Massively-Parallel Simulation of Biochemical Systems

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Understanding biological evolution prompts for a detailed understanding of the realized phenotype. Biochemical and gene regulatory dynamics are a cornerstone for the physiology of the cell and must therefore be regarded as one of the major aspects of such a phenotype. Experimental insight into molecular parameters is, however, hard to come by. Model development therefore requires computational parameter estimation. At the same time, design of cellular dynamics is highly efficient when done in-silico. We therefore developed a computational approach to allow for massively parallel simulation of biological molecular networks that leverage the massively-parallel computing power of modern graphics cards and other many-core programming paradigms. Our system can automatically compile standard SBML files into CUDA code, using analytic derivatives, and computing standard measures of complex dynamics like the Lyapunov exponent.

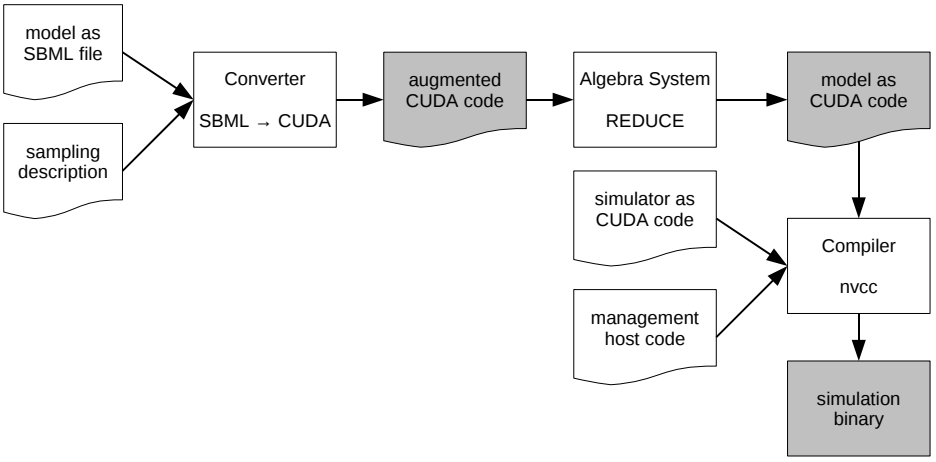

Figure 1: Overview over the pipeline. Gray boxes indicate automatically created files, while white parts are fixed elements.

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