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Some experiences in mixed finite element formulations for (model-free) data-driven computational mechanics

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Résumé — Recently, the so-called (model-free) data-driven computational mechanics (DDCM) has established an alternative paradigm allowing to completely bypass explicit constitutive models. Such method. The DDCM solver relies exclusively on a finite dataset of gradient-fluxes pairs and consists of two steps : i) a continuous constrained minimisation problem and ii) a nearest neighbour search (of finite nature). In this work, we explore alternative choices to rephrase Problem i) into an unconstrained format via Lagrange Multipliers, leading to different DDCM algorithms.

Mots clés — (Model-free) data-driven computational mechanics (DDCM) ; Mixed Finite Element ; Poisson problem ; Raviart-Thomas ; Brezzi-Douglas-Marini.

1 Introduction

Following the societal general trend, experimental data (in several forms) has become more widely available to the computational mechanics community. Concerning data-driven techniques for dealing with material behaviour, we can distinguish two families of approaches : i) the creation of surrogate models by machine learning techniques (e.g [1, 2]), and ii) the complete bypass constitutive models by the exclusive use of material dataset, such as the so-called data-driven computation mechanics (DDCM) paradigm [3] or the manifold learning [4]. Given the sound mechanical formulation of DDCM and motivated by recent extensions (e.g. finite strains [5], inelasticity [6], material identification [7], frequency domain [8], among others), the present work focuses on revisiting and exploring alternative variational formulations for the standard DDCM.

In a nutshell, DDCM proposes a generalisation at the governing field equation's level. The generalised formulation is such that it ensures relevant conservation principles, which are independent of material behaviour, while the nearest neighbour search guarantees the interplay with experimental material data. Hence, the DDCM solver is respectively composed of i) a constrained minimisation problem and ii) a nearest neighbour search (of finite nature). The weakly enforcing of balance equations via Lagrange Multipliers [9] allows the conversion of a constrained minimisation problem into an unconstrained one (more tractable) . Such a procedure resembles mixed finite element formulations used for example in the Darcy flow (analogous to the Poisson equation) context. Note that in the former case, there is a certain flexibility in the variational formulation choice, i.e., different functional space combinations for the primal and dual variables. In this work, we apply these choices in the context of DDCM to solve the Poisson problem.

Remark 1 (Notice on notations) *Let us consider the following conventions. As usual, the unit vectors $\{\mathbf{e}_i\}_{i=1}^d$ refer to the canonical basis for \mathbb{R}^d . We also use the font convention $\mathbf{a} \in \mathbb{R}^d$, $\mathbf{A} \in \mathbb{R}^{d \times d}$, $\mathbb{A} \in \mathbb{R}^{d \times d \times d \times d}$ to discern between vectors, second- and fourth-order tensors, respectively. Single dot (\cdot) and double dots $(:)$ designate single or double contractions of the most internal indexes, e.g. $\mathbf{a} \cdot \mathbf{b} = a_i b_i$, $\mathbf{A} : \mathbf{B} = A_{ij} B_{ij}$, etc. Standard matrix-vector and fourth-second-order tensor multiplication are assumed in the absence of any sign, i.e., $\mathbf{A}\mathbf{b} := \mathbf{A} \cdot \mathbf{b}$, $\mathbb{A}\mathbf{B} := \mathbb{A} : \mathbf{B}$. Spaces $\mathbb{R}_{\text{sym}}^{d,d}$ and $\mathbb{R}_{\text{skw}}^{d,d}$ denote symmetric and skew real-valued second-order tensors respectively, and the superscript $(\cdot)^s$ (or $(\cdot)^w$) stands for the symmetric (or $(\cdot)^w$) part of some given object. particularly we also have $\nabla(\cdot) = [\nabla(\cdot)]^s$, and $\nabla^w(\cdot) = [\nabla(\cdot)]^w$.*

2 Mixed formulations for the Poisson problem

Let us introduce the physical problem we address. Consider a domain $\Omega \subset \mathbb{R}^2$ and the partition of its boundary $\partial\Omega = \partial\Omega_N \cup \partial\Omega_D$. For the sake of simplicity, we focus on an elliptic scalar PDE given by the following Poisson problem : find u such that

$$\begin{cases} -\operatorname{div} \mathbf{K} \nabla u = s & \text{in } \Omega, \\ u = \bar{u} & \text{on } \partial\Omega_D, \\ -\mathbf{K} \nabla u \cdot \mathbf{n} = \bar{q} & \text{on } \partial\Omega_N \end{cases} \quad (1)$$

where u is the primal variable of the problem (pressure in the Darcy flow, temperature in the heat equation, etc), \mathbf{K} a positive definite symmetric tensor, \bar{q} the normal flux along $\partial\Omega_N$, \bar{u} a Dirichlet boundary condition along $\partial\Omega_D$, and s is a source term. Let us refer to the former problem as the primal formulation for the Poisson problem, for the sake of differentiation from the mixed formulation described below.

Now, let us create the auxiliary variable $\mathbf{q} = \mathbf{K} \nabla u$, the so-called dual variable, which represents a flux. The mixed equivalent problem now becomes : find u, \mathbf{q} such that

$$\begin{cases} -\operatorname{div} \mathbf{q} = s & \text{in } \Omega, \\ \mathbf{q} = \mathbf{K} \nabla u & \text{in } \Omega, \\ u = \bar{u} & \text{on } \partial\Omega_D, \\ \mathbf{q} \cdot \mathbf{n} = -\bar{q} & \text{on } \partial\Omega_N. \end{cases} \quad (2)$$

In the weak sense, we can derive two different (equivalent) variational formulations : M1 (Problem 1) and M2 (Problem 2). We can state them as follows.

Problem 1 (M1) Find $(u, \mathbf{q}) \in \mathcal{U} \times Q$ such that

$$a(\mathbf{q}, \boldsymbol{\tau}) + b(\boldsymbol{\tau}, u) + b(\mathbf{q}, v) = f(\boldsymbol{\tau}) + g(v) \quad \forall (v, \boldsymbol{\tau}) \in \mathcal{V} \times \mathcal{T} \quad (3)$$

with

$$\begin{cases} a(\mathbf{q}, \boldsymbol{\tau}) &= (\mathbf{K}^{-1} \mathbf{q}, \boldsymbol{\tau})_{L^2(\Omega)}, \\ b(\boldsymbol{\tau}, v) &= -(\boldsymbol{\tau}, \nabla v)_{L^2(\Omega)}, \\ f(\boldsymbol{\tau}) &= 0, \\ g(v) &= -(s, v)_{L^2(\Omega)} - (\bar{q}, v)_{L^2(\partial\Omega_N)}, \\ Q &= \mathcal{T} = [L^2(\Omega)]^2, \\ \mathcal{U} &= \{w \in H^1(\Omega); w = \bar{u} \text{ on } \partial\Omega_D\}, \\ \mathcal{V} &= \{w \in H^1(\Omega); w = 0 \text{ on } \partial\Omega_D\}. \end{cases} \quad (4)$$

Problem 2 (M2) Find $(u, \mathbf{q}) \in \mathcal{U} \times Q$ such that

$$a(\mathbf{q}, \boldsymbol{\tau}) + b(\boldsymbol{\tau}, u) + b(\mathbf{q}, v) = f(\boldsymbol{\tau}) + g(v) \quad \forall (v, \boldsymbol{\tau}) \in \mathcal{V} \times \mathcal{T} \quad (5)$$

with

$$\begin{cases} a(\mathbf{q}, \boldsymbol{\tau}) &= (\mathbf{K}^{-1} \mathbf{q}, \boldsymbol{\tau})_{L^2(\Omega)}, \\ b(\boldsymbol{\tau}, v) &= (\operatorname{div} \boldsymbol{\tau}, v)_{L^2(\Omega)}, \\ f(\boldsymbol{\tau}) &= (\bar{u}, \boldsymbol{\tau} \cdot \mathbf{n})_{L^2(\partial\Omega^D)}, \\ g(v) &= -(s, v)_{L^2(\Omega)}, \\ \mathcal{U} &= \mathcal{V} = L^2(\Omega), \\ Q &= \{\mathbf{w} \in H(\operatorname{div}, \Omega); \mathbf{w} \cdot \mathbf{n} = -\bar{q} \text{ on } \partial\Omega^N\}, \\ \mathcal{T} &= \{\mathbf{w} \in H(\operatorname{div}, \Omega); \mathbf{w} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega^N\}. \end{cases} \quad (6)$$

Note that M1 and M2 were obtained using the standard process of multiplying each side of strong equations by adequate test function and after proceeding with the necessary integration by parts. While in the infinite-dimensional setting both formulations are equivalent, when finite-dimensional subspaces $\mathcal{U}_h \subset \mathcal{U}$ and $\mathcal{Q}_h \subset \mathcal{Q}$ are taken (mixed finite element setting), M1 and M2 are different. In particular, formulation M2 has the advantage of providing locally conservative fluxes (in each element). Moreover, the approximation for the dual variable is privileged with respect to the primal variable. Such features are the main motivations to apply M2 to the DDCM (see Section 2.1). Hence, thereafter we focus on formulation M2 since it provides better properties for the problem at hand.

2.1 Data-driven computational mechanics in mixed formulations

In this section, we briefly revisit the (model-free) data-driven mechanics formulation, originally proposed in [3], but in the mixed formulations framework. Although DDCM has been originally proposed in a solid mechanics context, its extension to other similar physics is straightforward (e.g. poroelasticity [12], piezo-electricity [13], among others). Our formulation follows more closely the work of [9], which is more suited for continuum problems in a variational (weak) format, allowing a straightforward implementation using the finite element method.

In the DDCM framework, material information is given exclusively in the form of a dataset composed of gradient-flux pairs, say $D = \{(\hat{\mathbf{g}}_i, \hat{\mathbf{q}}_i) \in \mathbb{R}^d \times \mathbb{R}^d \text{ for } i = 1, \dots, N_d\}$. We call $\mathbb{Z} = \mathbb{R}^d \times \mathbb{R}^d$ as the local phase-space, whose elements are represented by $\hat{\mathbf{z}} = (\hat{\mathbf{g}}, \hat{\mathbf{q}})$ (with a hat). Accordingly, $\mathcal{Z} = L^2(\Omega; \mathbb{Z})$ denotes the global phase-space such that $\mathbf{z} = (\mathbf{g}, \mathbf{q})$ (hat-free) is a field in Ω . The notion of distance in \mathcal{Z} is given by the metric $\text{dist}(\mathbf{z}, \mathbf{z}^*) = (\int_{\Omega} \|\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x})\|_{\text{loc}}^2)^{1/2}$, whilst $\|\hat{\mathbf{z}}\|_{\text{loc}}^2 = \mathbf{M}\hat{\mathbf{z}} \cdot \hat{\mathbf{z}}$ defines a norm for \mathbb{Z} , with \mathbf{M} a constant symmetric and positive definite second-order tensor. In practice, $\text{dist}^2(\mathbf{z}, \mathbf{z}^*) = \sum_{i=1}^{N_g} \omega_i \|\hat{\mathbf{z}}_i - \hat{\mathbf{z}}_i^*\|_{\text{loc}}^2$, where N_g is the number of integration points and ω_i its weight at point \mathbf{x}_i , both taken with respect to the adopted finite element formulation and discretization. Finally, the DDCM problem amounts to seek

$$\min_{\mathbf{z} \in \mathcal{Z}_E} \min_{\mathbf{z}^* \in \mathcal{Z}_D} \text{dist}(\mathbf{z}, \mathbf{z}^*), \quad (7)$$

where $\mathcal{Z}_E, \mathcal{Z}_D \subset \mathcal{Z}$ are respectively the physically admissible manifold and D -compatible subset¹, defined as

$$\mathcal{Z}_E = \{\mathbf{z} = (\mathbf{g} := \nabla u, \mathbf{q}) \in \mathcal{Z}; \text{ satisfying (2)}\}, \quad (8a)$$

$$\mathcal{Z}_D = \{\mathbf{z} \in \mathcal{Z}; \mathbf{z}(\mathbf{x}_i) = \hat{\mathbf{z}}_i \in D; \mathbf{x}_i \in \Omega, \forall i = 1, \dots, N_g\}. \quad (8b)$$

Note that to extend the local notion of D to $\mathcal{Z}_D \subset \mathcal{Z}$, we should restrict the phase functions to have point-valued images corresponding to data points at disposal in D . The unconstrained version of the "data-to-equilibrium" subproblem yields as follows : given $\mathbf{z}^* \in \mathcal{Z}_D$, find

$$(u, \mathbf{q}, \eta) = \arg \min_{u' \in \mathcal{U}} \min_{\mathbf{q}' \in \mathcal{Q}} \max_{\eta' \in \mathcal{W}} \mathcal{L}(u', \mathbf{q}', \eta'), \quad (9)$$

with the Lagrangian functional

$$\mathcal{L}(u, \mathbf{q}, \eta) = \frac{1}{2} \text{dist}^2((\mathbf{g}(u), \mathbf{q}), \mathbf{z}^*) + \frac{1}{2} a(\mathbf{q}, \mathbf{q}) + b(\mathbf{q}, \eta) - f(\mathbf{q}) - g(\eta), \quad (10)$$

and $\mathcal{U}, \mathcal{W}, \mathcal{Q}$ should be defined appropriately accordingly to variational formulation chosen. The original DDCM formulation amounts for choosing all the ingredients as in formulation M1. On the other hand, if we choose to use M2 as reference, we have to adjust some ingredients. First, we note that primal variable u only appears in the first contribution for the Lagrangian (the distance to \mathbf{z}^*), while in the remaining terms it has been replaced by the Lagrange Multiplier η . Therefore \mathcal{U} and \mathcal{W} can be chosen independently. In particular it is required to take gradients of u , so let us consider $\mathcal{U} = \{w \in H^1(\Omega); w = \bar{u} \text{ on } \partial\Omega_D\}$ and $\mathcal{W} = \{w \in H^1(\Omega); w = 0 \text{ on } \partial\Omega_D\}$. Finally, as η should vanish on $\partial\Omega_D$, it yields that $f(\tau) = 0$. The remaining ingredients are taken identical to M2. These choices are condensed in the problems below :

1. This notion is analogous to the so-called Data-functions space introduced in [9].

Problem 3 (DDCM-M1 (standard formulation)) Let the ingredients as in Problem 1 and $\mathbf{M}_{qg} = \mathbf{M}_{gq} = \mathbf{0}$. Given $\mathbf{z}^* \in \mathcal{Z}_D$, and $\mathcal{W} = \mathcal{V}$, find $(u, \mathbf{q}, \boldsymbol{\eta}) \in \mathcal{U} \times \mathcal{Q} \times \mathcal{V}$ such that

$$\begin{cases} (\mathbf{M}_{gg} \nabla u, \nabla v) = (\mathbf{M}_{gg} \mathbf{g}^*, \nabla v) \quad \forall v \in \mathcal{V} \\ (\mathbf{q}, \nabla \xi) = -g(\xi) \quad \forall \xi \in \mathcal{V}, \\ (\mathbf{M}_{qq} \mathbf{q}, \boldsymbol{\tau}) - (\boldsymbol{\tau}, \nabla \boldsymbol{\eta}) = (\mathbf{M}_{qq} \mathbf{q}^*, \boldsymbol{\tau}) \quad \forall \boldsymbol{\tau} \in \mathcal{T}. \end{cases} \quad (11)$$

For appropriate choices for $Q_h = \mathcal{T}_h \subset Q = \mathcal{T}$ and $\mathbf{M}_{qq} = \mathbf{M}_{gg}^{-1}$, we get

$$\begin{cases} (\mathbf{M}_{gg} \nabla u, \nabla v) = (\mathbf{M}_{gg} \mathbf{g}^*, \nabla v) \quad \forall v \in \mathcal{V} \\ (\mathbf{M}_{gg} \nabla \boldsymbol{\eta}, \nabla \xi) = g(\xi) - (\mathbf{q}^*, \nabla \xi) \quad \forall \xi \in \mathcal{V}, \\ \mathbf{q} = \mathbf{q}^* + \mathbf{M}_{gg} \nabla \boldsymbol{\eta}. \end{cases} \quad (12)$$

Problem 4 (DDCM-M2) Let the ingredients as in Problem 2 and $\mathbf{M}_{qg} = \mathbf{M}_{gq} = \mathbf{0}$. Given $\mathbf{z}^* \in \mathcal{Z}_D$, find $(u, \mathbf{q}, \boldsymbol{\eta}) \in \mathcal{U} \times \mathcal{Q} \times \mathcal{W}$ such that

$$\begin{cases} (\mathbf{M}_{gg} \nabla u, \nabla v) = (\mathbf{M}_{gg} \mathbf{g}^*, \nabla v) \quad \forall v \in \mathcal{V} \\ (\operatorname{div} \mathbf{q}, \xi) = g(\xi) \quad \forall \xi \in \mathcal{W}, \\ (\mathbf{M}_{qq} \mathbf{q}, \boldsymbol{\tau}) + (\operatorname{div} \boldsymbol{\tau}, \boldsymbol{\eta}) = (\mathbf{M}_{qq} \mathbf{q}^*, \boldsymbol{\tau}) \quad \forall \boldsymbol{\tau} \in \mathcal{T}. \end{cases} \quad (13)$$

It is worth noticing that classical finite-dimensional choices for DDCM-M2 $\mathcal{W}_h \subset \mathcal{W}$ are constant by part functions or Lagrangian basis discontinuous between elements, while for $Q_h \subset Q$ (same for \mathcal{T}_h) Raviart-Thomas [10] or BDM [11] spaces are the most common choices. Stability conditions require the latter to have polynomials of one order higher than the former space.

3 Numerical Results

We have considered an unitary square $\Omega = [0, 1]^2 \subset \mathbb{R}^2$ (we have used dimensionless quantities). Let us denote $\partial\Omega_N^L$ and $\partial\Omega_N^T$ the left and top boundary respectively, and $\partial\Omega_D$ the remaining of the boundary. As boundary conditions, we have imposed the normal fluxes $q_L = 100$ and $q_T = 10$ on $\partial\Omega_N^L$ and $\partial\Omega_N^T$, respectively, and homogeneous conditions for the primal variable on $\partial\Omega_D$ ($\bar{u} = 0$). The source term was chosen as $s = c_3 \sin c_1 x \cos c_2 y$, with $c_1 = 6, c_2 = 3, c_3 = 500$. We have used a nonlinear flux constitutive law

$$\mathbf{q} = \alpha_0 (1 + \beta \|\mathbf{g}\|^2) \mathbf{g}, \quad (14)$$

with $\alpha_0 = 1000.0$ and $\beta = 1e2$. The reference solution was obtained in a 20×20 homogeneous mesh with alternated triangles using standard (primal) finite elements with linear continuous lagrangian shape functions.

Concerning the DDCM, firstly a material dataset with $N_d = 1000$ points was generated using the same nonlinear flux law sampled uniformly on the gradient parameter space $[-0.09, -0.05] \times [0.05, 0.15]$ (these ranges were found *a posteriori* to correspond approximately to those attained by the reference solution). The solutions obtained by DDCM-M1 and DDCM-M2 are shown in form of scatter plots in figures 1 and 2, respectively. Errors are reported in Table 1. We can that both approaches reproduced the reference test, DDCM-M1 leading to more accurate results than DDCM-M2.

Formulations	$\ u^{DDCM} - u^{FE}\ $	$\ \mathbf{q}^{DDCM} - \mathbf{q}^{FE}\ $
DDCM-M1	4.623696e-02	2.179316e-02
DDCM-M2	1.241739e-01	9.391753e-02

TABLE 1 – Comparisons with the reference solution (non-DDCM with a known constitutive law).

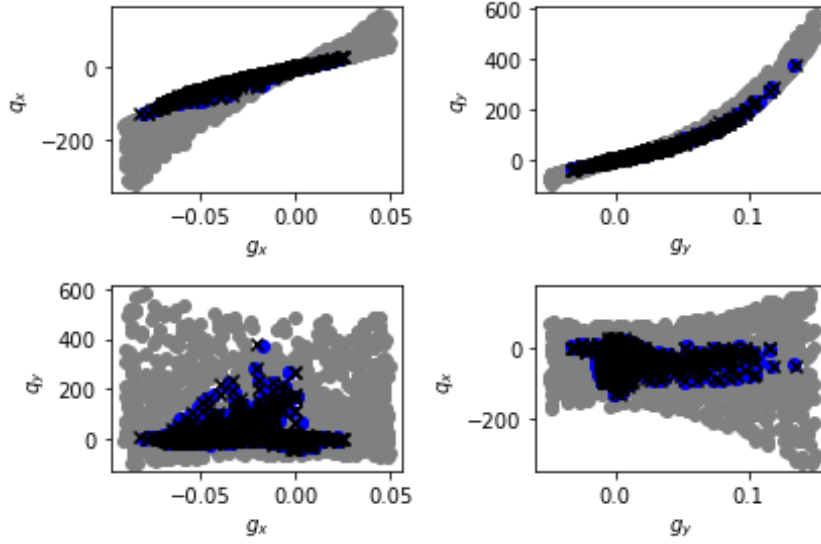


FIGURE 1 – Scatter plots of numerical results on DDCM-M1 phase-space (legend : Z_E (black cross), Z_D (blue bullets), D (gray bullets)).

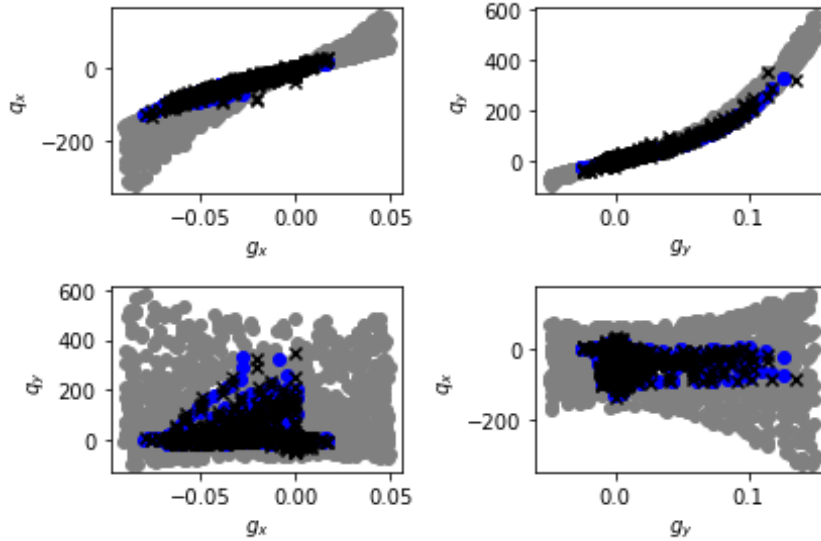


FIGURE 2 – Scatter plots of numerical results on DDCM-M2 phase-space (legend : Z_E (black cross), Z_D (blue bullets), D (gray bullets)).

4 Concluding Remarks

In this work we have explored different mixed formulations for the DDCM method applied to the Poisson equation. In the DDCM-M2, Lagrange Multiplier is able to enforce locally conservative fluxes. Also, fluxes live in richer space the Lagrange Multiplier, which is coherent with the physical importance of the variables. These are strong advantages of this method if compared to DDCM-M1. The drawback is that a larger linear system needs to be solved given the impossibility of statically condensate fluxes. This drawback can be minimised since the same left-hand-side factorisation can be reused in all DDCM iterations. In terms of numerical errors with reference solution, we have noticed that DDCM-M1 has performed better than DDCM-M2. This might be linked with the form of the reference solution which was obtained by the standand primal formulation, so it might be biased to privilege the DDCM-M1 accuracy. More tests are being performed to assess in more scrutinity such differences.

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