

Simbios R01 Collaborations: Process and Content

Simbios executive committee

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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. A potential collaborating investigator contacts a Simbios participating investigator (listed on the Simbios website <http://simbios.stanford.edu/people.htm>), with an indication of interest in Simbios collaboration. (2 months prior to the submission deadline)
2. The Simbios investigator will alert the Executive Director or PIs. A summary of Simbios research and development activities, active areas of research interests, and current driving biological problems are available for download at simbios.stanford.edu (under collaborating with Simbios). This summary is suitable as a starting point for the summary required with R01 and R21 applications, as described in [PAR-08-184](#) and [PAR-08-183](#). 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 document (that you are reading) is also available for download at simbios.stanford.edu. 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.
3. 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. A copy will be sent to the Simbios program officer and lead scientific officer (Peter Lyster, Jennie Larkin, respectively: lysterpe@NIGMS.NIH.GOV, larkinj2@nhlbi.nih.gov). (1 month prior to the submission deadline)
4. The Simbios executive committee will read this, and suggest a Simbios investigator with appropriate expertise for comment and coordination, for the collaborating investigator to contact. Potential interactions, resources required, and scientific merit and impact should be explored. (1 month prior to submission deadline)
5. The Simbios executive committee will discuss applications with its program and lead scientific officer to determine the fit to Simbios goals, and to write a letter of collaboration for the collaborating investigators proposal.

Types of Collaborations

The R01 and R21 programs outline 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 RNA dynamics, protein folding, neuromuscular biomechanics, and cardiovascular fluid dynamics. We welcome collaborations in closely related areas where existing technologies can be directly tested with little modification.

2. Adoption of our APIs. We release an API for molecular dynamics, designed to take hardware acceleration via Graphic Processor Units (GPUs) into account. We will incorporate this API into Gromacs and Amber and are actively seeking collaborators to incorporate this API into a wide range of additional Molecular Dynamics codes. The collaboration could be at an algorithmic level or could focus on the use of the MD code to solve a particular biological problem.

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 datamining 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 four biological application areas. We would welcome collaborations that introduce new biological areas, and extend and test code we develop for our four initial areas to new areas.

8. Develop novel methods to deliver SimTK functionality. We are interested in ensuring that the broadest possible base of biomedical researchers has access to adequate computational and human resources to use SimTK software.

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>), bug tracking, daily backups, mailing lists, surveys, document manager and more.
2. Consultation on how to submit new computational capabilities, models, and datasets to SimTK as part of your project.
3. Consultation on how to engineer software to interact with the SimTK core offering, including how to address multiplatform build, testing, download and installation issues.
4. Access to SimTK core numerical methods at simtk.org/home/simtkcore, (including consultation on effective use on your small cluster or low-cost multiprocessors).

Code and Data Sharing

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