Biophysiological Applications – Cardiovascular simulations

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The Model

The modelling and simulation of cardiovascular phenomena is a coupled multi-physics problem that consists of electrophysiology (excitation pattern in the heart), of non-linear elasticity (deformation of heart tissue) and of fluid dynamics (blood flow through heart chambers).

The **electrophysiology** is described via the bidomain equations that consist of two PDEs coupled with a system of ODEs (non-linear coupled PDE-ODE system):

$$
\begin{bmatrix} -\nabla \cdot (\bar{\sigma}_i + \bar{\sigma}_e)\nabla\phi_e \\ -\nabla \cdot \sigma_b \nabla\phi_e \end{bmatrix} = \begin{bmatrix} \nabla \cdot \bar{\sigma}_i \nabla V_m \\ I_e \end{bmatrix}
$$

$$
\frac{\partial V_m}{\partial t} = \frac{1}{\beta C_m}\left(\nabla \cdot \bar{\sigma}_i \nabla V_m + \nabla \cdot \bar{\sigma}_i \nabla\phi_e\right) - \frac{1}{C_m} i_{ion}(V_m, \vec{\eta})
$$

$$
\frac{d\vec{\eta}}{dt} = g(V_m, \vec{\eta})
$$

Here φ_e and V_m are the extracellular potential and transmembrane voltage respectively; $\tilde{\eta}$ represents the ionic current variables; $\bar{\sigma}_i$ and $\bar{\sigma}_e$ are conductivity tensors of intracellular and extracellular spaces respectively; σ_b is the isotropic conductivity of the fluid in which the heart is immersed (bath and cavities); C_m is the capacitance per unit area and β is surface to volume ratio; i_{ion} and g model ionic currents and specify the cell membrane model.

There are cheaper models as the monodomain equations or the Eikonal equation available in case only the arrival time of the excitation wave (=stimulation time of the heart muscles) is needed.

Cardiac electromechanics couple electrophysiology with the non-linear deformation, i.e., the bidomain equations are extended with the elasticity equation for large deformations and for non-linear material laws. The deformation is governed by the equilibrium equation

$$-\text{div}_\sigma(\mathbf{u}) = \mathbf{b},$$

with unknown displacement field $\mathbf{u}$. The stress tensor $\sigma = \sigma_p + \sigma_a$ consists of a passive contribution σ_p and an active contribution σ_a, while the latter depends on the normalized myocyte orientation. The passive contribution requires the right Cauchy-Green tensor taking into account the deformation gradient and a nonlinear function Ψ describing the strain energy density of the specific material.

The full cardiovascular model requires a **Fluid-Structure interaction** (FSI) and adds the **Navier-Stokes equations** to the coupled system from electro mechanics including coupling terms at the interfaces between fluid domain and deformation domain. The fluid (blood) is assumed as incompressible.

$$\rho \left(\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} \right) = -\nabla p + \mu \Delta \vec{v} + \vec{f}.$$
$$\nabla \cdot \vec{v} = 0,$$

The conditions on the interface between fluid domain and deformation domain have to guarantee continuity of pressure and deformation via the related physical quantities. The FSI has to be performed on changing computational domains which requires some caution in the numerical realization, especially a high quality mesh deformation for the moving discretized computational domains.

Discretization and numerical realization

The overall computational framework is embedded in the Cardiac Arrhythmia Research Package (CARP) (G. Plank, Graz and E. Vigmond, Bordeaux) [1] where the University of Graz contributes with parallel solvers (G. Haase, Graz; MontBlanc3) [2,3] and image processing [C. Bredies, Graz].

The computational domain is determined a priori by image processing (registration + segmentation) and physiological mapping. This continuous domain is discretized by finite elements (tetrahedrons) that define the computational domains. We have to distinguish between the fluid domain, the deformation domain and the electrical domain.
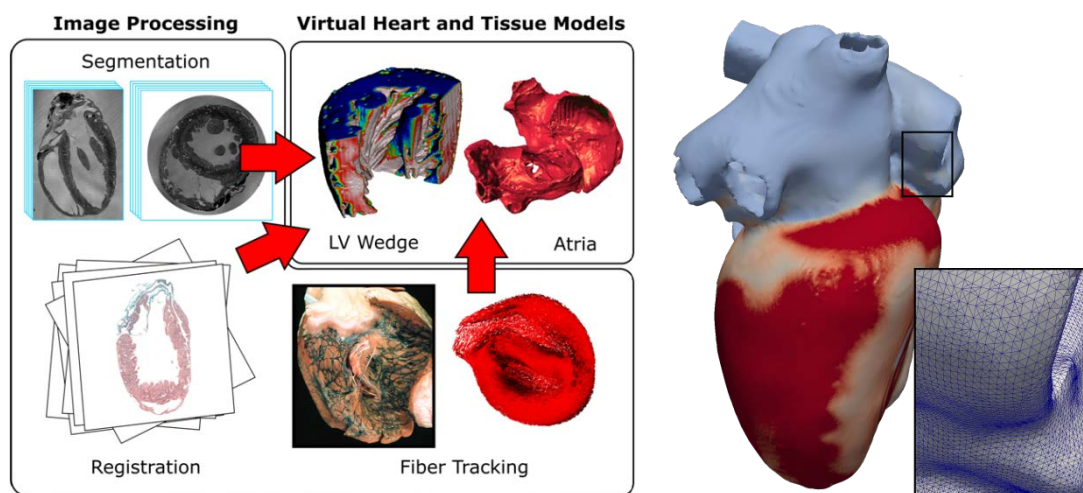
From images to the heart geometry (left) and an electrical excitation wave on a discretized heart (right).

The finite element discretization of the PDEs uses linear elements, stable elements for saddle point problems and higher order elements regarding the regularity requirements on the solution (that is analysis of PDEs).

Independently of the model under investigation we always have to solve a huge linear system of linear equations in each time step and in each step of the outer non-linear iteration. Solving the (block) systems takes advantage of the sparse matrix structure and the

properties of the originating PDEs (symmetric?, positive definite?). The solution methods for the linear systems of equations are preconditioned Krylov subspace as the conjugate gradient (cg) or the generalized minimal residual (gmres) method with algebraic multigrid (AMG) as preconditioner.

Thanks to the Mont-Blanc 3 project, we have been able to improve our solver package and parts of it (AMG, Jacobi smoother, Eikonal solver) with performance tools from other workgroups in MontBlanc3 on available and brand-new hardware as the Arm Clusters at BSC.

High Performance Computing

Solving the discretized (coupled) problems from above requires a lot of compute power, e.g., it takes 8 minutes on 16192 CPU cores (SuperMuc in Munich, Germany) to simulate a full electromechanic heart beat on a realistic discretization with 45 Million tetrahedrons. The Implementation is usually done in C++ and uses shared memory parallelization (OpenMP, OpenSs) as well as distributed memory parallelization (MPI) and occasionally GPU-parallelization (CUDA, OpenACC) [2,3].
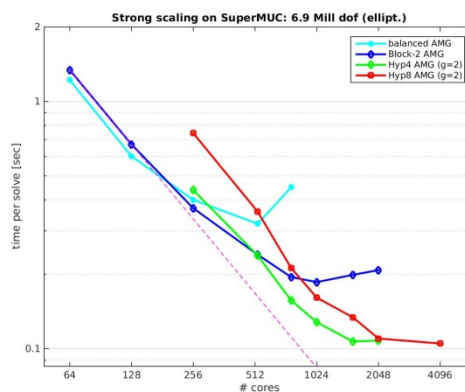
A 4x4 domain decomposition (left) and some strong scaling results for the electrophysiological subproblem on SuperMuc (right).

Further topics (ongoing research)

In contrast to engineering applications, the material parameters (σ *etc.*) are only roughly known because dead tissue can be measured but behaves different than living tissue and experiments on beating human hearts are forbidden by themselves.

Therefore, simulation results have to be compared to measurable data (here, the ECG at 12 spots on the torso) and the material data will be calibrated such the computed ECG gets closer to the measured ECG. We follow currently several approaches for an automatic calibration (with reduced sets of equations) which contain

- optimization approaches

- deep learning approaches

- combinations of the two.

Here the highly optimized Eikonal solver [4] (based on several simplification of the bidomain equations) is the first choice to calculate a fast and sufficiently accurate electrical excitation wave, see figure. The Arm cluster outperforms the performance of other hardware platforms for our Eikonal solver in terms of power consumption.
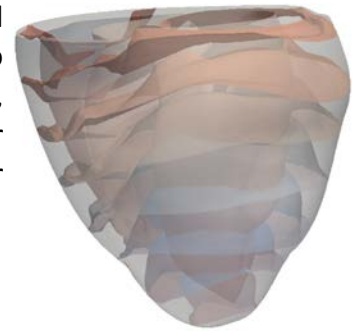
References

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[2] G. Plank, M. Liebmann, R. Weber dos Santos, E.J. Vigmond and G. Haase: "Algebraic Multigrid Preconditioner for the Cardiac Bidomain Model", IEEE Transactions on Biomedical Engineering, Vol 54, Issue 4, pp. 585-596 (2007).

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