A fast solver for the Navier-Stokes equations

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1

Outline

- 1. Introduction
- 2. Problem
- 3. Krylov solvers and preconditioners
- 4. ILU-type preconditioners
- 5. Block preconditioners (SIMPLE, Augmented Lagrangian)
- 6. Maritime Applications
- 7. Conclusions





2

1. Introduction



Streamlines around the stern and the axial velocity field in the wake.



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3

2. Problem

$$-\nu \nabla^2 \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = f \quad \text{in} \quad \Omega$$
$$\nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega.$$

 ${\bf u}$ is the fluid velocity vector

p is the pressure field

 $\nu > 0$ is the kinematic viscosity coefficient (1/Re).

 $\Omega \subset \mathbf{R}^{2 \text{ or } 3}$ is a bounded domain with the boundary condition:

$$\mathbf{u} = \mathbf{w} \text{ on } \partial \Omega_D, \quad \nu \frac{\partial \mathbf{u}}{\partial \mathbf{n}} - \mathbf{n}p = 0 \text{ on } \partial \Omega_N.$$

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4

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Linear system

Matrix form after linearization and discretization:

$$\begin{bmatrix} F & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

where $F \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{m \times n}$, $f \in \mathbb{R}^n$ and $m \leq n$

- $F = \nu A$ in Stokes problem, A is vector Laplacian matrix
- $F = \nu A + N$ in Picard linearization, N is vector-convection matrix
- $F = \nu A + N + W$ in Newton linearization, W is the Newton derivative matrix
- *B* is the divergence matrix
- Sparse linear system, Symmetric indefinite (Stokes problem), nonsymmetric otherwise.
- Saddle point problem having large number of zeros on the main diagonal



5

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3. Krylov Solvers and preconditioners

Direct method:

To solve Ax = b, factorize A into upper U and lower L triangular matrices (LUx = b) First solve Ly = b, then Ux = y

• <u>Classical Iterative Schemes:</u> Methods based on matrix splitting, generates sequence of iterations $x_{k+1} = M^{-1}(Nx_k + b) = Qx_k + s$, where $\mathcal{A} = M - N$ Jacobi, Gauss Seidel, SOR, SSOR

• Krylov Subspace Methods:

 $x_{k+1} = x_k + \alpha_k p_k$ Some well known methods are CGNR[1975], QMR[1991], CGS[1989], Bi-CGSTAB[1992], GMRES[1986], GMRESR[1994], GCR[1986], IDR(s)[2007]



6

IDR and IDR(s) (Induced Dimension Reduction)

- Sonneveld developed IDR in the 1970's. IDR is a finite termination (Krylov) method for solving nonsymmetric linear systems.
- Analysis showed that IDR can be viewed as Bi-CG combined with linear minimal residual steps.
- This discovery led to the development of first CGS, and later of Bi-CGSTAB (by van der Vorst).



7

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IDR and IDR(s) (continued)

- As a result of these developments the basic IDR-idea was abandoned for the Bi-CG-approach.
- Recently, Sonneveld and van Gijzen discovered that the IDR-approach was abandoned too soon and proposed a generalization of IDR: IDR(s).
- P. SONNEVELD AND M.B. VAN GIJZEN IDR(s): a family of simple and fast algorithms for solving large nonsymmetric systems of linear equations SIAM J. Sci. Comput., 31, pp. 1035-1062, 2008

More information: http://ta.twi.tudelft.nl/nw/users/gijzen/IDR.html

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8

4. ILU-type Preconditioners

A linear system Ax = b is transformed into $P^{-1}Ax = P^{-1}b$ such that

- $P \approx \mathcal{A}$
- Eigenvalues of $P^{-1}A$ are more clustered than A
- Pz = r cheap to compute

Several approaches, we will discuss here

- ILU preconditioner
- Preconditioned IDR(s) and Bi-CGSTAB comparison
- Block preconditioners



9

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SILU preconditioners

New renumbering Scheme

- Renumbering of grid points:
 - Sloan algorithm [Sloan 1986]
 - Cuthill McKee algorithms [Cuthill McKee 1969]
- The unknowns are reordered by p-last or p-last per level methods
 - In p-last reordering, first all the velocity unknowns are ordered followed by pressure unknowns. Usually it produces a large profile but avoids breakdown of LU decomposition.
 - In **p-last per level reordering**, unknowns are reordered per level such that at each level, the velocity unknowns are followed by the pressure unknowns.

what are the levels ?

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10

SILU preconditioner

 4×4 Q2-Q1 grid





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Numerical experiments (SILU preconditioner)



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12

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Numerical experiments (SILU preconditioners)

Stokes Problem in a square domain with Bi-CGSTAB, $accuracy = 10^{-6}$, Sloan renumbering

	Q	2-Q1	Q	2 - P1
Grid size	p-last p-last per leve		p-last	p-last per level
16×16	36(0.11)	25(0.09)	44(0.14)	34(0.13)
32×32	90(0.92)	59(0.66)	117(1.08)	75(0.80)
64×64	255(11.9)	135(6.7)	265(14)	165(9.0)
128×128	472(96)	249(52)	597(127)	407(86)



13

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Numerical Experiments (IDR(s) vs Bi-CGSTAB)

SILU preconditioned: Comparison of iterative methods for increasing stretch factor for the driven cavity Stokes problem.



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14

Numerical Experiments (IDR(s) vs Bi-CGSTAB(l))

SILU preconditioned: Comparison of iterative methods

Grid	Bi-CGSTAB(<i>l</i>)	IDR(s)	
	MatVec.(ts) l		MatVec.(ts)	s
128×128	1104(36.5)	4	638(24.7)	6
256×256	5904(810)	6	1749(307)	8

Driven Cavity Stokes problem, stretch factor 10

Channel flow Stokes problem, length 100

Grid	Bi-CGSTAB(<i>l</i>)	IDR(s)	
	MatVec.(ts) l		MatVec.(ts)	s
64×64	1520(12)	4	938(8.7)	8
128×128	NC	6	8224(335)	8



15

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5. Block preconditioners

$$\mathcal{A} = \mathcal{L}_b \mathcal{D}_b \mathcal{U}_b = \begin{bmatrix} F & B^T \\ B & 0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ BM_l^{-1} & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I & M_u^{-1}B^T \\ 0 & I \end{bmatrix}$$

 $M_l = M_u = F$ and $S = -BF^{-1}B^T$ is the Schur-complement matrix.

$$\mathcal{U}_{bt} = \mathcal{D}_b \mathcal{U}_b = \begin{bmatrix} F & B^T \\ 0 & \hat{S} \end{bmatrix}, \quad \mathcal{L}_{bt} = \mathcal{L}_b \mathcal{D}_b = \begin{bmatrix} F & 0 \\ B & \hat{S} \end{bmatrix}$$

Preconditioners are based on combination of these blocks involve:

 $Fz_1 = r_1$ The velocity subsystem

$$S \longrightarrow \hat{S}$$

 $\hat{S}z_2 = r_2$ The pressure subsystem

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16

Block preconditioners

Block triangular preconditioners

$$P_t = \mathcal{U}_{bt} = \left[\begin{array}{cc} F & B^T \\ 0 & \hat{S} \end{array} \right]$$

- Pressure convection diffusion (PCD) [Kay et al, 2002] $\hat{S} = -A_p F_p^{-1} Q_p$, Q_p is the pressure mass matrix
- Least squares commutator (LSC) [Elman et al, 2002] $\hat{S} = -(BQ_u^{-1}B^T)(BQ_u^{-1}FQ_u^{-1}B^T)^{-1}(BQ_u^{-1}B^T), Q_u \text{ is the velocity mass}$ matrix
- Augmented Lagrangian approach (AL) [Benzi and Olshanskii, 2006] F is replaced by $F_{\gamma} = F + \gamma B W^{-1} B^T$ $\hat{S}^{-1} = -(\nu \hat{Q}_p^{-1} + \gamma W^{-1}), W = \hat{Q}_p$



17

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Block preconditioners (SIMPLE)

SIMPLE-type preconditioners[Vuik et al-2000]

SIMPLE	SIMPLER
$z = \mathcal{U}_b^{-1} \mathcal{L}_{bt}^{-1} r$	$z = \mathcal{U}_{bt}^{-1} \mathcal{L}_{b}^{-1} r$
	$z = z + \mathcal{U}_b^{-1} \mathcal{L}_{bt}^{-1} (r - \mathcal{A}z)$
$M_u = D$	$M_l = M_u = D$, $D = diag(F)$
$\hat{S} = B D^{-1} B^T$	$\hat{S} = BD^{-1}B^T$
One Poisson solve	Two Poisson solves
One velocity solve	Two velocity solves

Lemma: In the SIMPLER preconditioner/algorithm, both variants (one or two velocity solves) are identical .

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18

Improvements in SIMPLE-type preconditioners

We use approximate solvers for subsystems, so flexible Krylov solvers are required (GCR, FGMRES, GMRESR)

- hSIMPLER
- MSIMPLER

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19

Improvements in SIMPLE(R) preconditioners

hSIMPLER preconditioner:

In hSIMPLER (hybrid SIMPLER), first iteration of Krylov method preconditioned with SIMPLER is done with SIMPLE and SIMPLER is employed afterwards.



- Faster convergence than SIMPLER
- Effective in the Stokes problem

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20

Improvements in SIMPLE(R) preconditioners

MSIMPLER preconditioner:

Making the following changes in SIMPLER leads to the MSIMPLER preconditioner. LSC: $\hat{S} \approx -(B\hat{Q_u}^{-1}B^T)(B\hat{Q_u}^{-1}\underbrace{F\hat{Q_u}^{-1}}_{F\hat{Q_u}^{-1}}B^T)^{-1}(B\hat{Q_u}^{-1}B^T)$

assuming $F\hat{Q_u}^{-1} \approx I$ (time dependent problems with a small time step)

 $\hat{S} = -B\hat{Q_u}^{-1}B^T$

MSIMPLER uses this approximation for the Schur complement and updates scaled with $\hat{Q_u}^{-1}$.

-Convergence better than other variants of SIMPLE -Cheaper than SIMPLER (in construction) and LSC (per iteration)



21

Numerical Experiments (comparison)

3D Backward facing step: Preconditioners used in the Stokes problem with preconditioned GCR(20) with *accuracy* of 10^{-6} (SEPRAN) using Q2-Q1 hexahedrons

Grid	SIMPLE	SIMPLE LSC					
	iter. $(t_s)\frac{\text{in-it-}u}{\text{in-it-}p}$						
$8 \times 8 \times 16$	44(4) $\frac{97}{342}$	16(1.9) <u>41</u> <u>216</u>	14(1.4) $\frac{28}{168}$				
$16 \times 16 \times 32$	84(107) <u>315</u> <u>1982</u>	29(51) $\frac{161}{1263}$	17(21) $\frac{52}{766}$				
$24 \times 24 \times 48$	99(447) $\frac{339}{3392}$	26(233) $\frac{193}{2297}$	17(77) <u>46</u> <u>1116</u>				
$32 \times 32 \times 40$	132(972) <u>574</u> 5559	37(379) <u>233</u> 2887	20(143) $\frac{66}{1604}$				

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22

Numerical Experiments (comparison)

3D Lid driven cavity problem (tetrahedrons):The Navier-Stokes problem is solved with accuracy 10^{-4} , a linear system at each Picard step is solved with accuracy 10^{-2} using preconditioned Krylov subspace methods. Bi-CGSTAB is used as inner solver in block preconditioners(SEPRAN)

Re	LSC	MSIMPLER	SILU			
	GCR iter. (t_s)	GCR iter. (t_s)	Bi-CGSTAB iter. (t_s)			
$16 \times 16 \times 16$						
20	30(20)	20(16)	144(22)			
50	57(37)	37(24)	234(35)			
100	120(81)	68(44)	427(62)			
		$32 \times 32 \times 32$				
20	38(234)	29(144)	463(353)			
50	87(544)	53(300)	764(585)			
100	210(1440)	104(654)	1449(1116)			



23

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Numerical Experiments (comparison)

2D Lid driven cavity problem on 64×64 stretched grid: The Stokes problem is solved with accuracy 10^{-6} . PCG is used as inner solver in block preconditioners (SEPRAN).

Stretch factor	LSC MSIMPLER		SILU
	GCR iter.	GCR iter.	Bi-CGSTAB iter.
1	20	17	96
8	49	28	189
16	71	34	317
32	97	45	414
64	145	56	NC
128	NC	81	NC

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24

 $\begin{bmatrix} F & B^T \\ B & O \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \text{ is transformed into}$ $\begin{bmatrix} F + \gamma B^T W^{-1} B & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} \hat{f} \\ g \end{bmatrix} \text{ or } \mathcal{A}_{AL} \mathbf{x} = \hat{b},$

with $\hat{f} = f + \gamma B^T W^{-1} B g$, where W is a non-singular matrix. The *Ideal* AL preconditioner proposed for \mathcal{A}_{AL} is

$$\mathcal{P}_{IAL} = \begin{bmatrix} F + \gamma B^T W^{-1} B & 0\\ B & -\frac{1}{\gamma} W \end{bmatrix}.$$

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25

$$\mathcal{A}_{AL} = \begin{bmatrix} F + \gamma B^T W^{-1} B & B^T \\ B & 0 \end{bmatrix} \qquad (S_{AL} = -B(F + \gamma B^T W^{-1} B)^{-1} B^T \\ \mathcal{P}_{IAL} = \begin{bmatrix} F + \gamma B^T W^{-1} B & 0 \\ B & -\frac{1}{\gamma} W \end{bmatrix} \qquad (F_{\gamma} = F + \gamma B^T W^{-1} B)$$

- The Schur complement S_{AL} of \mathcal{A}_{AL} is approximated by $-\frac{1}{\gamma}W$.
- The block F_{γ} becomes increasingly ill-conditioned with $\gamma \to \infty$.
- In practice it is often chosen as $\gamma = 1$, or $\gamma = O(1)$, and $W = \hat{Q}_P$.
- Open question: fast solution methods for systems with F_{γ} , which is denser than F and consists of mixed derivatives.

[1] M. Benzi and M.A. Olshanskii. An augmented Lagrangian-based approach to the

Oseen problem. SIAM J. Sci. Comput., 28:2095-2113, 2006.

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26

The transformed coefficient matrix $\mathcal{A}_{AL} = \begin{bmatrix} F + \gamma B^T W^{-1} B & B^T \\ B & 0 \end{bmatrix}$ and the ideal AL precondition $\mathcal{P}_{IAL} = \begin{bmatrix} F + \gamma B^T W^{-1} B & 0 \\ B & -\frac{1}{\gamma} W \end{bmatrix}$ includes (in 2D)

• the convection-diffusion block: $F = \begin{bmatrix} F_{11} & O \\ O & F_{11} \end{bmatrix}$,

• the (negative) divergence matrix: $B = [B_1 \ B_2]$,

• the modified pivot block
$$F_{\gamma} = \begin{bmatrix} F_{11} + \gamma B_1^T W^{-1} B_1 & \gamma B_1^T W^{-1} B_2 \\ \gamma B_2^T W^{-1} B_1 & F_{11} + \gamma B_2^T W^{-1} B_2 \end{bmatrix}$$
.

One approximation of F_{γ} is $\widetilde{F}_{\gamma} = \begin{bmatrix} F_{11} + \gamma B_1^T W^{-1} B_1 & O \\ \gamma B_2^T W^{-1} B_1 & F_{11} + \gamma B_2^T W^{-1} B_2 \end{bmatrix}$, which leads to the modified AL preconditioner \mathcal{P}_{MAL} for \mathcal{A}_{AL} .

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27

$$\mathcal{P}_{IAL} = \begin{bmatrix} F_{\gamma} & 0 \\ B & -\frac{1}{\gamma}W \end{bmatrix} \qquad (F_{\gamma} = \begin{bmatrix} F_{11} + \gamma B_1^T W^{-1} B_1 & \gamma B_1^T W^{-1} B_2 \\ \gamma B_2^T W^{-1} B_1 & F_{11} + \gamma B_2^T W^{-1} B_2 \end{bmatrix})$$
$$\mathcal{P}_{MAL} = \begin{bmatrix} \tilde{F}_{\gamma} & 0 \\ B & -\frac{1}{\gamma}W \end{bmatrix} \qquad (\tilde{F}_{\gamma} = \begin{bmatrix} F_{11} + \gamma B_1^T W^{-1} B_1 & 0 \\ \gamma B_2^T W^{-1} B_1 & F_{11} + \gamma B_2^T W^{-1} B_2 \end{bmatrix})$$

- systems with \widetilde{F}_{γ} are easier to be solved, compared to F_{γ} .
- the number of iterations by using the ideal and modified AL preconditioners are both independent of the mesh refinement, and nearly independent of the Reynolds (viscosity) number.
- by using the modified AL preconditioner, there exists an optimal value of γ, which minimises the number of Krylov subspace iterations. The optimal γ is problem dependent, but mesh size independent.



28

Numerical experiments (Lid driven cavity)

2D lid driven cavity problem. the domain is $[0,1] \times [0,1]$. The Reynolds number is $Re = UL/\nu$, and here U = 1 and L = 1. The stretched grids are generated based on the uniform Cartesian grids with $n \times n$ cells. The stretching function is applied in both directions with parameters a = 1/2 and b = 1.1

$$x = \frac{(b+2a)c - b + 2a}{(2a+1)(1+c)}, \ c = (\frac{b+1}{b-1})^{\frac{\bar{x}-a}{1-a}}, \ \bar{x} = 0, 1/n, 2/n, ..., 1.$$

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29

Numerical experiments (Lid driven cavity)

Re	100	400	1000	2500^{*}	5000*		
modified AL preconditioner							
Picard iterations:	14	27	33	66	286		
GCR iterations:	5	9	11	17	19		
total time:	22.7	65.1	119.6	457.7	2636.3		
modified 'grad-div' preconditioner							
Picard iterations:	13	27	31	51	308		
GCR iterations:	7	11	16	28	24		
total time:	10.8	35.8	64.4	159.5	812.5		
ideal SIMPLER preconditioner							
Picard iterations:	14	27	31	51	325		
GCR iterations:	40	53	63	92	107		
total time:	81.5	235.2	508.4	929.7	9548.7		

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30

Numerical experiments (Lid driven cavity)

Re	100	400	1000	2500*	5000*		
modified AL preconditioner							
Newton iterations:	6	7	7	8	9		
GCR iterations:	8	14	21	33	50		
total time:	14.8	26.2	74.6	194.2	277.1		
modified 'grad-div' preconditioner							
Newton iterations:	6	7	8	9	9		
GCR iterations:	10	17	28	53	77		
total time:	8.5	15.7	32.7	119.1	167.9		
modified SIMPLER preconditioner							
Newton iterations:	10	8*	8*	11	15		
GCR iterations:	43	82	84	80	90		
total time:	68.3	102.9	232.8	203.2	561.6		

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31

6. Maritime Applications

Container vessel (unstructured grid)



RaNS equations k- ω turbulence model $y^+ \approx 1$

Model-scale: $Re = 1.3 \cdot 10^7$ 13.3m cells max aspect ratio 1 : 1600



Tanker (block-structured grid)



Model-scale: $Re = 4.6 \cdot 10^6$ 2.0m cells max aspect ratio 1 : 7000

Full-scale:

 $\mathrm{Re} = 2.0 \cdot 10^9$

2.7m cells max aspect ratio 1 : 930 000





Discretization

Co-located, cell-centered finite volume discretization of the steady Navier-Stokes equations with Picard linearization leads to linear system:

$$\begin{bmatrix} Q_1 & 0 & 0 & G_1 \\ 0 & Q_2 & 0 & G_2 \\ 0 & 0 & Q_3 & G_3 \\ D_1 & D_2 & D_3 & C \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ p \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ g \end{bmatrix}$$
for brevity:
$$\begin{bmatrix} Q & G \\ D & C \end{bmatrix} \begin{bmatrix} f \\ g \end{bmatrix}$$

with $Q_1 = Q_2 = Q_3$.

 \Rightarrow Solve system with FGMRES and SIMPLE-type preconditioner Turbulence equations (*k*- ω model) remain segregated



34

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SIMPLE-method

Given u^k and p^k :

- 1. solve $Qu^* = f Gp^k$
- 2. solve $(C DQ^{-1}G)p' = g Du^* Cp^k$
- 3. compute $u' = -Q^{-1}Gp'$
- 4. update $u^{k+1} = u^* + u'$ and $p^{k+1} = p^k + p'$

with the SIMPLE approximation $Q^{-1} \approx \operatorname{diag}(Q)^{-1}$.

 \Rightarrow "Matrix-free": only assembly and storage of Q and $(C - DQ^{-1}G)$. For D, G and C the action suffices.

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35

SIMPLER: additional pressure prediction

Given u^k and p^k , start with a pressure prediction:

1. solve
$$(C - D \operatorname{diag}(Q)^{-1}G)p^* = g - Du^k - D \operatorname{diag}(Q)^{-1}(f - Qu^k)$$

2. continue with SIMPLE using p^* instead of p^k

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36

Some practical constraints

Compact stencils are preferred on unstructured grids:

• neighbors of cell readily available; neighbors of neighbors not

Also preferred because of MPI parallel computation:

• domain decomposition, communication

Compact stencil?

- ✓ Matrix $Q_1 (= Q_2 = Q_3)$, thanks to defect correction
- \checkmark Stabilization matrix C
- \Rightarrow modify SIMPLE(R) such that C is not required on the l.h.s.



37

Treatment of stabilization matrix

• In SIMPLE, neglect *C* in l.h.s. of pressure correction equation

$$(C - D\operatorname{diag}(Q)^{-1}G)p' = g - Du^* - Cp^k$$
$$\Downarrow$$
$$-D\operatorname{diag}(Q)^{-1}Gp' = g - Du^* - Cp^k$$

• In SIMPLER, do *not* involve the mass equation when deriving the pressure prediction p^*

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38

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Container vessel

Tables show number of non-linear iterations and wall clock time needed to converge to machine precision, starting from uniform flow.

grid	CPU cores	SIMPLE		KRYLOV-SIMPLER	
		# its	Wall clock	# its	Wall clock
13.3m	128	3187	5h 26mn	427	3h 27mn

Model-scale $\text{Re} = 1.3 \cdot 10^7$, max cell aspect ratio 1:1600





39

Tanker

grid	CPU cores	SIMPLE	SIMPLE		KRYLOV-SIMPLER	
		its	Wall clock	its	Wall clock	
0.25m	8	1379	25mn	316	29mn	
0.5m	16	1690	37mn	271	25mn	
1m	32	2442	57mn	303	35mn	
2m	64	3534	1h 29mn	519	51mn	

Model-scale $Re = 4.6 \cdot 10^6$, max cell aspect ratio 1:7000

Full-scale $Re = 2.0 \cdot 10^9$, max cell aspect ratio $1:930\,000$

grid	CPU cores	SIMPLE	SIMPLE		KRYLOV-SIMPLER	
		its	Wall clock	its	Wall clock	
2.7m	64	29578	16h 37mn	1330	3h 05mn	





7. Conclusions

- MSIMPLER is at present the fastest of all SIMPLE-type preconditioners.
- In our experiments, MSIMPLER proved to be cheaper than SILU, especially when the problem is solved with high accuracy.
- MSIMPLER shows better performance than LSC. Both have similar convergence characteristics.
- For academic problems, Modified Augmented Lagrangian (MAL) and grad-div are nearly independent of the grid size and Reynolds number
- MAL/grad-div are faster than (M)SIMPLER
- Future research: MAL/grad-div for industrial (Maritime) applications



41

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October 6, 2014



42