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ON SOME COMPOSITE SCHEMES OF TIME INTEGRATION IN STRUCTURAL DYNAMICS

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Abstract: Numerical simulations of time-dependent behaviour of advances structures need the analysis of systems of partial differential equations of hyperbolic type, whose semi-discretization, using the Fourier multiplicative decomposition together with the finite element or similar techniques, leads to large sparse systems of ordinary differential equations. Effective and robust methods for numerical evaluation of their solutions in particular time steps are required; thus still new computational schemes occur in the engineering literature. This paper presents certain classification of such approaches, together with references to their expectable accuracy and some practical applications.

Keywords: structural dynamics, time-integration schemes

MSC: 74H15, 65M20, 65D30

1. Introduction

Physical formulations of computational tasks in continuum mechanics, motivated by the analysis of advanced structures, needed in civil engineering, result in the initial and boundary value problems for certain hyperbolic systems of partial differential equations of second order, in the simplest case linear, but frequently containing some nonlinear terms. Such problems can be handled using the multiplicative Fourier decomposition of their solutions to functions of Cartesian coordinates in the (in general) 3-dimensional Euclidean space \mathbb{R}^3 and to functions of time on certain finite time interval, starting from zero time. The complete evaluation using orthogonal Fourier (or similar) series is available just in sufficiently simple cases like [6], otherwise some discretization technique in \mathbb{R}^3 is needed, which leads to large systems of ordinary differential equations; for a possible approach to the convergence analysis see [7].

Numerical analysis relying (at least for appropriate linearized formulations) on the knowledge of exact solutions of such problems, analogous to [10] for a parabolic

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(heat transfer) problem, suffer from their general complex forms. Consequently robust, stable, reliable and effective direct integration algorithms for the construction of approximate solutions, step by step in time, are needed – cf. [3], Chap. 9. Most existence, uniqueness, convergence, etc. proofs utilize finite differences for the approximation of time derivatives of vectors of unknown variables, as sketched in [21]. An original idea of Newmark [18] is to solve a system including second time derivatives from Taylor series (approximate ones, motivated by the mean value theorem), constructed for both function values and first time derivatives, in particular time steps; for its modern convergence analysis see [13]. Attempts to increase numerical damping without degrading the order of accuracy can be documented on [8], [11] and [1]; [14] shows even a (rather complicated) possibility to improve even the order of accuracy. Other class of algorithms, based on operator splitting, comes from [9].

Unlike all one-step methods derived from [18], an intermediate time step by Bathe is hidden in [2] and [4]: the first half-step is based on the simple rectangular integration rule, the second one on the one-side formula for numerical differentiation, formally the same for function values and first time derivatives. Although this approach brings no improvement of the order of accuracy, some computational advantages can be registered. Recently 2 new relevant papers occurred: [17] brings a further improvement of [2] and [4], whereas the new Wen algorithm by [23] suggests a special division of h into 3 substeps. We shall sketch the expectable numerical benefits of the above sketched approaches, together with certain unified formulation of such class of algorithms, open to further generalizations, and with some references to the original numerical experiments.

2. Physical, mathematical and computational considerations

For the introduction of a model problem, let \mathbb{R}^3 be supplied by the Cartesian coordinate system $x=(x_1,x_2,x_3)$. Let Ω be some domain, representing a construction, or its selected part, in \mathbb{R}^3 , with its (sufficiently smooth) boundary $\partial\Omega$, whose supported part is $\Theta\subseteq\partial\Omega$, the remaining one $\Gamma=\partial\Omega\setminus\Theta$. (The possible simplifications for \mathbb{R}^2 or \mathbb{R}^1 are evident.) Moreover, let $\mathcal{I}=[0,\tau]$ be a time interval where τ denotes its positive length ($\tau\to\infty$ is not forbidden). Any time t will be considered from I; the upper dots will refer to d/dt briefly. Let $u(x,t)=(u_1(x,t),u_2(x,t),u_3(x,t))$ be the (a priori unknown) displacement on $\Omega\times\mathcal{I}$, related to the initial geometrical configuration (with t=0), connected with certain strain tensor $\varepsilon(u)\in\mathbb{R}^{3\times3}_{\mathrm{sym}}$ and also with the stress tensor $\sigma\in\mathbb{R}^{3\times3}$ satisfying

$$\sigma = \mathcal{S}(\varepsilon(u)) \text{ on } \Omega \times \mathcal{I} \tag{1}$$

where S refers to some algebraic constitutive relation; the above sketched symmetry can be interpreted as the property of Boltzmann continuum. The geometrical linearization (appropriate at least for the first estimate) of (1) is based on the formula $\varepsilon_{ij}(u) = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$ for every $i, j \in \{1, 2, 3\}$, whereas the physical linearization

$$S(\varepsilon(u)) = E\varepsilon(u) \text{ on } \Omega \times \mathcal{I},$$
 (2)

containing $E \in \mathbb{R}^{(3\times3)\times(3\times3)}_{\mathrm{sym}}$ defined on Ω , comes from the empirical Hooke law (very special for orthotropic or even isotropic materials, homogeneity is not necessary here). The material density ρ will be considered as time-independent on Ω .

We shall work with the standard Cauchy initial conditions

$$u(.,0) = u_0, \quad \dot{u}(.,0) = \hat{u}_0 \quad \text{on } \Omega$$
 (3)

for some prescribed \bar{u}_0 and \hat{u}_0 on Ω (zero-valued frequently, except seismic simulations). The time development of u is then influenced by

- i) the volume load $f = (f_1, f_2, f_3)$ on $\Omega \times \mathcal{I}$,
- ii) the surface (or, alternatively, interface contact) load $g = (g_1, g_2, g_3)$ on $\Gamma \times \mathcal{I}$,
- iii) the forced support motion $w = (w_1, w_2, w_3)$ on $\Theta \times \mathcal{I}$.

Clearly ii) refers to the Neumann (or similar) boundary conditions and iii) to the Dirichlet ones. In general, the dependence of f, g and w on u is also possible, although this typically disturbs any linearization.

We shall now work with the notation

$$(\omega, \varpi)(t) = \int_{\Omega} \omega(x, t) \ \varpi(x, t) \ dx, \quad \langle \omega, \varpi \rangle(t) = \int_{\partial \Omega} \omega(x, t) \ \varpi(x, t) \ ds(x)$$

for any scalar functions ω and ϖ integrable in the required sense; the generalization of this notation for vector and tensor functions (needed here, too) is straightforward. Following [5], using a virtual (arbitrary admissible) displacement $v = (v_1, v_2, v_3)$ on Ω , zero-valued on Θ , assuming a closed physical system, we can formulate the principle of conservation of energy

$$(\varepsilon(v), \sigma) = (v, f - f_{\diamond}) + \langle v, g \rangle \text{ on } \mathcal{I}$$
 (4)

where

$$f_{\diamond} = \rho \ddot{u} \text{ on } \Omega \times \mathcal{I} \,.$$
 (5)

is the force of inertia. Consequently (1), (2), (4) and (5) yield

$$(v, \rho \ddot{u}) + (\varepsilon(v), \alpha E \dot{\varepsilon}(u_{\star})) = F(v) \text{ on } \mathcal{I}$$
 (6)

with

$$F(v) = (v, f) + \langle v, g \rangle$$
 on \mathcal{I} . (7)

Nevertheless, the formulation (6) with (7) is not realistic because of the irreversible energy lost by damping, explained as the transformation of mechanical energy to thermal one on the contact between Ω and its surrounding in any time from \mathcal{I} . Two simplest models incorporating this effect are

$$f_{\diamond} = \rho(\ddot{u} + \beta \dot{u}) \text{ on } \Omega \times \mathcal{I},$$
 (8)

known as mass damping, and

$$S(\varepsilon(u)) = E(\varepsilon(u) + \alpha \dot{\varepsilon}(u)) \text{ on } \Omega \times \mathcal{I},$$
(9)

known as structural damping, referring to the Kelvin viscoelastic model; α and β here must be seen as certain new material characteristics. Both these linear models are combined frequently; for more such considerations see [22]. Another useful technique relies on the implementation of an additive decomposition $u_{\star} = u - w$, working with some reasonable extension of w from $\Theta \times \mathcal{I}$ to $\Omega \times \mathcal{I}$. Consequently, instead of (6) with (7), now (1), (9), (4) and (8) yield

$$(v, \rho \ddot{u}_{\star}) + (v, \beta \rho \dot{u}_{\star}) + (\varepsilon(v), \alpha E \dot{\varepsilon}(u_{\star})) + (\varepsilon(v), E \varepsilon(u_{\star})) = F(v) \text{ on } \mathcal{I}$$
(10)

with

$$F(v) = (v, f) + \langle v, g \rangle - (v, \rho \ddot{w}) - (v, \beta \rho \dot{w}) - (\varepsilon(v), \alpha E \varepsilon(\dot{w})) - (\varepsilon(v), E \varepsilon(w)) \text{ on } \mathcal{I}.$$
 (11)

Assuming $w(.,0) = u_0$ and $\dot{w}(.,0) = \hat{u}_0$ on Ω , the Cauchy initial conditions (3) for u_{\star} and \dot{u}_{\star} become homogeneous.

For numerical evaluations some approximations of functions on Ω and $\partial\Omega$ of a finite dimension n are needed; the study of convergence properties refers to the limit passage $n \to \infty$. For (almost) every $x \in \Omega$ and $t \in I$ the generalized Fourier decomposition $u_{\star}(x,t) = \phi_k(x)\psi_k(t)$, applying an Einstein summation index $k \in \{1,2,\ldots,n\}$, is available. All functions $\phi_1,\phi_2,\ldots,\phi_n$ are a priori known (mostly not orthogonal in a corresponding unitary space, but usually with a small compact support, typically in the finite element method). Let us choose, step-by-step, $v = \phi_j$ in (10) for all $j \in \{1,2,\ldots,n\}$, and consider (for simplicity, thanks to the appropriate choice of $\phi_1,\phi_2,\ldots,\phi_n$) $\psi_k(t) \approx u_{\star}(x_k,t)$ in selected points $x_k \in \Omega$. Consequently, in the remaining text, similarly to [13], [4], [17] and [23], we can understand $\mathcal{U}(t)$ as the vector of length n composed from $\psi_1(t),\psi_2(t),\ldots,\psi_n(t)$. In the analogous way, $\mathcal{F}(t)$ can denote the vector of the same length generated by the right-hand side of (10).

Thus we receive, instead to (10), some large (typically sparse) system of ordinary differential equations

$$M\ddot{\mathcal{U}} + C\dot{\mathcal{U}} + K\mathcal{U} = \mathcal{F} \text{ on } \mathcal{I}$$
 (12)

The matrices M, C and K from $\mathbb{R}^{n \times n}_{\text{sym}}$ here, well-known as the mass, damping and stiffness matrices, are crucial for the numerical analysis of the problem.

Clearly (10) corresponds to just one part of structure, connected with its other parts by some interface conditions. For simplicity, let us suppose that all such conditions can be written in the same form as those boundary ones on Γ or Θ using $\sigma - \sigma_{\times}$, $u - u_{\times}$, etc., instead of σ , u, etc., in (4) and the following relations; \cdot_{\times} refers to some neighbour domain. Consequently, (10) is transformed from 1 partial differential equation to a system of such equations, whose number corresponds to the number of structural parts. Therefore the size of the system (12) increases dramatically (in comparison with a model problem), the choice of functions ϕ determines the number

and location of non-zero elements in particular square blocks (whose overlapping comes from interface conditions) in all square matrices occurring in (12) and also in (13), as presented lower (needed for practical calculations), and the numbering of domains influences the positions of such blocks. Moreover, the results of optimization of such properties for the sequential algorithms need not be valid in the case of parallel processing, depending on the available hardware and software support.

3. Classical and novel time integration schemes

Most engineering papers start their theoretical and computational analysis with the semi-discretized system (12), although for nearly all applications some relations like $K = n^2 \bar{K}$ and $C = n\bar{C}$ with bounded $\bar{K}, \bar{C}, M \in \mathbb{R}^{n \times n}_{\text{sym}}$ hold, namely for regular and semi-regular families of decompositions to finite elements, which is important for the convergence properties and stability of computational algorithms. Also the analysis of nonlinear effects, forcing the dependencies $C(\mathcal{U})$, $K(\mathcal{U})$ or even $\mathcal{F}(\mathcal{U})$ and $M(\mathcal{U})$, making use of some quasi-Newton iterations, is non-trivial, as sketched in [21]: certain quasi-linearity conditions from [20] must be satisfied. However, such considerations will be omitted in this short paper.

We shall now present a unified form of above mentioned approaches. We shall work just with the decomposition of I to m equidistant subintervals of length $h = \tau/m$, i. e. to the subintervals $\mathcal{I}_s = ((s-1)h, sh]$ where $s \in \{1, \ldots m\}$, with the final aim $m \to \infty$. For the brevity we shall use the notation $\mathcal{U}_s = \mathcal{U}(sh) \in \mathbb{R}^n$ and analogously some \mathcal{F}_s , taken as $\mathcal{F}(sh)$, as the mean value of $\mathcal{F}(.)$ over \mathcal{I}_s , or in some similar way, to optimize the error of numerical quadrature. All algorithms come from the fully discretized modification of (12)

$$M\ddot{\mathcal{U}}_s + C\dot{\mathcal{U}}_s + K\mathcal{U}_s = \mathcal{F}_s \text{ on } \mathcal{I}_s \text{ for each } s \in \{1, \dots, m\},$$
 (13)

derived from some formulae for numerical differentiation or quadrature based on appropriate relations between u_s , \dot{u}_s and \ddot{u}_s and other quantities. Their computational efficiency depends on the possibility to evaluate \mathcal{U}_s , $\dot{\mathcal{U}}_s$ and $\ddot{\mathcal{U}}_s$ applying (13), just from \mathcal{U}_{s-1} , $\dot{\mathcal{U}}_{s-1}$ and $\ddot{\mathcal{U}}_{s-1}$, which is true for all following schemes except the classical finite difference one (which is the well-known drawback of such scheme, utilizing an additive fictive node, in our case related to s=-1, i. e. to the hypothetical time -h). The above sketched homogenization of the Cauchy initial conditions (3) is not obligatory here, i. e. we are able to work also with the modified versions of (10) containing u instead of u_* and of (11) where all additive terms including w are missing, forcing $u(., sh) \approx w(sh)$ on Θ by another computational technique. The appropriate vectors $\bar{\mathcal{U}}$ and $\hat{\mathcal{U}}$ can be then derived from the Cauchy initial conditions (3) with \bar{u} and \hat{u} .

We are now ready to compare the above introduced algorithms, together with some remarks to their expectable convergence quality. All symbols I refer to the unit matrix from $\mathbb{R}^{n\times n}$; zeros mean also the zero vectors and matrices from \mathbb{R}^n or $\mathbb{R}^{n\times n}$. The MAPLE software support has been utilized. For the brevity, all

schemes here take the unified form $\mathcal{KU} = \mathfrak{F}$ where \mathcal{K} is some real square matrix of integer order p and \mathcal{U} , \mathfrak{F} are vectors of length p containing various real functions. Only the necessary first steps $s \in \{1, 2, \ldots\}$ are presented for easy comparison of different schemes. However, all schemes start with s = 0 in (13) formally to set some reasonable $\ddot{\mathcal{U}}_0$, unlike \mathcal{U}_0 and $\dot{\mathcal{U}}_0$ induced by (3); we shall see that the finite difference algorithm needs still another artificial step.

a) The finite difference algorithm works with the simplest formulae of numerical differentiation to obtain $\dot{\mathcal{U}}_s$ and $\ddot{\mathcal{U}}_s$. We have

$$\mathcal{K} = \begin{bmatrix} -I & 0 & 0 & I & 0 & 0 & 0 \\ 0 & M & C & K & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & M & C & K \\ I & 0 & 0 & -2I & -h^2I & 0 & I \\ 0 & 0 & 0 & -I & 0 & -hI & I \end{bmatrix}, \quad \mathfrak{U} = \begin{bmatrix} \mathcal{U}_{-1} \\ \ddot{\mathcal{U}}_0 \\ \dot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_1 \\ \dot{\mathcal{U}}_1 \\ \ddot{\mathcal{U}}_1 \end{bmatrix}, \quad \mathfrak{F} = \begin{bmatrix} 2h\hat{\mathcal{U}}_0 \\ \mathcal{F}_0 \\ \hat{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_0 \\ \mathcal{F}_1 \\ 0 \\ 0 \end{bmatrix}.$$

Its simplicity (1st and 2nd derivatives are replaced by 1st and 2nd differences formally) supports the transparency of all convergence proofs, as sketched in [21]. However, all numerical implementations suffer from the above mentioned drawback. The hypothetical alternative of exact solution of (13) cannot avoid the expensive evaluation of complex eigenvalues and eigenvectors of sparce matrices, although the resulting solution is real. The convergence $\mathcal{O}(h^2)$ of the differentiation formulae (under certain additional data smoothness assumptions) in any s-th step forces the convergence $\mathcal{O}(h)$ (at least) for a finite \mathcal{I} . This is true (in slight modifications) for b) and c) and partially even to d), too, although some such formulae are replaced by certain numerical quadrature rules.

b) The motivations for the **Newmark algorithm** and its practical implementations are studied in [15] in details; for its convergence properties cf. [21]. The principle idea is to express \mathcal{U}_s and $\dot{\mathcal{U}}_s$ ($s \in \{1, 2, \ldots\}$ again) using the Taylor polynomials separately, with $\ddot{\mathcal{U}}_s$ occurring in the additive error terms. We have

$$\mathcal{K} = \begin{bmatrix} M & C & K & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & M & C & K \\ hI & I & 0 & hI & -2I & 0 \\ h^2I & 2hI & 2I & 0 & 0 & -2I \end{bmatrix}, \quad \mathfrak{U} = \begin{bmatrix} \ddot{\mathcal{U}}_0 \\ \dot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_1 \\ \dot{\mathcal{U}}_1 \\ \ddot{\mathcal{U}}_1 \end{bmatrix}, \quad \mathfrak{F} = \begin{bmatrix} \mathcal{F}_0 \\ \hat{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_0 \\ \ddot{\mathcal{F}}_1 \\ 0 \\ 0 \end{bmatrix}.$$

Various modifications of this algorithms, preserving the same accuracy and efficiency can be found in the literature: e.g. the last row of the left-hand-side matrix can be replaced by $\begin{bmatrix} h^2I & 4hI & 4I & h^2I & 0 & -4I \end{bmatrix}$, which is motivated by the fact that the evaluation of u_s can work even with linear Taylor polynomials, similarly to that of $\dot{\mathcal{U}}_s$, or even by $\begin{bmatrix} 0 & hI & I & 0 & hI & -2I \end{bmatrix}$, substituting this by the rectangular quadrature rule.

c) The composed **Bathe algorithm** uses (in general) the rectangular quadrature rule for the odd steps and the Euler backward differentiation formula for the even steps. We have

$$\mathfrak{U} = \left[egin{array}{c} \ddot{\mathcal{U}}_0 \\ \dot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_1 \\ \dot{\mathcal{U}}_1 \\ \ddot{\mathcal{U}}_2 \\ \dot{\mathcal{U}}_2 \\ \mathcal{U}_2 \end{array}
ight], \quad \mathfrak{F} = \left[egin{array}{c} \mathcal{F}_0 \\ \dot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_0 \\ \mathcal{F}_1 \\ 0 \\ 0 \\ \mathcal{F}_2 \\ 0 \\ 0 \end{array}
ight].$$

The convergence in particular steps $O(h^2)$ can be guaranteed, similarly to b); thus various combinations with b) in particular steps are available. Some variable positive step lengths, namely h_1 instead of h in the 5th and 6th lines of K and h_2 in its 8th and 9th lines can be implemented, too.

d) The Wen algorithm tries to improve c) joining an additional step (thus the typical triple of steps occur). Such step relies on the Houbolt backward differentiation formula, with the guaranteed convergence $\mathcal{O}(h^3)$, in addition to the Euler one in the preceding step. We have

$$\mathfrak{U} = \left[egin{array}{c} \ddot{\mathcal{U}}_0 \\ \dot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_1 \\ \dot{\mathcal{U}}_1 \\ \dot{\mathcal{U}}_1 \\ \dot{\mathcal{U}}_2 \\ \dot{\mathcal{U}}_2 \\ \ddot{\mathcal{U}}_2 \\ \ddot{\mathcal{U}}_3 \\ \dot{\mathcal{U}}_3 \\ \ddot{\mathcal{U}}_3 \end{array} \right], \quad \mathfrak{F} = \left[egin{array}{c} \mathcal{F}_0 \\ \dot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_0 \\ \ddot{\mathcal{U}}_1 \\ \ddot{\mathcal{U}}_1 \\ \ddot{\mathcal{U}}_1 \\ \mathcal{F}_2 \\ \ddot{\mathcal{U}}_2 \\ \ddot{\mathcal{U}}_2 \\ \ddot{\mathcal{U}}_2 \\ \ddot{\mathcal{F}}_3 \\ \ddot{\mathcal{U}}_3 \\ \ddot{\mathcal{U}}_3 \end{array} \right].$$

The variable positive step lengths, namely h_1 instead of h in the 5th and 6th lines of K, h_2 in its 8th and 9th and h_3 in its 11th and 12th lines, make the last formula still more complicated, but offer a possibility of algorithm optimization.

4. Conclusions with references to applications

In general, no formal proof of the better convergence of c) or d) than b) is available. However, many numerical experiments have been performed using the software package RFEM. Their results seem to justify good properties of c) namely in the case of seismic response where non-zero oscillating values of w in (11) occur, as demonstrated by [16], but one cannot ignore the increased number of arithmetic operations in particular steps of c) in comparison with b). The practical implementation of d) is still in development. Also the parallel computations can lead to quite other priorities, even to the rehabilitation of selected explicit algorithms – cf. [19].

A more extensive proper theoretical study comparing the convergence properties of a), b), c), d) is being prepared. Consequently the continuing work on further practical applications based on RFEM (contact problems, brittle and quasi-brittle fracture, ...), with the participation of Ph.D. students at Brno University of Technology, should lead to the validation of theoretical results, related to both projects from *Acknowledgements*.

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