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An efficient iterative scheme for the highly constrained augmented Stokes problem for the numerical simulation of flows in porous media

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ABSTRACT

In this work, we present a new efficient iterative solution technique for large sparse matrix systems that are necessary in the mixed finite-element formulation for flow simulations of porous media with complex 3D architectures in a representative volume element. Augmented Stokes flow problems with the periodic boundary condition and the immersed solid body as constraints have been investigated, which form a class of highly constrained saddle point problems mathematically. By solving the generalized eigenvalue problem based on block reduction of the discrete systems, we investigate structures of the solution space and its subspaces and propose the exact form of the block preconditioner. The exact Schur complement using the fundamental solution has been proposed to

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implement the block-preconditioning problem with constraints. Additionally, the algebraic multigrid method and the diagonally scaled conjugate gradient method are applied to the preconditioning sub-block system and a Krylov subspace method (MINRES) is employed as an outer solver. We report the performance of the present solver through example problems in 2D and 3D, in comparison with the approximate Schur complement method. We show that the number of iterations to reach the convergence is independent of the problem size, which implies that the performance of the present iterative solver is close to O(N).

Key Words: Flow in porous media, Representative volume element (RVE), Iterative solver, Block preconditioning, Algebraic multigrid method

1. Introduction

In this work, we consider a fast and efficient iterative solution technique for the numerical simulation of flows in porous media with complex micro-architectures to investigate the flow behaviors such as the permeability, the mobility of fluids with shear-dependent viscosity or the flow resistance of viscoelastic fluids, which has various industrial applications: e.g. liquid molding in composite manufacturing, the packed-bed reactor in chemical engineering, the secondary-oil recovery in petroleum industries and various filters in automobile industries. Due to its repeated structure, it is necessary to introduce a representative volume element containing a small number of microstructures with periodic boundary conditions for effective numerical simulations. Good examples are the works of one of the authors' group (Wang and Hwang, 2008; Liu and Hwang, 2009; Hwang and Advani, 2010; Liu and Hwang, 20 12) in which the authors modeled 2D and 3D structures in bi-periodic or tri-periodic unit cells containing fibers or fiber tows to predict the permeability of complex porous microstructures for the application to the composite manufacturing. There are two necessary ingredients in dealing with this class of porous media flows: one is the treatment of the periodic boundary condition and the other is the introduction of the solid bodies within the flow. As we will introduce later, mathematical treatments for these two lead to highly constrained flow problem, the so-called augmented Stokes problem, particularly with mixed formulation of the finite-element method. A suitably preconditioned iterative scheme is essential for successful flow simulations of large-scale problems, as the use of a direct solver is impractical and even impossible for large 3D problems. In this work, we aim to develop a new efficient iterative solution technique for the highly constrained large sparse matrix system using specific choices of block-preconditioning, which is specifically tailored for flow simulations of porous media within a unit cell.

To introduce the problem, let us first consider the standard Stokes problem in a domain Ω. Since fluid inertia is often neglected on scale of interest with flows in porous media, the Stokes flow is usually assumed as follows:

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

subjected to the following boundary conditions:

$$\boldsymbol{u} = \bar{\boldsymbol{u}}, \quad \text{on} \quad \Gamma_u \quad \text{and} \quad \boldsymbol{t} = \bar{\boldsymbol{t}}, \quad \text{on} \quad \Gamma_t. \tag{2}$$

The stress is $\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta \boldsymbol{D}$ with the pressure p, the identity tensor $\boldsymbol{I}$, the viscosity η and the rate-of-the deformation tensor $\boldsymbol{D} = 1/2\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right)$. Suppose that the domain boundary $\Gamma (= \partial\Omega)$ be composed of the Dirichlet-type boundary Γ_u and the Neumann-type Γ_t boundary and $\Gamma = \Gamma_u \bigcup \Gamma_t$. From the standard Galerkin approximation with the velocity and the pressure as the primitive variables, one can obtain the following weak form for this problem: Find $(\boldsymbol{u}, p)$ such that

$$-\int_\Omega p(\nabla \cdot \boldsymbol{v})\, d\Omega + \int_\Omega 2\eta \boldsymbol{D}[\boldsymbol{u}] : D[\boldsymbol{v}]\, d\Omega = \int_{\Gamma_t} \boldsymbol{t} \cdot \boldsymbol{v}\, d\Gamma, \tag{3}$$

$$\int_\Omega q(\nabla \cdot \boldsymbol{u})\, d\Omega = 0, \tag{4}$$

for all the admissible weighting functions $(\boldsymbol{v}, q)$. The discrete finite element matrix system for Eqs. (3) and (4) can be written in a block-matrix form with a suitable combination of discretized spaces for the velocity and the pressure as

$$\begin{bmatrix} K & G \\ G^T & 0 \end{bmatrix}\begin{pmatrix} \tilde{u} \\ \tilde{p} \end{pmatrix} = \begin{pmatrix} \tilde{f} \\ 0 \end{pmatrix}, \quad A_{Stokes} = \begin{bmatrix} K & G \\ G^T & 0 \end{bmatrix}. \tag{5}$$

The variable $\tilde{u}$ is a collective unknown for the discrete velocity variables, $\tilde{p}$ for the discrete pressure variables and $\tilde{f}$ is the work equivalent nodal force due to the traction boundary condition. (The symbols with tilde indicate the discretized variables throughout this work.)

The linear system shown in Eq.(5) is already highly constrained and can be classified as the saddle point problem, which means that the matrix A_{Stokes} is indefinite though symmetric and it will have positive and also negative eigenvalues and pivots while elimination (Strang, 2007). (We will consider additional constraints to the discrete Stokes problem in Eq. (5) in this work and therefore the class of the flow problem of interest in the present work may be best called highly constrained augmented Stokes problem.) This complication has originated from the presence of the incompressibility constraint. Although the basic methods for solving large sparse indefinite problems are the minimum residual (MINRES) and the generalized minimum residual (GMRES), the iterative method does not behave satisfactory or even does not converge without a suitable choice of the preconditioner. An extremely efficient, indeed $O(N)$, iterative scheme for the discrete Stokes problem of Eq. (5) has been proposed by Silverster and Wathen (1994). This approach formulates a block structured preconditioner and uses appropriate techniques for each block system such that it can be solved with optimal efficiency. They employed the outer MINRES iteration along with the inner iterations of the algebraic multigrid and conjugate gradient (CG) methods.

It is worthwhile to briefly introduce their Krylov subspace/multigrid method, as we will further extend their method in this work for much more complex highly constrained system with the presence of the immersed solid bodies or the periodic boundary condition. For the discrete Stokes problem, Silverster and Wathen (1994) introduced a finite element mass matrix as a block preconditioner for the pressure unknowns and the discrete Laplacian as a preconditioning block for the velocity unknowns. The mass matrix has been shown to be spectrally equivalent to the exact Schur complement $S = GK^{-1}G^{T}$ and it can be solved by a diagonally scaled CG method within a fixed number of iterations (Elman et al., 2005). Also, the discrete Laplacian can be optimally inverted by the multigrid method for the preconditioning problem of the velocity unknowns. They showed that this combination of the approximate preconditioners clusters the eigenvalue spectrum independent of the mesh size and thereby the convergence of the Krylov subspace outer iterative scheme (MINRES) can be guaranteed within a fixed number of iterations. The CPU time as well as the memory usage is observed to scale linearly with the number of degree of freedom. That is, the ultimate $O(N)$ performance of the solution scheme has been established.

In this work, we aim to develop a new efficient iterative solution technique for the highly constrained large sparse matrix system using specific choices of block-preconditioning. Augmented Stokes flow problems with the periodic boundary condition and the immersed solid body as additional constraints have been investigated. By solving the generalized eigenvalue problem in block matrix form, we propose an exact form of the block preconditioner to achieve the $O(N)$ performance of the iterative solution technique. The exact Schur complement using the fundamental solution has been proposed to implement the block preconditioner with the constraints. The paper is organized as follows. In Sec. 2, we introduce the mathematical framework for the two highly constrained Stokes problem by presenting the weak form and the structure of the block matrices in their discretized form. Sec.3, we investigate the solution space of the discretized weak form by solving the generalized eigenvalue problem with block reduction and then propose an exact form of the block preconditioner that guarantees fixed number of iteration for convergence. In Sec. 4, we introduce the implementation techniques for this preconditioned iterative method, particularly the exact Schur complement method using the fundamental solution. Finally, the performance of the present solver will be presented through example problems in 2D and 3D, in comparison with the approximate Schur complement method. We show that the number of iterations to reach the convergence is independent of the problem size, which implies that the performance of the present iterative solver is close to $O(N)$.

2. Highly constrained Stokes flow problems

2.1. The augmented Stokes flow problem with periodic boundary conditions

The first problem of the two highly constrained Stokes problems of interest in this work is the flow with the periodic boundary condition. Let us first consider a simple 2D problem in a rectangular domain of $[0, L]\times[0, H]$ with the periodic boundary condition in the horizontal direction such that the velocity on the left boundary is the same as the that on the right boundary: i.e.,

$$u(0, y) = u(L, y), \quad y \in [0, H]. \tag{6}$$

To combine the periodic boundary condition with the weak form, one usually introduces a Lagrangian multiplier $\boldsymbol{\lambda}$ on the left boundary Γ_{left}: i.e., $\boldsymbol{\lambda} \in L^2\left(\Gamma_{left}\right)$ and the periodic boundary condition can be expressed as an additional constraint. Then the weak form for the Stokes flow can be rewritten as: Find $(\boldsymbol{u}, p, \boldsymbol{\lambda})$ such that

$$-\int_\Omega p(\nabla\cdot\boldsymbol{v})d\Omega + \int_\Omega 2\eta\boldsymbol{D}[\boldsymbol{u}]:D[\boldsymbol{v}]d\Omega + \int_{\Gamma_{left}}\boldsymbol{\lambda}\cdot\left(\boldsymbol{v}(0, y) - \boldsymbol{v}(L, y)\right)d\Gamma = 0, \tag{7}$$

$$\int_\Omega q(\nabla\cdot\boldsymbol{u})d\Omega = 0, \tag{8}$$

$$\int_{\Gamma_{left}}\boldsymbol{\mu}\cdot\left(\boldsymbol{u}(0, y) - \boldsymbol{u}(L, y)\right)d\Gamma = 0. \tag{9}$$

for all the admissible weighting functions $(\boldsymbol{v}, q, \boldsymbol{\mu})$. Comparing with Eq. (3) and Eq. (7), one can find the identity between the Lagrangian multiplier for the periodicity and the traction force. Introducing approximate interpolations for the velocity, the pressure and the Lagrangian multiplier, Eqs. (7-9) can be written as the matrix equation:

$$\begin{bmatrix} K & G^T & \Lambda^T \\ G & 0 & 0 \\ \Lambda & 0 & 0 \end{bmatrix}\begin{pmatrix} \tilde{u} \\ \tilde{p} \\ \tilde{\lambda} \end{pmatrix} = \begin{pmatrix} \tilde{f} \\ 0 \\ 0 \end{pmatrix}, \quad A = \begin{bmatrix} K & G^T & \Lambda^T \\ G & 0 & 0 \\ \Lambda & 0 & 0 \end{bmatrix}. \tag{10}$$

Dimensions and entries of the block matrix K, G and Γ are determined by the choice of the spatial discretization and we chose a quadrilateral element with the bi-periodic velocity and the discontinuous pressure interpolations ($Q_2 - P_1$ Crouzeix-Raviert element). Construction of the block matrices K and G is obvious in the standard Galerkin formalism and therefore we only consider the entries of the block matrix Γ. Among several possible interpolation schemes for the Lagrangian multiplier $\boldsymbol{\lambda}$, we consider only two of them: (i) interpolation with the Delta function at every node (nodal collocation) and (ii) a linear continuous interpolation. (The implementation with the weak form of the integrals in Eqs. (7) and (9) involved with the periodic boundary is called the mortar element method (Laursen, 2002)). To deliver the idea easily, we selected a simple 2D model mesh as shown in Fig. 1.

<u>**Nodal Collocation**</u> Using the nodal collocation, the collocation at all nodes, the boundary integral in Eq. (9) can be written as

$$\int_{\Gamma_{left}} \boldsymbol{\mu} \cdot \left(\boldsymbol{u}(0,y) - \boldsymbol{u}(L,y) \right) d\Gamma = \sum_{k=1}^{5} \boldsymbol{\mu}_k \cdot \left(\boldsymbol{u}_k - \boldsymbol{u}_{k+30} \right), \quad \text{for all } k. \tag{11}$$

Refer to Fig. 1 for example nodal numbering scheme used in Eq. (11). In this case the block matrix Γ, which is a 10×70 matrix, for this specific problem in a symbolic form can be expressed as follows:

$$\Gamma = \left[I_{10\times10} \quad O_{10\times50} \quad -I_{10\times10} \right], \tag{12}$$

where the sub-block matrix $I_{10\times10}$ indicates the identity matrix of the size 10×10 and $O_{10\times50}$ is the null block matrix of the corresponding dimension. Considering the following product of the matrix Γ

$$\Gamma\Gamma^T = 2I_{10\times10} \quad \text{and} \quad \Gamma^T\Gamma = \begin{bmatrix} I_{10\times10} & O_{10\times50} & -I_{10\times10} \\ O_{50\times10} & O_{50\times50} & O_{50\times10} \\ -I_{10\times10} & O_{10\times50} & I_{10\times10} \end{bmatrix}, \tag{13}$$

we notice that the matrix $\Gamma\Gamma^T$ is a full-rank matrix, whereas $\Gamma^T\Gamma$ is not with rank deficiency.

<u>**Linear Continuous Interpolation**</u> A standard mortar element discretization is much more involved in this case. Introducing the linear interpolation of the Lagrangian multiplier along the 1D element boundary (see Fig. 2),

$$\boldsymbol{\lambda} = \lfloor N_\lambda \rfloor (\tilde{\lambda}) = \lfloor \phi_1 \quad \phi_2 \rfloor \begin{pmatrix} \boldsymbol{\lambda}_1 \\ \boldsymbol{\lambda}_2 \end{pmatrix},$$

the integral in Eq. (9) along the element boundary can be written as follows:

$$\int_{\Gamma_{left}} \boldsymbol{\mu} \cdot \left(\boldsymbol{u}(0,y) - \boldsymbol{u}(L,y)\right) d\Gamma = \sum_{e=1}^{2} (\tilde{\mu})_e^T \int_{\Gamma_{e,left}} \lfloor N_\lambda \rfloor^T [N] d\Gamma \left((\tilde{u})_{e,left} - (\tilde{u})_{e,right}\right). \tag{14}$$

The symbol $[N]$ is the interpolation function for the velocity unknowns and the subscript $'e'$ indicates the variable defined within an element. Using the local numbering in Fig. 2, the block matrix Γ in the specific mesh of Fig. 1 can be expressed in a symbolic form as

$$\Gamma = \begin{bmatrix} U_{3\times5} & O_{3\times5} & O_{3\times5} & -U_{3\times5} & O_{3\times5} \\ O_{3\times5} & U_{3\times5} & O_{3\times5} & O_{3\times5} & -U_{3\times5} \end{bmatrix}, \tag{15}$$

where a sub-block matrix $U_{3\times5}$ is

$$U_{3\times5} = \begin{bmatrix} 1/3 & 2/3 & 0 & 0 & 0 \\ 0 & 2/3 & 2/3 & 2/3 & 0 \\ 0 & 0 & 0 & 2/3 & 1/3 \end{bmatrix}.$$

Again considering the following two products of the block matrix Γ:

$$\Gamma\Gamma^T = \begin{bmatrix} 2U_{3\times3}^2 & 0 \\ 0 & 2U_{3\times3}^2 \end{bmatrix} \quad \text{and} \quad \Gamma^T\Gamma = \begin{bmatrix} \left(U^T\right)_{5\times5}^2 & O_{5\times5} & O_{5\times50} & -\left(U^T\right)_{5\times5}^2 & O_{5\times5} \\ O_{5\times5} & \left(U^T\right)_{5\times5}^2 & O_{5\times50} & O_{5\times5} & -\left(U^T\right)_{5\times5}^2 \\ O_{50\times5} & O_{50\times5} & O_{50\times50} & O_{50\times5} & O_{50\times5} \\ -\left(U^T\right)_{5\times5}^2 & O_{5\times5} & O_{5\times50} & \left(U^T\right)_{5\times5}^2 & O_{5\times5} \\ O_{5\times5} & -\left(U^T\right)_{5\times5}^2 & O_{5\times50} & O_{5\times5} & \left(U^T\right)_{5\times5}^2 \end{bmatrix}, \tag{16}$$

the matrix $\Gamma\Gamma^T$ is found to be a full-rank matrix, whereas $\Gamma^T\Gamma$ is not with rank deficiency.

2.2. The augmented Stokes flow problem with immersed solid bodies

The second highly constrained Stokes problem of interest in this study is the Stokes flow with immersed solid bodies. To model this problem, we use the so-called rigid-ring (or rigid-shell in 3D) description, one of the fictitious domain methods, such that the interior of the solid body is considered as a part of the fluid with the same constitutive equation as the fluid domain with the zero velocity condition on the solid boundary (Wang and Hwang, 2008; Liu and Hwang, 2009; Liu and Hwang, 2012). As fluid inertia is neglected in the Stokes flow, the zero velocity condition on the solid boundary ensures vanishing velocity inside the body. There are three advantages of the rigid-shell description with the fictitious domain method in simulation of flow in porous media: first, one does not have to consider the interface conditions between solid and fluid, as the entire problem is essentially the fluid problem. The second one is the easiness in discretization of the immersed body using its boundary information only and, as will be shown later, one needs just points on the solid boundary. Thirdly, as the entire problem is the fluid flow problem, one can use the regular mesh which facilitates simple implementation for the mortar element technique for the periodic boundary condition of the representative volume element.

The zero boundary condition on the solid boundary ∂B can be expressed as

$$\boldsymbol{u} = 0, \quad \text{on} \quad \partial B. \tag{17}$$

As was done with the periodic boundary condition, we define the Lagrangian multiplier $\boldsymbol{\lambda}$ on ∂B and the zero velocity condition on the boundary can be treated as the constraint in the weak form in exactly the same form as previous: Find $(\boldsymbol{u}, p, \boldsymbol{\lambda})$ such that

$$-\int_\Omega p(\nabla \cdot \boldsymbol{v})\, d\Omega + \int_\Omega 2\eta \boldsymbol{D}[\boldsymbol{u}] : D[\boldsymbol{v}]\, d\Omega + \int_{\partial B} \boldsymbol{\lambda} \cdot \boldsymbol{v}\, d\Gamma = \int_{\Gamma_t} \boldsymbol{t} \cdot \boldsymbol{v}\, d\Gamma, \tag{18}$$

$$\int_\Omega q(\nabla \cdot \boldsymbol{u})\, d\Omega = 0, \tag{19}$$

$$\int_{\partial B} \boldsymbol{\mu} \cdot \boldsymbol{u}\, d\Gamma = 0 \tag{20}$$

for all the admissible weighting functions $(\boldsymbol{v}, q, \boldsymbol{\mu})$. We employ the point collocation method to implement the integral over the solid boundary in Eqs. (18) and (20). For example, the integral in Eq. (20) can be approximated as

$$\int_{\partial B} \boldsymbol{\mu} \cdot \boldsymbol{u}\, d\Gamma \approx \sum_{k=1}^{M} \boldsymbol{\mu}_k \cdot \boldsymbol{u}(\boldsymbol{x}_k), \tag{21}$$

where M, $\boldsymbol{x}_k$ and $\boldsymbol{\mu}_k$ are the number of collocation points on ∂B, the position of the *k*-th colocation point and the collocated Lagrangian multiplier at $\boldsymbol{x}_k$, respectively. The resulting matrix equation appears exactly the same as the previous periodic boundary condition in Eq. (10). Though not presented here, the product of the corresponding off-diagonal sub-block matrix Γ satisfies the same characteristics: the matrix $\Gamma\Gamma^T$ is a full-rank matrix, whereas $\Gamma^T\Gamma$ is not with rank deficiency.

3. Block-preconditioning strategy and the generalized eigenvalue problem

For the solution of the matrix equation in Eq. (10), we propose a block preconditioner P similar to (or motivated by) the Schur complement in the discrete Stokes problem: i.e.,

$$P = \begin{bmatrix} K & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & T \end{bmatrix}, \quad \text{with} \quad S = GK^{-1}G^T \quad \text{and} \quad T = \Gamma K^{-1}\Gamma^T. \tag{22}$$

The matrix K is a square matrix of the size $n_u \times n_u$ and is a full rank matrix $\left(\text{rank}\left(K\right) = n_u\right)$; the matrix G is a non-square matrix of the size $n_p \times n_u$ is of a full rank $\left(\text{rank}\left(G\right) = n_p\right)$; and the matrix Γ is a non-square matrix of the size $n_\lambda \times n_u$ is of a full rank $\left(\text{rank}\left(\Gamma\right) = n_\lambda\right)$. The symbols n_u, n_p and n_λ are the numbers of the velocity, pressure and Lagrangian multiplier unknowns, respectively. The adequateness and performance of the proposed preconditioner can be analyzed by the eigenvalue problem of the preconditioned system $P^{-1}A$ and therefore the generalized eigenvalue problem, $P^{-1}Ax = \xi x$ with the eigenvalue ξ, can be stated as follows:

$$\begin{bmatrix} K & G^T & \Lambda^T \\ G & 0 & 0 \\ \Lambda & 0 & 0 \end{bmatrix} \begin{pmatrix} \tilde{u} \\ \tilde{p} \\ \tilde{\lambda} \end{pmatrix} = \xi \begin{bmatrix} K & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & T \end{bmatrix} \begin{pmatrix} \tilde{u} \\ \tilde{p} \\ \tilde{\lambda} \end{pmatrix}. \tag{23}$$

To solve the generalized eigenvalue problem in Eq. (23), we divide the solution space of the discretized velocity vectors V_h into four subspaces. Now consider the following four subspaces (Fig. 3):

- Space I: $V_h^I = N(G) \cap N(\Gamma)$,
- Space II: $V_h^{II} = N(G) \cap N(\Gamma)^c$,
- Space III: $V_h^{III} = N(G)^c \cap N(\Gamma)$,
- Space IV: $V_h^{IV} = N(G)^c \cap N(\Gamma)^c$.

We have some remarks on the four subspaces.

(i) The space $N(G)$ is the right null space of the matrix G, which satisfies $G\tilde{u} = 0$ for all $u \in N(G)$, and the dimension of $N(G)$ is $(n_u - n_p)$, since the matrix G is of full rank.

(ii) Similarly, the right null space of the full rank matrix Γ, denoted by $N(\Gamma)$, satisfies $\Gamma\tilde{u} = 0$ and has the dimension of $(n_u - n_\lambda)$.

(iii) The dimension of the subspace V_h^{IV} is no larger than n_λ or n_p, which means that

$$\dim\left(N(G)^c \cap N(\Gamma)^c\right) \le \min\left(n_p, n_\lambda\right).$$

(iv) The number of unknowns related with the constraint (the periodic boundary condition or the zero velocity condition) can be safely considered much smaller than the primitive variables $\tilde{u}$ and $\tilde{p}$, since the dimension where the constraint is one-order lower than those of $\tilde{u}$ and $\tilde{p}$: i.e., $n_\lambda \ll n_p < n_u$.

The eigenvalue problem in Eq. (23) can be solved exactly for the mutually exclusive four subspaces. The general procedures involve the block Gaussian elimination process and we summarize the results below.

<u>Subspace I</u> In this space, $G\tilde{u} = 0$ and $\Gamma\tilde{u} = 0$. Therefore from Eq. (23) we have a single eigenvalue $\xi = 1$ and the corresponding eigenvector is $\lfloor \tilde{u} \quad 0 \quad 0 \rfloor^T$ with $\tilde{u}$ satisfying $G\tilde{u} = \Gamma\tilde{u} = 0$. The multiplicity of the eigenvalue is $\dim\left(V_h^I\right) = \dim\left(N(G) \cap N(\Gamma)\right)$.

<u>Subspace II</u> In this case, $G\tilde{u} = 0$ and $\Gamma\tilde{u} \ne 0$ and the eigenvector can be expressed as

$\lfloor \tilde{u} \quad 0 \quad \tilde{\lambda} \rfloor^T$ with $G\tilde{u} = 0$. By using block Gaussian elimination with $G\tilde{u} = 0$ and $T = \Gamma K^{-1}\Gamma^T$, the eigenvalue problem can be reduced to

$$\left(\xi^2 - \xi - 1\right)T\tilde{\lambda} = 0. \tag{24}$$

Since the matrix T is symmetric and positive-definite, we have two distinct eigenvalues $1/2 \pm \sqrt{5}/2$ whose multiplicity is $\dim\left(V_h^{II}\right)$.

<u>Subspace III</u> In this case, $G\tilde{u} \neq 0$ and $\Gamma\tilde{u} = 0$ and the eigenvector can be expressed as $\lfloor \tilde{u} \quad \tilde{p} \quad 0 \rfloor^T$ with $\Gamma\tilde{u} = 0$. Similarly to the space II, one can obtain the reduced eigenvalue problem with $\Gamma\tilde{u} = 0$ and $S = GK^{-1}G^T$ as follows:

$$\left(\xi^2 - \xi - 1\right)S\tilde{p} = 0. \tag{25}$$

Again, we have two distinct eigenvalues $1/2 \pm \sqrt{5}/2$ whose multiplicity is $\dim\left(V_h^{III}\right)$, since the Schur complement matrix S is symmetric and positive-definite.

<u>Subspace IV</u> This is the hardest problem. We notice that $\tilde{u} \notin N(G)$ implies $\tilde{u} \in \mathrm{range}\left(G^T\right)$ at least in the eigenvector space of $\tilde{u}$, since the null space and the row space are mutually orthogonal. In the same way $\tilde{u} \notin N(\Gamma)$ implies $\tilde{u} \in \mathrm{range}\left(\Gamma^T\right)$. Further, as the space IV is $N(G)^c \cap N(\Gamma)^c$, the row space of the two matrices can be identified.

$$\mathrm{range}\left(G^T\right) = \mathrm{range}\left(\Gamma^T\right), \quad \text{when} \quad \tilde{u} \in V_h^{IV}. \tag{26}$$

The eigenvector in V_h^{IV} has the form $\lfloor \tilde{u} \quad \tilde{p} \quad \tilde{\lambda} \rfloor^T$ and $\tilde{u}$ should satisfy $\tilde{u} \notin N(G)$ and $\tilde{u} \notin N(\Gamma)$. By the block Gaussian elimination with Eq. (26), one gets the reduced form of the eigenvalue problem in V_h^{IV}:

$$\left\{\left(\xi^2 - \xi - 1\right)^2 - 1\right\}T\tilde{\lambda} = 0. \tag{27}$$

We have four distinct eigenvalues $(-1, 0, 1, 2)$, whose multiplicity is $\dim\left(V_h^{IV}\right)$, since the Schur complement matrix T is symmetric and positive-definite.

In summary, the preconditioned matrix $P^{-1}A$ has only six eigenvalues $\left(-1,\left(1-\sqrt{5}\right)/2,0,1,\left(1+\sqrt{5}\right)/2,2\right)$ and therefore, once K^{-1}, S^{-1} and T^{-1} are computed exactly by any means, the solution of the iterative scheme converges to the exact solution within maximum six iterations, independent of the problem size. Further, if the solution methods to obtain K^{-1}, S^{-1} and T^{-1} satisfy the $O(N)$ performance, the iterative scheme for the entire problem will show the ultimate $O(N)$ performance.

4. Implementation techniques

Although the preconditioner P in Eq. (22) is theoretically optimal, one cannot employ the preconditioner as is, since the Schur complement $S = GK^{-1}G^T$ and $T = \Gamma K^{-1}\Gamma^T$ involves the inverse of K which is prohibitively expensive by themselves. Therefore one needs further approximation of the preconditioning matrix P. In this section, we seek implementation techniques for the preconditioning problem. As the preconditioners K and S, which are related with the velocity and the pressure unknowns respectively, are the same as the Stokes flow problem, we can follow the approach outlined for the Stokes systems (Silvester and Wathen, 1994; Elman et al., 2005; Hwang et al., 2011a). For the approximation of the preconditioning block matrix , we employ the discrete Laplace operator $\hat{K}$, which can be inverted by an algebraic multigrid (AMG) V-cycle to provide a fast and efficient solution. Details of analyses on the choice of the discrete Laplace operator has been presented by the authors' previous work (Hwang et al., 2011a). The block preconditioner S, the Schur complement matrix of the Stokes problem, is spectrally equivalent to a mass matrix M in the pressure space (Elman et al., 2005). Therefore we adopt the mass matrix M in the discrete pressure space as the approximation of the Schur complement S in the present study and the mass matrix can always be easily solved within a fixed number of iteration with the diagonally scaled CG, independent of the number of unknowns.

From the above statement, the approximation of the preconditioner, denoted by $\hat{P}$, can be expressed as

$$\hat{P} = \mathrm{diag}\left(\hat{K}, M, T\right). \tag{28}$$

The last remaining problem is the sub-preconditioning problem with T, which can be written as

$$Tz = r, \quad \text{with} \quad T = \Gamma K^{-1} \Gamma^T. \tag{29}$$

The problem with Eq. (29) is that the block matrix Γ is not a square matrix and its inverse is not obvious. In this work, we propose an exact solution method for Eq. (29) using the fundamental solution and present the performance of our scheme in comparison with the approximation method for the matrix Γ proposed by Elman (1996).

4.1. Implementation of block preconditioning with an approximate solution of the Schur complement

First we start presenting the approximation method for the solution of Eq. (29), which was originally developed of Elman (1996) and is called as the 'BFBt' preconditioner. It is relatively easy to implement but at the same time the number of iterations for the convergence scales with $O\left(\sqrt{N}\right)$ and therefore the CPU time scales with $O\left(N\sqrt{N}\right)$. Here we present a little bit modified implementation scheme to clearly show the procedures, which are composed of three steps as below.

Step 1 [Solution of $\Gamma y = r$] This can be done by taking $y = \Gamma^T y^*$. Firstly solve for y^*

$$\Gamma \Gamma^T y^* = r, \tag{30}$$

and find y from $y = \Gamma^T y^*$. As illustrated in Eqs. (13) and (16), the matrix $\Gamma\Gamma^T$ is small and easily invertible for both the constrained problems. Especially with the nodal collocation, the matrix $\Gamma\Gamma^T$ is simply twice of the identity matrix.

Step 2 [Solution of $A^{-1} x = y$] The solution x can be obtained by a simple matrix-vector multiplication though hugh:

$$x = Ay \tag{31}$$

Step 3 [Solution of $\Gamma^T z = x$] This problem can be transformed into a trivial problem by multiplying Γ on both sides, since $\Gamma\Gamma^T$ is easily invertible.

$$\Gamma\Gamma^T z = x \tag{32}$$

The whole solution process requires two matrix inversions in the form of $\Gamma\Gamma^T x = b$ and three matrix-vector multiplications among which one is hugh $x = Ay$ and the other two are small. Though it looks concise and clear, the final solution of Eq. (32) is not exact but only an approximation. The reason is that x in Eq. (32) does not reside in the range of Γ^T in general and the equation in the third step $\Gamma^T z = x$ does not have exact solution. Therefore, one may expect minor improvement in iterative performance and as will be seen later the number of iterations scales with $O\left(\sqrt{N}\right)$.

4.2. Implementation of block preconditioning with the fundamental solutions

In the present work, we propose an exact solution of Eq. (29) using the fundamental solutions and with this method we start rewriting Eq. (29) as follows: Find z satisfying

$$\Gamma^T z = Ky, \tag{33}$$

subjected to the constraint of

$$\Gamma y = r. \tag{34}$$

In this method, we represent the solution z in terms of y which resides in the column space of $K^{-1}\Gamma^T$, or range$\left(K^{-1}\Gamma^T\right)$. Let γ_i be the *i*-th column vector of Γ^T, which is an $n_u \times n_\lambda$ matrix.

$$\Gamma^T = \begin{bmatrix} | & | & & | \\ \gamma_1 & \gamma_2 & \cdots & \gamma_{n_\lambda} \\ | & | & & | \end{bmatrix}. \tag{35}$$

We notice that $n_\lambda \ll n_u$ in the constrained problems of this study, since the Lagrangian multiplier is defined on the space which has one order lower dimension than the velocity unknowns. Note also that the γ_i vectors are independent each other as the matrix Γ^T is of a full rank. That is, $\mathrm{rank}\left(\Gamma^T\right) = n_\lambda$.

Now one can express the right-hand side of Eq. (33) as a linear combination of the γ_i vectors with the constant coefficient z_i's:

$$\Gamma^T z = \sum_{i=1}^{n_\lambda} z_i \gamma_i . \tag{36}$$

Let y_i^* be the fundamental solution of the problem.

$$K y_i^* = \gamma_i , \quad \left(i = 1, \cdots, n_\lambda\right) \tag{37}$$

The name 'fundamental solution' seems to be proper for two reasons: one is that y_i^* is the solution for each column vector of Γ^T and the other is that the solution of Eq. (34) can be represented as a linear combination of y_i^* such that

$$y = \sum_{i=1}^{n_\lambda} z_i y_i^* . \tag{38}$$

Finally one can get the exact solution of Eq. (34) subjected to the constraint of Eq. (35) by solving the linear system below:

$$Tz = r, \quad \text{with} \quad T = \Gamma Y \quad \text{and} \quad Y = \begin{bmatrix} | & | & & | \\ y_1^* & y_2^* & \cdots & y_{n_\lambda}^* \\ | & | & & | \end{bmatrix}. \tag{39}$$

The matrix T is the exactly Schur complement defined in Eq. (22) and is an $n_\lambda \times n_\lambda$ square matrix whose component is a simply inner product of γ_i and y_i^*:

$$T_{ij} = \gamma_i \cdot y_j^* , \quad \left(i, j = 1, \cdots, n_\lambda\right). \tag{40}$$

From Eq. (40) one identifies that the matrix T is unsymmetric and almost full matrix. We have several remarks on this method.

(i) This scheme is based on the fact that the number of Lagrangian multipliers is much smaller that that of the velocity unknowns, which is valid in the periodic boundary condition and the immersed solid body problem with the rigid-ring or rigid-shell description.

(ii) The most time-consuming step is Eq. (37) for the solution of the complete fundamental solution set y_i^*'s. However one can construct the AMG matrix only once and use it repeatedly for all right hand side vectors γ_i's with the splitted AMG method. This facilitates significant saving in computation time and moreover the AMG method has the $O(N)$ performance. (The memory usage and CPU time scales linearly with the number of unknowns.)

(iii) For the problems of interest in this work, the matrix Γ does not change even in the time dependent problem or problems with nonlinear material properties (e.g. shear-thinning viscosity) and this means that one can construct the Schur complement T once and use it for all.

(iv) As every fundamental solution y_i^* is independent, it is not necessary to build the matrix Y explicitly, which is a hugh matrix. In practice, one can introduce a temporary vector as a fundamental solution and use it to build the *j*-th column of the matrix T by using Eq. (40).

(v) As the Schur complement matrix T is completely full, there is no advantage to use a sparse matrix storage and related solution technique in solving Eq. (39). We use a simple LU decomposition provided in LINPACK. The LU decomposition can be used for all repeated, which invokes significant reduction in computation time as well. Therefore, this method does not require any additional storage other than the matrix T itself.

5. Numerical examples

The first test problem is a 3D cubic channel Stokes flow of the size $1\times1\times1$ with the pressure drop in one direction, where the periodic boundary condition is applied. We tested the two interpolation schemes for the Lagrangian multipliers, the nodal collocation and the linear continuous interpolation. Three different finite element meshes have been employed from coarse to fine: $5\times5\times5$, $10\times10\times10$ and $20\times20\times20$. Note that the number of unknowns increases by the factor of 64. In all the computational results presented here, the number of V-cycles in the AMG is set to six and the convergence tolerance for the norm of the residual vector has been set to 10^{-7} relative to the norm of the original right-hand side vector b, i.e. $\|r\|/\|b\| \le 10^{-7}$ as the convergence criteria.

Plotted in Fig. 4 are the convergence behaviors of the iterative scheme based on the approximation of the Schur complement discussed in Sec. 4.1. In both the results, the number of iteration for the convergence is found to increase with the number of unknowns and more specifically results show that the number of iterations indeed scales with $O\left(\sqrt{N}\right)$, which is consistent to the result presented by Elman (1996).

Having validated the correctness of our code, we tested the proposed exact Schur complement method using the fundamental solution and the results are presented in Fig. 5. Plotted in Fig. 5 are the convergence behaviors for the same 3D Stokes problem in a cubic channel with the periodic boundary condition implemented with the exact Schur complement scheme using the fundamental solution for the linear continuous interpolation of the Lagrangian multipliers. Fig. 5 shows monotonic exponential convergence (nearly straight line) and that the number of iterations of the outer MINRES algorithm to reach convergence is roughly constant irrespective of the problem size. As was already shown in Hwang et al. (2011a) and Eq. (28), the AMG algorithm for the preconditioning velocity unknowns $\left(\hat{K}z = r\right)$ has $O(N)$ expenses in both memory and CPU time and the preconditioning for the pressure variable $(Mz = r)$ with the diagonally scaled CG converges within a single iteration for this specific choice of the pressure discretization, the overall performance can be expected to be close to $O(N)$ in both the memory usage and computation time. It is close to the ultimate $O(N)$ convergence, since there is one exception in the proposed iterative scheme. The only exception is the solution of the preconditioning problem in (39) involving the LU decomposition and related full matrix construction. (A hugh problem with Eq. (37) involves the inverse of the matrix K but we employ the AMG as mentioned in Sec. 4.2 which has the $O(N)$ performance by itself.) However, since the Lagrangian multiplier is defined in the space one order lower than those of the velocity and the pressure, the increase in memory and CPU time in the preconditioning for the

Lagrangian multiplier variables can be expected minor. In summary, the iterative solution technique with the fundamental solution for the exact Schur complement shows nearly the $O(N)$ convergence, because the outer MINRES iteration converges within the fixed number of iteration and, among the three block preconditioning schemes, two large problems related to the velocity and pressure unknowns has the $O(N)$ convergence.

Finally we present the convergence behavior of the Stokes flow problem with an immersed solid body in Fig. 6. A circle of radius 0.15 is centered in a domain of the size 1×1 in the 2D problem and a sphere of radius 0.15 is centered in a domain of the size $1\times1\times1$ as for the 3D problem. The particle boundary is discretized with uniformly distributed (collocation) points and non-trivial task in obtaining uniformly spaced points on a spherical surface has been performed by using the spiral point-set method (Saff and Kuijlaars, 1997). The numbers of collocation points were 21 with a 20×20 mesh in 2D and 81 with a $10\times10\times10$ mesh in 3D and they were chosen to scale with the number of elements for larger or smaller problems. The same pressure difference boundary condition as previous is applied such that the circle (or sphere) is an obstacle for flow separation. In 2D problem (Fig. 6a), one can again observe monotonic exponential convergence along with the fixed number of iteration for both 10×10 and 20×20 meshes indicating mesh-independent number of outer iterations, as in the previous periodic boundary problems. However, we observed convergence stalling, around the residual value of 10^{-5}, though global convergence behavior is somewhat satisfactory. We need further investigation for the origin of the convergence stalling. From our previous experience on the Stokes flow, this phenomenon might be related with modification of the singularity behavior by introducing the (non-singular) preconditioner (Hwang et al. 2011a), where the pressure specification to remove singularity in all Dirichlet boundary conditions invokes adverse effects such as convergence stalling (delay in the convergence rate) counter to common wisdom. Similarly, Elman et al. (2005) reported that rank deficiency for an enclosed flow does not prevent convergence to a consistent solution for Stokes and Navier-Stokes problem. The optimal number of collocation points in direct solver might yield additional constraints to the matrix system to be an over-constrained problem.

6. Conclusions

In this work, we have presented a new efficient iterative scheme to apply large-scale 3D simulations of flows in porous media, using on the optimal block-preconditioning and the combination of the Krylov-subspace/AMG method and the exact Schur complement method with the fundamental solution. The use of the exact Schur complement can be justified by the fact that the Lagrangian multipliers are defined in the space one order lower than those of the primitive variables, which is particularly true for the periodic boundary constraint and the zero velocity condition on the immersed solid body boundary which are the two main ingredients for successful flows simulations in porous media with the representative volume element (unit cell). The block preconditioner has been proposed by solving the generalized eigenvalue problem to result in only six different eigenvalues of the preconditioned matrix system. Further, we proposed the exact Schur complement method using the fundamental solution. We illustrated the performance of the present solver through example problems in 2D and 3D, in comparison with the approximate Schur complement method. We reported that the number of iterations to reach the convergence is independent of the problem size, which implies that the performance of the present iterative solver is close to $O(N)$.

Further development of the iterative solution techniques of this class is necessary particularly for flow simulations with complex fluids such as viscoelastic fluids, particle suspensions, droplet emulsions and/or fiber suspensions, in which one always wants to solve large-scale 3D flow problems to understand hydrodynamic interactions, particle-particle/droplet-droplet interactions in various ranges. The next step would be the development of a similar iterative solution method for massive 3D simulations of particle or fiber suspensions (e.g., Hwang et al., 2011a). The periodic boundary conditions and the treatment of immersed solid body in this work can be extended to solve particle suspension flow simulations without any significant modifications.

Acknowledgement

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References

Elman, H.C., 1996, Preconditioning for the steady-state Navier-Stokes eqautions with low viscosity, *SIAM J. Sci. Comput.*, **20**, 1299-1316.

Elman, H.C., D.J. Silvester, A.J. Wathen, 2005, Finite Elements and Fast Iterative Solvers with Applications in Incompressible Fluid Dynamics, Oxford University Press, New York.

Hwang, W.R., S.G. Advani, 2010, Numerical simulations of Stokes-Brinkman equations for permeability prediction of dual-scale fibrous porous media, *Physics of Fluids*, **22**, 113101.

Hwang, W.R., M.A. Walkley, O.G. Harlen, 2011a, A fast and efficient iterative scheme for viscoelastic flow simulations with the DEVSS finite element method, *J. Non-Newtonian Fluid Mech.*, **166**, 354-362.

Hwang, W.R., W.R. Kim, E.S. Lee and J.H. Park, 2011, Direct simulations of orientational dispersion of platelet particles in a viscoelastic fluid subjected to a partial drag flow for effective coloring of polymers," *Korea-Australia Rheol. J.* **23**, 173-181.

Laursen, T.A., 2002, Computational Contact and Impact Mechanics, Springer, Berlin.

Saff E.B., and A.B.J. Kuijlaars, 1997, Distributing many points on a sphere, *Mathematical Intelligencer*, **19**, 5-11.

Silvester, D.J. and A. J. Wathen, 1994, Fast iterative solution of stabilized Stokes systems. Part II: Using general block preconditioner, *SIAM J. Numer. Anal.*, **31**, 1352-1367.

Strang, G., 2007, Computational Science and Engineering, Wellesley, Cambridge.

Wang, J.F., and W.R. Hwang, 2008, Permeability prediction of fibrous porous media in a bi-periodic domain, *J. Compos. Mater.*, **43**, 909-929.

Liu, H.L., and W.R. Hwang, 2009, Transient filling simulations in unidirectional fibrous porous media, *Korea-Australia Rheol. J.*, **21**, 71-79.

Liu, H.L., and W.R. Hwang, 2012, Permeability prediction of fibrous porous media with complex 3D architectures, *Compos. Part A*, **43**, 2030-2038.

List of Figure Captions

Figure 1: A 2D model mesh (left) and local node numbering in an element (right).

Figure 2: An example 1-D element for the linear interpolation of the Lagrangian multipliers.

Figure 3: Subspaces of the solution space V_h of the velocity unknowns.

Figure 4: Convergence behaviors of the iterative technique for 3D Stokes problem with the periodic boundary condition implemented with the approximate Schur complement scheme for both nodal collocation and linear continuous interpolation of the Lagrangian multipliers. 'p1n' indicates results from the nodal collocation and 'p1c' is for the linear continuous interpolation.

Figure 5: Convergence behaviors of the iterative technique for 3D Stokes flow with the periodic boundary condition implemented with the exact Schur complement scheme using the fundamental solution for the linear continuous interpolation of the Lagrangian multipliers.

Figure 6: Convergence behaviors for 2D (a) and 3D (b) Stokes flow with an immersed solid body implemented with exact Schur complement scheme using the fundamental solution.

Figure 1: Hwang et al.

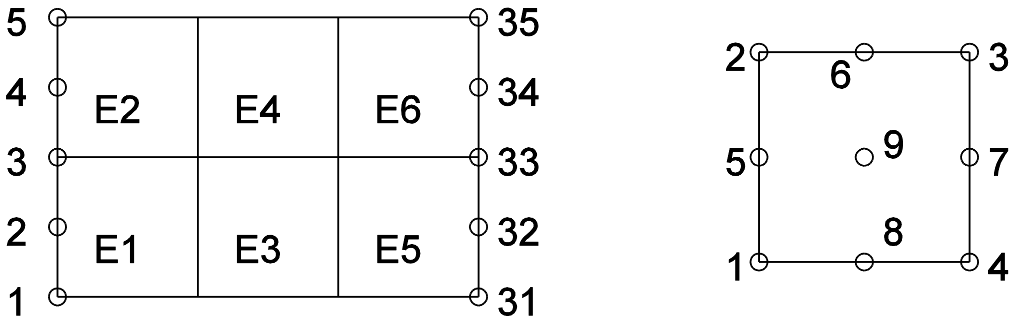


Figure 2: Hwang et al.

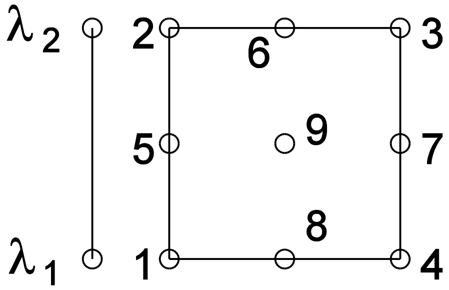


Figure 3: Hwang et al.

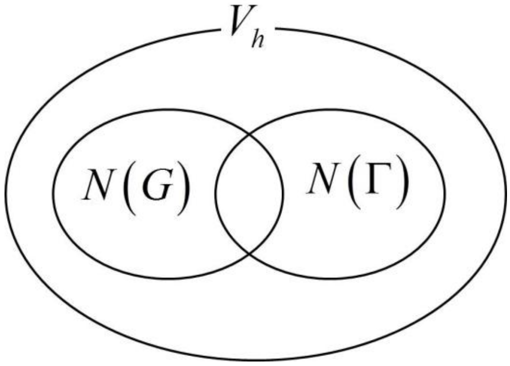
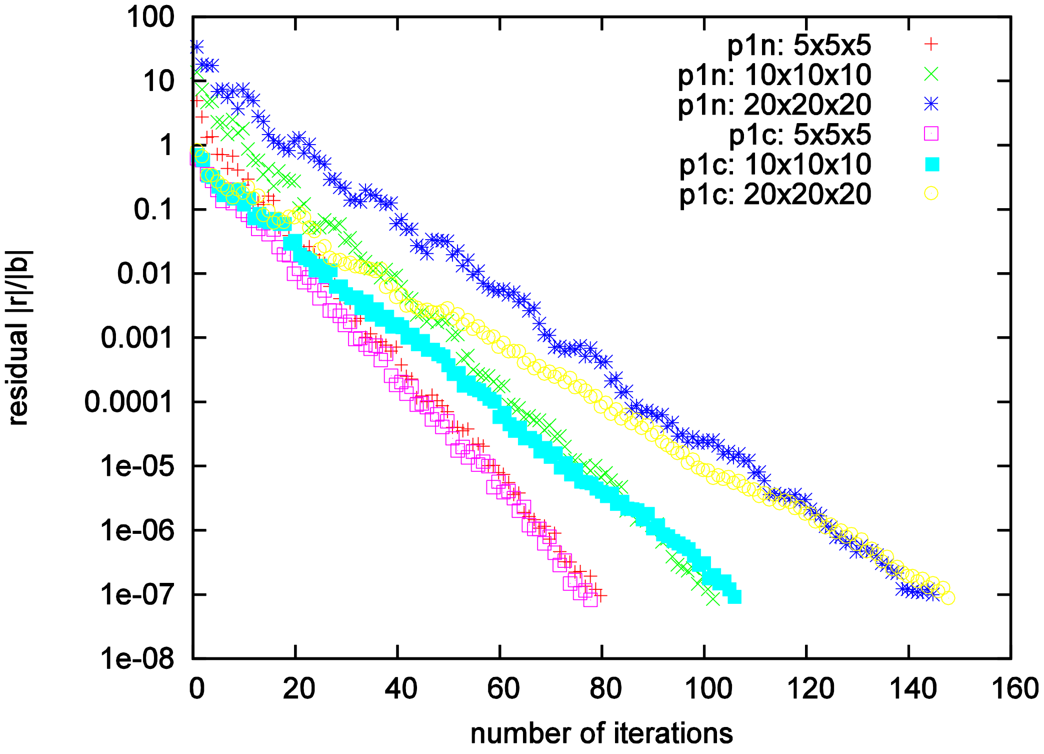


Figure 4: Hwang et al.



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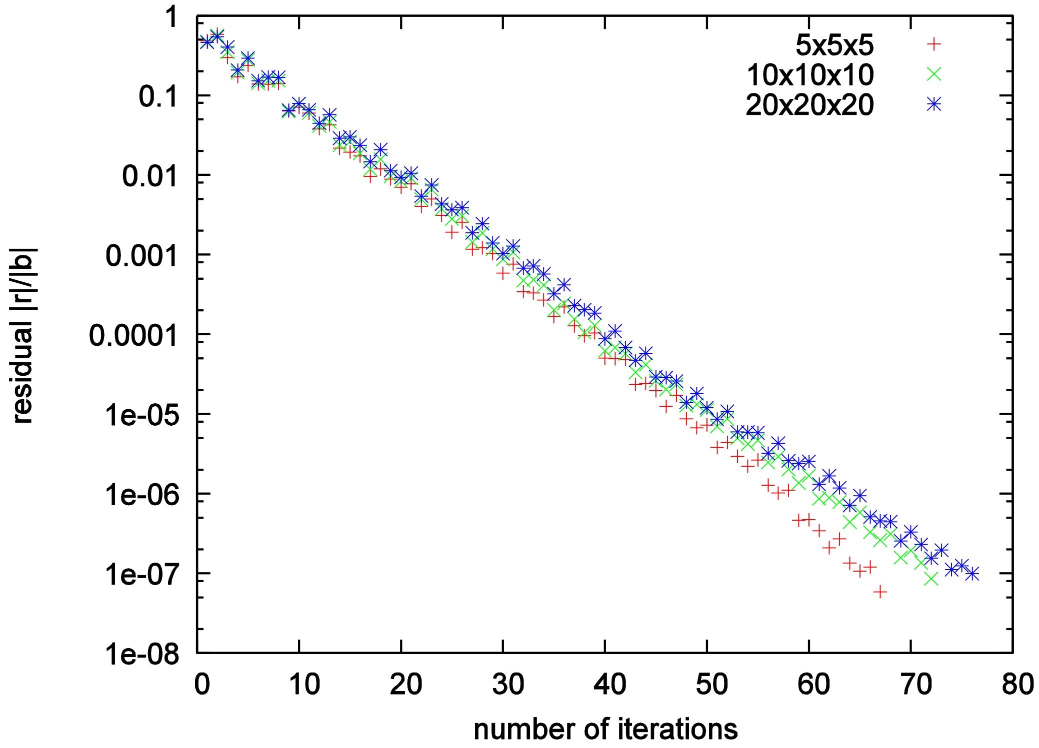
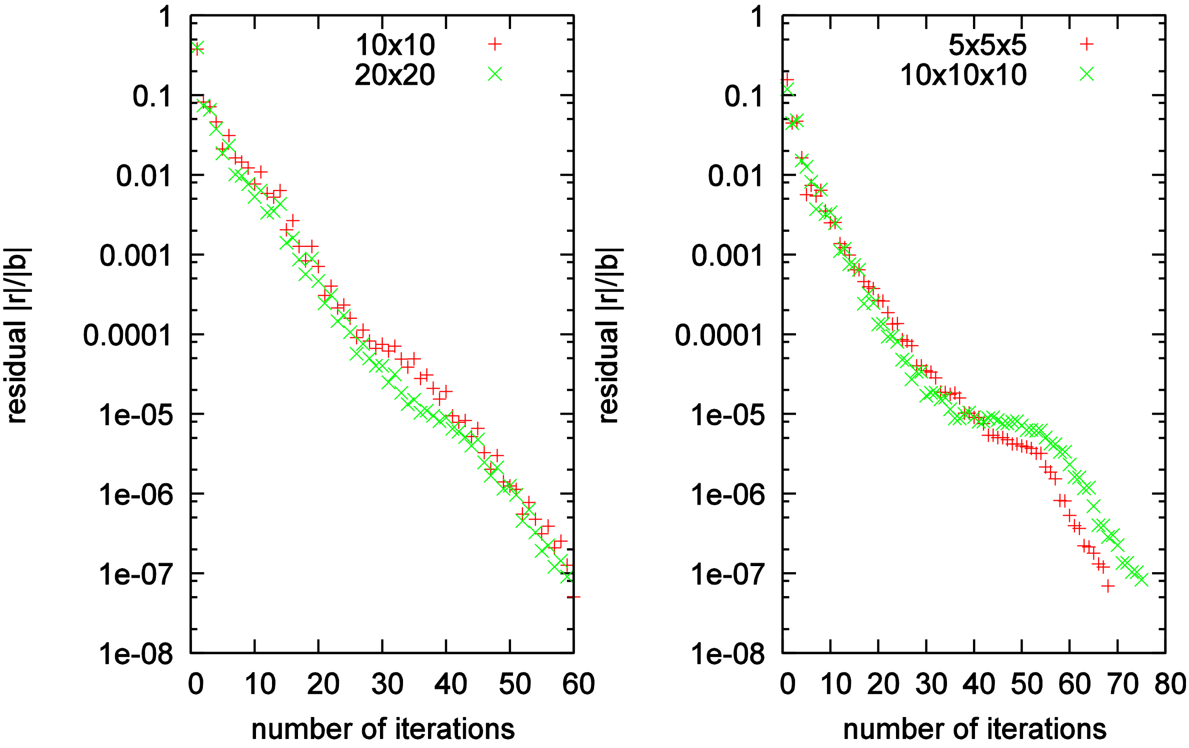


Figure 6: Hwang et al.



(a) (b)