Finite Element Method Analysis in insilicoIDE

Hideki Oka[1], Li LI[1], Tatsuhide Okamoto[1], Takahito Urai[2], Takeshi Abe[1], Yoshiyuki Kido[1],Yoshiyuki Asai[3], Taishin Nomura[4]
[1] The Center for Advanced Medical Engineering and Informatics, Osaka University
[2]Intasect communications Ltd.
[3]Okinawa Institute of Science and Technology
[4]Department of Medical Science and Bioengineering, Osaka University

Abstract: insilicoIDE function is being enhanced to make the finite element method analysis available. The preprocessing window for morphology definition and the initial, boundary, constraint conditions and the material values setup window were developed. Preparing various primitives, we can build an arbitrary morphology. Also, external morphology file can be specified. Segment specification where the boundary conditions are imposed is able to be done visually. Numerical definition or the external file where the node values are stored is available for the initial/boundary conditions and the material definition. Solver of the finite element method is a general-purpose script based tool, FreeFem++. Primitive script library is pre-installed and the equation converter to the weak form type is also functioned. FreeFem++ script for a target insilicoML can be generated from insilicoIDE directly. Several examples for setting initial condition, boundary conditions and material definition are demonstrated.
Keywords: Physiome, Integrated Development Environment, insilicoIDE, insilicoML, Finite Element Method

1. Introduction

insilicoIDE is Integrated Development Environment for physiome biological modeling based on medlling description language insilicoML[1,2]. It can handle ODE, DDE, SDE and PDE. Here, we focus to a finite element method to solve partial differential equations by which complex morphology based problem can be solved.

2. Simulation flow

Typical simulation flow is morphology definition, mesh generation, define equation, set initial and boundary conditions, set material values, solve the equation and post-processing. Following this flow, insilicoIDE has corresponding menus.

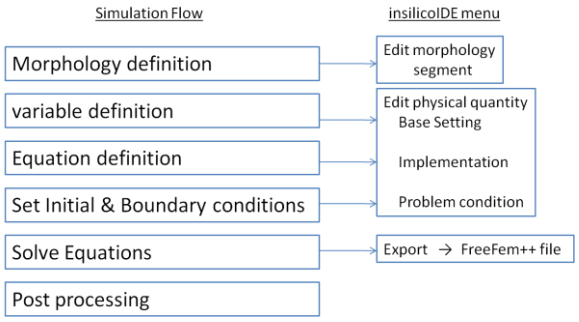

Fig. 1. Simulation flow and insilicoIDE menu

3. Morphology definition

To define target morphology, four methods are ready to use in insilicoIDE, Primitive, vertex, parametric and external. 2D and 3D basic primitives such as triangle, cuboid and sphere can be defined with parameters. Combining these primitives, complex structure can be built as CAD tools can do it. If morphology can be expressed by mathematical equation with parameters such as a spline function, "parametric" definition is suitable. Nodes and corresponding elements are assigned directly in "vertex" menu to build a complex structure when both methods are useless. "External" mesh file can be assigned if it is available. Fig. 2 is a insilicoIDE morphology definition window.

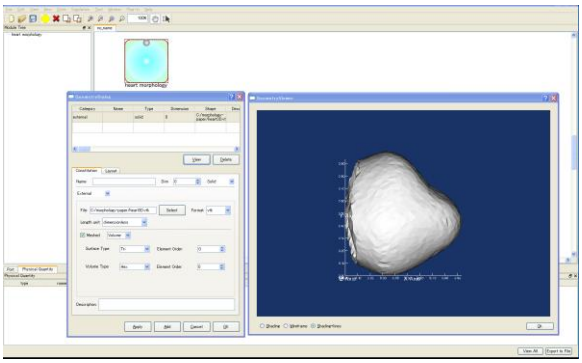

Fig. 2. Morphology definition window

4. Finite Element Method

To solve partial differential equations, we use a finite element method because of its adaptability to a complex structure and high numerical accuracy. Finite element method code is so complex especially for 3D case, we adopt a script based solver FreeFem++[3]. Only writing a simple script can do the finite element method simulation. It can greatly reduce the elaborate task to write a huge scratch source code or a long input data.

5. FreeFem++

If weak form equations are presented, FreeFem++ can solve any problems. Its generality is one of reasons why we adopt FreeFem++. We have developed inhouse FreeFem++ libraries, for example, morphology primitive function (.idp file) library. If target equation is given by a normal strong form equation, it is converted to a weak form equation automatically. Representative equations such as a Navier Stokes equation and solving algorithm are so complex that they are pre-installed in insilicoIDE. Only specifying problem equation's name, its equations' definition are automatically included into insilicoML.

6. Segmentation tool

Initial and boundary conditions and material values are typically space dependent. Target node and element assignment tool has

been developed. Mouse picking and rubber band selection can select nodes or elements on which above conditions are imposed. These nodes or elements are labeled per group by segment-id. Also, external files can be specified for both conditions and material. For primitives, default segments are predefined. User only specify the labels to set both conditions.

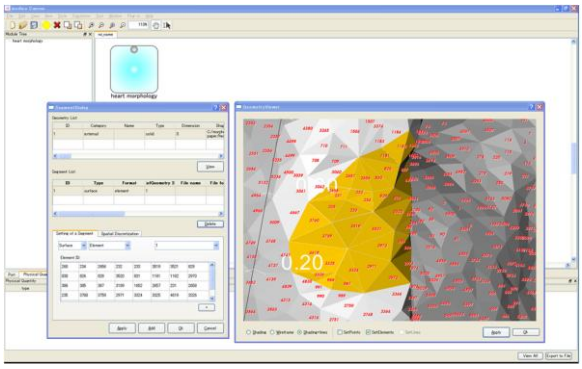

Fig.3. Segmentation tool

7. Example1 - initial condition -

Cardiac reentry simulation: Cardiac stimulus propagation was simulated by Fitzher-Nagumo model. Initial stimulus was applied to a part of surface elements. Then, another stimulus was added with a certain time delay. Such time dependent condition was described by an initial condition function. Excitement propagation shows a reentry phenomena.

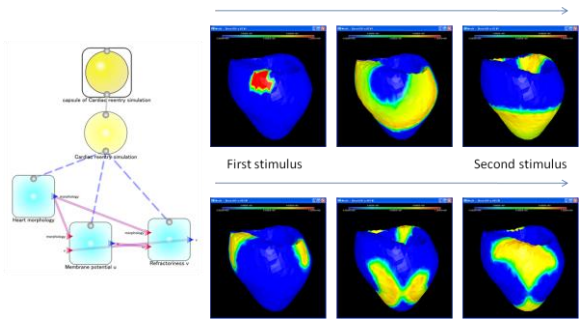

Fig. 4. Cardiac reentry simulation

8. Example2 - boundary conditions -

Thigh bone stress-strain simulation: Load force was applied to top part of a thigh bone and bottom part was fixed. Load was treated as a boundary condition and fixed position was a constraint condition. Elasticity equation was solved under these conditions. Stress component distribution was shown in Fig. 5.

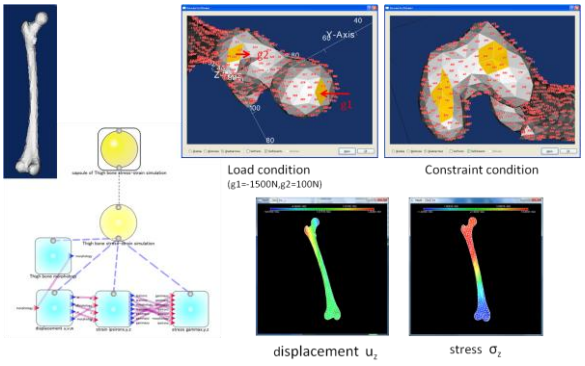

Fig.5. Thigh bone simulation

Blood vessel simulation: Blood fluid simulation was done imposing velocity and pressure boundary conditions on wall, inlet and outlet of the blood vessel. In this case, three boundary mesh files are constructed and each boundary conditions are applied to these boundaries through these mesh files.

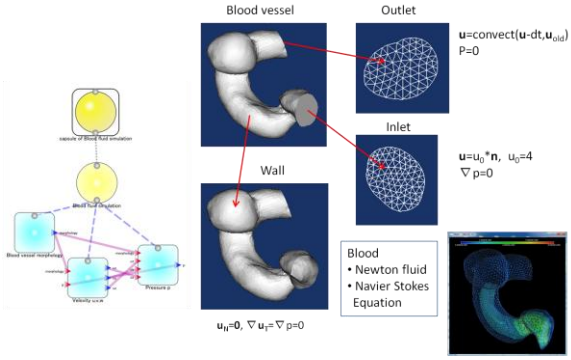

Fig. 6. Blood vessel fluid simulation

9. Example 3 - material definition -

Electric field in brain: Electric field in brain from a dipole current source was simulated (EEG problem). In this case, conductivity distribution is essential because white matter, grey matter, cfs, and skull bone have different conductivities. These conductivities are stored in each material files and insilicoIDE assigned these files for material definition. Giving time dependent vibrating current source densities of the dipole, electric field was calculated by Poisson's equation.

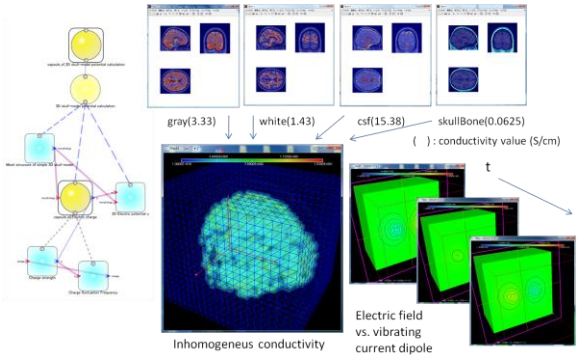

Fig. 7. Electric field in brain.

10. Summary

insilicoIDE is being developed adding new features. Advanced boundary condition such as moving boundaries, coupled simulation, multi-scale (time and space) simulation and parallel processing will be available in insilicoIDE.

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Reference

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[3] http://www.freefem.org