

Simbios R01 Collaborations: Process and Content

Simbios Executive Committee

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Updated 01/15/2013

Process and Schedule

In order to track requests for collaborations and to have information necessary to prioritize activities, the Simbios executive team has designed a process for managing collaboration requests. This process can be summarized here:

1. **Contact Simbios investigator (2 months prior to the submission deadline):** A potential collaborating investigator contacts a Simbios PI (listed above) with an indication of interest in Simbios collaboration.

Available resources: A summary of Simbios research and development activities, active areas of research interests, and current driving biological problems are available for download from Simbios' collaboration page (<http://simbios.stanford.edu/collab.htm>). This summary is suitable as a starting point for the summary required with R01 applications, as described in [PAR-12-001: Collaborations with National Centers for Biomedical Computing \(R01\)](#). It is recommended that the summary be modified to clearly describe the precise nature of the collaboration with Simbios or to describe the collaboration elsewhere in the proposal.

The collaborating grant process document (that you are reading) is also available for download from the Simbios' collaboration page (<http://simbios.stanford.edu/collab.htm>). It summarizes the process and provides a discussion of the general types of collaborations that are possible and how they fit into the Simbios plan.

2. **Submit draft of "specific aims" (1 month prior to the submission deadline):** The potential collaborating investigator should then send a 1-2 page draft of proposed "specific aims" for the research to be conducted to Simbios. This should also contain a summary of the intellectual and other resources (software/hardware) at the collaborating institution, the expected resources required from Simbios for the collaboration, and the expected additional resources for the proposed collaboration that will be requested by the potential collaborating institution.

3. **Proposal review by Simbios (1 month prior to submission deadline):** The Simbios executive committee will read the proposal and explore potential interactions, resources required, and scientific merit and impact with the collaborating investigator.
4. **Simbios provides a letter of collaboration:** The Simbios executive committee will determine the fit to Simbios goals and write a letter of collaboration for the collaborating investigators' proposal.

Types of Collaborations

The R01 program outlines a number of possible interaction types with NCBCs, and we list and expand on them here. Contributions of algorithms and data types should be delivered as self-contained libraries with appropriate documentation. The Simbios software is hosted at and disseminated from <https://simtk.org>.

1. **Extend the application of existing Simbios efforts in the same biological realm:** We are currently focusing on neuroprosthetics dynamics and drug target dynamics. In the past, we have studied RNA folding, protein folding, myosin dynamics, neuromuscular dynamics, and cardiovascular dynamics. We welcome collaborations in closely related areas where existing technologies can be directly tested with little modification.
2. **Adoption of our APIs:** We have released three APIs and welcome collaborations that utilize them. These collaborations could be at an algorithmic level or could focus on the use of the code to solve a particular biological problem. Our APIs include:
 - [OpenMM](#) – an API for molecular dynamics, designed to take hardware acceleration via Graphical Processor Units (GPUs) into account. We have incorporated this API into GROMACS, CHARMM, and TINKER, have developed an AMBER (Sander)-compatible interface to this API, and are actively seeking collaborators to incorporate this API into a wide range of additional Molecular Dynamics (MD) codes.
 - [OpenSim](#) – an API to simulate the movement of musculoskeletal structures. The API enables individuals to extend and customize the OpenSim application, including adding new components to a model, creating new types of probes to extract values from a simulation, and developing new types of analyses. We welcome collaborators who leverage this API to create new algorithms or workflows that help solve a particular biological problem.
 - [Simbody](#) – a high-performance multibody dynamics API that delivers accuracy suitable for scientific and engineering applications with real-time interactive capabilities suitable for virtual worlds and games. We have used it for internal coordinate modeling of molecules and for coarse-grained models. Simbody has also been used for neuromuscular models of human gait and for robotics applications. We are actively seeking collaborators to incorporate this API into other applications, particularly those for biosimulation.

3. **Introduce new models and other data into the Simbios capabilities:** We are interested in sharing data and models produced by other groups, as part of a dissemination repository.
4. **Develop basic relevant algorithms.** We are interested in breakthroughs at the basic algorithmic level that will help facilitate faster or more accurate simulations at any scale, as well as multiscale simulations. We are also interested in algorithms that can be significantly accelerated using GPUs, which has become one of our focus areas for Molecular Dynamics.
5. **Provide applications that can be downloaded from Simtk.org.** We are interested in providing applications (using novel models, methods and algorithms) that end users (scientists and clinicians) can download from Simtk.org and use in their research.
6. **Develop ways to perform data mining and analysis of Simbios output.** We are interested in methods to analyze simulations, visualize them, and pull out useful new biomedical knowledge.
7. **Run experimental projects to be additional driving biological problems.** We are currently focusing on two biological application areas. We would welcome collaborations that introduce new biological areas, and extend and test code we developed for our previous application areas to new areas.

Resources

Simbios resources are currently devoted to infrastructure development and research support for our driving biological problems. Costs for new collaborations, therefore, should be built in to new applications. Subcontracts to Simbios investigators are permitted, if they can be justified.

Simbios is able to provide the following collaborative resources as part of its core mission:

1. Stable project hosting environment on Simtk.org --- this includes consultation on setting up and managing your project on Simtk.org, source control (using subversion, see <http://svnbook.red-bean.com> and <https://simtk.org/cvs2svn.html>), download statistics, bug tracking, daily backups, mailing lists, wikis, and more.
2. Consultation on how to submit new computational capabilities, models, and datasets to Simtk.org as part of your project.
3. Consultation on how to engineer software to interact with Simbios software offerings, including how to address multiplatform build, testing, download and installation issues.

Code and Data Sharing

Simbios adheres to the code and data sharing rules specified in the RFA. Collaborators should ensure that they are compatible with these rules in order for collaborations to proceed smoothly.