Data-Parallel Techniques for Agent-Based Hepatic Drug Disposition Models

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Abstract

We present a set of algorithms for simulating agent-based hepatic drug disposition models using data-parallel techniques. These algorithms have been implemented using NVIDIA CUDA, an extension to the C programming language which allows for data-parallel Graphics Processing Unit (GPU) programming through the use of computation kernels. We implemented the In-Silico Liver (ISL) model developed by Hunt et al. to demonstrate the capabilities of our algorithms. Our implementation is able to compute over one million mobile agents and over five million static grid points in real-time.

References

[1] C Anthony Hunt, Glen E P Ropella, Li Yan, Daniel Y Hung, and Michael S Roberts, "Physiologically based synthetic models of hepatic disposition" (2006). Journal of Pharmacokinetics and Pharmacodynamics. 33 (6), pp. 737-772. Postprint available free at: http://repositories.cdlib.org/postprints/2226

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