

Konrad-Zuse-Zentrum
für Informationstechnik Berlin

Takustraße 7
D-14195 Berlin-Dahlem
Germany

MARTIN WEISER AND SIMONE SCACCHI

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Telefon: 030-84185-0
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Spectral Deferred Correction methods for adaptive electro-mechanical coupling in cardiac simulation

Martin Weiser and Simone Scacchi*

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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 (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

*Department of Mathematics, University of Milan, via Saldini 50, 20133 Milano, Italy, simone.scacchi@unimi.it

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 model Let us denote the material coordinates of the undeformed or reference cardiac domain by $\mathbf{X} = (X_1, X_2, X_3)^T$, the spatial coordinates of the deformed cardiac domain by $\mathbf{x} = (x_1, x_2, x_3)^T$ and the region occupied by the undeformed and deformed, at time t , cardiac domains by $\hat{\Omega}$ and $\Omega(t)$, respectively. We denote by Div and Grad the material divergence of a vector and gradient of a scalar field, respectively. From a mechanical point of view, the cardiac tissue is modeled as a non-linear elastic material. Let us denote by \mathbf{F} and J the deformation derivative tensor and its determinant, respectively. The Cauchy-Green deformation tensor \mathbf{C} and Lagrange-Green strain tensor \mathbf{E} are $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ and $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$, with identity matrix \mathbf{I} .

We first assume that the time-dependent inertial term in the governing elastic wave equation may be neglected, see e.g. [9, 14]. Thus, the steady-state force equilibrium equation reads

$$\text{Div}(\mathbf{F}\mathbf{S}) = \mathbf{0}, \quad \mathbf{X} \in \hat{\Omega}, \quad (1)$$

where \mathbf{S} is the second Piola-Kirchoff stress tensor. We close the quasi-static mechanical model (1) by imposing a prescribed displacement on a Dirichlet boundary $\mathbf{x}(\mathbf{X}) = \hat{\mathbf{x}}(\mathbf{X})$, $\mathbf{X} \in \partial\hat{\Omega}_D$ and no traction force on a Neumann boundary $\mathbf{F}\mathbf{S}\mathbf{N} = \mathbf{0}$, $\mathbf{X} \in \partial\hat{\Omega}_N$.

The tensor $\mathbf{S} = \mathbf{S}^{pas} + \mathbf{S}^{vol} + \mathbf{S}^{act}$ is given by the sum of a passive elastic component \mathbf{S}^{pas} , a volumetric component \mathbf{S}^{vol} and a biochemically generated active component \mathbf{S}^{act} , cf. [8, 9, 13].

The passive component \mathbf{S}^{pas} is computed from a suitable strain energy function

W^{pas} and the Green Lagrange strain \mathbf{E} as

$$S_{ij}^{pas} = \frac{1}{2} \left(\frac{\partial W^{pas}}{\partial E_{ij}} + \frac{\partial W^{pas}}{\partial E_{ji}} \right) \quad i, j = 1, 2, 3.$$

In this paper, the myocardium is modeled as a transversely isotropic hyperelastic material, with the exponential strain energy function introduced in [13]. The near-incompressibility of the myocardium is modeled by an additive volume change penalization term.

The contraction of the ventricles results from the active tension generated by the model of myofilements dynamics activated by calcium. We assume that the generated active force acts only in the direction of the fiber, as in the other works [12, 14], hence, according to [7, Ch. 10], the second Piola-Kirchhoff active stress component is given by

$$\mathbf{S}^{act} = J \mathbf{F}^{-1} \boldsymbol{\sigma}^{act} \mathbf{F}^{-T} = T_a \frac{\hat{\mathbf{a}}_l \otimes \hat{\mathbf{a}}_l}{\hat{\mathbf{a}}_l^T \mathbf{C} \hat{\mathbf{a}}_l}.$$

The biochemically generated active stress T_a is modeled as *stretch and stretch-rate independent*. Thus, we assume as in [6, 11] that the dynamics of T_a depends only on the transmembrane potential v according to a simple twitch-like rule, see [6, 11] for details.

Electrical model As electrical model we consider the monodomain model using the Aliev-Panfilov membrane model [1] on the reference cardiac domain $\hat{\Omega}$ [11, 12, 14]. Given an applied current per unit volume $I_{app} : \hat{\Omega} \times (0, T) \rightarrow \mathbb{R}$, and initial conditions $v_0 : \hat{\Omega} \rightarrow \mathbb{R}$, $w_0 : \hat{\Omega} \rightarrow \mathbb{R}$, find the transmembrane potential $v : \hat{\Omega} \times (0, T) \rightarrow \mathbb{R}$ and the gating variable $w : \hat{\Omega} \times (0, T) \rightarrow \mathbb{R}$ such that

$$c_m \frac{\partial v}{\partial t} - J^{-1} \text{Div}(J \mathbf{F}^{-1} D_m \mathbf{F}^{-T} \text{Grad } v) + I_{ion}(v, w) = I_{app} \quad \text{in } \hat{\Omega} \times (0, T), \quad (2)$$

$$\frac{\partial w}{\partial t} - R(v, w) = 0 \quad \text{in } \hat{\Omega} \times (0, T), \quad (3)$$

where \mathbf{F} is the deformation gradient tensor and the functions $I_{ion}(v, w)$, $R(v, w)$ are given by the Aliev-Panfilov membrane model [1]. Insulating boundary conditions on v are prescribed.

The computation of the tensors $\mathbf{F}^{-1}(\mathbf{X}) D_m(\mathbf{x}) \mathbf{F}^{-T}(\mathbf{X})$ must be performed on the reference configuration $\hat{\Omega}$. Denoting by $\hat{\mathbf{a}}_l(\mathbf{X})$ the unit vector parallel to the local fiber direction in the reference configuration, it holds

$$(\mathbf{F}^{-1} D_m \mathbf{F}^{-T})(\mathbf{X}) = \sigma_t^m \mathbf{C}^{-1}(\mathbf{X}) + (\sigma_l^m - \sigma_t^m) \frac{\hat{\mathbf{a}}_l(\mathbf{X}) \hat{\mathbf{a}}_l^T(\mathbf{X})}{\hat{\mathbf{a}}_l^T(\mathbf{X}) \mathbf{C}(\mathbf{X}) \hat{\mathbf{a}}_l(\mathbf{X})}, \quad (4)$$

where $\sigma_{l,t}^m$ are the Monodomain axisymmetric conductivities, see e.g. [4].

3 Numerical methods

Spectral deferred correction methods Spectral deferred correction methods [5] 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 $0 = \tau_0 < \dots < \tau_n = \tau$ 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

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

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

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

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 (2), the gating variables (3), 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 excitation 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.

Interleaved mesh refinement Here 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 [10], 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

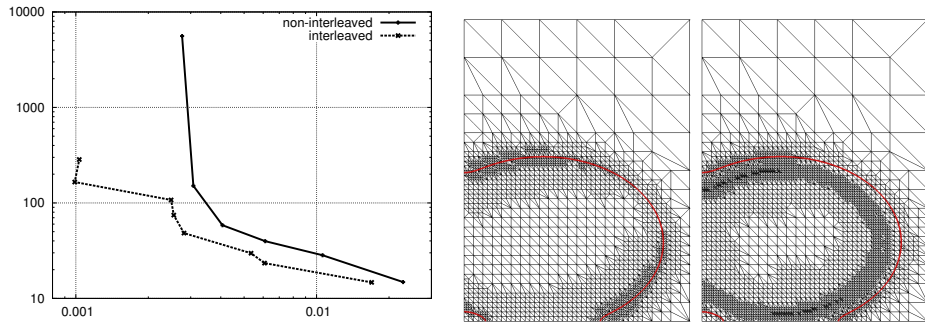


Figure 1: *Left*: Wall clock time vs. achieved error for different tolerances. *Right*: Grid maladaptation by mesh refinement based on the first sweep. Front position is marked.

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.

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*).

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., Deuffhard, 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)

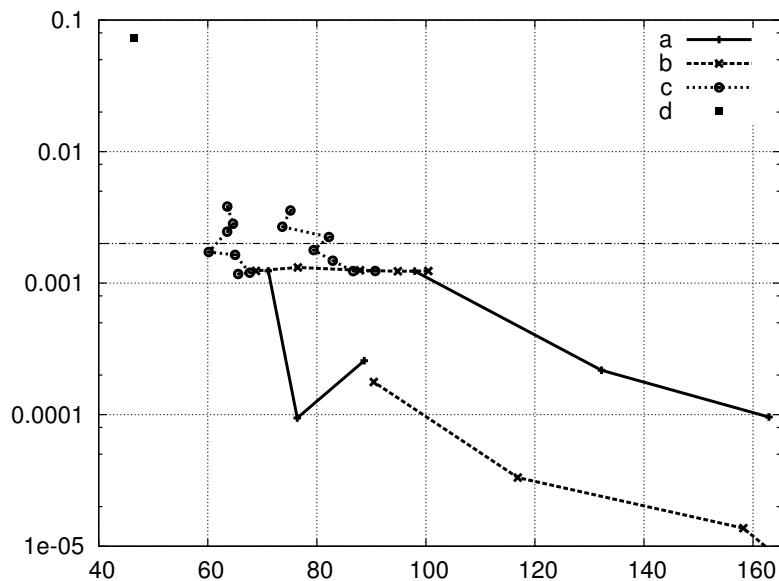


Figure 2: Total error vs. run time for inexact solution of displacement.

- [4] Colli Franzone, P., Pavarino, L.F.: A parallel solver for reaction-diffusion systems in computational electrocardiology. *Math. Mod. Meth. Appl. Sci.* **14**, 883–911 (2004)
- [5] Dutt, A., Greengard, L., Rokhlin, V.: Spectral deferred correction methods for ordinary differential equations. *BIT* **40**(2), 241–266 (2000)
- [6] Göktepe, S., Kuhl, E.: Electromechanics of the heart – a unified approach to the strongly coupled excitation-contraction problem. *Comp. Mech.* **80**, 227–243 (2010)
- [7] Humphrey, J.D.: *Cardiovascular Solid Mechanics, Cells, Tissues and Organs*. Springer, New York (2001)
- [8] Hunter, P.J., McCulloch, A.D., ter Keurs, H.E.D.J.: Modelling the mechanical properties of cardiac muscle. *Progr. Biophys. Molec. Biol.* **69**, 289–331 (1998)
- [9] 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 asynchrony of depolarization: a model study. *Ann. Biomed. Eng.* **31**, 536–547 (2003)

- [10] Lang, J.: Adaptive Multilevel Solution of Nonlinear Parabolic PDE Systems, *Lecture Notes in Computational Science and Engineering*, vol. 16. Springer (2001)
- [11] Nash, M.P., Panfilov, A.V.: Electromechanical model of excitable tissue to study reentrant cardiac arrhythmias. *Progr. Biophys. Molec. Biol.* **85**, 501–522 (2004)
- [12] Pathmanathan, P.J., Whiteley, J.P.: A numerical method for cardiac mechano-electric simulations. *Ann. Biomed. Engrg.* **37**, 860–873 (2009)
- [13] 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)
- [14] 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)