JOHN BOWMAN, University of Alberta
Conservative, Symplectic, and Exponential Integrators

Novel integration algorithms for initial value problems can be formed by applying conventional explicit discretizations in a transformed space. One can devise integration methods that respect desired properties of ordinary differential equations such as first integrals, positivity, or unitary structure. For example, traditional numerical integration algorithms, which are polynomials in the time step, typically lead to systematic drifts of nonlinear first integrals. For a 4-body classical mechanics problem, we compare conservative integration with conventional symplectic discretization, which conserves only an approximate Hamiltonian.

One can also develop new numerical integration methods that preserve analytical structure by discretizing perturbations of exactly solvable differential equations. For example, exponential integrators are ideal for solving linearly stiff first-order ordinary differential equations, where the nonlinearity varies slowly on the time scale of the linearized equations.

We use the stiff-order criteria of Hochbruck and Ostermann [2005] to derive efficient embedded exponential pairs of high- and low-order estimates to support dynamic time-step adjustment. A key requirement is that the pair be robust: if the nonlinear source function has a nonzero total time derivative, the order of the low-order estimate should never exceed its design value. Robust exponential Runge–Kutta (3,2) and (4,3) embedded pairs that are well-suited to initial value problems with a dominant linearity are constructed.