A Note on the Effect of the Choice of Weak Form on GMRES Convergence for Incompressible Nonlinear Elasticity Problems

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The generalized minimal residual (GMRES) method is a common choice for solving the large nonsymmetric linear systems that arise when numerically computing solutions of incompressible nonlinear elasticity problems using the finite element method. Analytic results on the performance of GMRES are available on linear problems such as linear elasticity or Stokes' flow (where the matrices in the corresponding linear systems are symmetric), or on the nonlinear problem of the Navier–Stokes flow (where the matrix is block-symmetric/block-skew-symmetric); however, there has been very little investigation into the GMRES performance in incompressible nonlinear elasticity problems, where the nonlinearity of the incompressibility constraint means the matrix is not block-symmetric/block-skew-symmetric. In this short paper, we identify one feature of the problem formulation, which has a huge impact on unpreconditioned GMRES convergence. We explain that it is important to ensure that the matrices are perturbations of a block-skew-symmetric matrix rather than a perturbation of a block-symmetric matrix. This relates to the choice of sign before the incompressibility constraint integral in the weak formulation (with both choices being mathematically equivalent). The incorrect choice is shown to have a hugely detrimental effect on the total computation time. [DOI: 10.1115/1.4000414]

1 Introduction

This short report is concerned with the rate of convergence of the generalized minimal residual (GMRES) method when used in numerical computations in incompressible nonlinear elasticity. It is standard procedure when computing large nonlinear deformations to discretize using the finite element (FE) method [1] and solve the resultant nonlinear system using the Newton (or Newton-like) method, which converts the nonlinear system into a sequence of nonsymmetric linear systems. GMRES [2] is a common choice of iterative solver for large sparse nonsymmetric systems. This report highlights one particular feature in the weak formulation of the problem that has far-reaching consequences on the total computation time. Specifically, we shall see that the choice of sign before the term in the weak formulation representing the incompressibility constraint (both choices being mathematically equivalent) has a huge effect on GMRES convergence, and thus, on the total computation time. As we shall describe, the Jacobian matrices arising from a Newton linearization of a finite element discretization of a nonlinear elastic problem have the form

$$\mathcal{J}=\begin{bmatrix} P & Q \\ R^T & 0 \end{bmatrix}$$

for some matrices P, Q, and R, with Q and R being dependent on the choice of weak form. The same 2×2 block structure occurs in problems such as incompressible linear elasticity, incompressible Stokes' flow, or incompressible Navier–Stokes' flow, with the latter in particular having attracted a great deal of analytic and numerical research into the GMRES performance and effective preconditioning. However, for the Navier–Stokes flow $Q=\pm R$ (the matrix is block-symmetric/block-skew-symmetric), due to the linearity of the incompressibility constraint $\nabla\cdot\mathbf{u}=0$, and for the linear problems, P is also symmetric and positive-definite. None of these conditions are true for nonlinear elasticity problems, and there has been very little investigation into the GMRES performance in nonlinear elasticity problems.

We discuss this in the context of what we term as the *backward problem*—the problem of computing the undeformed state of a body given a deformed state and body forces[2] (arising in, for example, soft tissue modeling of the breast [3,4]), as well as the standard elasticity problem (which we call the *forward problem*). Both are used in order to illustrate the points made, and also because, with the backward problem, the "natural" choice of weak form (using the positive sign) is the "incorrect" choice, in contrast to the forward problem where the natural choice is the "correct" choice. As such, the observation made here is vital for the backward problem, but equally relevant to the forward standard problem.

2 Computing Large Deformations Using the FE Method

2.1 Mathematical Formulation. Let $\Omega_0,\Omega\subset\mathbb{R}^3$ denote an elastic body in its undeformed and deformed configurations, respectively, and let $\mathbf{X}$ and $\mathbf{x}(\mathbf{X})$ represent equivalent points in these regions. The deformation gradient is defined as $F^i_M=\partial x^i/\partial X^M$ and the right Cauchy–Green deformation tensor as $C_{MN}=F^i_M F^i_N$. The Cauchy stress tensor σ^{ij} represents the force measured per unit deformed area acting on the deformed body, and second, the Piola–Kirchhoff stress T^{MN} is defined as the force measured per unit undeformed area acting on a surface in the undeformed body. σ and T are related by the expression $\sigma=(1/\det F)FTF^T$ [5]. For incompressible materials, the constraint $\det F=1$ has to be imposed, and this introduces an internal pressure p, which acts as a Lagrange multiplier and contributes to the total stresses [5]

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[2]This is a mathematical inverse problem, but we use the terminology "backward problem" rather than "inverse problem," as the latter is generally taken to mean the problem of determining material parameters given a deformation.

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$$\sigma^{ij} = \bar{\sigma}^{ij} - p\delta^{ij} \quad \text{and} \quad T^{MN} = \bar{T}^{MN} - p(C^{-1})^{MN}$$

where $\bar{\sigma}^{ij}$ and $\bar{T}^{MN}$ are the material-dependent parts of the stresses. We assume hyperelasticity, which relates stress and strain through a strain energy function $W(C)$, such that $T = 2\,\partial W/\partial C$.

The equations governing the static equilibrium of an incompressible nonlinear elastic body under body force $\mathbf{b}$ are [5]

$$\frac{\partial}{\partial X^M}\left(T^{MN}\frac{\partial x^i}{\partial X^N}\right) + \rho_0 b^i = 0$$

$$\det F = 1 \tag{1}$$

where ρ_0 is the density, with appropriate boundary conditions. The corresponding full weak formulation, assuming zero surface traction (for simplicity—this assumption has no effect on the results in this paper), is then [6]

$$\int_{\Omega_0} T^{MN}\frac{\partial x^i}{\partial X^M}\frac{\partial(\delta x_i)}{\partial X^N}dV_0 - \int_{\Omega_0}\rho_0 b^i \delta x_i dV_0 + \int_{\Omega_0}\delta p(\det F - 1)dV_0 = 0 \quad \forall\ \delta\mathbf{x}, \quad \delta p \tag{2}$$

where $\delta\mathbf{x}$ and δp are arbitrary functions from suitable vector spaces.

In the backward problem, $\mathbf{x}$ and Ω are known and $\mathbf{X}$ and Ω_0 are unknown. Let $G_i^M = \partial X^M/\partial x^i$ be the deformation gradient of the inverse (backward) map. $G = F^{-1}$, so incompressibility implies that $\det G = 1$. The weak formulation for the backward problem is just the Eulerian formulation (i.e., involving derivatives with respect to x^i and integrals over Ω) that is equivalent to the Lagrangian formulation Eq. (2), that is [6,7]

$$\int_{\Omega}\sigma^{ij}(\mathbf{X}(\mathbf{x}),p(\mathbf{x}))\frac{\partial(\delta x_j)}{\partial x^i}dV - \int_{\Omega}\rho_0 b^i \delta x_i dV + \int_{\Omega}\delta p(\det G - 1)dV = 0 \quad \forall\ \delta\mathbf{x}, \quad \delta p \tag{3}$$

2.2 Numerical Computation With the FE Method: Newton's Method and GMRES. To compute numerical solutions of the forward and backward problem, we can use the finite element method to convert the problem into a finite set of nonlinear equations [6]. Unless stated otherwise, a hexahedral mesh is used, with linear basis functions for position and piece-wise constant basis functions for pressure. Let this nonlinear system be represented by $\mathcal{F}(\mathbf{a}) = 0$, where $\mathbf{a}$ are the nodal unknowns (position and pressure). The nonlinear system can be solved using Newton's method, for which the Jacobian of the system

$$\mathcal{J}_{ij} = \frac{\partial \mathcal{F}_i}{\partial a_j} \tag{4}$$

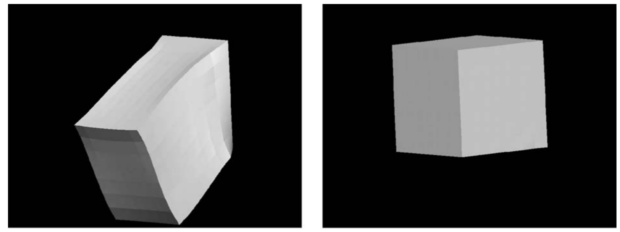
is required. Without going into the derivation of the exact values of the components of $\mathcal{J}$, it is important to consider the block structure of the Jacobian. Suppose the vector of unknowns is ordered so that all the pressure unknowns follow all the position unknowns. Then $\mathcal{J}$, for both types of problem, has a natural 2×2 block structure

$$\mathcal{J} = \begin{bmatrix} P & Q \\ R^T & 0 \end{bmatrix} \tag{5}$$

for some matrices[3] P, Q, and R. Note that $\mathcal{J}$ is not symmetric (P is not symmetric, and $Q \neq R$), although $\mathcal{J}$ would be symmetric if linear elasticity was used (together with the linearized version of the incompressibility constraint $\nabla \cdot \mathbf{u} = 0$).

Newton's method[4] reduces the nonlinear system into a sequence of linear problems, on which we use the iterative (restarted) GMRES method. In full GMRES, the residual norm decreases monotonically (not necessarily strictly), but unfortunately, very little can be said in general about the convergence, as many counterexamples can be constructed, where convergence is poor or stagnation occurs [8]. In the restarted GMRES method, denoted GMRES(p), the algorithm is restarted after p iterations to avoid large storage costs. Even less can be said in general about GMRES(p), not even that convergence is faster as p increases [9].

A sample computation, which we will use to investigate computation time in Sec. 3, is displayed in Fig. 1. Here, we initially solve the forward problem on a cube (using a Mooney–Rivlin [10] material law), letting it hang under gravity (Fig. 1(*a*)), and then use the result as the initial deformed state for a backward computation. The solution of the backward computation—which should obviously be the cube again—is shown in Fig. 1(*b*).



(*a*) (*b*)

Fig. 1 Solving the backward problem on a sheared cube: (*a*) shape taken as the deformed starting state for a backward problem computation (obtained by solving a forward problem on a cube), (*b*) result of the backward computation

Table 1 Total computation times for forward, original backward, and modified backward simulations on a number of meshes

	Computation time		
No. of nodes	Forward (s)	Backward (s)	Modified backward (s)
2^3	0.5	0.5	0.5
4^3	15	19	18
6^3	88	111	98
8^3	204	345	279
10^3	451	1555	535
12^3	1077	7428	1214
14^3	1884	48,054	2426

3 The Effect of the Choice of Weak Form on GMRES Convergence

The computation time for the forward and backward problems (as currently set up) on the simulation displayed in Fig. 1 are given in the first two columns of Table 1. The computation time for the backward problem is significantly higher than for the forward problem. This is due to the rate of convergence of GMRES in the backward problem: Fig. 2 displays the rate of convergence of GMRES(50) on a linear system from the first Newton iteration of a forward and backward problem, illustrating that the rate of decrease is much slower with the backward problem.

[3]The zero block occurs because, if i corresponds to an index of a pressure unknown in $\mathbf{a}$, then (considering the forward problem only) $\mathcal{F}_i = \int_{\Omega_0}\psi(\det F - 1)dV_0$ (for some basis function ψ), which is independent of the pressure p.

[4]In this paper, we only consider the full Newton method (i.e., where the full Jacobian defined by Eq. (4) is used in each iteration).

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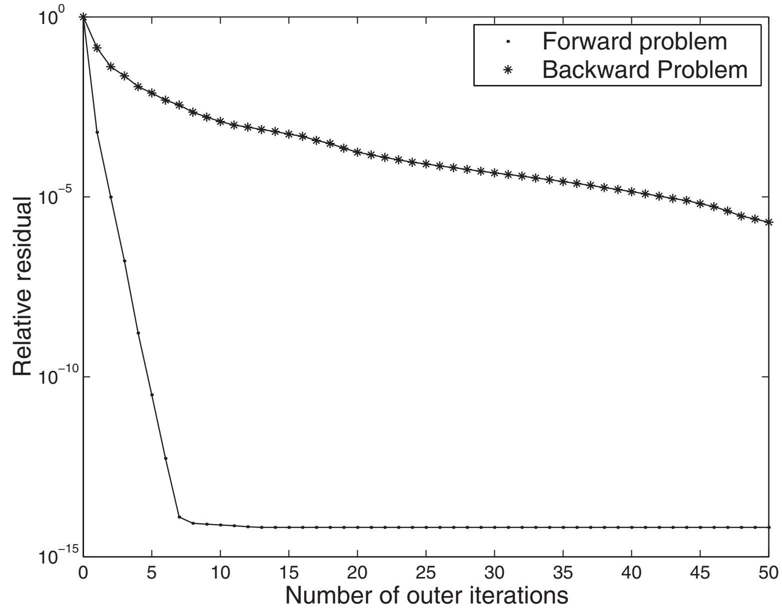

Fig. 2 Convergence histories for GMRES(50) on linear systems arising from a forward and backward problem

Consider the general form for matrices arising from saddle-point problems as

$$\mathcal{A} = \begin{bmatrix} A & B_1 \\ B_2^T & 0 \end{bmatrix} \tag{6}$$

where A is $m\times m$ and B_1 is $m\times(n-m)$, and define, for the cases $B_1 = \pm B_2$ as

$$\mathcal{A}_+ = \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \quad \text{and} \quad \mathcal{A}_- = \begin{bmatrix} A & B \\ -B^T & 0 \end{bmatrix}$$

Note that when A is symmetric and B has a full rank, then: $\mathcal{A}_+$ is symmetric and indefinite, with real eigenvalues, of which m are positive and $n-m$ are negative [11]; however $\mathcal{A}_-$ is block-skew-symmetric and has complex eigenvalues, but all eigenvalues have positive real parts [11].

As stated earlier, most research on GMRES convergence or on preconditioning is restricted to the cases where $\mathcal{A}$ has extra structure—in particular, A being symmetric and positive-definite (which is true for linear elasticity or Stokes' flow), or $B_1=B_2$ (true for linear elasticity, Stokes' flow, or Navier–Stokes' flow). Neither of these are true for nonlinear elasticity problems. However, the nonlinear elasticity Jacobians can be viewed as perturbations of matrices of the form $\mathcal{A}_\pm$, as illustrated in Fig. 3, in which the spectra of some of the matrices encountered in the forward and backward problems are plotted. For the forward problem Jacobian (Fig. 3(a)), the eigenvalues all have positive real parts, whereas for matrices arising from the backward problem (Figs. 3(b) and 3(c)), the eigenvalues are real or close to being real, and have negative real parts. The spectra illustrate that matrices for the forward and backward problems can be considered to be perturbations of matrices $\mathcal{A}_-$ and $\mathcal{A}_+$, respectively. In this case, where we are looking at the first or second Newton iterations where the displacement is small, the spectra are dominated by the spectra of the linearized problem.

Although the convergence behavior of GMRES or GMRES(p) cannot be characterized by the spectrum of the matrix (matrices can be constructed which have n eigenvalues of 1, for which GMRES stagnates until the n-th step [8]), it has been observed that for linear systems arising from physical problems, GMRES will typically converge faster if the matrix has clustered eigenvalues away from the origin, which is the case for matrices of the form $\mathcal{A}_-$, compared with those of the form $\mathcal{A}_+$. Since the fundamental difference between the (fast) forward problem and (slow) backward problem is the type of matrix they are perturbations of, the difference in computation time can be removed by transforming backward problem Jacobians from perturbations of $\mathcal{A}_+$ to perturbations of $\mathcal{A}_-$, by changing the sign of the appropriate block. This is of course equivalent to applying a simple preconditioner, but also identical to replacing the backward weak formulation, Eq. (3), with the completely equivalent weak formulation

$$\int_\Omega \sigma^{ij}\frac{\partial(\delta x_j)}{\partial x^i}dV - \int_\Omega \rho_0 b^i \delta x_i dV - \int_\Omega (\det G - 1)\delta p dV = 0 \quad \forall\ \delta\mathbf{x}, \quad \delta p$$

(just the sign before the last integral having changed). The spectrum of a modified backward problem Jacobian is shown in Fig. 3(d), and lies wholly in the right-half plane. Figure 4 plots the convergence history of GMRES(50) on the modified backward problem Jacobian and displays convergence at the same rate for both the forward and backward problem.

Finally, the computations in the second column of Table 1 are repeated and given in the third column. The time for solving backward problems now grows at the same rate as the forward problems. Note that this table gives the computation time for solving a *full nonlinear problem*, showing that the modification works for linear systems in *all* the Newton iterations, even later Newton iterations where the displacement is not small and the Jacobian will look least like $\mathcal{A}_+$ or $\mathcal{A}_-$.

This observation that the choice of sign before the incompressibility constraint term affects the GMRES convergence applies to forward problems, as well as to backward problems. In the forward problem, had we chosen the weak formulation

$$\int_{\Omega_0} T^{MN}F_M^k\frac{\partial(\delta x^k)}{\partial X^N}dV_0 - \int_{\Omega_0} \rho_0 b^i \delta x_i dV_0 - \int_{\Omega_0} (\det F - 1)\delta p dV_0 = 0 \quad \forall\ \delta\mathbf{x}, \quad \delta p$$

instead of Eq. (2), both of which are completely equivalent (this weak form corresponds to an identical problem to the original

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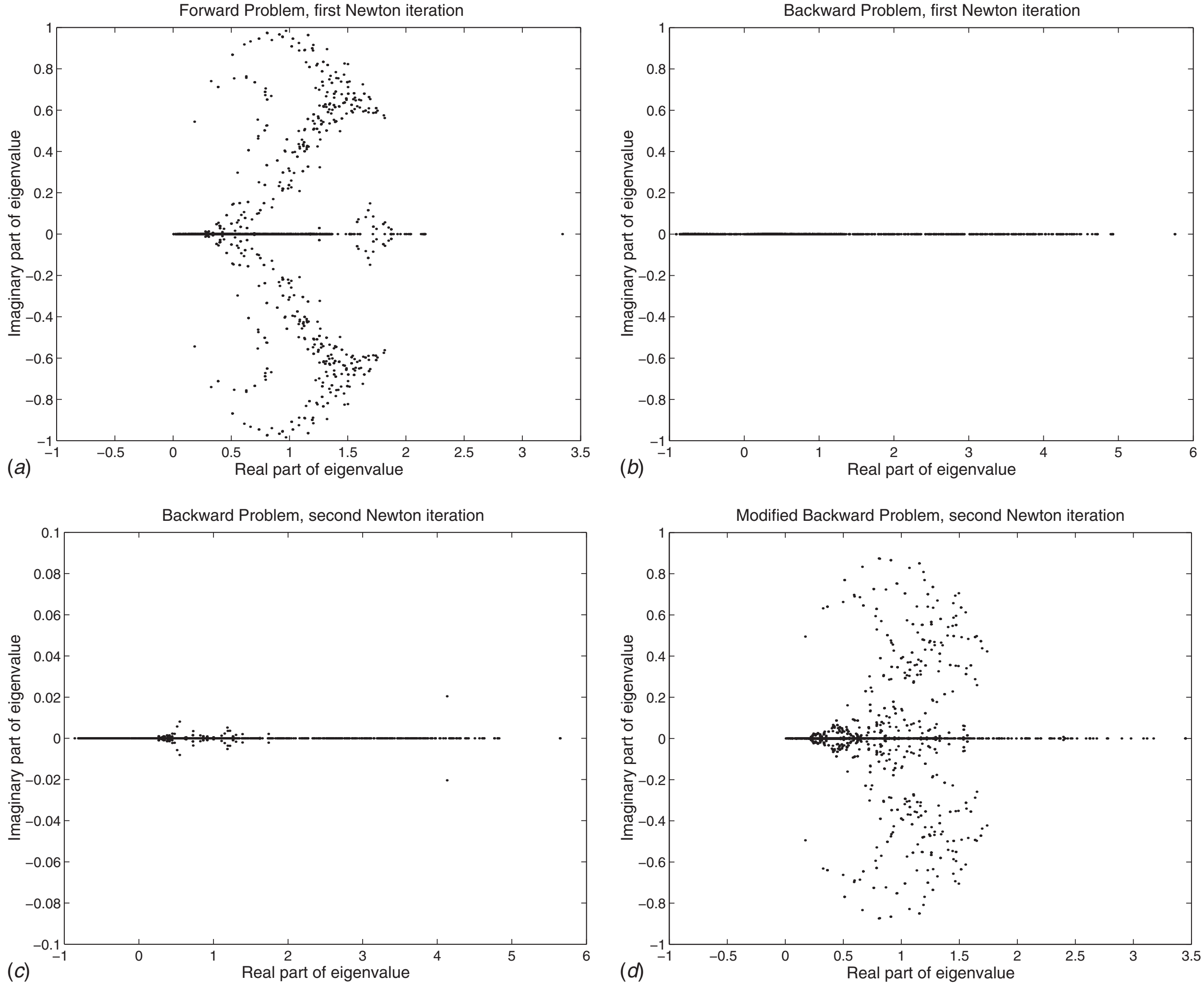

Fig. 3 Spectra of some matrices: (*a*) forward problem; (*b*) backward problem, first Newton iteration; (*c*) backward problem, second Newton iteration; (*d*) modified backward problem, second Newton iteration

weak form—both weak forms reduce to the same strong form of the problem, i.e., Equation (1), then forward problem Jacobians would be perturbations of $\mathcal{A}_+$ with indefinite spectra, and GMRES convergence would be as slow for the forward problem as it had been for the backward problem.

To verify this and illustrate that the observations made are not restricted to the single case studied, we have computed the solution of a number of different forward problems using both the correct and incorrect choice of sign; the results of which are shown in Fig. 5. This figure displays the average number of GMRES(100) outer iterations required per Newton iteration for a number of simulations. Simulations 1–3 are two-dimensional and solve for the incompressible deformation $\mathbf{x}=(X+\alpha X^2/2, Y(1+\alpha X)^{-1})^T$ on the unit square with a Neo-Hookean material (by applying appropriate body forces and tractions—see Ref. [12]), using various values of α and numbers of elements. Simulation 4 solves for the 3D deformation $\mathbf{x}=(X+\alpha X^2/2, Y+\alpha Y^2/2, Z(1+\alpha X)^{-1}(1+\alpha Y)^{-1})^T$. In each of these simulations, we use triangular/tetrahedral elements with quadratic basis functions for position and linear bases for pressure (in contrast to the earlier simulations). The average number of GMRES iterations using the negative sign in the weak form is at least an order of magnitude greater than that using the positive sign in all the simulations, even those such as simulation 3, where the deformation is highly nonlinear—in this simulation the principal values of the nonlinear Lagrangian strain tensor are ± 1.5, i.e., the strains are certainly not small. Note that between all the simulations run in this paper, problems with: hexahedral/tetrahedral/triangular elements, quadratic/linear displacement basis functions, linear/constant pressure basis functions, two/three dimensions, small and large strains, body forces with/without surface tractions, and small to medium numbers of elements, have all been encountered, and in all cases, GMRES was found to be significantly less effective with the wrong choice of sign.

4 Discussion

GMRES is a common choice for solving large nonsymmetric linear systems in incompressible nonlinear elasticity using a displacement-pressure formulation. We have illustrated that the matrices which arise in such problems can be viewed as perturbations of symmetric or block-skew-symmetric matrices corresponding to linearized versions of the problem, and that the block structure of the matrix has a huge impact on GMRES convergence. The choice of block structure corresponds to the choice of sign before the incompressibility term in the weak form of the problem.

The importance of using a weak form in nonlinear elasticity, which leads a matrix which is a perturbation of a block-skew-symmetric matrix does not seem to be well-known; we have found no mention of it in the literature. Studies of iterative solver per-

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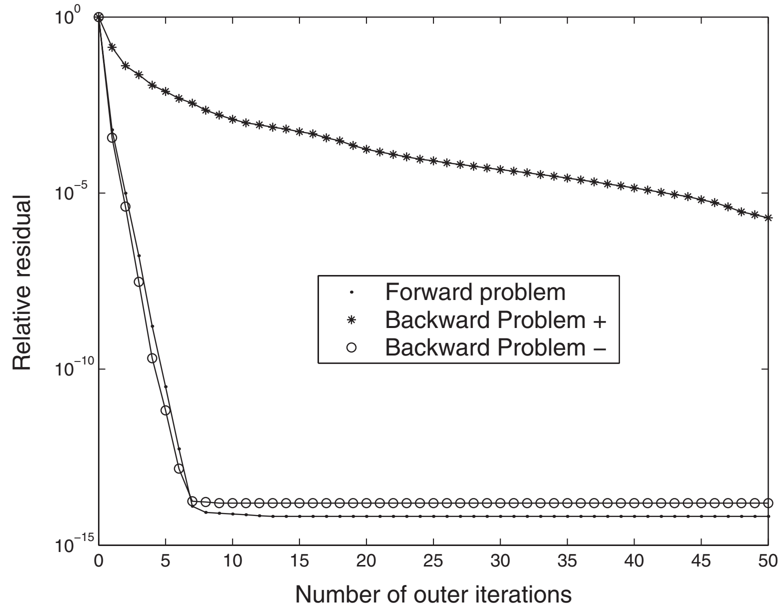

Fig. 4 Convergence histories for GMRES(50) on the forward problem and two versions of a backward problem matrix. "Backward problem +" represents the original backward problem matrix: a perturbation of $\mathcal{A}_{+}$, and "backward problem −" represents the modified backward problem matrix: a perturbation of $\mathcal{A}_{-}$.

formance in the context of block structure are restricted to fluid dynamics problems, for example, for the Stokes flow [13] or the Navier–Stokes equations [14], each of which has a linear incompressibility constraint. There has been very little investigation into the GMRES performance on the "more" nonlinear problem of nonlinear elasticity, and, to our knowledge, it has not been observed that the particular choice of Jacobian block structure from the two alternatives has a huge impact on the total computation time. Although it may have been expected that the transformation from a block-symmetric-type matrix to a block-skew-symmetric-type matrix might improve GMRES performance for small enough strains, it has not previously been demonstrated that this transformation will improve GMRES performance by an order of magnitude (or more), even with finite strains. Note that we have only considered unpreconditioned GMRES. In problems with purpose-built preconditioners, the choice of block structure will be less important, and this is perhaps the reason why the choice of weak form appears less important in Navier–Stokes problems, where there has been significant research into preconditioning. In nonlinear elasticity, the relative lack of advanced preconditioners means that this observation can be fundamental to reducing computation time, especially for inverse (backward) problems. We leave a precise mathematical explanation of why this is the case, or an analysis, which bounds the GMRES convergence rate as a function of the nonlinear terms, as an open problem.

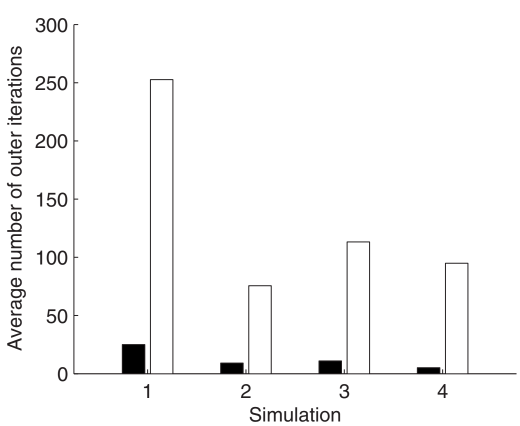

Fig. 5 The average number of outer GMRES iterations per Newton iteration in various forward simulations. Black bars: positive choice of sign in incompressibility term. White bars: negative choice of sign. Simulations 1–3 are on the unit square, with solution $\mathbf{x}=(X+\alpha X^2/2, Y(1+\alpha X)^{-1})^T$: (1) $\alpha=0.2$, 800 triangular elements; (2) $\alpha=0.4$, 800 elements; (3) $\alpha=1$, 200 elements. Simulation (4) is on the unit cube, with solution $\mathbf{x}=(X+\alpha X^2/2, Y+\alpha Y^2/2, Z(1+\alpha X)^{-1}(1+\alpha Y)^{-1})^T$, with $\alpha=0.1$ and 750 tetrahedral elements.

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