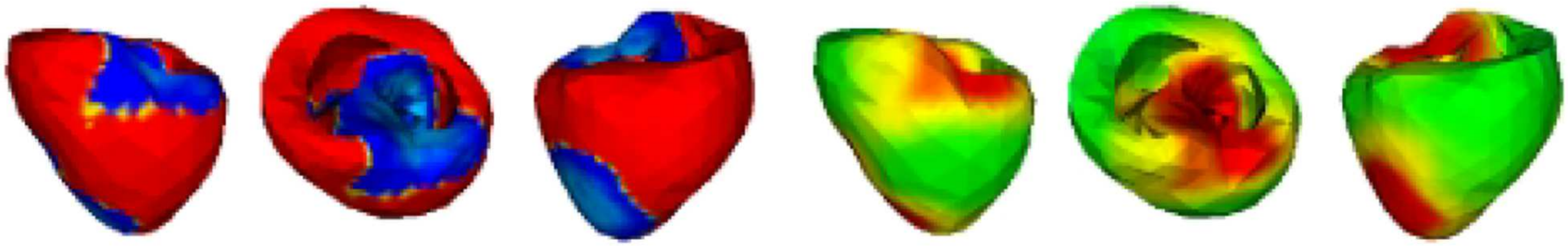
jh200036-MDHI

High resolution simulation of cardiac electrophysiology on realistic whole-heart geometries



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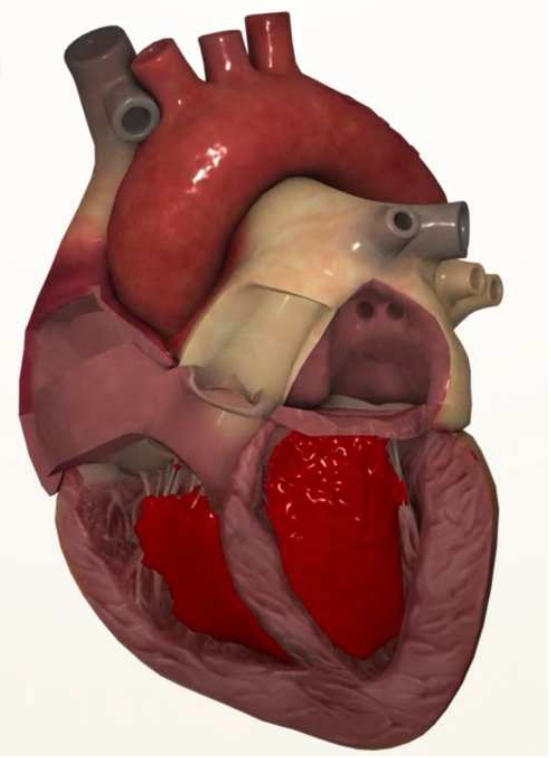
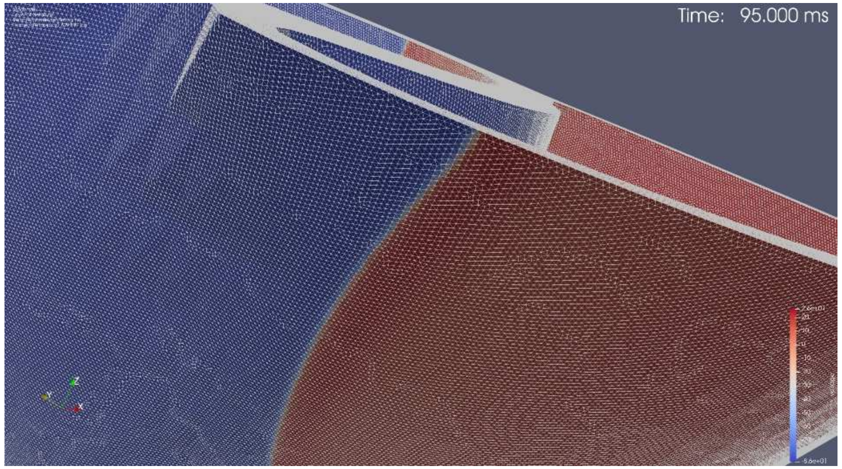
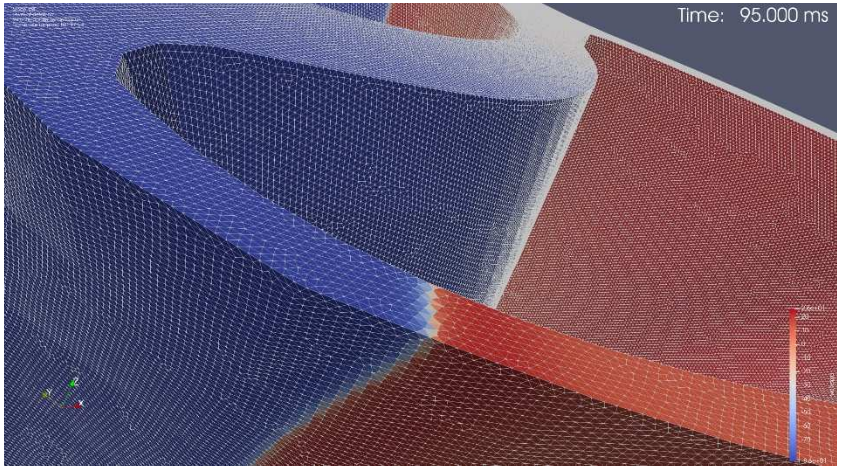
Background

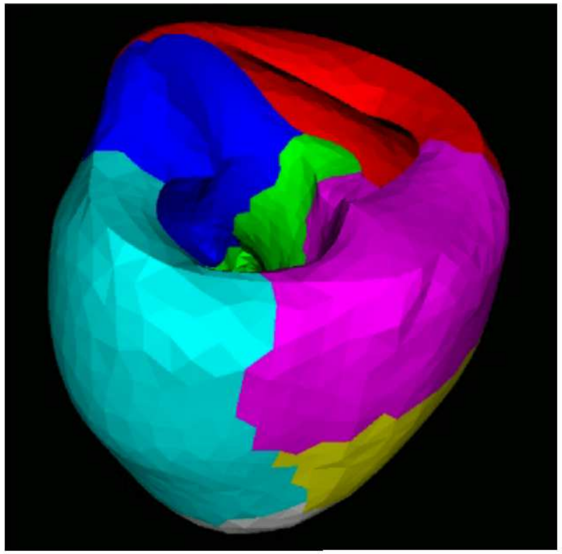


- Coordinated electrical activities in the heart rely on proper calcium handling at the cellular and subcellular levels.
- Many questions about cardiac electrophysiology remain unanswered.
- We need advances in the realism of mathematical models and simulation resolutions.
- These require developing simulators of electrophysiology that can effectively use modern supercomputers to do “in-silico” experiments.





Governing equations & numerical scheme



- The 3D solution domain, of an irregular shape, represents an entire heart.
- The mathematical model consists of two parts:
  - The PDE part is a diffusion equation with variable conductivity properties;
  - The ODE part determines I_{ion} based on a system of nonlinear ODEs modeling a set of state variables inside each cell.

$$\frac{\partial V_m}{\partial t} = \frac{-I_{\mathrm{ion}}}{C_m} + \nabla \cdot (\mathbf{D} \nabla V_m)$$

- The irregular 3D domain is discretized by an unstructured tetrahedral mesh.
- There already exists a simulator based on explicit time integration:
  - A 2^{nd}-order finite volume method is used to discretize the PDE part;
  - The ODE part is also solved explicitly.
- The simulator’s efficiency and parallel scalability need an extensive study for improvements.

FY2020 research plan

Single-node optimization of the explicit-method based simulator (month 1 – month 6), so that it can effectively use both a single Xeon-Phi Knights Landing processor and a single node of Oakbridge-CX.

- For the PDE part, OpenMP threads will be used for the parallelization, with special emphasis on ensuring good data locality.
- Different data element re-ordering schemes will be investigated.
- For the ODE part, we aim to decrease the number of special mathematical function calls and to enable AVX-512 code vectorization.
- A simple performance model will be established to verify the actually obtained single-node performance.
- Fast file caches will be tested for in-situ data analysis tasks.

FY2020 research plan (cont'd)

Scale-out optimization of the explicit simulator (month 7 – month 12), to allow scalable use of multiple nodes on Oakforest-PACS and Oakbridge-CX.

- Adding MPI parallelization to the simulator:
  1. Hardware-aware partitioning of unstructured tetrahedral meshes;
  2. Overlapping MPI communication with useful computation.
- Combining OpenMP threads and MPI processes.
- Delegating special tasks (communication, coordination, internal boundary handling etc.) to a small selection of threads while the remaining threads carry out the main computational tasks.

Investigation of an implicit version of the simulator (month 7 – month 12), which uses global-synchronization-free variants of Krylov subspace methods for efficiently solving linear systems related to the PDE part.