11^{th} World Congress on Structural and Multidisciplinary Optimization
7^{th} - 12^{th}, June 2015, Sydney Australia

Design optimization of multi-point constraints in structures

Daniel N. Wilke[1], Schalk Kok[2]

[1] Department of Mechanical and Aeronautical Engineering, University of Pretoria, South Africa, nico.wilke@up.ac.za
[2] Department of Mechanical and Aeronautical Engineering, University of Pretoria, South Africa, schalk.kok@up.ac.za

1. Abstract

Multi-point constraints have been used in analysis of structures, since the early 1970's. However, limited research regarding the sensitivity analysis and design optimization of multi-point constraints have been done. We recently showed for the master-slave elimination approach that for the analysis using Newton's method, the exact consistent tangent contribution requires the second derivative contribution of the multi-point constraint relations. However, the second-order contribution is often omitted when conducting the analysis resulting in an inexact consistent tangent contribution.

In this study, we investigate whether the exact consistent tangent contribution is essential when designing multi-point constraints for structural applications. The multi-point constraint design problem is to design a frictionless roller guide for a center loaded simply supported beam. The unconstrained design problem aims to find the geometry of a frictionless roller guide such that the centroid of the beam follows a prescribed load path . We compute the exact analytical gradients of the objective function using the the exact consistent tangent contribution of the multi-point constraints. In addition, we also compute the approximate analytical gradients of the objective function, where the only approximation in the sensitivity analysis is the inexact consistent tangent contribution of the multi-point constraints.

We then investigate the difference in design optimization performance when supplying the exact and approximate analytical gradients. We compare the ability and performance of steepest descent and BFGS conjugate gradient algorithms with a cubic line search strategy to design the multi-point constraints when both the exact and inexact gradients are supplied.

2. Keywords: Multi-point constraint, exact consistent tangent, inexact consistent tangent, design optimization, analytical sensitivities.

3. Introduction

Finite element based multi-point constraint (MPC) research was introduced in the middle seventies by the well known Gallagher textbook [2]. This textbook was supplemented by a number of papers from the late seventies [3, 4] to early eighties [5, 6, 7]. These papers mainly included discussions on the analysis of linear and nonlinear MPCs for the master-slave elimination and Lagrangian approaches. The discussion on MPCs got rekindled in the nineties and early 2000s, with papers that mainly focussed on linear MPCs [8, 9, 10, 11, 12]. These papers touched on implementation approaches [9, 10, 11], programming abstractions that are well suited to implement MPCs [8] or specific applications [12].

Unfortunately, not much work has been conducted on the sensitivity analysis or the use of sensitivities in the design of nonlinear MPCs. We recently showed [1] that for the analysis of MPCs using Newton's method in the master-slave elimination approach the exact consistent tangent contribution requires the second derivative contribution of the multi-point constraint relations. However, the second-order contribution is often omitted when conducting the analysis resulting in an inexact consistent tangent contribution that are often employed with inexact Newton strategies. The inexact consistent tangent contribution is sufficient to efficiently analyze nonlinear MPCs. It however remains unclear whether they are sufficient to approximate design sensitivities for the efficient design of MPCs.

In this paper, we investigate whether the design sensitivities requires the exact consistent tangent or whether the inexact consistent tangent is sufficient to design MPCs efficiently or at all using conventional gradient based algorithms. Instead of using the master-slave elimination approach we conduct all analyses using the Lagrangian approach to enforce MPCs. To the best of our knowledge this is the first time that the design sensitivities computed using the exact consistent tangent from the primary analysis for MPCs is investigated.

In this study, we indicate vectors by $\{\cdot\}$ and matrices using $[\cdot]$.

4. Sensitivity Analysis

Consider the partitioning of the nonlinear system of equations into free (f), prescribed (p) and MPC (c) degrees of freedom,

$$\{\mathscr{R}_f\} = \{\mathscr{F}_f^{\text{int}}\} - \{\mathscr{F}_f^{\text{ext}}\} = \{0\} \tag{1}$$
$$\{\mathscr{R}_c\} = \{\mathscr{F}_c^{\text{int}}\} - \{\mathscr{F}_c^{\text{ext}}\} = \{0\} \tag{2}$$
$$\{\mathscr{R}_p\} = \{\mathscr{F}_p^{\text{int}}\} - \{\mathscr{F}_p^{\text{ext}}\} = \{0\}, \tag{3}$$

which we solve using Newton's algorithm. The MPC (c) degrees of freedom are all the degrees of freedom that are associated with the MPC equations. The prescribed displacements are applied at the start of the iterative process, which leaves only the free and MPC degrees of freedom to solve

$$\{\mathscr{R}_f\} = \{\mathscr{F}_f^{\text{int}}\} - \{\mathscr{F}_f^{\text{ext}}\} = \{0\}, \tag{4}$$
$$\{\mathscr{R}_c\} = \{\mathscr{F}_c^{\text{int}}\} - \{\mathscr{F}_c^{\text{ext}}\} = \{0\}, \tag{5}$$

in addition, to the nonlinear MPC equations that are written in residual form

$$\{\mathscr{R}_c^{mpc}\} = \{0\}. \tag{6}$$

The Lagrangian approach allows us to formulate the problem using the potential energy approach [2]. The potential energy for elastic media is given by the sum of the strain energy or equivalently the work conducted by the external loads, and the work potential of the external loads [13],

$$\Pi(U_f, U_c) = \int \{\mathscr{F}_f^{\text{int}}\}^{\mathrm{T}} d\{U_f\} + \int \{\mathscr{F}_c^{\text{int}}\}^{\mathrm{T}} d\{U_c\} - \{\mathscr{F}_f^{\text{ext}}\}^{\mathrm{T}}\{U_f\} - \{\mathscr{F}_c^{\text{ext}}\}^{\mathrm{T}}\{U_c\}, \tag{7}$$

which we can augment with the nonlinear MPC equations to obtain the Lagrangian functional

$$\mathscr{L}(U_f, U_c, \lambda) = \int \{\mathscr{F}_f^{\text{int}}\}^{\mathrm{T}} d\{U_f\} + \int \{\mathscr{F}_c^{\text{int}}\}^{\mathrm{T}} d\{U_c\} - \{\mathscr{F}_f^{\text{ext}}\}^{\mathrm{T}}\{U_f\} - \{\mathscr{F}_c^{\text{ext}}\}^{\mathrm{T}}\{U_c\} + \{\lambda\}^{\mathrm{T}}\{\mathscr{R}_c^{mpc}(U_c)\}. \tag{8}$$

Note the presence of the additional unknowns $\{\lambda\}$, the Lagrange multipliers. The stationary point of (8) is given by the first order optimality conditions

$$\begin{aligned}
\left\{\frac{d\mathscr{L}(U_f,U_c,\lambda)}{d\{U_f\}}\right\} &= \{\mathscr{F}_f^{int}\} - \{\mathscr{F}_f^{ext}\} = \{0\}, \\
\left\{\frac{d\mathscr{L}(U_f,U_c,\lambda)}{d\{U_c\}}\right\} &= \{\mathscr{F}_c^{int}\} - \{\mathscr{F}_c^{ext}\} + \{\lambda\}^{\mathrm{T}}\frac{d\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}} = \{0\}, \\
\left\{\frac{d\mathscr{L}(U_f,U_c,\lambda)}{d\{\lambda\}}\right\} &= \{\mathscr{R}_c^{mpc}\} = \{0\}.
\end{aligned} \tag{9}$$

The resulting system of equations (9), can then be solved using Newton's method to obtain the following update formula

$$\begin{bmatrix}
\frac{d\{\mathscr{F}_f^{\text{int}}\}}{d\{U_f\}} & \frac{d\{\mathscr{F}_f^{\text{int}}\}}{d\{U_c\}} & \{0\} \\
\frac{d\{\mathscr{F}_c^{\text{int}}\}}{d\{U_f\}} & \frac{d\{\mathscr{F}_c^{\text{int}}\}}{d\{U_c\}} + \{\lambda\}^{\mathrm{T}}\frac{d^2\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}^2} & \left(\frac{d\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}}\right)^{\mathrm{T}} \\
\{0\} & \frac{d\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}} & \{0\}
\end{bmatrix}
\left\{\begin{array}{c} \triangle\{U_f\} \\ \triangle\{U_c\} \\ \triangle\{\lambda\} \end{array}\right\} = -\left\{\begin{array}{c} \{\mathscr{R}_f\} \\ \{\mathscr{R}_c\} + \{\lambda\}^{\mathrm{T}}\frac{d\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}} \\ \{\mathscr{R}_c^{mpc}\} \end{array}\right\}, \tag{10}$$

which needs to be solved at each iterate until convergence.

Note the presence of the second derivative $\frac{d^2\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}^2}$ of the MPC relations in (10). Similarly, we can compute the second derivative of the i^{th} constraint equation w.r.t. all $\{U_c\}$ and multiply the result by the i^{th} Lagrange multiplier. This process is then repeated for all the constraint equations to finally obtain the symmetric matrix $\left[\{\lambda\}^{\mathrm{T}}\frac{d^2\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}^2}\right]$.

However, the second derivative is ofte omitted in the consistent tangent contribution that results in an inexact consistent tangent. In this study inexact consistent tangent is taken to imply the omission of $\left[\{\lambda\}^{\mathrm{T}}\frac{d^2\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}^2}\right]$ in the consistent tangent, whereas the exact consistent tangent includes this term.

The sensitivity analysis for the design of an MPC can be computed using the direct sensitivity or adjoint sensitivity approach. Consider the sensitivity analysis for the unconstrained objective function $f(\{U\}(\{x\}))$

$$\left\{\frac{df}{d\{x\}}\right\} = \left\{\frac{df}{d\{U\}}\right\}\left[\frac{d\{U\}}{d\{x\}}\right]. \tag{11}$$

As usual in implicit sensitivity calculations, $\left[\frac{d\{U\}}{d\{x\}}\right]$ can be computed from the consistent tangent computed during the Newton step of the primary analysis and the explicit dependency of the non-linear equations w.r.t. the design variables $\{x\}$. For the design of MPCs, only the MPC equations depend explicitly on $\{x\}$. Hence, right-hand side vectors of the explicit dependency of the residual equations with respect to $\{x\}$ is then given by multiple right-hand sides stored in a right-hand side matrix

$$-\begin{bmatrix} [0] \\ \left[\{\lambda\}^{\mathrm{T}} \frac{d}{dx}\left(\frac{d\{\mathscr{R}_c^{mpc}\}}{d\{U_c\}}\right)\right] \\ \left[\frac{d\{\mathscr{R}_c^{mpc}\}}{d\{x\}}\right] \end{bmatrix}, \tag{12}$$

with each column associated with a design variable.

In computing these sensitivities we consider the exact and inexact consistent tangent from the primary analysis to compute the exact and inexact gradients used in the design optimization of the MPCs.

5. Numerical example

We demonstrate the optimal design of MPCs on a slender beam with a nonlinear tip path that is modelled using a MPC, as depicted in Figure 1. The left edge is clamped. The aim is to find the required frictionless tip path defined by a MPC constraint that best predicts a prescribed load path of the centroid at which the load is applied.

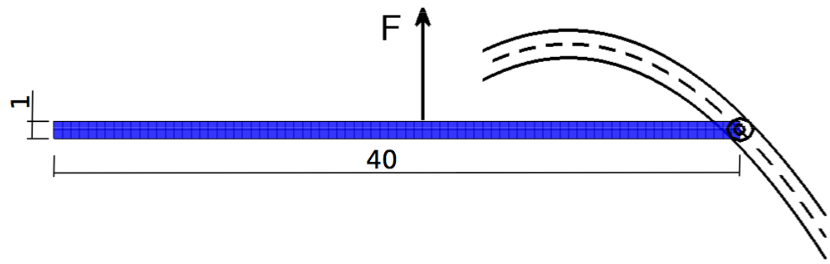


Figure 1: A slender beam with a predefined nonlinear tip path parameterized by a quadratic MPC relation.

The slender beam has a length of 40 mm, height of 1mm and a thickness of 10 mm. The slender beam is modeled using non-linear elastic finite elements in plane strain, with an applied vertical load at the centroid of the beam. The load depicted in Figure 1 indicates the positive direction. The plane strain linear elastic material properties are Young's modulus of 200 GPa and Poisson's ration of 0.3. The load path is specified by the centroid position for five load cases. The five load cases are $-1,\ldots,-5$ kN and the required centroid positions tabulated in Table 2. The non-linear geometrical problem is solved using load control. The x- and y-displacements are respectively indicated under the column headings ($\{U\}_{xc}$ and $\{U\}_{yc}$). The optimal MPC solution is depicted in Figure 2. Also depicted is the deformed structure under the five load cases, in addition to the requested centroid positions for each load case.

The nonlinear tip path modeled by a MPC is parameterised by the following simple quadratic relation

$$y = a(x-b)^2 - c, \tag{13}$$

with a, b and c the design variables for the MPC design optimisation problem.

To allow us to assess the quality of the MPC design optimization solutions, we choose the parameters $a = 0.05$, $b = 30$ and $c = 5$ to compute the desired tip displacements for the five load cases given in Table 2. Hence, the optimal solution for this simple problem is known. We formulate the MPC design optimization problem as a least squares minimization problem of the error between the desired and actual centroid displacements. To ensure the points weighted properly, we normalize the centroid displacements by the solution given in Table 2 when computing the least squares error.

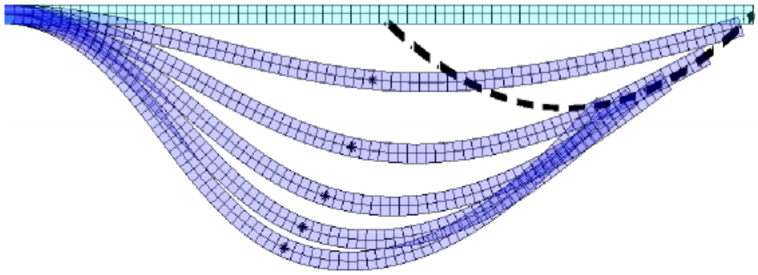


Figure 2: The optimal MPC design indicated by the dashed line. The desired centroid positions for each load case is indicated by the star markers together with the deformed structure for each load case. The undeformed structure is depicted in cyan.

Table 1: Desired tip displacement for five prescribed loadings.

Loading (kN)	$\{U\}_{xc}$ (mm)	$\{U\}_{yc}$ (mm)
-1	-0.352054942516627	-3.498394714046134
-2	-1.474966653993082	-7.072093243279817
-3	-2.868280374657851	-9.677838609719000
-4	-4.086135653307218	-11.353803264917335
-5	-5.051015315558891	-12.449137211538474

We consider two optimization algorithms that employ a cubic line search strategy. Firstly, the steepest descent (SD) algorithm and secondly the well-known Quasi-Newton Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. For each algorithm we supply the exact analytical gradient using the exact consistent tangent indicated by SD-EG and BFGS-EG. In addition we also have the algorithms indicated by SD-IG and BFGS-IG for which the inexact gradients are supplied. The inaccuracies result solely from using the incomplete consistent tangent from the primary analysis in the sensitivity analysis. Lastly, to quantify the effective computational savings we indicate the SD-FD and BFGS-FD algorithms to only use numerically computed finite difference gradients.

All algorithms start from the initial guess $\{x_0\} = [0.1,\ 25,\ 10]$. The four convergence criteria used in this study are

1. $\|\{\Delta x\}\| \leq 10^{-6}$,
2. $\Delta f \leq 10^{-6}$,
3. $\|\{\nabla f\}\| \leq 10^{-6}$,
4. the maximum number of function evaluations is 300.

As an initial investigation we compute the exact ∇f_{exact} and inexact $\nabla f_{inexact}$ gradients at the starting point for the objective function, as well as the complex-step ∇f_{cs} computed sensitivities using a complex step size of 10^{-20} [14]. For this problem, the inexact consistent tangent contribution is surprisingly inaccurate when compared to the exact and complex-step computed sensitivities. Since our MPC relation is quadratic, the second order consistent tangent contribution that is neglected is $2a$ multiplied by the Lagrange multiplier. The Lagrange multiplier scales with the reaction force required to enforce the MPC, and consequently amplifies this neglected contribution.

Table 2: Desired tip displacement for five prescribed loadings.

∇f	∇f_{exact}	$\nabla f_{inexact}$	∇f_{cs}
$\frac{\partial f}{\partial x_1}$	20.020650821600508	29.629165450470268	20.020650813878873
$\frac{\partial f}{\partial x_2}$	-0.220751984034818	-0.399390566601492	-0.220751983922336
$\frac{\partial f}{\partial x_3}$	0.096695873252482	0.060859843096620	0.096695873297742

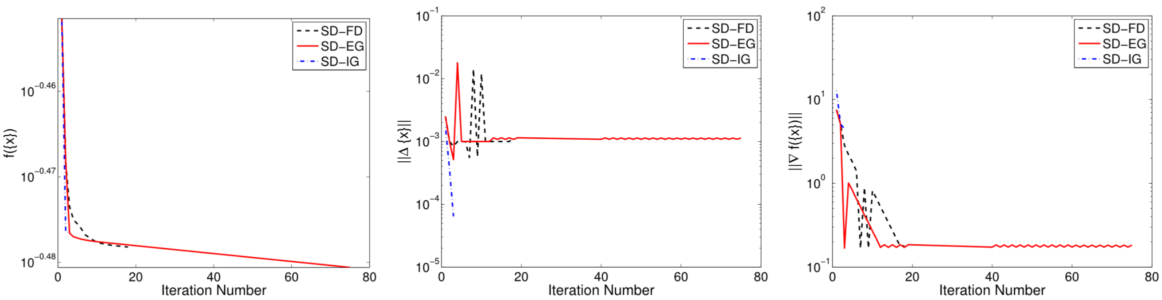
The results for all six algorithms are summarized in Table 3. The steepest descent algorithms all terminated prematurely before reaching a stationary point. The SD-EG and SD-FD terminated due to the maximum number of function values being reached. The SD-IG terminated the computed descent direction failed to indicate descent. We note that convergence is very slow for steepest descent directions. Although not explored in this study, this indicates that appropriate scaling might play a significant role to improve the results. However, both the SD-EG and SD-FD is continuously improving the solution as opposed to terminating like SD-IG. Here, it is clear that the inexact gradient is insufficient to solve this problem using conventional gradient based algorithms. The BFGS algorithms using exact gradients be it analytical (BFGS-EG) or numerical (BFGS-FD) converged to the optimum. In turn, BFGS-IG terminated since the computed descent direction failed to indicate descent. The computational benefit of using analytical gradients as opposed to numerically computed finite differences is also evident, even if the problem has only three design variables.

Table 3: Optimization results.

Parameter	SD-EG	SD-IG	SD-FD	BFGS-EG	BFGS-IG	BFGS-FD
Iterations	75	4	19	41	3	41
Function Evaluations	300	39	300	46	19	184
$\|\|\{x\}^* - \{x\}^{\text{target}}\|\|$	7.063	7.070	7.067	3.557×10^{-7}	7.070	1.685×10^{-6}
$\|\|\nabla f(\{x\}^*)\|\|$	0.254	4.473	0.255	2.902×10^{-8}	1.508	2.173×10^{-6}
f^*	0.331	0.334	0.332	9.184×10^{-16}	0.336	3.029×10^{-13}

The convergence histories for the steepest descent algorithms are depicted in Figures 3 (a)-(c), and the BFGS algorithms in Figures 4 (a)-(c). Figures 3 (a) and 4(a) indicate the function value histories. Figures 3 (b) and 4 (b) indicate the step size norm at the various iterations. Figures 3(c) and 4 (c) indicate the gradient norm history.

From Figure 3(a), the steady improvement by the steepest descent algorithms and dramatic improvement by the BFGS algorithms is evident in Figure 4(a), when the exact gradient is made available.



(a) (b) (c)

Figure 3: (a) Function value, (b) step size norm and (c) gradient norm history for the SD-FD, SD-IG and SD-EG algorithms.

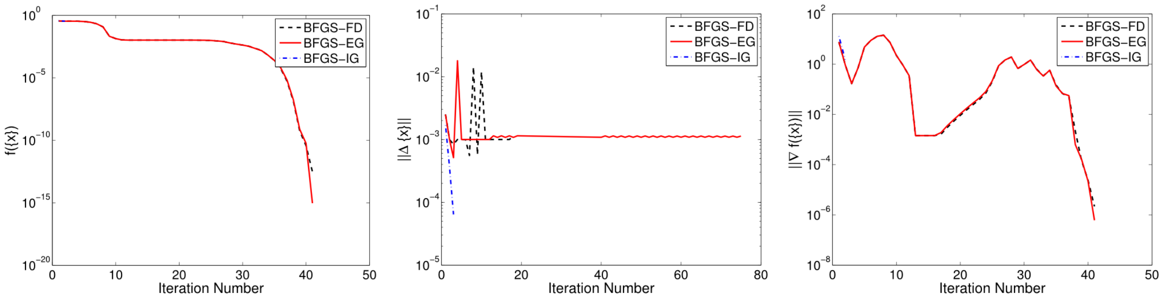
5. Conclusions

We demonstrated that the inexact consistent tangent contribution from the primary analysis is not reliable to compute design sensitivities for MPC design. The inexact gradients were not able to compute descent directions and consequently the conventional gradient based algorithms terminated. The second order contribution often omitted for the primary analysis cannot be omitted when using the consistent tangent from the primary analysis for the sensitivity analysis to design MPCs. It is essential that the exact consistent tangent contribution be used to compute reliable design sensitivities, which requires the second derivative of the MPC constraint relation to be computed.

6. References

[1] S. Kok and D.N. Wilke, Understanding linear and non-linear multi-point constraints in finite element analysis, *9th South African Conference on Computational and Applied Mechanics*, Somerset West, 14 - 16 January 2014.

[2] R. Gallagher, *Finite element analysis: Fundamentals*, John Wiley & Sons, Ltd, 1975.



(a) (b) (c)

Figure 4: (a) Function value, (b) step size norm and (c) gradient norm history for the BFGS-FD, BFGS-IG and BFGS-EG algorithms.

[3] J. Curiskis and S. Valliappan, A solution algorithm for linear constraint equations in finite element analysis, *Computers & Structures*, 8, 117 - 124, 1978.

[4] J. F. Abel and M. S. Shephard, An algorithm for multipoint constraints in finite element analysis, *International Journal for Numerical Methods in Engineering*, 14, 464- 467, 1979.

[5] J. Barlow, Constraint relationships in linear and nonlinear finite element analyses, *International Journal for Numerical Methods in Engineering*, 18, 521 - 533, 1982.

[6] M. S. Shephard, Linear multipoint constraints applied via transformation as part of a direct stiffness assembly process, *International Journal for Numerical Methods in Engineering*, 20, 2107 - 2112, 1984.

[7] O. S. Narayanaswamy, Processing nonlinear multipoint constraints in the finite element method, *International Journal for Numerical Methods in Engineering* 21, 1283 - 1288, 1985.

[8] Y. Dubois-Pélerin and P. Pegon, Linear constraints in object-oriented finite element programming, *Computer Methods in Applied Mechanics and Engineering*, 154, 31 - 39, 1998.

[9] R.-P. Mechnik, Consideration of constraints within the finite element method by means of matrix operators, *International Journal for Numerical Methods in Engineering*, 31, 909 - 926, 1991.

[10] H. L. Schreyer and D. A. Parsons, Direct application of constraints to symmetric algebraic systems, *Communications in Numerical Methods in Engineering*, 11, 563 - 573, 1995.

[11] E. Chow, T. A. Manteuffel, C. Tong and B. K. Wallin, Algebraic elimination of slide surface constraints in implicit structural analysis, *International Journal for Numerical Methods in Engineering*, 57, 1129 - 1144, 2003.

[12] L. Jendele and J. Cervenka, On the solution of multi-point constraints: application to FE analysis of reinforced concrete structures, *Computers & Structures* 87, 970 - 980, 2009.

[13] M. Silhavy, *The Mechanics and Thermodynamics of Continuous Media*, Springer, 1997.

[14] J. Martins, P. Sturdza, J.J. Alonso, The Complex-Step Derivative Approximation, *ACM Transactions on Mathematical Software*, 29, 245-262, 2003.