

### Featured Application:

## BioSim: Bio-electric Simulator for Whole Body Tissues

**ABSTRACT:** This application is designed to simulate the response of a "whole body tissue" model to potential/current stimulus through direct electrode contact. The Electrical and Computer Engineering and Office of Computing and Communications Services departments at Old Dominion University are using SURAggrid to grid-enable this application to utilize concepts such as workflow and virtual data methods. The Bio-electric Simulator, which is both computation and data intensive, has been demonstrated to scale with the number of processors and can thus benefit from the accessibility to the additional computational resources of SURAggrid.

### Understanding the Science

Electrical stimulation of the central and peripheral nervous system has a variety of diagnostic and therapeutic applications. An important first step in accurately predicting the bio-response to an electrical stimulation is the development of realistic and accurate numerical models for quantifying the currents and potential induced electrically within whole-body systems. The Bio-electric Simulator for Whole Body Tissue models (BioSim application) is used to perform numerical simulations of electro-stimulation of tissues and full body bio-models [1]. Response to electrical stimulus and the resulting potential distribution within the bio mass is very dynamic and is dependent on several factors. These systems are very complex and consist of a multitude of tissues, organs and sub-components with diverse properties. Researchers of electrical stimulation at Old Dominion University (ODU) analyze the measurement data from a complex set of variables with simulation models that use simple and efficient numerical implementations. Based on the LU decomposition method for solving a system of linear equations, these implementations for BioSim were developed for execution on distributed memory architectures such as those available in the SURAggrid environment.

### Application Characteristics

Whole-body simulation models are mapped onto a mesh by placing the points that form the outline of the system onto the lines of the mesh. For accuracy, whole-body simulation models must be discretized into a very fine-grained mesh and this can lead to a very large number of points on the mesh, especially for a three-dimensional entity. Processing a data set of millions of mesh points creates prohibitively large requirements for system memory and computation times. To address this problem, ODU researchers have demonstrated that BioSim scales well with the increased computational resources of distributed systems such as high-performance compute clusters. By grid-enabling BioSim and deploying it in the SURAggrid environment, ODU's

researchers have gained access to the HPC clusters that are part of SURAggrid's collective resources and have increased their ability to process the mesh point data in their large whole-body model simulations. LU decomposition in BioSim is performed with SuperLUDIST [2], a general-purpose library for the direct solution of large, sparse, non-symmetric systems of linear equations on high performance machines. SuperLUDIST has to be preinstalled on each resource based on the availability of compilers and linear algebra routines. BioSim also uses METIS [3] libraries for data reorganization.

### SURAggrid Deployment

ODU's work to grid-enable BioSim is a joint effort between their department of Electrical and Computer Engineering and the Office of Computing and Communications Services. In addition to deploying BioSim on SURAggrid, ODU has dedicated a four-node compute cluster, Mileva, to SURAggrid. Mileva has served as a staging platform for BioSim's deployment on other SURAggrid resources and also functions as a gateway for ODU's users to access SURAggrid's collective resources. For the latter purpose, ODU has established an X.509-standard based Certification Authority (CA) and cross-certified with the SURAggrid Bridge CA. User accounts, compatible with the ODU Unix environment, are created on Mileva for ODU grid users. These users are then given a SURAggrid account by ODU's SURAggrid User Administrator. In the absence of an ODU cross-certified CA, BioSim users would need to have local accounts created for them on each SURAggrid resource they want to use. ODU's cross-certified CA thus makes SURAggrid resource access simpler for BioSim users as well as for SURAggrid users at other institutions that want to run their applications on Mileva. Management of authorization to Mileva is based on group membership. User accounts created in the SURAggrid centralized user management system can also access Mileva and are synchronized on a timely basis. Mileva also provides MyProxy services for SURAggrid Portal<sup>1</sup> users.

<sup>1</sup> <https://gridportal.sura.org/gridsphere/gridsphere>

## Grid Workflow

To date, BioSim is grid-enabled in that it is being used to run multiple, large and computationally intensive jobs both independently and simultaneously on numerous SURAGrid resources. Before submitting their jobs, BioSim researchers manually check the SURAGrid portal to determine which resources have the smallest load and are available at a given time. BioSim researchers can then use the command line and GSISSH or SSH to logon to remote resources, generate proxies using grid-proxy-init, transfer files with globus-url-copy, and submit jobs using the Globus job manager. Alternately, users can access the SURAGrid Portal to carry out the same activities. To use the portal for their jobs, BioSim users create proxies with their user certificates by using the MyProxy utility either at the command-line (myproxy-init) or a Java MyProxy upload utility. Once the proxies are uploaded into their SURAGrid portal account, the user is able to use the portal's file transfer and job submission GUIs. In both the approaches, the Globus job manager will forward the jobs to the local resource manager and scheduler (e.g., LSF, PBS, SGE) installed on the SURAGrid resource. Job output is stored in text files and visualized using MATLAB®.

The project team sees their current use of BioSim on SURAGrid as their first stage of grid-enabling BioSim. Even though they're presently carrying out some application workflow steps manually, ODU researchers are making significant headway on their initial grid-enabling goal - to test the scalability of BioSim on large compute clusters with hundreds of processors and fast interconnects (e.g., InfiniBand®, Myrinet®.) In the next stage of grid enabling BioSim ODU will modify BioSim so that it will make use of the SURAGrid portal for data and job management and, when fully grid-enabled, BioSim will be able to automatically detect the best available resources and dynamically manage jobs. The ODU project team is currently investigating various methods for grid-enabling BioSim, in particular, Java CoG Kit, MPICH-G2 and Grid Application Toolkit (GAT) are being evaluated for their potential to perform resource detection, data transfer, job staging and clean-up.

As one of the first production applications to fully exercise SURAGrid's access management infrastructure, ODU found their biggest challenge in BioSim's grid deployment to be integrating their newly created campus CA and user accounts into the external grid trust fabric. Since SURAGrid's flexibility enables both SURAGrid BCA-cross-certified and non-cross-certified institutions to participate, providing BioSim user access through several newly upgraded SURAGrid authentication and authorization features was not trivial. ODU's efforts in this area have not only helped pave the way for future quick and smooth application grid-deployments on their own campus, they've provided SURAGrid with the necessary collaborative testing of its infrastructure that is already

benefiting other SURAGrid users and will continue to do so in the future.

## Lessons Learned

While the advantages of grid computing to applications like BioSim are significant, grid computing should not be considered a simple, straight-forward problem. A considerable amount of time and effort needs to be invested in grid-enabling an application, especially in finding the right expertise in the functional domain, along with computational and grid skills. In order to ensure an appropriate cost-benefit ratio, applications being considered for grid deployment should be considered in detail for suitability.

## Conclusion

Though some of the data errors inherent to real-world experiments for electrical stimulation of bio mass can be minimized, the prohibitive sizes of computational models can make numerical simulations arduous. ODU's grid enabling of BioSim and its deployment on SURAGrid is easing the burden of these simulations by helping them harness the power of compute resources they might otherwise not have access to. ODU researchers will continue their development of grid-enabled, multilevel-models of both larger scale and greater detail, such as the rat models with a 1-mm spatial resolution that they have successfully developed and tested on 32-node clusters. In addition, the project team at ODU will also use BioSim as a prototype to demonstrate the potential advantages of grid computing for numerous other computationally intensive applications in use on the ODU campus and beyond.


## References

- [1] A Mishra, R Joshi, K Schoenbach and C Clark, "A Fast Parallelized Computational Approach Based on Sparse LU Factorization for Predictions of Spatial and Time-Dependent Currents and Voltages in Full-Body Biomodels", IEEE Trans. Plasma Science, August 2006, Volume 34, Number 4.
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- [3] G. Karypis and V. Kumar, "A fast and high quality multilevel scheme for partitioning irregular graphs", SIAM Journal on Scientific Computing, 1999, Volume 20, Numer 1.

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 SURAGrid is developing an infrastructure for access to heterogeneous resources and support for a dynamic and diverse application set.

For more information, or to join SURAGrid:

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