

**Speaker:** Elena Akhmatskaya, Basque Center for Applied Mathematics, Spain

**Title:** Problem-specific Multistage Splitting Integration Schemes for Hybrid/Hamiltonian Monte Carlo with Applications

**Abstract:** We discuss an alternative to fix-parameter multistage splitting integration schemes commonly used in the popular Hybrid (molecular simulation)/Hamiltonian (Bayesian inference) Monte Carlo (HMC) methods.

The proposed new family of numerical integrators includes one-/two-parameter 2-/3-stage splitting integrators, with the parameters being a function of a simulation step size, a number of splitting stages and angular frequencies present in a simulated system. Such a family of model-specific integration schemes is generated by the Adaptive Integration Approach which we developed for molecular simulation (AIA) and Bayesian statistical inference (s-AIA) applications. Given a model (frequencies), a step size and a number of splitting stages (s)-AIA detects a splitting integrator, which provides the best conservation of energy for harmonic forces. The methods rely on the analysis of univariate/multivariate Gaussian model and make use of simulation data collected at the burn-in stage of an HMC simulation.

The AIA methods have been formulated for a range of HMC algorithms, which simulate either constrained or unconstrained dynamics, and sample with Hamiltonians or modified Hamiltonians. They can be implemented in a MD / HMC software code, without introducing computational overheads in the simulations.

Numerical tests show that the methods successfully realise the fail-safe strategy. In all experiments, and for each of the criteria employed, the (s-)AIA is at least as good as, and often significantly outperforms the standard Verlet scheme, as well as fixed-parameter multistage splitting integrators.

The ideas underlying the (s-)AIA can be also used for a rational choice of simulation parameters. The impact of problem-specific integrators on the performance of HMC methods in energy and medical applications is also discussed.

This is a joint work with M. Fernández-Pendás, L. Nagar and J.M. Sanz-Serna.