

Discontinuous collocation

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The `RATTLE` algorithm is one of the most widely used integrators for constrained Hamiltonian systems (in particular in molecular dynamics). Its natural extension to higher order is the partitioned Runge-Kutta method, based on the Lobatto IIIA–IIIB pair. In this talk we give a new interpretation of this integrator as “discontinuous collocation” method. This allows us to get new elegant proofs for their superconvergence and symplecticity.