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Long time averaging using symplectic solvers, with applications to molecular dynamics

Molecular simulation often leads to the computation of certain averaged quantities, in order to recover macroscopic coefficients (like, say, transport coefficients). The averaging procedure should in principle be done over the whole phase-space. In practice however, assuming ergodicity of the underlying dynamics allows to replace the averaging over the whole phase-space, which involves high-dimensional integration, by a time averaging of the dynamics over sufficiently large time intervals.

From a numerical point of view, it is thus tempting to compute the relevant averages in time (rather than in space). This raises the question of defining numerical schemes that preserve the ergodicity properties of the system, so as to approximate the time average by the space average.

In this talk, we prove that symplectic schemes do preserve ergodicity when the underlying dynamics is Hamiltonian, completely integrable, and ergodic. Using this idea together with appropriate filtering procedures to eventually compute the time averages, we devise schemes that approximate the quantity to be computed with an error which may be an arbitrary power of both $1/T$ and h , where h is the (small) time step used for computing the dynamics, and T is the (large) time truncation used to approximate the space average by the time average.

This talk reflects a joint work with E. Cancès, P. Chartier, E. Faou, C. Le Bris, F. Legoll, G. Turinici.