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Anatomically accurate high resolution modeling of human whole heart electromechanics: A strongly scalable algebraic multigrid solver method for nonlinear deformation ☆

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ABSTRACT

Electromechanical (EM) models of the heart have been used successfully to study fundamental mechanisms underlying a heart beat in health and disease. However, in all modeling studies reported so far numerous simplifications were made in terms of representing biophysical details of cellular function and its heterogeneity, gross anatomy and tissue microstructure, as well as the bidirectional coupling between electrophysiology (EP) and tissue distension. One limiting factor is the employed spatial discretization methods which are not sufficiently flexible to accommodate complex geometries or resolve heterogeneities, but, even more importantly, the limited efficiency of the prevailing solver techniques which is not sufficiently scalable to deal with the incurring increase in degrees of freedom (DOF) when modeling cardiac electromechanics at high spatio-temporal resolution.

This study reports on the development of a novel methodology for solving the nonlinear equation of finite elasticity using human whole organ models of cardiac electromechanics, discretized at a high para-cellular resolution. Three patient-specific, anatomically accurate, whole heart EM models were reconstructed from magnetic resonance (MR) scans at resolutions of 220 μm, 440 μm and 880 μm, yielding meshes of approximately 184.6, 24.4 and 3.7 million tetrahedral elements and 95.9, 13.2 and 2.1 million displacement DOF, respectively. The same mesh was used for discretizing the governing equations of both electrophysiology (EP) and nonlinear elasticity. A novel algebraic multigrid (AMG) preconditioner for an iterative Krylov solver was developed to deal with the resulting computational load. The AMG preconditioner was designed under the primary objective of achieving favorable strong scaling characteristics for both setup and solution runtimes, as this is key for exploiting current high performance computing hardware.

Benchmark results using the 220 μm, 440 μm and 880 μm meshes demonstrate efficient scaling up to 1024, 4096 and 8192 compute cores which allowed the simulation of a single

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heart beat in 44.3, 87.8 and 235.3 minutes, respectively. The efficiency of the method allows fast simulation cycles without compromising anatomical or biophysical detail.

1. Introduction

Electromechanical function of the heart emerges from a complex cascade of processes, which interact across a broad range of spatial and temporal scales. Despite the large body of experimental and theoretical research accumulated, our current understanding of how alterations in subcellular function affect whole organ pumping performance or, conversely, how changes at the systemic level influence subcellular function, remains incomplete. Computational modeling bears high promise as a methodology for integrating experimental data into a mechanistic framework which enables the quantitative observation of complex cause–effect relationships across a broad range of spatio-temporal scales.

While the potential gains from modeling approaches are significant, the challenges to be addressed are daunting. Historically, the development of EP and mechanical models of cardiac function proceeded rather independently than in tandem. The vast majority of EP modeling studies ignored any effects due to mechanical deformation, and, vice versa, most mechanical modeling studies did not represent explicitly any feedback of deformation on EP. While such a simplified EM coupling has proven suitable for addressing a variety of questions [85,53,60], the assumption of a unidirectional coupling between EP and mechanical deformation is inaccurate as there is strong evidence that EP is modulated by tissue distension via mechano–electric feedback (MEF) mechanisms [58,62,63]. However, from a model development point of view, it is attractive to assume that MEF can be neglected, as this allows to develop EP and mechanical models independently which reduces the complexity of implementation. This effective split into two separate sequentially executed solution steps is reflected in a notable divergence in the employed methodologies between EP and mechanics modeling communities.

State of the art organ scale EP finite element or finite volume models are discretized at a high spatio-temporal resolution using tetrahedral [112] or hybrid elements [100]. High resolutions are not only necessary to capture the fast transients and steep depolarization wavefronts, but also to resolve fine microscopic scale structural detail [93,122] as well as functional heterogeneities [78,18,57]. In contrast, mechanical models build on the assumption that cardiac deformation is governed by smoother spatial and slower temporal scales, suggesting that the use of much coarser spatio-temporal discretizations may yield sufficient accuracy. Thus the use of higher order cubic Hermite elements became popular [24] as they allow tessellation of stylized ventricular anatomy using a very small number of elements and they avoid *volumetric locking*, however, their major drawback is the limited capacity to accommodate complex geometries. This issue is being addressed now with the use of tetrahedral $P_1 - P_0$, $P_2 - P_0$ or mixed formulation $P_2 - P_1$ elements, which have been introduced only very recently for modeling cardiac mechanics [43,42,32]. In general, finite element discretizations with tetrahedral and hexahedral elements of the same order showed similar results in terms of precision and efficiency [19].

Unsurprisingly, as a consequence the cost of model execution has been addressed quite differently as well. In EP modeling, due to a large number of DOF, a pressing need for strongly scalable iterative solvers has emerged [82,97], whereas for the lower dimensional mechanical models this has not been the case. While high resolution models and corresponding scalable solver algorithms have been developed for vascular applications [61,3], for cardiac mechanics direct solvers, executed on a very small number of compute cores [32], prevail.

The use of higher spatial resolutions and more flexible tetrahedral or hybrid finite element meshes is also driven by the needs of clinical modeling applications. Generation pipelines for individualized EM models rely increasingly on reconstruction from tomographic imaging [111] which provide an ever increasing level of anatomical detail [68]. Multimodal clinical imaging also facilitates more accurate tissue classification. Clinically important delineation of viable myocardium, fat deposits, cleft spaces and vascularization, as well as substrate abnormalities such as infarct scars [103] or the presence of fibrosis [76,77] is becoming feasible. These are known to be important factors influencing cardiac deformation, however, the spatial resolutions and methodology currently used impede their elucidation in modeling studies.

Spatial resolution also becomes an important factor when considering bidirectionally coupled, anatomically accurate EM models. A bidirectional link between EP and mechanics demands information being passed back and forth between EP and mechanics solver components. With tomographically reconstructed models the bidirectional projection of data may constitute a significant technical challenge when markedly different spatio-temporal resolutions are used. Either one resorts to using simplified, stylized anatomical representations for both physics to ensure an exact overlap of both domains, a refined electrical mesh is derived from spatial refinement of finite elements forming the mechanical mesh [15], or one opts to use the same high resolution mesh for both physics and accepts the increase in computational load. The advantage of the latter approach is that convergence studies with bidirectionally coupled EM models are feasible as discretization errors are governed by the spatio-temporal discretization of the EP problem. When attempting to build human whole organ EM models the use of high resolution meshes becomes particularly challenging due to the larger size of a human heart compared to other species used in many previous EM modeling studies [83], and the overall increase in DOF needed for discretizing both ventricles as well as the thin-walled atria [11].

This study reports on the development of a novel methodology for modeling of human whole organ cardiac electromechanics at a high para-cellular resolution. A clinical magnetic resonance (MR) scan was segmented to generate a