
Explicit stabilized integrators for stiff problems: the interplay of geometric integration and stochastic integration

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Résumé

The preservation of geometric structures by numerical methods, such as the symplecticity of the flow for the long time solution of deterministic Hamiltonian systems, often reveals essential for an accurate numerical integration, and this is the objective of geometric numerical integration.

In this talk, we highlight the role that some key geometric integration tools originally introduced in the deterministic setting, such as modified differential equations, processing techniques, Butcher trees, B-series and their generalizations, play in the design of high-order stochastic integrators, in particular for sampling the invariant distribution of ergodic stochastic partial differential equations or high-dimensional ergodic stochastic systems that typically arise in Langevin dynamics in the context of molecular dynamics simulations.

We show that this approach reveals decisive in particular for the construction of efficient explicit stabilized integrators for stiff stochastic problems, which are a popular alternative to implicit methods to avoid the severe timestep restrictions faced by standard explicit integrators.

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