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Time step estimates for explicit dynamics with reciprocal mass matrices

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ABSTRACT

In this contribution, a novel local, node-based time step estimate for reciprocal mass matrices is proposed. Element-based estimates turn out to be not generally conservative and are consequently inadequate. Therefore, the nodal time step estimate for diagonally lumped mass matrices based on Gershgorin's theorem is further developed for application to reciprocal mass matrices. Additionally, simplifications of the proposed time step estimate that improve computational efficiency, especially for contact problems with the penalty method, are discussed and evaluated by numerical examples.

1. Introduction

Recently, *reciprocal mass matrices*, i.e. directly assembled inverse mass matrices, were proposed by Lombardo and Askes [1], Tkachuk and Bischoff [2] and Gonzalez et al. [3] as an efficient alternative to diagonally lumped mass matrices in explicit dynamics. These reciprocal mass matrices allow trivial computation of the nodal acceleration from the total force vector. The latter two were developed in the context of selective mass scaling, i.e. they increase the stable time step of explicit integration without deteriorating the low frequency response. Though these papers show that a substantial speed-up with respect to lumped mass can be obtained, accurate and efficient time step estimates remain an open issue. In both the earlier work of the authors' group [2] and in the work of Gonzalez et al. [3] inefficient global estimates were used. In the paper of Lombardo and Askes [1] element-based time step estimates were proposed, but their possible non-conservativeness is shown in this work. An efficient, accurate and conservative estimate, however, is indispensable to exploit the full capacity of the increased time step and make these methods attractive for practical applications.

For the central difference method, the time step Δt is limited by the critical time step Δt_{crit} through the stability criterion

$$\Delta t < \Delta t_{\text{crit}} = \frac{2}{\omega_{\max}}, \tag{1}$$

where $\omega_{\max}$ is the maximum eigenfrequency. Existing time step estimates to determine the critical time step Δt_{crit} can be categorized into two groups, namely global and local time step estimates. The latter can again be categorized as element-based and node-based estimates. Element-based estimates require data from the element level, like a characteristic element length, whereas node-based estimates require data from the degree-of-freedom-level, like the mass or stiffness associated with the degree of freedom. Global time step estimates determine the maximum eigenfrequency of the global system by solving the standard eigenvalue problem (EVP). For reciprocal mass matrices this is

$$(\mathbf{C}^{\circ}\mathbf{K} - \lambda_i \mathbf{I})\boldsymbol{\phi}_i = \mathbf{0} \quad \text{with} \quad \lambda_i = \omega_i^2, \tag{2}$$

where $\mathbf{C}^{\circ}$ and $\mathbf{K}$ are the reciprocal mass matrix and the stiffness matrix and λ_i, ω_i and $\boldsymbol{\phi}_i$ are the ith eigenvalue, eigenfrequency and the right eigenvector, respectively. Note that the symbol $\mathbf{C}^{\circ}$ is used for the reciprocal mass matrix in consistence with earlier publications on reciprocal mass matrices and it should not be confused with the damping matrix. Damping is ignored within this work. The standard EVP can be solved by iterative algorithms, like forward iteration. Since global estimates are computationally expensive, local estimates are preferred in practical applications. Element-based local estimates make use of the element eigenvalue inequality by Fried [4], which states that the global eigenvalue λ is bounded by the element eigenvalues λ_i^e,

$$|\lambda^{\max}| \leqslant |\lambda_E^{\max}| \quad \text{where} \quad \lambda_E^{\max} = \max_{i,e} \lambda_i^e. \tag{3}$$

The maximum element eigenfrequencies can be estimated by considering the strain-displacement operator as proposed by Flanagan and Belytschko [5] or by geometric considerations (as used in LS-DYNA [6]) through the Courant-Friedrichs-Lewy-criterion [7] with

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$$\max_{i,e} \omega_i^e = \frac{c}{l_e}. \tag{4}$$

Here, c is the characteristic wave speed, which depends on the dimensionality, the stress assumptions and the material properties and l_e is the characteristic length of the element.

Note that the inequality from Eq. (3) is valid for a generalized symmetric eigenvalue problem only as it exists for the lumped or consistent mass $\mathbf{M}$ with

$$(\mathbf{K} - \lambda_i \mathbf{M})\boldsymbol{\phi}_i = \mathbf{0} \quad \text{with} \quad \lambda_i = \omega_i^2, \tag{5}$$

and results from the inequality of the Rayleigh quotient on the local and global level with

$$\begin{aligned} \max_i \omega_i^2 = \max_i \lambda_i = \max_i \frac{\boldsymbol{\phi}_i^{\mathrm{T}} \mathbf{K} \boldsymbol{\phi}_i}{\boldsymbol{\phi}_i^{\mathrm{T}} \mathbf{M} \boldsymbol{\phi}_i} \leqslant \max_{i,e} (\omega_i^e)^2 = \max_{i,e} \lambda_i^e \\ = \max_{i,e} \frac{\boldsymbol{\phi}_i^{e\mathrm{T}} \mathbf{k}_e \boldsymbol{\phi}_i^e}{\boldsymbol{\phi}_i^{e\mathrm{T}} \mathbf{m}_e \boldsymbol{\phi}_i^e}, \end{aligned} \tag{6}$$

where $\boldsymbol{\phi}_i^e, \mathbf{k}_e, \mathbf{m}_e$ are the ith eigenvalue, the stiffness matrix and the mass matrix on the element level. The eigenvalues on the global and element level for the product eigenvalue problem given in Eq. (2) can also be obtained from the Rayleigh quotient using additionally the global left eigenvectors $\boldsymbol{\phi}_i^{\mathrm{L}}$ and the local left eigenvectors $\boldsymbol{\phi}_i^{\mathrm{L},e}$ with

$$\begin{aligned} \max_i \omega_i^2 = \max_i \lambda_i = \max_i \frac{\left(\boldsymbol{\phi}_i^{\mathrm{L}}\right)^{\mathrm{T}} \mathbf{C}^{\circ} \mathbf{K} \boldsymbol{\phi}_i}{\left(\boldsymbol{\phi}_i^{\mathrm{L}}\right)^{\mathrm{T}} \boldsymbol{\phi}_i} \quad \not\leqslant \quad \max_{i,e} (\omega_i^e)^2 \\ = \max_{i,e} \lambda_i^e = \max_{i,e} \frac{\left(\boldsymbol{\phi}_i^{\mathrm{L},e}\right)^{\mathrm{T}} \mathbf{c}_e^{\circ} \mathbf{k}_e \boldsymbol{\phi}_i^e}{\left(\boldsymbol{\phi}_i^{\mathrm{L},e}\right)^{\mathrm{T}} \boldsymbol{\phi}_i^e}. \end{aligned} \tag{7}$$

However, the inequality does not necessarily hold for the product eigenvalue problem. This is confirmed by a simple illustrative example in Appendix A. As a consequence, element-based estimates for reciprocal mass matrices may be non-conservative and they are thus inappropriate. Alternative, node-based local estimates are based on Gershgorin's theorem [8], which bounds the spectrum of a square matrix. For a square matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$, the Gershgorin's circles that belong to the ith diagonal entry A_{ii} of the matrix are defined by

$$\begin{aligned} &\overline{S}_i\left(A_{ii}, \sum_{j=1, j\neq i}^{n} |A_{ij}|\right), \; i = 1..n(\text{row-wise}) \quad \text{and} \quad \overline{S}_i\left(A_{ii}, \sum_{j=1, j\neq i}^{n} |A_{ji}|\right), \\ &i = 1..n(\text{column-wise}), \end{aligned} \tag{8}$$

where $\overline{S}(\Re(z), r)$ defines a circle with center $\Re(z)$ and radius r in the complex plane. Gershgorin's theorem states that all eigenvalues are found inside the circles defined in Eq. (8). Based on Gershgorin's theorem Kulak [9] proposed a nodal estimate to determine the maximum eigenfrequency for diagonally lumped mass matrices

$$\omega_{\max}^{\mathrm{LMM}} = \max_i \sqrt{\frac{\sum_{j=1}^{n} |K_{ij}|}{M_i}}, \tag{9}$$

where M_i is the lumped mass at degree of freedom i. In case of penalty contact the estimate can be supplemented by the absolute row sum K_i^p at degree of freedom i of the penalty stiffness matrix (see Belytschko and Neal [10])

$$\omega_{\max}^{\mathrm{LMM,pen}} = \max_i \sqrt{\frac{\sum_{j=1}^{n} |K_{ij}| + K_i^p}{M_i}}. \tag{10}$$

The assumption on the penalty stiffness is an upper bound in general. In the special case of rigid wall contact it is exact.

In the following, Gershgorin's time step estimate for lumped mass matrices is extended to reciprocal mass matrices. Moreover, some modifications on the algorithm to increase computational efficiency are proposed. The objective is to meet the requirements.

- to be conservative,
- to be efficient and
- to provide satisfactory results for irregular and distorted meshes.

Efficiency implies both reasonable computational effort to compute the time step and an estimate that is not too conservative, i.e. not too small compared to the exact critical time step.

2. Node-based time step estimate and further assumptions for efficient implementation

In this section, the extension of Gershgorin's time step estimate to reciprocal mass matrices is systematically explored. First, row-wise, column-wise and symmetric estimates for the non-symmetric eigenvalue problem stated in Eq. (2) are discussed. Secondly, the extension of the row-wise estimate to penalty contact is developed. Thirdly, the time step estimate for penalty contact is rearranged. The rearrangements allow efficient recomputation of the time step with the time varying active contact set and are based on several consequent assumptions using sub-additivity and sub-multiplicativity of vector and matrix norms.

2.1. Time step estimates for problems without contact

The maximum eigenfrequency of eigenvalue problem (2) with reciprocal mass matrices is bounded according to Gershgorin's theorem by

$$\omega_{\max}^{\text{row-wise}} = \max_i \sqrt{\sum_{j=1}^{n} |(\mathbf{C}^{\circ}\mathbf{K})_{ij}|}. \tag{11}$$

The matrix-product $\mathbf{C}^{\circ}\mathbf{K}$ is non-symmetric and a row-wise Gershgorin's circle is used in Eq. (11). Alternatively, a column-wise Gershgorin's circle

$$\omega_{\max}^{\text{column-wise}} = \max_i \sqrt{\sum_{j=1}^{n} |(\mathbf{K}\mathbf{C}^{\circ})_{ij}|} = \max_i \sqrt{\sum_{j=1}^{n} |(\mathbf{C}^{\circ}\mathbf{K})_{ji}|} \tag{12}$$

may be used. The use of a non-symmetric matrix $\mathbf{C}^{\circ}\mathbf{K}$ may be avoided by a Cholesky decomposition of the reciprocal mass matrix, $\mathbf{C}^{\circ} = \mathbf{L}^{\mathrm{T}}\mathbf{L}$. It can be used to apply Gershgorin's theorem to the symmetric EVP

$$(\mathbf{L}^{\mathrm{T}}\mathbf{K}\mathbf{L} - \omega_i^2 \mathbf{I})\boldsymbol{\varphi}_i = \mathbf{0} \rightarrow \omega_{\max}^{\text{symm}} = \max_i \sqrt{\sum_{j=1}^{n} |(\mathbf{L}^{\mathrm{T}}\mathbf{K}\mathbf{L})_{ij}|}, \tag{13}$$

which has different eigenvectors but the same eigenvalues as the EVP stated in Eq. (2).

Eqs. (11)–(13)$_2$ are the basic estimates of the eigenfrequency. From this, the time step estimates for the central difference method are obtained with Eq. (1). The proposed novel nodal time step estimate for reciprocal mass matrices resulting from Eq. (11) is thus

$$\Delta t_{\text{crit}}^{\text{row-wise}} = \min_i \Delta t_{\text{crit}}^{i,\text{row-wise}} = \min_i \sqrt{\frac{4}{\sum_{j=1}^{n} |(\mathbf{C}^{\circ}\mathbf{K})_{ij}|}}. \tag{14}$$

The choice of the row-wise version is justified in some more detail in the following section.