

On the use of exponential integrators for large-scale Hamiltonian systems

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Hamiltonian systems are differential equations that exhibit a particular structure. This structure leads to geometric attributes e.g. energy conservation or symplectic flow maps. Such systems come along in physical problems like Maxwell's equations, molecular dynamics or wave equations. Simulating and analyzing these systems lead to differential equations of a high dimension that are computationally expensive to solve. We consider large and sparse Hamiltonian systems

$$\dot{y}(t) = J\nabla\mathcal{H}(y(t)), \quad y(0) = y_0, \quad J = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}, \quad (1)$$

where $\mathcal{H} : \mathbb{R}^{2n} \rightarrow \mathbb{R}$ is a C^2 -function and $0_n, I_n$ are the zero and identity matrix of order n . A natural approach is to consider Krylov subspace based methods to approximate the solution of the original system by one of smaller dimension. In this work, only structure preserving approximation methods and a structure preserving integrator are considered in order to let the smaller systems and their solution of the differential equation inherit the relevant geometric properties of the original system. We recapitulate existing methods of this type and compare these with respect to the error in the energy conservation and the global error. We suggest to use such a method in combination with model order reduction techniques for the studies of Hamiltonian systems to reduce the computational effort.