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Recent Advances in the Numerical Solution of Hamiltonian PDEs

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Abstract. The numerical solution of Hamiltonian PDEs has been the subject of many investigations in the last years, specially concerning the use of multi-symplectic methods. We shall here be concerned with the use of energy-conserving methods in the HBVMs class, when a spectral space discretization is considered.

Keywords: Hamiltonian Partial Differential Equations, Fourier discretization, Energy-conserving Runge-Kutta methods, Hamiltonian Boundary Value Methods.
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INTRODUCTION

The efficient numerical solution of Hamiltonian PDEs has been the subject of many investigations in recent years (see, e.g., [15, 1]) especially in connection with the use of multi-symplectic methods [13, 14]. Here, we shall be concerned with the use of energy-conserving methods in the HBVMs class [5, 6, 8], which are methods based on the concept of discrete line integral [10, 11, 12], when they are coupled with a spectral space discretization (see, e.g., [9]). We shall sketch the approach when periodic boundary conditions are prescribed, even though the used approach can be generalized to the case of general boundary conditions. For simplicity, though without loss of generality, we shall consider the 1D nonlinear wave equation,

$$\begin{array}{rcl} u_{tt}(x,t) & = & u_{xx}(x,t) - f'(u(x,t)), \qquad (x,t) \in (0,1)\times(0,\infty), \\ u(x,0) & = & \psi_0(x), \qquad u_t(x,0) \;=\; \psi_1(x), \qquad x \in (0,1), \\ u(0,t) & = & u(1,t), \qquad t > 0. \end{array} \tag{1}$$

As usual, subscripts denote partial derivatives, and the functions f, ψ_0 and ψ_1 are supposed to be sufficiently smooth, so they define a regular solution $u(x,t)$ (f' denotes the derivative of f). By setting $v = u_t$, and defining the functional

$$\mathscr{H}[u,v](t) = \int_0^1 \left[\frac{1}{2}v^2(x,t) + \frac{1}{2}u_x^2(x,t) + f(u(x,t))\right] \mathrm{d}x \equiv \int_0^1 E(x,t)\,\mathrm{d}x, \tag{2}$$

we can rewrite (1) as the infinite-dimensional Hamiltonian system

$$\begin{array}{rcl} u_t(x,t) & = & v(x,t), \qquad (x,t) \in (0,1)\times(0,\infty), \\ v_t(x,t) & = & u_{xx}(x,t) - f'(u(x,t)), \end{array}$$

that is, the first-order formulation of the first equation in (1), for which (2) is a conserved quantity. In view of applying a Fourier spatial discretization for problem (1), let us consider the following orthonormal functions in $[0,1]$:

$$c_0(x) \equiv 1, \qquad c_k(x) = \sqrt{2}\cos(2k\pi x), \quad s_k(x) = \sqrt{2}\sin(2k\pi x), \qquad k = 1,2,\ldots, \tag{3}$$

so that

$$\int_0^1 c_i(x)c_j(x)\mathrm{d}x = \int_0^1 s_i(x)s_j(x)\mathrm{d}x = \delta_{ij}, \qquad \int_0^1 c_i(x)s_j(x)\mathrm{d}x = 0, \qquad \forall i,j, \tag{4}$$

δ_{ij} being the Kronecker symbol. Then, the following expansion of the solution of (1) is a slightly different way of writing the usual Fourier expansion in space:

$$u(x,t) = c_0(x)\gamma_0(t) + \sum_{n\ge 1}\left[c_n(x)\gamma_n(t) + s_n(x)\eta_n(t)\right] \equiv \gamma_0(t) + \sum_{n\ge 1}\left[c_n(x)\gamma_n(t) + s_n(x)\eta_n(t)\right], \quad x \in [0,1],\ t \ge 0. \tag{5}$$

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Consequently, by taking into account (3)–(4), the first equation in (1) can be rewritten as:

$$\begin{aligned}
\ddot{\gamma}_n(t) &= -(2\pi n)^2\gamma_n(t) - \int_0^1 c_n(x) f'\left(\gamma_0(t) + \sum_{j\geq 1}\left[c_j(x)\gamma_j(t) + s_j(x)\eta_j(t)\right]\right)\mathrm{d}x, \quad n \geq 0,\\
\ddot{\eta}_n(t) &= -(2\pi n)^2\eta_n(t) - \int_0^1 s_n(x) f'\left(\gamma_0(t) + \sum_{j\geq 1}\left[c_j(x)\gamma_j(t) + s_j(x)\eta_j(t)\right]\right)\mathrm{d}x, \quad n \geq 1,
\end{aligned} \tag{6}$$

where the dot denotes, as usual, the time derivative. By introducing the infinite vectors

$$\mathbf{q}(t) = (\gamma_0(t), \gamma_1(t), \eta_1(t), \gamma_2(t), \eta_2(t), \ldots)^\top, \quad \mathbf{p}(t) = \dot{\mathbf{q}}(t), \quad \boldsymbol{\omega}(x) = (c_0(x), c_1(x), s_1(x), c_2(x), s_2(x), \ldots)^\top, \tag{7}$$

the infinite matrix $D = \mathrm{diag}\left(0, (2\pi)^2, (2\pi)^2, (4\pi)^2, (4\pi)^2, \ldots\right)$, and considering that $u(x,t) = \boldsymbol{\omega}(x)^\top \mathbf{q}(t)$, problem (6) can be cast in vector form as the following Hamiltonian problem:

$$\dot{\mathbf{q}}(t) = \mathbf{p}(t), \qquad \dot{\mathbf{p}}(t) = -D\mathbf{q}(t) - \int_0^1 \boldsymbol{\omega}(x) f'(\boldsymbol{\omega}(x)^\top \mathbf{q}(t))\mathrm{d}x, \qquad t \geq 0,$$

with Hamiltonian

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^\top\mathbf{p} + \frac{1}{2}\mathbf{q}^\top D\mathbf{q} + \int_0^1 f(\boldsymbol{\omega}(x)^\top\mathbf{q})\mathrm{d}x, \tag{8}$$

which is easily seen to be equivalent to the Hamiltonian (2), via the expansion (5).

TRUNCATED FOURIER APPROXIMATION

In the computational practice, it is mandatory to truncate the infinite expansion (5) to a finite sum:

$$u(x,t) \;\approx\; \gamma_0(t) + \sum_{n=1}^{N}\left[c_n(x)\gamma_n(t) + s_n(x)\eta_n(t)\right] \;\equiv\; u_N(x,t). \tag{9}$$

This reflects in the fact that the differential equations (6) now reduce to a finite number, i.e., $2N+1$. Correspondingly, one defines the vectors $\mathbf{q}_N(t), \mathbf{p}_N(t), \boldsymbol{\omega}_N(t) \in \mathbb{R}^{2N+1}$ given by the leading parts of the corresponding infinite vectors in (7), and the principal submatrix D_N of dimension $2N+1$ of matrix D. Then, considering that $u_N(x,t) = \boldsymbol{\omega}_N(x)^\top \mathbf{q}_N(t)$, the equations which must be satisfied by (9) can be cast in vector form as:

$$\dot{\mathbf{q}}_N(t) = \mathbf{p}_N(t), \qquad \dot{\mathbf{p}}_N(t) = -D_N\mathbf{q}_N(t) - \int_0^1 \boldsymbol{\omega}_N(x) f'(\boldsymbol{\omega}_N(x)^\top \mathbf{q}_N(t))\mathrm{d}x, \qquad t \geq 0, \tag{10}$$

which is again in Hamiltonian form, with Hamiltonian

$$H(\mathbf{q}_N,\mathbf{p}_N) = \frac{1}{2}\mathbf{p}_N^\top\mathbf{p}_N + \frac{1}{2}\mathbf{q}_N^\top D_N\mathbf{q}_N + \int_0^1 f(\boldsymbol{\omega}_N(x)^\top\mathbf{q}_N)\mathrm{d}x. \tag{11}$$

This latter is glaringly equivalent to a truncated Fourier expansion of the Hamiltonian (2), that is, by truncating the expansion (5) as done in (9). For approximating problem (10), one can consider the use of a HBVM(k,s) method, which is the k-stage Runge-Kutta method defined by the following Butcher tableau [6, 8]:

$$\begin{array}{c|c} c_1 & \\ \vdots & \left[b_j \sum_{\ell=0}^{s-1} P_\ell(c_j) \int_0^{c_i} P_j(\tau)\mathrm{d}\tau\right]_{i,j=1,\ldots,k} \\ c_k & \\ \hline & b_1 \;\ldots\; b_k \end{array}, \qquad \int_0^1 P_i(x)P_j(x)\mathrm{d}x = \delta_{ij}, \quad P_i \in \Pi_i, \quad i,j = 0,\ldots,k,$$

with P_i, P_j the normalized and shifted Legendre polynomials, and $(b_i, c_i)_{i=1,\ldots,k}$ the Legendre weights and abscissae. For such methods, which reduce to the s-stage Gauss-Legendre collocation methods when $k = s$, the following result holds true [4].

Theorem 1 *For all $k \geq s$, a HBVM(k,s) method applied to problem (10)–(11):*

- *has order $2s$;*

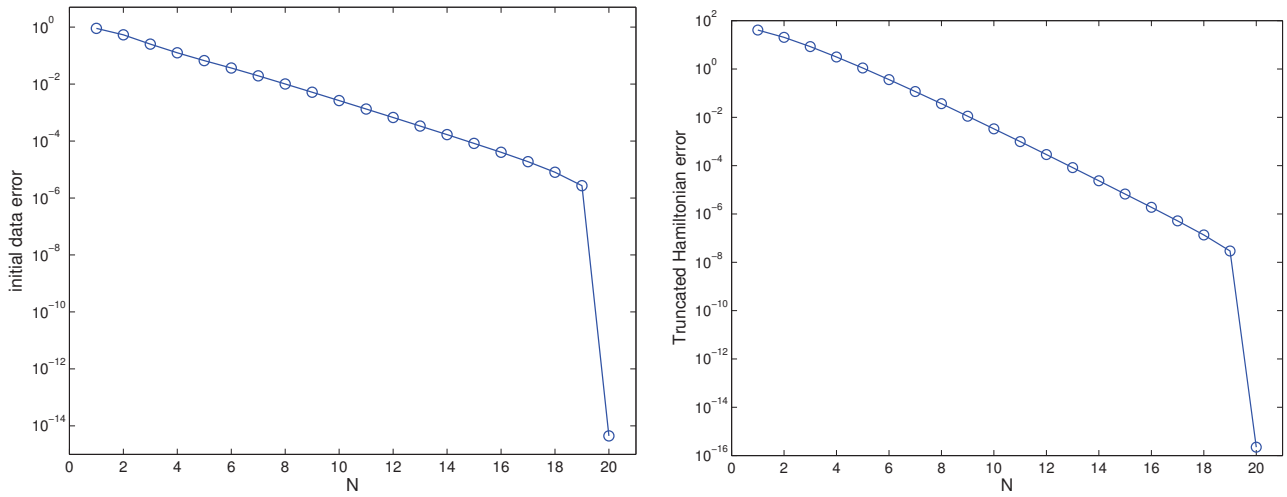

FIGURE 1.

- *is energy conserving when f is a polynomial of degree $\nu \leq \lfloor 2k/s \rfloor$;*
- *for general and suitably regular functions f, the energy error at each step is $O(h^{2k+1})$.*

This, in turn, implies that a (at least *practical*) conservation of energy is obtained, provided that f is suitably regular (which will be assumed hereafter), by choosing k large enough, also considering that the computational cost for implementing a HBVM(k,s) method depends essentially on s, rather than on k [7, 2, 3]. Clearly, the integrals appearing at the right-hand side in (10) and (11) can be computed accurately, by using a composite trapezoidal rule, the argument being a periodic function: fo sake of brevity, we shall omit here the handling of such a standard stuff.

We end this section, by stressing that the above arguments can be extended to cope with different kind of boundary conditions, by suitably modifying the Hamiltonian function defining the problem [4].

NUMERICAL TESTS

The use of energy-conserving methods is quite well understood, proving to be very useful, when speaking about Hamiltonian ordinary differential equations. Their use in the framework of Hamiltonian partial differential equations is fairly less obvious and deserves further investigations. We here just report a few numerical tests, showing that the proposed truncated Fourier space discretization, coupled with a HBVM solution in time, allows to obtain energy-conservation, as above described. We consider problem (1) with:

$$f(u) = u^4 - u, \qquad \psi_0(x) = \sum_{n=1}^{20} 2^{-n} \left[\sin(2n\pi x) - \cos(2n\pi x)\right], \qquad \psi_1(x) \equiv 0, \tag{12}$$

for which the Hamiltonian (2) has a value $H_0 \approx 62.93$. In Figure 1, left-plot, we show the error in the initial data, depending on the value N for the truncation in (9). The right-plot in the same figure displays the error of the corresponding truncated Hamiltonian (11), with respect to the exact Hamltonian (8): as one may infer from the initial data in (12), the error at $N = 20$ has to be of the order of round-off errors in both cases.

Let us now solve the same problem, by using a sixth-order HBVM(k,3) method, over the interval [0,100]. For this purpose, we fix a stepsize $h = 10^{-1}$. In the left-plot of Figure 2 we plot the absolute error in the numerical Hamiltonian ($|H - H_0|$) when $k = 3, 5, 7$:[1] as one may see, the larger k the smaller the error, which is within round-off for $k = 7$. In the right-plot in the same figure, one finds the maximum error in the numerical Hamiltonian (line with circles),

$$E_H(k) = \max_{n=1,\ldots,1000} |H_n - H_0|, \qquad k = 3, \ldots, 9,$$

[1] By the way, when $k = 3$, HBVM(3,3) coincides with the symplectic 3-stage Gauss-Legendre collocation method

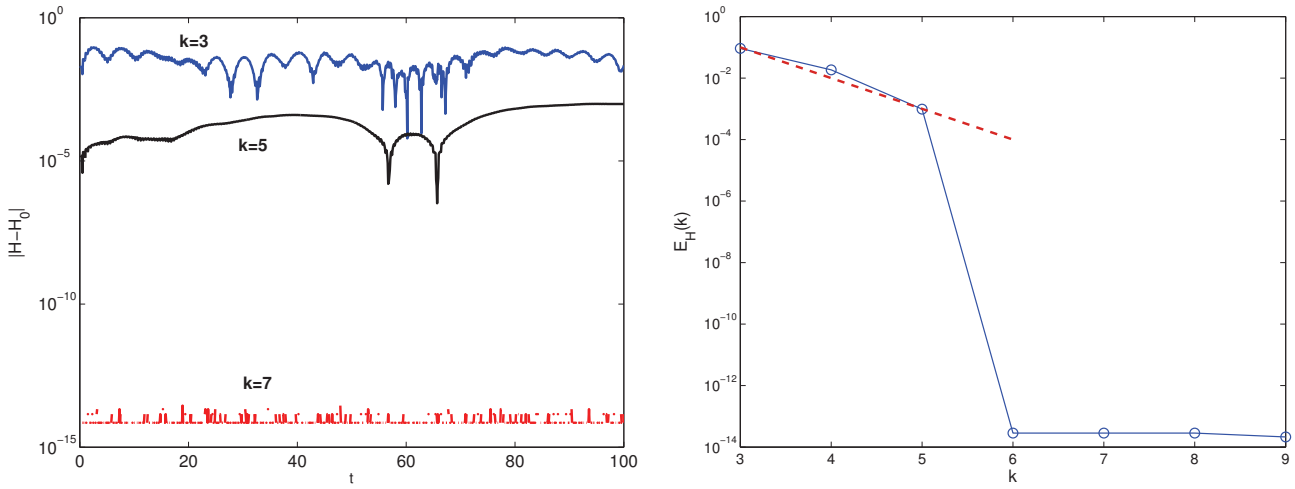

FIGURE 2.

where H_n is the value of the numerical Hamiltonian at the time-step n. In the same sub-plot, one finds a dashed-line, showing a decrease proportional to h^{2k} ($h = 10^{-1}$, in our case). It is then clear that the $E_H(k)$ behaves as h^{2k}, for $k = 3,4,5$, whereas it is of the order of round-off errors, for $k \geq 6$, according to Theorem 1. Indeed, in the present case the function f in (12) is a polynomial of degree 4, and $2k \geq 4s \equiv 12$, for $k \geq 6$.

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