

High Performance Computing using libRoadRunner

We present libRoadrunner, an open-source and cross-platform C/C++ library for the JIT compilation, simulation and analysis of models expressed in SBML. As simulations of cellular systems become more complex and larger, particularly in multicellular and multiscale or whole cell models, the need for reusable and high performance simulation engines is becoming clear. The libRoadrunner library has been designed to be extensible and offers superior performance to standard desktop simulators. Here we describe the architectural design of the library, the challenges involved in JIT compilation of declarative languages, and an overview of the interactive Python API.

To our knowledge, libRoadrunner is the first SBML JIT compilation engine. JIT compilers are rare for declarative languages. Declarative languages present unique challenges for dynamic compilation and many of the constructs, such the symbol table from traditional compiler design are expanded to deal with the challenging scoping issues present in SBML. We will give an overview of SBML semantic analysis and intermediate code generation, and finally machine code generation.

The JIT compiled model is combined with variety of plug-able integrators and an extensive API designed for both interactive and high performance use to form the libroadrunner library. libRoadRunner currently runs on Windows, Linux, Mac and uniquely on ARM based computers.