Block Preconditioning for a Coupled Model of Transport with Sorption in Porous Media

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Reactive transport models lead to a set of coupled partial differential equations, coupled with algebraic equations. The system may be very large, as the number of unknowns is the number of grid points times the number of chemical species. In Amir and Kern [1] a method was introduced where the chemical equations are eliminated, and a set of transport equations are solved, with a source term implicitly representing the effect of chemistry. The resulting problem is solved by the Newton–Krylov method, where the linear system is solved by an iterative method. It was seen that an efficient preconditioning was a crucial component of the method. However, finding a preconditioner is difficult, as no matrix is constructed in the Newton–Krylov method, and one would like to preserve the decoupling between transport and chemistry that is the main advantage of the formulation in Amir and Kern [1].

In this work, we consider a simplified model with one species undergoing a sorption reaction, given by a known equilibrium isotherm. This choice is motivated by the facts that the resulting mathematical problem has the same structure as that considered in the more general multicomponent model, that it is amenable to a more complete analysis, and that it can still be seen as representative of a physically relevant model

The model couples the aqueous concentration c of the chemical species, with its fixed concentration $\bar{c}$. he mathematical model given by writing the mass balance equation, and the adsorption relation is:

$$\begin{aligned} &\omega\partial_t c + \omega\partial_t \bar{c} - \nabla.(D\,\nabla c - qc) = 0 \\ &\bar{c} = \psi(c) \end{aligned} \qquad \text{in } \Omega \times [0,T] \tag{1}$$

with appropriate initial and boundary conditions. Here Ω is a bounded domain in $\mathbf{R}^d$, $1 \le d \le 3$, $[0,T]$ a fixed time interval, q is the Darcy velocity, ω is the porosity and D is the diffusion–dispersion tensor. The *sorption isotherm* ψ in equation (1) will be taken as the Langmuir isotherm:

$$\psi(c) = \sigma \frac{Kc}{1+Kc}, \tag{2}$$

where σ and K are two constants.

After discretization, the following non-linear algebraic system is obtained:

$$\begin{aligned} &AC^{n+1} = g^n - M\bar{C}^{n+1} \\ &\bar{C}^{n+1} = \psi(C^{n+1}), \end{aligned} \tag{3}$$

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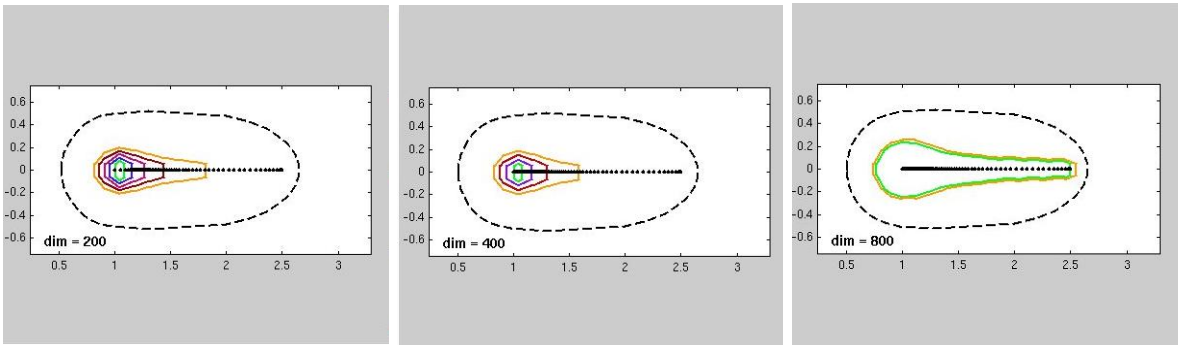

Figure 1: Field of values of the Jacobian matrix, for different mesh sizes

where A is a stiffness matrix representing the spatially discretrized transport operator, M a (diagonal) mass matrix, and g^n is a know term that lumps together the boundary conditions and the initial conditions. For simplicity, in the following we drop the time superscripts from the notation.

It is possible to eliminate one of the unknowns in the previous non-linear system. It turns out that the most efficient alternative is to eliminate the aqueous concentration C (this assumes that one can efficiently invert the transport operator), which leads to the new system:

$$\bar{C} = \psi(A^{-1}(g - M\bar{C})). \tag{4}$$

Even though this system is written in fixed–point form, we still want to use Newton's method for its solution. As the function defined in (4) involves A^{-1}, it is not practical to compute the full Jacobian, and we turn to a Newton–Krylov method, as this only requires the action of the Jacobian on a vector, and this in turn means solving a transport problem over one time step.

We investigate preconditioners that respect the block structure inherent in system (3). The simplest choices are to use either block Jacobi, or block Gauss–Seidel preconditioners. It is worthwhile to note that the Jacobian of the function in (4) is the same as that obtained by taking the Schur complement of C in the linearized coupled system, using Gauss-Seidel preconditioning.

It is possible to compute the eigenvalues of the various matrices. We denote by $\mu_j,\ j = 1, N$ the eigenvalues of the (generalized) eigenproblem $Aw = \mu M D^k w$ (the μ_j are real positive numbers because M was assumed diagonal and D^k is diagonal and positive, if ψ is an increasing function). We assume that, for large N, μ_j behaves as $1/h^2$, where h is a measure of the mesh-size. This is a natural assumption since the matrix A approximates a diffusion operator. For Gauss–Seidel preconditioning, and also for the matrix obtained after elimination of C, the eigenvalues of the preconditioning matrix are of the form $\lambda_j = 1 + \dfrac{1}{\mu_j},\ j = 1, \ldots, N$, with the addition of 1, with multiplicity N, for Gauss–Seidel.

As the matrix in (the linearization of) (3) is non-symmetric, the performance of GMRES is theoretically not determined by the eigenvalues. Nevertheless, the fact that they are tightly clustered

around 1 gives a good indication that convergence of GMRES will be mesh-independent. This is confirmed by the behavior of the field of values, which for the moment we have only been able to approximate numerically. Figure 1 shows the field of values for the Jacobian of (4)for several mesh sizes. The field of values is the inside of the dashed curves, and one sees it is bounded away from zero, independently of h.

We have compared the performance of the Newton–Krlyov method, with different preconditioners. In the tables below, "None" refers to no preconditioning, "BJ" and "GS" refer to block Jacobi (resp. block Gauss–Seidel) preconditioning and "Elim. of C" means using (4)

	h		$h/2$		$h/4$		$h/8$		$h/16$	
Mesh / PC	NNI	NLI	NNI	NLI	NNI	NLI	NNI	NLI	NNI	NLI
None	3	104	3	167	3	275	3	453	—	—
BJ	3	68	3	67	3	63	3	60	3	62
BGS	3	48	3	48	3	47	3	45	3	44
Elim. of C	3	41	3	41	3	41	3	40	3	40

Table 1: Performance of preconditioners, constant forcing term: NNI is Number of Nonlinear Iterations, NLI is Number of Linear Iterations

It can be seen that when using non preconditioner, the number of linear iterations grows quickly when the mesh is refined. When a preconditioner where transport is eliminated is used, the number of linear iterations becomes almost independent of the mesh, as predicted by the spectral analysis.

References

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