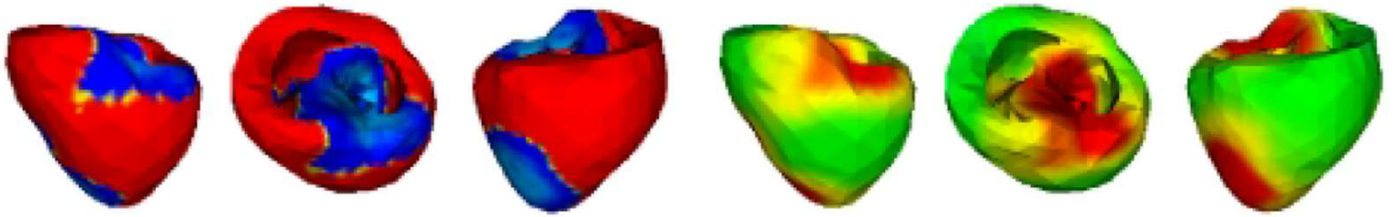
jh210021-MDHI

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



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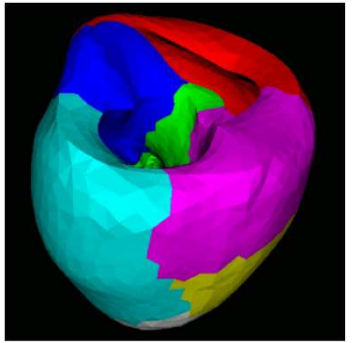
Computational Overview

- Mathematical model: a 3D nonlinear reaction-diffusion equation

$$\frac{\lambda}{1+\lambda}\nabla\cdot(\boldsymbol{\Sigma}_i\nabla v) = \chi\left(C_m\frac{\partial v}{\partial t} + I_{\text{ion}}\right)$$

- Operator splitting results in a “PDE” part and an “ODE” part
  - PDE part: 3D diffusion equation for v (transmembrane potential) with an inhomogeneous and anisotropic conductivity tensor
  - ODE part: a system of nonlinear ODEs to model transmembrane ionic current I_{ion}
- Unstructured tetrahedral mesh used to represent the heart geometry
  - Mesh partitioning used for distributed-memory (MPI) parallelization
  - OpenMP threads used for shared-memory parallelization



FY.2021 Research Activity 1

Improve the current parallel diffusion equation solver (explicit time integration & cell-centered finite volume discretization)

- Appropriate combination of MPI processes and OpenMP threads
  - What's the ideal number of MPI processes per compute node?
  - Non-default scheduling of the OpenMP threads?
  - Should some of the OpenMP threads be exclusively reserved for communication tasks?
  - Better ordering of the degrees of freedom within each MPI process?
- Overlap between computation and MPI communication
  - Replacement of MPI_Neighbor_alltoallv with MPI_Ineighbor_alltoallv for halo exchange?
  - Other ways of optimizing the MPI communication?

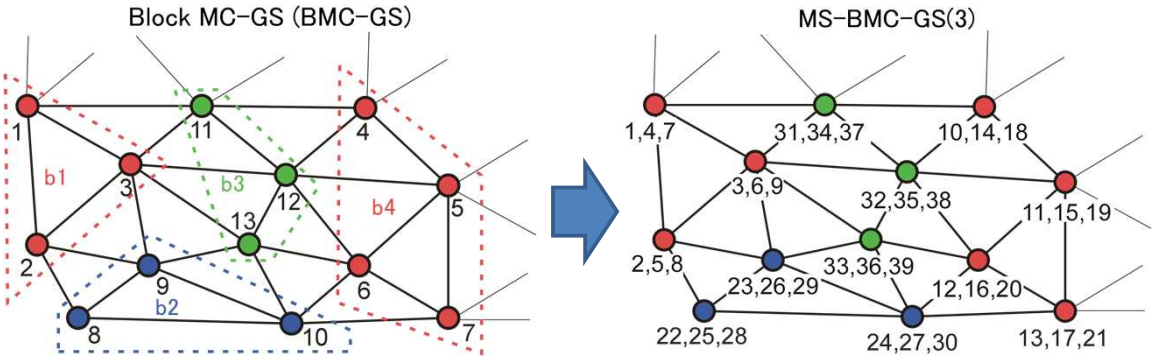
FY.2021 Research Activity 2
Implement a new parallel diffusion equation solver

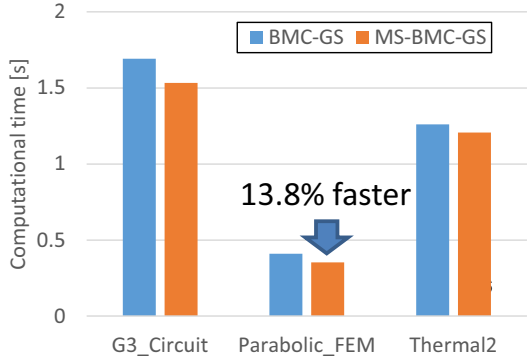
- Implicit time integration + cell-centered finite volume discretization
- Better numerical stability and possibly better accuracy
  - Can use larger step sizes
  - However, each time step will be more time consuming
- Need to efficiently solve a sparse linear system during each time step
  - Can reuse the same mesh partitioning strategy
  - Can reuse the same SpMV implementation and the associated halo-exchange
  - Need to incorporate a parallel MPI+OpenMP Conjugate Gradient iterative solver
  - Need an effective parallel MPI+OpenMP preconditioner

FY.2021 Research Activity 3

Parallel Algebraic Multigrid (AMG) Preconditioner

- Need to be high-performance and compatible with the MPI+OpenMP parallelization
  - Multiplicative Schwartz type block multi-color parallelization for Gauss-Seidel smoother†1 → Improving convergence rate, Reducing amount of communication





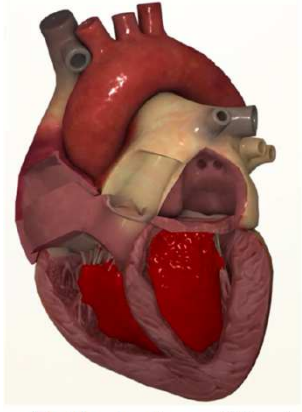
[Kawai et al. HPC Asia 2020]

- Need to find suitable AMG parameters for sparse matrices that arise from discretizing 3D diffusion equation on unstructured heart meshes

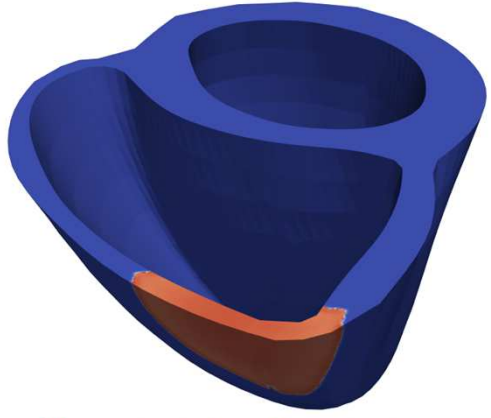
FY.2021 Research Activity 4

Realistic whole-heart simulations of cardiac electrophysiology

- $O(10^8)$ tetrahedra to represent realistic whole-heart geometries
- Effective use of $O(100)$-$O(1000)$ powerful compute nodes for close-to-real-time parallel simulations
- Goal: To be able to carry out detailed, in-silico experiments of cardiac electrophysiology, in both healthy and diseased states



(a) Illustration of the heart



(b) Tetrahedral mesh for the heart ventricles

FY.2021 Research Activity 5

Port the simulator of cardiac electrophysiology to Wisteria/BDEC-01 (Odyssey)

- Performance benchmarking on the A64FX architecture
  - Single node
- Performance tuning/optimization on the A64FX architecture
  - Single node
  - Many nodes