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Symplectic algorithms for viscoelastic and viscoplastic systems

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ABSTRACT

Standard numerical integration schemes neglect important features of the dynamics. Thus, they inevitably imply artificial dissipation and other parasitic artifacts. The paper presents some applications of symplectic integrators to the viscoelastic and viscoplastic systems and shows the advantages of such numerical schemes for long time periods. The mid - point rule, a simpler scheme of symplectic algorithm avoid the incremental method used until now in viscoelasticity and plasticity.

1. INTRODUCTION

Almost all the numerical methods used for nonlinear evolution mechanical phenomena are incremental. Loads or time interval are decomposed in a serie of small increments. Large time increment method as remarked by Ladevèze [1], Simo, Tarnow [2], Simo, Vu - Quoc [3] is an iterative procedure issues by an elastic calculus.

As presented by Ladevèze [4] the method is based on three principles: a division of equations in two groups, the first one concerning the separation of difficulties, i.e., one group of local equations in space variables (possible nonlinear) and one group of linear equations (possible globales in space variables); the second principle concerns an iterative procedure into two steps. We build alternately a solution from the first group and other solution from the second group. The first solution is local in space variable, possible nonlinear, while the second is linear generally global; the third principle uses a time - space approximation for the global approach. Ladevèze proofs that for numerous problems in plasticity and viscoplasticity this method converges in the case of certain values of parameters. The iterative processus may be controlled by means of a posteriori errors estimation.

But, the above considerations concern only a mathematical strategy. In dynamics, standard integration techniques are useful in the investigation of short - time qualitative phenomena, but may be severely limited in the study of long time qualitative phenomena.

Also, typically standard numerical integrators induce an artificial damping (or exciting) of the systems. In many applications the salient features of the solutions appear only after long time or large number of iterations; in these applications spurious damping or excitation may lead to misleading results.

Standard numerical integration schemes neglect important special features of the dynamics, in particular the time Δt - map of the phase space is symplectic (e.g. the motion of the space points from time 0 to time t preserves the Poincaré invariants). A new study method is named "conformal stability" that means the preservation of global structure and qualitative phenomena. It is possible to devise numerical integration algorithms that approximate the time Δt - map of the exact dynamics to any desired order in the time step and that are exactly symplectic.

The general symplectic algorithms are related to numerical integration of Hamiltonians and some authors like Sanz - Serna [5] consider that symplectic algorithms are members of the Runge - Kutta methods.

For elastodynamic systems the symplectic algorithms conserve the energy or momentum. Tarnow and Simo considered a general class of second order accurate algorithms, fourth order accurate that retain the stability and conservation properties. The mid - point rule is the simplest symplectic algorithm. The present paper applies this symplectic algorithm to a Maxwell body and for a viscoplastic system with isotropic hardening.

2. SYMPLECTIC RUNGE - KUTTA METHODS

For the system of differential equations, in general

$$\frac{dx}{dt} = f(x) \qquad 0 \le t \le \tau \tag{1}$$

An s stage Runge - Kutta method (generally implicit) which is a natural generalisation of the classical 4^{th} order one, is defined as follows. First, vectors k_i are determined by solving the simultaneous algebraic equations

$$k_i = f(x + \tau \sum_{j=1}^{s} a_{ij} k_j) \qquad i = 1,\dots,s \tag{2}$$

then the mapping $x \to x'$ is

$$x' = x + \sum_{j=1}^{s} b_j k_j \tag{3}$$

where a_{ij} and b_j are scalar constants which characterise the scheme. The so called Butcher table which lists a_{ij} and b_j as an s+1 by s matrix is often used to specify a given Runge-Kutta method.

Note that if $a_{ij} = 0$ for $i < j$, then the scheme is implicit. For general Runge - Kutta methods, the mapping (3) is not symplectic.

If we suppose that the differential system (1) is hamiltonian, i.e.

$$\dot{p} = -\frac{\partial H}{\partial q} \qquad \dot{q} = \frac{\partial H}{\partial p} \qquad p = \dot{q}$$

we have the relations

$$P_i = p_n + h \sum_{j=1}^{s} a_{ij} f(P_j, Q_j) \qquad p_{n+1} = p_n + h \sum_{i=1}^{s} b_i f(P_i, Q_i)$$

$$Q_i = q_n + h \sum_{j=1}^{s} a_{ij} g(P_j, Q_j) \qquad q_{n+1} = q_n + h \sum_{i=1}^{s} b_i g(P_i, Q_i)$$

$$1 \le i \le s$$

where f and g respectively denote the m - vectors with components $\partial H/\partial q_i$ and $\partial H/\partial p_i$ and P_i and Q_i are the interval stages corresponding to the p and q variables.

Sanz - Serna and Lasagni found that if the constants satisfy the conditions

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0; \qquad 0 \le 1, j \le s \tag{4}$$

identically, then the mapping is symplectic. Notice that for (4) to be satisfied, the scheme must be implicit.

The simplest solution (1 - stage, s = 1) which satisfies the conditions (4) is given by (for Runge - Kutta, order 2)

$$a_{11} = 1/2 \qquad b_1 = 1$$

and we have the scheme

$$k_1 = f(x + \frac{1}{2} \tau k_1) \qquad x' = x + \tau k_1 \tag{5}$$

or more concisely

$$x' = x + \tau f\left(\frac{x + x'}{2}\right) \tag{6}$$

which is known as the implicit midpoint rule and has order 2.

For the 2 -stage method we have, order 4 table

$$a_{ij} = \begin{bmatrix} 1/4 & 1/4 - \sqrt{3}/6 \\ 1/4 + \sqrt{3}/6 & 1/4 \end{bmatrix}; \qquad b = \{1/2 \quad 1/2\}$$

and the order 4. These schemes are the simplest examples of the family of Gauss - legendre method and the s - stage Gauss - Legendre method has order 2s. This family has a good stability.

3. SYMPLECTIC ALGORITHMS FOR VISCOELASTIC AND VISCOPLASTIC SYSTEMS

a) We consider a Maxwell body in 3D - space with notations from fig. 1.

The Hooke's and Newton's relations for spring and damper written for spherical and deviatonic tensor components are the following

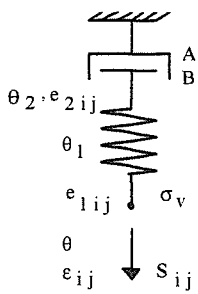

Fig. 1

$$\frac{1}{3}\sigma_v = \alpha\theta_1 \; S_{ij} = \beta e_{1ij} \tag{7}$$

$$\frac{1}{3}\sigma_v = A\,\dot{\theta}_2 \qquad S_{ij} = B\,\dot{e}_{2ij}$$

from which

$$\dot{\theta} = \dot{\theta}_1 + \dot{\theta}_2 = \frac{\dot{\sigma}_v}{3\alpha} + \frac{\sigma_v}{3A} \qquad \text{is the velocity of cubic dilation}$$

$$\dot{e}_{ij} = \dot{e}_{1ij} + \dot{e}_{2ij} = \frac{\dot{S}_{ij}}{\beta} + \frac{S_{ij}}{B} \qquad \text{is the distortion velocity.}$$

We may write the above relations with respect to the stress and strain tensor components, σ_{ij}, ε_{ij} as

$$\dot{\theta} = \dot{\varepsilon}_{11} + \dot{\varepsilon}_{22} + \dot{\varepsilon}_{33} = \frac{1}{3\alpha}(\dot{\sigma}_{11} + \dot{\sigma}_{22} + \dot{\sigma}_{33}) + \frac{1}{3A}(\sigma_{11} + \sigma_{22} + \sigma_{33}) \tag{8}$$

We have the general relation

$$\dot{e}_{ij} - \frac{1}{3}\dot{\theta} = \frac{1}{\beta}(\dot{\sigma}_{ij} - \frac{1}{3}\dot{\sigma}_v) + \frac{1}{B}(\sigma_{ij} - \frac{1}{3}\sigma_v) \tag{9}$$

Finally, for i = j = 1 and i = j = 2

$$\frac{1}{\beta}(\dot{\sigma}_{11} - \dot{\sigma}_{22}) + \frac{1}{B}(\sigma_{11} - \sigma_{22}) = \dot{\varepsilon}_{11} - \dot{\varepsilon}_{22}$$

Similar by, for i = j = 1 and i = j = 3 respectively i = j = 2, i = j = 3, it results

$$\frac{1}{\beta}(\dot{\sigma}_{11} - \dot{\sigma}_{33}) + \frac{1}{B}(\sigma_{11} - \sigma_{33}) = \dot{\varepsilon}_{11} - \dot{\varepsilon}_{33} \tag{10}$$

$$\frac{1}{\beta}(\dot{\sigma}_{22} - \dot{\sigma}_{33}) + \frac{1}{B}(\sigma_{22} - \sigma_{33}) = \dot{\varepsilon}_{22} - \dot{\varepsilon}_{33}$$

or matricial

$$\frac{d\boldsymbol{\sigma}}{dt} = -\frac{h\beta}{B}\boldsymbol{\sigma} + \dot{\mathbb{E}} \tag{11}$$

The differential motion system may be discretized in symplectic form

$$\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^n = -\frac{h\beta}{B}\boldsymbol{\sigma}^{n+1/2} + \dot{\mathbb{E}}^{n+1/2} \tag{12}$$

where

$$\dot{\mathbb{E}}^{n+1/2} = \frac{1}{2}(\dot{\mathbb{E}}^{n+1} + \dot{\mathbb{E}}^{n})$$

b) we consider a viscoplastic material with an isotropic hardening with the constitutive law:

[4]

$$\begin{bmatrix} \dot{\mathbb{E}}_p \\ -\dot{p} \end{bmatrix} = \dot{\lambda}_p \begin{bmatrix} \frac{\sigma}{\|\sigma\|} \\ -1 \end{bmatrix} \tag{13}$$

where

$$\dot{\lambda}_p = kz^m = k(\|\sigma\| - R - R_0)^m \tag{14}$$

$R = \lambda_p$ is the linear hardening law, λ - plastic coefficient

From the relation (13) we obtain the symplectic form by means of mid - point rule

$$\dot{\lambda}_p^{n+1/2} \begin{bmatrix} \frac{\sigma^{n+1/2}}{\|\sigma\|^{n+1/2}} \\ -1 \end{bmatrix} + \frac{1}{\lambda\tau} \begin{bmatrix} \sigma^{n+1/2} - \sigma^n \\ R^{n+1/2} - R^n \end{bmatrix} + \frac{1}{E\tau} \begin{bmatrix} tr(\sigma^{n+1/2} - \sigma^n) \\ 0 \end{bmatrix} = \begin{bmatrix} \dot{\mathbb{E}}_p^n \\ -\dot{p}^n \end{bmatrix} \tag{15}$$

where τ is a characteristic time, from which we determine

$$\begin{aligned} tr\sigma^{n+1/2} &= \frac{E\sigma}{3} tr\, \dot{\mathbb{E}}_p^n + tr\sigma^n \\ -\dot{\lambda}_p^{n+1/2} + \frac{R^{n+1/2}}{\lambda\tau} &= -\dot{p}^n + \frac{R^n}{\lambda\tau} \\ \sigma^{n+1/2} \left[\frac{1}{\lambda\tau} + \frac{\dot{\lambda}_p^{n+1/2}}{\|\sigma^{n+1/2}\|} \right] &= \dot{\mathbb{E}}_p + \frac{\sigma^n}{\lambda\tau} \end{aligned} \tag{16}$$

It results

$$z^{n+1/2} = -2\, \dot{\lambda}_p^{n+1/2} \lambda\tau + (\left\| \lambda\tau\, \dot{\mathbb{E}}_p^n + \sigma^n \right\| + \lambda\tau\, \dot{p}^n - R^n - R_0)$$

where

$$\gamma_n = (\left\| \lambda\tau\, \dot{\mathbb{E}}_p^n + \sigma^n \right\| + \lambda\tau\, \dot{p}^n - R^n - R_0)$$

If $\gamma_n < 0$, $z^{n+1/2} < 0$ and $\dot{\lambda}_p^{n+1/2} = 0$.

For $\gamma_n \geq 0$ i.e. viscoplastic case, we obtain the iterative system

$$\begin{aligned} \sigma^{n+1/2} &= (1 - \frac{\dot{\lambda}_p^{n+1/2} \lambda\tau}{\left\| \lambda\tau\, \dot{\mathbb{E}}_p^n + \sigma^n \right\|})(\lambda\tau\, \dot{\mathbb{E}}_p^n + \sigma^n) \\ tr\sigma^{n+1/2} &= \frac{E\tau}{3} \dot{\mathbb{E}}_p^n + tr\sigma^n \\ R^{n+1/2} &= \lambda\tau\, \dot{\lambda}^{n+1/2} + \lambda\tau(-\dot{p}^n + \frac{R^n}{\lambda\tau}) \end{aligned}$$

The convergence of the iterations are studied by means of a posteriori indicators based on the differences

$$\Delta s_n = s_n - s_e$$
$$\Delta s_{n+1/2} = s_{n+1/2} - s_e$$

where $s = (\dot{\mathbb{E}}_p, \dot{p}, \sigma, R)$, s_e - "exact" solution

4. NUMERICAL EXAMPLE

We consider a viscoplastic Chaboche's model one dimensional bar for which:

$$z = |\sigma - \beta| + \frac{a}{c}\beta^2 - R - R_0; \qquad R = \lambda\,[1 - \exp(-\delta p)]$$

$$R = \lambda p = \lambda \int_0^p \delta^{1/2} \exp(-\frac{1}{2}\delta p) = \frac{2\lambda}{\delta^{1/2}}[1 - \exp(-\frac{1}{2}\delta p)]$$

The potential plastic function

$$\phi(\sigma, \beta, R) = \frac{k}{m+1} z^{m+1}$$

and we select $\delta = 10$, $m = 12$, $R_0 = 6$ MPa, $a = 300$ MPa, $k = 1/150^m$, $c = 24800$ MPa, $\beta = C\alpha$, $\lambda = 80$ MPa, $E = 137600$ MPa, $\varepsilon_{max} = 1{,}2 \cdot 10^{-3}$.

We compute first the elastic solution and the next iterations in symplectic mid - point rule form.

The error indicator is selected by the expression:

$$e = \frac{\|s_{n+1/2} + s_n\|}{\frac{1}{2}(\|s_{n+1/2}\| + \|s_n\|)}$$

The final results obtained by a gradient method are illustrated in fig. 2 and the errors evolution in fig. 3.

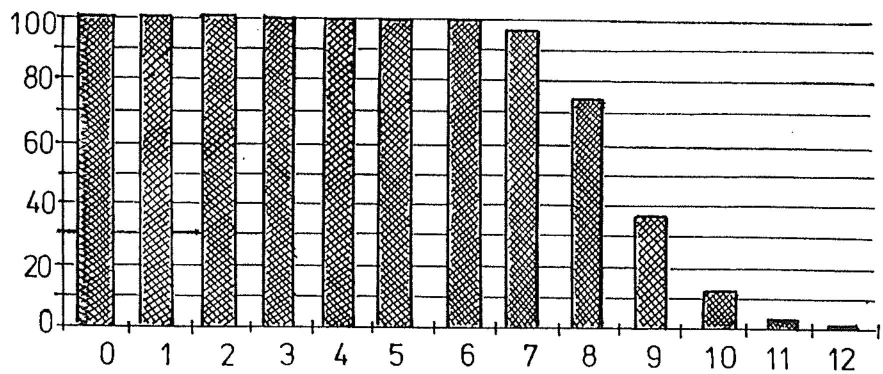

Fig. 2

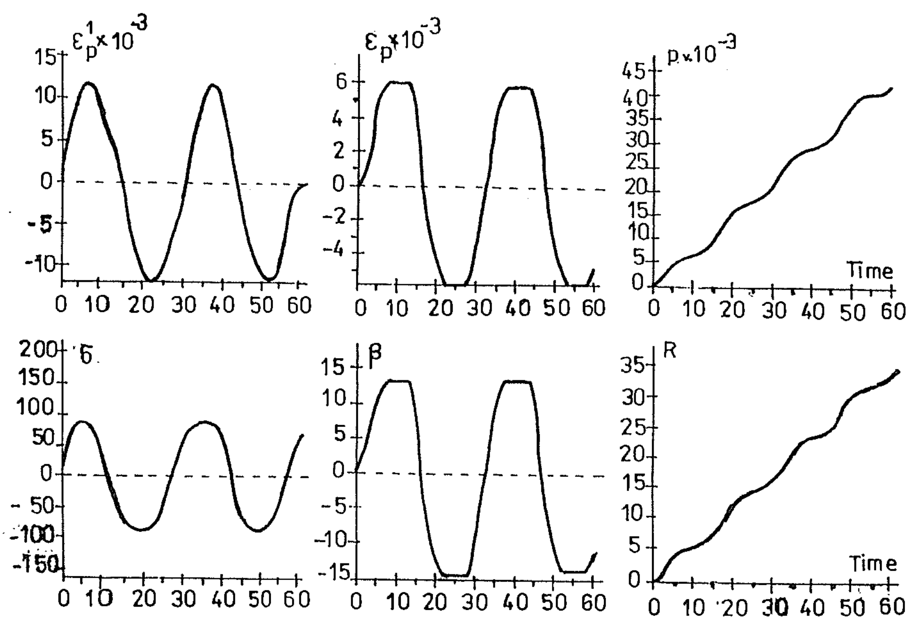

Fig. 3

5. CONCLUSIONS

The symplectic integration presents an alternative computation for large displacements and long time behaviour more effective than incremental method. These type of computations preserves some invariants and have a physical means some of them explained in the basic body paper different from other approaches purely mathematics. The numerical experiences must be extended to other examples.

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