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ASYNCHRONOUS/MULTIPLE TIME INTEGRATORS FOR MULTI-FRACTURING SOLIDS AND DISCRETE SYSTEMS

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Summary. *The current work presents an asynchronous/multiply time stepping integration scheme for the simulation of dynamic systems exhibiting multi-fracture and discrete features. It is a novel extension of existing methodologies to the discrete element simulation and several fundamental developments in both theoretical and implementation aspects are achieved that are essential for the success of the approach. It is shown that the resulting AVI/MTS discrete element method can achieve a nearly optimal speed-up for typical discrete systems. However, the stability is the issue that needs to be further addressed.*

1 INTRODUCTION

Significant advances have been made over the last decade in the modelling of practical problems that exhibit strong discrete/discontinuous phenomena by employing combined finite/discrete element solution strategies [1]. Typical examples include multi-fracturing solids under high speed impact and granular/particulate materials in the processing industry and geo-mechanics. The highly nonlinear contact dynamic/impact nature of these systems dictates that explicit time integration, such as central difference schemes, are almost the only feasible option to be employed to compute the system response. The stability issue associated with explicit time integration, however, imposes a severe constraint on the maximum time step that can be used. In many impact problems, finite elements with different sizes, often achieved by mesh adaptivity, are present and constantly change in order to optimally model the structural response. In many discrete particulate systems, a wide range of particulate size distribution must be employed so that the underlying physical features can be captured to a certain degree. In both cases the smallest element controls the maximum time-step that can be employed, leading to extremely intensive computations involved in the simulations.

There has been a continuous interest over the last two decades in the development of time integration schemes that can inherently exploit different time scales in many science and engineering problems. In addition to the cases of the finite element analysis of structural dynamic systems where the sizes of elements can be significantly different, which lead to different dynamic scales of the elements, multi-scale dynamic features also exist in problems where highly heterogenous materials and/or different physical phenomena are present.

Since 1980's, some effort has been made to develop so called multiple/sub-cycling time step (MTS) methods [2] where larger time steps may be used for the regions with larger finite elements. More recently a more flexible approach, termed the Asynchronous Variational Integrator (AVI) [3], is proposed within the general framework of symplectic integrators for conservative (Hamiltonian) systems. Limited numerical examples have demonstrated their potential for significantly reducing computations in structural dynamic analysis. Note that similar MTS methods have also been proposed in molecular dynamic simulations [4].

The current work attempts to extend both MTS and AVI to discrete element simulations so that a substantial improvement in terms of computational costs can also be gained for the problems concerned. However, the extension is not trivial, due primarily to the nature of the continuously changing configuration of the discrete systems. Several fundamental developments are made to overcome the difficulties. In addition, several theoretical and implementation issues are identified that are essential for the success of the approach. It is shown that the resulting AVI/MTS discrete element method can achieve a nearly optimal speed-up for typical discrete systems. However, the stability is the issue that needs to be further addressed.

2 MTS/AVI APPROACHES FOR FINITE ELEMENT SYSTEMS

2.1 Node/Element Update

AVI is so called element-partition based while MTS/subcycling approaches are node-partition based and there exist several variants. For their suitability for discrete systems currently concerned, only the non-integer ratio constant-velocity subcycling scheme [2] is considered. The node/element update procedures for both MTS and AVI are illustrated in Fig.1. Note that both approaches can be viewed as an "event-driven" time stepping scheme.

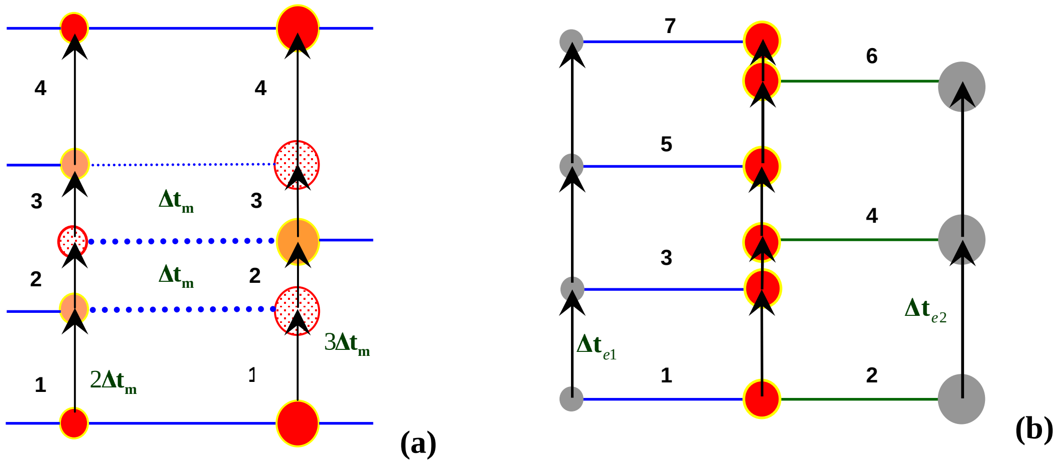

Fig.1. Node/element update: (a) MTS/Subcycling – constant velocity; (b) AVI

2.2 Stability

One important issue associated with MTS and AVI is their numerical stability in comparison with the original single time step counterpart (the central difference algorithm). The stability is examined numerically for simple spring-mass models as shown in Fig2. For the model (a), the critical time step associated with each node (mass) is

$$\Delta t_1^{cr} = 2/\omega_1 = 2\sqrt{m_1/k_1} = 2;\quad \Delta t_2^{cr} = 2/\omega_2 = 2\sqrt{m_2/k_2} = 2\sqrt{m_2} \tag{1}$$

Assuming $m_2 \geq 1$, the actual time steps for the two nodes in MTS are chosen to be

$$\Delta t_1 = \lambda \Delta t_1^{cr};\ \Delta t_2 = n\Delta t_1 \quad (\text{interger } n = [\omega_1/\omega_2]) \tag{2}$$

where $0 < \lambda < 1$is the time step factor. Fig.1(a) depicts the (capped) energy increase of MTS for the system after 1000 time steps for different values of λ and nodal frequency/time ratio ω_1/ω_2, revealing the existence of a complex unstable region within the standard stable limit. A similar result is also obtained for AVI for the model (b) and shown in Fig.2(b). In this case $m_1 + m_2 = 1$. By varying the ratio of m_1/m_2, different element frequency ratios can be achieved. Again a complex unstable region is emerged. Note however that the unstable region can be reduced by introducing the system damping.

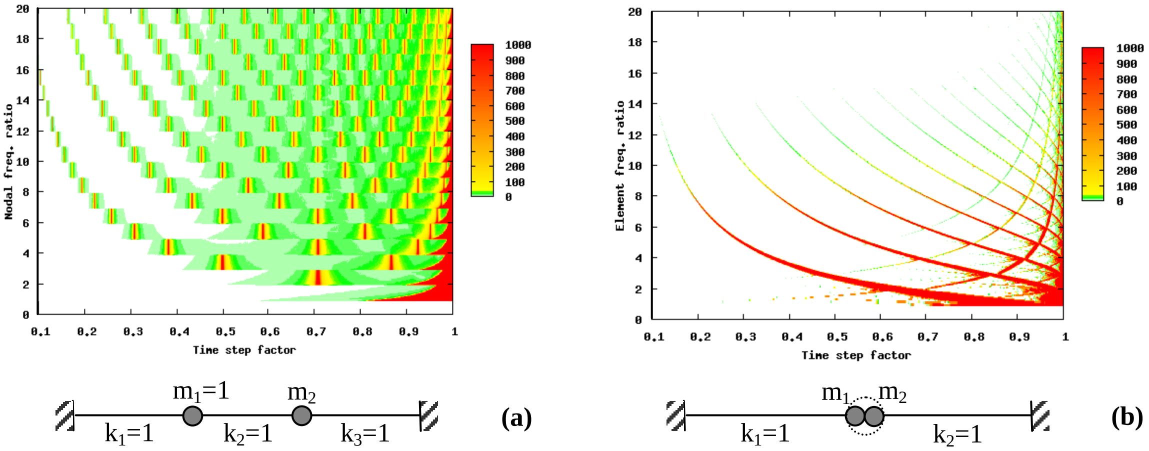

Fig.2. Numerical stability: (a) MTS/Subcycling – constant velocity; and (b) AVI

3 MTS/AVI APPROACHES FOR DSICRETE ELEMENT SYSTEMS

3.1 Algorithmic issues

MTS and AVI methods for finite element systems cannot be directly applied to discrete element cases without important modifications to be made to the discrete element method. The difficulty lies in the feature of continuous changing configurations of discrete systems which requires the constant update of the contact list between discrete objects. As both MTS and AVI advance only a (small) part of the objects at each step, a global search algorithm should be able to effectively deal with this situation. Unfortunately most of currently used search methods are not suitable for this purpose and a new effective approach has been development. In addition, the improved computational efficiency is achieved in MTS and AVI mainly by the reduction of the number of internal force computations but at the expense of an increased overhead for additional data processing. To maximise the speed-up several operations are agglomerated at each internal force calculation.

3.2 Priority queue for AVI

Although AVI has an advantage over MTS for its flexibility to choose desirable time steps for elements, an efficient scheduling procedure, or a priority queue, has to be applied to determine the order of element operation. The elements in the priority queue are ordered according to the next time when they are to become active. The order of complexity of maintaining a priority queue is however $N \log N$ which may lead to a possible computational bottleneck for large scale applications. To overcome this problem, a bin-type algorithm is implemented which regroups the elements into a limited number of bins and thus avoids the use of priority queue and also provides a unified implementation of MTS and AVI.

4 NUMERICAL ILLUSTRATIONS

Both MTS and AVI approaches developed are numerically assessed by two test cases: hopper filling and particle compaction. The element size is distributed evenly in the range of [1,10] and both disks and ellipses are considered. The speed-up of the methods over the standard central difference scheme is listed in Table 1. Note that the maximum speed-up that can be achieved is about 3.40.

Case	**Problem size**	**Particle shape size**	**Speed-up**	
			MTS	AVI
Case 1	3000	disk	2.15	2.01
		ellipse	3.23	3.12
Case 2	3000	disk	2.26	2.12
		ellipse	3.24	3.15

Table 1 : Speed-up of MTS and AVI for two test cases

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