Higher-order integration schemes for jump-diffusion models of biomolecular reaction networks

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The work of this master thesis revolves around jump-diffusion approximations of pure Markovian jump processes used to model biomolecular interaction networks if molecule counts are low. Recently error bounds for such an approximations were derived and based on them an adaptive simulation algorithm was developed that dynamically partitions reactions into fast and slow ones and applies the diffusion approximation to the fast ones as the stochastic simulation unfolds [1]. In order to obtain noticeable speed-up between the simulation of the pure jump process and of that hybrid model, efficient higher-order integrators need to be employed for the diffusion part. A potential candidate solver is S-ROCK2, a second weak order explicit integrator [2].

Goal of the master thesis project is to obtain a fast and robust integrator for jump-diffusion models with adaptive reaction partitioning. It involves reimplementing S-ROCK2 in Matlab and later on scaling it up using C++ on parallel architecture using openMP, or equivalent. The incorporation into the jump-diffusion simulation requires a clever re-initialization procedure of the integrator after a re-partitioning event. The algorithm will be benchmarked on large kinetic models from the systems and synthetic biology domain.

Good programming skills are required and a certain willingness to absorb the underlying mathematics will be necessary.

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References

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[2] A. Abdulle, G. Vilmart, and K.C. Zygalakis. Second weak order explicit stabilized methods for stiff stochastic differential equations. *SIAM J. Sci. Comput.*, 35(4), 17921814, 2013.