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A NOTE ON ENERGY CONSERVATION FOR HAMILTONIAN SYSTEMS USING CONTINUOUS TIME FINITE ELEMENTS

PETER HANSBO

Abstract. In this note we suggest a new approach to ensure energy conservation in time-continuous finite element methods for nonlinear Hamiltonian problems.

1. Introduction

In this note, we consider the Hamiltonian problem

$$\ddot{u} + F'(u) = 0 \tag{1.1}$$

where $t \in [0, T]$ and $u(t) \in \mathbb{R}$, supplemented with initial conditions for u and $\dot{u}$. Our approach for solving (1.1) numerically works equally well for systems of equations, but for notational simplicity we choose to work with a scalar problem.

Several authors, e.g., French and Schaeffer [3] and Betsch and Steinmann [1], have proposed the use of the time-continuous Galerkin (CG) method for the approximate solution of (1.1). The CG method is inherently energy-conserving, but in the case of nonlinear problems this property hinges on the exact evaluation of integrals and may be lost when quadrature is used. In [1] this was achieved only in the special case of linear-in-time finite elements. The general case can be treated either using a Lagrange multiplier technique as proposed by Hughes, Caughey, and Liu [4], which may not be so useful in case there is dissipation in the system, or by a special adaptive quadrature rule devised by French and Schaeffer [3].

In this paper, we propose a third alternative which does not use multipliers and allows for the use of any quadrature rule (as applied to the nonlinear term).

2. Continuous Time Elements and Energy Conservation

For solving (1.1) numerically using finite elements, we introduce the space $P^k(I_n)$ of k:th degree polynomials on $I_n = (t_n, t_{n+1})$. On each interval I_n we pose the problem of finding

$$(U, V) \in (P^k(I_n) \times P^k(I_n)) \cap (C^0([0, T]) \times C^0([0, T]))$$

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such that

$$\int_{t_n}^{t_{n+1}} \left(\dot{U} - V\right) \xi \, dt = 0 \quad \forall \xi \in P^{k-1}(I_n), \tag{2.1}$$

and

$$\int_{t_n}^{t_{n+1}} \left(\dot{V} + F'(U)\right) \cdot \eta \, dt = 0 \quad \forall \eta \in P^{k-1}(I_n). \tag{2.2}$$

Since U and V are continuous, the number of unknowns equals the number of equations, and the problem is uniquely solvable, see, e.g., Eriksson et al. [2].

In particular, by setting $\eta = \dot{U}$ and $\xi = \dot{V}$, we find that

$$\int_{t_n}^{t_{n+1}} \dot{U}\,\dot{V}\, dt - \int_{t_n}^{t_{n+1}} \frac{1}{2}\frac{d}{dt}\|V\|^2 \, dt = 0$$

and

$$\int_{t_n}^{t_{n+1}} \dot{V}\,\dot{U}\, dt + \int_{t_n}^{t_{n+1}} \frac{d}{dt}F(U) \, dt = 0$$

from which it follows that the discrete energy $E := \frac{1}{2}\|V\|^2 + F(U)$ is conserved at discrete time levels.

The problem from a practical point of view is that since

$$\int_{t_n}^{t_{n+1}} F'(U)\,\dot{U} dt = F(U(t_{n+1})) - F(U(t_n)),$$

our chosen quadrature rule must, in order to conserve, also fulfill

$$\sum_i \omega_i F'(U(t_i))\,\dot{U}(t_i) = F(U(t_{n+1})) - F(U(t_n)),$$

where ω_i are quadrature weights and t_i are quadrature points. This is not generally the case (unless suitable modifications of the weights are introduced, cf. French and Schaeffer [3]). However, we in fact only need to fulfill the relation

$$\int_{t_n}^{t_{n+1}} \dot{V}\,\dot{U}\, dt + (F(U(t_{n+1})) - F(U(t_n))) = 0$$

which can be done in a nonlinear iteration algorithm using coordinate transformations. We have

$$\int_{t_n}^{t_{n+1}} \left(\dot{V} + F'(U)\right) \eta \, dt = 0$$

for all η expressed in a basis spanning $P^{k-1}(I_n)$. We begin by defining an arbitrary normalized basis $\{\phi_1, \phi_2, \ldots, \phi_k\}$ for $P^{k-1}(I_n)$. One natural choice is

$$\{1, 2\,\tau, 3\,\tau^2, \ldots, k\,\tau^{k-1}\}, \tag{2.3}$$

where $\tau = t/(t_{n+1} - t_n)$. Next, we change the basis (in each iteration) to $\{\varphi_1, \varphi_2, \dots, \varphi_k\}$ in such a way that $\dot{U}$ is explicitly contained in the basis. Since $\dot{U} = \sum_j \alpha_j \phi_j$, this can be achieved by simply finding k corresponding to $\max_k |\alpha_k|$ and setting

$$\varphi_i = \begin{cases} \dot{U} & \text{if } i = k, \\ \varphi_i & \text{if } i \neq k. \end{cases}$$

If $\max_k |\alpha_k| << 1$, we do not need to modify the basis. Once this is achieved, we can write (2.2) as

$$0 = \int_{t_n}^{t_{n+1}} \dot{V}\,\varphi_i\,dt + \begin{cases} F(U(t_{n+1})) - F(U(t_n)) & \text{if } i = k, \\ \displaystyle\int_{t_n}^{t_{n+1}} F'(U)\,\varphi_i\,dt & \text{if } i \neq k, \end{cases} \tag{2.4}$$

which clearly fulfills energy conservation irrespective of the quadrature rule used for the integral on the right-hand side. Note that this scheme is also viable in case dissipation is present; it only introduces exact integration of the crucial term and does not modify the scheme in the way enforced conservation does (cf. Hughes et al. [4]).

3. Numerical Example

Consider a pendulum of unit mass attached to a mass-free rigid rod of unit length under the action of normalized gravity. The equation describing the motion of this pendulum can be written

$$\frac{d}{dt}\left(\frac{1}{2}\dot{u}^2 + F(u)\right) = 0 \quad \text{with} \;\; F(u) = 1 - \cos(u),$$

which can be formulated as

$$\ddot{u} + \sin(u) = 0, \tag{3.1}$$

supplemented by initial conditions. We thus have that

$$F(u(t_{n+1})) - F(u(t_n)) = \cos(u(t_n)) - \cos(u(t_{n+1})).$$

Reformulating (3.1) as

$$\frac{d\boldsymbol{u}}{dt} + \boldsymbol{f}(\boldsymbol{u}) = 0, \quad \text{were} \;\; \boldsymbol{u} = \begin{bmatrix} u \\ v \end{bmatrix}, \; \boldsymbol{f} = \begin{bmatrix} -v \\ \sin(u) \end{bmatrix},$$

we can linearize around a known state $\boldsymbol{u}_0$, $\boldsymbol{u} = \boldsymbol{u}_0 + \boldsymbol{\delta}$, to obtain

$$\frac{d\boldsymbol{\delta}}{dt} + \boldsymbol{f}'(\boldsymbol{u}_0)\cdot\boldsymbol{\delta} \approx -\left(\frac{d\boldsymbol{u}_0}{dt} + \boldsymbol{f}(\boldsymbol{u}_0)\right),$$

which defines a Newton method for this problem: on each time interval $I_n = (t_n, t_{n+1})$ and for $i = 0, 1, \dots$ until convergence, set $\boldsymbol{u}_0 = \boldsymbol{u}(t_n)$, solve

$$\frac{d\boldsymbol{\delta}}{dt} + \boldsymbol{f}'(\boldsymbol{u}_i)\cdot\boldsymbol{\delta} = -\boldsymbol{r}(\boldsymbol{u}_i), \; \text{and let} \;\; \boldsymbol{u}_{i+1} = \boldsymbol{u}_i + \boldsymbol{\delta},$$

where $\boldsymbol{r}(\boldsymbol{u}) := d\boldsymbol{u}/dt + \boldsymbol{f}(\boldsymbol{u})$, $\boldsymbol{\delta}(t_n) = 0$, and

$$\boldsymbol{f}'(\boldsymbol{u}) = \begin{bmatrix} 0 & -1 \\ \cos(u) & 0 \end{bmatrix}.$$

Using the basis (2.3) for the approximation of $\boldsymbol{\delta}$ and $\boldsymbol{u}$, we let $\boldsymbol{\delta} \approx \mathbf{Ba}$ and

$$\boldsymbol{u} \approx \boldsymbol{U} = [U, V]^{\mathrm{T}} = \mathbf{Bb}$$

where

$$\mathbf{B} = \begin{bmatrix} \varphi_1 & 0 & \varphi_2 & 0 & \dots & \varphi_m & 0 \\ 0 & \varphi_1 & 0 & \varphi_2 & \dots & 0 & \varphi_m \end{bmatrix},$$

and $\mathbf{a}$ and $\mathbf{b}$ are vectors, each containing $2m$ coefficients. Note in particular that the two first components of $\mathbf{a}$ are zero by construction of the basis and the fact that $\boldsymbol{\delta}(t_n) = 0$. This motivates the introduction of the matrix

$$\mathbf{B}_{\mathrm{red}} = \begin{bmatrix} \varphi_2 & 0 & \varphi_3 & 0 & \dots & \varphi_m & 0 \\ 0 & \varphi_2 & 0 & \varphi_3 & \dots & 0 & \varphi_m \end{bmatrix}$$

and the corresponding vector $\mathbf{a}_{\mathrm{red}}$. With this notation, we can formulate the Newton scheme as to recursively find $\mathbf{a}_{\mathrm{red}}$ such that

$$\left(\int_{t_n}^{t_{n+1}} \dot{\bar{\mathbf{B}}}_{\mathrm{red}}^{\mathrm{T}} \left(\dot{\mathbf{B}}_{\mathrm{red}} + \boldsymbol{f}'(\boldsymbol{U}_i)\, \mathbf{B}_{\mathrm{red}} \right) dt \right) \mathbf{a}_{\mathrm{red}} = - \int_{t_n}^{t_{n+1}} \dot{\bar{\mathbf{B}}}_{\mathrm{red}}^{\mathrm{T}} \boldsymbol{r}(\boldsymbol{U}_i)\, dt,$$

where $\bar{\mathbf{B}}$ is the modified $\mathbf{B}$ ensuring conservation. We write this problem as

$$\mathbf{S}\mathbf{a}_{\mathrm{red}} = \mathbf{f},$$

and the solution is updated by $\boldsymbol{U}_{i+1} = \boldsymbol{U}_i + \mathbf{B}_{\mathrm{red}}\mathbf{a}_{\mathrm{red}}$.

To ensure energy conservation, we can thus formulate the following algorithm.

1. Iterate a few times in the Newton using the conservative basis (in the first iteration, this can be chosen as (2.3)).
2. Find the expression of the current value of $\dot{U}$ in the basis (2.3), i.e., find the set $\{\alpha_j\}$, by solving the problem
$$\int_{t_n}^{t_{n+1}} \dot{\varphi}_i \sum_{j\geq 2} \dot{\varphi}_j \alpha_j \, dt = \int_{t_n}^{t_{n+1}} \dot{\varphi}_i \dot{U}\, dt, \quad i = 2, 3, \dots$$
3. Replace the basis function $\dot{\varphi}_k$ by the current value of $\dot{U}$ in $\dot{\bar{\mathbf{B}}}_{\mathrm{red}}$, using the recipe described in the previous Section, and after setting up $\mathbf{f}$, modify position $2k$ to
$$(\mathbf{f})_{2k} = -\left(\int_{t_n}^{t_{n+1}} \dot{U}\dot{V}\, dt + \cos(U(t_n)) - \cos(U(t_{n+1})) \right).$$
4. Repeat from 1 until convergence.

Since $\mathbf{S}$ has to be set up anew in each iteration irrespective of whether we change the basis or not, the additional cost is low.

We solve the problem using a first and a second order polynomial approximation on the interval $T = [0, 16]$, using twenty equally distributed time-steps. The accuracy of the numerical integration has to be sufficient for the integration of the "mass matrix" corresponding to

$$\int_{t_n}^{t_{n+1}} \dot{\bar{\mathbf{B}}}_{\text{red}}^{\mathrm{T}} \dot{\mathbf{B}}_{\text{red}} \, dt,$$

so we choose one-point Gaussian integration in the linear case and two-point Gaussian integration in the second degree polynomial case.

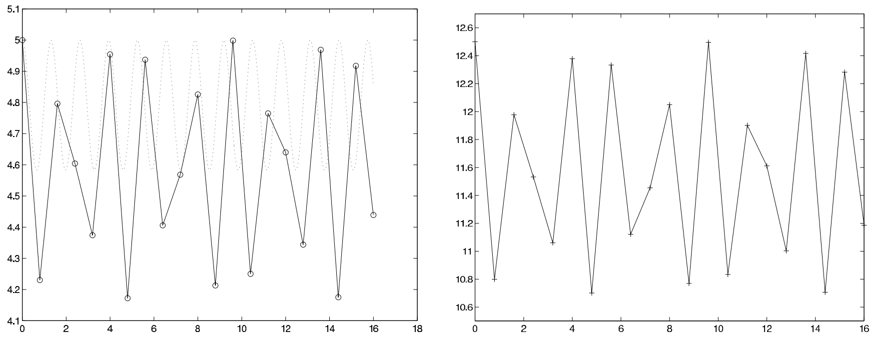

FIGURE 1. Linear polynomial solution and energy using one-point integration

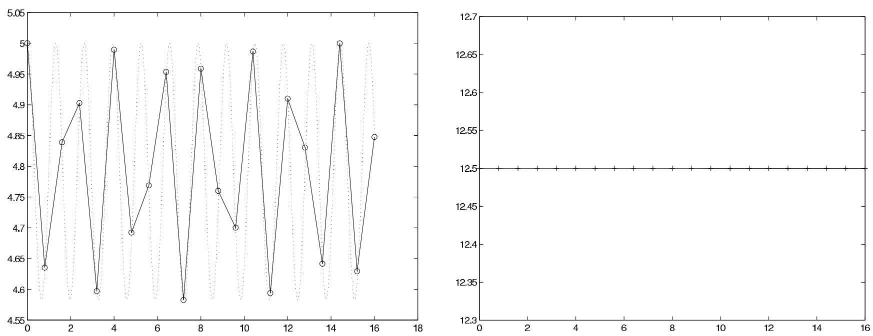

FIGURE 2. Linear polynomial solution and energy using the proposed method

In Fig. 1 we show the solution and the (interpolated) energy using a linear polynomial approximation without energy conservation, and in Fig. 2 we show the corresponding solution using the proposed method. Here, clearly, the conservation at the nodes is advantageous.

In Fig. 3 the solution and the (interpolated) energy using a second degree polynomial approximation without energy conservation is shown, and in Fig. 4 we find the corresponding solution using the proposed method. Here, we note that overshoots and undershoots

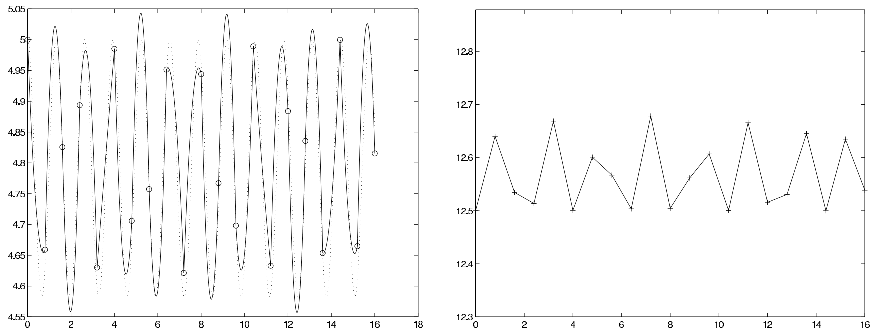

FIGURE 3. Second degree polynomial solution and energy using two-point integration

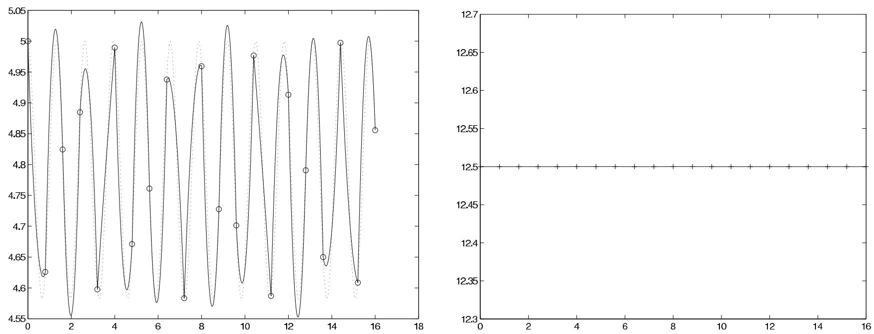

FIGURE 4. Second degree polynomial solution and energy using the proposed method

will still appear if the solution is plotted as a second degree polynomial; conservation is restricted to the discrete time levels.

4. Concluding Remarks

The basic continuous space–time finite element method only conserves energy exactly at discrete time-levels in case the numerical integration is (sufficiently) exact, which may be difficult to decide beforehand for nonlinear Hamiltonian problems. We have suggested a simple modification of the method which ensures energy conservation at discrete time-levels. In future work, we will make a more detailed study of the performance of the present approach compared with the different alternative methods proposed in the literature, in the case of vectorial Hamiltonian problems.

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