Are you stroked? Stroke prediction tool for doctors.

Group C

Abdi Essamade Saufi, Masamitsu Nakayama, Sameer Satish Deshmukh, and Yen Chen Chen
Mentors: Seiya Nishizawa, Rahul Bale

Abdi Essamade Saufi

Politecnico di Milano, Italy / PhD

(Presentation title)

Direct Numerical Simulation of the evaporation and combustion of suspended fuel droplets

(Research field / theme)

Computational Fluid Dynamics of Multiphase Flows

Masamitsu Nakayama

Tokai U, JPN / PhD

(Presentation title)

Prediction of bound Thrombin to Platelet Glycoprotein Ibα and von Willebrand Factor Complex using Molecular Dynamics Simulations

(Research field / theme)

Molecular dynamics simulation

Sameer Satish Deshmukh

Tokyo Tech, JPN / PhD

(Presentation title)

Distributed direct solvers for hierarchical matrices.

(Research field / theme)

Distributed LU factorization of hierarchical matrices

Yen Chen Chen

The U of Tokyo, JPN / PhD

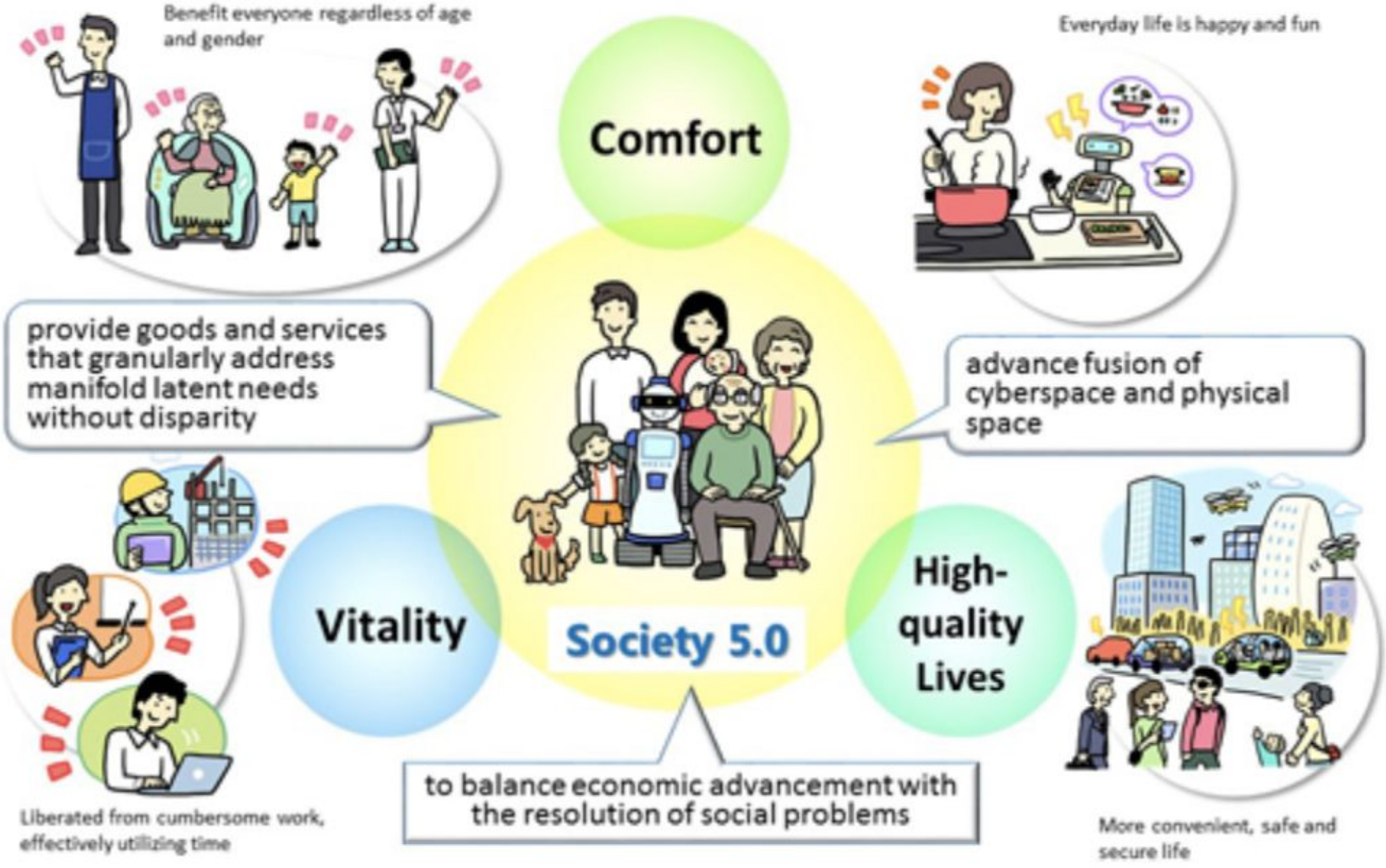
(Presentation title)

A Parallel-in-Space/ Time Method for Explicit Time-Marching Schemes

(Research field / theme)

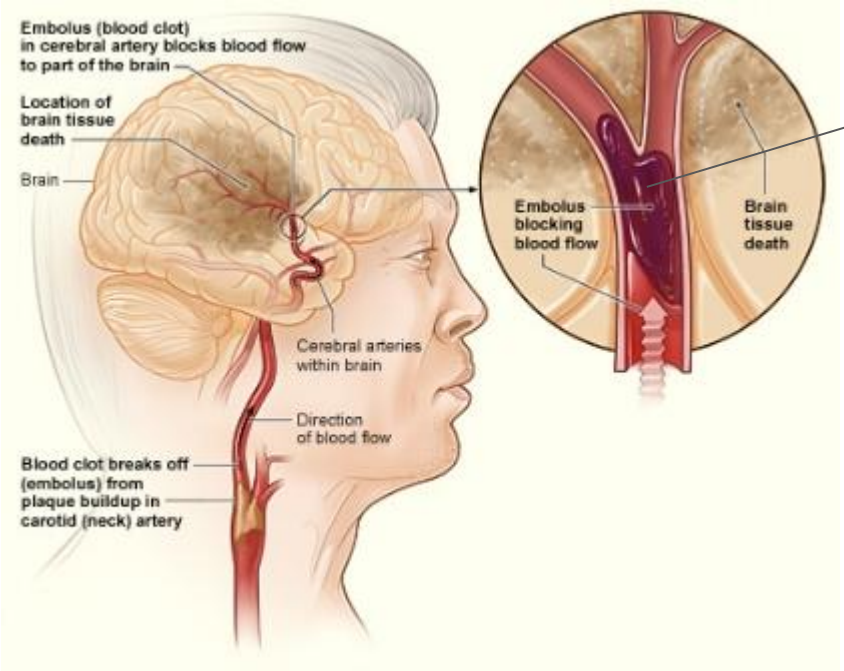
Parallel-in-Space/ Time Methods

Masamitsu

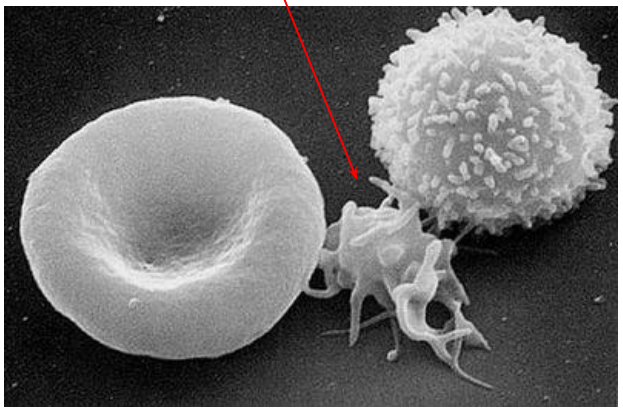

Benefit everyone regardless of age and gender
Everyday life is happy and fun
Comfort
provide goods and services that granularly address manifold latent needs without disparity
advance fusion of cyberspace and physical space
Vitality
Society 5.0
High-quality Lives
to balance economic advancement with the resolution of social problems
Liberated from cumbersome work, effectively utilizing time
More convenient, safe and secure life

Masamitsu

What is Stroke?



Thrombus is formed by Platelet



Stroke is a condition that affects the arteries leading to and within the brain. It is the No. 3 cause of death and a leading cause of disability in Japan. A stroke occurs when a blood vessel that carries oxygen and nutrients to the brain is either blocked by **Thrombus**.

Masamitsu

Prediction tool for stroke

Stroke happens suddenly in daily life. It is hard to predict precisely from medical data, because human body is very complicated.

We provide an AI-based tool for doctors to predict probability of stroke by combining **Molecular Dynamics, Computational Fluid Dynamics, Machine Learning and the power of Fugaku**.

The input data for prediction from patient test results, MRI image and blood pressure,etc.

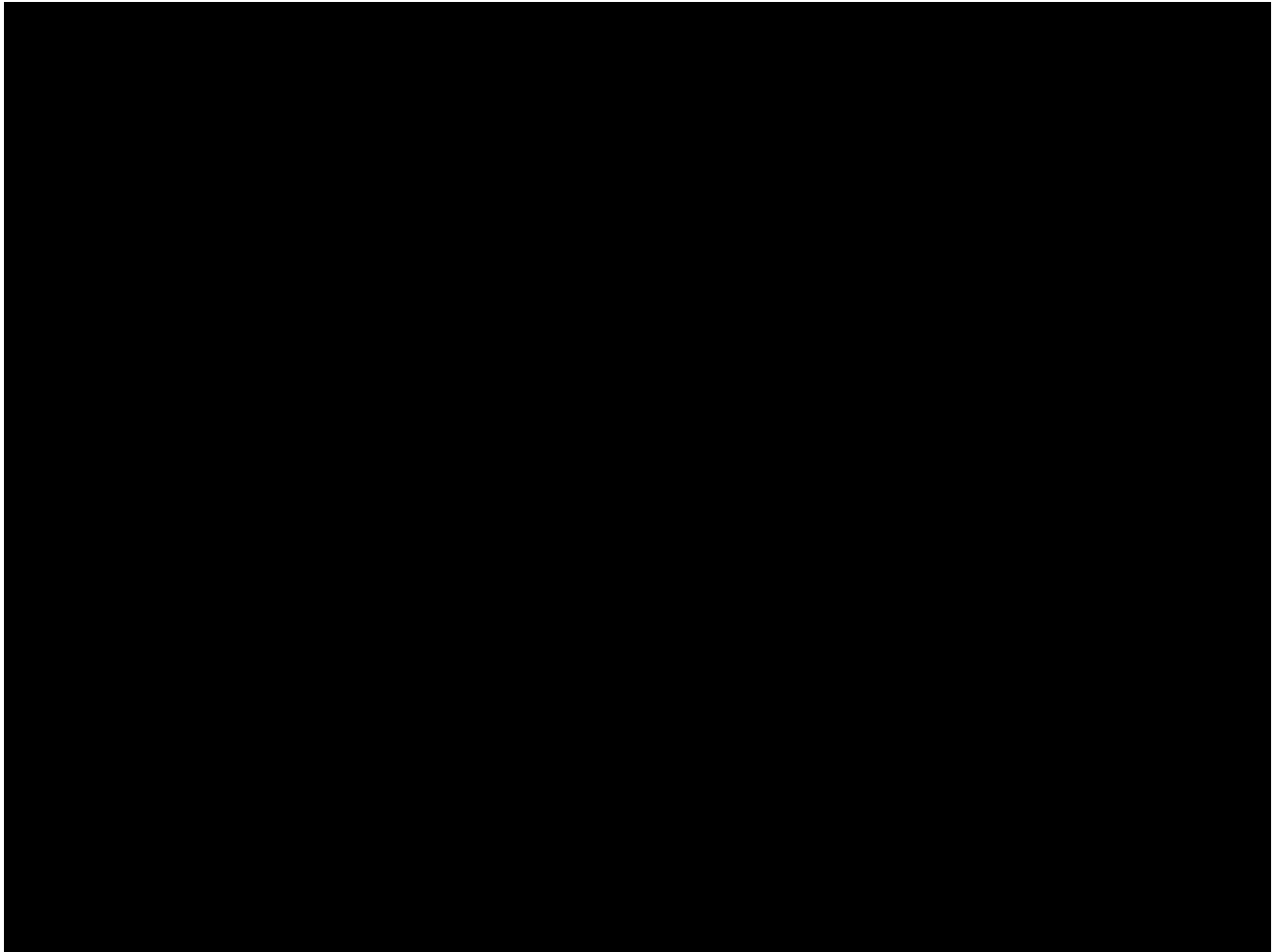
Masamitsu

Methodology

1. Thrombus formation accumulation by Molecular Dynamics
2. Machine learning interface
3. Computational fluid dynamics blood simulation
    a. Efficient matrix solver
    b. Parallel-in-time method
4. CFD based machine learning database for doctors

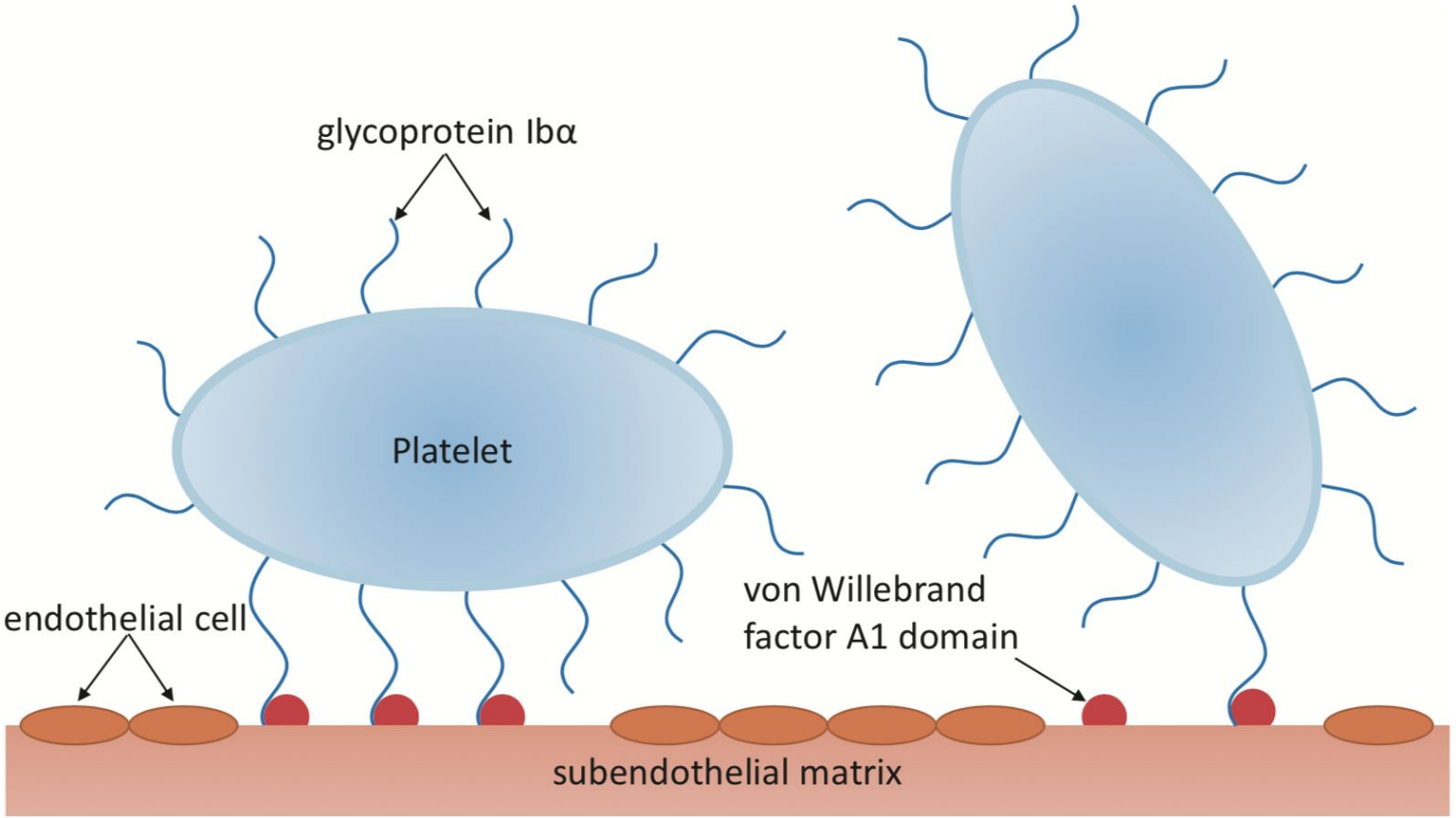
Masamitsu

Thrombus formation (platelet aggregation)



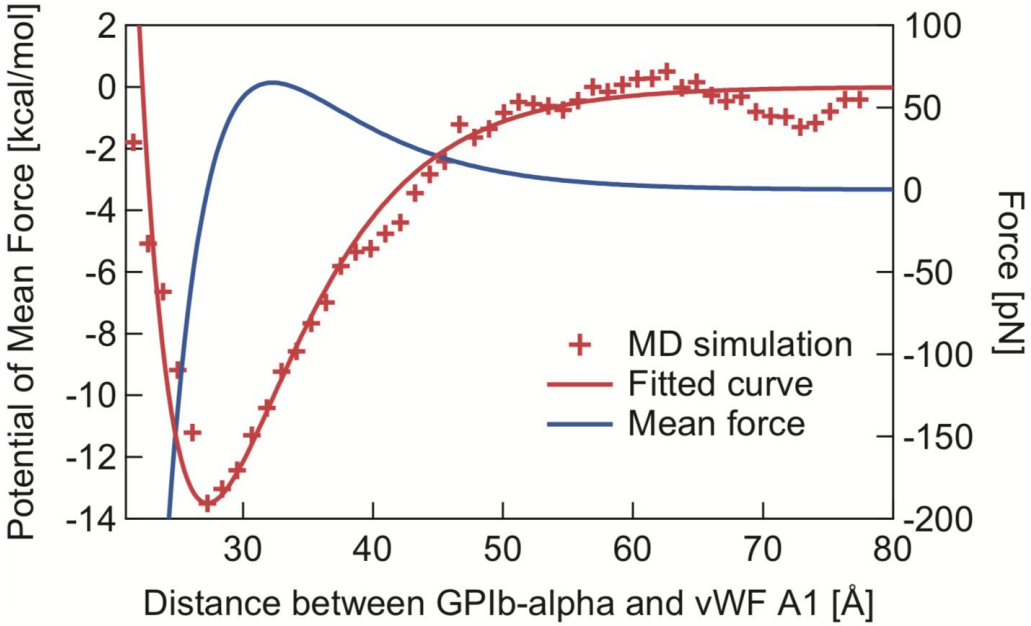
Masamitsu

Thrombus formation is occurred by protein interaction



Masamitsu

Thrombus formation is occurred by protein interaction

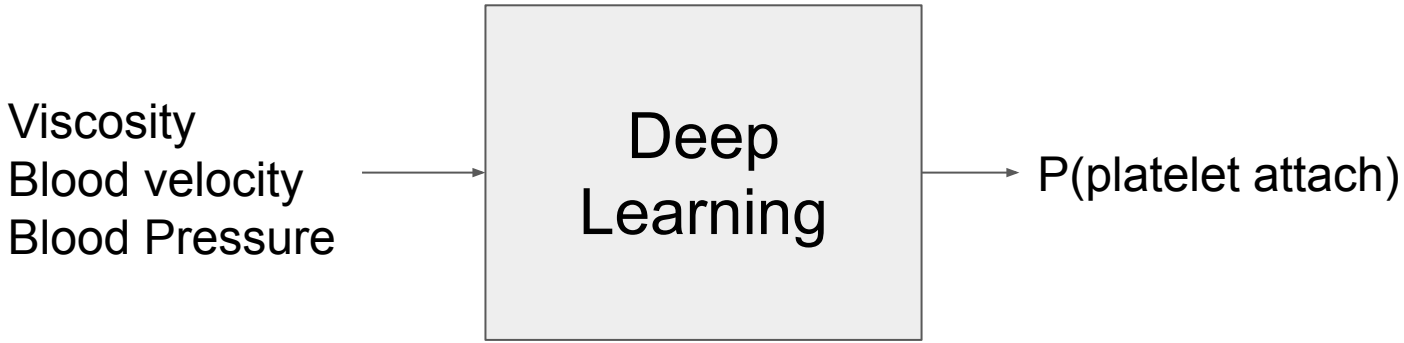


We will calculate the probability of the platelet attaching through MD simulation, in various parameters, viscosity, velocity and pressure changed.

Masamitsu

From Molecular Dynamics to CFD

- From the simulation data of Molecular Dynamics, we construct a machine learning interface that tells the attach rate of the platelet.

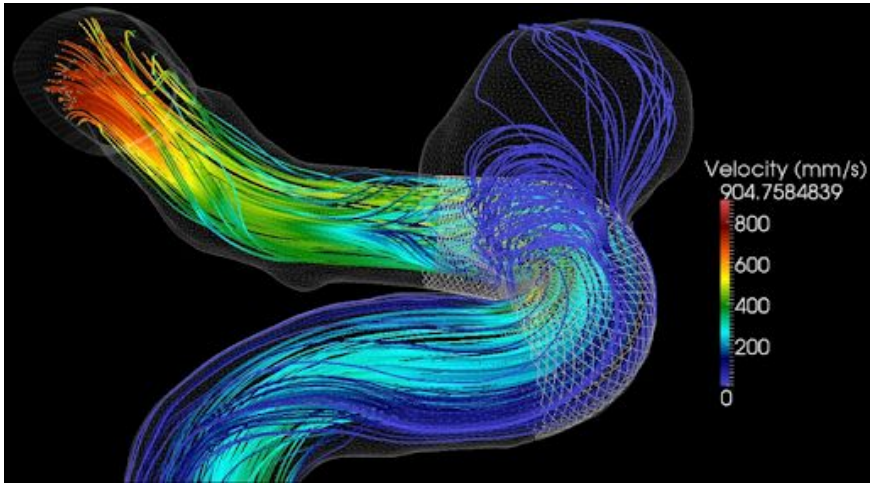


- From the platelet attach probability, we get the growth speed of the thrombus
- We expect that order of **100** datasets would be enough.

Yen

Blood fluid dynamics

Navier-Stokes equations can be numerically solved to obtain the **velocity and pressure fields** in arteries and veins.



Pressure Gradient

$$\rho\frac{\partial\vec{v}}{\partial t}+\rho(\vec{v}.\nabla)\vec{v}=-\nabla P+\vec{\gamma}\rho+\mu\nabla^2\vec{v}$$

Local Acceleration

Convective Acceleration

Body force term

Viscous term

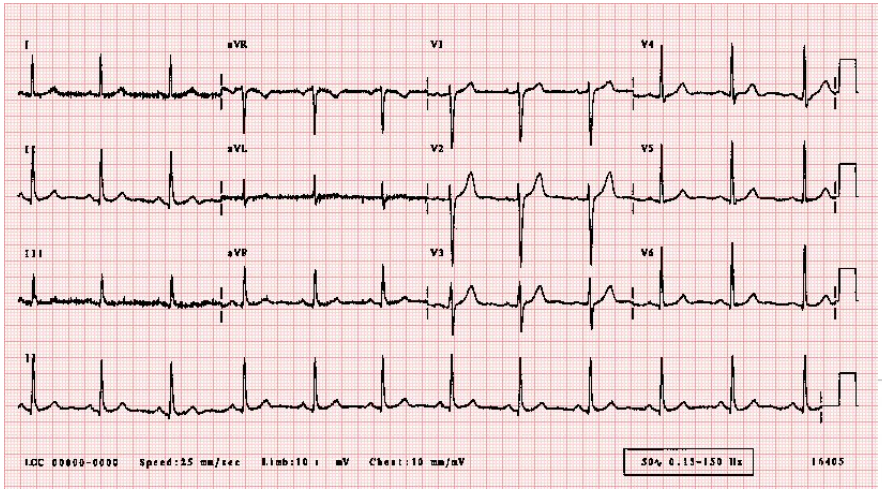
Problems: geometry definition
mesh construction
total simulation cost

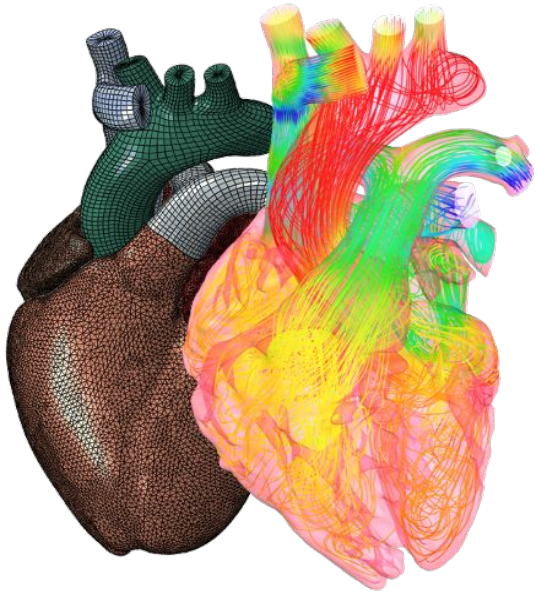
Sanji

Heart modeling

The heart acts as a pump. It is needed for blood circulation.

Its modeling is complex, but the research is advancing in this field





Sanji

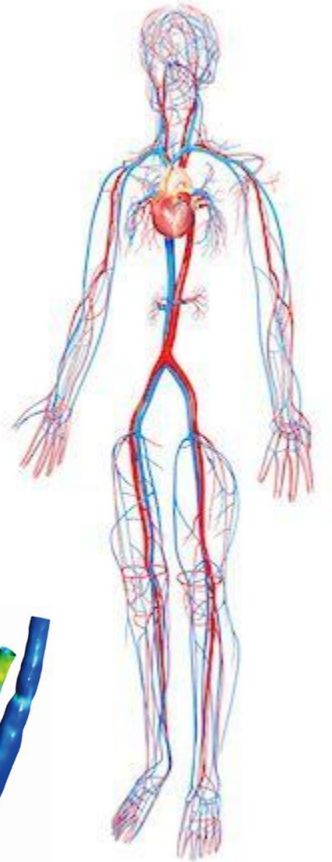
Mesh and geometry

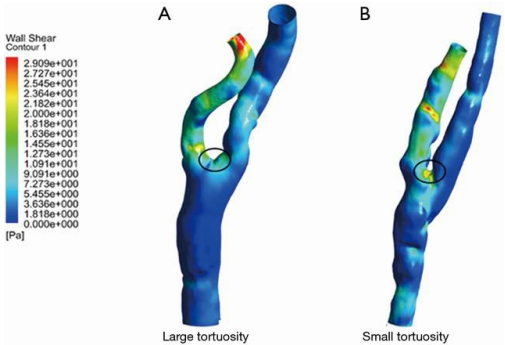
The geometry only accounts for the large arteries and veins, with a total length of 12 m.

N of cells: **1 x 10^8** (with AMR it can decrease even further)

N of CPUs: **~10^4** (Spatial parallelization saturation)

The stability condition involves the Courant number (it has to be lower than one). The relative time step is **2 x 10^4 s**. Total simulation time **10 h**.



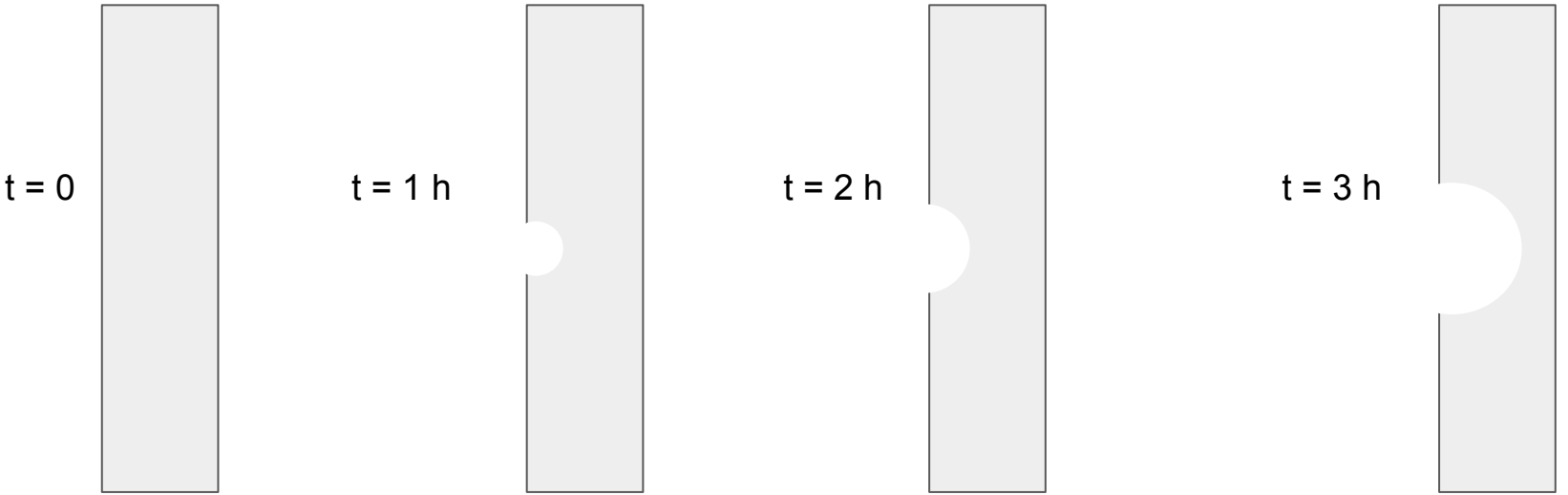


Sanji

Adaptive mesh for platelets accumulation

From the molecular dynamic simulation we obtain the **probability of particle attachment.**

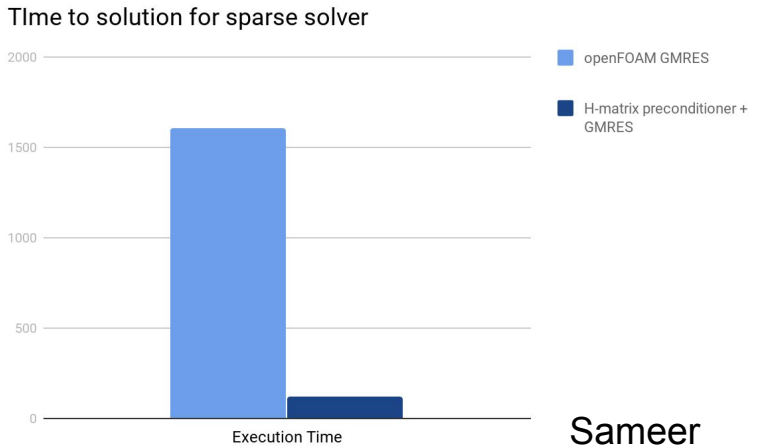
With this, we modify the geometry (at each time step) of the domain to account for the thrombus presence.



Sanji

Better convergence for the CFD solver

- The CFD simulation of the blood requires us to solve a large sparse matrix of the order 10^8 at 10^{-1} s per iteration.
- openFOAM GMRES would take about **10^8 seconds (about 3 years)**.
- H-matrix LU preconditioners along with parallelization can reduce the time to execute by **10 times (about 4 months)** and then more depending on number of compute resources.



Sameer

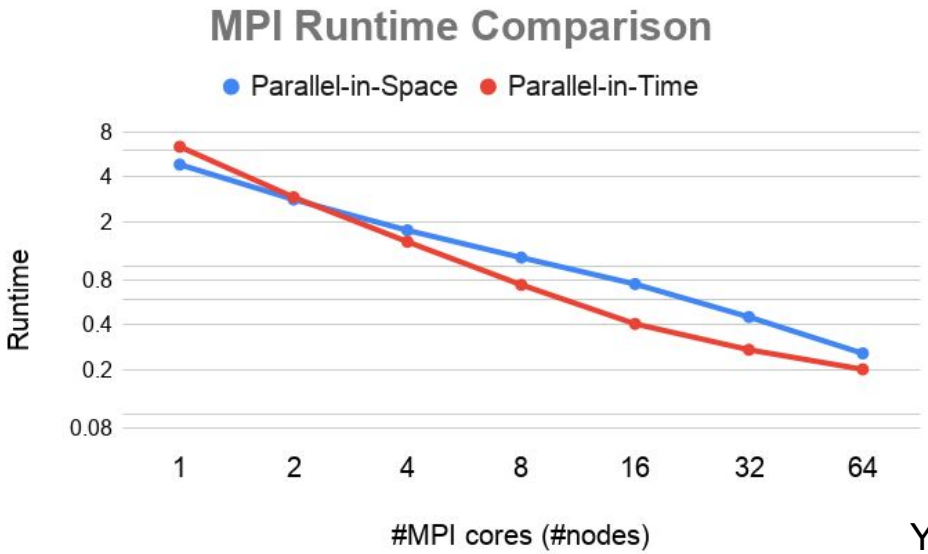
Using H-matrix LU factorization based preconditioners

The H-LU preconditioning changes the structure of the matrix and reduces the number of iterations for convergence. Approximation reduces time to compute.

Sameer

Parallel-in-Time acceleration

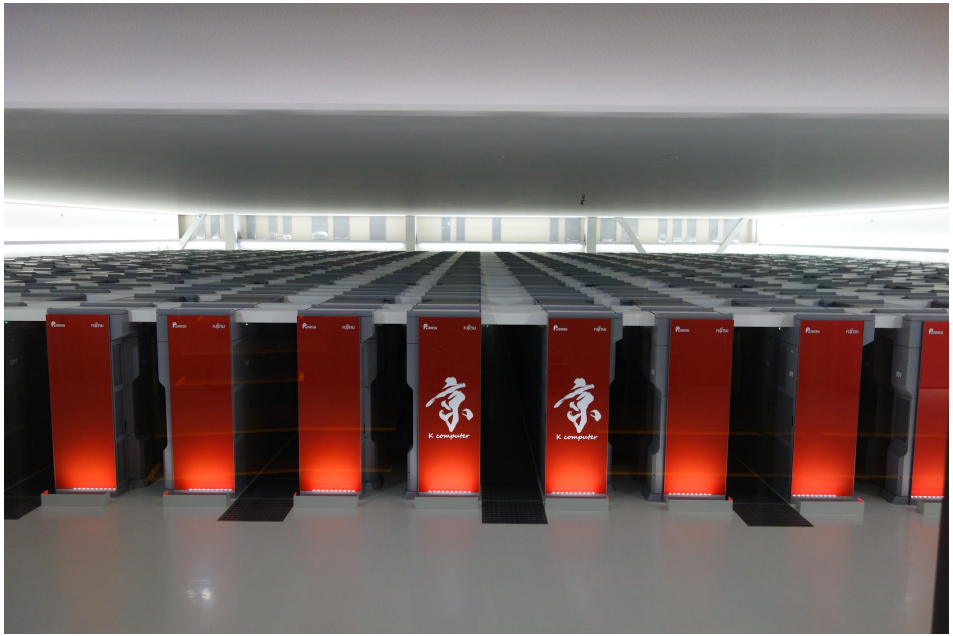
- Assuming we have enough computing power, it still takes 10^{-1} time per time step at saturation.
- By introducing Parallel-in-Time method to the solver, we can expect further acceleration.
- With some error tolerance, we could leverage similar parallelization with parallel-in-time method
- With 10^{6} CPUS, we could further accelerate the computation about **100** times



Yen

Using Fugaku for increased parallelization

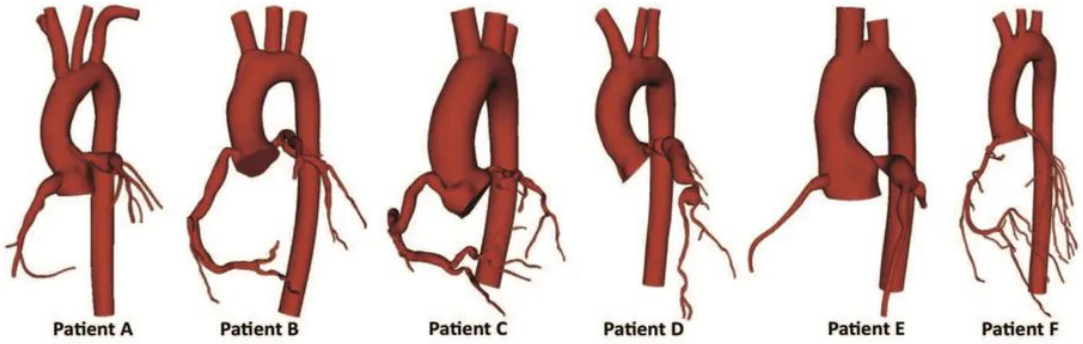
With Parallel-in-time method, we could further parallelize the problem and we expect that with **10%** of the Fugaku computation resource, we would be able to do a single calculation in **one day.**



Yen

Stroke prediction tool for doctors

- From the CFD prediction, we predict the accumulation speed of the thrombus formation given the patient information.
- From the prediction data, we could further build a Machine Learning model for doctors telling whether a patient would have a stroke.
- The parameters of the Deep Neural Network will be various factors determined by the simulation and other external factors.
- The depth of NN and number of parameters might vary depending on the detail we want to consider.



Prediction tool for stroke

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Yen