

A principle for constructing parallel AMG and its realization

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Contents

- Basic ingredients for multigrid and algebraic multigrid.
- Parallelization - Theory.
 - Domain decomposition data distribution and some theory.
 - Parallel multigrid.
 - Parallel setup in AMG.
- Parallelization - Realization.
- Applications.
- Summary.

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Assumptions on the linear equation

$$K_h u_h = f_h$$

- $K_h \in \mathbb{R}^{N_h \times N_h}$ is SPD
- K_h stems from an FE-discretization (G_h grid points)
- FE-discretization with Lagrange FE-functions
- Degrees of freedom per node ($n = \text{block-size}$)
- DOF: $N_h = G_h * n$

Notice: Although K_h is SPD we need this information in order to construct an appropriate AMG method!

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Parallelization

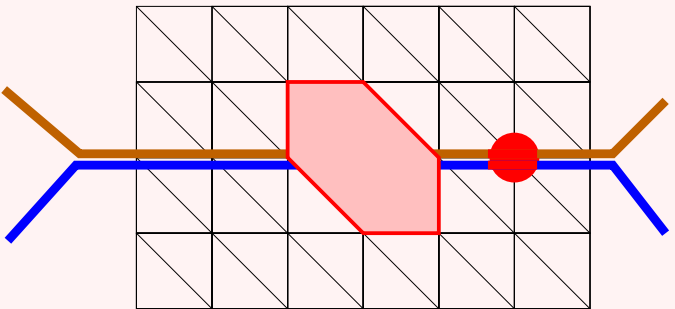
- General approach for iterative schemes (incl. conservation laws).
- Tool-box-like implementation.
- Mathematical theory as construction principle for **new parallel algorithms**.
- Data distribution by non-overlapping elements.
- Overlapping elements can also be used.

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Non-overlapping Domain Decomposition

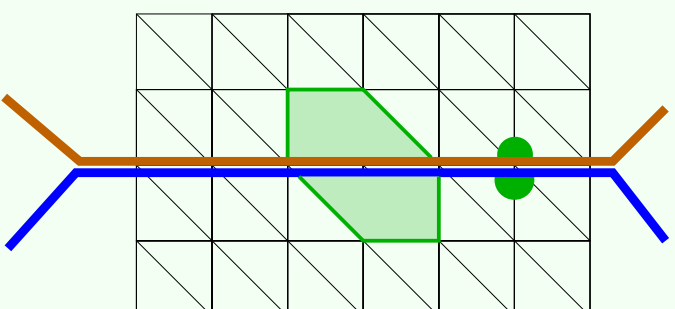
accumulated



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

$$\underline{m}_s = A_s \underline{m} A_s^T$$

distributed



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

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

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Overlapping Domain Decomposition

accumulated

$$\underline{\mathbf{u}}_s = A_s \underline{\mathbf{u}} \quad , \quad \mathbf{m}_s = A_s \mathbf{m} A_s^T$$

distributed

$$\underline{\mathbf{r}} = \sum_{s=1}^P A_s^T \underline{\mathbf{r}}_s \quad , \quad \mathbf{K} = \sum_{s=1}^P A_s \mathbf{K}_s A_s^T$$

BUT, how to choose \mathbf{K}_s ?

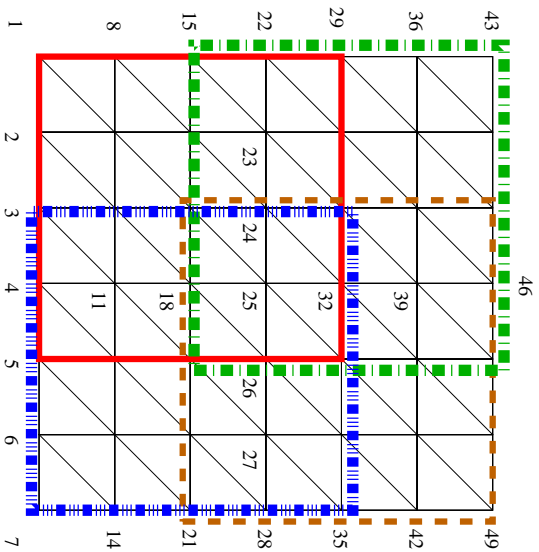
$$\mathbf{K}_s := \sum_{\delta^{(r)} \subseteq \Omega_s} \frac{1}{W^{(r)}} \cdot K^{\text{FEM},r}$$

$W^{(r)} := \# \Omega_s$ an element $\delta^{(r)}$ belongs to.

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Some Definitions



- subdomain 1
- - - - subdomain 2
- - - - subdomain 3
- - - - subdomain 4

Sets of subdomains :

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

Sets of indices/nodes :

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

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

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

Matrix patterns and operations

The following operations can be performed in parallel:

$$\underline{\mathbf{f}} = \mathbf{K} \cdot \underline{\mathbf{u}}$$

Matrix \mathfrak{M} fulfills pattern condition:

$$\forall i, j \in \omega : \sigma^{[i]} \not\subseteq \sigma^{[j]} \implies \mathfrak{M}^{[i,j]} = 0$$

$$\underline{\mathbf{u}} = \mathfrak{M} \cdot \underline{\mathbf{w}}$$

$$\underline{\mathbf{f}} = \mathfrak{M}^T \cdot \underline{\mathbf{r}}$$

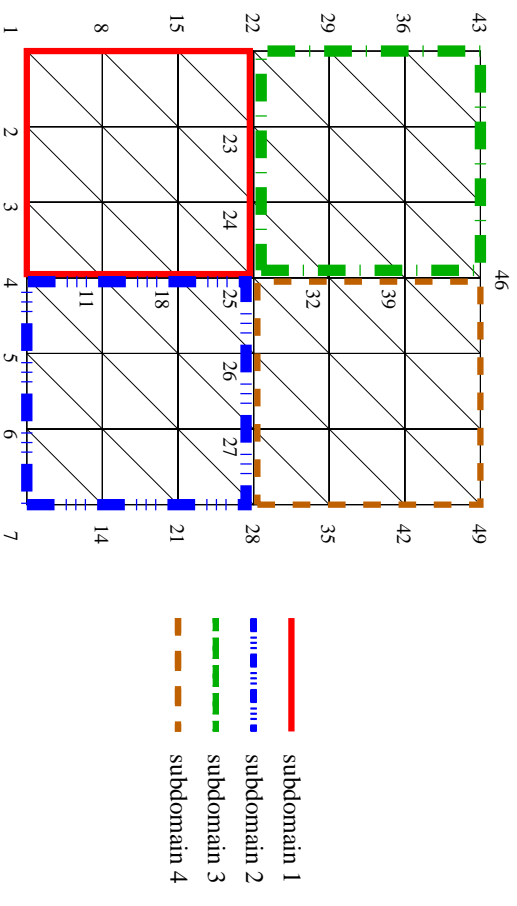
$$\mathbf{K}^H = \mathfrak{M}^T \cdot \mathbf{K} \cdot \mathfrak{M}$$

Non-overlapping Decomposition

$$\begin{aligned} \sigma^{[1]} &= \{1\}, & \sigma^{[7]} &= \{2\}, \\ \sigma^{[4]} &= \{1, 2\}, & \sigma^{[22]} &= \{1, 3\}, \\ \sigma^{[25]} &= \{1, 2, 3, 4\}. \end{aligned}$$

$$\begin{aligned} \omega(\sigma^{[1]}) &= \{1, 2, 3, 8, 9, 10, 15, 16, 17\}, \\ \omega(\sigma^{[4]}) &= \{4, 11, 18\}, \\ \omega(\sigma^{[22]}) &= \{22, 23, 24\}, \\ \omega(\sigma^{[25]}) &= \{25\}. \end{aligned}$$

$$\begin{aligned} \bar{\omega}(\sigma^{[1]}) &= \bar{\omega}(\{1\}) = \omega(\sigma^{[1]}) \cup \omega(\sigma^{[4]}) \cup \omega(\sigma^{[22]}) \cup \omega(\sigma^{[25]}) \\ &= \{1, 4, 8, 11, 15, 18, 22, 25\} =: \omega_1, \\ \bar{\omega}(\sigma^{[4]}) &= \omega(\sigma^{[4]}) \cup \omega(\sigma^{[25]}) = \{4, 11, 18, 25\}, \\ \bar{\omega}(\sigma^{[25]}) &= \omega(\sigma^{[25]}) = \{25\}. \end{aligned}$$



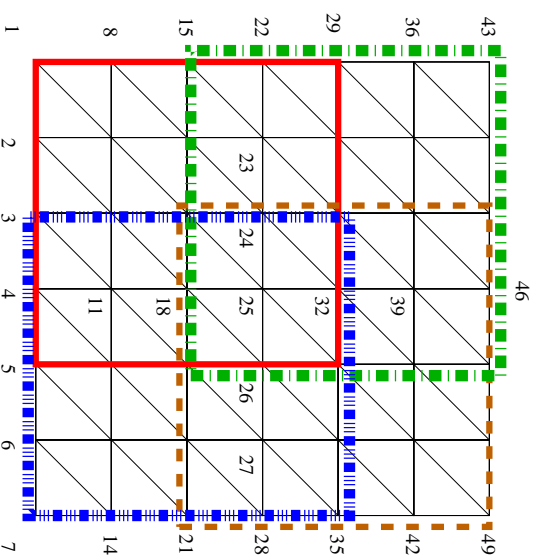
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Overlapping Decomposition

$$\sigma^{[3]} = \sigma^{[4]} = \sigma^{[5]} = \{1, 2\}$$

$$\begin{aligned} \omega(\sigma^{[1]}) &= \{1, 2, 8, 9\}, \\ \omega(\sigma^{[4]}) &= \{3, 4, 5, 10, 11, 12\}, \\ \omega(\sigma^{[22]}) &= \{15, 16, 22, 23, 29, 30\}, \\ \omega(\sigma^{[25]}) &= \{17, 18, 19, 24, 25, 26, 31, 32, 33\}. \end{aligned}$$



- subdomain 1
- ⋯ subdomain 2
- - - subdomain 3
- - - subdomain 4

$$\begin{aligned} \bar{\omega}(\sigma^{[1]}) &= \{1, 5, 8, 12, 15, 19, 22, 25, 29, 33\}, \\ \bar{\omega}(\sigma^{[4]}) &= \{3, 4, 5, 10, 11, 12, 17, 18, 19, 24, 25, 26, 31, 32, 33\}, \\ \bar{\omega}(\sigma^{[25]}) &= \omega(\sigma^{[25]}). \end{aligned}$$

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Patch Decomposition

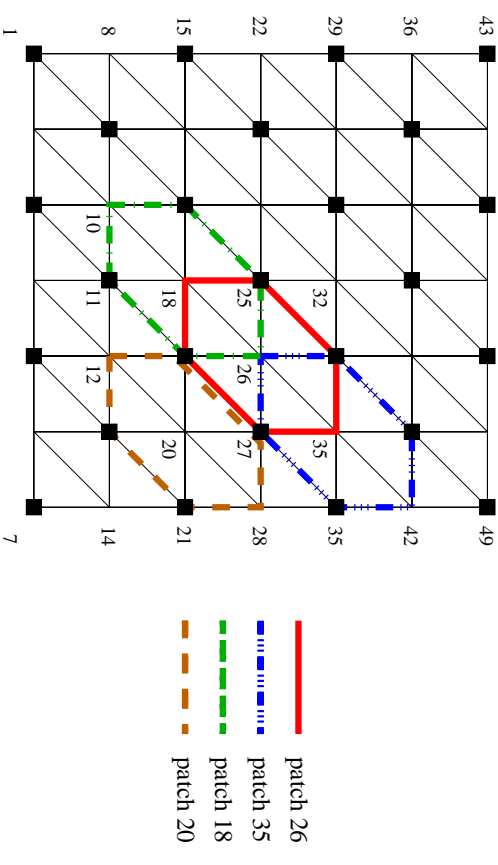
$$\begin{aligned} \sigma^{[18]} &= \{10, 18, 26\}, & \sigma^{[20]} &= \{12, 20, 28\}, \\ \sigma^{[26]} &= \{18, 26, 34\}, & \sigma^{[34]} &= \{26, 34, 42\}, \\ \sigma^{[19]} &= \{12, 18, 20, 26\} & \sigma^{[27]} &= \{20, 26, 28, 34\}. \end{aligned}$$

The sets of nodes contained in the patches are

$$\begin{aligned} \omega(\{18\}) &= \{10, 11, 17, 18, 19, 25, 26\} = \underline{\omega}(\{18\}), \\ \omega(\{20\}) &= \{12, 13, 19, 20, 21, 27, 28\} = \underline{\omega}(\{20\}), \\ \omega(\{26\}) &= \{18, 19, 25, 26, 27, 33, 34\} = \underline{\omega}(\{26\}), \\ \omega(\{34\}) &= \{26, 27, 33, 34, 35, 41, 42\} = \underline{\omega}(\{34\}). \end{aligned}$$

Derived index set for patch Ω_{26} are

$$\begin{aligned} \omega(\sigma^{[26]}) &= \underline{\omega}(\sigma^{[26]}) = \underline{\omega}(\sigma^{[26]}) \\ &= \{10, 11, 17, 18, 19, 25, 26, 27, 33, 34, 35, 41, 42\} \\ \underline{\omega}(\{26\}) &= \omega(\sigma^{[18]}) \cap \omega(\sigma^{[26]}) \cap \omega(\sigma^{[34]}) \\ &= \{2, 3, 9, 10, 11, 17, 18, 19, 25, 26, 27, 33, 34, 35, 41, 42, 49\}. \end{aligned}$$



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

```
if  $\ell == 1$  then
  solve  $\sum_{s=1}^P A_s^T K A_s \cdot \underline{u} = \underline{f}$ 
else
   $\hat{\underline{u}} \leftarrow \text{SMOOTH}(K, \underline{u}, \underline{f}, \nu)$ 
   $\underline{d} \leftarrow \underline{f} - K \cdot \hat{\underline{u}}$ 
   $\underline{d}^H \leftarrow \mathfrak{P}^T \cdot \underline{d}$ 
   $\underline{w}^H \leftarrow 0$ 
  PMG $^\gamma(K^H, \underline{w}^H, \underline{d}^H, \ell - 1)$ 
   $\underline{w} \leftarrow \mathfrak{P} \cdot \underline{w}^H$ 
   $\hat{\underline{u}} \leftarrow \hat{\underline{u}} + \underline{w}$ 
   $\underline{u} \leftarrow \text{SMOOTH}(K, \hat{\underline{u}}, \underline{f}, \nu)$ 
end if
```

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Main steps in AMG

(i) Coarsening procedure :

$$\omega^h = \omega_C^h \cup \omega_F^h .$$

(ii) Interpolation weights :

$$P = \{\alpha_{ij}\}_{i \in \omega^h, j \in \omega_C^h} : \mathbb{R}^H \mapsto \mathbb{R}^h .$$

(iii) Coarse grid matrix:

$$K^H = P^T \cdot K \cdot P \quad (\text{or } K^H = \tilde{P}^T \cdot K \cdot \tilde{P})$$

(iv) (i)-(iii) recursively.

(v) Apply mg-procedure.

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Coarsening in AMG

Arbitrary coarsening

$\text{COARSE}(K, \omega, \omega_C, \omega_F)$

$\omega_t \leftarrow \omega$

while $\omega_t \neq \emptyset$ **do**

 pick some $i \in \omega_t$ (strong connections in $K|_{\omega_t}$)

$\omega_C \leftarrow \omega_C \cup \{i\}$

 determine neighbors of $i \longrightarrow U_i$

$\omega_F \leftarrow \omega_F \cup (U_i \cap \omega_t)$

$\omega_t \leftarrow \omega_t \setminus (\{i\} \cup U_i \cap \omega_t)$

end while

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Interpolation weights in AMG

Here, we restrict the calculation of interpolation weights α_{ij} on a given index set. Again, we can use an arbitrary routine.

WEIGHTS($K, \omega_C, \omega_F, \alpha$)

```
for all  $i \in \omega_F$  do  
  determine neighbors of  $i \rightarrow U_i$   
  for all  $j \in U_i \cap \omega_C$  do  
    calculate  $\alpha_{ij}$   
  end for  
end for
```

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Coarse matrix calculation in AMG

$$(K^H)^{[ij]} = \sum_{k \in \omega} \sum_{l \in \omega} \alpha_{ki} \cdot K^{[kl]} \cdot \alpha_{lj} \quad \forall i, j \in \omega_C$$

GALERKIN($K^H, K, \omega_C, \omega_F, \alpha$)

Require: $K^H = 0$ before first call

for all $k \in \omega_F \cup \omega_C$ **do**

determine fine and coarse neighbors of $k \longrightarrow F^i, C^k$

for all $l \in F^k \cup C^k \cup \{k\}$ **do**

$T \leftarrow C^k \cup C^l \cup (\{l\} \cap \omega_C)$

for all $i \in T$ **do**

for all $j \in T$ **do**

$$(K^H)^{[ij]} \leftarrow (K^H)^{[ij]} + \alpha_{ki} \cdot (K)^{[kl]} \cdot \alpha_{lj}$$

end for

end for

end for

end for

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Parallelization idea for AMG

Parallel MG \Leftrightarrow interpolation \mathfrak{P} fulfills pattern condition

\Downarrow

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

\Downarrow

Idea

Control coarsening and interpolation such that pattern condition is fulfilled.

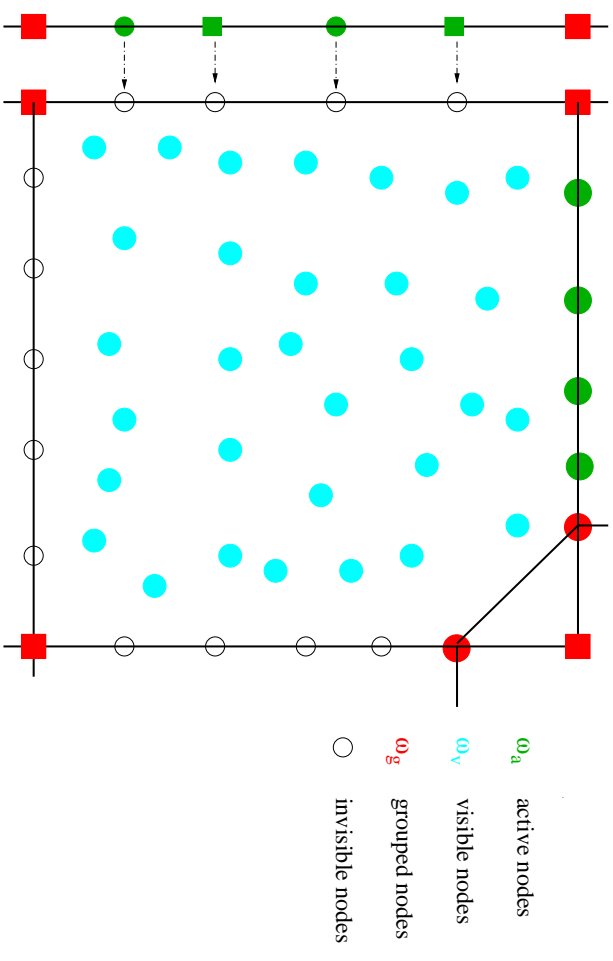
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Control of the coarsening pattern

COARSEP $(\{S^i\}, \omega_m, \omega_a, \omega_v, \omega_g, \omega_C, \omega_F)$

- K_i pattern $\rightarrow \tilde{K}_i$
- active nodes: $\omega_a := \{i \in \omega_s : \sigma^{[i]} \equiv \sigma_k\}$,
- visible nodes: $\omega_v := \{i \in \omega_s : \sigma^{[i]} \subset \sigma_k\}$,
- grouped nodes: $\omega_g := \{i \in \omega_s : \sigma^{[i]} \supset \sigma_k\}$,
- invisible nodes : $\omega_s \setminus (\omega_a \cap \omega_v \cap \omega_g)$.



PARCOARSE($\{S^i\}, \omega_s, \omega_G, \omega_F$)

Determine list $[\sigma_k]_{k=1, \dots, mc_s}$ (= communicator groups).

for all $k = 1, \dots, mc_s$ **do**

$\omega_a \leftarrow \{i \in \omega_s : \sigma^{[i]} \equiv \sigma_k\}$

$\omega_o \leftarrow \{i \in \omega_s : \sigma^{[i]} \subset \sigma_k\}$

$\omega_g \leftarrow \{i \in \omega_s : \sigma^{[i]} \supset \sigma_k\}$

$\omega_m \leftarrow \emptyset$

if $s == \text{ROOT}(\sigma_k)$ **then**

 COARSEP ($\{S^i\}, \omega_m, \omega_a, \omega_o, \omega_G, \omega_F$)

end if

$\omega_m \leftarrow \text{BROADCAST}(\sigma_k, \omega_G \cap \omega_a)$

if $s! = \text{ROOT}(\sigma_k)$ **then**

 COARSEP ($\{S^i\}, \omega_m, \omega_a, \omega_o, \omega_G, \omega_F$)

end if

for all $i \in \omega_a$ **do**

if $i \in \omega_F$ **then**

$S^i \leftarrow S^i \cap (\omega_a \cup \omega_g)$

else

$S^i \leftarrow S^i \cap (\omega_a \cup \omega_o)$

Parallel AMG: PARAMG($\mathbf{K}_h, \underline{\mathbf{u}}, \underline{\mathbf{f}}, \omega$)

```
for all  $s = 1, \dots, P$  do
 $\mathbf{K}_s^1 \leftarrow \mathbf{K}_s$ ,  $\omega_s^1 \leftarrow \omega_s$ ,  $\ell \leftarrow 1$ 
repeat
 $\tilde{\mathbf{R}} \leftarrow \left( \sum_{i=1}^P \mathbf{A}_i^T \tilde{\mathbf{K}}_i \mathbf{A}_i \right)$ ,  $\tilde{\mathbf{R}}_s \leftarrow \mathbf{A}_s \tilde{\mathbf{R}} \mathbf{A}_s^T$ 
 $S^i \leftarrow \text{GETSTRONG}(\tilde{\mathbf{R}}_s)$   $\forall i \in \omega_s$ 
 $\omega_C \leftarrow \emptyset$ ,  $\omega_F \leftarrow \emptyset$ 
PARCOARSE( $\{S^i\}^\ell$ ,  $\omega_s^\ell$ ,  $\omega_{C,s}$ ,  $\omega_{F,s}$ )
WEIGHTS( $\{S^i\}^\ell$ ,  $\tilde{\mathbf{R}}$ ,  $\omega_{C,s}$ ,  $\omega_{F,s}$ ,  $\mathfrak{R}_s^\ell$ ),  $\text{free}(\{S^i\}^\ell, \tilde{\mathbf{R}})$ 
 $\mathbf{K}_s^{\ell+1} \leftarrow 0$ 
GALERKIN( $\mathbf{K}_s^\ell$ ,  $\mathbf{K}_s^{\ell+1}$ ,  $\omega_{C,s}$ ,  $\omega_{F,s}$ ,  $\mathfrak{R}_s^\ell$ )
 $\omega_s^\ell \leftarrow \omega_{C,s}$ ,  $\ell \leftarrow \ell + 1$ 
until termination
end for
PMG-A( $\mathbf{K}, \underline{\mathbf{u}}, \underline{\mathbf{f}}, 1$ )
```

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Remarks and Conclusions

- ⊕ PMG-A and most of coarsening is fully parallel.
 - ⊕ Wide range of admissible decompositions.
 - ⊕ Coarsening terminates automatically if $|\omega(\sigma^{[i]})| = 1 \forall i \in \omega^\ell$.
 - ⊕ Arbitrary coarsening, interpolation on appropriate subsets.
 - ⊕ +/- Distributed matrix (e.g. element matrices) required.
 - ⊕ Successfull numerical tests:
Speedup 50 with 60 processors for MG and AMG
- FEPP and PEBBLES cover the full range from single PC via high-end workstation up to clusters of workstations/PC and high-end compute servers.

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