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Energy conservation in modified Nyström methods for separable Hamiltonian systems

Numerical integration methods that preserve structural properties of time dependent differential equations have often improved stability and smaller errors in long-term simulations than classical standard methods like Runge–Kutta or BDF. In the present paper an energy conserving Galerkin type approach of Betsch and Steinmann is generalized to modified Nyström methods for separable Hamiltonian systems. The benefits of this new class of methods are illustrated by numerical tests for a benchmark problem from celestial mechanics.

1. Structure preservation in separable Hamiltonian systems

Separable Hamiltonian systems

$$\dot{x}(t) = H_p^\top(x,p), \qquad \dot{p}(t) = -H_x^\top(x,p) \tag{1}$$

are characterized by a Hamiltonian $H(x,p) = V(x) + \frac{1}{2}p^\top M^{-1}p$ with a constant positive definite mass matrix M and a continuously differentiable potential $V : \mathbb{R}^d \to \mathbb{R}$.

The N-body problem may be considered as a typical example [2, Example IV.1.3]. Here we have $d = 3N$ and $x = (x^1, x^2, \ldots, x^N)^\top$ with $x^i \in \mathbb{R}^3$ denoting the position coordinates of the i-th particle that has mass m_i. The mass matrix is given by $M = \mathrm{blockdiag}_{1 \le i \le N} \, m_i I_3$. The interaction between particles is characterized by a distance potential $V(x) := \sum_{i=2}^{N} \sum_{j=1}^{i-1} V_{ij}(\|x^i - x^j\|_2)$ with continuously differentiable functions $V_{ij} : (0, \infty) \to \mathbb{R}$.

It is well known that the total energy $H(x,p)$, the total linear momentum $\sum_i p^i$ and the angular momentum $\sum_i x^i \times p^i$ are invariants of the N-body problem, i. e., for any given initial values x_0, p_0 these quantities remain constant for all $t \in [t_0, t_e]$. A 6-body problem with model data from [2, Table I.2.2] that describes the motion of the outer planets in the solar system will be used as test example.

The separable Hamiltonian systems (1) are equivalent to the system $M\ddot{x} = -\nabla V(x)$ that we rewrite in the form

$$\dot{x}(t) = y, \qquad \dot{y}(t) = g(x,y) := -M^{-1}\nabla V(x). \tag{2}$$

Any standard time integration method for ordinary differential equations (ODEs) may be applied to (2). Standard methods like Runge–Kutta methods or linear multi-step methods guarantee a small discretization error for sufficiently small time stepsizes h. But, in general, they do not preserve all invariants of the analytical solution.

This is illustrated by test results for two implicit Runge–Kutta methods. Fig. 1 shows the errors in three invariants for fixed stepsize computations. The three-stage Radau IIA method [3, Sect. IV.8] preserves only the linear invariants and has growing errors in $H(x,p)$ and in the angular momentum. The results are substantially improved using a simplectic method. The right plot of Fig. 1 illustrates that the four-stage Lobatto IIIA-IIIB pair [2, Sect. II.2.2] preserves linear and angular momentum up to machine precision and the error in $H(x,p)$ remains bounded.
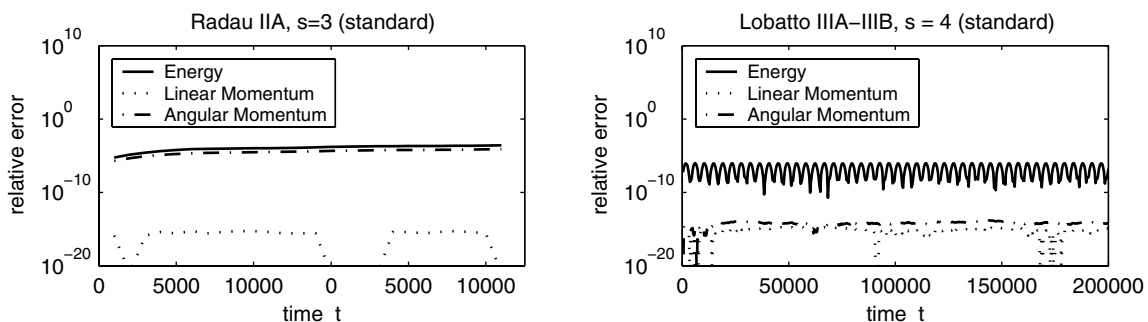

Figure 1: Errors in invariants of the 6-body problem if (2) is solved by classical Runge–Kutta methods.
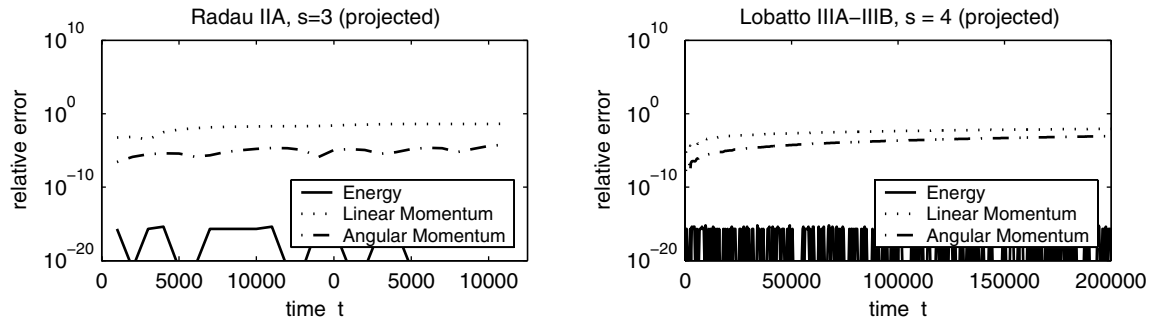
Figure 2: Errors in invariants of the 6-body problem. Classical Runge–Kutta methods with projection steps.

Energy conservation could be enforced by projection steps that project the numerical solution (x_n, p_n) after each time step back to the manifold $\{ (x, p) : H(x, p) = H(x_0, p_0) \}$ [3, pp. 470f]. However, Fig. 2 shows that these projection steps destroy other important inherent properties of the Runge–Kutta methods. For both methods the error in $H(x, p)$ is reduced to machine precision but now neither linear nor angular momentum are preserved.

2. Energy conserving modified Nyström methods

Betsch and Steinmann [1] study energy conserving Galerkin methods for solving (2) in a time step $t_n - h = t_{n-1} \to t_n$, $(n > 0)$. The known drawbacks of projected space variables (see Fig. 2) are avoided substituting $g(x, y)$ in the right hand side of (2) by $\kappa_n \cdot g(x, y)$ with a scalar $\kappa_n \approx 1$ that is adjusted such that $H(x_n, y_n) = H(x_{n-1}, y_{n-1})$. For a method of order p this condition determines implicitly a constant κ_n with $\kappa_n = 1 + \mathcal{O}(h^p)$ provided that $\nabla V(x_{n-1})^\top p_{n-1} \neq 0$ [4].

The methods of Betsch and Steinmann may be rewritten as modified Nyström methods

$$x_n = x_{n-1} + hy_{n-1} + h^2 \sum_{i=1}^s b_i \kappa_n g(X_{ni}, Y_{ni}), \quad y_n = y_{n-1} + h \sum_{i=1}^s w_i \kappa_n g(X_{ni}, Y_{ni}), \quad H(x_n, y_n) = H(x_{n-1}, y_{n-1})$$
$$(3)$$
$$X_{ni} = x_{n-1} + c_i h y_{n-1} + h^2 \sum_{j=1}^s a_{ij} \kappa_n g(X_{ni}, Y_{ni}), \quad Y_{ni} = y_{n-1} + h \sum_{j=1}^s \bar{a}_{ij} \kappa_n g(X_{ni}, Y_{ni}), \quad (i = 1, \ldots, s)$$

with special Runge–Kutta–Nyström parameters a_{ij}, $\bar{a}_{ij}$, b_i, w_i [4, Thm. 3.14]. All methods (3) conserve energy and linear momentum, see Fig. 3. Additionally, the angular momentum is preserved if the corresponding classical method ($\kappa_n := 1$ in (3)) has this property [4], see also [2, Sect. IV.2.3].
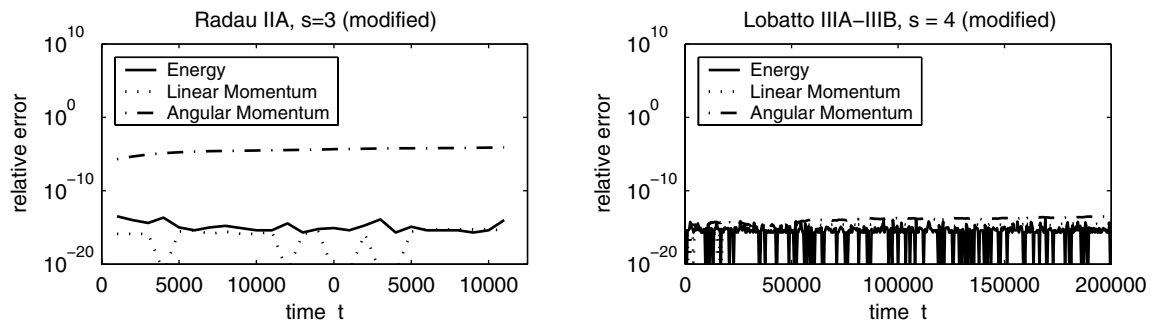

Figure 3: Errors in invariants of the 6-body problem if (2) is solved by modified Nyström methods.

3. References

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