

# **The Bi-CGSTAB Method with Red-Black Gauss-Seidel Preconditioner Applied to the Hermite Collocation Discretization of Subsurface Multiphase Flow and Transport Problems**

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## **Abstract**

The solution of the Hermite collocation discretization of the partial differential equations that govern subsurface multiphase flow and contaminant transport requires considerable computational effort. To minimize this burden, we solve these equations using the Bi-CGSTAB method with a red-black Gauss-Seidel preconditioning matrix. We find that our method of solution is virtually always much faster than the commonly used GMRES method with ILU preconditioning. In addition, our choice of preconditioner allows easy implementation on a parallel processing computer.

## **1 Introduction**

We report herein on a rapid and computationally efficient method of solution of the Hermite collocation discretization of the partial differential equations (PDEs) in two spatial dimensions that model multiphase flow and contaminant transport in porous media. The paper is organized as follows. First, we discuss the general governing

mass-balance equations and then introduce their final form and strategy of solution. We then briefly introduce the Hermite collocation discretization and our method of solution. Finally, we discuss the results of solving the multiphase equations via our method of solution compared to using GMRES/ILU, an alternative popular method for the solution of nonsymmetric systems of linear algebraic equations.

## 2 The PDEs of multiphase flow and transport

We solve the multiphase equations as implemented in the *NAPL* software described in [4]. In this simulator, we consider three fluid phases ( $W$  = water;  $N$  = NAPL (i.e., a non-aqueous phase liquid); and  $G$  = gas), each consisting of (at most) three constituent species ( $w$  = water,  $n$  = NAPL, and  $g$  = gas). Note the convention that capital letters indicate *phases* while lower case letters denote *species*.

The equation that gives the mass-balance for species  $i$  in phase  $\alpha$  in a porous medium is recognizable as an advection-dispersion equation with additional terms representing species decay, a source/sink of phase mass, and a source/sink of species mass moving across phase boundaries [4]. Because within each of the three phases ( $W, N, G$ ) there may exist three constituent species ( $w, n, g$ ), we begin with nine versions of this PDE.

After various manipulations to make the problem tractable (see [4] for details), we arrive at the final form of the multiphase equations. There are five of these, written in terms of known parameters and the five *primary variables*  $P^W$  = water phase pressure,  $S_W$ ,  $S_{T_w} = S_W + S_N$ ,  $\rho_n^W$ , and  $\rho_n^G$ . Here  $S_\alpha$  is the saturation of the  $\alpha$ -phase and  $\rho_i^\alpha$  is the mass concentration of species  $i$  in the  $\alpha$ -phase. As we advance from time step  $k$  to time step  $k + 1$ , the five equations are solved as described below. See [4] for details.

We first solve an elliptic-type equation for  $P^{W(k+1)}$ . We then arrive at the two coupled time-discrete *species transport* equations, which are solved iteratively as:

$$f_n^W \left( \rho_n^{W(k+1,m+1)}, \rho_n^{W(k+1,m)}, \rho_n^{W(k)}, \rho_n^{G(k+1,m)} \right) = 0 \quad (1)$$

$$f_n^G \left( \rho_n^{G(k+1,m+1)}, \rho_n^{G(k+1,m)}, \rho_n^{G(k)}, \rho_n^{W(k+1,m)} \right) = 0. \quad (2)$$

The notation  $\rho_n^{\alpha(k+1,m+1)}$  means the mass concentration of the NAPL species in the  $\alpha$ -phase at time step  $k + 1$  and iteration number  $m + 1$ .

The expression  $\rho_n^{\alpha(k)}$  refers to the mass concentration of the NAPL species in the  $\alpha$ -phase at time step  $k$ ; i.e., the value to which the iterates  $\rho_n^{\alpha(k,m)}$  converged. At time step  $k + 1$ , we solve (1) for  $\rho_n^{W(k+1,m+1)}$ , the concentration of the NAPL species in the water phase at time step  $k + 1$  and iteration number  $m + 1$ , using values of NAPL species concentration in the water phase at both the previous iteration and previous time step *and* the value of the NAPL species concentration in the *gas* phase at time step  $k + 1$  and iteration number  $m$ . Similarly, we solve (2) for  $\rho_n^{G(k+1,m+1)}$ , the concentration of the NAPL species in the gas phase at time step  $k + 1$  and iteration number  $m + 1$ , using values of NAPL species concentration in the gas phase at both the previous iteration and previous time step *and* the value of the NAPL species concentration in the *water* phase at time step  $k + 1$  and iteration number  $m$ . This coupled iterative solution technique continues until convergence is reached, i.e., until the changes in concentration from one iteration to the next are sufficiently minuscule.

Once this convergence is attained, i.e., we have values for  $\rho_n^{W(k+1)}$  and  $\rho_n^{G(k+1)}$ , we next arrive at two coupled time-discrete *phase saturation* equations, which are solved iteratively as:

$$f^W \left( S_W^{(k+1,m+1)}, S_W^{(k+1,m)}, S_W^{(k)}, S_{T_w}^{(k+1,m)} \right) = 0 \quad (3)$$

$$f^G \left( S_{T_w}^{(k+1,m+1)}, S_{T_w}^{(k+1,m)}, S_{T_w}^{(k)}, S_W^{(k+1,m)} \right) = 0. \quad (4)$$

The solution of the saturation equations (3),(4) is completely analogous to that of the transport equations (1),(2).

To summarize, at each time step we solve five equations for the five primary variables  $P^W$ ,  $S_W$ ,  $S_{T_w}$ ,  $\rho_n^W$ , and  $\rho_n^G$ . The equation for  $P^W$  is solved directly while the equations for the coupled parameter pairs  $(\rho_n^W, \rho_n^G)$  and  $(S_W, S_{T_w})$  are solved iteratively. It is worth noting that the pressure equation is independent of time step size. Also, should the scheme for the solution of  $\rho_n^W$  and  $\rho_n^G$  (respectively,  $S_W$  and  $S_{T_w}$ ) not converge in fewer than a prescribed maximum number of iterations, the time step size is reduced and the iterations begin again with the new time step size. It is therefore possible that many restarts and commensurate reductions in time step size may occur before convergence is actually reached at any particular time step.

### 3 Hermite collocation discretization of PDEs

We seek the solution  $u(x, y)$  of a time-discretized or time independent linearized PDE

$$\mathcal{L}\{u(x, y)\} = Q(x, y), \quad (5)$$

where  $\mathcal{L}$  is a second order linear differential operator. We solve (5) over a rectangular domain partitioned into a mesh of rectangular finite elements. The collocation discretization (see [1], [2], or [4] for details) proceeds by defining a bi-cubic Hermite interpolating polynomial  $\hat{u}$  to approximate  $u$ , and, after introducing boundary conditions, enforcing

$$\mathcal{L}\{\hat{u}(x, y)\} = Q(x, y)$$

at four “collocation points” in each finite element. In this paper, the collocation points within each finite element are chosen to coincide with its points of Gaussian quadrature, a selection which guarantees maximum accuracy [6].

The linearized, time-discrete form of the multiphase equations are discretized by the method given above for the general PDE (5). See [4] for details.

### 4 The Bi-CGSTAB method with block Red-Black Gauss-Seidel Preconditioner

The system of linear algebraic equations produced by the collocation discretization is neither symmetric nor diagonally dominant. To solve this system, which we write as

$$A\mathbf{x} = \mathbf{b}, \quad (6)$$

the *NAPL* software employs the SLATEC driver routine DSLUGM [8], which uses the GMRES [7] method with incomplete *LU* preconditioner. In an effort to obtain faster convergence, we propose replacing DSLUGM by the Bi-CGSTAB method [9] with a block Red-Black Gauss-Seidel preconditioner, which was introduced in [2]. The motivation for this change is previously published evidence [3] that Bi-CGSTAB is superior to GMRES for a wide range of problems and that Bi-CGSTAB lends itself more readily to parallel processing than does GMRES.

Our preconditioner is based upon a numbering of unknowns and collocation points that was introduced in [1] and analyzed for model problems in [2]. The system (6) is written in block form as

$$\begin{bmatrix} R & U \\ L & B \end{bmatrix} \begin{bmatrix} \mathbf{x}_R \\ \mathbf{x}_B \end{bmatrix} = \begin{bmatrix} \mathbf{b}_R \\ \mathbf{b}_B \end{bmatrix}$$

and the block Red-Black Gauss-Seidel preconditioner is  $\begin{bmatrix} R & \\ L & B \end{bmatrix}$ . As is seen in [1] and [2], our preconditioner has a structure which makes the Bi-CGSTAB method easily parallelizable.

## 5 Results

To compare the efficacy of the DSLUGM routine and the Bi-CGSTAB method with our preconditioner, we solved the multiphase equations using three example problems discussed in [4]. We augmented the *NAPL* code as follows. Every time DSLUGM (with restart parameter of 20, see [7] for explanation) solved a system (6), we then had Bi-CGSTAB (with our preconditioner) solve the identical system. Both methods of solution were timed on a serial computer.

### 5.1 Experiments

For all three experiments described below, refer to [4] for their implementation using the *NAPL* simulator. We note that for Experiments 1 and 2, the NAPL is assumed to be immiscible in both water and air, which obviates the necessity of solving the species transport equations (1) and (2).

#### 5.1.1 Experiment 1: LNAPL spill

The physical problem represented here is given in [10] and [11]. In part 1, a quasi-steady-state is reached by allowing an initially saturated sand to drain. Since no NAPL has been introduced yet, the only equations solved at each time step are the pressure equation and (3). In part 2, an LNAPL (i.e., a NAPL that is lighter than water) source is applied. At each time step we thus solve the pressure equation, (3), and (4). In part 3, the LNAPL source is discontinued and the system is allowed to redistribute and we thus solve the pressure equation, (3), and (4) at each time step.

	$D$ [secs]	$B$ [secs]	$D/B$	$D^*$	$B^*$	equation
Exp. 1,	657.1325	644.6898	1.0193	81	164	pressure
part 1	314.6103	156.0698	2.0158	2	344	(3)
	402.6298	378.9687	1.0624	41	106	pressure
Exp. 1,	365.8161	178.1669	2.0532	0	485	(3)
part 2	325.6655	114.7578	2.8379	0	485	(4)
	567.3365	572.4922	0.9910	105	99	pressure
Exp. 1,	287.1743	147.1151	1.9520	0	374	(3)
part 3	265.7106	107.3698	2.4747	0	374	(4)
Exp. 2,	631.6191	661.2326	0.9552	140	37	pressure
part 1	342.7492	192.1339	1.7839	1	276	(3)
	419.3771	379.5926	1.1048	32	77	pressure
Exp. 2,	552.1290	259.8333	2.1249	0	464	(3)
part 2	484.9935	184.8823	2.6233	0	463	(4)
	3448.8271	2312.8549	1.4912	59	674	pressure
Exp. 2,	1359.4818	606.2629	2.2424	0	1064	(3)
part 3	1319.4750	528.9365	2.4946	0	1064	(4)
	234.3932	121.5503	1.9284	0	96	pressure
	142.9025	56.0014	2.5518	0	262	(1)
	185.0255	71.0515	2.6041	0	256	(2)
	52.0629	39.4106	1.3210	0	96	(3)
Exp. 3	51.8614	37.8091	1.3717	0	96	(4)

Table 1: Comparison of DSLUGM ( $D$ ) and Bi-CGSTAB with our preconditioner ( $B$ ).  $D^*$  represents how many times method  $D$  was superior while  $B^*$  represents how many times method  $B$  was superior.

### 5.1.2 Experiment 2: DNAPL spill

The physical problem represented here, described in [4], is an artificial aquifer experiment conducted by M. Fishman. In part 1, a quasi-steady-state is reached after lowering the phreatic surface of an initially saturated sand. Since no NAPL has been introduced yet, the only equations solved at each time step are the pressure equation and (3). In part 2, a source of PCE, a DNAPL (i.e., a NAPL that is heavier than water), is applied. At each time step we thus solve the pressure equation, (3), and (4). In part 3, the PCE source is discontinued and the system is allowed to return to equilibrium and we thus solve the pressure equation, (3), and (4) at each time step.

### 5.1.3 Experiment 3: DNAPL vapor transport

This experiment is derived from one found in [5]. We make herein the change of eliminating the water table condition found in [5]. As the experiment begins, the water saturation profile of a sand column is in static equilibrium. A container filled with sand and residual TCE is placed at the top of the center of the sand column to act as a contaminant vapor source.

## 5.2 Interpretation of results

With reference to Table 1, each row provides data about the solution all the equations of a specified type (e.g., the pressure equation) for the indicated part of a particular experiment. For each row, the second,  $D$ , (respectively, third,  $B$ ) column gives the time (in seconds) required for DSLUGM (respectively, Bi-CGSTAB with our preconditioner) to solve all the equations relevant to that row. The fourth column,  $D/B$ , gives the ratio of the second and third columns. The fifth column,  $D^*$ , gives the total number of times DSLUGM solved a system (6) more quickly than did Bi-CGSTAB (with our preconditioner). The sixth column,  $B^*$ , gives the total number of times Bi-CGSTAB (with our preconditioner) solved a system (6) more quickly than did DSLUGM. We find, for the pressure equation, that Bi-CGSTAB is at worst competitive and and at best almost twice as fast as DSLUGM. For the other four equations, Bi-CGSTAB is almost always twice as fast as DSLUGM and, in one instance, almost three times as fast.

## 6 Conclusion

We demonstrated herein the efficacy of using a new preconditioner for the Bi-CGSTAB method for the solution of the Hermite collocation discretization of the PDEs which model multiphase flow and contaminant transport in porous media. We find that our method, compared to the DSLUGM solver currently used, is always competitive and often more than twice as fast. Further, our method has the added advantage of being easily utilized in a parallel processing mode.

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