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A Comparison of Solver Performance for Complex Gastric Electrophysiology Models

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Abstract

Computational techniques for solving systems of equations arising in gastric electrophysiology have not been studied for efficient solution process. We present a computationally challenging problem of simulating gastric electrophysiology in anatomically realistic stomach geometries with multiple intracellular and extracellular domains. The multiscale nature of the problem and mesh resolution required to capture geometric and functional features necessitates efficient solution methods if the problem is to be tractable. In this study, we investigated and compared several parallel preconditioners for the linear systems arising from tetrahedral discretisation of electrically isotropic and anisotropic problems, with and without stimuli. The results showed that the isotropic problem was computationally less challenging than the anisotropic problem and that the application of extracellular stimuli increased workload considerably. Preconditioning based on *block Jacobi* and algebraic multigrid solvers were found to have the best overall solution times and least iteration counts, respectively. The algebraic multigrid preconditioner would be expected to perform better on large problems.

I. INTRODUCTION

Motility in the gastrointestinal tract is controlled and coordinated by an underlying electrical activity termed slow waves. Networks of specialized cells called interstitial Cells of Cajal (ICC) generate and propagate these slow waves, and they are conducted to the surrounding smooth muscle cells (SMC) which in turn drives the muscle contraction [1]–[3]. The bidomain reaction-diffusion equations, commonly used in cardiac modeling do not capture the effects of intermingled ICC and SMC cells coupled through gap junctions [4], [5]. Recently, a continuum modeling framework was proposed capable of incorporating two intracellular domains (communicating through gap junctions) and an extracellular space [5].

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The framework was further refined and was utilized for simulating gastric electrophysiology and effects of pacing [6].

Simulating gastric electrophysiology on a large anatomically realistic geometrical model coupled with multi-scale continuum modeling approaches is computationally expensive. Moreover, gastric simulations typically span over temporal scale up to several minutes, necessitating the search for efficient methods and tools for solving such problems. There have been extensive studies developing and defining efficient solvers for solving the linear system arising from the bidomain equations [7]–[9]. However, the efficiency of solvers for the system of equations arising from equations arising in gastric electrophysiology context have not been studied [5], [6]. For bidomain problems, preconditioned conjugate gradient solvers with preconditioners ranging from symmetric successive over relaxation to incomplete LU factorization, block Jacobi and multigrid techniques [7] have been proven to be successful. In addition, several problem specific preconditioning techniques that take into account the structure of systems of equations have been proposed and investigated [10].

Previous studies have shown that for intracellular stimuli, incomplete LU factorization is a valid choice for a bidomain type of problems [10]. However, when extracellular stimuli are applied, problem specific preconditioners accounting the structure of the system are required for computational efficiency. Furthermore, mesh-independence has been found to be an important factor for determining effective preconditioning for very-high resolution meshes [9].

In this study of useful preconditioning strategies for multiple domain gastric problems, we have compared the effectiveness of preconditioners with a range of complexities for solving gastric electrophysiology problems. Gastric electrophysiology simulations with varying electrical anisotropy and extracellular stimuli in anatomically realistic stomach models were considered [6]. Specifically, we have compared *Jacobi*, *block Jacobi* and the *BoomerAMG* algebraic multigrid method [11] and implemented these in the Chaste [12] modeling framework.

II. Methods

A. Continuum model for gastric electrophysiology

The gastric tissue syncytium can be effectively divided into three domains: (1) an intracellular domain corresponding to the ICC; (2) an intracellular domain corresponding to the SMC cells; and (3) the extracellular space. The conservation of current in and between these three domains following previous studies [5], [6] can be expressed as:

$$\chi^{(ICC)} \left(\xi^{(ICC)} \frac{\partial V_m^{(ICC)}}{\partial t} + I_{ion}^{(ICC)} \left(u^{(ICC)}, \phi_i^{(ICC)}, \phi_e \right) \right) - \nabla \cdot \left(\sigma_i^{(ICC)} \nabla \left(V_m^{(ICC)} + \phi_e \right) \right) + \chi^{(ICC)} I_{stim}^{(ICC)} - \chi^{gap} I_{gap} = 0$$

(1)

$$\chi^{(SMC)} \left(\xi^{(SMC)} \frac{\partial V_m^{(SMC)}}{\partial t} + I_{ion}^{(SMC)} \left(u^{(SMC)}, \phi_i^{(SMC)}, \phi_e \right) \right) - \nabla \cdot \left(\sigma_i^{(SMC)} \nabla \left(V_m^{(SMC)} + \phi_e \right) \right) + \chi^{(SMC)} I_{stim}^{(SMC)} + \chi^{gap} I_{gap} = 0 \quad (2)$$

$$-\nabla \cdot \left(\sigma_i^{(ICC)} \nabla V_m^{(ICC)} \right) - \nabla \cdot \left(\sigma_i^{(SMC)} \nabla V_m^{(SMC)} \right) - \nabla \cdot \left(\sigma_i^{(SMC)} + \sigma_i^{(ICC)} + \sigma_e \right) \nabla \phi_e = I^{totalstim} \quad (3)$$

Here $\sigma_i^{(ICC)}$, $\sigma_i^{(SMC)}$ and σ_e are the intracellular conductivity tensors for the ICC, SMC and the extracellular domain respectively. The transmembrane potential for ICC and SMC domain are given by the variables $V_m^{(ICC)}$, $V_m^{(SMC)}$ and ϕ_e is the extracellular potential. The variables χ^{gap} and I_{gap} are the surface to volume ratio of the space and the associated gap junction current; I_{ion} with superscripts (ICC) and (SMC) are the total membrane ionic current flowing between the respective intracellular and extracellular spaces; and ξ is the membrane capacitance per unit area. The total sum of the applied stimuli is $I^{totalstim}$.

A semi-implicit finite-element discretisation of this coupled continuum model formulation generates a large, highly sparse system of linear equations in the form of $Ax = b$ [6] to be solved for each discrete time-step. x forms the vector of unknowns $V_m^{(ICC)}$, $V_m^{(SMC)}$ and ϕ_e . Matrix A has entries from the FEM discretisation which is constant over time, and has dimensions corresponding to the number of solution points in the problem.

B. Benchmark for computational analysis

The effects of extracellular stimuli and electrical conductivity anisotropies on computational performance were determined on an anatomically realistic stomach model (Fig. 1) recently developed for studying gastric pacing [6]. A finite-element tetrahedral mesh was generated with an average edge length of 0.3 mm, resulting in a problem with 0.5 million nodes and 2.5 million tetrahedral elements. The model setup configurations are listed in Table 1. This model was used for both isotropic, anisotropic and external pacing cases. For pacing, an extracellular stimulus with amplitude of 5 mA and pulse duration of 200 ms was applied at time $t = 200$ ms at the pacing site as shown in Fig. 1.

C. Preconditioning extended-bidomain problem

Preconditioned conjugate gradient algorithms have been shown to be the best choice for solving such systems [13]. The gastric model equations system is preconditioned with *Jacobi*, *blockJacobi* and *BoomerAMG* and solved using a conjugate gradient (CG) solver. Left preconditioning was used, i.e. $P^{-1}Ax = P^{-1}b$, where P^{-1} is the preconditioner.

The solution options were implemented in the open source computational framework Chaste and this framework was used for all the simulations [14]. The number of iterations and elapsed wall clock time spent on each solution time step were recorded. The PETSc package implementations of *CG*, *Jacobi*, *blockJacobi* and *BoomerAMG* were used [<http://www.mcs.anl.gov/petsc/>]. The *BoomerAMG* algorithm included in the HYPRE library through the PETSc interface was used with the number of V-cycles set to 1 to reduce the overhead in setting up the preconditioner. An absolute tolerance of 0.0002 mV was specified.

The simulations were performed on the NeSI Auckland PAN cluster with 128 Intel Westmere cores operating at 2.7–2.8 GHz with 4 GB RAM.

III. Results

For a normal slow wave simulation with anisotropic conductivities *block Jacobi* showed better time performance than the *Jacobi* preconditioner. However, the iteration counts were better controlled for *BoomerAMG* as shown in Fig. 2A. The time spent by solver for each iteration for 450 time-steps had a 75th percentile value of 0.58 s, 0.68 s and 0.16 s for *BoomerAMG*, *Jacobi* and *block Jacobi* respectively. The iteration count over 500 time-steps had a 75th percentile value of 6,286 and 38 for *BoomerAMG*, *Jacobi* and *block Jacobi* respectively. Although the iteration counts are considerably different for *BoomerAMG* and *Jacobi*, the solver solution time were comparable. This can be attributed to the additional overhead in implementing the *BoomerAMG* algorithm over each solver iteration.

With the application of an extracellular stimulus, there was a sharp increase in the iteration count and hence the solution time. The peak count occurs at the stimulus onset and also at the end of the stimulus time as shown in Fig. 2B. The 200 ms and 400 ms time-steps show a peak close to 5000 iterations and solution time of 12 ms. The 75th percentile value of 0.55 s, 0.68 s and 0.16 s for *boomerAMG*, *Jacobi* and *block Jacobi* are similar to a normal simulation as explained in Fig. 2A. The iteration count 75th percentile values were also similar with values of 7, 290 and 41 respectively. The *BoomerAMG* was better in terms of convergence even at the time of stimulus.

For isotropic simulation, the *block Jacobi* was the best preconditioner choice as it was stable in terms of iteration counts and had a comparatively low solution time. Importantly, the total solution time was considerably lower compared to the anisotropic cases for all the three cases. The 75th percentile value was 0.55 s, 0.39 s and 0.03 s respectively for *BoomerAMG*, *Jacobi* and *block Jacobi*. The iteration count 75th percentile values were also similar with 7, 162 and 7 iterations respectively.

IV. Discussion

In this study, we present and evaluate different preconditioners for solving problems arising in gastric electrophysiology. The *block Jacobi* preconditioner was the most suitable choice for the majority of simulations with its efficient performance, however, the *BoomerAMG* preconditioner may be a better choice when considering the iteration count together with the

solving time. The *Jacobi* preconditioner was an inefficient and poor choice for the cases considered in this study.

As the problem size increases, with the availability of more detailed anatomical information incorporated in the mesh, the *BoomerAMG* preconditioner may be a better alternative considering its excellent parallel scaling capability [7]. The study presented here only considered 1 AMG V-cycle for the approximation in addition to BoomerAMG default configuration. The trade-off between using multiple V-cycles and its impact on efficiency will be investigated in a future study.

The increased iteration count and thus the solution time at the application of an extracellular stimulus can be explained with the residual associated with each of $V_m^{(1)}$, $V_m^{(2)}$ and ϕ_e evaluated as (continuing from a previous analysis [10])

$$A \begin{pmatrix} x_{V_1} \\ x_{V_2} \\ x_{\phi_e} \end{pmatrix} = \begin{pmatrix} b_{V_1} \\ b_{V_2} \\ 0 \end{pmatrix} \quad (4)$$

The residual in an iteration of preconditioned CG can be expressed in V_1 , V_2 and ϕ_e as

$$\begin{pmatrix} r_{V_1} \\ r_{V_2} \\ r_{\phi_e} \end{pmatrix} = \begin{pmatrix} b_{V_1} \\ b_{V_2} \\ 0 \end{pmatrix} - A \begin{pmatrix} x_{V_1} \\ x_{V_2} \\ x_{\phi_e} \end{pmatrix} \quad (5)$$

such that

$$\|r\|^2 = \|r_{V_1}\|^2 + \|r_{V_2}\|^2 + \|r_{\phi_e}\|^2 \quad (6)$$

The application of extracellular stimulus induces sudden changes in extracellular domain which increases the $\|r_{\phi_e}\|$. Future works includes investigating more problem specific preconditioners. Block diagonal and LDU preconditioners have been shown to be efficient for solving bidomain problems [10] and these may be candidates for further study. Additionally, combinations of different parameters for the *BoomerAMG* preconditioner will be investigated to determine if additional computational efficiencies can be found.

V. Conclusion

This study evaluated the performance of different preconditioning techniques for solving gastric electrophysiology simulation models. The algebraic multigrid based preconditioners were evaluated to have least solver iteration counts and *block Jacobi* to have best overall solver solution time. Over the coming years, identifying efficient preconditioners and developing problem specific preconditioners for gastric electrophysiology problems will be

an active area of interest as these models continue to become more complex and anatomically detailed.

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Figure 1. Simulated slow wave propagation on the benchmark model with anisotropic propagation. Pacing site defines the site of application of extracellular stimulus.

Figure 2.

Plot of time spent and iteration count over time-step. (A) corresponds to anisotropic case with no stimulus application. (B) corresponds to anisotropic case with stimulus of duration 200 ms applied at $t = 200$ ms. (C) corresponds to isotropic case with extracellular stimulus applied at $t = 200$ ms and for duration of 200 ms. Row 1 corresponds to the variation in time-spent by the linear solver at each time step for cases A, B and C. Rows 2 and 3 corresponds to the variation in number of solver iterations per time step represented by line and box plot respectively. The box plot whiskers in all cases represent the standard deviation, '+' is the mean and box ends corresponds to 25th and 75th quartiles.

Table 1

Study Configurations

Configuration	Value
Simulation duration	500 ms
PDE time-step	1 ms
ODE time-step	0.1 ms
Cell model for ICC	FSM-ICC CB model
Cell model for SMC	Passive with no active ionic current