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DEFLATED ICCG METHOD SOLVING THE POISSON EQUATION DERIVED FROM 3-D MULTI-PHASE FLOWS

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Abstract. *Simulating bubbly flows is a very popular topic in CFD. These bubbly flows are governed by the Navier-Stokes equations. In many popular operator splitting formulations for these equations, solving the linear system coming from the discontinuous Poisson equation takes the most computational time, despite of its elliptic origins. Sometimes these singular linear systems are forced to be invertible leading to a worse (effective) condition number. If ICCG is used to solve this problem, the convergence is significantly slower than for the case of the original singular problem.*

In this paper, we show that applying the deflation technique, which leads to the DICCG method, remedies the worse condition number and the worse convergence of ICCG. Moreover, some useful equalities are derived from the deflated variants of the singular and invertible matrices, which are also generalized to preconditioned methods. It appears that solving the invertible and singular linear systems with DICCG leads to exactly the same convergence results. Numerical experiments considering air-bubbles in water emphasize these theoretical results. This means that the deflation method is well-applicable for singular linear systems. In addition, from the numerical experiments it appears that DICCG is insensitive for the geometry of the density field, which is an important advantage of the deflation method.

1 Introduction

Recently, moving boundary problems have received much attention in literature due to their applicative relevance in many physical processes. One of the most popular moving boundary problems is modelling bubbly flows, see e.g. [12]. These bubbly flows can be simulated by solving the Navier-Stokes equations using for instance the pressure correction method [5]. The most time-consuming part of this method is solving the symmetric and positive semi-definite (SPSD) linear system on each time step, which is coming from a second-order finite-difference discretization of the Poisson equation with possibly discontinuous coefficients and Neumann boundary conditions:

$$\left\{ \begin{array}{rcl} \nabla \cdot \left(\frac{1}{\rho(\mathbf{x})} \nabla p(\mathbf{x}) \right) & = & f(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \frac{\partial}{\partial \mathbf{n}} p(\mathbf{x}) & = & g(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega, \end{array} \right. \tag{1}$$

where $p, \rho, \mathbf{x}$ and $\mathbf{n}$ denote the pressure, density, spatial coordinates and the unit normal vector to the boundary $\partial\Omega$, respectively. The resulting singular linear system is

$$Ax = b, \quad A = [a_{i,j}] \in \mathbb{R}^{n \times n}, \tag{2}$$

where the coefficient matrix A is SPSD. If $b \in \text{Col } A$ then the linear system (2) is consistent and infinite number of solutions exists. Due to the Neumann boundary conditions, the solution x is determined up to a constant, i.e., if x_1 is a solution then $x_1 + c$ is also a solution where $c \in \mathbb{R}^n$ is an arbitrary constant vector. This situation presents no real difficulty, since pressure is a relative variable, not an absolute one. In this paper we concentrate on the linear system (2), which can also derived from other problems besides the bubbly flow problems. The precise requirements can be found in the next section of this paper.

In many computational fluid dynamics packages, see also [1,4,11], one would impose an invertible A, denoted by $\widetilde{A}$. This makes the solution x unique which can be advantageous in computations, for instance,

- direct solvers like Gaussian elimination can only be used to solve the linear systems when A is invertible;
- the original singular system may be inconsistent as a result of rounding errors whereas the invertible system is always consistent;
- the deflation technique requires an invertible matrix $E := Z^T AZ$ which will be explained later on in this paper. The choice of Z is straightforward if A is non-singular.

One common way to force invertibility of matrix A in literature is to replace the last element $a_{n,n}$ by $\tilde{a}_{n,n} = (1 + \sigma)a_{n,n}$ with $\sigma > 0$. In fact, a Dirichlet boundary condition is imposed in one point of the domain Ω. This modification results in an invertible linear system

$$\widetilde{A}x = b, \quad \widetilde{A} = [\tilde{a}_{i,j}] \in \mathbb{R}^{n \times n}, \tag{3}$$

where $\widetilde{A}$ is SPD.

The most popular iterative method to solve linear systems like (3) is the Preconditioned Conjugate Gradient (CG) method. It is well-known that the error during the iterations of CG is bounded by an expression with the spectral condition number κ of $\widetilde{A}$. A smaller κ leads asymptotically to a faster convergence of the CG method. In practice, it appears that the condition number κ is relatively large, especially when σ is close to 0. Hence, solving (3) with the CG method shows slow convergence, see also [4, Section 4] and [11, Section 6.7]. The same holds if the ICCG method [7] is used. ICCG shows good performance for relatively small and easy problems. However, it appears that ICCG still does not give satisfactory results in more complex models, for instance when the number of grid points becomes very large or when there are large jumps in the density of (1). To remedy the bad convergence of ICCG, deflation techniques are proposed, originally from Nicolaides [10]. The idea of deflation is to project the extremely large or small eigenvalues of $\widetilde{M}^{-1}\widetilde{A}$ to zero, where M denotes the IC preconditioner. This leads to a faster convergence of the iterative process. The deflation technique has been exploited by several other authors, e.g., [2, 8, 9]. The resulting linear system which has to be solved is

$$\widetilde{P}\widetilde{M}^{-1}\widetilde{A}x = \widetilde{P}\widetilde{M}^{-1}b, \tag{4}$$

where $\widetilde{P}$ denotes the deflation matrix based on $\widetilde{A}$.

It is known that forcing invertibility of A leads always to a worse condition number. As a consequence, the convergence of the CG method applied to the system with A is theoretically faster than with $\widetilde{A}$. In practice, this is indeed the case and it holds also for ICCG. In this paper, we investigate this issue for the deflated variants of the matrix $\widetilde{A}$ and the singular matrix A. Most papers on deflation deal only with invertible systems. Applications of deflation to singular systems are described in [6, 15, 16]. In these papers, some suggestions have been given how to combine singular systems with a deflation technique, but the underlying theory has not yet been developed. In this paper, relations between the singular matrix A and the invertible matrix $\widetilde{A}$ will be worked out using the deflation matrices P and $\widetilde{P}$ to gain more insight into the application of the deflation technique for singular systems.

The outline of this paper is as follows. In Section 2 we introduce some notations and definitions and we give some preliminary results. Furthermore, we show that the condition number of $\widetilde{A}$ is always worse than the effective condition number of A. In Section 3 the proof is given of the equality $\widetilde{P}\widetilde{A} = PA$, which is an unexpected result. This will also be generalized to $\widetilde{P}\widetilde{M}^{-1}\widetilde{A}$ and $PM^{-1}A$. Results of numerical experiments will be presented in Section 4 to illustrate the theory. For more details we refer to [14].

2 Definitions and Preliminary Results

We first define the notations for standard matrices and vectors, see Table 1. Next, the $n \times n$ matrix A satisfies two assumptions which are given below.

Notation	Meaning
$\mathbf{e}_p^{(r)}$	r-th column of the $p \times p$ identity matrix I
$\mathbf{e}_{p,q}^{(r)}$	$p \times q$ matrix with q identical columns $\mathbf{e}_p^{(r)}$
$\mathbf{1}_{p,q}$	$p \times q$ unit matrix
$\mathbf{1}_p$	column of $\mathbf{1}_{p,q}$
$\mathbf{0}_{p,q}$	$p \times q$ zero matrix
$\mathbf{0}_p$	column of $\mathbf{0}_{p,q}$

Table 1: Notations for standard matrices and vectors where $p, q, r \in \mathbb{N}$.

Assumption 1. *Matrix $A \in \mathbb{R}^{n \times n}$ is SPSD and singular. Moreover, the algebraic multiplicity of the zero-eigenvalue of A is equal to one.*

Assumption 2. *Matrix A satisfies $A\mathbf{1}_n = \mathbf{0}_n$.*

Now, matrix $\widetilde{A}$ is defined in the following way.

Definition 1. *Let A be given which satisfies Assumptions 1 and 2. Then $\widetilde{A}$ is defined by $\widetilde{a}_{n,n} = (1+\sigma)a_{n,n}$ where $\sigma > 0$, and $\tilde{a}_{i,j} = a_{i,j}$, for the other indices i and j.*

Some consequences of Definition 1 can be found in the following two corollaries.

Corollary 1. *Matrix $\widetilde{A}$ is invertible and SPD.*

Corollary 2. *Matrix A satisfies $\widetilde{A}\mathbf{1}_n = \sigma a_{n,n} \mathbf{e}_n^{(n)}$.*

Next, let the computational domain Ω be divided into open subdomains Ω_j, $j = 1, 2, \ldots, r$, such that $\Omega = \cup_{j=1}^r \overline{\Omega}_j$ and $\cap_{j=1}^r \Omega_j = \emptyset$ where $\overline{\Omega}_j$ is Ω_j including its adjacent boundaries. The discretized domain and subdomains are denoted by Ω_h and Ω_{h_j}, respectively. Then, for each Ω_{h_j} with $j = 1, 2, \ldots, r$, we introduce a deflation vector z_j as follows:

$$(z_j)_i := \begin{cases} 0, & x_i \in \Omega_h \setminus \overline{\Omega}_{h_j}; \\ 1, & x_i \in \Omega_{h_j}, \end{cases} \tag{5}$$

where x_i is a grid point in the discretized domain $\Omega_h$and $z_0 = \mathbf{1}_n$.

Subsequently, we define the so-called deflation subspace matrices Z and $\widetilde{Z}$ and also the deflation matrices P_r and $\widetilde{P}_r$.

Definition 2. *For $r > 1$, we define $Z := [z_1 \ z_2 \ \cdots \ z_{r-1}] \in \mathbb{R}^{n \times (r-1)}$ and $\widetilde{Z} := [Z \ z_r]$. Moreover, the deflation matrices are defined by $P_r := I - AZE^{-1}Z^T$, $E := Z^T A Z$ and $\widetilde{P}_r := I - \widetilde{A}\widetilde{Z}\widetilde{E}^{-1}\widetilde{Z}^T$, $\widetilde{E} := \widetilde{Z}^T \widetilde{A} \widetilde{Z}$. Finally, we define $\widetilde{P}_1 := I - \widetilde{A} z_0 \widetilde{E}_0^{-1} z_0^T$, $\widetilde{E}_0 := z_0^T \widetilde{A} z_0$.*

Next, the eigenvalues λ_i of a symmetric $n \times n$ matrix are always ordered increasingly, i.e., $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. In addition, let B be an arbitrary $n \times n$ SPSD matrix with rank $n - r$, so that $\lambda_1 = \ldots = \lambda_r = 0$. Note that in this case all eigenvalues of B are real-valued due to the symmetry of B. Then its effective condition number $\kappa_{\text{eff}}(B)$ is defined by $\kappa_{\text{eff}}(B) := \lambda_n(B)/\lambda_{r+1}(B)$.

We end this section with some preliminary results from the theory of deflation and linear algebra.

Lemma 1 (Thm. 2.6, [8])**.** $\lambda_1(\widetilde{P}_r\widetilde{A}) = \lambda_2(\widetilde{P}_r\widetilde{A}) = \ldots = \lambda_r(\widetilde{P}_r\widetilde{A}) = 0.$

Based on other results in [8], we derive the next lemma.

Lemma 2. *P_rA and $\widetilde{P}_r\widetilde{A}$ are SPSD matrices.*

Subsequently, we give Lemma 3 [17, pp. 94–97].

Lemma 3. *Suppose $K = L + \tau cc^T$ where $L \in \mathbb{R}^{n\times n}$ is symmetric, $c \in \mathbb{R}^n$ has unit 2-norm and $\tau > 0$. Then*

$$\lambda_i(L) \leq \lambda_i(K) \leq \lambda_{i+1}(L), \quad i = 1, 2, \ldots, n-1. \tag{6}$$

Moreover, there exist $m_1, m_2, \ldots, m_n \geq 0$ such that

$$\lambda_i(K) = \lambda_i(L) + m_i\tau, \quad i = 1, 2, \ldots, n, \tag{7}$$

with $m_1 + m_2 + \ldots + m_n = 1$.

Using Lemma 3, we can derive Theorem 1 which says that forcing invertibility of A leads automatically to a worse condition number.

Theorem 1. *Inequality $\kappa(\widetilde{A}) \geq \kappa_{\text{eff}}(A)$ holds for all $\sigma \geq 0$.*

Proof. To prove the theorem, we apply Lemma 3. Note that $\widetilde{A} = A + \tau cc^T$, with $c = \mathbf{e}_n^{(n)}$ and $\tau = \sigma a_{n,n}$. Therefore, from Eq. (6) we have $\lambda_i(A) \leq \lambda_i(\widetilde{A}) \leq \lambda_{i+1}(A)$ for $i = 1, 2, \ldots, n-1$, so in particular $\lambda_1(A) \leq \lambda_1(\widetilde{A}) \leq \lambda_2(A)$. On the other hand, from Eq. (7) we obtain $\lambda_i(\widetilde{A}) \geq \lambda_i(A)$ with $i = 1, 2, \ldots, n$, since $m_i\tau \geq 0$ for all i. So in particular, this implies $\lambda_n(\widetilde{A}) \geq \lambda_n(A)$. Combining these facts, the theorem follows immediately. $\square$

3 Comparison of the Preconditioned Deflated Singular and Invertible Matrix

In this section, we first show that the condition number of $\widetilde{A}$ is reduced to the condition number of A by a simple deflation technique. Thereafter, we show that even the deflated variants of $\widetilde{A}$ and A are equal. Finally, we generalize this also to preconditioned deflated variants. As a consequence, solving $Ax = b$ and $\widetilde{A}x = b$ with DICCG leads in theory to the same convergence results.

3.1 Comparison of $\widetilde{P}_1\widetilde{A}$ and A

Before proving the equality $\widetilde{P}_1\widetilde{A} = A$, we show that $\widetilde{P}_1$ is the identity matrix except for the last row. This is stated in Lemma 4 which can be easily proven.

Lemma 4. $\widetilde{P}_1 = I - \boldsymbol{e}_{n,n}^{(n)}$.

Next, applying Lemma 4, we obtain the following theorem.

Theorem 2. *Equality $\widetilde{P}_1\widetilde{A} = A$ holds.*

Proof. The exact form of $\widetilde{P}_1$ is given in Lemma 4. Obviously, $\widetilde{P}_1\widetilde{A} = A$ for all rows except the last one, since the rows 1 to $n-1$ of $\widetilde{P}_1$ are equal to the corresponding rows of the identity matrix.

The analysis of the last row of $\widetilde{P}_1\widetilde{A}$, which is $(\mathbf{e}_n^{(n)} - \mathbf{1}_n)^T\widetilde{A}$, is as follows. The sum of each column of A is zero due to symmetry and Assumption 2 leading to $\mathbf{1}_n^T A = \mathbf{0}_n^T$. On the other hand, using Definition 1 we have $(\mathbf{e}_n^{(n)} - \mathbf{1}_n)^T\widetilde{A} = (\mathbf{e}_n^{(n)} - \mathbf{1}_n)^T A$, because A and $\widetilde{A}$ differs only in the last element. Combining these facts yields $(\mathbf{e}_n^{(n)} - \mathbf{1}_n)^T\widetilde{A} = (\mathbf{e}_n^{(n)} - \mathbf{1}_n)^T A = \mathbf{e}_n^{(n)T} A$. Hence, the last rows of $\widetilde{P}_1\widetilde{A}$ and A are also equal which proves the theorem. □

Theorem 2 implies that, after applying deflation with $r = 1$, the invertible matrix $\widetilde{A}$ becomes equal to the original singular matrix A. Now, intuitively it is clear that subdomain deflation with $r \geq 1$ acting on A and $\widetilde{A}$ leads to the same convergence results, since the constant deflation vector is in the span of the subdomain deflation vectors. In the remaining of this section, we will prove this idea.

3.2 Comparison of $\widetilde{P}_r\widetilde{A}$ and P_rA

Theorem 3 is the main result of this section, which shows that the deflated singular system based on A is equal to the deflated variant of the invertible system $\widetilde{A}$. This is a rather unexpected result, since Z consists of one vector less compared to $\widetilde{Z}$. In order to prove this theorem, a set of auxiliary results is required. We start with Lemma 5 which can be easily proven.

Lemma 5. *Define* $B := (\beta_1,\ \beta_2,\ \ldots,\ \beta_n)^T\, \boldsymbol{1}_n^T,\ \beta_i \in \mathbb{R},\ i = 1, 2, \ldots, n.$

(i) For some β_i we have that $P_r - \widetilde{P}_r = B$ is satisfied, i.e., each row of $P_r - \widetilde{P}_r$ contains the same elements.

(ii) The last column of $\widetilde{P}_r$ is the zero-vector $\boldsymbol{0}_n$.

Now, we can prove Lemma 6 which show that deflation matrix $\widetilde{P}_r$ is invariant by right-multiplication with deflation matrix $\widetilde{P}_1$ and that deflated systems $\widetilde{P}_rA$ and P_rA are identical.

Lemma 6. *The following equalities holds:*

(i) $\widetilde{P}_r \widetilde{P}_1 = \widetilde{P}_r$;

(ii) $\widetilde{P}_r A = P_r A$.

Proof. Corollary 2 implies $\widetilde{A}\mathbf{1}_{n,n} = \sigma a_{n,n} \mathbf{e}_{n,n}^{(n)}$. From Lemma 5, we have the result that the last column of $\widetilde{P}_r$ is $\mathbf{0}_n$. This implies that $\widetilde{P}_r \widetilde{A}\mathbf{1}_n = \mathbf{0}_n$, for arbitrary $\sigma > 0$. Using this fact, we obtain immediately $\widetilde{P}_r \widetilde{P}_1 = \widetilde{P}_r(I - \alpha \widetilde{A}\mathbf{1}_n) = \widetilde{P}_r - \alpha \widetilde{P}_r \widetilde{A}\mathbf{1}_n = \widetilde{P}_r$. This proves part (i).

Furthermore, define $B = [b_{i,j}]$ as in Lemma 5. In the same lemma, it has been shown that each row i of $\widetilde{P}_r - P_r$ has the same elements, i.e., $B = \widetilde{P}_r - P_r$. Then this yields $(\widetilde{P}_r - P_r)A = BA = \mathbf{0}_{n,n}$, since $\mathbf{1}_n^T A = \mathbf{0}_n^T$ holds due to Assumption 2. This completes the proof of part (ii) of the lemma. □

Finally, our main result $\widetilde{P}_r \widetilde{A} = P_r A$ can be shown.

Theorem 3. $\widetilde{P}_r \widetilde{A} = P_r A$ *holds for all* $\sigma > 0$ *and* $r \geq 1$.

Proof. In Theorem 2 and Lemma 6, we have derived the equalities $\widetilde{P}_1 \widetilde{A} = A$, $\widetilde{P}_r \widetilde{P}_1 = \widetilde{P}_r$ and $\widetilde{P}_r A = P_r A$, respectively, which hold for all $\sigma > 0$ and $r \geq 1$. Hence, $\widetilde{P}_r \widetilde{A} = \widetilde{P}_r \widetilde{P}_1 \widetilde{A} = \widetilde{P}_r A = P_r A$. □

3.3 Comparison of $\widetilde{M}^{-1}\widetilde{P}_r\widetilde{A}$ and $\widetilde{M}^{-1}P_r A$

Although $\widetilde{P}_r \widetilde{A} = P_r A$ holds, the preconditioned variant of this equality is not valid generally, i.e., $\widetilde{M}^{-1}\widetilde{P}_r \widetilde{A} \neq M^{-1} P_r A$. Moreover, in Section 2 we have seen $\lim_{\sigma \to 0} \kappa(\widetilde{A}) = \infty$, whereas obviously $\lim_{\sigma \to 0} \kappa_{\text{eff}}(\widetilde{P}_r \widetilde{A}) = \kappa_{\text{eff}}(P_r A)$. The topic of this section is to show that $\lim_{\sigma \to 0} \kappa_{\text{eff}}(\widetilde{M}^{-1}\widetilde{P}_r \widetilde{A}) = \kappa_{\text{eff}}(M^{-1}P_r A)$ holds, which is also equivalent to prove that $\lim_{\sigma \to 0} \kappa_{\text{eff}}(\widetilde{M}^{-1}P_r A) = \kappa_{\text{eff}}(M^{-1}P_r A)$. In this paper, we restrict ourselves to the incomplete Cholesky (IC) preconditioners. First we deal with the comparison of the effective condition numbers of $M^{-1}A$ and $\widetilde{M}^{-1}A$ and thereafter we generalize these results to $M^{-1}P_r A$ and $\widetilde{M}^{-1}P_r A$.

It can be proved that if $\sigma \to 0$ then the effective condition numbers of $M^{-1}A$ and $\widetilde{M}^{-1}A$ are the same, see Theorem 4. The proof is omitted here, but it can be found in [14].

Theorem 4. *Let* M^{-1} *and* $\widetilde{M}^{-1}$ *be the corresponding IC preconditioners to* A *and* $\widetilde{A}$. *Then* $\lim_{\sigma \to 0} \ \kappa_{\mathit{eff}}(\widetilde{M}^{-1}A) = \kappa_{\mathit{eff}}(M^{-1}A)$.

Next, we compare the effective condition numbers of $M^{-1}P_r A$ and $\widetilde{M}^{-1}P_r A$. Note that both A and $P_r A$ are SPSD matrices, see also Lemma 2. So in particular, we can subsitute $P_r A$ into A in Theorem 5, which implies immediately $\lim_{\sigma \to 0} \kappa_{\text{eff}}(\widetilde{M}^{-1}P_r A) = \kappa_{\text{eff}}(M^{-1}P_r A)$. In other words, the theory given in Theorem 4 still holds if we replace A by $P_r A$ in the whole analysis. This has been summarized in the next theorem.

Theorem 5. *Let M^{-1} and $\widetilde{M}^{-1}$ be the corresponding IC preconditioners to A and $\widetilde{A}$. Then* $\lim_{\sigma \to 0}\ \kappa_{\textit{eff}}(\widetilde{M}^{-1} P_r A) = \kappa_{\textit{eff}}(M^{-1} P_r A)$.

4 Numerical Experiments

In this section we give the results of some numerical experiments. These experiments will illustrate the theoretical results obtained in the previous sections.

4.1 Test Problem

We consider the 3-D Poisson problem as given in Eq. (1) with two fluids Λ_0 and Λ_1, see also [12]. Specifically, we consider two-phase bubbly flows with air and water in a unit domain. In this case, ρ is piecewise constant with a relatively high contrast:

$$\rho = \begin{cases} \rho_0 = 1, & \mathbf{x} \in \Lambda_0, \\ \rho_1 = 10^{-3}, & \mathbf{x} \in \Lambda_1, \end{cases}$$

where Λ_0 is water, the main fluid of the flow around the air bubbles, and Λ_1 is the region inside the bubbles. In the first part of the numerical experiments, we choose $m = 2^3 = 8$ bubbles with the same radii. In Figure 1 one can find the geometry of this test case.

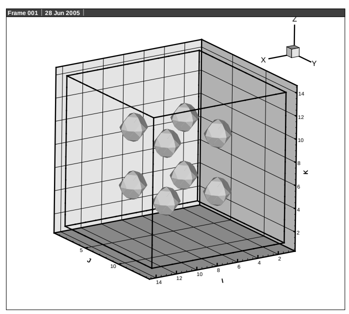


Figure 1: Geometry of an air-water problem with eight air bubbles in the domain.

The resulting singular linear system $Ax = b$ and also the invertible linear system $\widetilde{A}x = b$ are ill-conditioned due to the presence of the bubbles. We apply ICCG and DICCG$-k$ to solve the linear system, where DICCG$-k$ denotes DICCG with k deflation vectors. The relative tolerance $||M^{-1}P(b - A\tilde{x}_k)||_2/||M^{-1}b||_2$ is chosen to be smaller than $\epsilon = 10^{-8}$. It is easy to see that this choice of relative tolerance for DICCG is equivalent to the relative tolerance of $||M^{-1}(b - Ax_k)||_2/||M^{-1}b||_2$ for ICCG. We vary the perturbation parameter σ and the number of deflation vectors k in our experiments.

4.2 Results

The results of the above described test problem with $\widetilde{A}$ can be found in Table 2. In the case of ICCG, the results of the singular matrix A are added for comparison.

From this table, one observes immediately that the results of DICCG$-k$ are completely independent of σ, as expected from the previous sections. Furthermore, if $\sigma = 0$ then the original singular problem has been solved. In this case, we see that the required number of iterations for ICCG is equal to the number for DICCG-1 when the problem with arbitrary $\sigma > 0$ is solved. Moreover, note that increasing the number of deflation vectors k leads to a non-decreasing number of iterations for DICCG$-k$. All these observations are in agreement with the theoretical results.

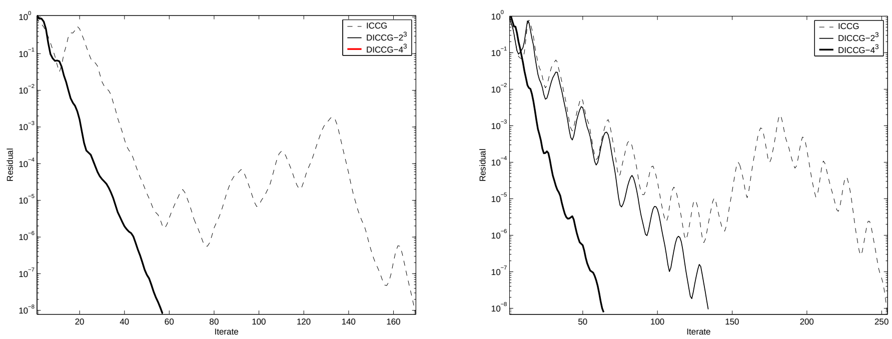
(a) ICCG.

σ	# Iterations $n = 32^3$	# Iterations $n = 64^3$
0	118	200
10^{-1}	163	329
10^{-3}	170	350

(b) DICCG$-k$.

σ	k	# Iterations $n = 32^3$	# Iterations $n = 64^3$
10^{-1}	1	118	200
10^{-1}	2^3	57	106
10^{-1}	4^3	57	106
10^{-3}	1	118	200
10^{-3}	2^3	57	106
10^{-3}	4^3	57	106

Table 2: Number of iterations of ICCG and DICCG$-k$ to solve the invertible linear system $\widetilde{A}x = b$ with $m = 2^3$ bubbles.



(a) $m = 2^3$ bubbles. (b) $m = 3^3$ bubbles.

Figure 2: Plots of the update residuals of ICCG, DICCG-2^3 and DICCG-3^3 in the test cases with $n = 32^3$ and $\sigma = 10^{-3}$.

In Figure 2(a) one can find a plot of the residuals of ICCG and DICCG$-k$ for our test case. From this figure, it can be observed that ICCG shows an erratic convergence behavior, while DICCG$-k$ converges almost monotonically. Apparently, the approximations of the eigenvectors corresponding to the small eigenvalues are very good. Moreover, we note that the residuals of DICCG-2^3 and DICCG-4^3 coincide. However, from Table

3, it appears that if we take $m = 3^3$ bubbles, then the results with $k = 4^3$ is much better than with $k = 2^3$ (see Table 3).

(a) ICCG.

σ	# Iterations
0	160
10^{-1}	234
10^{-3}	254

(b) DICCG$-k$.

σ	k	# Iterations
10^{-1}	1	160
10^{-1}	2^3	134
10^{-1}	4^3	64
10^{-3}	1	160
10^{-3}	2^3	134
10^{-3}	4^3	64

Table 3: Number of iterations of ICCG and DICCG$-k$ to solve the invertible linear system $\widetilde{A}x = b$ with $m = 3^3$ bubbles and $n = 32^3$.

In Figure 2(b) one can find a plot of the residuals of ICCG and DICCG$-k$ for this test case. Now, the residuals of DICCG-4^3 decrease more or less monotonically, whereas the residuals of both ICCG and DICCG-2^3 are still erratic. Obviously, in this case the small eigenvalues are worse approximated by the deflation technique compared by the case with $m = 2^3$ bubbles (cf. Figure 2(a)). The reason is not only the position of the bubbles with respect to the subdomains, but also the increased number of bubbles is more difficult to treat with a constant number of deflation vectors.

In the above experiments, we have not yet tested DICCG$-k$ in cases for singular linear systems. In Table 4 we have compared these to the results using the invertible linear systems. Recall that in the singular case, DICCG$-k$ applies $k-1$ instead of k deflation vectors. Note further that DICCG-1 is not defined in this case.

(a) $Ax = b$.

	# Iterations	
k	$n = 32^3$	$n = 64^3$
2^3	57	106
4^3	57	106

(b) $\widetilde{A}x = b$ with both $\sigma = 10^{-1}$ and $\sigma = 10^{-3}$.

	# Iterations	
k	$n = 32^3$	$n = 64^3$
2^3	57	106
4^3	57	106

Table 4: Number of iterations of DICCG$-k$ to solve the singular linear system $Ax = b$ and the invertible linear system $\widetilde{A}x = b$ with $m = 2^3$ bubbles.

From Table 4 we observe immediately that the results considering singular matrices are the same as the results of the corresponding test cases with invertible matrices. Indeed, the two different approaches of the deflation technique considering both the singular and invertible matrices are equivalent, which confirms the theory.

5 Conclusions

In this paper, we have analyzed a singular matrix coming from for instance the Poisson equation. This matrix can be made invertible by modifying the last element, while the solution of the resulting linear system is still the same. Invertibility of the matrix gives several advantages for the iterative solver. The drawback, however, is that the condition number becomes worse compared to the effective condition number of the singular matrix. It appears that this problem with a worse condition number has completely been remedied by applying the deflation technique with just one deflation vector. Moreover, the deflated singular and invertible matrices have been related to each other. For special choices of the deflation vectors, these matrices are even identical. These results can also be generalized for the preconditioned singular and invertible matrices. This means that two variants of deflated and preconditioned linear systems can be solved resulting in the same convergence results. Results of numerical experiments considering bubbly flows confirm the theoretical results and show the good performance of the iterative method including the deflation technique, also for cases of complex geometries of the bubbly flows.

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