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Consideration of nonlinear multipoint constraints in finite element analyses based on a master-slave elimination scheme operating at the global level

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A method to consider nonlinear multipoint constraints in finite element analysis based on a master-slave elimination scheme operating at the global level is presented. We focus on systems with nonlinear constraints in which the number of constraints is of the same order of magnitude as the number of degrees of freedom. Therefore, we rely on the master-slave elimination which gives us the huge benefit of drastically reducing the problem size. In the literature the presented master-slave elimination schemes for linear constraints are based on the manipulation of the system equations (global level), but the master-slave elimination schemes for nonlinear constraints are based on manipulation of the element formulation (local level). In contrast to that we use a global approach for which the nonlinear constraints are applied directly on the system equations in analogy to linear constraints. Thus, the method is independent of the underlying element formulation and the type of constraints which makes it more flexible.

1 Introduction

Nonlinear multipoint constraints can be used to model a wide range of features in engineering structures like joints [1, 2] or coupling of elements [3]. Therefore, efficient and accurate methods for the consideration of such constraints in finite element analyses are needed. This is particularly important for systems in which the number of constraints n_c is of the same order of magnitude as the number of degrees of freedom n_{dof}, i.e. $n_c = \mathcal{O}(n_{\text{dof}})$.

Constraints can be considered in the resulting system of equations (global level) or under certain circumstances at the element level of the underlying finite element approach (local level). In the following we focus on a treatment of constraints at global level. Thus, the discussed methods are independent of the underlying element formulation and the type of constraints which make them more flexible.

The following three equations describe a general nonlinear FE model with nonlinear constraints:

$$\text{nonlinear equilibrium equation:} \quad \mathbf{R}(\mathbf{V}) = \mathbf{0}\,; \quad \text{vector of dofs } \mathbf{V} \in \mathbb{R}^{n_{\text{dof}}}, \text{residual vector } \mathbf{R} \in \mathbb{R}^{n_{\text{dof}}} \tag{1}$$

$$\text{linearization of equilibrium equation:} \quad \mathbf{K}\Delta\mathbf{V} = -\mathbf{R}\,; \quad \text{tangential stiffness matrix } \mathbf{K} \in \mathbb{R}^{n_{\text{dof}} \times n_{\text{dof}}} \tag{2}$$

$$\text{nonlinear constraint equation:} \quad \mathbf{c}(\mathbf{V}) = \mathbf{0}\,; \quad \text{vector of constraint equations } \mathbf{c} \in \mathbb{R}^{n_c} \tag{3}$$

Four methods can be found in the literature to incorporate multipoint constraints in finite element analyses: Lagrange multipliers, penalty method, augmented Lagrange multipliers and master-slave elimination. In the following each method is presented briefly and its advantages and disadvantages are discussed.

The overview and notation is based on the widely used book by Belytschko et al. [4]. The following three quantities are needed for all methods:

- constraint vector $\mathbf{c}$
- constraint jacobian $\mathbf{G} = \frac{\partial \mathbf{c}}{\partial \mathbf{V}}$
- constraint hessian $\mathbf{H}_i = \frac{\partial^2 c_i}{\partial \mathbf{V}^2}$ with $i = 1, \ldots, n_c$

1.1 Lagrange Multipliers

In the Lagrange multiplier method n_c additional unknowns in form of the Lagrange multipliers $\boldsymbol{\lambda}$ are introduced. This leads to the following modified system:

$$\begin{bmatrix} \mathbf{K} + \lambda_i \mathbf{H}_i & \mathbf{G}^T \\ \mathbf{G} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{V} \\ \Delta\boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -\mathbf{R} - \boldsymbol{\lambda}^T\mathbf{G} \\ -\mathbf{c} \end{bmatrix} \quad ; \qquad \boldsymbol{\lambda} \in \mathbb{R}^{n_c} \tag{4}$$

Usage of Lagrange multipliers satisfies the constraints exactly and gives direct information on the constraint forces. However, Lagrange multipliers lead to a larger system of equations which is a huge drawback for systems with a large number of constraints. Without additional modification the resulting matrix is not positive definite [4].

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1.2 Penalty Method

In the penalty method additional terms with the penalty factor β are introduced. This leads to the following modified system:

$$\left(\mathbf{K} + \beta \mathbf{G}^T \mathbf{G} + \beta c_i \mathbf{H}_i\right) \Delta \mathbf{V} = -\mathbf{R} - \beta \mathbf{c}^T \mathbf{G} \ ; \qquad \beta \in \mathbb{R};\ \beta \gg 0 \tag{5}$$

Penalty methods are very easy to implement but they exhibit two main drawbacks. Firstly, the constraints are not fulfilled exactly. Secondly, choosing the proper penalty values is difficult, as small values worsen the problem of not fulfilling the constraints and large values can lead to an ill-conditioned stiffness matrix and therefore a deterioration of the convergence of the solution and numerical stability issues [4].

1.3 Augmented Lagrange Method

There also exists a mixture of the Lagrange multiplier method and the penalty method, the so called augmented Lagrange method. Here both Lagrange multipliers $\boldsymbol{\lambda}$ and penalty terms with penalty factor β are introduced:

$$\begin{bmatrix} \mathbf{K} + \lambda_i \mathbf{H}_i + \beta \mathbf{G}^T \mathbf{G} + \beta c_i \mathbf{H}_i & \mathbf{G}^T \\ \mathbf{G} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Delta \mathbf{V} \\ \Delta \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -\mathbf{R} - \boldsymbol{\lambda}^T \mathbf{G} - \beta \mathbf{c}^T \mathbf{G} \\ -\mathbf{c} \end{bmatrix} \ ; \qquad \boldsymbol{\lambda} \in \mathbb{R}^{n_c} \ ; \qquad \beta \in \mathbb{R};\ \beta \gg 0 \tag{6}$$

This augmentation leads to an improved numerical stability [4].

1.4 Master-Slave Elimination

Master-slave elimination schemes partition the degrees of freedom into $n_{\text{dof}} - n_c$ master dofs, denoted with m, and n_c slave dofs, denoted with s, see the following equation:

$$\begin{bmatrix} \mathbf{K}_{mm} & \mathbf{K}_{ms} \\ \mathbf{K}_{sm} & \mathbf{K}_{ss} \end{bmatrix} \begin{bmatrix} \Delta \mathbf{V}_m \\ \Delta \mathbf{V}_s \end{bmatrix} = - \begin{bmatrix} \mathbf{R}_m \\ \mathbf{R}_s \end{bmatrix} \tag{7}$$

For each constraint there is no more than one slave dof. A standard master-slave elimination scheme operating at the global level developed by Shephard [5] which leads to a symmetric modified matrix is presented in the following:

$$\left(\mathbf{K}_{mm} + \mathbf{G}_m^T \mathbf{K}_{sm} + \mathbf{K}_{ms} \mathbf{G}_m + \mathbf{G}_m^T \mathbf{K}_{ss} \mathbf{G}_m\right) \Delta \mathbf{V}_m = -\mathbf{R}_m - \mathbf{G}_m^T \mathbf{R}_s - \mathbf{K}_{ms} \mathbf{c} - \mathbf{G}_m^T \mathbf{K}_{ss} \mathbf{c} \tag{8}$$

$$\Delta \mathbf{V}_s = \mathbf{G}_m \Delta \mathbf{V}_m - \mathbf{c} \tag{9}$$

The master-slave elimination also satisfies the constraints exactly and leads to a smaller resulting system of equations. However, this approach relies on heavy manipulation of the system matrix and system vector which can, under certain circumstances, lead to a loss of favorable properties of the system matrix e.g. a small bandwidth. By using modern mathematical libraries, highly efficient functions are available for these manipulations. Thus, the computational cost of these manipulation is small compared to the gain of efficiency by reduction of the number of equations. However, the master-slave elimination schemes operating at the global level found in the literature are limited to linear constraints, e.g. [5]. In contrast there are master-slave elimination schemes operating at the local level that are designed to handle nonlinear constraints but they are limited to constraints due to joints [1, 2].

Through the discussion, it becomes clear that there is no master-slave elimination scheme operating at the global level that is capable of handling nonlinear constraints. In the following such a new master-slave elimination scheme operating at the global level is presented which can be used to consider nonlinear multipoint constraints in contrast to the existing schemes.

2 New Master-Slave Elimination Scheme

Due to the constraints additional constraint forces are induced in the system. These constraint forces perturb the equilibrium defined by equation (1). Therefore the premise of the new method is to include the constraint forces $\mathbf{C}$ in the equilibrium equations which is similar to the approach by Narayanaswamy [6]. However, the constraints are introduced in the equilibrium equation (1) and not in the linearization (2). In constrast to [6] this results in a consistent linearization of the constraint forces. In the following the new method is derived in a compact manner. For more details, see [7].

The new approach leads to the following modified equilibrium equation:

$$\mathbf{R}_{\text{mod}} = \mathbf{R} + \mathbf{C} \ ; \qquad \mathbf{C} \in \mathbb{R}^{n_{\text{dof}}} \tag{10}$$

The constraint forces $\mathbf{C}$ can be separated into different parts $\mathbf{C}_i$ for each individual constraint i:

$$\mathbf{C} = \sum_{i=1}^{n_c} \mathbf{C}_i \ ; \qquad \mathbf{C}_i \in \mathbb{R}^{n_{\text{dof}}} \tag{11}$$

The constraint forces $\mathbf{C}$ are additional unknowns. Thus, to calculate these n_{dof} unknowns n_{dof} additional equations are needed. By numerical experiments the following relationship between constraint forces at master dofs and slave dofs could be identified:

$$-G_{i,s}C_{i,m_j} + G_{i,m_j}C_{i,s} = 0 \qquad \Longleftrightarrow \qquad C_{i,m_j} = \frac{G_{i,m_j}}{G_{i,s}}C_{i,s} \tag{12}$$

The theoretical justification of this relationship (12) is part of ongoing research.

In a first step the relationship (12) can be used to express constraint forces at master dofs with constraint forces at slave dofs. For the sake of simplicity this is only shown for one constraint with n master dofs, i.e. $n_c = 1$:

$$c(V_{m_1}, \ldots, V_{m_n}, V_s) = 0 \tag{13}$$

Incorporating equation (12) in equation (10) yields the following expression for the modified equilibrium equations:

$$\begin{bmatrix} R_{m_1} + C_{m_1} \\ \ldots \\ R_{m_n} + C_{m_n} \\ R_s + C_s \end{bmatrix} = \begin{bmatrix} R_{m_1} + \frac{G_{m_1}}{G_s}C_s \\ \ldots \\ R_{m_n} + \frac{G_{m_n}}{G_s}C_s \\ R_s + C_s \end{bmatrix} = \begin{bmatrix} R_{m_1} - \frac{G_{m_1}}{G_s}R_s \\ \ldots \\ R_{m_n} - \frac{G_{m_n}}{G_s}R_s \\ R_s + C_s \end{bmatrix} = \mathbf{0} \tag{14}$$

Thus, the constraint force at the slave dof C_s remains as the only unknown variable in equation $(14)_{n+1}$. It can be shown that the last equation in (14) is linearly dependent on all the other equations in (14). To show this the equations in $(14)_{n+1}$ are scaled.

$$R_s + C_s = 0 \quad \Leftrightarrow \quad \frac{G_{m_1}}{G_s}R_s + \frac{G_{m_1}}{G_s}C_s = 0 \quad \Leftrightarrow \quad \ldots \quad \Leftrightarrow \quad \frac{G_{m_n}}{G_s}R_s + \frac{G_{m_n}}{G_s}C_s = 0 \tag{15}$$

Thus, equation $(14)_{n+1}$ can now be replaced

$$\begin{bmatrix} R_{m_1} - \frac{G_{m_1}}{G_s}R_s \\ \ldots \\ R_{m_n} - \frac{G_{m_n}}{G_s}R_s \\ \frac{G_{m_1}}{G_s}R_s + \frac{G_{m_1}}{G_s}C_s + \ldots \frac{G_{m_n}}{G_s}R_s + \frac{G_{m_n}}{G_s}C_s \end{bmatrix} = \begin{bmatrix} R_{m_1} - \frac{G_{m_1}}{G_s}R_s \\ \ldots \\ R_{m_n} - \frac{G_{m_n}}{G_s}R_s \\ \frac{G_{m_1}}{G_s}R_s - R_{m_1} + \ldots + \frac{G_{m_n}}{G_s}R_s - R_{m_n} \end{bmatrix} = \mathbf{0} \tag{16}$$

As equation $(16)_{n+1}$ is linearly dependent on the other equations in (16), it has to be replaced by another equation. This can only be done by the constraint (13) itself. The modified equilibrium equations are:

$$\begin{bmatrix} R_{m_1} - \frac{G_{m_1}}{G_s}R_s \\ \ldots \\ R_{m_n} - \frac{G_{m_n}}{G_s}R_s \\ c \end{bmatrix} = \mathbf{0} \tag{17}$$

The summation of the constraint forces for different constraints (11) leads to the following expression for the modified equilibrium equations for an arbitrary number of constraints:

$$\mathbf{R}_{\text{mod}} = \begin{bmatrix} \mathbf{R}_{\text{mod, m}} \\ \mathbf{R}_{\text{mod, s}} \end{bmatrix} = \begin{bmatrix} \mathbf{R}_m - \mathbf{G}_m^T\mathbf{G}_s^{-1}\mathbf{R}_s \\ \mathbf{c} \end{bmatrix} = \mathbf{0}\ ; \qquad \mathbf{R}_{\text{mod}} \in \mathbb{R}^{n_{\text{dof}}} \tag{18}$$

Therefore, the total constraint forces at the master dofs can be calculated as follows:

$$\mathbf{C}_m = -\mathbf{G}_m^T\mathbf{G}_s^{-1}\mathbf{R}_s \tag{19}$$

Remark: The jacobian of the constraint equations with respect to the slave dofs $\mathbf{G}_s$ is a diagonal matrix. This is computationally beneficial because the inversion of the matrix can be computed very easily.

$$\mathbf{G}_s = \text{diag}\left(\frac{\partial c_i}{\partial V_{s,i}}\right)\ ; \qquad \mathbf{G}_s \in \mathbb{R}^{n_c \times n_c};\ i = 1, \ldots, n_c \tag{20}$$

If the modified equilibrium equation (18) is solved by a NEWTON-RAPHSON scheme, the linearization is needed:

$$\mathbf{K}_{\text{mod}} = \frac{\partial \mathbf{R}_{\text{mod}}}{\partial \mathbf{V}}\ ; \qquad \mathbf{K}_{\text{mod}} \in \mathbb{R}^{n_{\text{dof}} \times n_{\text{dof}}} \tag{21}$$

The modified linearized equilibrium equation is given by:

$$\begin{bmatrix} \mathbf{K}_{\text{mod},mm} & \mathbf{K}_{\text{mod},ms} \\ \mathbf{G}_m & \mathbf{G}_s \end{bmatrix} \begin{bmatrix} \Delta \mathbf{V}_m \\ \Delta \mathbf{V}_s \end{bmatrix} = \begin{bmatrix} -\mathbf{R}_{\text{mod},m} \\ -\mathbf{c} \end{bmatrix} \tag{22}$$

As a second step the dimension of the system is reduced by elimination of the increment of the slave dofs $\Delta\mathbf{V}_s$. This is done by a static condensation on the global level. This leads to the following reduced system of equations:

$$\mathbf{K}_{\text{red}} \Delta \mathbf{V}_m = \mathbf{R}_{\text{red}} \tag{23}$$

$$\mathbf{K}_{\text{red}} = \mathbf{K}_{\text{mod},mm} - \mathbf{K}_{\text{mod},ms} \mathbf{G}_s^{-1} \mathbf{G}_m \; ; \qquad \mathbf{K}_{\text{red}} \in \mathbb{R}^{(n_{\text{dof}}-n_c)\times(n_{\text{dof}}-n_c)} \tag{24}$$

$$\mathbf{R}_{\text{red}} = -\mathbf{R}_{\text{mod},m} + \mathbf{K}_{\text{mod},ms} \mathbf{G}_s^{-1} \mathbf{c} \; ; \qquad \mathbf{R}_{\text{red}} \in \mathbb{R}^{n_{\text{dof}}-n_c} \tag{25}$$

It can be shown that the reduced tangential stiffness matrix $\mathbf{K}_{\text{red}}$ is symmetric. As already mentioned more details can be found in [7].

3 Example

In the following the performance of the new method is compared to established methods. The example is a simple tensile test as shown in figure 1 with the following parameters: $E = 1, A = 1, L = 1$. The nonlinear constraint takes the form of:

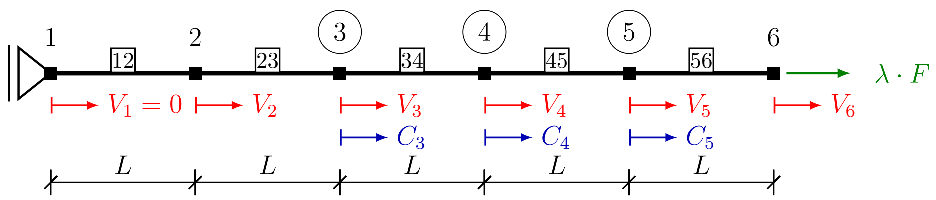

Fig. 1: tensile test with nonlinear constraint

$$c(V_4, V_3, V_5) = V_4^{1+\gamma} - \frac{1}{2} V_3^{1+\alpha} - \frac{1}{2} V_5^{1+\beta} = 0 \tag{26}$$

In terms of the master-slave elimination V_4 is the slave dof, V_3 and V_5 are the master dofs. The underlying finite element formulation is linear and the load F is increased linearly. The parameters α, β and γ control the nonlinearity of the constraint (26). For three sets of these parameters the results of the example are shown in table 1.

In the first row the constraint force at the slave dof for the master-slave elimination is shown. It can be seen that the results are in good agreement for different load steps. This demonstrates the robustness of the new method.

In the second row the error e_C is shown for the master-slave elimination and the penalty method. It is defined as the relative error in the constraint force at the slave dof in comparison to the result for the Lagrange multiplier method which is used as a reference because it fulfills the constraints exactly:

$$e_C = \frac{|C_4 - C_{4,\text{Lagrange}}|}{|C_{4,\text{Lagrange}}|} \tag{27}$$

The diagram shows that the error for the master-slave elimination is of the same order as the achievable computational accuracy. It can be deduced that the master-slave elimination gives the same results for the constraint force as the Lagrange multiplier method and is therefore of similar accuracy. For comparison the result for the penalty method for different values of the penalty parameter β are plotted, too. As expected the penalty method is not as accurate as the other methods.

In the third row the absolute value of the constraint equation is shown. Here the master-slave elimination and the Lagrange multiplier method give results of the same order as the achievable computational accuracy. As a result it can be shown that both methods fulfill the constraint exactly with respect to the achievable accuracy. As expected the penalty method does not fulfill the constraints exactly.

In the fourth row the number of iteration per load step is shown. Here the master-slave elimination shows similar behavior as the Lagrange multiplier method. From this it can be concluded that the master-slave elimination is of similar robustness as the Lagrange multiplier method. It performs slightly better than the penalty method.

In the fifth row the norm of the residual during the NEWTON-RAPHSON iteration for the last load step for the master-slave elimination is shown. It can be seen clearly that the new method exhibits quadratic convergence.

Table 1: Results for the tensile test. Last row shows the norm of the residual vector of the last load step for the master-slave elimination.

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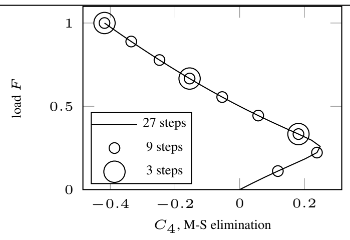
<td>
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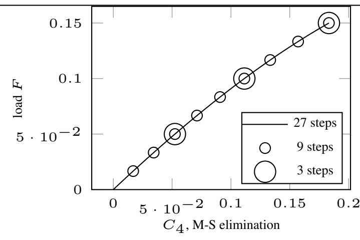
<td>
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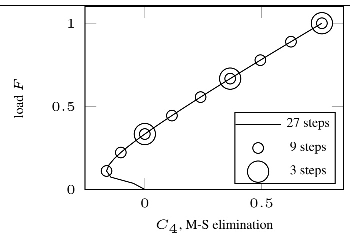
<td>
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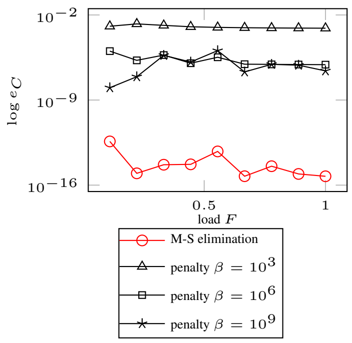
<td>
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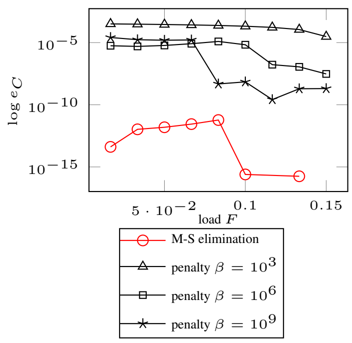
<td>
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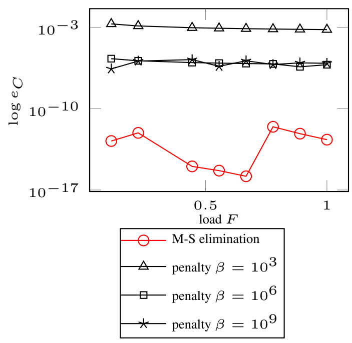
<td>
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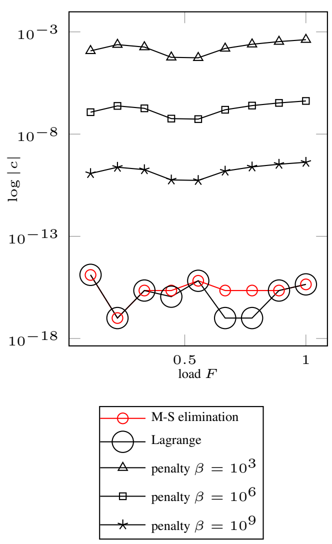
<td>
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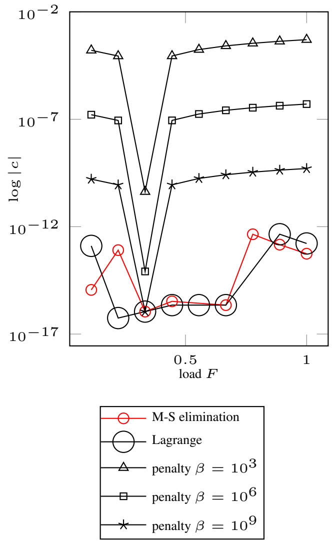
<td>
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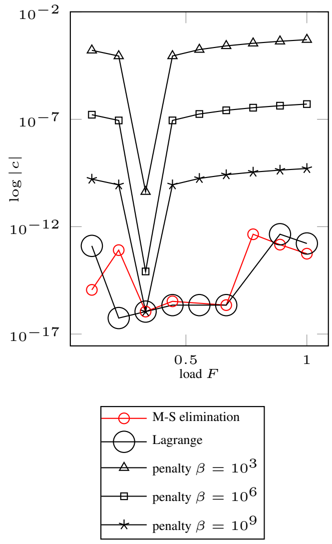
<td>
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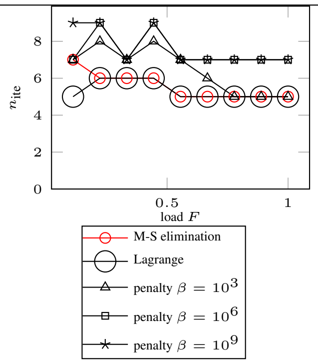
<td>
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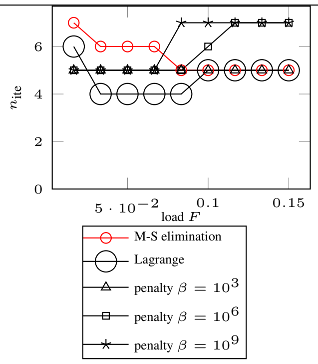
<td>
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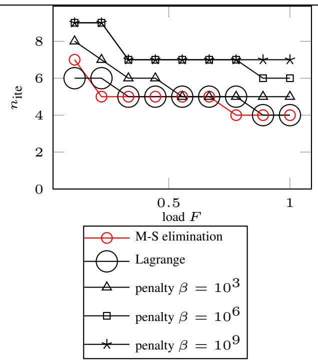
<td>
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4 Conclusion

A new method for the consideration of linear and nonlinear multipoint constraints in finite element analyses was presented. It is a modification of the well established master-slave elimination. In contrast to the existing master-slave elimination schemes operating at the global level it is capable of handling nonlinear constraints. In contrast to the penalty method the constraints are fulfilled exactly. In contrast to the Lagrange multiplier method no additional unknowns are introduced. On the contrary, the problem size is even reduced by the number of constraints n_c. This is computationally beneficial especially for problems in which the number of constraints is of the same order of magnitude as the number of degrees of freedom $n_c = \mathcal{O}\left(n_{\mathrm{dof}}\right)$. The new method is of similar accuracy and robustness and more efficient as the Lagrange multiplier method.

The theoretical justification of the relationship between the constraint forces at the master and the slave dofs (12) is part of ongoing research. The presented method will be used to quantify the influence of constraints for highly nonlinear problems and realistic applications. Additionally the applicability of the new method for transient problems is investigated. These results will be available in [7].

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