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BFGS quasi-Newton finite element solver for the penalty constrained contact problems

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Micro Abstract
A solution scheme for the penalty constrained contact problems is presented. The algorithm employes popular quasi-Newton solver for FE applications-the BFGS (Broyden-Fletcher-Goldfarb-Shanno) method with contact constraints enforced by the penalty method. The effectiveness of proposed solution strategy is tested by means of benchmark examples including bending dominated problems. Finally, the capability of contact solver is demonstrated in creep analysis of high pressure steam turbine casing.

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Introduction

The iteration scheme used most frequently for the solution of nonlinear finite element (FE) equations is the Newton-Raphson method. It is well known that the local convergence property of the Newton iteration is difficult to achieve even when an emphasis is laid on the use of consistent tangent stiffness matrices for contact analysis [3–5] based on the correct derivation of gradient matrix. Moreover, excessive changes in the active constraint set may occur during the iteration process and totally change the basic system of equations. In this case, quadratic convergence can no longer be expected.

A very good alternative is offered by a class of methods known as the quasi-Newton methods. The quasi-Newton solvers construct an algorithmic secant matrix based on the series of successive approximations to the solution, using the current and previous iteration steps. Therefore, no full linearization of the contact constraint is required in the solution of contact problems within the framework of the quasi-Newton strategies.

In this work, the most popular quasi-Newton solvers for FE applications, the BFGS (Broyden-Fletcher-Goldfarb-Shanno) method is considered [2]. The modification of the BFGS method is outlined for constrained non-linear system that results from the FE discretization of contact problem. The contact conditions are enforced by the penalty method [1]. The effectiveness of proposed solution strategy is tested by means of benchmark examples including two cubes contact and bending of two cantilever beams. Finally, the capability of contact solver is demonstrated in creep analysis of high pressure steam turbine casing.

1 A simple model problem

In order to demonstrate the behaviour of the proposed solution scheme, we now present a solution of a simple model problem [1]. We consider a one-dimensional, one degree of freedom mechanical system, subject to a single constraint: a simple linear spring with stiffness k, whose right end contacts against an obstacle. The spring is loaded by external force F_{ext} (see Fig. 1). This contact imposes a unilateral constraint on unknown displacement u, allowing a gap to open but preventing from penetration. The solution to this system is apparent: if $F_{\mathrm{ext}} < 0$, then

$u = F_{\text{ext}}/k$; if $F_{\text{ext}} \geq 0$, then $u = 0$ to avoid penetration.

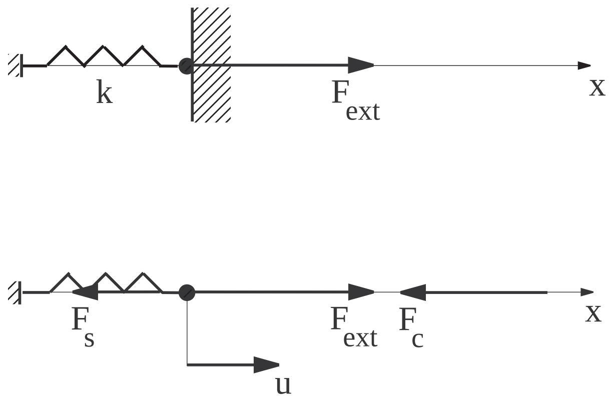

Figure 1. Simple one dimensional spring system subject to a single constraint.

Denoting by F_{s} the force produced by the spring and $F_c = \xi d$ the penalty force expressed as a linear function of the penetration depth d multiplied by penalty parameter ξ, equilibrium is enforced through the definition of the residual force G

$$G = F_{\text{s}} + F_{\text{c}} - F_{\text{ext}}. \tag{1}$$

When $G = 0$, the equilibrium condition is satisfied. In addition to the equilibrium condition (1), u and F_c are subject to the contact conditions

$$u \leq 0 \quad F_{\text{c}} \geq 0 \quad F_{\text{c}}\, u = 0. \tag{2}$$

A graphical illustration of solution of this example with penalty constraint, plotted as the residual force G versus u, is shown in Fig. 2, which represents polygonal characteristic (solid line) with slopes given by the penalty parameter ξ (for $u > 0$) and the spring stiffness k (for $u < 0$), denoted by $\texttt{KCS} = 1$. We should emphasize that the final numerical solution ($G = 0$) is always entailed by undesirable penetration d_{final}, which violates conditions (2).

Now, we demonstrate the BFGS and modified Newton-Raphson (MNR) iteration process. Both methods start at point '0' directed by initial stiffness k toward point '1' corresponding to elastic solution u_{elastic} for unconstrained spring. There contact force F_c induces an increase of the residual G. As a result, the spring rebounds to point '2', from where the MNR method keeping initial direction regresses to point '1' and the cycle is repeated. The BFGS method using algorithmic secant based on the curent and previous iteration step gradually drifts to the solution but the convergence is very slow (points '3', '4',...).

In order to improve the convergence properties we fix spring to obstacle by penalty force after initial bounce has been encountered. In graphical interpretation it represents the replacement of the spring part of characteristic with penalty one for $u < 0$ (dash-and-dot line), denoted by $\texttt{KCS} = 0$ in Fig. 2. Then, the solution of the spring model is obtained in three steps for the BFGS method (points '2*', '3*'), whereas the MNR method still diverges.

2 The modified BFGS algorithm

Now, we generalize the discussion of this simple model by considering the multiple degrees of freedom discrete system of governing equilibrium equations (see equation (18) in [1]), which is useful to rewrite in the form of the residual vector $\mathbf{g}(\mathbf{u}_i)$

$$\mathbf{g}(\mathbf{u}_i) = \mathbf{F}(\mathbf{u}_i) - \mathbf{R}(\mathbf{u}_i) - \mathbf{R}_{c1}(\mathbf{u}_i) - \mathbf{R}_{c2}(\mathbf{u}_i) \tag{3}$$

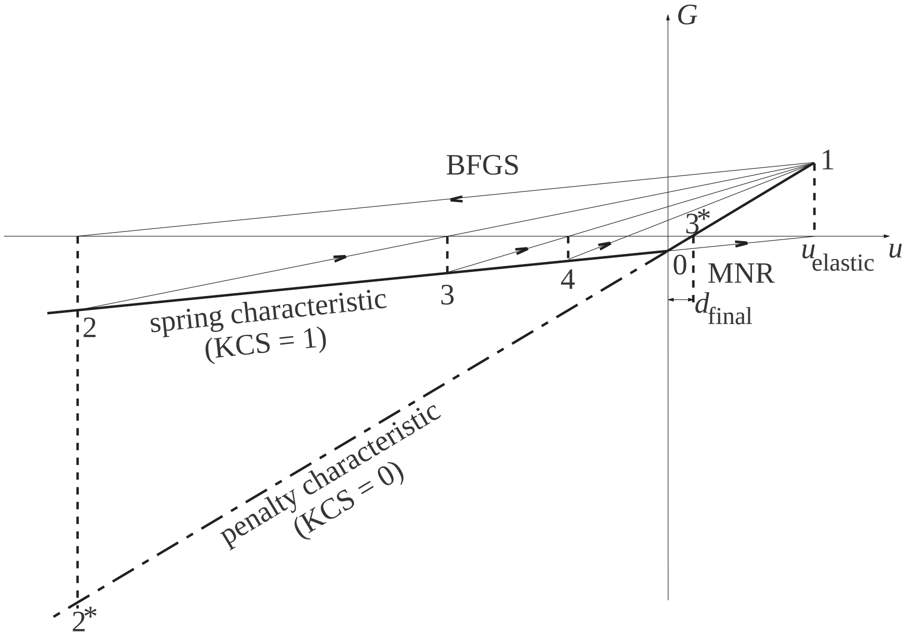

Figure 2. The BFGS and MNR iterations for a single degree of freedom system with penalty constraint.

or briefly

$$\mathbf{g}_i = \mathbf{F}_i - \mathbf{R}_i - \mathbf{R}_{c1i} - \mathbf{R}_{c2i}. \tag{4}$$

The vectors $\mathbf{u}, \mathbf{F}, \mathbf{R}$ and $\mathbf{R}_{c1}, \mathbf{R}_{c2}$ are of length `LSOL`. The vectors $\mathbf{R}_{c1}, \mathbf{R}_{c2}$ contain penalty forces resulting from FE discretization. Similarly, as in one dimensional example the iteration process is controlled by setting of key `KCS`: $\texttt{KCS} = 1$ means that contact search is performed while $\texttt{KCS} = 0$ corresponds to the case when existing contact surfaces are only re-established regardless of sign the penetration d_{IG} [1]. The implementation of the BFGS algorithm for constrained nonlinear system is outlined in Template 1.

The crucial point of the algorithm is the following: after the contact search has been performed in the evaluation of $\mathbf{g}(\mathbf{u}_0)$ the assigned contact surfaces are sticked together by penalty tractions ($\texttt{KCS} = 0$) regardless of their signs. In a general 3D case it cannot be expected that the next approximation will find solution $\mathbf{g}(\mathbf{u})$ as in the model example, thus the calculation must be performed until the equilibrium is reached. Then, the verification of the correct contact state (step 3) is necessary since tension tractions can occur on contact boundaries. All the penalty constraints are removed and the convergence condition is tested again with $\texttt{KCS} = 1$. If it is not satisfied, the algorithm continues with the iteration process with re-initialization $\tilde{\mathbf{K}}_0 = \mathbf{K}_{\text{elastic}}, \mathbf{u}_0 = \mathbf{u}_{\text{c}}$ and $\texttt{KCS} = 1$ by returning to step 2.

In fact, the box is virtually identical to the BFGS implementation [2], which is executed twice, firstly with $\texttt{KCS} = 0$ and then again with $\texttt{KCS} = 1$. The converged solution of the first run $\mathbf{u}_{\text{c}}$ serves as an approximation for the second one. The capability of this procedure was confirmed in a number of problems [1].

3 Numerical examples

3.1 Two cubes contact

Let us consider the two cubes shown in Fig. 3 subjected to uniformly distributed pressure p, interacting over their common contact interface. The pressure acting on bottom face is replaced with the equivalent reactions introduced by appropriate boundary conditions. The top cube is suspended on soft regularization springs of total stiffness k.

Template 1, The modified BFGS algorithm for constrained nonlinear system.

1. **Initialize** the iteration process
   (a) Set initial parameters: $i = 0, \texttt{KCS} = 1$
   (b) Initialize values: $\mathbf{R}_0, \tilde{\mathbf{K}}_0 = \mathbf{K}_{\text{elastic}}, \mathbf{u}_0 = \mathbf{u}_{\text{elastic}}$ (initial guess)
   (c) Evaluate: $\tilde{\mathbf{K}}_0^{-1}, \mathbf{g}(0), \mathbf{g}(\mathbf{u}_0)$
   (d) Set key: $\texttt{KCS} = 0$
2. **Loop** on i (iteration counter) for equilibrium
   (a) Compute search direction: $\tilde{\mathbf{K}}_i \mathbf{d}_{i+1} = \mathbf{g}(\mathbf{u}_i)$
   (b) Line search and solution vector update:
      i. Evaluate $G(0) = \mathbf{d}_{i+1}^{\text{T}} \mathbf{g}(\mathbf{u}_i)$
      ii. **Loop** over β; $\beta \in \{\beta_k\} = \{1, 2, 4, 8, 16\}$
         - Evaluate: $G(\beta) = \mathbf{d}_{i+1}^{\text{T}} \mathbf{g}(\mathbf{u}_i + \beta \mathbf{d}_{i+1})$
         - IF $G(\beta) \leq \texttt{STOL} * G(0)$ THEN go to step iii
         - IF $G(\beta)$ changed its sign THEN
           – finer adjustment of $\beta \in \langle \beta_{k-1}, \beta_k \rangle$ by means of accelerated secant method (*Illinois* algorithm [2])
           ENDIF
      iii. Update: $\mathbf{u}_{i+1} = \mathbf{u}_i + \beta \mathbf{d}_{i+1}$
   (c) Equilibrium check IF $(\|\mathbf{g}(\mathbf{u}_{i+1})\| < \texttt{RTOL}\|\mathbf{g}(0)\|)$ THEN
      - IF $(\texttt{KCS} = 1)$ THEN equilibrium achieved $\rightarrow$ EXIT
      - go to step 3

      ENDIF
   (d) Increment iteration counter: $i = i + 1$
   (e) Stability check
      i. Evaluate the condition number: $c = \sqrt{\dfrac{\beta G_0}{G_0 - G(\beta)}}$
      ii. IF $c > c_{\text{crit}} \approx 5$ THEN
         - Take previous quasi-secant matrix: $\tilde{\mathbf{K}}_i = \tilde{\mathbf{K}}_{i-1}$
         - go to step 2a
   (f) Perform BFGS update
      i. Evaluate: $\Delta \mathbf{u}_i = \mathbf{u}_i - \mathbf{u}_{i-1}$, $\Delta \mathbf{g}_i = \mathbf{g}(\mathbf{u}_i) - \mathbf{g}(\mathbf{u}_{i-1})$
      ii. Compute BFGS auxiliary vectors:
      $$\mathbf{v}_i = -\sqrt{\frac{\Delta \mathbf{u}_i^{\text{T}} \Delta \mathbf{g}_i}{\Delta \mathbf{u}_i^{\text{T}} \tilde{\mathbf{K}}_{i-1} \Delta \mathbf{u}_i}} \tilde{\mathbf{K}}_{i-1} \Delta \mathbf{u}_i - \Delta \mathbf{g}_i$$
      $$\mathbf{w}_i = \frac{\Delta \mathbf{u}_i}{\Delta \mathbf{u}_i^{\text{T}} \mathbf{g}_i}$$
      iii. Compute the inverse quasi-secant matrix:
      $$\tilde{\mathbf{K}}_i^{-1} = (\mathbf{I} + \mathbf{w}_i \mathbf{v}_i^{\text{T}}) \tilde{\mathbf{K}}_{i-1}^{-1} (\mathbf{I} + \mathbf{v}_i \mathbf{w}_i^{\text{T}})$$
      iv. go to step 2a
3. **Check on** correct contact state on contact boudaries
   (a) Re-initialize values: $\tilde{\mathbf{K}}_0 = \mathbf{K}_{\text{elastic}}, \mathbf{u}_0 = \mathbf{u}_{\text{c}}$
   (b) go to step 2

This example demonstrates a generalization of a simple one-dimensional spring model described in Section 1. We investigated an accuracy of the numerical solution for various values of the penalty parameter ξ and for different stiffnesses of the regularization springs k. The stiffness k was by several orders of magnitude smaller than the stiffnesses of the cubes so that the results were not significantly affected. The performace of both linear and quadratic isoparametric serendipity elements was tested.

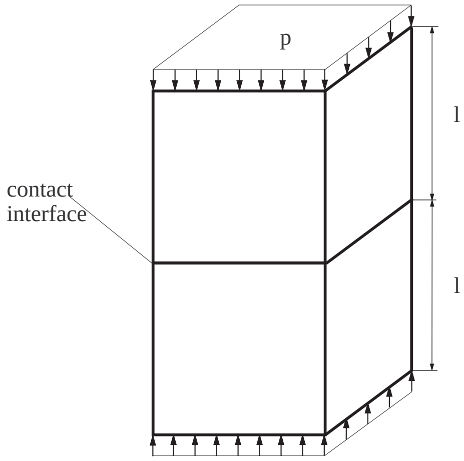

Figure 3. Two cubes subjected to uniformly distributed pressure p, interacting over their common contact interface. Geometry: length $l = 1$ [m]. Material properties: Young modulus $E = 2.1\times\ 10^5$ [MPa], Poisson's ratio $\nu = 0.3$. Loading: $p = 10$ [MPa].

The results are summarized in Tab. 1, where relative displacement errors ϵ calculated as the magnitudes of penetrations related to the displacements of cubes and the numbers of iterations `NITER` (linear elements/quadratic elements) are shown. The divergence of calculation is denoted by symbol '***', the results were obtained within one load step.

k	ξ[N/m^3]									
	10^{12}		10^{13}		10^{14}		10^{15}		10^{16}	
[N/m]	NITER	ϵ[%]	NITER	ϵ[%]	NITER	ϵ[%]	NITER	ϵ[%]	NITER	ϵ[%]
10^6	5/11	20	8/16	2	11/***	0.2	***/***	***	***/***	***
10^7	5/9	20	5/15	2	8/***	0.2	11/***	0.02	***/***	***
10^8	5/7	20	5/12	2	8/14	0.2	9/***	0.02	9/***	0.002
10^9	4/5	20	4/9	2	5/13	0.2	9/17	0.02	8/***	0.002

Table 1. Relative displacement errors ϵ and numbers of iterations `NITER`.

Similarly, as in one dimensional example the initial rebound of the top cube arose. Its amount, which was directly proportional to ξ and inversely proportional to k, was enormous (e.g. for $\xi = 10^{14}$ [N/m^3] and $k = 10^7$ [N/m] the initial rebound was 10^7 [m]). Although it was reduced by the line search the nodal diplacements were affected by round-off errors leading to the distortion of the contact plane. This explains the increase of number of iterations `NITER` or even the divergence of the calculation of normal vector with increasing ξ or with decreasing k in Tab. 1. This effect is particulary apparent for quadratic mesh since a larger distortion of contact plane occurs. Note that a number of iterations is always greater than three in contrast to one dimensional spring model. It is caused by the 3D effect when besides huge rebound large compression of the top cube occurs due to presence of regularization springs.

3.2 Contact between two cantilever beams

Let us consider the contact between two cantilever beams shown in Fig. 4. The example was adopted from Reference [6]. The problem was treated as plane stress one discretized using eight-node quadratic serendipity elements. The FE analysis took into account large displacements and rotations in the total Lagrangian formulation (TLF). The value of the penalty parameter was set to $\xi = 10^9[\mathrm{N/m^3}]$.

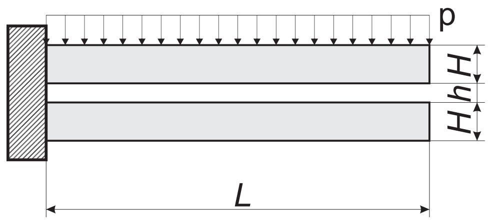

Figure 4. Contact of two cantilever beams. Geometry: length $L = 1000$ [mm], height $H = 20$ [mm], inital gap $h = 10$ [mm], thickness $t = 20$ [mm]. Material properties: Young modulus $E = 2.1 \times\ 10^5$ [MPa] and Poisson's ratio $\nu = 0.3$. Loading: $p = 0.5$ [MPa]

The deformed configuration of FE model for large displacement analysis is shown in Fig. 6. For illustration, the elastic solution which serves as initial guess is plotted in Fig. 5. It is clear that starting approximation is very far from final contact solution. Alternatively, approximated contact matrix can be more convenient used instead of initial elastic matrix as it will be shown in the presentation. Note that the total load was applied within ten load substeps. This example nicely demonstrates the the capability of the modified BFGS algorithm for the solutions of bending dominated problems.

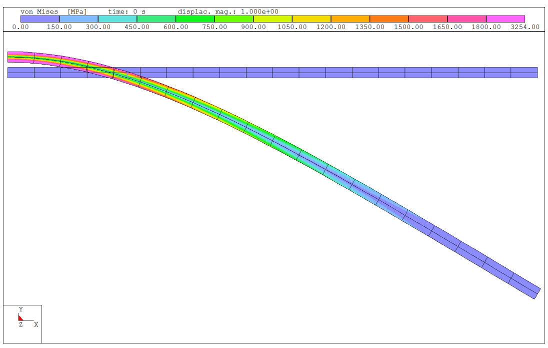

Figure 5. The deformed configuration of the beams—initial linear solution.

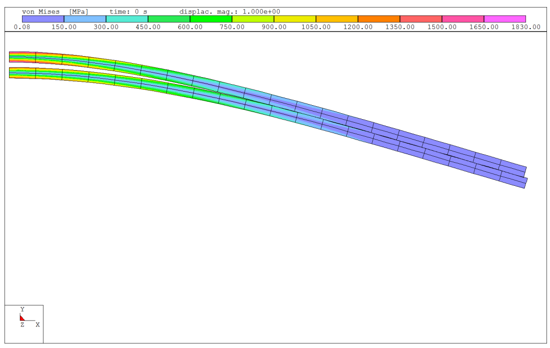

Figure 6. The deformed configuration of the beams—contact solution including large displacement.

Conclusions

In this work, a solution scheme for the FE solution of contact problems was presented. The proposed technique uses the BFGS method modified for constrained nonlinear system enforced by the penalty method. For the improvement of the convergence properties the iteration process was divided into two steps. After the contact search had been performed the assigned contact surfaces were connected together by the penalty tractions regardless of the sign of the reaction forces. The converged solution of this run served as an approximation for the second one, where the contact search was applied as usual. The effectiveness of proposed solution strategy was tested by means of benchmark examples including two cubes contact and bending of two cantilever beams. In the presentation, the capability of contact solver will be demonstrated in creep analysis of high pressure steam turbine casing.

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