Algebraic Multigrid Methods on GPU-Accelerated Hybrid Architectures

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January 25, 2016

(6) Bidomain Equations with Elasticity Coupling

The elastic coupling is realized with the parameters $\mathbf{a}$ and the Cauchy-Green deformation tensor $\mathbf{C}$, calculated from the deformation model [Pathmanathan/Whiteley 2009], with the equilibrium equations of large elastic deformations describing the mechanic behavior.

$$-\nabla \cdot \boldsymbol{\sigma}_e \mathbf{C}^{-1} \nabla \phi_e = \nabla \cdot \boldsymbol{\sigma}_i \mathbf{C}^{-1} \nabla \phi_i + I_e \tag{1}$$

$$\beta I_m = \nabla \cdot \boldsymbol{\sigma}_i \mathbf{C}^{-1} \nabla \phi_i \tag{2}$$

$$I_m = C_m \frac{\partial V_m}{\partial t} + I_{ion}(V_m, \boldsymbol{\eta}, \mathbf{a}) - I_i \tag{3}$$

$$\frac{d\boldsymbol{\eta}}{dt} = f(t, \boldsymbol{\eta}, \mathbf{a}) \tag{4}$$

$$V_m = \phi_i - \phi_e \tag{5}$$

Large Elastic Deformations

$$-\mathrm{div}\,\boldsymbol{\sigma}(u) = f, \quad \boldsymbol{\sigma} = 2J^{-1}\mathbf{F}\frac{\partial\Psi(\mathbf{C})}{\partial\mathbf{C}}\mathbf{F}^{\top} \tag{6}$$

$$\mathbf{C} = \mathbf{F}^{\top}\mathbf{F}, \quad J = \det\mathbf{F}, \quad \mathbf{F} = \mathbf{F}(u) \tag{7}$$

$$\tag{8}$$

Where

$$\Psi = U(J) + \overline{\Psi}_{\text{iso}} + \overline{\Psi}_{\text{aniso}} + \overline{\Psi}_{\text{act}}(\boldsymbol{a}, \eta(V_m)), \quad U(J) = \frac{\kappa}{2}(J-1)^2 \ . \tag{9}$$

is the Helmholtz free energy including both the isotropic and anisotropic response, and an active part due to the excitation–induced contraction during the course of depolarization. [Kroon/Holzapfel 2009; Pathmanathan/Whiteley 2009]

Nonlinear Elasticity: A Sketch

Solve the nonlinear system of equations

$$K(u) \cdot u = f$$

with u describing the elastic deformation with Newtons method.

In every Newton iteration we have to solve the system

$$A'(u) \cdot \Delta u = g(u) \tag{10}$$

where

$$\begin{aligned} A'(u) &= \frac{\partial K(u)}{\partial u} \cdot u + K(u) \\ g(u) &= f - K(u) \cdot u \end{aligned} \tag{11}$$

Nonlinear Elasticity: Algorithmic View I

Newton solver for the nonlinear elasticity problem:

1. Calculate $K(u)$, $A'(u)$, $g(u)$

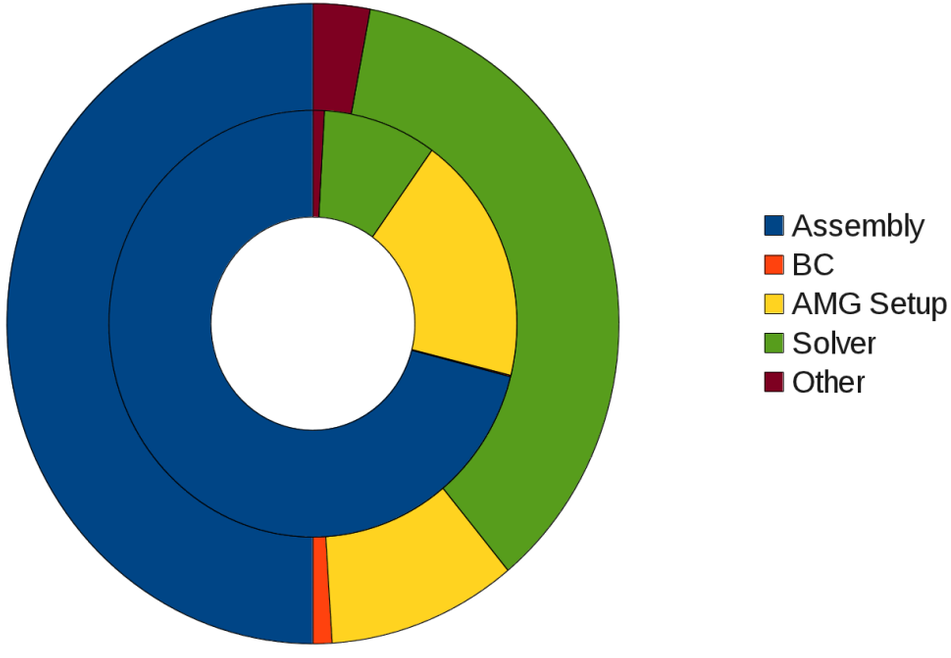
2. Solve the Newton system with AMG-PCG

   (a) Setup of AMG-preconditioner wrt. $A'(u)$
      i. Find coarse/fine nodes
      ii. Calculate interpolation operators
      iii. Calculate coarse grid operators
   (b) Apply AMG-PCG solver

3. Update $\widehat{u} = u + \Delta u$

4. Goto 1

CARP-PT Performance of Elasticity Solver



	CPU %	GPU %
Assembly	50	71
AMG Setup	10	19
AMG-PCG Solver	36	9

Table 1: Percentage of time spent in the components of the nonlinear elasticity solver

Nonlinear Elasticity: Algorithmic View II

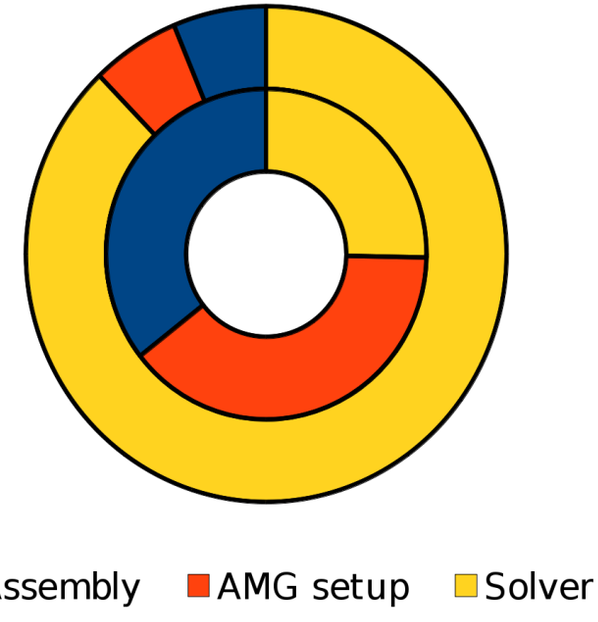
1. Setup of operators performed once
   (a) Calculate sparsity pattern of $K(u)$, $A'(u)$
   (b) Calculate $K(u)$, $A'(u)$, $g(u)$
   (c) Setup of AMG-preconditioner wrt. $A'(u)$

2. Solve the Newton system with AMG-PCG
   (a) Setup of AMG-preconditioner wrt. $A'(u)$ with fixed sparsity pattern
      i. No setup wrt. coarse/fine nodes
      ii. Update interpolation operators
      iii. Update coarse grid operators
   (b) Apply AMG-PCG solver

3. Update $\widehat{u} = u + \Delta u$
   Update $K(\widehat{u})$, $A'(\widehat{u})$, $g(\widehat{u})$ with fixed sparsity pattern

4. Goto 2

CARP-PT Performance of Optimized Elasticity Solver



	Original		Optimized	
	CPU %	GPU %	CPU %	GPU %
Assembly	50	71	6	36
AMG Setup	10	19	6	39
PCG-AMG Solver	36	9	88	25

Table 2: Percentage of time spent in the components of the nonlinear elasticity solver

(7) AMG for Elasticity Revisited

- Solve $K\,u = f$ using a hierarchy of equation systems

$$K^{\ell}\,\bar{u}^{\ell} = \bar{f}^{\ell} \quad ,\ell = 0,\ldots,L$$

- Hierarchy is constructed from *algebraic* operator K

$$K^{\ell+1} = R^{\ell} K^{\ell} P^{\ell}$$

Exact Two-Grid Method

- Block System

$$\begin{bmatrix} K_{CC} & K_{CF} \\ K_{FC} & K_{FF} \end{bmatrix} \begin{bmatrix} u_C \\ u_F \end{bmatrix} = \begin{bmatrix} f_C \\ f_F \end{bmatrix}$$

- Schur decomposition

$$\begin{bmatrix} K_{CC} & K_{CF} \\ K_{FC} & K_{FF} \end{bmatrix} = \begin{bmatrix} I & K_{CF}K_{FF}^{-1} \\ & I \end{bmatrix} \begin{bmatrix} S_C & \\ & K_{FF} \end{bmatrix} \begin{bmatrix} I & \\ K_{FF}^{-1}K_{FC} & I \end{bmatrix}$$

$$S_C = K_{CC} - K_{CF}\,K_{FF}^{-1}\,K_{FC} = RKP$$

- Exact two grid method

$$R := \begin{pmatrix} I & -K_{CF}K_{FF}^{-1} \end{pmatrix}, \quad P := \begin{pmatrix} I \\ -K_{FF}^{-1}K_{FC} \end{pmatrix}$$

Standard AMG Coarsening

- Strong connection criterion

$$|K_{ij}| > \epsilon |K_{ii}|$$

- Construction of Prolongation operator

$$P := \begin{pmatrix} I_{CC} \\ P_{FC} \end{pmatrix}$$

$$\begin{aligned} n_i &:= \#\{j \in C : |K_{ij}| > \epsilon |K_{ii}|\} \\ (P_{FC})_{ij} &:= \begin{cases} 1/n_i & \text{if } |K_{ij}| > \epsilon |K_{ii}| \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

Adaptation of AMG for Elasticity Problems

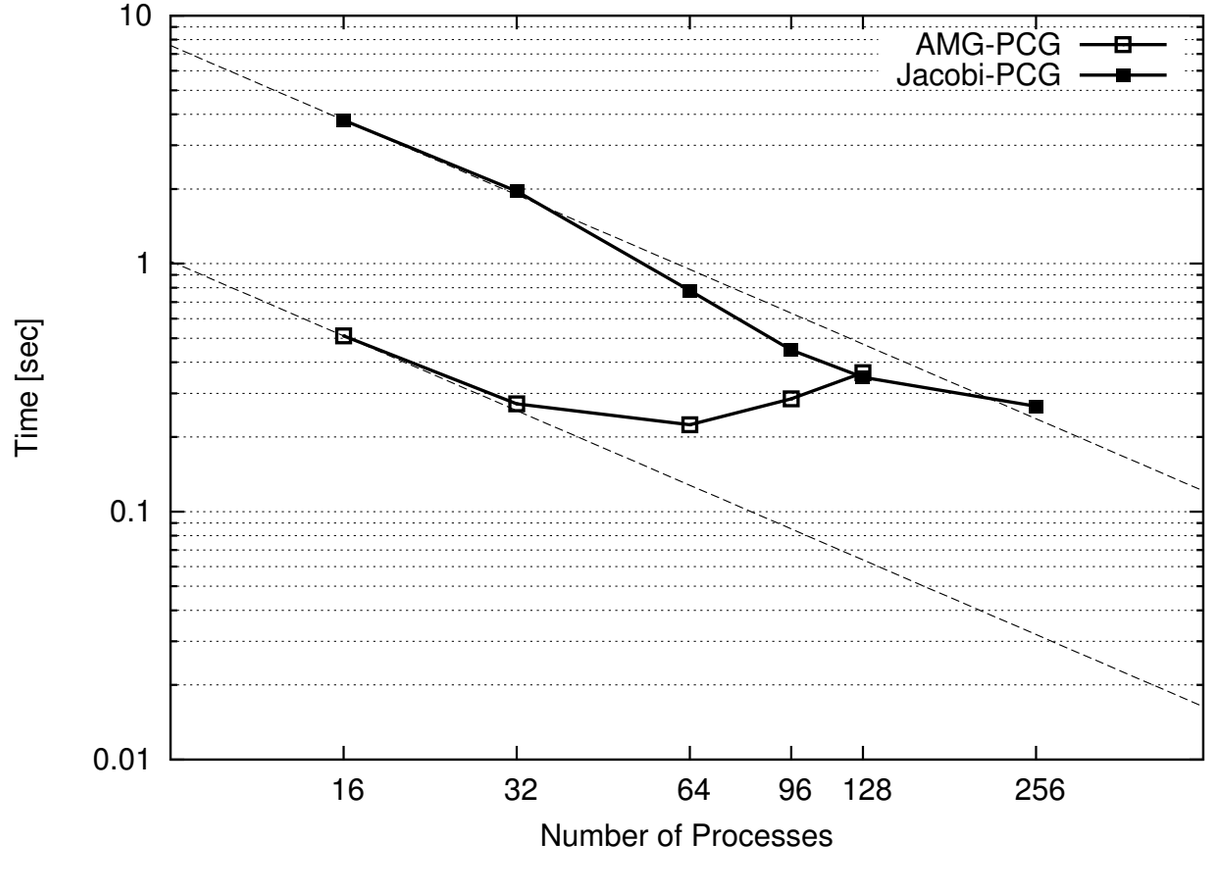
- Extension of the standard AMG algorithm
- The matrix K has a 3×3 block struckture
- Define an auxiliary matrix $\tilde{K}$ by taking matrix norms of the 3×3 blocks of K
- Calculate coarsening with auxiliary matrix $\tilde{K}$
- Extended prolongation operator based on auxiliary matrix $\tilde{K}$

(8) Parallel Scaling: Redistribution of AMG Hierarchy

- Multigrid methods efficient as solvers and preconditioners:
  Stable convergence w.r.t. grid refinement and spatial resolution
- Main concern with modern hardware architectures: **Parallel scalability**
- **Main bottleneck is communication on intermediate grids**

Scaling Problems

Comparison of AMG-PCG and Jacobi-PCG as a limit case.



Scaling Problems

- Fine-Grid
  - Big subdomains, interfaces, message sizes
  - Sparse communication pattern
- Intermediate Grids
  - Small subdomains, interfaces, message sizes
  - Still most processes, accumulate interface values
- Coarse-Grid
  - Small subdomains, interfaces, message sizes
  - Few processes, accumulate interface values

Redistribution of multigrid hierarchy

- Common solution: Reduce parallelism
  - Redistribute parallel data on fewer processes
- Open questions:
  - When to redistribute: Once, multiple times, systematic?
  - Redistribution pattern: Based an which criteria?

Proposed Method

- Systematic reduction of processes with configurable rate
- Redistribution in a block-pattern matching the domain decomposition

Reasoning:

- Systematic:
  - Logarithmic reduction of processes
  - Robust configuration, doesn't need fine tuning.
- Block-Pattern:
  - Should match hardware layout
  - Intermediate levels redistributed in local memory.

Block Pattern

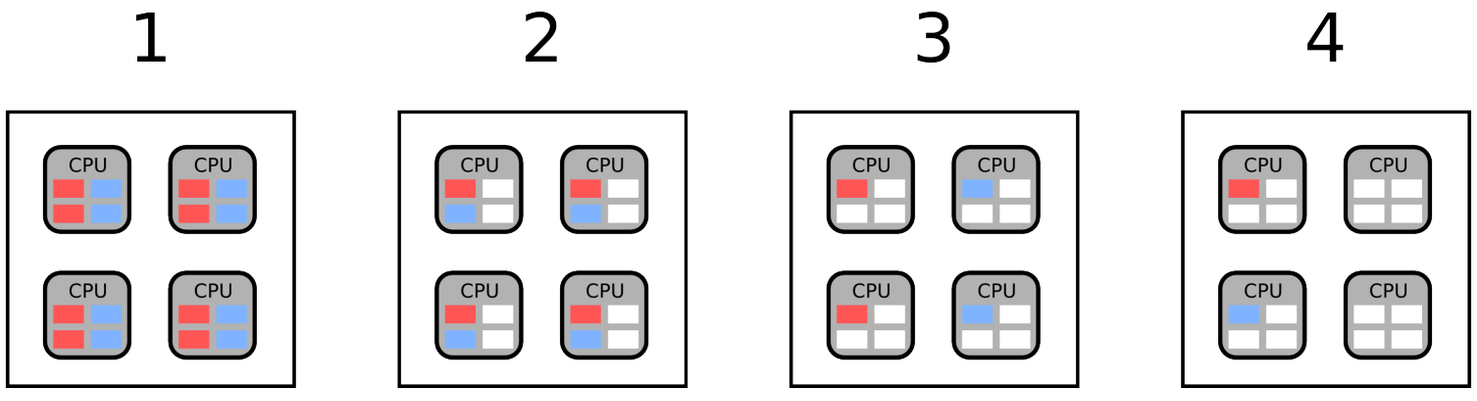


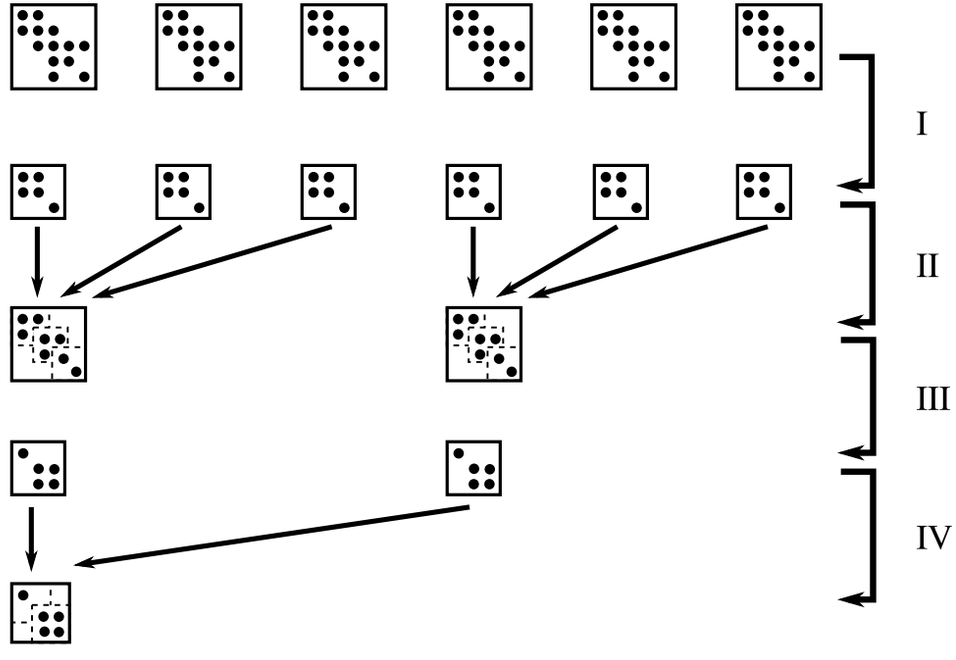
Figure 1: Redistribution pattern for a blocksize **2**. **Red:** Active Ranks, **Blue:** Idle Ranks

- Can be computed based on process rank if the assignment to computing units is systematic.
- In case of 16 processes per compute node, the first 4 redistributions are in shared memory!

Modified AMG Setup and Algorithm

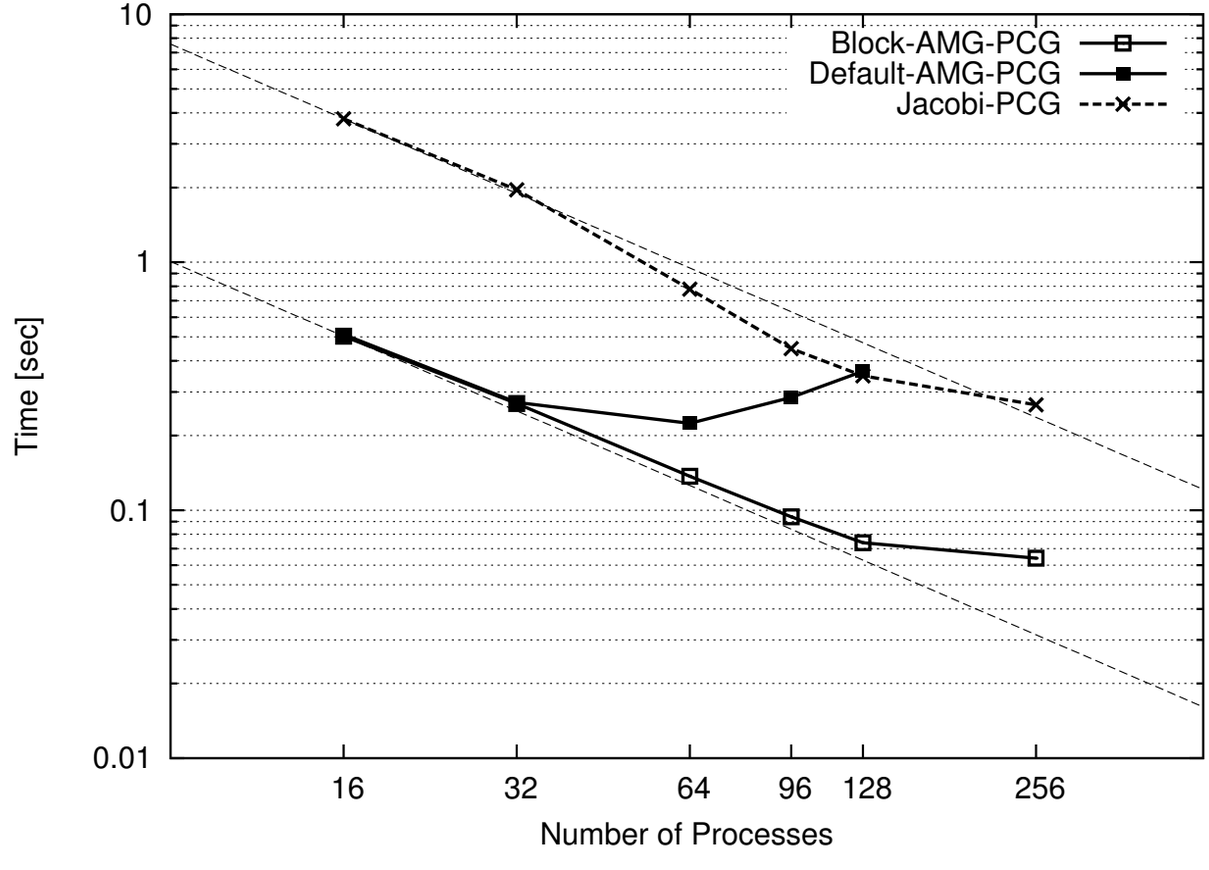
1. Coarsening
   (a) Coarse-grid selection
   (b) Construct Prolongation/Restriction
   (c) Triple-matrix-product

2. Redistribution
   (a) Active-idle selection
   (b) Data transfer
   (c) Matrix accumulation

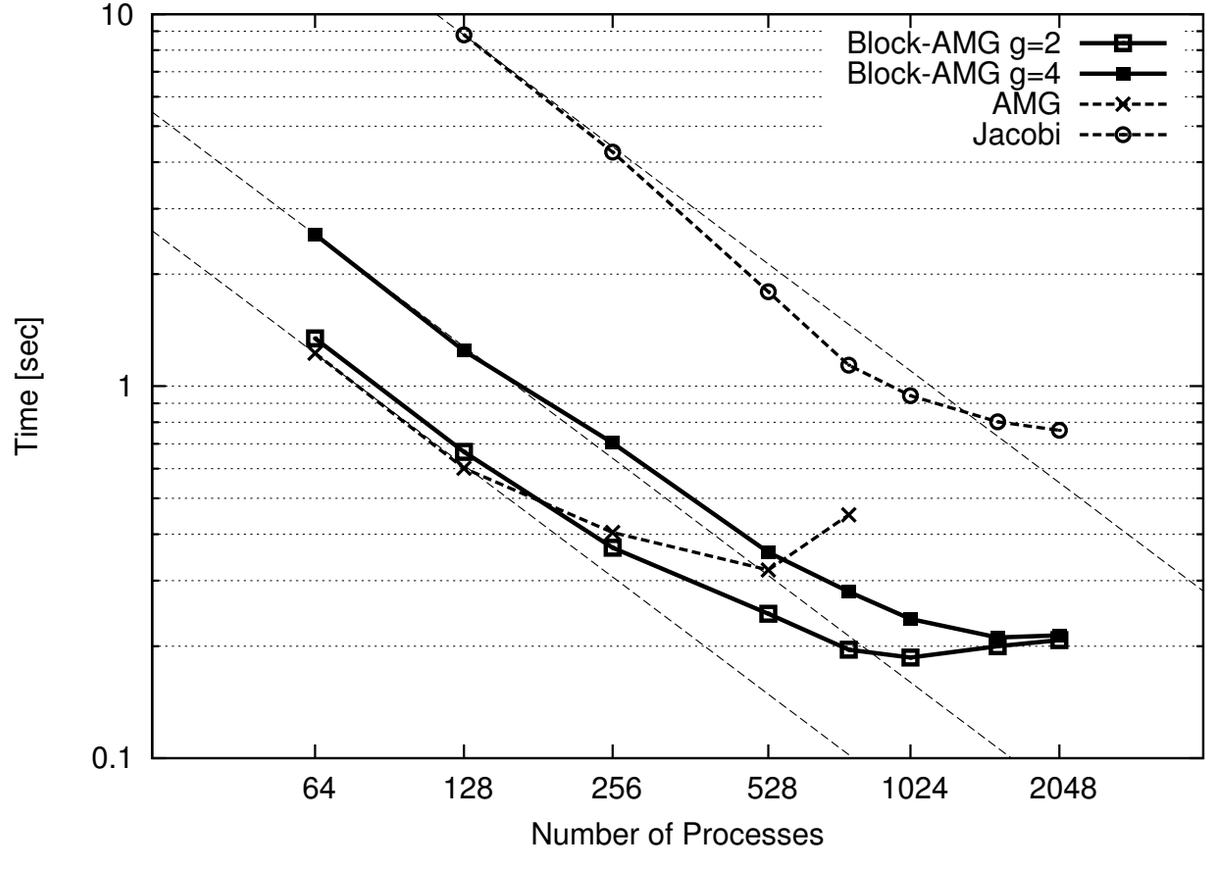


Require: $\mathsf{K}_p^\ell, \underline{\mathsf{f}}_p^\ell, \underline{\mathsf{u}}_p^\ell, \underline{\mathsf{r}}_p^\ell, P_p^\ell, J_p^\ell, G, a \in G, A_p, active_p; \ell = 1, \ldots, L$
  if $\ell < L$ **then**
    if $active_p[\ell] = true$ **then**
      $\underline{\mathsf{u}}_p^\ell \leftarrow 0$
      $\underline{\mathsf{u}}_p^\ell \leftarrow J_p^\ell(\underline{\mathsf{u}}_p^\ell, \underline{\mathsf{f}}_p^\ell)$ {Pre-smooth}
      $\underline{\mathsf{r}}_p^\ell \leftarrow \underline{\mathsf{f}}_p^\ell - \mathsf{K}_p^\ell \underline{\mathsf{u}}_p^\ell$ {Compute residual}
      $\underline{\mathsf{f}}_p^{\ell+1} \leftarrow (P_p^\ell)^T \underline{\mathsf{r}}_p^\ell$ {Restrict residual}
      $\underline{\mathsf{f}}_a^{\ell+1} \leftarrow \sum_{i \in G} \hat{A}_a A_i^T \underline{\mathsf{f}}_i^{\ell+1}$ {Gather}
    end if
    multigrid($\ell + 1$) {Recursion}
    if $active_p[\ell] = true$ **then**
      $\underline{\mathsf{u}}_i^{\ell+1} \leftarrow A_i \hat{A}_a^T \underline{\mathsf{u}}_a^{\ell+1} \quad i \in G$ {Scatter}
      $\underline{\mathsf{c}}_p^\ell \leftarrow P_p^\ell \underline{\mathsf{u}}_p^{\ell+1}$ {Prolongate correction}
      $\underline{\mathsf{u}}_p^\ell \leftarrow \underline{\mathsf{u}}_p^\ell + \underline{\mathsf{c}}_p^\ell$ {Add correction}
      $\underline{\mathsf{u}}_p^\ell \leftarrow J_p^\ell(\underline{\mathsf{u}}_p^\ell, \underline{\mathsf{f}}_p^\ell)$ {Post-smooth}
    end if
  else
    if $active_p[L] = true$ **then**
      $\underline{\mathsf{u}}_p^L \leftarrow (\mathsf{K}_p^L)^{-1} \underline{\mathsf{f}}_p^L$ {Direct solve}
    end if
  end if

Benchmarks 1



Benchmarks 2



Hybrid MPI/OpenMP Parallelization

- Increase the number of OpenMP threads per MPI process
  - SuperMuc Thin Node: 16 cores, 32 GB RAM
  - SuperMuc Fat Node: 40 core, 256 GB RAM
- Pin OpenMP threads to computing tasks
  - Desktop: OpenMPI rankfiles
  - Server: OpenMPI rankfiles, Custom modules
- Advantage: More computing tasks with less communication

Motivation

Matrix-Vector benchmarks:

	runtime		speedup	
# cores	OMP	MPI	OMP	MPI
1	4.579	4.336	1.00	1.00
2	2.306	2.161	1.99	2.01
4	1.347	1.123	3.40	3.86
6	1.133	1.009	4.04	4.30
12	0.565	0.378	8.10	11.48

OpenMP kernels show reduced computational efficiency

Implementation

- OpenMP parallelization only for computational kernels
- Independent of MPI parallelization
- Scheduler of choice: **guided**
  - Background load should be assumed $\rightarrow$ dynamic scheduling usually better
  - Optimal chunksize unknown or varying $\rightarrow$ guided scheduling decreases the chunksize linearly to a defined minimum size
- Optimal number of threads per process is hardware and problem dependent
- Parallelization across multiple CPUs disadvantageous

Benchmarks

Reduced number of MPI processes is advantageous for a large number of threads.