Software Engineering for the SimVascular Project

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Background

Stanford Research Computing Center

Manage and support more than

- 35 petabytes of data
- 2,000 HPC servers
- 40,000 CPU cores, 2,040 GPUs
- 13,000 user accounts

20 team members (two research software engineers)

- Help researchers transition their analyses and models from the desktop to HPC systems
- Manage a variety of compute clusters for various Stanford schools, departments, and/or labs

My background

- BS Computer Science (GaTech), PhD Biomechanics (Stanford)
- Visualization, Computational mechanics, Scientific computing, Biomechanics, Biophysics, Bioinformatics, Geometric computation, Structural biology
- Industry: Centric Engineering, Autodesk, Thermo Fisher, ...
- Academia: GaTech, Stanford (Vascular Surgery, SimBios)



Background

Marsden Research Group

Develops fundamental computational methods for the study of

- Cardiovascular disease progression
- Surgical methods
- Treatment planning and medical devices

Focus on patient-specific modeling in pediatric and congenital heart disease, as well as adult cardiovascular disease

Develops open-source modeling and simulation tools to enable clinical and basic science research

- **SimVascular** Interactive image-based modeling (C++, Python)
- **svSolver** Computational fluid dynamics solver (Fortran, C++)
- **svFSI** Fluid-structure interaction solver (Fortran)
- **svOneDSolver** Flow in deformable 1D hemodynamic networks (C++, Python)



SimVascular

Open-source image-based modeling application

- Initial release in 2007
- Rewritten in 2013 with NSF support
- Hosted on GitHub (<u>https://github.com/SimVascular/SimVascular</u>)
- 1,700 user and 4,386 unique downloads
- 100 citations in publications/abstracts
- Used in coursework for project-based learning
- Download installers from SimTK for MacOS, Ubuntu and Windows

Web-based documentation (<u>http://simvascular.github.io/</u>)

- Tutorial-based guides
- No user manual

User forum hosted on SimTK



SimVascular





Marsden research group - Cardiovascular Biomechanics Computation Lab

SimVascular Modeler

SimVascular software

- 300K lines of C++
- Depends on 12 externals packages (MITK, Qt, VTK, ITK, ...)
- Build installers for MacOS, Ubuntu and Windows using CMake

Implementation

- No software engineering best practices
- No error handling
- No design documents and no code comments

Software management

- No bug tracking
- No automated testing



Improving SimVascular

Implementation

- Adding implementation documents and code comments
- Replace C-like array data structures with containers
- Remove using object pointers when possible
- Implement error handling using exceptions
- Add unit tests

Software management

- Use GitHub Issues for bug and feature tracking
- Establish strict criteria for merging code
- Jenkins for automated testing
- Add component tests
- Scripting for manual testing of GUI and graphics



Education

Training for for students, post-docs and PI's

- Presentations
- Example code
- Resources

Git and GitHub for sharing and safely storing code

- Workflows: how to use Git in a consistent and productive manner
- Forking and branch strategies to isolate development
- GitHub Issues for providing a history of implementation decisions

Software development

- Software best practices (comments, code structure, etc.)
- Designing for extensibility and maintainability
- Setting lab software standards
- C++ and Python best practices



SimVascular Python API

Access SimVascular functionality using Python

- Add functionality not supported by GUI
- Prototyping new methods
- Automate parameter-based generation of models
- Testing core components (modeling, meshing, etc.)

Implementation

- Implemented in C++ using Python C API
- Define Python classes for all SimVascular tools: path planning, segmentation, modeling, meshing and simulation
- Execute scripts in GUI Python console or from the command line
- Visualize geometry using VTK



SimVascular Python API

"Test TetGen local edge (face) refinement.

from pathlib import Path import sv import vtk

Create a TetGen mesher.
mesher = sv.meshing.TetGen()

Load solid model into the mesher. home = str(Path.home()) file_name = home + "/SimVascular/DemoProject/Models/demo.vtp" mesher.load_model(file_name)

Set the face IDs for model walls.
mesher.set_walls([1, 2])

Set meshing options.
options = sv.meshing.TetGenOptions(global_edge_size=0.8, surface_mesh_flag=True,
volume_mesh_flag=True)

Generate the mesh.
mesher.generate_mesh(options)

Get the mesh as a vtkUnstructuredGrid. mesh = mesher.get_mesh()

Get the mesh surface as VTK PolyData.
mesh_surface = mesher.get_surface()





Challenges

Convincing people that good software is important

- Poor design and implementation
 - Produces fragile code that is not usable
 - Wasted time spent trying to understand and modify code
 - Short project life time
- Good software practices can make a big difference

Accountability

- How to enforce software policies
- Post-docs are a big problem

Leadership

- PI's must take an active role in managing software
- NSF needs to better monitor software coming out of grants



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Computing Resources

XSEDE Extreme Science and Engineering Discovery Environment

