Preconditioned Krylov methods for incompressible flow problems

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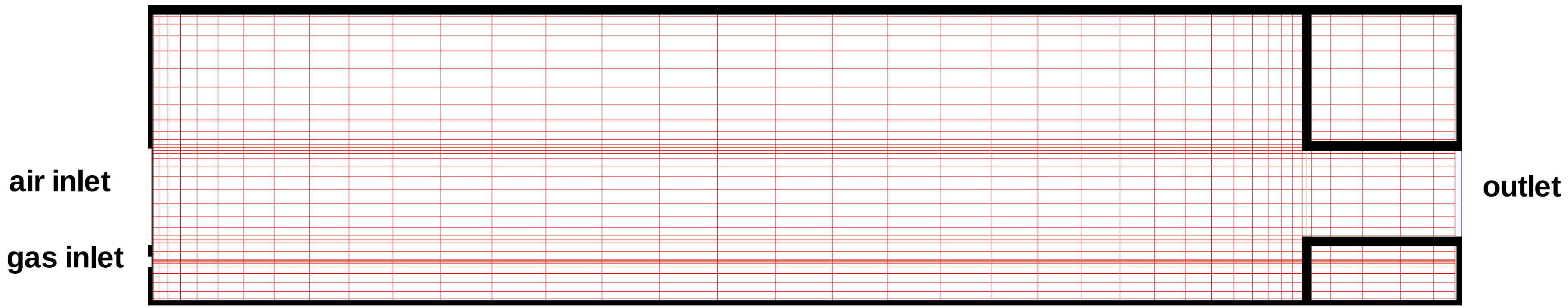
Gas-fired glass melting furnace   Combustion process

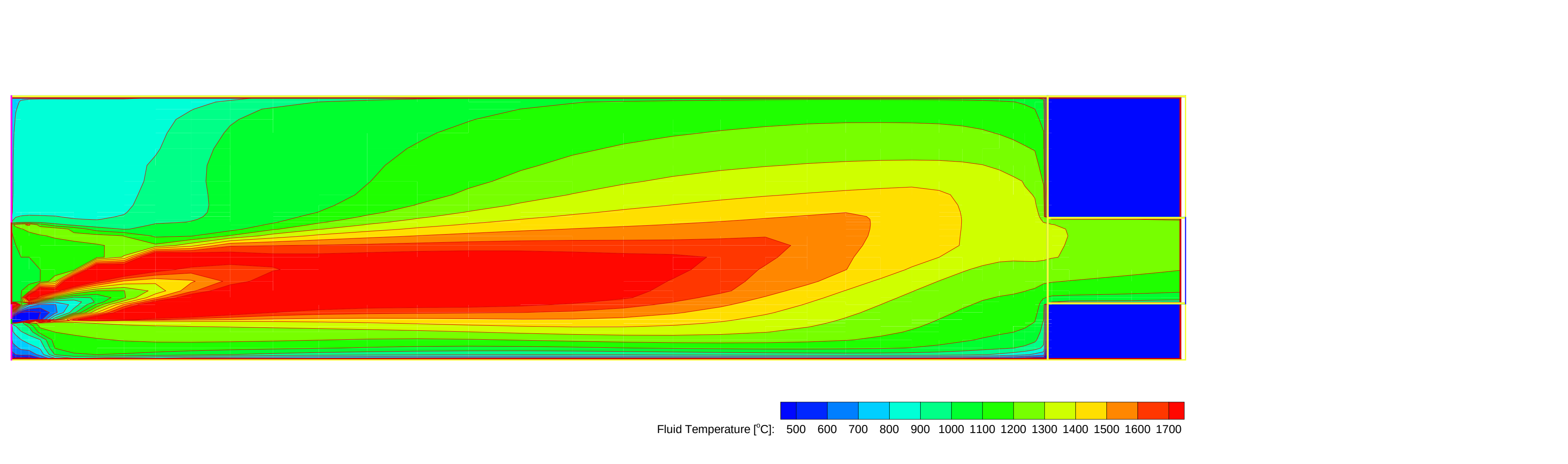
The symmetry plane of the furnace Grid: $42 \times 37 \times 27$



1. Introduction

Gas-fired glass melting furnace Combustion process

The symmetry plane of the furnace Grid: $42 \times 37 \times 27$



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Mathematical model

3D incompressible Navier-Stokes

Turbulence ($k - \varepsilon$)

Combustion

Chemistry (one step global reaction)

Radiative heat transfer

NO_x postprocessor

Soot formation

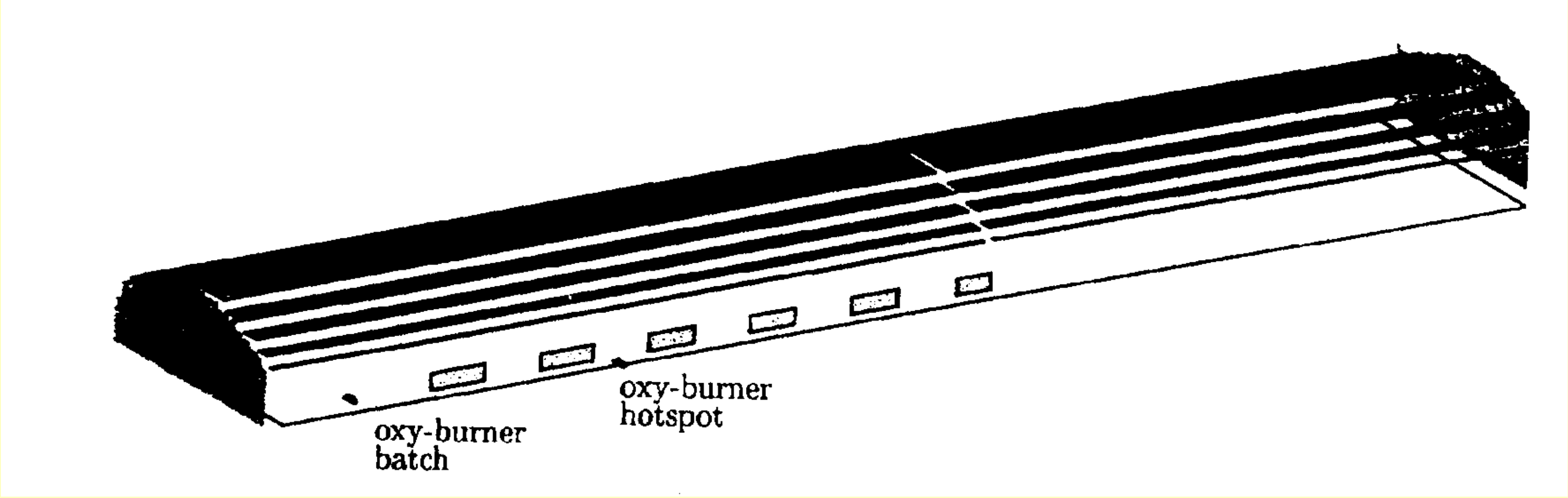
Results for the IFRF furnace

The IFRF furnace (Grid $24 \times 20 \times 16$)

method	$niter$	CPU time (hours)
SIMPLE	2047	4.8
SIMPLER	2415	6.9
GCR-SIMPLE	623	2.4
GCR-SIMPLER	578	2.0

The Ford Nashville furnace

combustion chamber dimensions: $34.7 \times 10.1 \times 2.3\ m$



grid $130 \times 40 \times 40$ = 208000 points

GCR-SIMPLER: 3390 iteration, CPU time ≈ 3.3 days

SIMPLER: not converged after 7.5 days

2. SIMPLE method

Incompressible Navier Stokes equation

$$\begin{aligned} -\nu\Delta\mathbf{u} + \mathbf{u}\cdot\text{grad}\mathbf{u} + \text{grad}p &= \mathbf{f}, \\ \text{div}\mathbf{u} &= 0. \end{aligned}$$

Finite volumes, staggered grid

$$\begin{pmatrix} \mathbf{Q}_{11} & \mathbf{Q}_{12} & \mathbf{Q}_{13} & \mathbf{G}_1 \\ \mathbf{Q}_{21} & \mathbf{Q}_{22} & \mathbf{Q}_{23} & \mathbf{G}_2 \\ \mathbf{Q}_{31} & \mathbf{Q}_{32} & \mathbf{Q}_{33} & \mathbf{G}_3 \\ \mathbf{G}_1^T & \mathbf{G}_2^T & \mathbf{G}_3^T & \mathbf{O} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ p \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Solution of the linear system

$$\begin{pmatrix} \mathbf{Q} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}, \; u \in \mathbb{R}^n \text{ and } p \in \mathbb{R}^m$$

Difficulties due to zero block

- Traditional iterative solvers fail
- SIMPLE(R) converges slowly — Patankar
- Krylov method and ILU preconditioner — Dahl, Wille, Segal, Vuik
- Multigrid acceleration — Gjesdal, Wesseling, Wittum
- Saddle point preconditioner — Elman, Silvester, Wathen

SIMPLE methods

$\mathbf{D} = diag(\mathbf{Q})$ and $\mathbf{R} = -\mathbf{G}^T\mathbf{D}^{-1}\mathbf{G}$

SIMPLE algorithm

1. Choose an initial estimate p^*.
2. Solve $\mathbf{Q}u^* = b_1 - \mathbf{G}p^*$.
3. Solve $\mathbf{R}\delta p = b_2 - \mathbf{G}^T u^*$.
4. Compute $u = u^* - \mathbf{D}^{-1}\mathbf{G}\delta p$
   and $p := p^* + \delta p$.
5. If not converged take $p^* = p$ and go to 2.

Systems are solved by a TDMA solver, use of relaxation parameters

Patankar, Spalding, Wittum, Van Doormaal, Raithby, Ferziger, Peric

Algebraic view of SIMPLE

Definitions

$$\mathbf{A} = \begin{pmatrix} \mathbf{Q} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{pmatrix}, \mathbf{B} = \begin{pmatrix} \mathbf{I} & -\mathbf{D}^{-1}\mathbf{G} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

Problem

$$\mathbf{A}x = b$$

Right-preconditioned system

$$\mathbf{AB}y = b, x = \mathbf{B}y$$

Algebraic view of SIMPLE (continued)

$$\mathbf{AB} = \begin{pmatrix} \mathbf{Q} & \mathbf{G} - \mathbf{QD}^{-1}\mathbf{G} \\ \mathbf{G}^T & R \end{pmatrix}$$

Splitting method (Gauss-Seidel)

$$\mathbf{AB} = \mathbf{M} - \mathbf{N}, \quad \mathbf{M} = \begin{pmatrix} \mathbf{Q} & \mathbf{0} \\ \mathbf{G}^T & R \end{pmatrix}$$

SIMPLE method

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

distributive iterative method Hackbusch, Wittum, Wesseling

3. Comparison with related method

A saddle point preconditioner proposed by Elman, Silvester, Wathen:

$$\mathbf{P_E} = \begin{pmatrix} \mathbf{Q} & \mathbf{G} \\ \mathbf{0} & -\mathbf{X} \end{pmatrix}^{-1}.$$

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It is easy to show that

$$\mathbf{AP_E} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{G}^T\mathbf{Q}^{-1} & \mathbf{G}^T\mathbf{Q}^{-1}\mathbf{G}\mathbf{X}^{-1} \end{pmatrix},$$

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so that the eigenvalues are: $\{1\} \cup \sigma(\mathbf{G}^T\mathbf{Q}^{-1}\mathbf{G}\mathbf{X}^{-1})$, where the algebraic multiplicity of eigenvalue 1 is equal to n.

Comparison with related method (continued)

For the SIMPLE preconditioner we have:

$$\mathbf{M}^{-1} = \begin{pmatrix} \mathbf{Q}^{-1} & \mathbf{0} \\ -\mathbf{R}^{-1}\mathbf{G}^T\mathbf{Q}^{-1} & \mathbf{R}^{-1} \end{pmatrix}.$$

Comparison with related method (continued)

For the SIMPLE preconditioner we have:

$$\mathbf{M}^{-1} = \begin{pmatrix} \mathbf{Q}^{-1} & \mathbf{0} \\ -\mathbf{R}^{-1}\mathbf{G}^T\mathbf{Q}^{-1} & \mathbf{R}^{-1} \end{pmatrix}.$$

So the iteration matrix $\mathbf{ABM}^{-1}$ can be written as:

$$\begin{pmatrix} \mathbf{I} - (\mathbf{I} - \mathbf{QD}^{-1})\mathbf{GR}^{-1}\mathbf{G}^T\mathbf{Q}^{-1} & (\mathbf{I} - \mathbf{QD}^{-1})\mathbf{GR}^{-1} \\ \mathbf{0} & \mathbf{I} \end{pmatrix},$$

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The eigenvalues of $\mathbf{ABM}^{-1}$ are: $\{1\} \cup \sigma(\mathbf{I} - (\mathbf{I} - \mathbf{QD}^{-1})\mathbf{GR}^{-1}\mathbf{G}^T\mathbf{Q}^{-1})$,

where the multiplicity of eigenvalue 1 is at least m.

Comparison with related method (continued)

SIMPLE $\begin{pmatrix} \mathbf{I} - (\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1}\mathbf{G}^T\mathbf{Q}^{-1} & (\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$

If $\mathbf{D} \to \mathbf{Q}$, the SIMPLE iteration matrix goes to $\mathbf{I}$.

Comparison with related method (continued)

SIMPLE $\begin{pmatrix} \mathbf{I} - (\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1}\mathbf{G}^T\mathbf{Q}^{-1} & (\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$

If $\mathbf{D} \rightarrow \mathbf{Q}$, the SIMPLE iteration matrix goes to $\mathbf{I}$.

Saddle point $\begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{G}^T\mathbf{Q}^{-1} & \mathbf{G}^T\mathbf{Q}^{-1}\mathbf{G}\mathbf{X}^{-1} \end{pmatrix}$

For $\mathbf{X} \rightarrow \mathbf{G}^T\mathbf{Q}^{-1}\mathbf{G}$, the Saddle point iteration matrix goes to

$$\begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{G}^T\mathbf{Q}^{-1} & \mathbf{I} \end{pmatrix}$$

Relation spectrum and convergence of Krylov solvers

Example

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad x = \begin{pmatrix} -1 \\ 1 \\ -1 \\ 1 \end{pmatrix}, \quad b = e_4 := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Relation spectrum and convergence of Krylov solvers

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Krylov space

$K_1\{A;b\} = \text{span}\{e_4\}$

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$K_1\{A;b\} = \text{span}\{e_4\}$
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$K_3\{A;b\} = \text{span}\{e_2, e_3, e_4\}$

Full GMRES requires n iterations, before convergence sets in.

4. Spectral analysis

$J := D^{-1}(D - Q)$ is the Jacobi iteration matrix for Q.

Proposition

1. 1 is an eigenvalue with algebraic multiplicity at least of m, and
2. the remaining eigenvalues are $1 - \mu_i,\ i = 1, 2, \cdots, n$, where μ_i is the i the eigenvalue of the generalized eigenvalue problem

$$Bx = \mu Zx,$$

where,

$$B = GR^{-1}G^T \in \mathbb{R}^{n \times n},\ \ Z = QJ^{-1} \in \mathbb{R}^{n \times n}.$$

Alternative analysis

The eigenvalue problem $AP^{-1}x = \lambda x$ has the same spectrum as the generalized eigenvalue problem $Ax = \lambda Px$.

For SIMPLE

$$P = MB^{-1} = \begin{pmatrix} \mathbf{Q} & \mathbf{0} \\ \mathbf{G}^T & \mathbf{R} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{D}^{-1}\mathbf{G} \\ \mathbf{0} & \mathbf{R} \end{pmatrix} = \begin{pmatrix} \mathbf{Q} & \mathbf{Q}\mathbf{D}^{-1}\mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{pmatrix}$$

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So the generalized eigenvalue problem can be written as

$$\begin{pmatrix} \mathbf{Q} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{Q} & \mathbf{Q}\mathbf{D}^{-1}\mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix}$$

Eigenvalue 1

Writing out and rearrangement yields:

$$\begin{cases} (1-\lambda)u &= -Q^{-1}Gp + \lambda D^{-1}Gp, \\ G^T(1-\lambda)u &= 0. \end{cases}$$

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Eigenvalue 1

Writing out and rearrangement yields:

$$\begin{cases} (1-\lambda)u &= -Q^{-1}Gp + \lambda D^{-1}Gp, \\ G^T(1-\lambda)u &= 0. \end{cases}$$

So 1 is an eigenvalue and the corresponding eigenvectors are

$$v_i = \begin{pmatrix} u_i \\ 0 \end{pmatrix} \in \mathbb{R}^{(n+m)}, u_i \in \mathbb{R}^n, \ i = 1, 2, \cdots, n,$$

where, $\{u_i\}_{i=1}^n$ is an arbitrary linearly independent base of $\mathbb{R}^n$.

Other eigenvalues

For $\lambda \neq 1$, combining the two equations leads to

$$-G^T Q^{-1} G p = -\lambda G^T D^{-1} G p.$$

Note that $S = -G^T Q^{-1} G$ is the Schur complement of the matrix A.

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$$-G^T Q^{-1} G p = -\lambda G^T D^{-1} G p.$$

Note that $S = -G^T Q^{-1} G$ is the Schur complement of the matrix A.

Proposition
For the SIMPLE preconditioned matrix

1. 1 is an eigenvalue with multiplicity of n, and
2. the remaining eigenvalues are defined by the generalized eigenvalue problem

$$Sp = \lambda R p.$$

Q is symmetric positive definite

The extreme eigenvalues of the generalized eigenvalue problem $Sp = \lambda Rp$ are the extreme values of:

$$\frac{p^T S p}{p^T R p} = \frac{p^T G^T Q^{-1} G p}{p^T G^T D^{-1} G p}, \quad p \neq 0, p \in \mathbb{R}^m$$

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Since G has full column rank

$$\lambda_{\max} = \max_{y \neq 0} \frac{y^T Q^{-1} y}{y^T D^{-1} y}.$$

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Since G has full column rank

$$\lambda_{\max} = \max_{y \neq 0} \frac{y^T Q^{-1} y}{y^T D^{-1} y}.$$

This implies

$$\min\left\{1, \frac{d_n}{\mu_1}\right\} \leqslant \lambda \leqslant \max\left\{1, \frac{d_1}{\mu_n}\right\}$$

where $d_n \leq \sigma(D) \leq d_1$ and $\mu_n \leq \sigma(Q) \leq \mu_1$.

5. GCR acceleration

LSQR	Paige and Saunders
GMRES	Saad and Schultz
CGS	Sonneveld
Bi-CGSTAB	Van der Vorst and Sonneveld

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5. GCR acceleration

LSQR	Paige and Saunders
GMRES	Saad and Schultz
CGS	Sonneveld
Bi-CGSTAB	Van der Vorst and Sonneveld
GCR	Eisenstat, Elman and Schultz
GMRESR	Van der Vorst and Vuik

GCR-SIMPLE

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

for k = 0, 1,...,$ngcr$

$$s^{k+1} = \mathbf{BM}_k^{-1} r^k$$
$$v^{k+1} = \mathbf{A}s^{k+1}$$

for i = 1, 2,...,k

$$v^{k+1} = v^{k+1} - (v^{k+1}, v^i)v^i, \qquad s^{k+1} = s^{k+1} - (v^{k+1}, v^i)s^i$$

end for

$$v^{k+1} = v^{k+1}/\|v^{k+1}\|_2, \qquad s^{k+1} = s^{k+1}/\|v^{k+1}\|_2$$
$$x^{k+1} = x^k + (r^k, v^{k+1})s^{k+1}$$
$$r^{k+1} = r^k - (r^k, v^{k+1})v^{k+1}$$

end for

Diagonal scaling

Dirichlet boundary conditions (velocity)

$$u_P = g_P$$

Add c_{max} to the main diagonal, add $c_{max} g_P$ to the right-hand side

GCR-SIMPLE: bad results

Diagonal scaling $\Rightarrow$ GCR-SIMPLE: good results

Eigenvalue analysis of diagonal scaling

Scale the matrix A by left multiplying with the diagonal matrix

$$\widehat{D} := \begin{pmatrix} \mathbf{D}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_R^{-1} \end{pmatrix}$$

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Eigenvalue analysis of diagonal scaling

Scale the matrix A by left multiplying with the diagonal matrix

$$\widehat{D} := \begin{pmatrix} \mathbf{D}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_R^{-1} \end{pmatrix}$$

$$\widehat{A} = \begin{pmatrix} \mathbf{I} - (\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1}\mathbf{G}^T\mathbf{Q}^{-1} & \mathbf{D}^{-1}(\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1}\mathbf{D}_R \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

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$$A = \begin{pmatrix} \mathbf{I} - (\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1}\mathbf{G}^T\mathbf{Q}^{-1} & (\mathbf{I} - \mathbf{Q}\mathbf{D}^{-1})\mathbf{G}\mathbf{R}^{-1} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

6. Numerical experiments

Incompressible Oseen equation

$$\begin{aligned} -\nu\Delta\mathbf{u} + \mathbf{w}\cdot\text{grad}\mathbf{u} + \text{grad}p &= \mathbf{f}, \\ \text{div}\mathbf{u} &= 0. \end{aligned}$$

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6. Numerical experiments

Incompressible Oseen equation

$$\begin{aligned} -\nu\Delta\mathbf{u} + \mathbf{w}\cdot\text{grad}\mathbf{u} + \text{grad}p &= \mathbf{f}, \\ \text{div}\mathbf{u} &= 0. \end{aligned}$$

Consider a channel flow for a channel with width 2 and varying length.

The Dirichlet b. c. are included as extra equations in the linear system.

We start GCR with $x_0 = 0$ and stop if $\frac{||r_k||}{||b||} \leq \epsilon$.

Influence of diagonal scaling

Staggered grid, 16×16, exact inverses are used

Stokes flow

Length	2	20	200
no scaling	26	35	17
scaling	18	22	9

Influence of diagonal scaling

Staggered grid, 16×16, exact inverses are used

Stokes flow

Length	2	20	200
no scaling	26	35	17
scaling	18	22	9

Oseen, $\nu = 0.01$, $0.1 * w$

Length	2	20	200
no scaling	21	29	15
scaling	20	30	17

Influence of diagonal scaling

Staggered grid, 16×16, exact inverses are used

Stokes flow

Length	2	20	200
no scaling	26	35	17
scaling	18	22	9

Oseen, $\nu = 0.01$, $0.1 * w$

Length	2	20	200
no scaling	21	29	15
scaling	20	30	17

Oseen, $\nu = 1$, $10 * w$

Length	2	20	200
no scaling	29	45	30
scaling	20	30	17

Comparison for Stokes

Number of iterations of the preconditioned GCR method

As Saddle Point preconditioner we take $\mathbf{X} = \gamma \mathbf{I}$ (Elman 1999).

Length	2	20	200
ILU	57	62	91
SIMPLE	18	22	9
SIMPLER	9	11	6
Elman	12	22	31

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Comparison for Oseen

Oseen, $\nu = 0.01$, $0.01 * w$

Length	2	20	200
ILU	57	63	94
SIMPLE	19	24	11
SIMPLER	9	13	7
Elman	12	25	39

Comparison for Oseen

Oseen, $\nu = 0.01,\ 0.01 * w$

Length	2	20	200
ILU	57	63	94
SIMPLE	19	24	11
SIMPLER	9	13	7
Elman	12	25	39

Oseen, $\nu = 0.01,\ 0.1 * w$

Length	2	20	200
ILU	53	91	101
SIMPLE	20	30	17
SIMPLER	8	16	12
Elman	26	49	53

Convergence plot

Incompressible Oseen equation: $\nu = 0.01$, $0.1 * w$ and Length = 200

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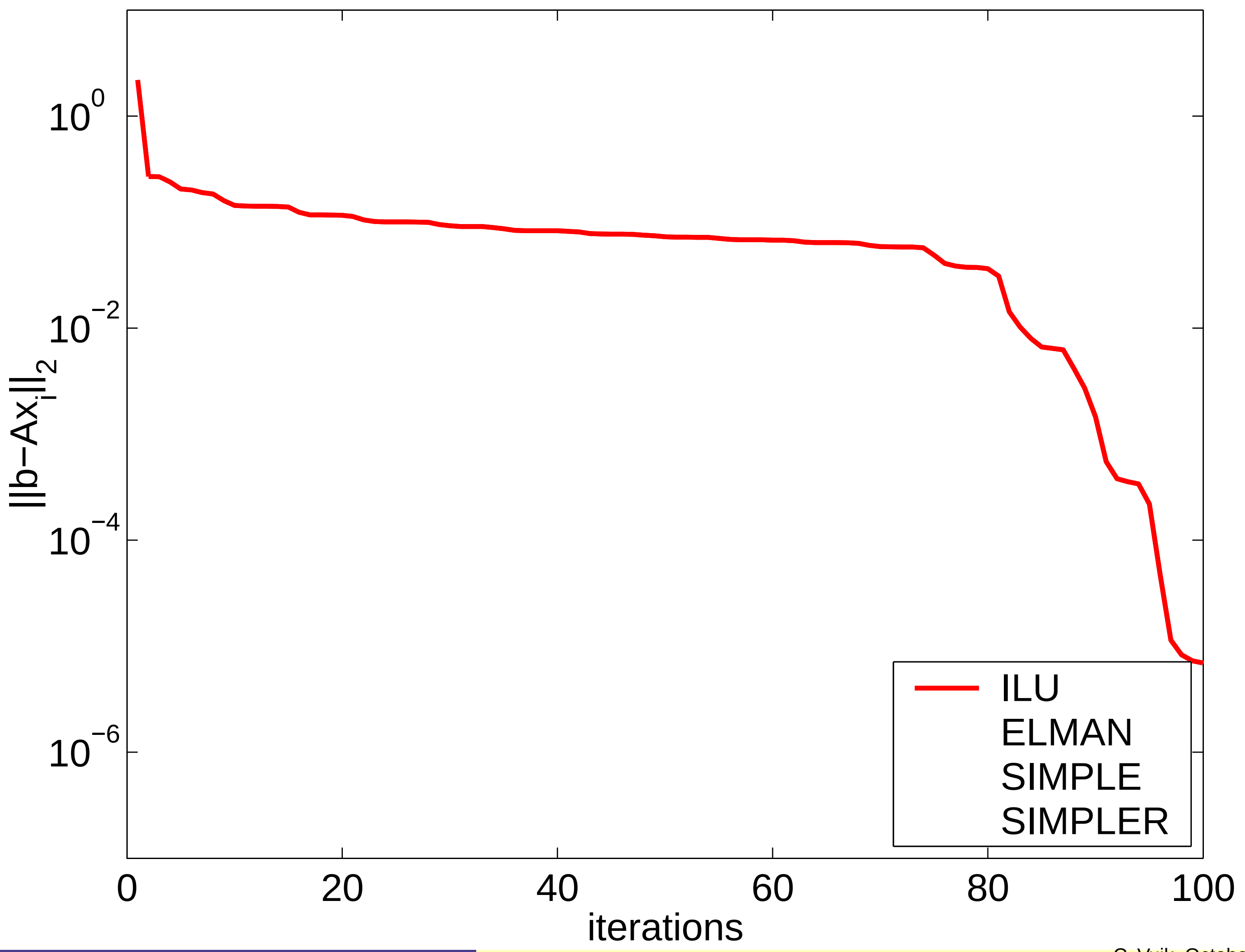
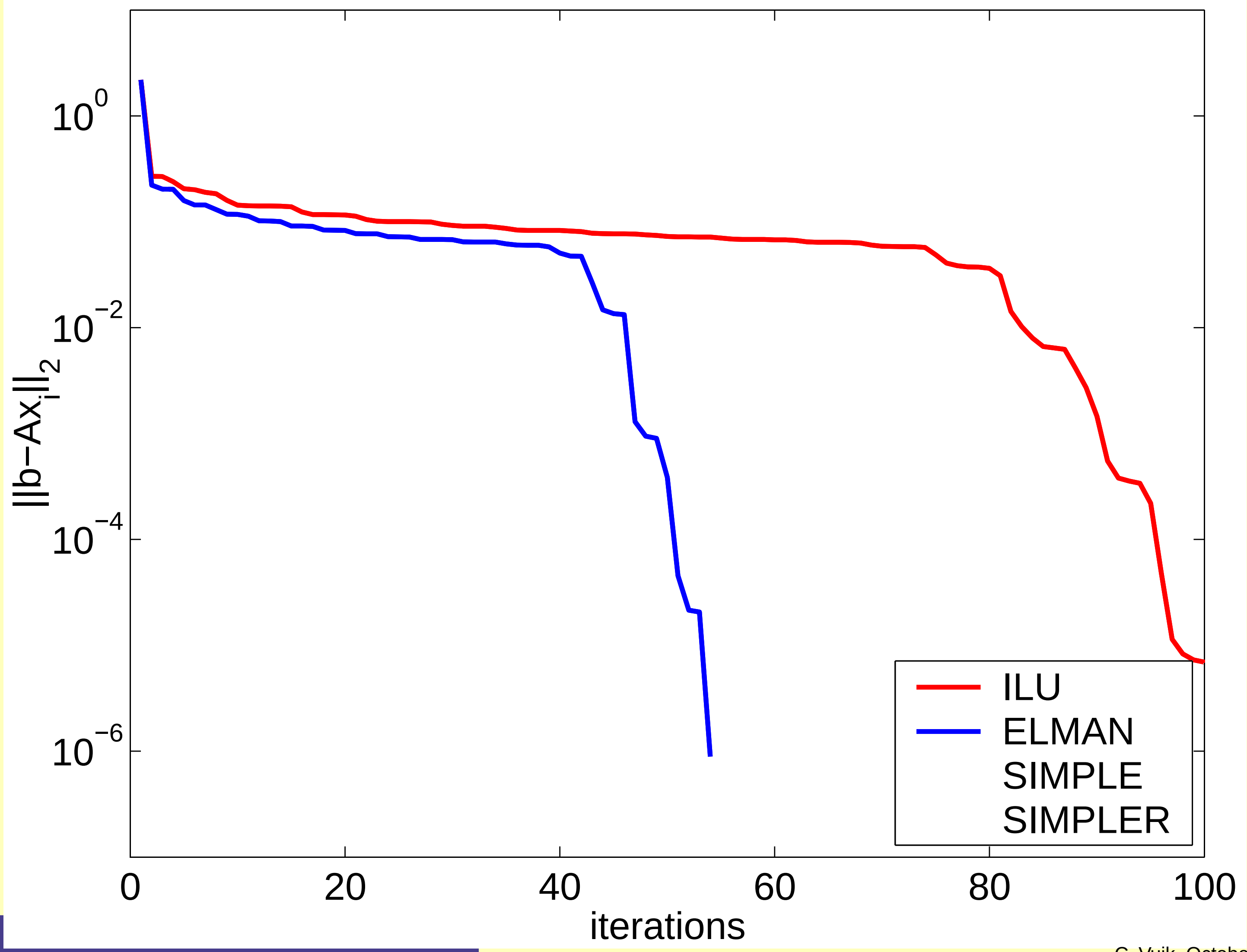
Convergence plot

Incompressible Oseen equation: $\nu = 0.01$, $0.1 * w$ and Length = 200



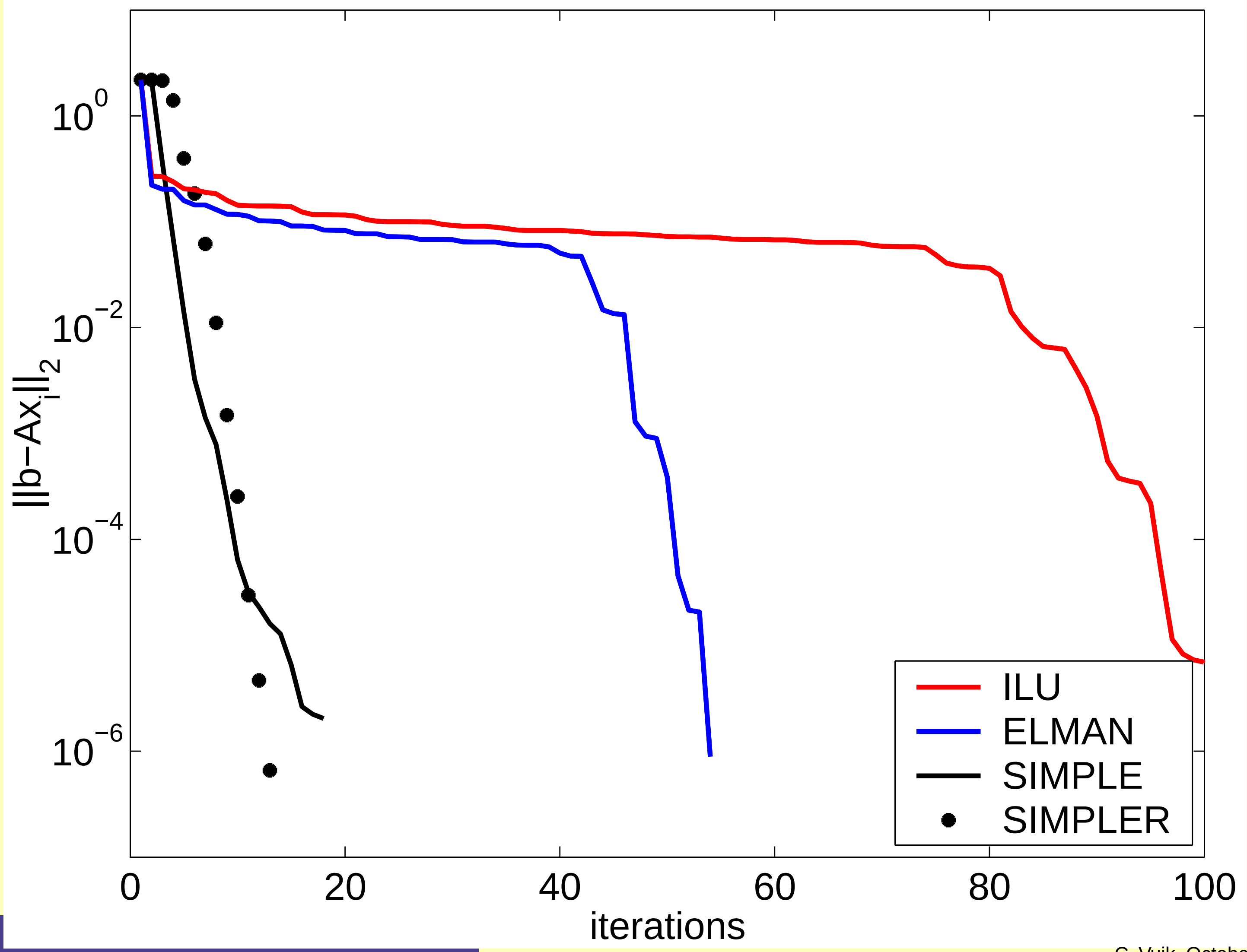
Convergence plot

Incompressible Oseen equation: $\nu = 0.01$, $0.1 * w$ and Length = 200



Convergence plot

Incompressible Oseen equation: $\nu = 0.01$, $0.1 * w$ and Length = 200



Backward facing step problem

The length is 25 and the width is 2.

We have a parabolic profile at the upper half part of the inflow boundary.

Oseen: $\mathbf{w}$ is equal to zero in the lower part of the channel and equal to the Poiseuille flow velocities in the upper part of the channel.

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The length is 25 and the width is 2.

We have a parabolic profile at the upper half part of the inflow boundary.

Oseen: $\mathbf{w}$ is equal to zero in the lower part of the channel and equal to the Poiseuille flow velocities in the upper part of the channel.

Preconditioner	Stokes	Oseen	
		$\nu = 0.25$	$\nu = 0.025$
ILU	77	77	136
SIMPLE	47	52	66
SIMPLER	16	17	18
Elman	34	41	105

7. Conclusions

- GCR-SIMPLE(R) is an efficient and robust method to simulate incompressible flows (glass-melting furnaces)
- GCR-SIMPLE(R) allows large relaxation factors
- The GCR acceleration can easily be added in an existing CFD code
- GCR-SIMPLE(R) is robust with respect to variations in the Reynolds number and stretching of the grid cells.

Further information

C. Vuik, A. Saghir and G.P. Boerstoel
The Krylov accelerated SIMPLE(R) method for flow problems in industrial furnaces
International J. for Numer. Methods in Fluids, 33, pp. 1027-1040, 2000.

C. Vuik and A. Saghir
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