Systems biology

**SBSI: an extensible distributed software infrastructure for parameter estimation in systems biology**

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**ABSTRACT**

**Summary:** Complex computational experiments in Systems Biology, such as fitting model parameters to experimental data, can be challenging to perform. Not only do they frequently require a high level of computational power, but the software needed to run the experiment needs to be usable by scientists with varying levels of computational expertise, and modellers need to be able to obtain up-to-date experimental data resources easily. We have developed a software suite, the Systems Biology Software Infrastructure (SBSI), to facilitate the parameter-fitting process. SBSI is a modular software suite composed of three major components: SBSINumerics, a high-performance library containing parallelized algorithms for performing parameter fitting; SBSIDispatcher, a middleware application to track experiments and submit jobs to back-end servers; and SBSIVisual, an extensible client application used to configure optimization experiments and view results. Furthermore, we have created a plugin infrastructure to enable project-specific modules to be easily installed. Plugin developers can take advantage of the existing user-interface and application framework to customize SBSI for their own uses, facilitated by SBSI’s use of standard data formats.

**Availability and implementation:** All SBSI binaries and source-code are freely available from http://sourceforge.net/projects/sbsi under an Apache 2 open-source license. The server-side SBSINumerics runs on any Unix-based operating system; both SBSIVisual and SBSIDispatcher are written in Java and are platform independent, allowing use on Windows, Linux and Mac OS X. The SBSI project website at http://www.sbsi.ed.ac.uk provides documentation and tutorials.

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**Supplementary information:** Supplementary data are available at Bioinformatics online.

Received on June 28, 2012; revised on November 22, 2012; accepted on January 12, 2013

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Our use of standard data formats such as the Systems Biology Markup Language [SBML, Hacka et al. (2003)] provides a stable basis for plugin development. Plugins can be downloaded and installed from an update site (http://www.sbsi.ed.ac.uk/update) with minimal user input. Plugins developed to date enable access to project-specific databases and editing support for standard data formats such as SBML and SED-ML (Adams et al., 2012; Adams, 2012).

3 CONCLUSIONS

The main focus of SBSI is the task of parameter estimation, which by its nature is computationally intensive. Progress of long-running jobs can be monitored by observing cost function values, and downloading intermediate result files. At the end of a parameter fitting, the user can download the fitted model, together with simulation results generated from the model, and a full log of the explored search space. Since it is beyond our resources to provide computational time for everyone wishing to use SBSI, we have endeavoured to package the software in a form that can be easily installable on other servers. SBSIDispatcher, which acts as a task manager for remotely running jobs, is deployed as a regular Java web application, and only requires configuration of database access in order to be useable on other application servers.

ACKNOWLEDGEMENT

The authors thank Kevin Stratford for consultancy on SBSINumerics.

Funding: UK Biotechnology and Biological Sciences Research Council, and Engineering and Physical Sciences Research Council (to SynthSys, a Centre for Integrative and Systems Biology) (BB/D019621/1).

Conflict of Interest: none declared.

REFERENCES


