

SimVascular Gateway for Education and Research

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ABSTRACT

Over the last two decades, science gateways have become essential tools for supporting both research and education. The SimVascular application is an open source software package providing a complete pipeline from medical image data segmentation to patient-specific blood flow simulation and analysis. With an ever-increasing user base of students, educators, clinicians, and researchers, the development group wanted a user-friendly web portal for users to run SimVascular flow simulations and to be able to support a large number of users with minimum effort and also hide complexity of using HPCs. This paper discusses how the SimVascular Science Gateway became a tool for students, educators, and researchers of all levels and continues to gather and grow a strong research community.

CCS CONCEPTS

• **Social and professional topics** → *Computational science and engineering education*; • **Computer systems organization** → **Cloud computing**; • **Computing methodologies** → **Simulation environments**.

KEYWORDS

SimVascular, Cardiovascular, Apache Airavata, Science Gateways, Solver

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1 INTRODUCTION

SimVascular is NSF- and NIH-supported open source software that is used to model and simulate blood flow in patient-specific anatomical geometries. It supports users from all over the world for applications such as cardiovascular disease research, medical device design, and virtual surgery. There are two main parts to the software: a) a front-end graphical user interface that is used to load medical image data and construct the patient-specific geometry (Fig. 1) and b) a finite element-based flow solver for performing high-fidelity simulations of blood flow in those geometries. The front-end interface can be run on Windows, Mac, and Linux operating systems even on the most modest personal computers and laptops [12]. The flow solver, on the other hand, often requires a high-performance computing (HPC) resource to produce reliable and accurate results. Simplifying access to and use of HPC resources for the SimVascular solver component using a science gateway [4] is highly desirable.

The SimVascular supercomputing gateway [14] was deployed in 2017 in collaboration with XSEDE Extended Collaborative Support Services (ECSS) [13] to support the growing number of classrooms around the country using the SimVascular application in their coursework. The gateway is deployed on the Science Gateway Platform as a Service (SciGaP) [7] with Apache Airavata [5] as the middleware. SciGaP is a hosted, multi-tenant service platform integrated with national, institutional, cloud, and private HPC resources. In addition to managing the execution of simulations on multiple remote HPC resources, the gateway provides federated authentication and user management [2] [9], a software application catalog [8], computational experiment/job sharing [6] and an admin module for gateway administrators to assist users.

2 THE SIMVASCULAR GATEWAY AS AN EDUCATIONAL TOOL

Students in academic courses in cardiovascular modeling use the SimVascular flow solver to run a simulation on a patient-specific

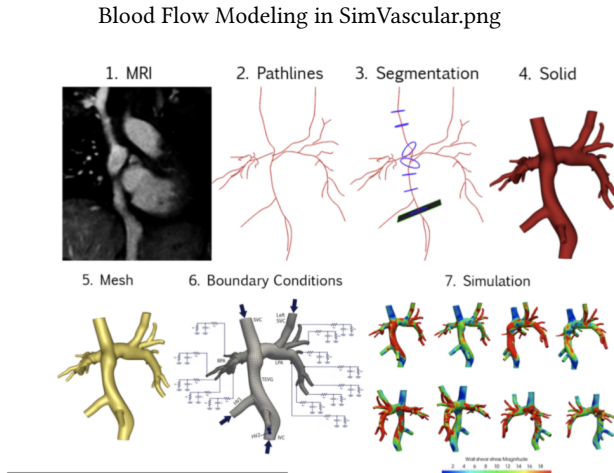


Figure 1: Patient-Specific Blood Flow Modeling in SimVascular produces high-fidelity, finite element-based simulations (7) based initially on patient MRI data (1) through several input preparation steps.

geometry, then analyze the simulation results to draw conclusions about the patient’s biomechanics. It has been successfully integrated at multiple institutions, including Stanford, UC Berkeley, UC San Diego, Purdue, Marquette, CSU Long Beach, and CSU Fullerton, among others (Fig. 2). The students in these classes mostly did not have exposure to or training in HPC resources.

The gateway’s initial requirements were that it be easy to use through a web interface, provide access to all of the HPC resources needed to run the flow simulations, and provide safeguards to prevent any user from accidentally depleting the shared XSEDE allocation. The SimVascular gateway provides a web interface for the students to upload their simulation files, select the cluster settings, run the simulation, and download the results. Users are able to make an account on the gateway using their institutional login information through CILogon [2], which provides secure and robust user authentication. The gateway uses Apache Airavata’s group management features to manage a classroom as a group within the gateway. This allows administrators to manage default settings for computational resource properties such as number of nodes, CPUs, and computational time for jobs. Managing users within the groups is the responsibility of an assigned group member, and group members can share their gateway work with other group members. Most educational users will run three to seven simulations with relatively modest computational cost as part of their course requirements, so the group management feature can be used to prevent such users from accidentally requesting too many hours and depleting the allocation. The gateway supports multiple XSEDE allocations at a given time, so different allocations can be assigned for different user groups.

Educational allocations from XSEDE provided all of the computational resources needed for the students without any downtime. Because of the large number of educational users with access to the gateway, it is much more difficult to train and supervise all of the users in proper use of an allocation. The ability to place users

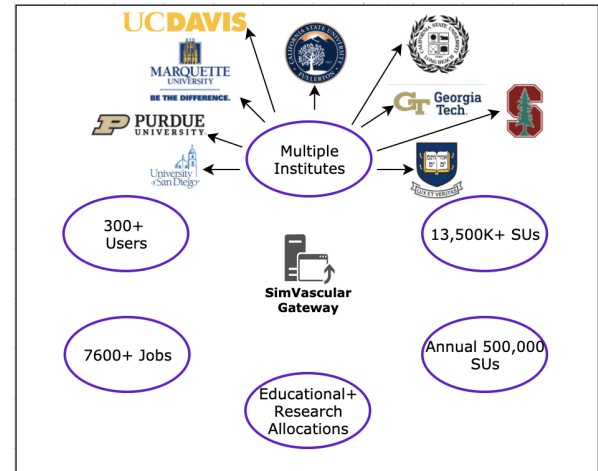


Figure 2: The SimVascular Gateway in Numbers

in groups with restrictions provides a safeguard for administrators to ensure that the computational allocation’s use is maximized.

3 SIMVASCULAR GATEWAY AS A RESEARCH TOOL

Compared to educational users, research users have much larger and complex computational requirements. Their goal in running simulations is to perform novel research on engineering or clinical problems, with computational demands far greater than an educational simulation. These simulations have to be run on a much finer mesh, with much more complex boundary conditions, and sometimes with additional physics included. It is common for a single simulation of a research user to be at least one order of magnitude more costly than an educational user in terms of computing hours. Research users may also run hundreds more simulations than an educational user. We have a couple of research users who have run more than 1000 simulations since the research usage of the gateway was started in January of 2021. We can place our research users into groups with fewer usage restrictions than our educational users with very liberal computational resources.

Naturally, the gateway administrative support needed for research users is different from the educational user. Since research users will be using the gateway much more, the issues that they typically run into involve needing larger computational resource power and more storage capacity for their output files. Research users also require longer-term support for their research projects, which can take months or up to a year to complete, and they may also require support in using more advanced features of SimVascular that the typical educational user does not use.

The gateway has a few features that are more ideal for advanced research users than for educational users. The research users have the option of sharing their computational allocation and computational inputs and outputs with their fellow researchers. This is particularly useful when working on common research problems. Advanced researchers’ jobs are computationally very expensive as they need a lot of resources, so the gateway provides checking of

output files as they are generated, while the job is running, so if it is not as expected the users can start over. This saves resources compared to waiting for jobs to complete to check the outputs. The gateway admins can also have solvers restricted by user groups and have them dedicated for advanced researchers or even for specific research groups or projects. This way, users can focus on their work with minimum to no disturbances from other gateway users. These custom solvers can be deployed as separate applications within the gateway.

4 USAGE EXAMPLES AND USER TESTIMONIALS

The SimVascular gateway is in a steady path, growing in terms of users, use of computing resources, number of jobs, number of service units (SUs), etc. (Fig. 2). There are many success stories that have bloomed through the years of the SimVascular gateway being in production. They speak in volumes in showing how important the gateway is for both educational and research users.

The XSEDE research allocation's current PI (Tran) was an educational user at the early stages of the gateway. All of the students in that class were able to run a flow simulation of blood flow for their final projects thanks to the gateway, which was the first time most of them had ever run a simulation with that level of detail and complexity. But the introductory HPC knowledge that they gained from using the gateway (i.e., concepts of parallel computing, scheduling, and processing files) led to some of them pursuing more training and usage of HPC resources.

As the gateway gained users from courses at different institutions, it started to garner interest from students outside of engineering. One example is students from the Stanford School of Medicine, who started using the gateway to support clinical research. Because blood flow is so difficult to measure and observe, researchers and clinicians from the engineering and medical communities are interested in the ability to model blood flow for their projects, yet do not have the background to understand all of the technical details of HPC. The gateway provides an excellent opportunity to reap the benefits of running flow simulations on an HPC resource without extensive training in computational engineering and would facilitate collaborative research across many disciplines.

The gateway has also been instrumental in enabling the completion of student theses and dissertation work, especially when the students do not have much time to complete their projects. For example, a typical MS thesis student in the Mechanical Engineering department at CSU Fullerton has only one to four semesters to finish their project in order to graduate on time. During this time, students are typically also taking full course loads and sometimes working a job on the side. There is not much time to spend on training, so usually the aim is to maximize the student's time as much as possible by teaching them only the most essential skills and knowledge needed to get the project done.

Another case of the gateway enabling research was at Marquette University in the group of Dr. John LaDisa to support masters, doctoral, and postdoctoral research. The gateway was used to conduct research involving computational modeling of patients with anomalous aortic origin [10] [11], fractional flow reserve in patients with

multi-vessel coronary disease [3], and patients who have undergone aortic reconstruction as part of the Norwood procedure [1], as well as other masters, dissertation, and postdoctoral work. The gateway allowed groups fast and easy access to the HPC resources they needed to complete their research and run simulations in a timely manner. This was especially helpful during periods where HPC resources and personnel were not available locally. Without the gateway, the same amount of simulations would have taken months as opposed to weeks. The group at Marquette also noted how technical support staff responded to questions and resolved issues quickly. Several graduate students from this group have since moved on to different institutions as postdoctoral researchers and continue to work with the gateway for their research.

5 FUTURE DIRECTIONS FOR THE GATEWAY

We plan to develop the gateway further to add additional features, improve the user interface, and add additional training resources based on feedback we have received from our users. We wish to improve the web interface to make it more intuitive. We commonly hear that when a simulation fails, the error messaging is not particularly helpful or actionable to the common user. Enabling actionable and meaningful messages for gateway users is in the pipeline for implementation. Another feature to be added is automated post-processing of simulation results on the gateway. Currently when a simulation finishes on the gateway, the user is required to download the raw simulation result files to their personal machine, where they must perform additional processing before they can view the results. Also, some of our research users run hundreds of jobs at once with small variations in the boundary condition parameters, so adding tools on the gateway where they can submit arrays of jobs would improve their experience.

Another major area where we would like to improve the gateway is in adding extensive training materials on the website since we would like to open the gateway more broadly to local and international users. To support these users, we need to develop comprehensive tutorials and training resources that will teach them how to run simulations on the gateway, how to use available features such as sharing, using their own allocation, etc. We plan for these to be in the form of interactive text tutorials that are linked directly on the website as well as video tutorials that show users the process step-by-step.

SimVascular currently has more than 6000 unique users from all around the world who use it in the classroom to support learning of cardiovascular biomechanics or to perform novel research. We would like for SimVascular to be used as a tool for industry and the clinic as well. When we release the SimVascular gateway for public use, we plan to place users into a new "trial" group that will let them try out the gateway in a limited capacity. Once the user proves that they can use the gateway responsibly and have clear and focused research goals, they can be moved to a suitable allocation by the administrators. These users will be required to share any publications that they produce with the gateway's resources. Tracking the publications that result from use of the gateway is important for assessing its impact on producing novel research in our community.

To ensure the gateway is maximizing its use among the several community of users it supports, we plan to form an administrative board to discuss future directions and address further improvements and any new feature implementations with the gateway. The board will consist of PI's, staff, and power users who have been instrumental in the deployment and maintenance of the gateway. The board will be finalized and formed by mid-2022 and will be at the helm of taking the gateway to the next level for its growing user community.

6 CONCLUSION

The SimVascular gateway started in 2017 as an educational tool allowing access to HPC resources to complete course projects. Since then, the number of students and courses that use the gateway grew, while support for research users expanded. Being used by students with well-defined use cases and adding value to their education and research was a great recipe for a successful gateway. This was an early advantage of SimVascular gateway and catered for its rapid growth. These experiences can be useful for other potential gateways looking to get started or grow. This allowed the gateway to be live-tested early with the exact group of users it was targeting and their feedback was essential in ensuring the experience was as smooth as possible. Many of these students continued their research in the field after the course, and a gateway from a hosted platform such as SciGaP provides them with the resources and support they need.

The continuous availability of compute resources was made possible through the XSEDE Resource Allocation System (XNAS) process and XSEDE ECSS support was essential for the gateway project. They provided the technical support necessary to bring the gateway into existence, and their continued support is instrumental in the maintenance and growth of the gateway.

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