Spectral Deferred Correction methods for adaptive electro-mechanical coupling in cardiac simulation

Martin Weiser and Simone Scacchi

Abstract We investigate spectral deferred correction (SDC) methods for time stepping and their interplay with spatio-temporal adaptivity, applied to the solution of the cardiac electro-mechanical coupling model. This model consists of the Monodomain equations, a reaction-diffusion system modeling the cardiac bioelectrical activity, coupled with a quasi-static mechanical model describing the contraction and relaxation of the cardiac muscle. The numerical approximation of the cardiac electro-mechanical coupling is a challenging multiphysics problem, because it exhibits very different spatial and temporal scales. Therefore, spatio-temporal adaptivity is a promising approach to reduce the computational complexity. SDC methods are simple iterative methods for solving collocation systems. We exploit their flexibility for combining them in various ways with spatio-temporal adaptivity. The accuracy and computational complexity of the resulting methods are studied on some numerical examples.

1 Introduction

The spread of the electrical impulse in the cardiac muscle and the subsequent contraction-relaxation process is quantitatively described by a mathematical model called electro-mechanical coupling. The electrical model consists of the Monodomain system (a reduction of the Bidomain model), which is a reaction-diffusion equation describing the evolution of the transmembrane voltage. The PDE is coupled through the reaction term with a stiff system of ordinary differential equations

Martin Weiser
Zuse Institute Berlin, Bereich Numerische Mathematik, Taku strasse 7, D-14195 Berlin-Dahlem, Germany, e-mail: weiser@zib.de

Simone Scacchi
Department of Mathematics, University of Milan, via Saldini 50, 20133 Milano, Italy, e-mail: simone.scaccchi@unimi.it

(ODEs), the so-called *membrane model*, describing the flow of the ionic currents through the cellular membrane. The mechanical model consists of quasi-static finite elasticity, coupled with a system of ODEs modeling the development of biochemically generated active stress.

The numerical approximation of the cardiac electro-mechanical coupling is a challenging multiphysics problem, because the space and time scales associated with the electrical and mechanical models are very different. Therefore, spatial and temporal adaptivity is a promising approach to reduce the computational complexity [2, 3]. However, spatial adaptivity by local mesh refinement incurs a substantial overhead for error estimation, grid manipulation, repeated integration until spatial accuracy is achieved, and reassembly of mass and stiffness matrices, which reduces the performance gain.

In this work, we investigate the use of spectral deferred correction (SDC) methods for time stepping and their interplay with spatial and temporal adaptivity. SDC methods are simple iterative methods for solving collocation systems. Their flexibility allows to combine them in various ways with spatio-temporal adaptivity. We explore interleaving mesh refinement with SDC iterations for improved convergence and local time stepping. In particular, we develop SDC methods for strong electro-mechanical coupling including mechano-electrical feedback and their potential for multi-rate integration. The properties of the resulting methods in terms of accuracy and computational complexity are discussed at a simple numerical example.

2 Mathematical models

Mechanical deformation

Let us denote the region occupied by the undeformed myocardium by Ω. Fow now we consider a simple two-dimensional square domain. The myocard undergoes a time-dependent deformation with displacement $u : \Omega \times (0,T) \to \mathbb{R}^2$, such that point $x \in \Omega$ is moved to $x + u(x,t)$ at time $t \in (0,T)$. As usual, $\mathbf{F} = \mathbf{I} + u_x$ denotes the deformation derivative, $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ the Cauchy-Green deformation tensor, and $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$ the Green-Lagrange strain tensor, with identity matrix $\mathbf{I}$.

The cardiac tissue is modeled as a transversely isotropic nonlinear hyperelastic material with exponential strain energy function

$$W_{\text{pas}}(\mathbf{E}) = c_1 \exp(b_1 E_{11}^2 + 4b_2 E_{22}^2 + 4b_3 E_{12}^2).$$

introduced in [11], where the muscle fiber direction is just x_1. The near-incompressibility is modeled by an additive volume change penalization term

$$W_{\text{com}}(\det \mathbf{F}) = c_2((\det \mathbf{F})^2 + (\det \mathbf{F})^{-2} - 2),$$

which ensures orientation preservation. The contraction of the ventricles results from the active tension T_a generated by the myofilements, which are activated by

calcium release. We assume that the generated active stress acts only in the direction of the fibers [6, 10, 12]. This leads to a third term in the variational functional:

$$W_{\text{act}}(\mathbf{E}, T_a) = T_a E_{11}.$$

The biochemically generated active stress T_a is modeled as *stretch and stretch-rate independent*. Thus, we assume as in [5, 9] that the dynamics of T_a depends only on the transmembrane voltage v according to a simple twitch-like rule,

$$\frac{\partial T_a}{\partial t} = \varepsilon(v)(k_{T_a}(v - v_r) - T_a), \tag{1}$$

where $k_{T_a} > 0$ controls the saturated value of T_a for a given voltage v and a given resting voltage v_r, see [5, 9] for details.

We assume that the time-dependent inertial term in the governing elastic wave equation may be neglected, see, e.g., [7, 12]. At any point in time, the myocard then assumes the stationary minimizer of the internal energy, subject to essential boundary conditions on the Dirichlet part of $\partial\Omega$:

$$\min_{u(t)\in H^1(\Omega)^2} \int_\Omega W_{\text{pas}}(\mathbf{E}) + W_{\text{com}}(\det \mathbf{F}) + W_{\text{act}}(\mathbf{E}, T_a(t))\, dx \quad \text{s.t.} \quad u(t)|_{\partial\Omega_D} = 0. \tag{2}$$

Electrical excitation

The electrical excitation is described by the monodomain model using the Aliev-Panfilov membrane model [1] on the reference cardiac domain Ω [9, 10, 12]. Given an applied current per unit volume $I_{\text{app}} : \Omega \times (0,T) \to \mathbb{R}$, and initial conditions $v_0 : \Omega \to \mathbb{R}$, $w_0 : \Omega \to \mathbb{R}$, find the transmembrane potential $v : \Omega \times (0,T) \to \mathbb{R}$ and the gating variable $w : \Omega \times (0,T) \to \mathbb{R}$ such that

$$c_m \frac{\partial v}{\partial t} - \operatorname{div}(\mathbf{F}^{-1} D_m \mathbf{F}^{-T} \nabla v) + I_{\text{ion}}(v,w) = I_{\text{app}} \qquad \text{in } \Omega \times (0,T), \tag{3}$$

$$\frac{\partial w}{\partial t} = R(v,w) \qquad \text{in } \Omega \times (0,T), \tag{4}$$

holds. Note that the length changes due to tissue deformation change the diffusion tensor from D_m to $F^{-1} D_m F^{-T}$, neglecting the impact of volume changes. The functions

$$I_{\text{ion}}(v,w) = -g_a v(v-a)(v-1) - vw$$
$$R(v,w) = -\frac{1}{4}\left(\varepsilon_1 + \frac{\mu_1 w}{v+\mu_2}\right)(w + g_s v(v-a-1))$$

are given by the Aliev-Panfilov membrane model [1]. Insulating boundary conditions on v are prescribed.

3 Numerical methods

Spatial discretization: finite elements

A pure displacement discretization with P1-elements is used for computing the tissue deformation in reaction to active stress T_a. A Newton-like method is employed for minimizing (2). As hyperelastic energies can be nonconvex, the elemental matrices are modified during assembly to be positive definite. This ensures that the computed Newton step is a descent direction. Line search is applied to ensure monotone decrease of the elastic energy.

The transmembrane voltage is less smooth than the displacement, but easier to solve for. Thus, a finer spatial discretization is used. For implementation simplicity, we use P3-elements on the same mesh for transmembrane voltage, gating variables, and active stress generation. The transfer between different spatial discretizations is done by interpolation at quadrature nodes. Mesh refinement is based on an embedded energy error estimator for the transmembrane voltage, as this is the variable with dominating local dynamics.

Time discretization: spectral deferred correction methods

Spectral deferred correction methods [4] are simple iterative methods for solving ODE collocation systems, where each iteration consists of a sequence of time steps with a low order scheme, most often an Euler scheme. For simplicity of notation, we consider an initial value problem $\dot{u} = f(u)$ with initial value $u(0) = u_0$ and exact solution u^*. On a time step $[0,\tau]$ we define a collocation time subgrid $0 = \tau_0 < \cdots < \tau_n = \tau$ and a polynomial approximate solution $u^0 \in \mathbb{P}_n$ with values $u_i^k = u^k(\tau_i)$ at the collocation points τ_i. The defect $u^* - u^k$ satisfies the Picard equation

$$\frac{d}{dt}(u^* - u^k)(t) = \int_{s=0}^{t} (f(u^*) - \dot{u}^k)\,ds. \tag{5}$$

Linearizing f around u^k, integrating the implicit term in (5) approximately with the right-looking rectangular rule and the explicit terms by a quadrature rule on the collocation time grid gives approximate defect values

$$\delta u_{i+1}^k = \delta u_i^k + (\tau_{i+1} - \tau_i)\left(\sum_{j=0}^{n} S_j f(u_j^k) + f'(u_{i+1}^k)\delta u_{i+1}^k\right) - (u_{i+1}^k - u_i^k) \tag{6}$$

at the collocation nodes, which in turn define a polynomial defect approximation δu^k by interpolation. Note that (6) is a linearly implicit Euler scheme on the collocation time grid. Updating the approximation by $u^{k+1} = u^k + \delta u^k$ yields an iteration the fixed point of which satisfies the collocation condition $f(u_i) = \dot{u}_i$. In lack of better initialization, the starting iterate is the constant initial value: $u_i^0 = u_0$.

Interleaved SDC and mesh refinement

Popular diagonally linearly implicit Runge-Kutta schemes, such as Rosenbrock methods, can be combined with spatial adaptivity in two different ways. Error estimation and refinement can be performed either for the final result, or for the very first stage (essentially a linearly implicit Euler step) only. The first option is more conservative, but requires the recomputation of all stages from scratch, since order and accuracy of Rosenbrock schemes deteriorate when the stages are computed on different spatial grids. The second option is more efficient, as only the first stage is recomputed on mesh refinement, but assumes a sufficient similarity of Euler step and final Rosenbrock step to produce suitable meshes for the latter. As demonstrated in Section 4, this assumption can be quite wrong.

In contrast to Rosenbrock methods, SDC methods compute an independent correction in every sweep, wherever the approximation error originates, may it be the SDC iteration error or a spatial discretization error. Hence, spatial mesh refinement can be performed in between any SDC sweeps, creating meshes adapted to the final SDC step, and nevertheless the previously computed values can be reused.

Applied to the electromechanical model described in Section 2 above, the SDC iterations are performed for the transmembrane voltage (3), the gating variables (4), and the active stress generation in turn. After each sweep, the elastic displacement is updated at all collocation points by a simplified Newton method, followed by error estimation both for the spatial discretization error and the SDC iteration error. If the spatial error exceeds the iteration error, adaptive mesh refinement is performed.

Multi-rate integration

As the dynamics in the active stress generation and hence the mechanical displacement is slower than in the transmembrane voltage, a coarser time discretization of the displacement can be used. We exploit the continuous in time representation of approximate solutions by polynomial interpolation, using a finer collocation grid for the transmembrane voltage than for the displacement. Additionally, as after an SDC sweep the electrical state is still only an approximation, an exact solution of the nonlinear mechanic model is not required. The number of Newton steps can therefore be reduced. Finally, less than one Newton step per sweep effort can be achieved by solving for the elasticity part just every other SDC sweep. The induced inaccuracy in the displacement will have an impact on the convergence of the transmembrane voltage due to the mechano-electrical feedback.

4 Numerical results

We study the effect of the algorithmic variants in detail at a particularly simple example, the spread of an excitation wave in the 2D domain $\hat{\Omega} =]0,2[^2$ with an ex-

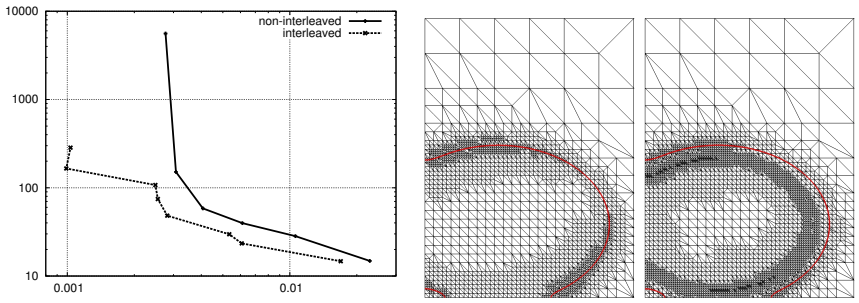

Fig. 1 *Left:* Wall clock time vs. achieved error for different tolerances. *Right:* Grid maladaptation by mesh refinement based on the first sweep. Front position is marked.

citation current in $[0.5,0.55]^2$ for 1 ms. For simplicity, the time step size is fixed to 1.5 ms on a Radau(4) collocation time grid, using cubic finite elements for the transmembrane voltage and linear FE for the displacement. Errors in u_h are quantified by the norm difference $\|u_h\|_{L^2(\hat{\Omega})} - \|u\|_{L^2(\hat{\Omega})}$ to the space-continuous collocation solution u, which is closely related to the error in the average conduction velocity.

First we study the performance impact of interleaving mesh refinement and SDC iterations. To this extent, we simulate the non-interleaving mode of operation by initializing the solution at all collocation points to the initial value after mesh refinement, in effect starting the SDC method only after a suitably refined grid has been constructed for the Euler solution. This mimics the approach used in some Rosenbrock schemes [8], where mesh adaptation is performed for the first stage only.

As shown in Fig. 1 left, the interleaved scheme is more efficient, roughly by a factor of two for large tolerances. The non-interleaved mode does not achieve high accuracy at all, independent of the tolerance. Fig. 1 right gives an explanation for this bad performance. It turns out that at the chosen time step size the first sweep results in a rather poor approximation of the front, in particular a too slow front speed and a significant overshoot. This leads to mesh refinement behind, and an insufficient refinement at the actual front position.

Next we turn to multi-rate integration for electromechanical coupling. With a fixed tolerance for spatial discretization error and SDC iteration error, we reduce the accuracy of displacement computation in each time step by reducing the collocation nodes from 4 to 1 (lines *a*), the number of simplified Newton steps from 10 to 1 (lines *b*), additionally skipping the displacement computation for up to 7 SDC sweeps (lines *c*), and report the deviation from the non-reduced reference solution in Fig. 2. The error of this reference solution is roughly $2 \cdot 10^{-3}$. Apparently, reduction of Newton iteration count and collocation points for the displacement computation introduce a coupling error well below the overall error tolerance. Additionally omitting the displacement computation during the first SDC sweeps exceeds this limit, without substantial run time reduction. Neglecting the mechano-electrical feedback completely yields an unacceptably large error (point *d*).

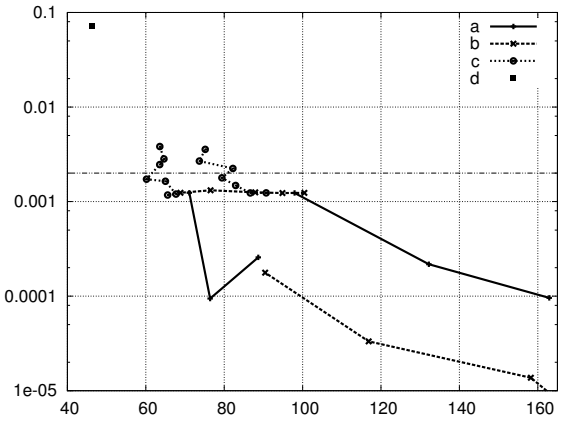

Fig. 2 Total error vs. run time for inexact solution of displacement.

References

1. Aliev, R.R., Panfilov, A.V.: A simple two-variable model of cardiac excitation. Chaos Sol. Fract. **7**, 293–301 (1996)
2. Bendahmane, M., Buerger, R., Ruiz-Baier, R.: A multiresolution space-time adaptive scheme for the bidomain model in electrocardiology. Num. Meth. Part. Diff. Eq. **26**, 13771404 (2010)
3. Colli Franzone, P., Deuflhard, P., Erdmann, B., Lang, J., Pavarino, L.F.: Adaptivity in space and time for reaction-diffusion systems in electrocardiology. SIAM J. Sci. Comput. **28**, 942–962 (2006)
4. Dutt, A., Greengard, L., Rokhlin, V.: Spectral deferred correction methods for ordinary differential equations. BIT **40**(2), 241–266 (2000)
5. Göktepe, S., Kuhl, E.: Electromechanics of the heart – a unified approach to the strongly coupled excitation-contraction problem. Comp. Mech. **80**, 227–243 (2010)
6. Humphrey, J.D.: Cardiovascular Solid Mechanics, Cells, Tissues and Organs. Springer, New York (2001)
7. Kerckhoffs, R.C.P., Bovendeerd, P.H.M., Kotte, J.C.S., Prinzen, F.W., Smits, K., Arts, T.: Homogeneity of cardiac contraction despite physiological asyncrony of depolarization: a model study. Ann. Biomed. Eng. **31**, 536–547 (2003)
8. Lang, J.: Adaptive Multilevel Solution of Nonlinear Parabolic PDE Systems, *Lecture Notes in Computational Science and Engineering*, vol. 16. Springer (2001)
9. Nash, M.P., Panfilov, A.V.: Electromechanical model of excitable tissue to study reentrant cardiac arrhythmias. Progr. Biophys. Molec. Biol. **85**, 501–522 (2004)
10. Pathmanathan, P.J., Whiteley, J.P.: A numerical method for cardiac mechanoelectric simulations. Ann. Biomed. Engrg. **37**, 860–873 (2009)
11. Vetter, F.J., McCulloch, A.D.: Three-dimensional stress and strain in passive rabbit left ventricle: a model study. Ann. Biomed. Engrg. **28**, 781–792 (2000)
12. Whiteley, J.P., Bishop, M.J., Gavaghan, D.J.: Soft tissue modelling of cardiac fibres for use in coupled mechano-electric simulations. Bull. Math. Biol. **69**, 2199–2225 (2007)