Stable Time Step Estimates for Mesh-Free Particle Methods

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SUMMARY

Real time computational biomechanics for medicine usually uses explicit time integration, due to its efficiency and suitability for parallel implementation. Explicit time integration is only conditionally stable and therefore requires an estimation of the maximum stable time step that can be used. In this paper we develop a method of estimating the stable time step for mesh-free particle methods for a specific case of mass lumping: the mass associated with an integration point is distributed equally to all nodes found in the support domain of that integration point. Two estimates of the stable time step for each integration point are developed: one which is very accurate but more costly to compute and one less accurate but easier to implement. The results are also valid for the finite element method and beyond computational biomechanics for medicine.

KEYWORDS: stability analysis, stable time step, mesh-free particle methods, maximum eigenvalue estimation

1. INTRODUCTION

In the past few years our research group developed a suite of finite element algorithms for computing soft tissue deformation based on the Total Lagrangian formulation and using explicit time integration [1-4]. By using artificial mass proportional damping in the explicit integration schemes such algorithms can not only be used for time accurate simulations, but also for fast computation of the steady state solution [5, 6]. Parallel implementations of these algorithms lead to real-time performance for intra-operative brain shift computations using comprehensive finite element models having more than 50,000 degrees of freedom and including different element types, nonlinear materials, large deformations and contacts [7].

While applying these algorithms for intra-operative image registration [8, 9], some important weakness of the finite element method became evident:

- In order to obtain good results and convergence of the simulation, a good quality mesh is needed. Such mesh is very hard to build for complicated organ shapes (such as the brain), and automatic generation is almost impossible for any element type except tetrahedrons.
- Even if a good quality mesh is used, the solution method may still fail in case of large deformations, due to problems such as element inversion.

In order to circumvent these problems we considered the use of mesh-free methods, such as the Mesh-free Total Lagrangian Explicit Dynamics (MTLED) algorithm based on the Element Free Garlekin method [10]. Such methods do not require a good quality mesh to be generated, as the shape functions are constructed based on a cloud of points, and they also perform much better in case of very large deformations. Therefore we propose to use mesh-free methods combined with explicit solution algorithms for more robust surgical simulations.

Explicit time integration can be used to perform dynamic simulations, leading to time accurate solutions, or for quasi-static simulations, to obtain the steady state solution. Because it does not require the solution of large systems of equations, explicit integration can be much more computationally efficient at finding the solution than other methods (implicit integration, static analysis). It also leads to solution algorithms that can be easily implemented on parallel hardware such as Graphics Processing Units (GPU) [7]. The main disadvantage of explicit integration is its conditional stability – the time step used for time integration must be smaller than a critical time step in order for the solution to converge [11].

In the case of the Finite Element Method (FEM) there are well established formulae for estimating the critical time step for each element type [11, 12]. These formulae are generally developed using the assumption of a homogenous isotropic material.

For mesh-free particle methods, there are few available methods for estimating the critical time step, and these methods are not generally valid. In [13] Belytschko et al. develop critical time step bounds for 1D and 2D mesh-free methods. Nevertheless, these bounds are valid in 2D only for uniformly distributed nodes, and they cannot be used for shape functions that have the Kronecker delta property and for shape functions that are not strictly positive, as they become indefinite (due to division by zero) [14]. Puso et al.

present in [14] an estimation of the critical time step for nodal integration methods. These formulae are also developed using the assumption of a homogenous isotropic material.

The critical time step is directly related to the maximum frequency of free vibration, which is determined by the mass and stiffness matrices of the system. Therefore, different lumping techniques used for obtaining a diagonal mass matrix lead to different critical time steps for the system. In this paper we consider that the mass associated with an integration point is distributed equally to all nodes found in the support domain of that integration point. The lumping technique has no influence on the results of a steady state analysis [6], as the mass matrix does not influence the steady state solution (for elastic materials). The correctness of results can be influenced by the lumping technique in case of dynamic analysis; therefore the analyst must check whether this lumping technique is appropriate.

In the next Section we develop a new method for estimating the critical time step for a mesh-free particle method. In Section 3 we assess the performance of the new method and Section 4 contains discussions and conclusions.

2. CRITICAL TIME STEP ESTIMATION

We consider a mesh-free particle method for which the displacement field is approximated by:

$$\mathbf{u}(\mathbf{x}) = \sum_{I \in N(\mathbf{x})} h_I(\mathbf{x}) \cdot \mathbf{u}^I \tag{1}$$

where $\mathbf{u}^I$ are the field variable values at node I, $N(\mathbf{x})$ is the set of nodes in the support domain of $\mathbf{x}$ and h_I is the shape function for node I.

The matrix of shape function derivatives is defined as:

$$\mathbf{B}_{jI}(\mathbf{x}) = \frac{\partial h_I(\mathbf{x})}{\partial x_j} \tag{2}$$

The stable critical time step for central difference integration can be obtained from the maximum frequency of free vibration as [15]:

$$\Delta t^{crit} = \frac{2}{\omega_{\max}} \tag{3}$$

Similar formulae are available for other explicit time integration methods [11].

The mass and stiffness matrices for the system are obtained by assembling the corresponding matrices from each integration point:

$$\mathbf{K} = \sum_{I=1}^{N} \mathbf{K}^I \tag{4}$$

$$\mathbf{M} = \sum_{I=1}^{N} \mathbf{M}^I \tag{5}$$

where N is the number of integration points.

The maximum free vibration frequency of the assembled system can be estimated using the eigenvalue inequality theorem [16]:

$$\min_I(\lambda^I_{Min}) \leq \lambda_{Min} \leq \lambda_{Max} \leq \max_I(\lambda^I_{Max}) \tag{6}$$

Therefore, a conservative estimate of the critical time step for the central difference method is given by:

$$\Delta t_{crit} = \frac{2}{\omega_{\max}} = \frac{2}{\sqrt{\lambda_{\max}}} \approx \frac{2}{\sqrt{\max_I(\lambda^I_{Max})}} = \min_I\left(\frac{2}{\sqrt{\lambda^I_{Max}}}\right) = \min_I(\Delta t^I_{crit}) \tag{7}$$

For a given integration point, the maximum eigenvalue can be estimated using the Rayleigh quotient as [16]:

$$\lambda_{Max}^{I} = \sup_{\mathbf{u}} \frac{\mathbf{u}^T \mathbf{K}^I \mathbf{u}}{\mathbf{u}^T \mathbf{M}^I \mathbf{u}} \quad (8)$$

Considering our specific mass lumping technique (mass associated to an integration point is distributed equally to all nodes found in the support domain of that integration point), the above relation can be re-written as:

$$\lambda_{Max}^{I} = \frac{N^I}{m^I} \sup_{\mathbf{u}} \frac{\mathbf{u}^T \mathbf{K}^I \mathbf{u}}{\mathbf{u}^T \mathbf{u}} = \frac{N^I}{m^I} \rho_{Max}(\mathbf{K}^I) \quad (9)$$

where N^I is the number of nodes in the support domain of integration point I, m^I is the mass allocated to integration point I and $\rho_{Max}(\mathbf{K}^I)$ is the maximum eigenvalue of the stiffness matrix for integration point I.

The stiffness matrix for integration point I is defined as:

$$\mathbf{K}_{iJlK}^{I} = \mathbf{B}_{jJ}(\mathbf{x}^I)\mathbf{C}_{ijkl}\mathbf{B}_{lK}(\mathbf{x}^I) \cdot V^I = \mathbf{B}_{jJ}^{I}\mathbf{C}_{ijkl}\mathbf{B}_{lK}^{I} \cdot V^I \quad (10)$$

where V^I is the volume allocated to integration point I [14]. For a homogenous isotropic material, the maximum eigenvalue of the stiffness matrix is developed in [14] as:

$$\rho_{Max}(\mathbf{K}^I) \le \left(\lambda \left\| \mathbf{B}^I \right\|_F^2 + 2\mu \cdot \left\| \mathbf{B}^I \right\|_2^2 \right) \cdot V^I \le (\lambda + 2\mu) \cdot V^I \cdot \left\| \mathbf{B}^I \right\|_F^2 \quad (11)$$

where λ and μ are the Lame constant, $||B||_F$ is the Frobenious norm:

$$\left\| \mathbf{B} \right\|_F^2 = \mathbf{B}_{jI}\mathbf{B}_{jI} \quad (12)$$

and $||B||_2$ is the matrix two norm, defined as:

$$\left\| \mathbf{B} \right\|_2^2 = \rho_{Max}(\mathbf{B}_{iJ}\mathbf{B}_{jJ}) \quad (13)$$

By replacing (11) in (9), and considering the definition of density, we get the bounds for the maximum eigenvalues of the stiffness matrix as:

$$\lambda_{Max}^{I} \le \frac{N^{I}}{\rho^{I}}\left(\lambda \mathbf{B}_{jl}^{I}\mathbf{B}_{jl}^{I} + 2\mu \cdot \rho_{Max}(\mathbf{B}_{iJ}^{I}\mathbf{B}_{jJ}^{I})\right) \tag{14}$$

$$\lambda_{Max}^{I} \le \frac{N^{I}}{\rho^{I}}(\lambda + 2\mu) \cdot \left\|\mathbf{B}^{I}\right\|_{F}^{2} = N^{I} c^{I^{2}} \cdot \mathbf{B}_{jl}^{I}\mathbf{B}_{jl}^{I} \tag{15}$$

where ρ is the material density and c is the dilatational wave speed. These can be used directly in Eq. (7) for estimating the critical time step. While Eq. (14) offers a better estimate, it involves the computation of the maximum eigenvalue of a 3x3 matrix (in 3D), and therefore Eq. (15) may be preferred in practice.

The bounds for the maximum eigenvalue of the stiffness matrix, as given by Eq. (14) and (15), are valid for 1D, 2D and 3D cases. They are also valid for finite elements, as long as the same mass lumping technique is used. For the uniform strain hexahedron and quadrilateral these bounds give the same result as the ones presented in [12].

3. PERFORMANCE EVALUATION

To evaluate the performance of the critical time step estimation algorithm for different numbers of nodes per integration point we use the nodal distribution presented in Fig. 1 for a 2D case and in Fig. 4 for a 3D case. For each node we define an influence domain based on the local node density. We use a dense grid of regularly distributed integration points to get different nodes-integration points associations. For the chosen parameters we have between 3 and 11 nodes associated to an integration point in 2D. We compute the Moving Least Squares (MLS) shape functions and their derivatives (matrix **B**, see Eq. 2) at each integration point. Using the **B** matrix we can compute the stiffness matrix (Eq. 10), find its maximum eigenvalue and compute the real value of the critical time step for a given integration point. We can compare the real value of the critical time step with estimates computed using Eq. 14 and Eq. 15. The obtained results are presented in Fig. 2 for a plane strain analysis and in Fig. 3 for a plane stress analysis.

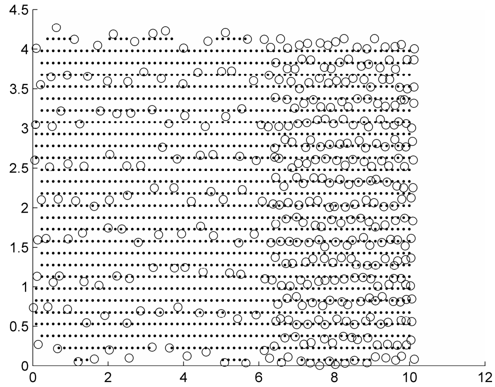
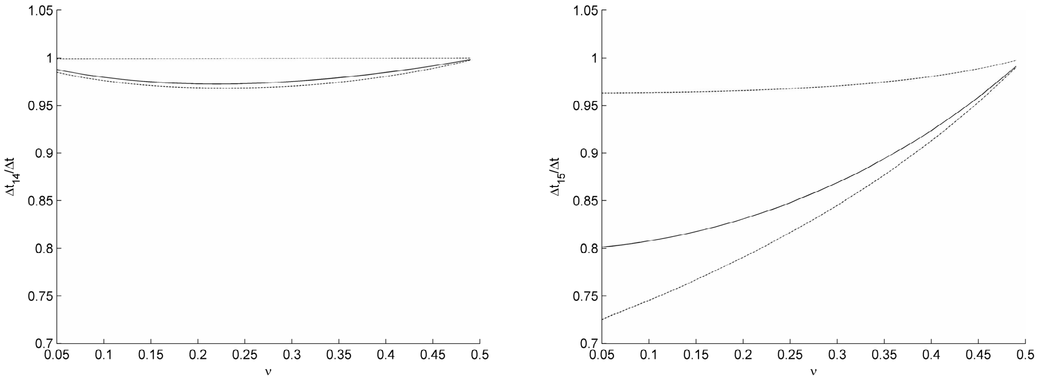
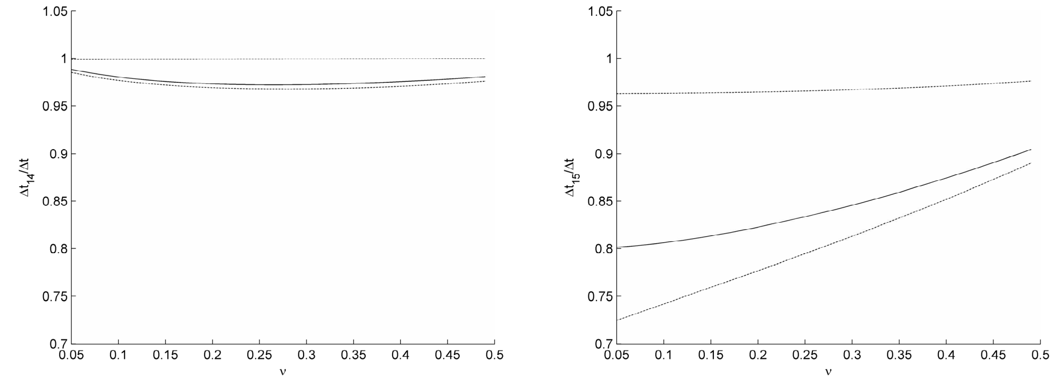


Fig. 1. The distribution of nodes (represented by circles) and integration points used for performance evaluation. MLS shape functions are computed for each integration point.



a) b)

Fig. 2. The ratio of critical time step estimates, as given by Eq. 14 (a) and Eq. 15 (b), to the real critical time step obtained based on the stiffness matrix is computed for all integration points. The maximum, minimum and average values of these ratios are plotted against material's Poisson's ratio, for a plane strain analysis.



a) b)

Fig. 3. The ratio of critical time step estimates, as given by Eq. 14 (a) and Eq. 15 (b), to the real critical time step obtained based on the stiffness matrix is computed for all integration points. The maximum, minimum and average values of these ratios are plotted against material's Poisson's ratio, for a plane stress analysis.

The obtained results show that Eq. 14 leads to a very good critical time step estimate, which is less than 5% lower than the actual value, for the entire range considered for the material's Poisson's ratio. The estimate of the critical time step given by Eq. 15 can be as much as 30% lower than the actual value, with a better prediction for higher values of the material's Poisson's ratio. Also the estimate given by Eq. 15 is better for plane strain than for plane stress analyses, especially at higher values of the material's Poisson's ratio.

We performed a similar evaluation for 3D shape functions using the nodes and integration points distributed as in Fig. 4, with a variable nodal influence domain leading to between 8 and 25 nodes associated to an integration point. The obtained results are presented in Fig. 5. The obtained results for 3D are very similar with those obtained for a plane strain analysis in 2D.

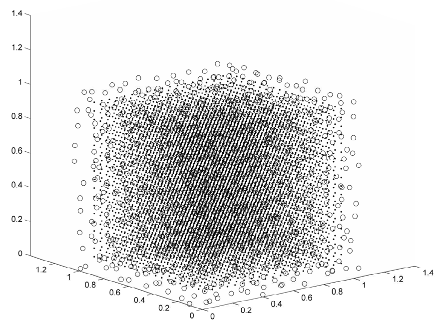
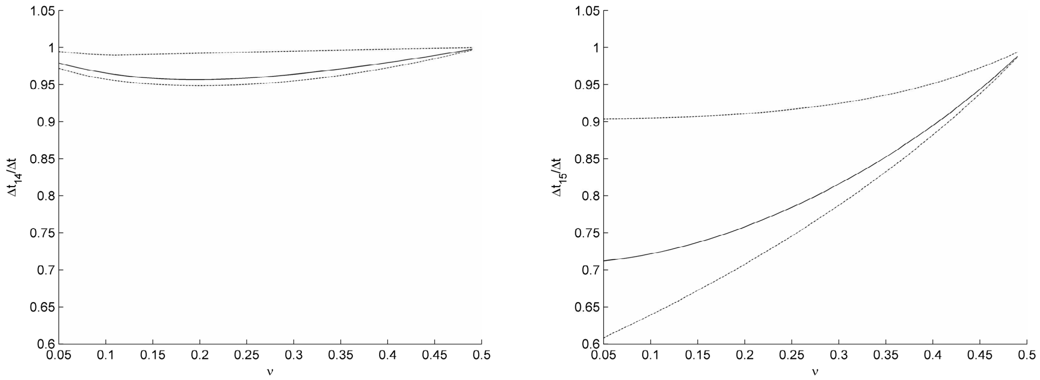


Fig. 4. The distribution of nodes (represented by circles) and integration points used for performance evaluation in 3D. MLS shape functions are computed for each integration point.



a) b)

Fig. 5. The ratio of critical time step estimates, as given by Eq. 14 (a) and Eq. 15 (b), to the real critical time step obtained based on the stiffness matrix is computed for all integration points. The maximum, minimum and average values of these ratios are plotted against material's Poisson's ratio, for a 3D analysis.

4. DISCUSSION AND CONCLUSSIONS

In this paper we present a method for estimating the critical time step for mesh-free particle methods. The estimates are valid for a specific case of mass lumping: the mass associated with an integration point is distributed equally to all nodes found in the support domain of that integration point. The same estimation method can also be used for finite elements if the mass lumping is done in the same way.

We present two formulas that can be used for estimating the critical time step. These formulas are obtained considering a homogenous isotropic material and are valid both in 2D and 3D. The first formula (Eq. 14) leads to a very good estimate, for any value of the material's Poisson's ratio, but it requires the computation of the maximum eigenvalue of a 2x2 (2D) or 3x3 (3D) matrix. The second formula (Eq. 15) is much simpler, but the accuracy of the estimates it provides is lower, especially for materials with a low Poisson's ratio. Nevertheless, this might be a better option for a large deformations non-linear solver implementation, as the critical time step might decrease during the analysis (because of changes in nodal positions and material properties due to the large deformations). The second formula would also be a good choice for almost incompressible materials, such as brain tissue, which have a very large Poisson's ratio.

The developed formulas offer a way of estimating the critical time step for mesh free methods, which can then be used together with explicit time integration algorithms to solve computational biomechanics problems in real time. Although developed in the context of linear elasticity, empirical evidence from the use of similar formulae with the finite element method suggests that these formulae are also useful for simulations involving large deformations and non-linear material models [11].

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