(Model-Free) Data-Driven Computational under Unilateral Constraints: application to contact

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Abstract — Model-Free Data-Driven Computational Mechanics (DDCM) departs from classical PDE-based formulations by replacing constitutive laws with raw material data, leading to a variational problem formulated as a double minimisation between mechanically admissible states and data-consistent states. While many of the mechanical admissibility constraints can be enforced naturally within a finite element setting, others require special treatment in the data-driven context. In this work, we focus on unilateral constraints arising in contact mechanics, formulated as nonlinear complementarity conditions of Signorini type. Such constraints have not yet been addressed within the DDCM framework, despite their practical relevance and nontrivial treatment. We first introduce a one-dimensional prototype problem to illustrate the main ideas and numerical challenges. The proposed formulation extends DDCM to contact problems and lays the groundwork for data-driven simulations involving inequality-constrained mechanics.
Mots clés — Unilateral Constraints, Nonlinear Complementarity Constraints, (Model-Free) Data-driven Computational Mechanics, Variational Formulations

1 Introduction

The so-called Model-Free Data-Driven Computational Mechanics (DDCM) [1] proposes a paradigm shift in computational mechanics. Instead of solving a PDE-based conservation principle supplemented by a constitutive law as a closure equation, DDCM replaces the constitutive law with raw material data. Applications include material identification [2] and acceleration of coupled computational homogenisation problems [3]. The problem is then reformulated as a double minimisation: one seeks the smallest distance between two pairs of strain/stress states (or, more generally, between gradients of potentials and flux-like quantities) that belong to two distinct spaces. The first is the mechanically admissible space, which satisfies linear momentum balance and kinematic compatibility (i.e., strains derived from displacements). The second is the data-driven space, which contains functions that are, pointwise, as close as possible to the given material dataset. It is worth mentioning that another class data-driven methods for constitutive modelling relies on the neural-network-based construction of surrogate models [4].

Regarding the finite element enforcement of the constraints defining the mechanically admissible space, many of these constraints can be incorporated straightforwardly by construction or through lagrange multipliers [1, 5]. However, some constraints that are naturally satisfied in a classical (non-DDCM) formulation require additional treatment in the DDCM setting. For example, in finite strains, the generalized symmetries of the first Piola-Kirchhoff tensor (pre-multiplied by the transpose of the deformation gradient), which are required for angular momentum conservation, cannot be easily enforced and typically require augmented Lagrangian formulations [6].

In this work, we investigate unilateral constraints expressed as nonlinear complementarity conditions, as arise in contact mechanics (the Signorini problem). To the best of the authors' knowledge, these constraints have not yet been explored within the DDCM framework, although its relevance and non trivial implementation. We therefore begin with a simple one-dimensional warm-up problem before deriving the full set of equations for three-dimensional continua.

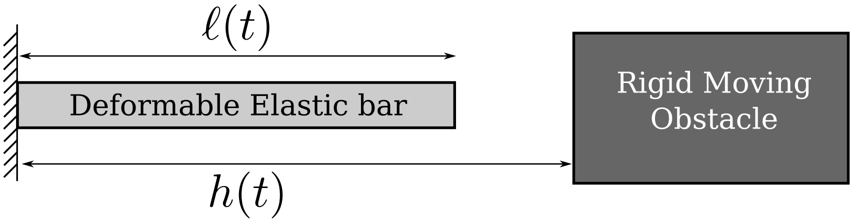


Figure 1: One dimensional bar with rigid moving obstacle scheme.

2 One dimensional problem (classical)

Let us consider a one dimensional bar (deformable body) with a rigid moving rigid obstacle as in Fig. 1. The bar is considered homogeneous with constant cross-section A and undeformed length ℓ_0. The current bar length is denoted $\ell(t)$ and the leftmost surface of the moving obstacle is parametrized by $h(t)$, where t is the (pseudo-)time, all positions being measured with respect to the fixed foundation on the left. Thereafter, we drop the t dependence as the problem is modeled in the quasi-static regime. As usual, it useful to write the equilibrium equations of the displacement $u = \ell - \ell_0$, as below

$$\begin{cases} \sigma + p = 0, \\ \sigma = E\varepsilon, \\ g_{h-\ell_0}(u) \geq 0, p \geq 0, p g_{h-\ell_0}(u) = 0 \end{cases}, \tag{1}$$

where $\varepsilon = \frac{u}{\ell_0}$ is the engineering strain measure, σ the axial stress, E the Young modulus, p the contact pressure, and $g_w(u) := w - u$ is the gap function ($w = h - \ell_0$). This problem admits an easy to find closed-form: $u = \min(0, h - \ell_0), p = -Eu/\ell_0$. The last three inequalities/equalities are named the Karush-Kunh-Tucker (KKT) conditions or nonlinear complementary constraints (NCC). This problem can be equivalently written by constrained minimizing of the potential energy (left) or in its dual form (right) as below

$$\inf_{g_{h-\ell_0}(u) \geq 0} \frac{EAL}{2} \left(\frac{u}{L}\right)^2 = \inf_u \sup_{p \geq 0} \frac{EAL}{2} \left(\frac{u}{L}\right)^2 - Apg_{h-\ell_0}(u). \tag{2}$$

Finding one stationary condition by deriving on u we get $Eu/L + p = 0$, which is essentially the first three equations of (1). The stationary condition by deriving on p gives rise to an inequality $g_{h-\ell_0}(u) \geq 0$, which confirms the equivalence of the dual formulation, but it is not suitable for numerical implementation. In fact, also the non-negativity constraint of p has non trivial numerical treatment. Generally, it is prefered to deal with a unconstrained minimisation at the price of adding nonlinear terms. Three possible approaches are:

Penalisation [7] Introducing a penalty parameter $\gamma >> 0$, find u such that

$$\inf_u \frac{EAL}{2} \left(\frac{u}{L}\right)^2 + A\frac{\gamma}{2} \langle -g_{h-\ell_0}(u) \rangle_+^2. \tag{3}$$

The stationary condition yields $Eu/L + \gamma \langle -g_{h-\ell_0}(u) \rangle_+ = 0$, and the contact pressure can retrieved as $p = \gamma \langle -g_d(u) \rangle_+$.

Augmented Lagrangian [7] Introducing a penalty parameter $\gamma > 0$, find u and p such that

$$\inf_u \sup_p \frac{EAL}{2} \left(\frac{u}{L}\right)^2 + \frac{A}{2\gamma} (\langle p - \gamma g_{h-\ell_0}(u) \rangle_+^2 - p^2), \tag{4}$$

where the stationary conditions leads to $Eu/L + \langle p - \gamma g_{h-\ell_0}(u) \rangle_+ = 0$ and $p = \langle p - \gamma g_{h-\ell_0}(u) \rangle_+$. In practice, these two nonlinear equations are solved alternatively by the the so-called Uzawa scheme : $Eu^{(k+1)}/L + p^k = 0$, $p^{k+1} = \langle p^k - \gamma g_{h-\ell_0}(u^{k+1}) \rangle_+$, for the iteration k, until convergence.

Fischer-Burmeister Find u and p such that

$$\begin{cases} (E/L)u + p = 0, \\ \Phi\left(\alpha g_{h-\ell_0}(u), \beta p\right) = 0 \end{cases}, \tag{5}$$

where KKT conditions has been replaced by finding the root the so-called of Fisher-Burmeister [8] function $\Phi : \mathbb{R}^2 \to \mathbb{R}$, defined as $\Phi(a,b) = \sqrt{a^2+b^2} - a - b$, that only admits solutions $a \geq 0, b \geq 0, ab = 0$ as property. The scaled positive normalizing constants α, β are introduced for the sake of numerical stability and physical dimensional consistency.

3 One dimensional problem (DDCM)

The DDCM problem is posed in terms of the double minimisation principle

$$\inf_{(\varepsilon,\sigma)\in Z_E} \inf_{(\varepsilon^*,\sigma^*)\in Z_D} \frac{AL}{2} d^2((\varepsilon,\sigma),(\varepsilon^*,\sigma^*)), \tag{6}$$

where the DDCM-distance is defined as $d^2((\varepsilon,\sigma),(\varepsilon^*,\sigma^*)) := c(\varepsilon-\varepsilon^*)^2 + c^{-1}(\sigma-\sigma^*)^2$, with c being a scaling parameter yielding energy per volume dimensions. Mechanically admissible states live in $Z_E := \{(\varepsilon,\sigma) : \varepsilon = u/\ell_0, \sigma = -p, (u,p) \in \mathbb{R}^2 \text{satifying KKT}\}$ and the $Z_D := \{(\varepsilon_i^*,\sigma_i^*)\}_{i=1}^{N_d}$ are the dataset of material states. We adopt the alternate minimisation scheme as usual in the DDCM literature. While the projection-onto-data subproblem is standard, the projection-onto-equilibrium subproblem formulation poses some complications due to the unilateral constraint enforcement. The standard way of relaxing the equilibrium by the incorporation of Lagrange Multiplier is not easily defined as it is not if the KKT restrictions should apply for the Lagrange Multiplier variable. Therefore, we follow the Fisher-Burmeister formulation rather than the penalization and the Augmented Lagrangian. The unconstrained version of the projection-onto-equilibrium problem reads as: given $(\varepsilon^*,\sigma^*) \in Z_D$, find $(u,p,\theta) \in R^3$ such as

$$\inf_u \inf_p \sup_\theta \frac{AL}{2} d^2((u/\ell_0,-p),(\varepsilon^*,\sigma^*)) + A\theta\Phi(\alpha g_{h-\ell_0}(u),\beta p). \tag{7}$$

The problem is solved by the Newton-Raphson scheme with residual vector $\mathbf{r} \in \mathbb{R}^3$ and Jacobian matrix $\mathbf{J} \in \mathbb{R}^{3\times3}$ formed by taking first and second derivatives of (7) as below

$$\mathbf{r}(u,p,\theta) = \begin{bmatrix} c(u/\ell_0 - \varepsilon^*) - \theta\alpha\Phi_{,a} \\ Lc^{-1}(p+\sigma^*) + \theta\beta\Phi_{,b} \\ \Phi \end{bmatrix}, \mathbf{J}(u,p,\theta) = \begin{bmatrix} c/\ell_0 + \alpha^2\theta\Phi_{,aa} & -\alpha\beta\theta\Phi_{,ab} & -\alpha\Phi_{,a} \\ -\alpha\beta\theta\Phi_{,ab} & \ell_0/c + \beta^2\theta\Phi_{,bb} & \beta\Phi_{,b} \\ -\alpha\Phi_{,a} & \beta\Phi_{,b} & 0 \end{bmatrix}, \tag{8}$$

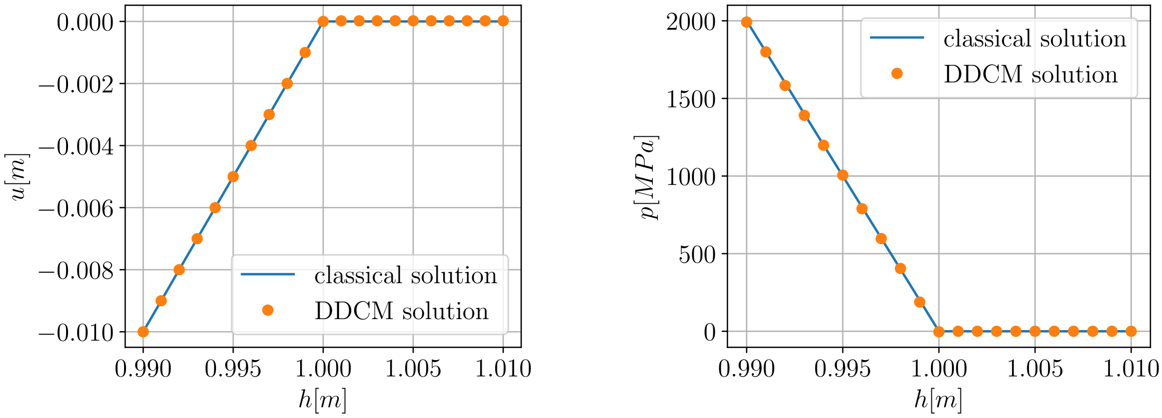
where the following shorthand notations concerning the Fisher–Burmeister function and its derivatives have been assumed

$$\begin{cases} \bar{a} = \alpha g_{h-\ell_0}(u), \quad \bar{b} = \beta p, \quad \bar{S} = \sqrt{\bar{a}^2+\bar{b}^2}, \\ \Phi := \bar{S} - \bar{a} - \bar{b}, \quad \Phi_{,a} := \bar{a}\bar{S}^{-1} - 1, \quad \Phi_{,b} := \bar{b}\bar{S}^{-1} - 1, \\ \Phi_{,ab} := -\bar{a}\bar{b}\bar{S}^{-3}, \Phi_{,aa} = (1-(\bar{a}\bar{S}^{-1})^2)\bar{S}^{-1}, \; \Phi_{,bb} = (1-(\bar{b}\bar{S}^{-1})^2)\bar{S}^{-1} \end{cases} \tag{9}$$

4 Numerical example

In order to validate our implementation we have contrasted classical and DDCM solution of the setting depicted in Fig. 1. We assume the following values for the variables: $E = 200GPa, \ell_0 = 1m$ and $h(t)$ linearly deacreasing from $1.01m$ to $0.99m$ in 21 (pseudo-)time steps. Specifically for the DDCM, 500 material states are sampled using the Hookean law with the same Young Modulus as in the classical case within the strain range of $\varepsilon \in [-0.05, 0.01]$, and the metric parameter is $c = 300GPa$. Finally, the Newton-Raphson tolerance is set 10^{-9} in the relative incremental norm of the variables (u,p,θ) and the normalising coefficients $\alpha = 100m^{-1}$ and $\beta = 1/c$.

Results contrasting classical and DDCM solutions are shown in Fig. 2, specifically comparing bar tip displacement in Fig. 2a and contact pressure in Fig. 2b. Both results perfectly matches the expected results. It is worth mentioning the linearity of constitutive law is assumed for the sake of simplicity, the DDCM being agnostic to this subject.



(a) Bar tip displacement versus obstacle position.

(b) Contact pressure versus obstacle position.

Figure 2: Classical versus DDCM solution.

5 Concluding Remarks

This work has presented an investigation of unilateral constraints formulated as nonlinear complementarity conditions within the framework of DDCM. By focusing on a one-dimensional prototype problem, we have demonstrated that contact conditions of Signorini type can be effectively incorporated into the data-driven setting using a Fischer–Burmeister reformulation. The numerical results obtained in this preliminary study are satisfactory and indicate that the proposed approach provides a robust and consistent means of enforcing inequality constraints without resorting to augmented Lagrangian technique.

Building on these encouraging results, future work will address the extension of the proposed formulation to three-dimensional hyperelastic continua, where additional challenges arise from finite-strain kinematics, stress symmetry requirements, and the increased complexity of contact search and projections. Numerical implementation will extend the current framework of [9]. Such an extension is expected to further broaden the applicability of data-driven computational mechanics to realistic contact problems encountered in engineering practice.

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