A General Concept for the Construction and Parallelization of Algebraic Multigrid Methods

Gundolf Haase Ulrich Langer Stefan Reitzinger

Department for Computational Mathematics and Optimization
Institute for Analysis and Computational Mathematics
Johannes Kepler University Linz

http://www.numa.uni-linz.ac.at http://www.sfb013.uni-linz.ac.at

{ghaase,ulanger}@numa.uni-linz.ac.at reitz@sfb013.uni-linz.ac.at

This work has been supported by the Austrian Science Found under the grand 'Fonds zur Förderung der wissenschaftlichen Forschung (FWF)' - SFB F013 'Numerical and Symbolic Scientific Computing'

Outline

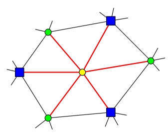
Problem Formulation - Linear System

Find $\underline{u}_h \in \mathbb{R}^{N_h}$ such that

$$K_h \underline{u}_h = \underline{f}_h$$

$$\begin{pmatrix} k_{ii} & 0 & 0 & 0 \\ 0 & k_{jj} & 0 & k_{jl} \\ 0 & 0 & k_{kk} & 0 \\ 0 & k_{lj} & 0 & k_{ll} \end{pmatrix}$$

1. System matrix $K_h \in \mathbb{R}^{N_h \times N_h}$ is
   (a) symmetric, positive definite (SPD)
   (b) sparse
   (c) stems from a finite element (FE) discretization
   (d) $(K_h)_{ij} = k_{ij} \in \mathbb{R}^{n \times n}$
2. Right-hand side $\underline{f}_h \in \mathbb{R}^{N_h}$
3. Number of unknowns $N_h = G_h \cdot n$
4. Construction of an iterative solver



Problem Formulation - Examples

Let $\Omega \subset \mathbb{R}^d$, $D \in \mathbb{R}^{m\times m}$ be SPD.

1. **Potential Equation**: $\int_\Omega \operatorname{grad} v^T D \operatorname{grad} u \, dx = \int_\Omega f v \, dx$

   $\mathbb{V} = H^1(\Omega)$, $\mathbb{V}_B = H^1_0(\Omega)$, $\mathbb{V}_h$: Lagrange FE-functions
   $\mathbb{V}_0 = \{b \,:\, b \in \mathbb{R}\}$

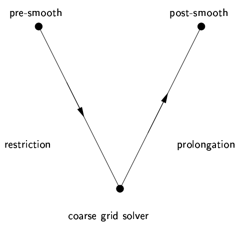
2. **Linear Elasticity**: $\int_\Omega \epsilon(\mathbf{v})^T D \epsilon(\mathbf{u}) \, dx = \int_\Omega \mathbf{f} \mathbf{v} \, dx$

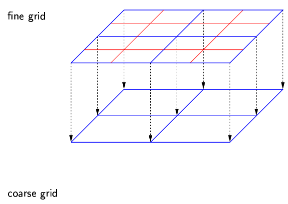
   $\mathbb{V} = (H^1(\Omega))^d$, $\mathbb{V}_B = (H^1_0(\Omega))^d$, $\mathbb{V}_h$: Lagrange FE-functions
   $\mathbb{V}_0 = \{\mathbf{a} \times \mathbf{x} + \mathbf{b} \,:\, \mathbf{a}, \mathbf{b} \in \mathbb{R}^d\}$

3. **Linear Magnetostatics**: $\int_\Omega \operatorname{curl} \mathbf{v}^T D \operatorname{curl} \mathbf{u} + \sigma \mathbf{u}\mathbf{v} \, dx = \int_\Omega \mathbf{f}\mathbf{v} \, dx$

   $\mathbb{V} = H(\operatorname{curl}, \Omega)$, $\mathbb{V}_B = H_0(\operatorname{curl}, \Omega)$, $\mathbb{V}_h$: Nedélćc FE-functions
   $\mathbb{V}_0 = \operatorname{grad} H^1_0(\Omega)$ if $\sigma = 0$

Multigrid Methods - Principle





Objective: Optimal iterative solver (memory, CPU-time)

Remark: A recursive application leads to a multilevel cycle

Algebraic Multigrid Methods - General

Objective: Construction of a multigrid cycle by using the system matrix and the right-hand side.

Motivation: no hierarchical grid, coarse grid is very large, ...

Selected papers:

1. A. Brandt, S. McCormick, J.W. Ruge [1982]
2. J.W. Ruge, K. Stüben [1986]
3. D. Braess [1995]
4. P. Vanek, J. Mandel, M. Brezina [1996]
5. F. Kickinger [1998], F. Kickinger, U. Langer [1998]
6. J. Jones et al. [2000]

Algebraic Multigrid Methods - Problems

1. M-matrix property is often lost
2. AMG method for systems of equations
3. AMG method for magnetostatic problems
4. Parallel version of AMG

Idea: We use additionally the **single grid information** (e.g. underlying PDE, FE-discretization, ...).

Components of an AMG Method

1. **Coarsening strategy**

   split the degrees of freedom into fine and coarse grid nodes

2. **Transfer operators**

   prolongation $P_h : V_H \mapsto V_h$, restriction $R_h = (P_h)^T : V_h \mapsto V_H$

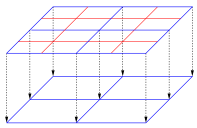
3. **Coarse grid operator**

   Galerkin's method: $K_H = P_h^T K_h P_h$

4. **Smoothing operator**

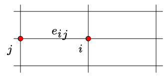
   Jacobi method
   Gauss-Seidel method

General Approach to AMG



Definition of an auxiliary matrix

$$(B_h)_{ij} = \begin{cases} b_{ij} \leq 0 & i \neq j \\ -\sum_{i \neq j} b_{ij} \geq 0 & i = j \end{cases}$$



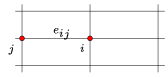
1. Distance of two grid points is represented
2. Operator D is represented

Example: anisotropic potential equation $b_{ij} = -\frac{1}{\|e_{ij}\|_D}$

Remark: B_h is by construction an M-matrix
If K_h is an M-matrix: $B_h \equiv K_h$

Auxiliary Matrix

Interpretation of B_h



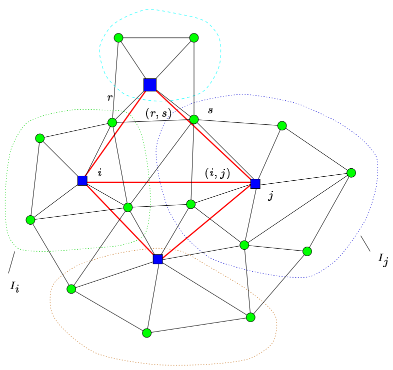
1. b_{ii} represents a node
2. b_{ij} represents an edge

Coarse auxiliary matrix (sparse, M-matrix)

$$B_H = (P_h^B)^T B_h P_h^B$$

1. Definition of P_h^{sys} depends on P_h^B
2. "Node to edge map" for edge FE-elements

Coarsening



Transfer Operators

We define 3 different prolongation operators:

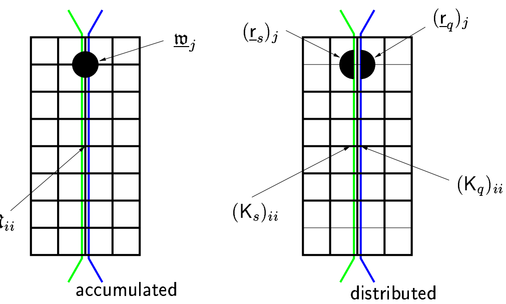
1. Prolongation for the system matrix: P_h^{sys}
2. Prolongation for the kernel of the system matrix: P_h^{ker}
3. Prolongation for the auxiliary system: P_h^B

Remark: A necessary condition for the prolongation operators can be shown, in order to preserve the "qualitative" properties of the underlying equation.

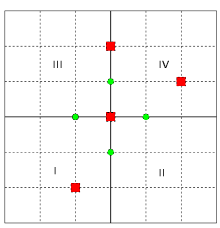
Transfer Operators - Examples

1. Potential Equation:
   $P_h^{sys} = P_h^{ker} = P_h^B \in \mathbb{R}^{N_h \times N_H}$
2. Linear Elasticity:
   $P_h^{sys} = P_h^{ker} \in \mathbb{R}^{N_h \times N_H}$, $P_h^B \in \mathbb{R}^{G_h \times G_H}$
3. Linear Magnetostatics:
   $P_h^{sys} \in \mathbb{R}^{N_h \times N_H}$, $P_h^{ker} = P_h^B \in \mathbb{R}^{G_h \times G_H}$

Parallel Version - Data Types



Parallel Version - Principle



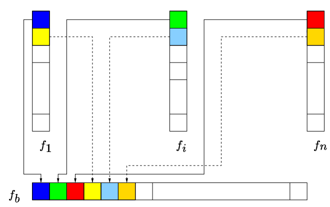
1. Coarsening is performed in an "hierarchical" way
2. Prolongation operator has to fulfill a pattern condition
3. A recursive application leads to a multilevel cycle

Simultaneous Right-Hand Sides

Motivation: Solution of a linear equation for n linear independent right-hand sides.

CPU-time for one right-hand side t: $t_n = n \cdot t$.

Memory management of the right-hand sides



Numerical Results

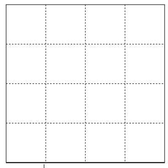
1. Implementation in the AMG program package PEBBLES
   Parallel **E**lement **B**ased grey **B**ox **L**inear **E**quation **S**olver
2. Interface to FE-codes
3. AMG preconditioner for the PCG method
4. $V(1,1)$ or $V(2,2)$ cycle
5. $K_h C_h^{-1} K_h$-energy norm, relative accuracy ε
6. SGI Octane or SGI ORIGIN 2000, 300 MHz

Anisotropic Equation

$\int_\Omega \operatorname{grad} v^T D \operatorname{grad} u \, dx$

$D = \begin{pmatrix} 1 & 0 \\ 0 & \epsilon \end{pmatrix}$

$\varepsilon = 10^{-8}$



$u = 0$

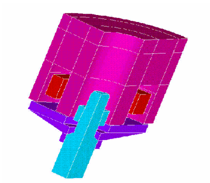
		AMG with AUX			AMG		
N_h	ϵ	it	OC	GC	it	OC	GC
10201		20	1.90	1.91	30	3.11	1.79
40401	10^{-1}	21	1.91	1.92	38	3.14	1.79
90601		33	1.91	1.92	47	3.16	1.80
10201		25	1.96	1.99	442	3.11	1.79
40401	10^{-3}	26	1.97	1.99	-	3.14	1.79
90601		25	1.98	2.00	-	3.16	1.80

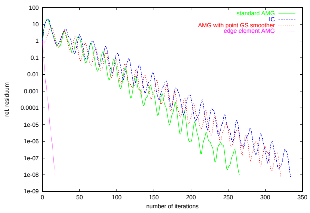
Magnetostatic Valve

$\int_\Omega \nu \operatorname{curl} \mathbf{u} \operatorname{curl} \mathbf{v} + \sigma \mathbf{uv} \, dx$

$\sigma = 10^{-4}$

$\varepsilon = 10^{-8}$





N_h	it	setup	solver
8714	14	0.53	2.49
65219	28	4.17	44.01
504246	63	34.49	792.49

Parallel Results - Crank Shaft

$\int_\Omega \operatorname{grad} u \operatorname{grad} v \, dx$

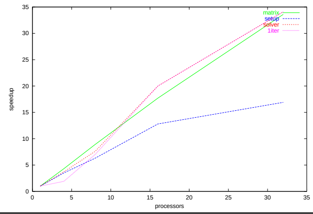
$\varepsilon = 10^{-4}$

$N_h = 576833$

SGI ORIGIN 2000

proc	it	matrix	setup	solver	solution
1	14	134.3	179.2	187.7	501.2
4	14	31.0	51.6	51.1	133.4
8	13	15.0	28.4	24.8	68.2
16	14	7.6	12.2	9.4	23.9
32	14	4.0	10.6	5.5	20.1

↑ CPU-times in seconds



← Speed up

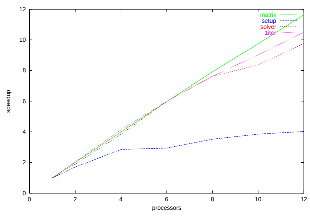
Parallel Results - Inverse Source Reconstruction

$\int_\Omega \mu \operatorname{grad} u \operatorname{grad} v \, dx$

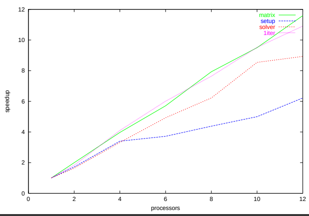
$\Omega =$ humain head

$\varepsilon = 10^{-8}$

SGI ORIGIN 200



↑ Tetrahedra, $N_h = 118299$



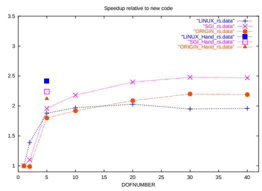
← Hexahedra, $N_h = 325384$

Simultaneous Right-Hand Sides

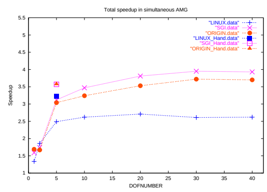
$\int_\Omega \mu \operatorname{grad} u \operatorname{grad} v \, dx$

$\Omega = (0,1)^2$

$\varepsilon = 10^{-8}$



↑ Simultaneous right-hand sides



← Total performance gain

Summary

1. General approach to AMG methods
2. Necessary condition for the prolongation operator
3. Parallel version
4. Simultaneous right-hand sides
5. Realized in the AMG software package PEBBLES
6. Numerical studies show an efficient and flexible preconditioner
7. Application to other discretization schemes (FIT, BEM, ...)