jh230018 Co-PI's: Kengo Nakajima (University of Tokyo), Xing Cai (Simula Research Laboratory, Norway)

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

Purpose & Organization: International Project under Japan-Norway Collaboration

To further advance the scientific understanding of the intricate electrical activities in the heart, which are of vital importance for the human body, more elaborate mathematical modeling is needed with the support of supercomputing. In this project, we propose to implement and optimize a new simulator of cardiac electrophysiology, based on the latest cell-resolved modeling approach. The expected level of physiological details and the resulting computational resolution can only be achieved by an effective use of modern supercomputers. By combining efficient numerical algorithms with hardware-compatible software implementations, we want to enable computational scientists to carry out novel "in-silico" experiments. Moreover, this project will consolidate the existing expertise of the project partners on large-scale simulations using realistic geometries and unstructured meshes, optimized parallel programming and use of non-x86 architecture (A64FX processors) and accelerator (Nvidia GPUs).

Information Technology Center, The University of Tokyo
Kengo Nakajima (HPC, Algorithms), Co-PI
Akihiro Ida (Algorithms) (⇒JAMSTEC)
Toshihiro Hanawa (HPC)
Masatoshi Kawai (HPC, Algorithms) (⇒Nagoya University)
Tetsuya Hoshino (HPC) (⇒Nagoya University)
Yohei Miki (HPC)
Masaharu Matsumoto (HPC) (⇒Fukushima University)

NVIDIA Japan
Akira Naruse (HPC)

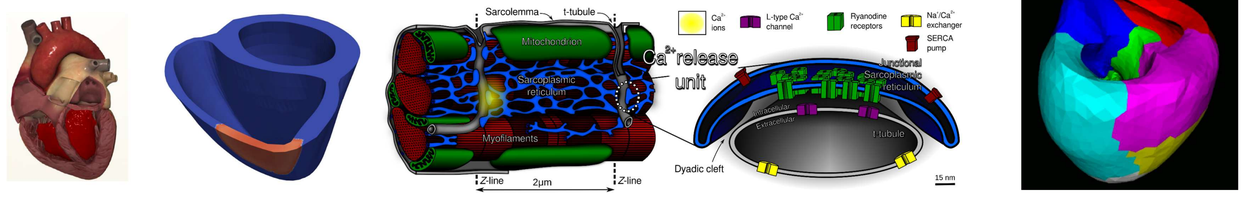
Simula Research Laboratory, Norway
Xing Cai (Simulations, Modeling, HPC), Co-PI (Norway)
Glenn Terje Lines (Modeling) (Norway)
Johannes Langguth (HPC) (Germany)
Kristian Gregorius Hustad (HPC) (Norway)
Hermenegild Arevalo (Simulations) (USA)
James Trotter (HPC) (Norway)
María Hernández Mesa (Simulations) (Spain)
Lena Myklebust (Simulations) (Norway)
Lisa Pankewitz (Simulations) (Germany)

3D Simulator for Cardiac Electrophysiology

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

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

- Operator splitting results in a "PDE" part and an "ODE" part
  - ✓ PDE part: 3D diffusion equation for V_m (membrane potential) with an inhomogeneous and anisotropic conductivity tensor D
  - ✓ 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



- The PDE part: 3D diffusion equation with variable coefficient
  - ✓ Fully explicit temporal discretization (Forward Euler scheme)
  - ✓ In space, the diffusion equation is discretized by a cell-centered FVM: 5pt. Stencil
  - ✓ During each time step, the PDE work translates to a sparse matrix-vector multiply (SpMV), where the vector contains the membrane potential values at all the computational cell centers
  - ✓ Unstructured mesh partitioning & MPI parallelization of the SpMV
- The ODE part: a system of nonlinear ordinary different equations
  - ✓ The ODE system (up to 39 state variables) applies to each computational cell
  - ✓ Explicit time integration (Forward Euler or Generalized Rush-Larsen scheme)
  - ✓ During each time step, the ODE work is to advance the ODE system separately on each computational cell
  - ✓ The ODE work is embarrassingly parallel, follows the mesh partitioning for work distribution
- Strategies of performance enhancement in the JHPCN project
  - ✓ Code optimiation, parallelization overhead reduction, more advanced numerical algorithm

Research Plan: FY.2023

A preliminary MPI-parallelized, cell-resolved simulator (Cai, Trotter, Hustad, Lines)

Based on an existing cell-resolved simulator that uses finite difference discretization and shared-memory parallelization [2], we will develop a new cell-resolved simulator that is based on finite element discretization where tetrahedral elements will be adopted and thus capable of handling irregular shapes of the extra-cellular and intra-cellular areas. Distributed-memory parallelization, programmed using MPI, will be enabled. The overall numerical strategy will otherwise follow the full operator-splitting approach adopted in [1,2], where the individual intra-cellular subdomains will be independently solved, while decoupled also from the extra-cellular subdomain and the cell membranes. During each time step, the ordinary differential equations applicable on the cell membranes will be integrated first, followed by solving the individual intra-cellular subdomain problems, and thereafter the overall extra-cellular subdomain problem.

Code optimization through overhead-aware partitioning (Cai, Trotter, Hustad, Langguth)

As mentioned above, there are three types of subdomains in the new cell-resolved modeling approach: the individual intra-cellular subdomains (each per cardiac cell), the cell membranes (surfaces surrounding the 3D intra-cellular subdomains) and the overall extra-cellular subdomain that is the exterior of all the intra-cellular subdomains. In the preliminary cell-resolved simulator (see above), partitioning of the three subdomain types will be made independent of each other. This implementation decision is conceptually simple, but may lead to unnecessarily large communication overhead. We will thus experiment in this task new partitioning schemes to achieve some coordination between the different partitioning sub-problems, thus reducing the communication overhead and achieving better parallel performance.

Optimization of the numerical schemes for the intra- and extra-cellular solvers (Nakajima, Cai, Trotter, Kawai, Ida, Matsumoto)

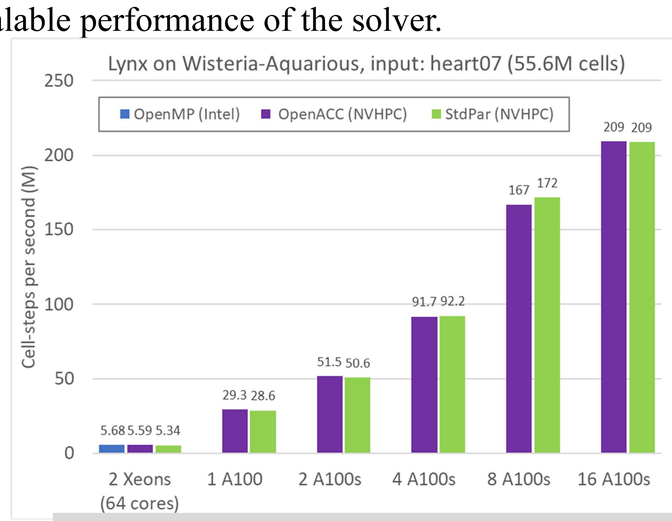
Each intra-cellular subdomain needs to independently solve a 3D Poisson equation per time step. The number of degrees of freedom per cell is expected to be no more than 10^4, thus a careful study will be carried out to find out whether a sparse direct solver should be used instead of a typical choice of the conjugate gradient iterative solver (possibly with a preconditioner). For the overall extra-cellular subdomain, another 3D Poisson equation needs to be solved per time step. The number of degrees of freedom (in the orders of 1010 or more) dictates the use of a parallel conjugate gradient solver. The question of concern is the appropriate parallel preconditioner. We expect a parallel algebraic multigrid (AMG) solver to be the correct choice, but research is needed regarding the actual linear-algebra library to be chosen and the internal AMG parameters to be tuned. Moreover, investigation for communication-computation overlapping will be continued in FY.2023

Porting to the GPU platform (Nakajima, Miki, Naruse, Hoshino, Trotter, Hanawa)

In a preceding JHPCN project during FY.2022, we had success with porting a conventional simulator of cardiac electrophysiology (based on the mondomain model) to Nvidia GPUs by using the Nvidia Software Development Kit (SDK) [3]. A similar effort will be made in this project to offload the main computational work of a cell-resolved simulator to Nvidia GPUs. Furthermore, AmgX library (AMG library for Nvidia GPUs, https://developer.nvidia.com/amgx) will be introduced for scalable performance of the solver.

Preliminary cell-resolved simulations of cardiac electrophysiology (Arevalo, Mesa, Myklebust, Pankewitz, Hustad, Lines)

During the last quarter of FY.2023, when the distributed-memory implementations of the cell-resolved simulator are properly tested and optimized, we will apply these to some carefully chose test cases. One of the goals will be to simulate one million fully resolved cardiac cells, requiring about 10^{11} mesh points in total. Such an achievement will considerably improve the state of the art.



Results of porting of Lynx code to Aquarius with NVIDIA A100 GPUs [3]

[1] K. H. Jæger, K. G. Hustad, X. Cai and A. Tveito. Efficient numerical solution of the EMI model representing the extracellular space (E), cell membrane (M) and intracellular space (I) of a collection of cardiac cells. Frontiers in Physics 8 (2021): 579461.
[2] K. H. Jæger, K. G. Hustad, X. Cai and A. Tveito. Operator Splitting and Finite Difference Schemes for Solving the EMI Model. In Modeling Excitable Tissue: The EMI Framework, 44-55. Vol. 7. Cham: Springer International Publishing, 2021
[3] A. Naruse, J.D. Trotter, J. Langguth, X. Cai, K. Nakajima, High resolution simulation of cardiac electrophysiology on realistic whole-heart geometries on Wisteria/BDEC-01 (Aquarius), 情報処理学会研究報告（2022-HPC-187-15）， 2022

Contact: Kengo Nakajima (nakajima@cc.u-toyo.ac.jp)
Information Technology Center (ITC), The University of Tokyo