A fast and robust solver for multi-phase flow

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Modelling and Measuring of Multi-phase Flow Phenomena in Micro-fluidic and Thin-film Systems
Lorentz Centre, Leiden University
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Some history

Developments of multi-phase flow

- Mach-uniform numerical methods
- Numerical methods for cavitation flows
- A mass conserving level set method for bubbly flows
- Fast solvers for bubbly flows
- Grid computing for multi-phase flow

Typical issues for solution of the linear systems

- Iterative methods for the coupled Navier-Stokes equations
- Iterative methods for methods for problems with discontinuos coefficients

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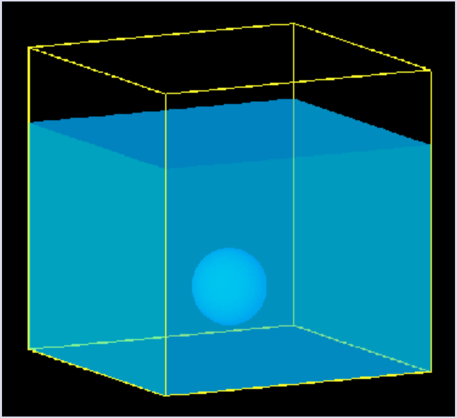
Bubbly Flow Problems

Simulation



Bubbly Flow Problems

Background

- Simulation of flows with bubbles and droplets
- Numerical models are used
- Flow governed by the Navier-Stokes equations with unknowns p and u:

$$\begin{cases} \frac{\partial u}{\partial t} + u \cdot \nabla u + \frac{1}{\rho} \nabla p = \frac{1}{\rho} \nabla \cdot \mu \left(\nabla u + \nabla u^T \right) + g \\ \nabla \cdot u = 0 \end{cases}$$

- Solution using operator-splitting methods

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Linear System

Most Time-Consuming Part in Operator-Splitting Methods

Solve the singular but consistent linear system

$$Ax = b, \quad A \in \mathbb{R}^{n \times n}$$

where A is large, sparse, SPSD, ill-conditioned

Origin of Linear System

Poisson equation with a discontinuous density ρ:

$$\text{div}\left(\frac{1}{\rho}\nabla p\right) = f$$

with Neumann boundary conditions

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Standard Iterative Methods

Preconditioned Conjugate Gradient Method (PCG)

Solve iteratively:

$$M^{-1}Ax = M^{-1}b$$

where M is a preconditioner

Bottleneck

The spectrum of $M^{-1}A$ consists of small eigenvalues due to presence of bubbles

Consequence

$\tilde{\kappa}(M^{-1}A)$ is large $\longrightarrow$ Slow convergence of the iterative process

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Aim of Research

Our Goal

Improve PCG to solve the linear system $Ax = b$ efficiently

Second-level Preconditioners

Idea

Incorporate a second-level preconditioner in the PCG method

Possibilities

- Deflation preconditioners
- Multigrid preconditioners
- Domain decomposition preconditioners

[1] R. Nabben and C. Vuik, SIAM J. Numer. Anal., **42**, pp. 1631–1647, 2004.
[2] R. Nabben and C. Vuik, SIAM J. Sci. Comput., **27**, pp. 1742–1759, 2006.
[3] R. Nabben and C. Vuik, Num. Lin. Alg. Appl., **4**, pp. 355–372, 2008.
[4] J.M. Tang, R. Nabben, C. Vuik and Y.A. Erlangga, Report 07-04, 2007. (submitted)
[4] J.M. Tang, S.P. MacLachlan, R. Nabben and C. Vuik , Report 08-05, 2008. (submitted)

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Idea of Deflation

Deflated PCG (DPCG)

Solve iteratively:

$$M^{-1}PAx = M^{-1}Pb$$

where M is a preconditioner and P is the deflation matrix

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P projects the small eigenvalues to exactly zero

Consequence

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Definition of Deflation Matrix

Notation

$$P := I - AZE^{-1}Z^T, \quad E := Z^T AZ, \quad Z \in \mathbb{R}^{n \times r}, \quad r \ll n$$

where Z is the deflation subspace matrix consisting of deflation vectors

Notes

- Space spanned by the columns of Z is the space to be projected out $\longrightarrow$ Success of deflation depends on the choice of Z
- Coarse matrix E has dimensions $r \times r$ $\longrightarrow$ E^{-1} is easy to compute

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Choices of Deflation Subspace

Ideal Choice of Z

Z consists of eigenvectors associated with small eigenvalues of $M^{-1}A$

Problem Ideal Choice of Z

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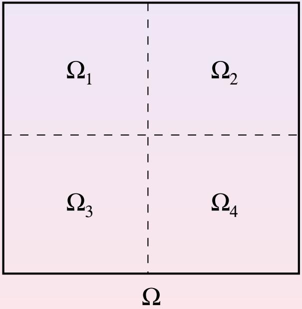
Alternatives

- **Approximated Eigenvector Deflation**: Yeremin et al. (1995), Padiy et al. (2000), Saad et al. (2000), Waisman (2005)
- **Solution / Recycling Deflation**: Clemens et al. (2004), Parks et al. (2006)
- **Subdomain Deflation**: Nicolaides (1987), Mansfield (1990,1991), Vuik, Nabben, Tang et al. (1999 – . . .)
- **Levelset Deflation**: Tang, Vuik (2007)

Subdomain Deflation

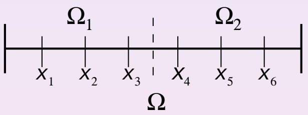


Deflation subspace matrix

$Z = [z_1 \; z_2 \; \cdots \; z_r]$ consists of

$$(z_j)_i = \begin{cases} 0, & x_i \in \Omega \setminus \bar{\Omega}_j \\ 1, & x_i \in \Omega_j \end{cases}$$

1-D Example of Subdomain Deflation



Example

Take $n = 6,\ r = 2$ and $\Omega = \{\Omega_1, \Omega_2\}$:

$$Z = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}$$

Subdomain Deflation

Advantages of Subdomain Deflation Vectors

- Easy approach
- Sparse structure
- Fixed at each time step
- Independent of geometry
- Approximate unfavorable eigenvectors
- Straightforward to parallellize

Alternatives of Subdomain Deflation

Density-related Deflation Vectors

Subdomains can also be chosen corresponding to bubbles

Observation

This does not lead to significant improvements compared to the original method (for sufficiently large number of subdomains)

Optimal Choice

Optimal choice of the number of deflation vectors depends on E^{-1}. Rule of thumb:

$$r \approx \sqrt{n}$$

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Theory of Subdomain Deflation

Known in Literature

Deflation method works well for linear systems with

- invertible matrices
- fixed density fields

Difficulties in Applications of Bubbly Flows

Can the deflation method deal with

- singular matrices?
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Deflation and Singular Systems

Problem

E^{-1} does not exist, since coarse matrix $E := Z^T AZ$ is singular

Solutions

- **Variant 1:** Delete one column of Z
- **Variant 2:** Force invertibility of A
- **Variant 3:** Solve systems with E iteratively

Which is the best?

All variants perform the same in theory and have the same original convergence properties

[1] J.M. Tang and C. Vuik, JCAM, **206**, pp. 603–614, 2007.
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Subdomains of Z are fixed, whereas the density fields can vary

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Performance of DPCG hardly depends on the value of the jumps and geometry of density fields

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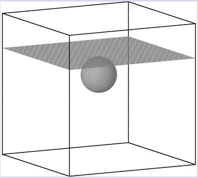
Simulations

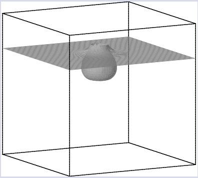
Problem Setting

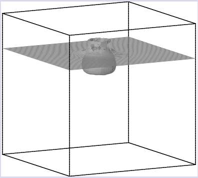
- Density jump $\rho_{\text{water}} / \rho_{\text{air}} = 1.000$
- Finite differences on a uniform Cartesian grid
- Grid sizes $n = 100^3 = 1.000.000$
- Comparison of PCG and DPCG with Incomplete Cholesky (IC) preconditioner
- Termination criterion $||r_j|| / ||r_0|| < 10^{-10}$

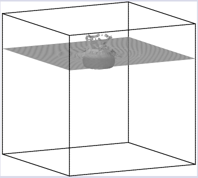
Simulation 1: Rising Bubble in Water

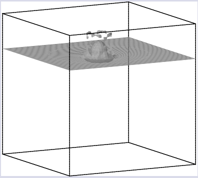
Plots of Simulation 1

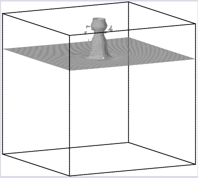

(a) $t = 0$


(b) $t = 50$


(c) $t = 100$

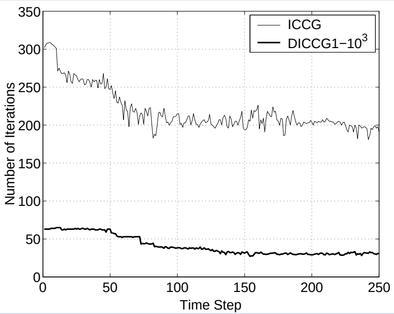

(d) $t = 150$


(e) $t = 200$

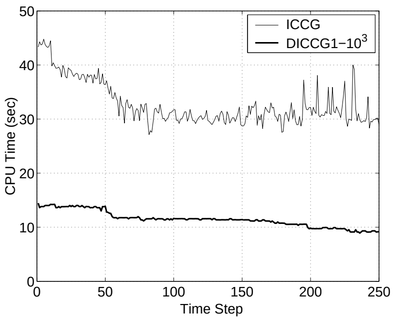

(f) $t = 250$

Results

Results for PCG and DPCG



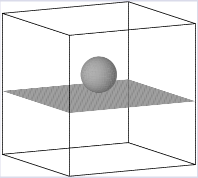
(a) Number of iterations



(b) CPU time (in seconds)

Simulation 2: Falling Droplet in Air

Plots of Simulation 2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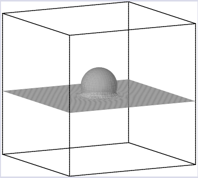
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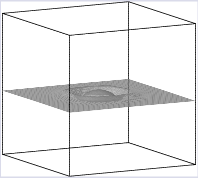
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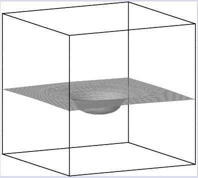
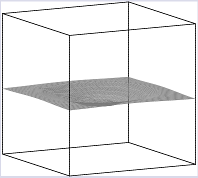

(d) $t = 150$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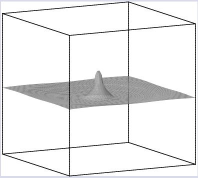
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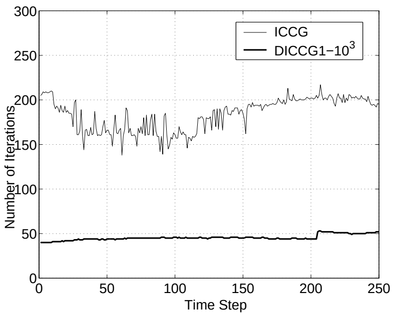

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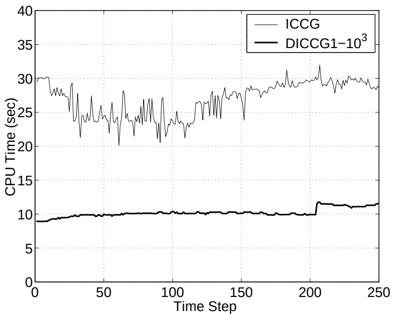

(b) CPU time (in seconds)

Discussion of the Results

Advantages of DPCG

- Performance is much better compared to PCG
- Depends hardly on the geometry of the problem
- Extremely robust in both simulations

Conclusions

Known Result

DPCG works well for problems with invertible matrices and fixed density fields

New Results

- DPCG can also be applied to problems with singular matrices
- Performance of DPCG hardly depends on the density fields

Main Conclusion

Simulation of bubbly flows can be accelerated and much more efficient using DPCG

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Current Research

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- Parallelization of deflation method

[1] S.P. MacLachlan, J.M. Tang and C. Vuik , Report 08-01, 2008. (submitted)