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Conservative single-step time-integration schemes with higher-order accuracy for multi-particle dynamics with local two-point potentials

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Abstract

A general framework for algorithms that conserve linear and angular momenta for problems of multi-particle mechanics is presented. Conditions for energy conservation are derived, and different manners in which this may be achieved are discussed. A detailed examination of the relative equilibrium states is carried out, and conditions under which algorithms preserve these states are given; in particular, algorithms can be designed to capture the *exact* solutions of relative equilibrium problems, although these algorithms are unlikely to be energy-conserving. Following on from the approach proposed by Argyris et al. [J.H. Argyris, P.C. Dunne, T. Angelopoulos, Dynamic response by large step integration, Earthquake Engrg. Struct. Dynam. 2 (1973) 185–203], the local accuracy characteristics of algorithms are investigated thoroughly, and it is shown that there is no limit to the order of accuracy that can be achieved by algorithms in this framework, even for problems with time-dependent forces. No extra stages of calculation or additional degrees of freedom are required to be present, although the sparsity of the resulting system of equations is compromised. A few examples of new algorithms are given, and their properties verified on some model problems.

Keywords: Higher-order accuracy; Conservation; Relative equilibria; Time reversibility

1. Introduction

In this work, we explore the possibilities for higher-order accuracy in the design of algorithms to solve non-linear, dynamic problems involving large displacements. The exact solutions to these problems are generally unavailable in closed form, existing only as power series in Δt. Our sphere of interest concerns undamped systems for which the forces are derived from a single scalar function, known as *monogenic* systems [2]. We are particularly interested in *Hamiltonian* systems, for which the external forces are *conservative*; in these cases, the Hamiltonian function H defining the total energy of the system is *constant* throughout the motion.

Fundamental to the accuracy of an algorithm is the concept of *stability*. There are many different definitions of algorithmic stability that exist; e.g., [3–6] and many more besides. Loosely speaking, each relates to whether or not an algorithm produces a solution that is bounded as the total time $T \to \infty$ (for some fixed Δt), assuming the exact solution to be bounded also. In any quest for accuracy, stability is essential; therefore we seek to ensure stability first, and subsequently concentrate on improving the accuracy of an algorithm. As a consequence, we will deal exclusively with *implicit* schemes,

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since explicit algorithms are known to be only conditionally stable [3,7]. For monogenic systems, we can formulate the definition of stability in terms of the change in energy within a single time-step, as was first done by Belytschko and Schoeberle [5]. Specifically, the internal energy of the system must not be allowed to increase beyond the amount of work done by the external forces during the time-step. It is possible to design algorithms that satisfy this condition for all time-step sizes; such algorithms are thus *unconditionally stable* for general non-linear problems.

For Hamiltonian systems, it is also possible to design algorithms that preserve the symplectic nature of the system: a detailed discussion of the construction of symplectic algorithms is given by Simo and Tarnow in Appendix II of [8], and also by Marsden and West [9]. It has been shown by Zhong and Marsden, however, that an algorithm cannot be symplectic and simultaneously conserve energy for a general non-integrable system, assuming the time-step size to be constant [10]. Also, algorithms which are spectrally stable and dissipate energy for linear problems cannot be symplectic, as demonstrated by Simo and Tarnow [8]. A choice must therefore be made, between the properties of symplecticity and energy conservation or dissipation, from the outset. Given the fact that a definition of stability is readily available in terms of energy growth, we elect to design algorithms based on energy criteria. In support of this decision, Simo and co-workers have shown that for stiff problems of non-linear elasticity, energy-conserving algorithms tend to perform better than symplectic algorithms [8,11,12].

Unconditional stability alone is not enough to ensure the overall accuracy of an algorithm. An extreme example of this was given by Ortiz [13], where a convergent, energy-conserving algorithm is shown to give completely inaccurate results after only a small number of time-steps. In the case of *systems with symmetries*, however, we have more information. These systems furnish two other constants of motion, namely the total linear momentum $\mathscr{L}$ and the total angular momentum $\mathscr{J}$, each of which gives information about the qualitative (as well as quantitative) nature of the solution. Algorithms can also be designed to conserve these momenta for such systems, in conjunction with energy conservation, with a view to achieving better accuracy. The importance of angular momentum conservation in regard to accuracy was noted by Betsch and Steinmann [14], and classic examples of such algorithms are given by Simo and co-workers [8,15].

As a consequence of having constant linear and angular momenta, an additional property of systems with symmetries is the existence of families of fully integrable solutions, each induced by a particular combination of initial conditions. These are known as *relative equilibrium states* (or *steady states*), and give further information about the stability of the system: see [16,17] for a detailed account. Algorithms that conserve momenta can be designed to preserve these relative equilibrium states (when the initial conditions arise): those that do give solutions to a steady-state problem that physically resemble the exact solution, and thus may have enhanced stability and accuracy properties for problems of *approximately* steady-state motion. An analysis of two popular time-integration schemes in this regard is given by Gonzalez and Simo [12] and further discussion on the importance of preservation of relative equilibrium orbits is provided by Armero and Romero [18]. Examples of algorithms designed to preserve relative equilibria include the energy–momentum algorithm of Simo and Tarnow [8], and subsequent algorithms that dissipate energy by Armero and co-workers [18–20].

One further property of dynamical systems in physics that we touch upon briefly is that of time-reversibility [21], which is closely related to the uniqueness of a dynamic response. In the discrete case, however, it is not certain that, at any given point on the solution, negating the time-step would recover the solution given at the previous point in time. Algorithms that guarantee this are described as *time-reversible*. An early citation of the importance of this property in the engineering context is due to Argyris et al. [1], and further examples of such algorithms relevant to our work are the energy-conserving algorithm proposed independently by Simo and Gonzalez [11] and Reich [22], as well as the symplectic mid-point rule [8,15,23,24] and the so-called assumed distance method [25].

It is widely accepted that an algorithm should be at least second-order accurate (e.g. [4]), and the energy–momentum algorithms of Simo et al. mentioned earlier all satisfy this requirement. Various ways to increase the order of accuracy have been proposed. These include *composition methods*, whereby greater accuracy is achieved by computing intermediate results at additional points within a single time-step; example algorithms include those given independently by Yoshida [21], Forest [26] and Tarnow and Simo [27]. A disadvantage is that the procedure involves stepping backwards in time, using a larger time-step size than the original algorithm; this makes the principle less attractive for algorithms that are not time-reversible, and increases the risk of instability or divergence during the non-linear iteration process. Another approach to enhancing accuracy can be taken by discretising the equations of motion using *finite elements in time*, where the accuracy can be prescribed by the degree of the polynomial basis functions chosen; example algorithms include those of Betsch and Steinmann [28] for non-linear dynamics. These schemes bear close resemblance to Gauss Runge–Kutta methods, as described in the Appendix of [28].

Both of these strategies to improve accuracy entail additional computation cost, due to the calculation of intermediate results or the presence of extra degrees of freedom in the temporal domain of the problem. A third approach, aimed at avoiding this additional cost, is based on *Taylor series expansions* of the state variables; for linear dynamics, this method is equivalent to using Padé approximations to the exact solution. Early work was done along these lines for non-linear analysis by Argyris et al. [1,29], who presented *arbitrarily* accurate algorithms that are time-reversible, although not conservative. They were followed by LaBudde and Greenspan, who produced arbitrarily accurate schemes that also conserve