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CONTROLLING THE CRITICAL TIME STEP WITH THE BI-PENALTY METHOD

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Abstract. *Penalty functions are a popular tool to add constraints to a system of equations, such as for instance Dirichlet boundary conditions or setting a relation between different degrees of freedom. Although implementation of the penalty method is simple, the commonly used stiffness-type penalties have a drawback in dynamics in that they increase the speed of sound locally. Thus, in conditionally stable time integration schemes the critical time step is lowered (often by orders of magnitude) if stiffness penalties are used. As an alternative, one may use inertia penalties that lower the speed of sound and therefore increase the critical time step, but in this paper we suggest the simultaneous use of stiffness and inertia penalties, which is called the bi-penalty method. In the bi-penalty method the relative magnitudes of stiffness penalty and inertia penalty can be tuned so that the net effect on the critical time step is neutral, thereby removing a major disadvantage of stiffness-type penalty methods.*

1 INTRODUCTION

Penalty functions are a popular technique to impose constraints in computational mechanics. Penalties can be used to enforce support conditions, tyings, interface conditions and/or contact. In mechanics, penalty functions are usually based on adding stiff springs to the system of equations. The accuracy of the constraint imposition depends on the magnitude of the penalty parameter, that is the stiffness of the added springs — the larger the penalty parameter, the more accurate the constraint is realised [1].

However, the penalty parameters cannot be chosen arbitrarily large: the condition number of the system matrix is affected adversely by increased penalty parameter, which deteriorates numerical accuracy. Furthermore, in dynamics an additional disadvantage is that stiffness-type penalties increase the speed of sound (at least locally where the penalty is applied). This becomes particularly significant in case a time domain analysis is performed with a conditionally stable time integration scheme; such schemes have a so-called *critical time step* which acts as an upper bound on the time step that can be used — larger time steps may (and usually do) lead to numerical instabilities. The critical time step is inversely proportional to the (local) speed of sound. Since the speed of sound increases with increased stiffness, applying stiffness penalties leads to increased speed of sound and decreased critical time steps [2].

As an alternative to stiffness-type penalties, it has more recently been suggested to use inertia-type penalties [3, 4]. Whereas stiffness-type penalties can be considered as stiff springs that prohibit displacement of the associated degree of freedom, inertia-type penalties act like heavy masses that prohibit acceleration of the corresponding degree of freedom. Although inertia penalties are not as accurate as stiffness penalties of equal magnitude, the beneficial effect of inertia penalties in dynamics is that they decrease the speed of sound and therefore increase the critical time step [4, 5].

To combine the benefits of stiffness penalties and inertia penalties, we suggest the simultaneous use of stiffness-type penalties and inertia-type penalties — a concept which is denoted as the bi-penalty method [5]. As explained above, stiffness penalties and inertia penalties have opposite effects on the critical time step; thus, critical ratios between the two penalty parameters can be derived such that their combined effect on the critical time step is neutral. The simultaneous use of inertia penalties and stiffness penalties has been suggested in the mid 1980s by Asano [6, 7, 8] for reasons of computational accuracy (and in fact penalties were also added to the damping matrix in these works), and more recently in [9] where the main focus was on frequency domain analysis.

In this paper, expressions will be given to compute the critical penalty ratio (CPR) described above. We will review the method to compute the CPR given in [5] and also present an alternative, much simpler method that has been developed recently. It will also be demonstrated that the critical time step remains unaffected if the penalty ratio is chosen not larger than the critical penalty ratio, whereas instabilities may occur otherwise. The bounds between stable and unstable simulations turn out to be very crisp, which is evidence for accuracy and relevance of the derived expressions for the critical penalty ratio.

2 BI-PENALISED EQUATIONS OF MOTION

We consider a linear elastic structure with stiffness matrix $\mathbf{K}$, mass matrix $\mathbf{M}$, external force vector $\mathbf{f}$ and degree of freedom (DOF) vector $\mathbf{u}$. A constraint $u_n - \overline{u} = 0$ is applied to the n^{th} DOF where $\overline{u}$ is the user-prescribed value of u_n. The constraint is enforced using stiffness and inertia penalty functions. For the former, the constraint in its usual form is added to the potential energy $\mathcal{U}$. For the latter, the rate format of the constraint is taken and added to the kinetic energy $\mathcal{T}$. The penalised potential and kinetic energy functionals thus read

$$\mathcal{U} = \frac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{u}^T\mathbf{f} + \frac{1}{2}\alpha_s\left(u_n - \overline{u}\right)^2 \tag{1}$$

and

$$\mathcal{T} = \frac{1}{2}\dot{\mathbf{u}}^T\mathbf{M}\dot{\mathbf{u}} + \frac{1}{2}\alpha_m\left(\dot{u}_n - \dot{\overline{u}}\right)^2 \tag{2}$$

where α_s and α_m are penalty parameters of the stiffness type (dimension N/m) and inertia type (dimension Ns^2/m), respectively. The equations of motion of the structure follow from

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{T}}{\partial\dot{\mathbf{u}}^T} + \frac{\partial\mathcal{U}}{\partial\mathbf{u}^T} = \left[\mathbf{M}+\mathbf{M}^P\right]\ddot{\mathbf{u}} + \left[\mathbf{K}+\mathbf{K}^P\right]\mathbf{u} - \left(\mathbf{f}+\mathbf{f}^P\right) = \mathbf{0} \tag{3}$$

The components of $\mathbf{M}^P$ and $\mathbf{K}^P$ are all zero except for the diagonal entries $M^P_{nn} = \alpha_m$ and $K^P_{nn} = \alpha_s$. Similarly, $f^P_n = \alpha_m\ddot{\overline{u}} + \alpha_s\overline{u}$ with all other components of $\mathbf{f}^P$ equal to zero.

3 COMPUTING THE CPR FROM THE BI-PENALISED SYSTEM

The critical time step Δt_{crit} of explicit time integration schemes, such as the central difference method, follows from

$$\Delta t_{\text{crit}} = \frac{2}{\omega_{\text{max}}} \tag{4}$$

where ω_{max} is the maximum eigenfrequency of the structure, which can be approximated (and is in fact bounded [10]) by the maximum eigenfrequency of the smallest element.

We require the critical time step to remain unaffected by the use of the bi-penalty method; thus, we require the maximum eigenfrequency of the bi-penalised system $\omega^{\text{BP}}_{\text{max}}$ to be not larger than the maximum eigenfrequency of the unpenalised system $\omega^{\text{UP}}_{\text{max}}$. We define the the critical penalty ratio (CPR) as the ratio α_s/α_m for which the maximum eigenfrequency of the bi-penalised system is identical to the maximum eigenfrequency of the unpenalised system. To find expressions for the CPR we proceed as follows:

1. Find $\omega^{\text{UP}}_{\text{max}}$ as the largest root from the unpenalised eigenvalue problem

$$\det\left(\mathbf{K} - \left(\omega^{\text{UP}}\right)^2\mathbf{M}\right) = 0 \tag{5}$$

2. Substitute $\omega^{\text{UP}}_{\text{max}}$ into the bi-penalised eigenvalue problem:

$$\det\left(\left[\mathbf{K}+\mathbf{K}^P\right] - \left(\omega^{\text{UP}}_{\text{max}}\right)^2\left[\mathbf{M}+\mathbf{M}^P\right]\right) = 0 \tag{6}$$

   The free parameters of the latter expression are the two penalty parameters α_s and α_m.

3. Define the CPR as CPR $= \alpha_s/\alpha_m$ and find an expression for the CPR from Equation (6).

This is the approach that was used in [5] to compute the CPR for linear bar elements, beam elements and two-dimensional four-noded square elements. Whilst valid results can be obtained with this approach, it is nevertheless somewhat cumbersome in that the eigenvalue problem of the bi-penalised system must be solved. The complexity of the expressions increases rapidly when more than one DOF is penalised. Thus, it is of interest to explore alternative methods to compute the CPR.

4 COMPUTING THE CPR FROM THE UNPENALISED SYSTEM

As it turns out, it is possible to compute the CPR without the need to consider the bi-penalised eigenvalue problem. Here, we will present some basic principles of the proofs — the full proofs are quite elaborate and will be published in detail elsewhere. The bi-penalised eigenvalue problem is written as

$$\left[\left(\mathbf{K}+\mathbf{K}^P\right)-\left(\omega^{\mathrm{BP}}\right)^2\left(\mathbf{M}+\mathbf{M}^P\right)\right]\mathbf{v}=\mathbf{0} \tag{7}$$

where $\mathbf{v}$ is an eigenvector of the bi-penalised system. The eigenvectors can be scaled such that they are $\mathbf{K}$-orthogonal and $\mathbf{M}$-orthonormal [1], that is

$$\mathbf{v}_I^T\left(\mathbf{K}+\mathbf{K}^P\right)\mathbf{v}_J = \left(\omega_I^{\mathrm{BP}}\right)^2\ \delta_{IJ} \qquad \text{(no summation over } I\text{)} \tag{8}$$

$$\mathbf{v}_I^T\left(\mathbf{M}+\mathbf{M}^P\right)\mathbf{v}_J = \delta_{IJ} \tag{9}$$

Taking $I = J$, we obtain for large values of α_s and α_m that $\alpha_s v_n^2 = \left(\omega_I^{\mathrm{BP}}\right)^2$ and $\alpha_m v_n^2 = 1$, where v_n is the penalised component of the I^{th} eigenvector $\mathbf{v}_I$. Elimination of v_n^2 then yields

$$\sqrt{\frac{\alpha_s}{\alpha_m}}=\omega_I^{\mathrm{BP}} \tag{10}$$

that is, for large values of the penalty parameters the square-root of the penalty ratio $\sqrt{\alpha_s/\alpha_m}$ is an eigenvalue of the bi-penalised system. It will be proven elsewhere that if $\sqrt{\alpha_s/\alpha_m}$ is chosen equal to the largest eigenvalue of the unpenalised system, then it is also equal to the largest eigenvalue of the bi-penalised problem, so that the overall conclusion is that by taking $\alpha_s = \left(\omega_{\max}^{\mathrm{UP}}\right)^2\alpha_m$ the maximum eigenfrequencies of the bi-penalised system and the unpenalised system are identical. Thus, the critical penalty ratio is

$$\mathrm{CPR}=\left(\omega_{\max}^{\mathrm{UP}}\right)^2 \tag{11}$$

This result is also valid for an arbitrary number of penalised DOF.

5 EXAMPLE

For illustration, we will consider the well-known case of one-dimensional linear bar elements. The lumped mass matrix and stiffness matrix are given as

$$\mathbf{M}=\frac{\rho A h}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} \qquad \text{and} \qquad \mathbf{K}=\frac{EA}{h}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix} \tag{12}$$

where A is the cross-sectional area, h is the element length, E is Young's modulus and ρ is the mass density. The unpenalised eigenvalue problem can be expanded as

$$\det\left(\mathbf{K}-\left(\omega^{\mathrm{UP}}\right)^2\mathbf{M}\right)=\left(\omega^{\mathrm{UP}}\right)^2\left(\left(\omega^{\mathrm{UP}}\right)^2-\frac{4E}{\rho h^2}\right)=0 \tag{13}$$

so that $\omega_{\max}^{\mathrm{UP}} = 2c_e/h$ where $c_e = \sqrt{E/\rho}$ is the one-dimensional speed of sound. The CPR is then found as CPR $= 4c_e^2/h^2$, which corresponds with the dimensionless CPR found earlier in [5]. For the consistent mass matrix, a similar procedure leads to CPR $= 12c_e^2/h^2$.

As a numerical example, we consider a bar of length $L = 100$ m and cross-sectional area $A = 1$ m^2. A force $F = 1$ N is applied at the left end from time $t = 0$ s onwards. Stiffness

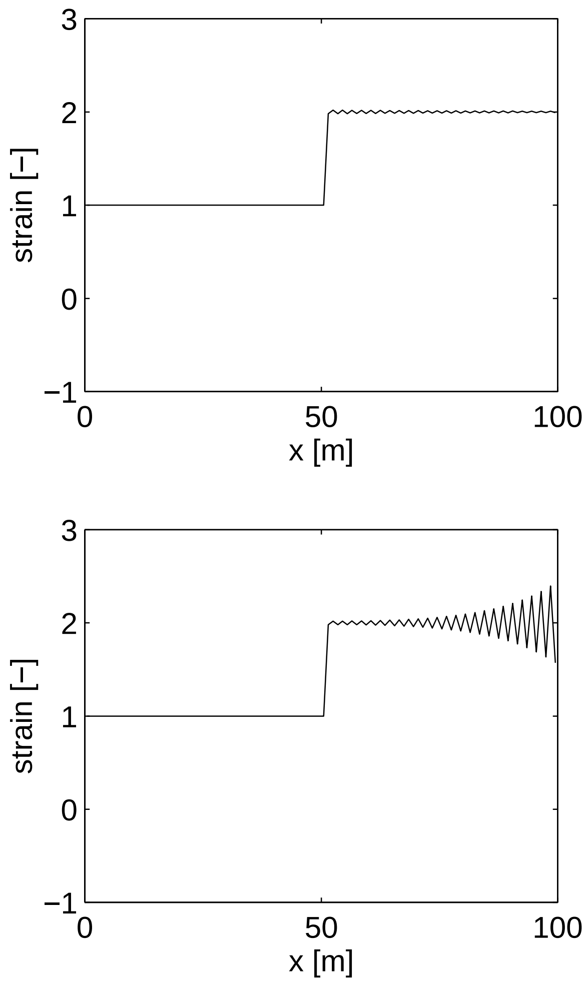

Figure 1: Wave propagation in a bar — strain profiles across the bar at time $t = 150$ s with critical penalty ratio (top) and super-critical penalty ratio (bottom)

and inertia penalties are applied at the right end of the bar to simulate fixed-end conditions. The material parameters are taken as $E = 1$ N/m^2 and $\rho = 1$ kg/m^3. The used finite element mesh consists of 100 two-noded bar elements. We apply a time step $\Delta t = \Delta t_{\text{crit}} = 1$ s, which means that the simulation should be numerically stable in the interior of the domain; if instabilities occur, they will occur due to the penalisation at the right end of the bar. The inertia penalty parameter $\alpha_m = 50$. Figure 1 shows the strain profiles across the bar at time $t = 150$ s for two values of the stiffness penalty: one whereby $\alpha_s/\alpha_m =$ CPR and one whereby $\alpha_s/\alpha_m = 1.002 \cdot$ CPR. It is clear that selecting a penalty ratio equal to the CPR leads to a simulation that is numerically stable. It can also be seen that if the penalty ratio is taken slightly larger than critical, instabilities are initiated at the penalised end of the bar.

6 CONCLUDING REMARKS

The bi-penalty method, in which inertia penalties are used simultaneously with the usual stiffness penalties, can be used in explicit dynamics to control the critical time step. The effects of stiffness penalties and inertia penalties on the critical time step are opposite, therefore their relative magnitudes can be tuned to obtain a zero net effect on the critical time step. We have also outlined procedures to compute so-called *critical penalty ratios* (CPRs) that set the stability limit for numerical simulations. An earlier method required that the bi-penalised eigenvalue problem was solved, but a new method has been formulated by which the CPR can be computed directly from the unpenalised eigenvalue problem.

In this paper, we have presented the computation of the CPR for simple one-dimensional bar elements. More sophisticated results for beam elements and two-dimensional square elements, obtained using the earlier method to compute the CPR, have been reported in [5], whereas the eigenfrequencies for unpenalised square elements (using plane various integration schemes) have also been given in [11].

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REFERENCES

[1] K.-J. Bathe. *Finite element procedures*. Prentice Hall, 1996.

[2] T. Belytschko and M.O. Neal. Contact-impact by the pinball algorithm with penalty and Lagrangian methods. *International Journal for Numerical Methods in Engineering*, 31:547–572, 1991.

[3] S. Ilanko. Introducing the use of positive and negative inertial functions in asymptotic modelling. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 461:2545–2562, 2005.

[4] J. Hetherington and H. Askes. Penalty methods for time domain computational dynamics based on positive and negative inertia. *Computers & Structures*, 87:1474–1482, 2009.

[5] H. Askes, M. Caramés-Saddler, and A. Rodríguez-Ferran. Bipenalty method for time domain computational dynamics. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 466:1389–1408, 2010.

[6] N. Asano. An approximate hybrid type of virtual work principle for two elastoimpact contact bodies. *Bulletin of the JSME*, 26(211), 1983.

[7] N. Asano. A Virtual Work Principle Using Penalty Function Method for Impact Contact Problems of Two Bodies. *Bulletin of the JSME*, 29(249), 1986.

[8] N. Asano. A penalty function type of virtual work principle for impact contact problems of two bodies. *Bulletin of the JSME*, 29(257), 1986.

[9] E.A. Paraskevopoulos, C.G. Panagiotopoulos, and G.D. Manolis. Imposition of time-dependent boundary conditions in FEM formulations for elastodynamics: critical assessment of penalty-type methods. *Computational Mechanics*, 45:157–166, 2010.

[10] T. Belytschko, P. Smolinski, and W.K. Liu. Stability of multi-time step partitioned integrators for first-order finite element systems. *Computer Methods in Applied Mechanics and Engineering*, 49:281–297, 1985.

[11] X. Ling and H.P. Cherukuri. Stability analysis of an explicit finite element scheme for plane wave motions in elastic solids. *Computational Mechanics*, 29:430–440, 2002.