Data-Driven simulation of inelastic materials using structured data sets and tangential transition rules

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Data-driven computational mechanics replaces phenomenological constitutive functions by performing numerical simulations based on data sets of representative samples in stress-strain space. The distance of modeling values, e.g. stresses and strains in Gauss-points of a finite element calculation, from the data set is minimized with respect to an appropriate metric, subject to equilibrium and compatibility constraints, see [1]. Although this method operates well for non-linear elastic problems, there are challenges dealing with history-dependent materials, since one point in stress-strain space might correspond to different material behaviour. In [2], this issue is treated by including local histories into the data set. However, there is still the necessity to include models for the evolution of internal variables. Thus, a mixed formulation is obtained consisting of a combination of classical and data-driven modeling.

In the presented approach, the data set is augmented with directions in the tangent space of points in stress-strain space. Moreover, the data set is classified into subsets corresponding to different material behaviour, e.g. elastic and inelastic. Based on the classification, transition rules map the modeling points to the various subsets. The approach and its performance will be demonstrated by applying it to a model of small strain elasto-plasticity with isotropic hardening.

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1 Data-driven approach

The distance-minimizing data-driven problem, introduced by [1], for a discretized system (e.g. by the finite element method) which undergoes displacements \( u \) subjected to applied forces \( f \), reads

\[
\begin{align*}
\text{Minimize} & \quad \sum_{e=1}^{m} w_e d(\hat{\varepsilon}_e, D_e) \quad \text{with} \quad \hat{\varepsilon}_e = (\varepsilon_e, \sigma_e), \\
\text{subject to} & \quad \hat{\varepsilon}_e = B_e u_e \quad \text{and} \quad \sum_{e=1}^{m} w_e B_e^T \sigma = f,
\end{align*}
\]

with an appropriate distance function \( d(\cdot, \cdot) \). In this case \( m \in \mathbb{N} \) is the number of material points, \( \{w_e\}_{e=1}^{m} \) are elements of volume, \( \{B_e\}_{e=1}^{m} \) are strain-displacement operators and \( D_e = \{ (\varepsilon_e, \sigma_e), i = 1, \ldots, n \in \mathbb{N} \} \) are data sets consisting of finite number of local material states. Thus, the aim of the data-driven computation is to find the closest point consistent with the kinematics and equilibrium laws to a material data set.

2 Extension to inelasticity using tangent spaces

An extension of the data-driven paradigm regards inelastic materials since points in stress-strain space might correspond to different material behaviour. Rather including local histories into the data set as in [2] the data set will be extended by the tangent space i.e.

\[
D_e := \{ (\varepsilon_e, \sigma_e, \Delta \varepsilon_e, \Delta \sigma_e), i = 1, \ldots, n \in \mathbb{N} \},
\]

where \( \Delta \varepsilon_e \) and \( \Delta \sigma_e \) are the tangential strain and stress increment. Furthermore the data sets will be separated in two sets of different material behavior e.g. elastic and inelastic \( D_e = D_e^{\text{elastic}} \cup D_e^{\text{inelastic}} \). By introducing the novel distance function

\[
d(\hat{\varepsilon}_e, D_e^{i}) = \min_{(\varepsilon_e, \sigma_e, \Delta \varepsilon_e, \Delta \sigma_e) \in D_e^{i}} \left\{ \frac{1}{2} \| \hat{\varepsilon}_e - \varepsilon_e - \Delta \varepsilon_e \|_2^2 + \frac{1}{2} \| \sigma_e - \sigma_e - \Delta \sigma_e \|_2^2 \right\}
\]

for \( \hat{\varepsilon}_e = (\hat{\varepsilon}_e, \hat{\sigma}_e) \), the resulting Euler-Lagrange equation with tangential stiffness \( C_e = \frac{\Delta \sigma_e}{\Delta \varepsilon_e} \) is given as

\[
\left( \sum_{e=1}^{m} w_e B_e^T C_e B_e \right) u = f - \sum_{e=1}^{m} w_e B_e^T (C_e - \frac{\Delta \sigma_e}{\Delta \varepsilon_e} \varepsilon_e).
\]

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The global state $z$ then follows by evaluating the local stress and strain for all material points as

$$
\dot{\varepsilon}_e = B_e u_e, \quad \forall e = 1, \ldots, m, \\
\dot{\sigma}_e = \sigma_e + C_e \Delta \varepsilon_e, \quad \forall e = 1, \ldots, m.
$$

(5) (6)

Given a list of modeling $\{\hat{z}_e^k\}_{k=1}^m$ and data points $\{z_e^m\}_{e=1}^m$, the material state at loading step $(k + 1)$ can be calculated by the data-driven solver in four steps:

- find values of modeling points $\{\hat{z}_e^{k+1}\}_{e=1}^m$ by solving the equations (4), (5) and (6) using the data points $\{z_e^m\}_{e=1}^m$;
- assign local data sets $\{\hat{D}_e^k\}_{e=1}^m$ by

$$
\hat{D}_e \equiv \begin{cases} 
D_e^\text{elastic}, & \text{if } \delta_y(\hat{\sigma}_e) < \sigma_0^e; \\
D_e^\text{inelastic}, & \text{if } \delta_y(\hat{\sigma}_e) \geq \sigma_0^e,
\end{cases}
$$

(7)

where $\sigma_0^e$ is the yield limit and $\delta_y(\cdot)$ is the yield stress;
- find closest data points $\{z_e^{k+1}\}_{e=1}^m$ in the data sets $\{\hat{D}_e^k\}_{e=1}^m$ to modeling points $\{\hat{z}_e^{k+1}\}_{e=1}^m$ with

$$
\min_{z_e^{k+1} \in \hat{D}_e} \left\{ \frac{1}{2} C_e \| \dot{\varepsilon}_e^{k+1} - \hat{\varepsilon}_e^{k+1} \|^2 + \frac{1}{2} C_e^{-1} \| \hat{\sigma}_e^{k+1} - \sigma_e^{k+1} \|^2 \right\};
$$

(8)

- if $\sigma_e \cdot \Delta \varepsilon_e < 0$ for all material points, set $\sigma_e^0 := \delta_y(\hat{\sigma}_e)$.

### 3 Numerical results for 3D problem

To visualize the convergence properties of the data-driven extension the problem of a cantilever beam subjected to a load causing plastic deformation is considered. Following [2], a virtual test is used to generate accurate coverage of suitable local material states; in this case 160 data sets samples. Thus, a standard data set is considered by randomizing an elasto-plasticity with isotropic hardening data set with isotropic hardening. First the load is applied from 0 to $1 \cdot 10^7$, down to 0 and then raised up again to $1.2 \cdot 10^7$. The material parameters of the reference solid used in the data-driven computing are Young’s modulus $E = 200 \cdot 10^3$ Pa, Poisson’s ratio $\nu = 0.3$ and initial yield stress $\sigma_0 = 200 \cdot 10^6$ Pa.

Figure 1a shows the data-driven based displacement solution at the maximum loading magnitude $1.2 \cdot 10^7$ using a data sample containing 10000 points. Figure 1b illustrates the convergence of the data-driven solution towards the reference elasto-plasticity with isotropic hardening model solution by increasing number of material data points.

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**Fig. 1**: Inelastic cantilever beam problem using data-driven solver. (a) Von Mises stress distribution at the maximum loading magnitude. (b) Maximum displacement with an applied force for different data resolution.

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**References**

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