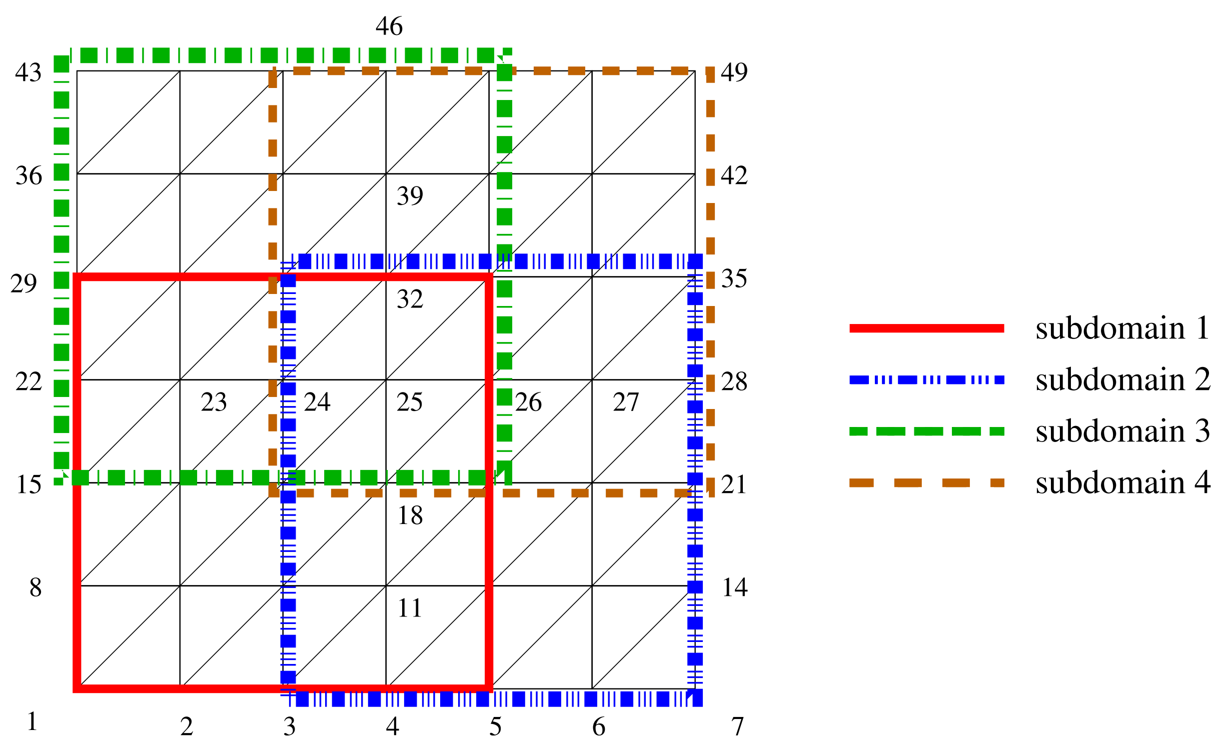

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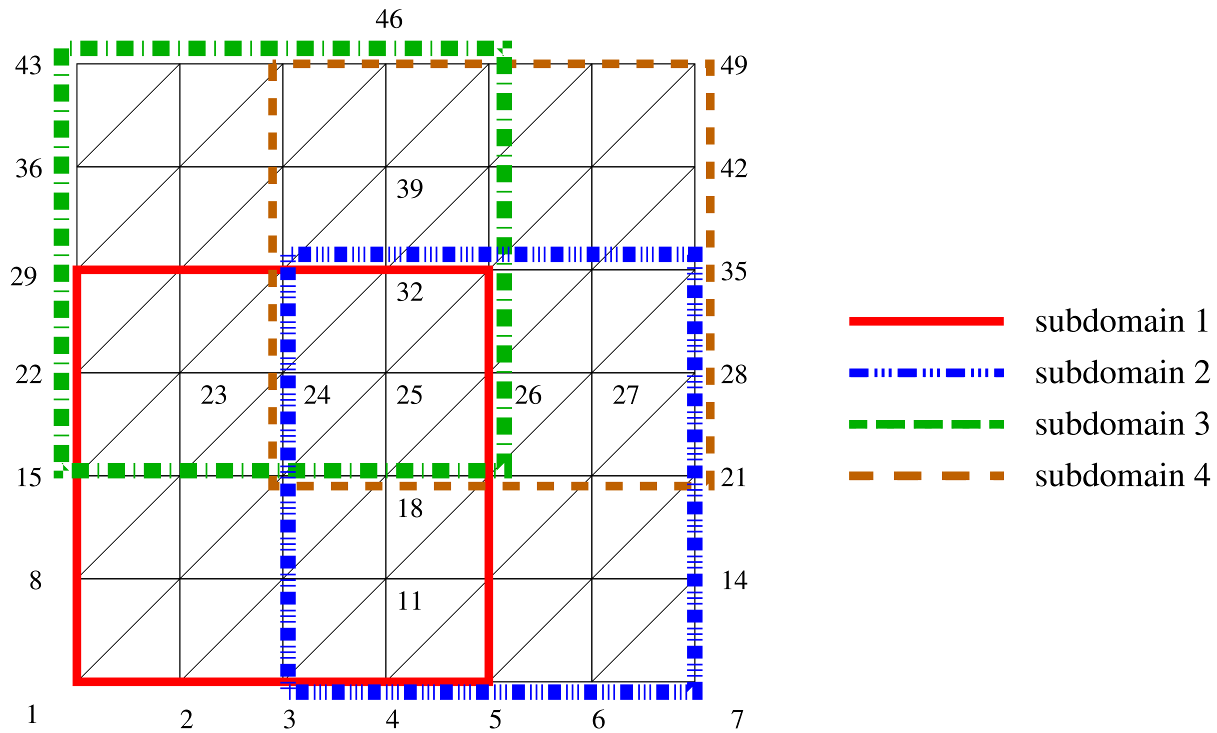

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$\sigma^{[14]} = \{2\}$ $\quad \omega(\{2\}) = \{6, 7, 13, 14\}$

Matrix Patterns and their Application

The following operations can be performed in parallel without any communication:

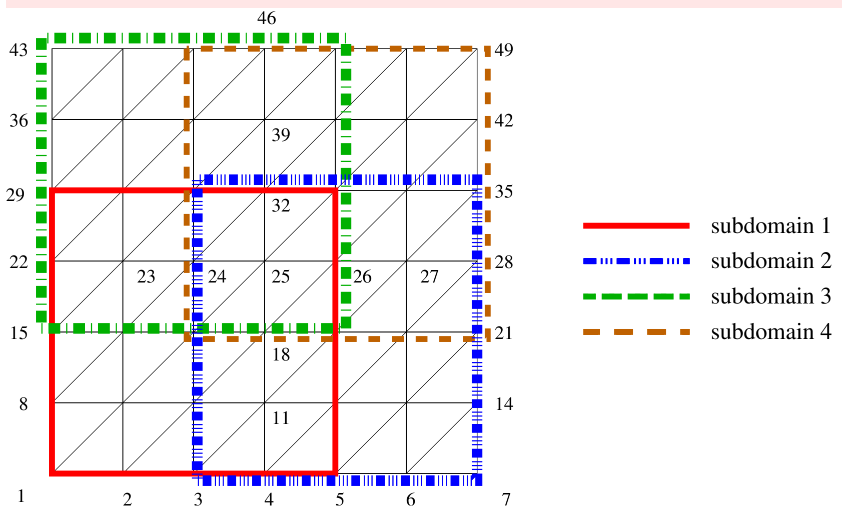
$$\underline{\mathsf{f}} = \mathsf{K} \cdot \underline{\mathfrak{u}}$$

Matrix $\mathfrak{M}$ fulfills the pattern condition: $\forall i,j \in \omega : \quad \sigma^{[i]} \not\subseteq \sigma^{[j]} \implies \mathfrak{M}^{[i,j]} = 0 \qquad i \not\longleftarrow j$

$$\underline{\mathfrak{u}} = \mathfrak{M} \cdot \underline{\mathfrak{w}}$$
$$\underline{\mathsf{f}} = \mathfrak{M}^T \cdot \underline{\mathsf{r}}$$

$$\boxed{\mathsf{K}^H = \mathfrak{M}^T \cdot \mathsf{K} \cdot \mathfrak{M}}$$

Theorems/Proofs **[Haase]**



Ex.:

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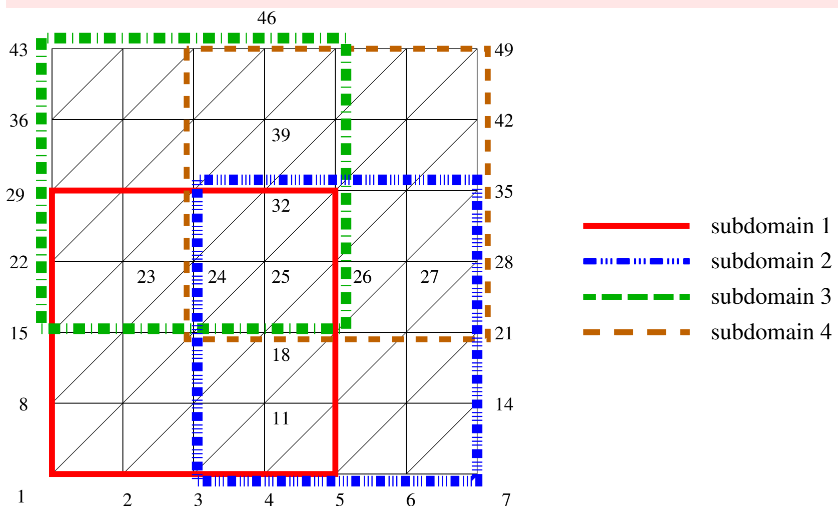

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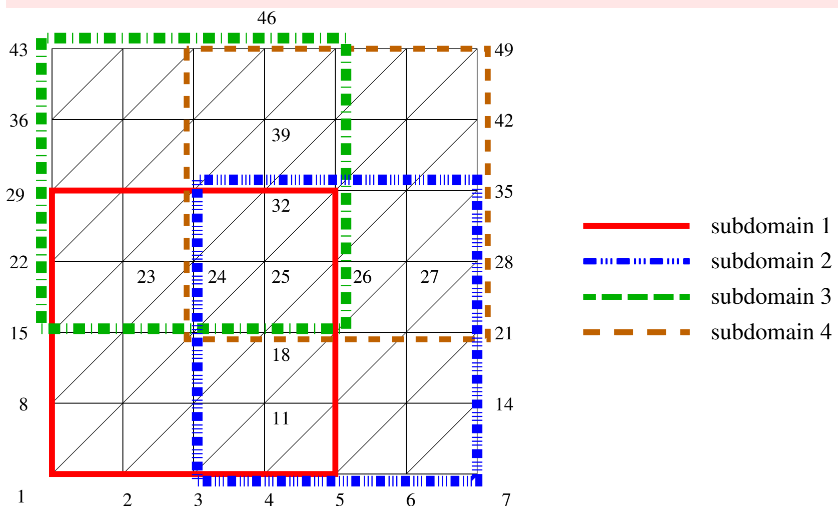

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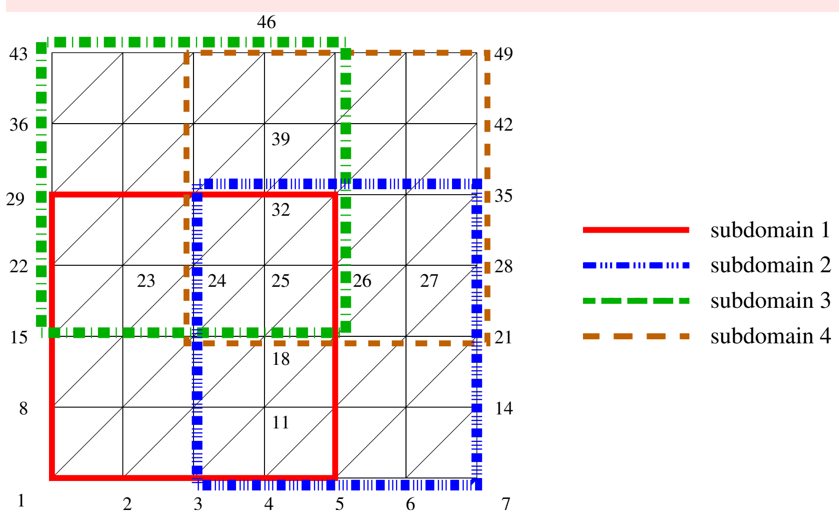

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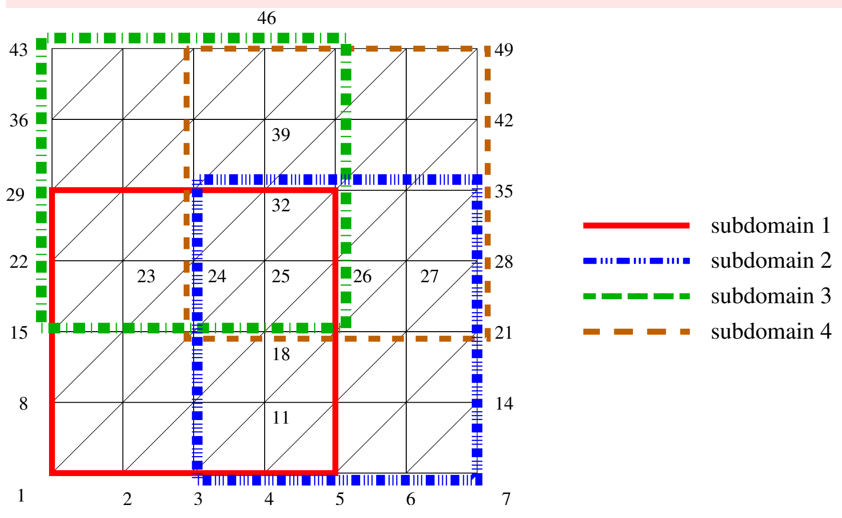

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$$\boldsymbol{\sigma}^{[27]} \not\subseteq \boldsymbol{\sigma}^{[14]} \Longrightarrow \mathfrak{M}^{[27,14]} = \mathbf{0} \qquad \mathbf{21} \not\longleftarrow \mathbf{14}$$

Admissible Matrix Operations

Vertex, **E**dge, **I**nner nodes

$$\mathfrak{M} = \begin{pmatrix} \mathfrak{M}_V & 0 & 0 \\ \mathfrak{M}_{EV} & \mathfrak{M}_E & 0 \\ \mathfrak{M}_{IV} & \mathfrak{M}_{IE} & \mathfrak{M}_I \end{pmatrix} = \mathfrak{M}_L + \mathfrak{M}_D \quad \Longrightarrow \quad \underline{\mathfrak{u}} = \mathfrak{M} \cdot \underline{\mathfrak{w}}$$

Pattern condition $\boldsymbol{\sigma}^{[i]} \not\subseteq \boldsymbol{\sigma}^{[j]} \implies \mathfrak{M}^{[i,j]} = \mathbf{0}$ has to be fulfilled in all submatrices!!

Allows operations as (Parallel ADI **[DouHaa]**)

$$\underline{\mathfrak{w}} = \mathfrak{M} \cdot \underline{\mathfrak{u}} := (\mathfrak{M}_L + \mathfrak{M}_D) \cdot \underline{\mathfrak{u}} + \sum_{s=1}^{P} A_s^T \mathfrak{M}_{U,s} R_s^{-1} \cdot \underline{\mathfrak{u}}_s$$

or, for $\mathfrak{M} = \mathfrak{L}^{-1} \cdot \mathfrak{U}^{-1}$ (**[Haase]**)

$$\underline{\mathfrak{w}} = \mathfrak{L}^{-1} \mathfrak{U}^{-1} \cdot \underline{\mathsf{r}} := \mathfrak{L}^{-1} \sum_{s=1}^{P} A_s^T \mathfrak{U}_s^{-1} \cdot \underline{\mathsf{r}}_s$$

Menü

Parallel Iteration Schemes to Solve $\mathsf{K} \cdot \underline{\mathfrak{u}} = \underline{\mathsf{f}}$

- Richardson iteration:

$$\underline{\mathfrak{u}}_s^{k+1} \;:=\; \underline{\mathfrak{u}}_s^{k} + \tau \sum_{q=1}^{P} \left(\underline{\mathsf{f}} - \mathsf{K} \cdot \underline{\mathfrak{u}}^{k}\right)_q$$

- Jacobi iteration with $\mathfrak{D} = \sum\limits_{s=1}^{P} \operatorname{diag}\{\boldsymbol{K_s}\}$:

$$\underline{\mathfrak{u}}_s^{k+1} \;:=\; \underline{\mathfrak{u}}_s^{k} + \omega \mathfrak{D}_s^{-1} \sum_{q=1}^{P} \left(\underline{\mathsf{f}} - \mathsf{K} \cdot \underline{\mathfrak{u}}^{k}\right)_q$$

- Incomplete factorization $\mathfrak{K} = \mathfrak{U} \cdot \mathfrak{L} + \mathfrak{R}$:

$$\underline{\mathfrak{u}}_s^{k+1} \;:=\; \underline{\mathfrak{u}}_s^{k} + \mathfrak{L}_s^{-1} \sum_{q=1}^{P} \mathfrak{U}_q^{-1} \left(\underline{\mathsf{f}} - \mathsf{K} \cdot \underline{\mathfrak{u}}^{k}\right)_q$$

Parallel Multigrid : PMG($\mathsf{K}, \underline{\mathfrak{u}}, \underline{\mathsf{f}}, \ell$)

if $\ell == 1$ **then**

LSSolve $\sum\limits_{s=1}^{P} \boldsymbol{A}_s^T \mathsf{K} \boldsymbol{A}_s \cdot \underline{\mathfrak{u}} \;=\; \underline{\mathsf{f}}$

else

$\underline{\widetilde{\mathfrak{u}}} \leftarrow$ SMOOTH($\mathsf{K}, \underline{\mathfrak{u}}, \underline{\mathsf{f}}, \boldsymbol{\nu}$)

$\underline{\mathsf{d}} \leftarrow \underline{\mathsf{f}} - \mathsf{K} \cdot \underline{\mathfrak{u}}$

$\boxed{\underline{\mathsf{d}}^{\boldsymbol{H}} \leftarrow \mathfrak{P}^{\boldsymbol{T}} \cdot \underline{\mathsf{d}}}$

$\underline{\mathfrak{w}}^{\boldsymbol{H}} \leftarrow \boldsymbol{0}$

PMG$^{\gamma}$($\mathsf{K}^{\boldsymbol{H}}, \underline{\mathfrak{w}}^{\boldsymbol{H}}, \underline{\mathsf{d}}^{\boldsymbol{H}}, \ell - 1$)

$\boxed{\underline{\mathfrak{w}} \leftarrow \mathfrak{P} \cdot \underline{\mathfrak{w}}^{\boldsymbol{H}}}$

$\underline{\widehat{\mathfrak{u}}} \leftarrow \underline{\widetilde{\mathfrak{u}}} + \underline{\mathfrak{w}}$

$\underline{\mathfrak{u}} \leftarrow$ SMOOTH($\mathsf{K}, \underline{\widehat{\mathfrak{u}}}, \underline{\mathsf{f}}, \boldsymbol{\nu}$)

end if

Menü

Application to LU-decomposition based on DD: Factorization

- Again, we have nodes which correspond to inner nodes (index **1**) and coupling nodes (index **2**) and a distributed sparse stiffness matrix $\mathsf{K} = \begin{pmatrix} \mathsf{K}_{11} & \mathsf{K}_{12} \\ \mathsf{K}_{21} & \mathsf{K}_{22} \end{pmatrix}$.
- property for set of subdomains $\sigma(\omega_1) \subset \sigma(\omega_2)$ is locally valid on all processors s.
- LU-decomposition:

$$
\begin{array}{llll}
\text{Get } \ \mathfrak{L}_{ij,s}, \mathfrak{U}_{ij,s} \ \text{ from} & \mathsf{K}_{11,s} & = & \mathfrak{K}_{11,s} = \mathfrak{L}_{11,s}\mathfrak{U}_{11,s};\, \mathsf{K}_{12,s} = \mathfrak{K}_{12,s} = \mathfrak{L}_{11,s}\mathfrak{U}_{12,s};\, \mathsf{K}_{21,s} = \mathfrak{K}_{21,s} = \mathfrak{L}_{21,s}\mathfrak{U}_{11,s}; \\
\text{Update remaining matrix} & \mathsf{K}_{22,s} & := & \mathsf{K}_{22,s} - \boxed{\mathfrak{L}_{21,s} \cdot \mathbf{I}_{22,s} \cdot \mathfrak{U}_{21,s}} \quad \text{with} \quad \mathbf{I}_{22,s} = R_{2,s}^{-1} \\
\text{Accumulate:} & \mathfrak{K}_{22} & := & \sum_{s=1}^{P} A_s \mathsf{K}_{22,s} A_s^T \\
 & \mathfrak{K}_{22,s} & := & A_s^T \mathfrak{K}_{22} A_s \\
\text{Get } \ \mathfrak{L}_{22}, \mathfrak{U}_{22} \ \text{ from} & \mathfrak{K}_{22,s} & = & \mathfrak{L}_{22,s}\mathfrak{U}_{22,s}
\end{array}
$$

- Above algorithm can be applied recursively but the lower right matrix block can be accumulated and decomposed only after the update of the remaining distributed matrix.

Application to LU-decomposition based on DD: Elimination

- Solving the (preconditioning) system: $\begin{pmatrix} \mathfrak{L}_{11} & 0 \\ \mathfrak{L}_{21} & \mathfrak{L}_{22} \end{pmatrix} \begin{pmatrix} \mathfrak{U}_{11} & \mathfrak{U}_{12} \\ 0 & \mathfrak{U}_{22} \end{pmatrix} \underline{\mathfrak{w}} = \underline{\mathsf{r}}$.
- LU-elimination:

$$
\begin{array}{rrcl}
\text{locally} & \underline{\mathsf{u}}_{1,s} & := & \mathfrak{L}_{11,s}^{-1} \underline{\mathsf{r}}_{1,s} \\
 & \underline{\mathsf{u}}_{2,s} & := & \boxed{\mathfrak{L}_{22,s}^{-1}} \left(\underline{\mathsf{r}}_{2,s} - \mathfrak{L}_{21,s} \underline{\mathsf{u}}_{1,s} \right) \\
\text{accumulate} & \underline{\mathfrak{u}} & := & \sum_{s=1}^{P} A_s \underline{\mathsf{u}} \\
\text{locally} & \underline{\mathfrak{w}}_{2,s} & := & \boxed{\mathfrak{U}_{22,s}^{-1}} \underline{\mathfrak{u}}_{2,s} \\
 & \underline{\mathfrak{w}}_{1,s} & := & \mathfrak{U}_{11,s}^{-1} \left(\underline{\mathfrak{u}}_{1,s} - \mathfrak{U}_{12,s} \underline{\mathfrak{w}}_{2,s} \right)
\end{array}
$$

- The matrices $\mathfrak{L}_{22}$ and $\mathfrak{U}_{22}$ have to fulfill the pattern condition if the boundary is assembled from pieces with different sets of subdomains σ. In this case, some entries have to be deleted in the accumulation phase of the matrix block (before the factorization of this block).
- restricted LU-dcomposition, ILU-decomposition, $\mathcal{H}$-LU-decomposition based on DD [Grasedyck]

Idea for Parallelizing AMG as realized in PEBBLES

parallel MG $\Leftrightarrow$ interpolation $\mathfrak{P}$ has to fulfill the pattern condition

$\Downarrow$

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$\mathsf{K}^{H} = \mathfrak{P}^{T} \cdot \mathsf{K} \cdot \mathfrak{P}$ can be used in PMG$(\mathsf{K}^{H}, \underline{\mathfrak{u}}^{H}, \underline{\mathsf{f}}^{H}, \ell - 1)$.

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$\Downarrow$

Idea

Control of coarsening and interpolation such that the pattern condition is fulfilled for $\mathfrak{P}$.

That requires identification and access to $\omega(\sigma)$.

Menu

Library: basic operations

Provide necessary data structures and functions to hide nasty details of communication from the user.
The user should be assisted to reuse as much as possible of his sequential routines.

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- Methods with communication:
  - setup of communicator(s) from **distributed f.e. mesh** information
  - inner product of vectors,
  - vector accumulation: $\underline{\mathfrak{w}} := \sum_{s=1}^{P} A_s^T \underline{\mathsf{r}}_s$,
  - matrix accumulation (blockwise, update of matrix pattern): $\mathfrak{M} := \sum_{s=1}^{P} A_s^T \mathsf{K}_s A_s$

Library: basic operations (cont.)

- Methods without communication
  - derive a distributed vector from an accumulated vector: $\underline{\mathsf{r}}_s := \mathsf{R}_s^{-1} \cdot \underline{\mathfrak{w}}_s$
  - determine subsets of nodes $\omega(\sigma)$ belonging to the same set of subdomains σ
  - derive new $\omega(\sigma)$ from the old one after refinement/coarsening
  - \# construct a local ordering of the σ-sets (subset property + unique ordering), **globally consistent!**
  - \# local node renumbering according to the ordering of the local σ-sets
  - \# renumbering of incoming and re-renumbering of outgoing data

- Data structures
  - array: local to global numbering
  - arrays: sequence of nodes belonging to σ-sets
  - array of communicators
  - vector for mult. right hand sides, blocks etc. `packed_vector<double> a(nnode, nrhs, nblock)`
    access as linear array $\Longrightarrow$ cache–aware programming
  - special intermediate sparse matrix format `[row, col, entry]`

Code example for setup in main–function

```
//  ----------------  read data from files  ---------------------------------------
string root("../Plank/TBunnyC2/");                  // directory for data
vector<int> hdr;
...
read_header(root, hdr);                             // size of arrays
read_partition(root, hdr, par);                     // partition mapping
read_connection(root, hdr, par, rcon);              // element connectivity
read_element(root, hdr, par, rele);                 // element matrices

// -----------------  setup communicator  ------------------------------------------
element_accumulation(hdr, rcon, row, col, rele);  // determine local nodes,elements
communicator<int, double> com(rcon);                // derive communicator

// -----------------  local matrix accumulation  ----------------------------------
idx_matrix<int, double> A(row, col, rele);          // intermediate matrix format

//  crs_matrix<int, double> D(cnt, col, rele);
GH_crs_matrix D(cnt, col, rele, com);               // derive user specific data format

// ------------------  call numerical algorithm  ----------------------------------
packed_vector<double> _X(_nnodes, _num, 1);
packed_vector<double> _B(_nnodes, _num, 1);

n = GS_iteration_merge(con, D, _X, _B , 1.0e-14, 512, stride);
```

Code example for applying parallel routines in preconditioned CG

```
 template<class T, class S>
 int conjugate_gradient(const matrix<T, S> &_K, const matrix<T, S> &_C,
                        packed_vector<S> &_u, const packed_vector<S> &_f,
const S _eps, const int _max,
                        communicator<T, S> &_com)
 {
   packed_vector<S> _r(_f);
   packed_vector<S> _s(_u);
   packed_vector<S> _v(_r.numnod(), _r.numrhs(), _r.numdof());

   multiply(_K, _s, _v);                          // sequ. matrix-vector
   sub_scale(_r, _v, alpha);                      // sequ. vector-vector
   multiply(_C, _r, _v);                          // parall. precond. [user]
   com.accumulate(_v);                            // parall. vector accu
   scalar_product(_v, _r, sigma);                 // sequ. vector-vector
   _com.collect(sigma);                           // parall. reduce operation
   scale_add(_s, _v, beta);                       // sequ. vector-vector
   ....
 }
```

Summary

- Toolbox works already well and efficient for one–level–methods
- Very fast communicator setup: (kepler:Infiniband, pregl/archimedes: Gigabit)

NP	kepler	pregl	archimedes
1	55.9	70.3	54.7
2	47.6	78.1	66.4
4	35.5	87.9	86.9
8	29.9	98.6	91.3
16	27.4	102.8	95.2
32	34.5	676.6	622.9

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Thank You for Your attention!!