Technische Universität Braunschweig

Partitioned Methods for Multifield Problems

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Motivating example: Heat equation

- Consider the one-dimensional heat equation

$$\dot{u} - u'' = -\exp(-t)(x^2 + 2)$$

  with Dirichlet boundary conditions
- Exact solution: $u(t) = 1 + \exp(-t)x^2$
- space discretisation: central differences
- time discretisation: fully implicit Runge–Kutta method with s internal stages
- Aim: Compute one timestep

Introduction

Coupled linear system:

$$\begin{pmatrix} A_{11} & \dots & A_{1n} \\ \vdots & & \vdots \\ A_{n1} & \dots & A_{nn} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \vdots \\ \mathbf{b}_n \end{pmatrix},$$

where $A_{ij} \in \mathbb{R}^{n_i, n_j}$ and $\mathbf{b}_i, \mathbf{x}_i \mathbb{R}^{n_i}$.

- Let $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top$ and $\mathbf{b} = (\mathbf{b}_1, \dots, \mathbf{b}_n)^\top$.
- Moreover A is the matrix containing of the blocks A_{ij}.
- Let the matrix A be regular.

Introduction

- monolythical approach: Solve $A\mathbf{x} = \mathbf{b}$ by a direct or an iterative method.
- Partitioned method: Solve

$$A_{ii}\mathbf{x}_i = \mathbf{b} - \sum_{\substack{j=0 \\ j \neq i}}^{n} A_{ij}\mathbf{x}_j$$

is solved w.r.t. $\mathbf{x}_i$.
Since the other components of $\mathbf{x}$ are not known in general, an iterative loop is needed to get an accurate numerical solution.

Example

2 × 2-block system:

$$A_{11}\mathbf{x}_1 + A_{12}\mathbf{x}_2 = \mathbf{b}_1 \tag{1}$$
$$A_{21}\mathbf{x}_1 + A_{22}\mathbf{x}_2 = \mathbf{b}_2. \tag{2}$$

In the first step we solve (1) w.r.t. $\mathbf{x}_1$, i. e.

$$\mathbf{x}_1 = A_{11}^{-1}(\mathbf{b}_1 - A_{12}\mathbf{x}_2).$$

Next we communicate the solution $\mathbf{x}_1$ from software 1 to software 2. Then we can solve equation (1) w.r.t. $\mathbf{x}_2$ and get

$$\mathbf{x}_2 = (A_{22} - A_{21}A_{11}^{-1}A_{12})^{-1}(\mathbf{b}_2 - A_{21}A_{11}^{-1}\mathbf{b}_1).$$

Block–Jacobi method

1. Set $\nu := 0$ and choose an initial guess $\mathbf{x}^{(0)} = (\mathbf{x}_1^{(0)}, \mathbf{x}_2^{(0)})$.
2. Solve (1) w.r.t. $\mathbf{x}_1$, i. e.
$$A_{11}\mathbf{x}_1^{(\nu+1)} = \mathbf{b}_1 - A_{12}\mathbf{x}_2^{(\nu)}.$$
3. Solve (2) w.r.t. $\mathbf{x}_2$, i. e.
$$A_{22}\mathbf{x}_2^{(\nu+1)} = \mathbf{b}_2 - A_{21}\mathbf{x}_1^{(\nu)}.$$
4. Set $\nu := \nu + 1$
5. Compute the residuum
$$r^{(\nu)} := A\mathbf{x}^{(v)} - \mathbf{b}.$$
6. If $\|r^{(\nu)}\|$ is sufficiently small, then stop. Otherwise compute $\mathbf{x}^{(v+1)}$.

This method is called Block–Jacobi method or simultaneous iteration method

Block-Gauß–Seidel method

1. Set $\nu := 0$ and choose an initial guess $\mathbf{x}^{(0)} = (\mathbf{x}_1^{(0)}, \mathbf{x}_2^{(0)})$.
2. Solve (1) w.r.t. $\mathbf{x}_1$, i. e.
$$A_{11}\mathbf{x}_1^{(\nu+1)} = \mathbf{b}_1 - A_{12}\mathbf{x}_2^{(\nu)}.$$
3. Solve (2) w.r.t. $\mathbf{x}_2$, i. e.
$$A_{22}\mathbf{x}_2^{(\nu+1)} = \mathbf{b}_2 - A_{21}\mathbf{x}_1^{(\nu+1)}.$$
4. Set $\nu := \nu + 1$
5. Compute the residuum
$$r^{(\nu)} := A\mathbf{x}^{(v)} - \mathbf{b}.$$
6. If $\|r^{(\nu)}\|$ is sufficiently small, then stop. Otherwise compute $\mathbf{x}^{(v+1)}$.

This method is called Block–Gauß–Seidel method or sucessive iteration method.

Example

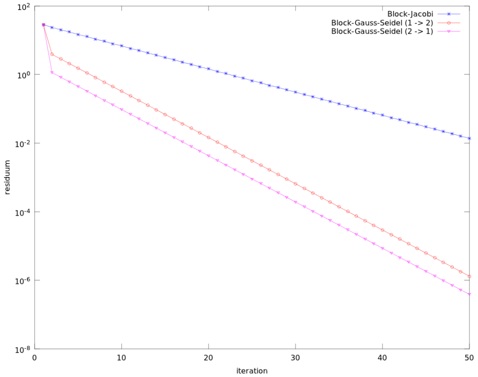
Let

$$A_{11} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}, \quad A_{12} = 0.4 \begin{pmatrix} 10 & 1 \\ 10 & 1 \end{pmatrix}$$
$$A_{21} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad A_{22} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

and let

$$b_1 = \begin{pmatrix} 17.6 \\ 18.6 \end{pmatrix}, \quad b_2 = \begin{pmatrix} 13 \\ 14 \end{pmatrix}.$$

Result


Block-Jacobi
Block-Gauss-Seidel (1 -> 2)
Block-Gauss-Seidel (2 -> 1)
residuum
iteration
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
0
10
20
30
40
50

Blockform of linear iteration methods

Notation:

- Let $A, B \in \mathbb{R}^{n,n}$ be given matrices.
- $A \geqslant B$, if $a_{ij} \geqslant b_{ij}$ holds for all $i, j \in \{1, \ldots, n\}$.
- $A \leqslant B$, if $a_{ij} \leqslant b_{ij}$ holds for all $i, j \in \{1, \ldots, n\}$.
- A is called nonnegative, if $A \geqslant 0$,
- A is called positive, if $A > 0$,
- A is called monotone, if $A\mathbf{x} \geqslant 0$ implies $\mathbf{x} \geqslant 0$.

Theorem: A matrix A is monotone, if and only if A is regular with $A^{-1} \geqslant 0$.

Proof: see Axelsson (1996)

Definition

- A matrix A with $A = (a_{ij})$ is called a (nonsingular) M-Matrix, if $a_{ij} \leqslant 0$ for $i \neq j$ and if it is monotone, i. e. $A^{-1} \geqslant 0$.
- By $M(A) = (m_{ij}(A))$ we denote the comparison matrix given by

$$m_{ij}(A) := \begin{cases} |a_{ij}|, & \text{if } i = j \\ -|a_{ij}|, & \text{if } i \neq j \end{cases} .$$

- If $M(A)$ is a M-Matrix, then A is called H-matrix.

Example

Let

$$A = \begin{pmatrix} 2 & -1 & 0 \\ -2 & 3 & 1 \\ -1 & 0 & 1 \end{pmatrix}.$$

Then

$$M(A) = \begin{pmatrix} 2 & -1 & 0 \\ -2 & 3 & -1 \\ -1 & 0 & 1 \end{pmatrix}$$

is a M-Matrix and it follows that A is an H-matrix.

Splittings

types of splittings: Let $C, \tilde{R} \in \mathbb{R}^{n,n}$ be matrices. Then the matrix $A = C - \tilde{R}$ is called:

- a regular splitting, if C is monotone and $\tilde{R} \geqslant 0$ (see Varga (1963))
- a weak regular splitting, if C is monotone and $C^{-1}\tilde{R} \geqslant 0$ (see Ortega and Rheinboldt (1970))
- a nonnegative splitting, if C is regular and $C^{-1}\tilde{R} \geqslant 0$ (see Beauwens (1979) and Song (1991))
- a convergent splitting, if C is regular and $\rho(C^{-1}\tilde{R}) < 1$.

Block-iterative methods

Let A be a M-matrix with $a_{ij} \leqslant 0$ for $i \neq j$. Moreover let A be of the form

$$A = \begin{pmatrix} D_1 & A_{12} & \dots & A_{1n} \\ A_{21} & D_2 & \dots & A_{2n} \\ \vdots & & \ddots & \vdots \\ A_{1n} & A_{n2} & \dots & D_n \end{pmatrix},$$

where $D_i \in \mathbb{R}^{n_i,n_i}$. It can be shown that D_i is regular and $D_i^{-1} \geqslant 0$.
Let $D_A := \operatorname{diag}(D_1, \dots, D_n)$. Then we have $D_A^{-1} \geqslant 0$.

Theorem

Let $A = C - \tilde{R}$ be a weak regular splitting. Then the splitting is convergent if and only if A is monotone.

Proof: Axelsson (1996)

Block–Jacobi method

- Splitting: $\tilde{R} = D_A - A$, i. e. $C := D_A$.
- Then it follows $C^{-1} = D_A^{-1} \geqslant 0$ and the matrix C is monotone.
- Moreover we have $\tilde{R} \geqslant 0$.
- All these conclusions show us that $C - \tilde{R}$ is a regular splitting.

(Block) Jacobi method or simultaneous iteration method:

$$D_A \mathbf{x}^{(k+1)} = (D_A - A)\mathbf{x}^{(k)} + \mathbf{b}.$$

Block–Gauß–Seidel method

Splitting: $A := D - L - U$ with $l_{ij} = -a_{ij}$ for $i < j$ and $u_{ij} = -a_{ij}$ for $i > j$. Let $C := D - L$. Then we have

$$C^{-1} = (D - L)^{-1} = \left[D\left(I - D^{-1}L\right)\right]^{-1}$$
$$= \left(I - D^{-1}L\right)^{-1} D^{-1} = \sum_{i=0}^{\infty} \left(D^{-1}L\right)^{i} D^{-1} \geqslant 0.$$

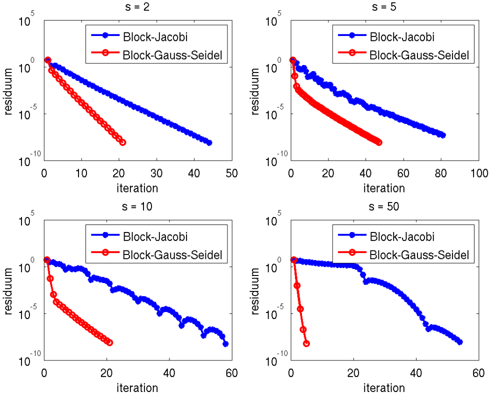
Moreover we have $U \geqslant 0$ and finally we have proven that $A = C - \tilde{R}$ with $\tilde{R} = U$ is a regular splitting. This approach is called (block) Gauß–Seidel method or sucessive iteration method and is given by

$$(D - L)\mathbf{x}^{(k+1)} = U\mathbf{x}^{(k)} + \mathbf{b}.$$

Contents

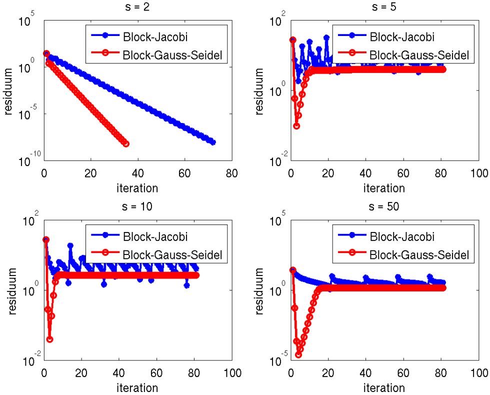
Heat equation

- space discretisation: $n = 20$
- time stepsize: $\tau = 0.01$



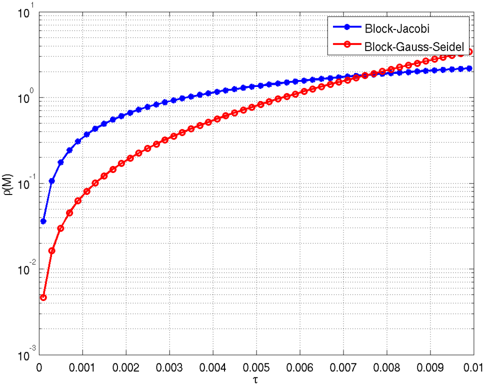
Heat equation

- space discretisation: $n = 50$
- time stepsize: $\tau = 0.01$



Heat equation: spectral radius

space discretisation: $n = 50$



Example

- Consider the problem

$$\begin{cases} -u'' &= f, \qquad x \in (0,1) \\ u &= 0, \qquad x \in \{0,1\} \end{cases}$$

- Exact solution:

$$u(x) = \frac{x(1-x)}{(x-1/4)+1/10}$$

- Then:

$$f(x) = -160\frac{3200x^3+3100x^2-3120x+351}{(80x^2-40x+13)^2}$$

- Space discretisation: central differences

Monolythical approach

discrete system: $A_h\mathbf{u}_h = \mathbf{f}_h$

n	$\|\mathbf{u}^h - \mathbf{u}\|$	CPU
100	2.9E-4	0.008
200	7.4E-5	0.04
400	1.9E-5	0.02

Partititioned approach (Block–Gauß–Seidel method)

discrete system:

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}^{(1)} \\ \mathbf{u}^{(2)} \end{pmatrix} = \begin{pmatrix} \mathbf{f}^{(1)} \\ \mathbf{f}^{(2)} \end{pmatrix}$$

with

$$A_{11} = A_{22} = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & & & 0 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 0 & & & 1 & -2 \end{pmatrix}$$

$$(A_{12})_{ij} = (A_{21})_{ij}^{\top} = \begin{cases} 1, & i = n, j = 1 \\ 0, & \text{else} \end{cases}$$

Partititioned approach

Block–Gauß–Seidel method:

n	$\|\mathbf{u}^h - \mathbf{u}\|$	Iterations	CPU	ρ
100	4.1E-4	472	0.04	0.98
200	1.0E-4	938	0.13	0.99
400	2.6E-5	1870	0.44	0.995

A parallel ansatz

- Idea: Split the domain into $(0, 1/2)$ and $(1/2, 1)$
- At $x = 1/2$ we require

$$u_{left}(1/2) = u_{right}(1/2),$$
$$u'_{left}(1/2) = u'_{right}(1/2),$$

Time-dependent problem

- Consider the problem

$$\begin{cases} \dot{u} - u'' = f, & (t,x) \in (0,1)^2 \\ u = 0, & t \in (0,1), x \in \{0,1\} \\ u = u_0(x), & x \in (0,1) \end{cases}$$

- Space discretisation: central differences
- Time discretisation: backward Euler method
- discrete problem:

$$(I - \tau A)\mathbf{u}_{m+1}^h = \mathbf{u}_m^h + \tau \mathbf{f}(t_{m+1})$$

- Here: spectral radius ρ depends on τ.

Literature

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- Yongzhong Song. Comparisons of nonnegative splittings of matrices. *Linear Algebra Appl.*, 154-156:433–455, 1991.
- R.S. Varga. *Matrix iterative analysis*. Series in Automatic Computation. Prentice-Hall, 1963.

BiCGStab method

- Iterative methods which convergece faster than the Jacobi, the Gauss–Seidel and SOR-method are cg-schemes (conjugient gradient schemes).
- These methods are based on optimization ideas, i.e. in each iteration step one or more search vectors are computed which minimises the residuum.
- In this lecture we only introduce the BiCGStab method.

BiCGStab method (I)

Let $\mathbf{x}^{(0)}$ be an initial guess for the solution of the linear system $A\mathbf{x} = \mathbf{b}$ and let

$$\mathbf{r}^{(0)} = A\mathbf{x}^{(0)} - \mathbf{b}$$

be the initial residuum. Set $\tilde{\mathbf{r}}^{(0)} := \mathbf{r}^{(0)}$ and $\mathbf{p}^{(0)} := \mathbf{r}^{(0)}$. Calculate $\rho^{(0)} := (\mathbf{r}^{(0)}, \tilde{\mathbf{r}}^{(0)})$.
Let ϵ be a given tolerance. If $\|\mathbf{r}^{(0)}\| \leqslant \epsilon$ then stop.

BiCGStab method (II)

Otherwise we iterate from $k = 0$ to $n - 2$ and compute

$$\mathbf{s}^{(k)} = A\mathbf{p}^{(k)}, \quad \sigma^{(k)} = (\mathbf{s}^{(k)}, \tilde{\mathbf{r}}^{(0)}), \quad \text{stop, if } \sigma^{(k)} = 0.$$

$$\alpha^{(k)} = \frac{\rho^{(k)}}{\sigma^{(k)}}, \quad \mathbf{w}^{(k)} = \mathbf{r}^{(k)} - \alpha^{(k)}\mathbf{s}^{(k)}, \quad \mathbf{v}^{(k)} = A\mathbf{w}^{(k)}, \quad \omega^{(k)} = \frac{(\mathbf{v}^{(k)}, \mathbf{w}_k)}{(\mathbf{v}^{(k)}, \mathbf{v}^{(k)}}$$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)}\mathbf{p}^{(k)} - \omega^{(k)}\mathbf{w}^{(k)}$$

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha^{(k)}\mathbf{s}^{(k)} - \omega^{(k)}\mathbf{v}^{(k)}$$

$$\rho^{(k+1)} = (\mathbf{r}^{(k+1)}, \tilde{\mathbf{r}}^{(0)})$$

If $\|\mathbf{r}^{(k+1)}\| \leqslant \epsilon \mathbf{r}^{(0)}$ then stop. Otherwise compute the new search vectors

$$\beta^{(k)} = \frac{\rho^{(k+1)}}{\rho^{(k)}} \frac{\alpha^{(k)}}{\omega^{(k)}}, \quad \mathbf{p}^{(k+1)} = \mathbf{r}^{(k+1)} + \beta^{(k)}(\mathbf{p}^{(k)} - \omega^{(k)}\mathbf{s}^{(k)}).$$

Example

- Consider the problem

$$\begin{cases} -u'' &= f, \qquad x \in (0,1) \\ u &= 0, \qquad x \in \{0,1\} \end{cases}$$

- Exact solution:

$$u(x) = \frac{x(1-x)}{(x-1/4)+1/10}$$

- Then:

$$f(x) = -160\frac{3200x^3+3100x^2-3120x+351}{(80x^2-40x+13)^2}$$

- Space discretisation: central differences

Example

Dimension: 100