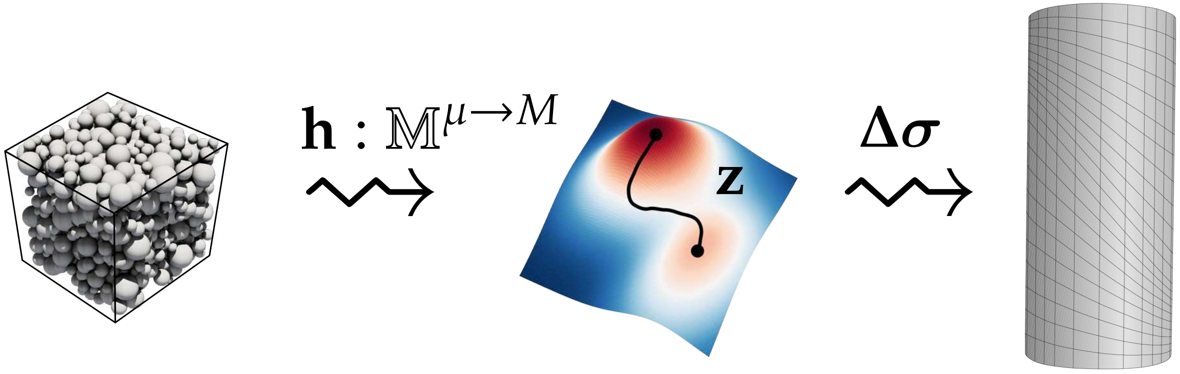
Thermodynamics- and data-driven scale bridging



Filippo Masi

Univ. Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK

Mécamat: Homogénéisation du comportement mécanique des matériaux hétérogènes
Aussois – Jan. 27-31, 2025

Scale-bridging

How to bridge the scales in inelastic, heterogeneous media


micro-

Macro-scale

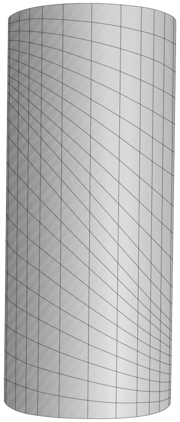
Scale-bridging

How to bridge the scales in inelastic, heterogeneous media

micro-

Macro-scale

BVP



$$\begin{cases} \nabla \boldsymbol{\sigma} + \rho \mathbf{b} = \rho \ddot{\mathbf{u}} \\ \boldsymbol{\varepsilon} = \mathrm{Sym}\left(\nabla \mathbf{u}\right) \end{cases}$$

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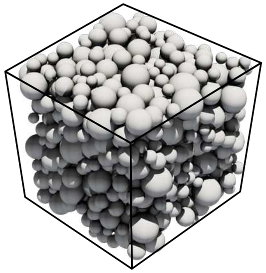
Macro-scale

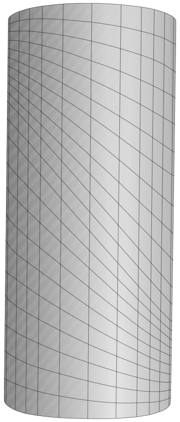
auxiliary problem

$\boldsymbol{\Delta\varepsilon}$

BVP



unit cell
implicit closure



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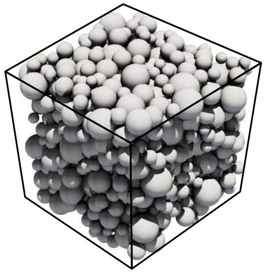


unit cell
implicit closure

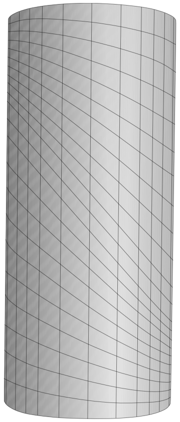
$\boldsymbol{\Delta\varepsilon}$

FE^2
FEM×DEM
FEM×...

Feyel 2003, Nitka et al. 2011, Nguyen et al. 2014

$\boldsymbol{\Delta\sigma}$

BVP



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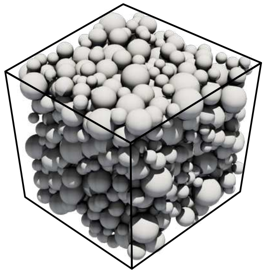
micro- → Macro-scale

auxiliary problem



unit cell
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$\boldsymbol{\Delta\varepsilon}$ ←

FE^2
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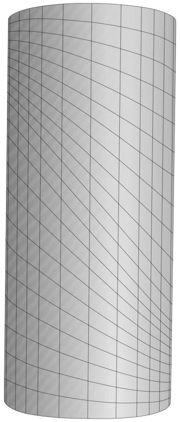
→ $\boldsymbol{\Delta\sigma}$

prohibitive computational cost

BVP



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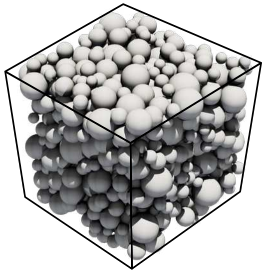
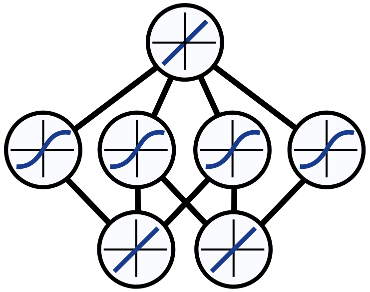


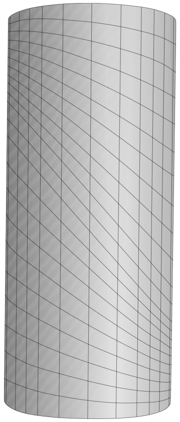
unit cell

ML (neural nets)



Ghaboussi et al. 1991,
Lefik & Schrefler 2003,
Mozaffar et al. 2019

BVP



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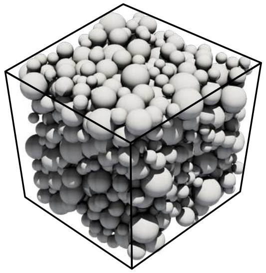
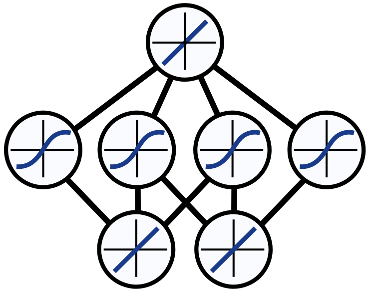


unit cell

measurement

ML (neural nets)



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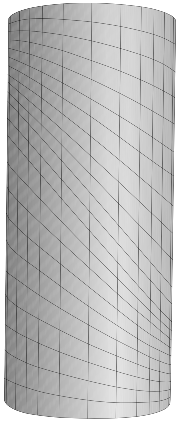

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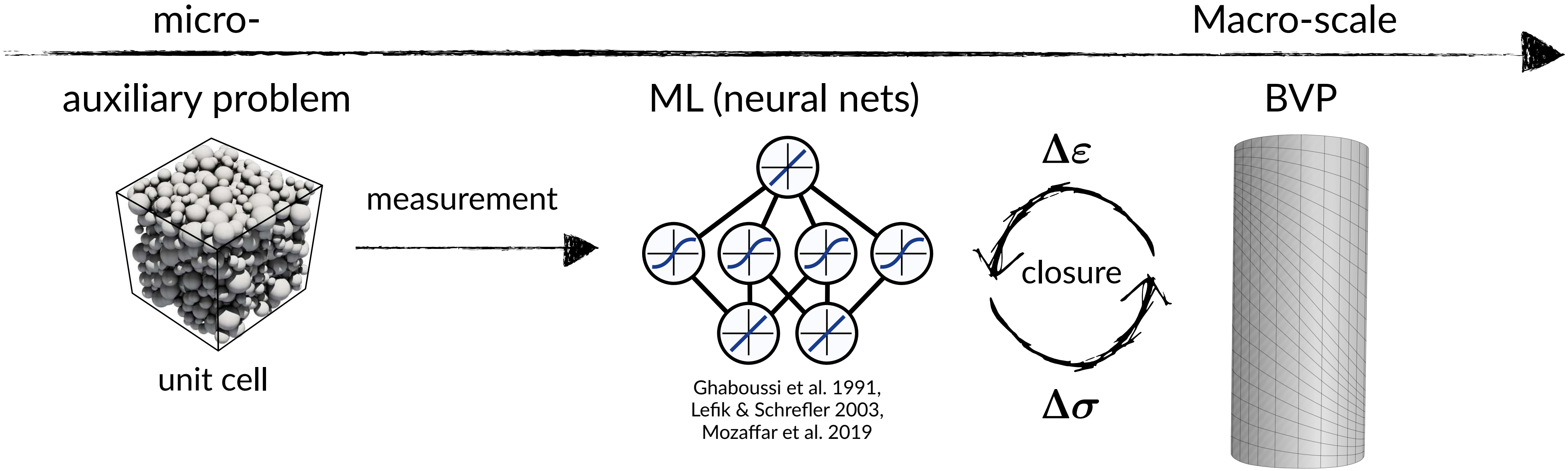

micro-

Macro-scale

auxiliary problem

ML (neural nets)

BVP

measurement

closure

$\boldsymbol{\Delta\varepsilon}$

$\boldsymbol{\Delta\sigma}$

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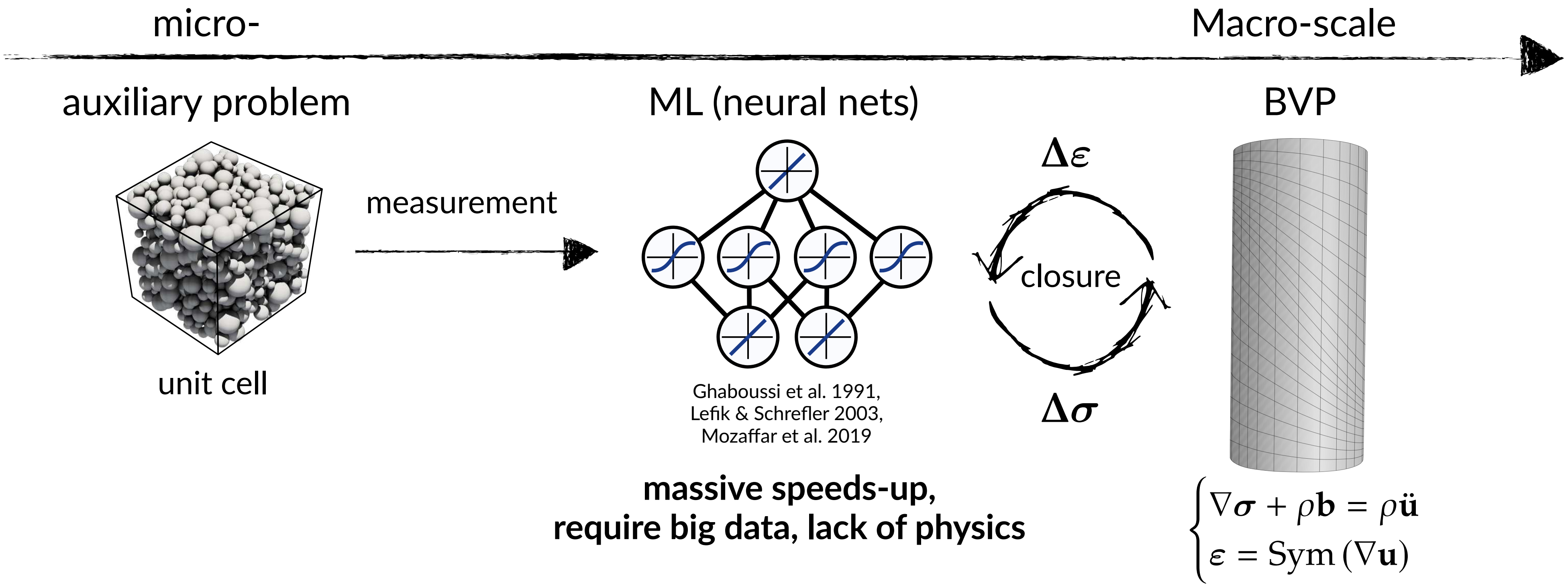

micro-

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**massive speeds-up,
require big data, lack of physics**

$\boldsymbol{\Delta\varepsilon}$

closure

$\boldsymbol{\Delta\sigma}$

BVP

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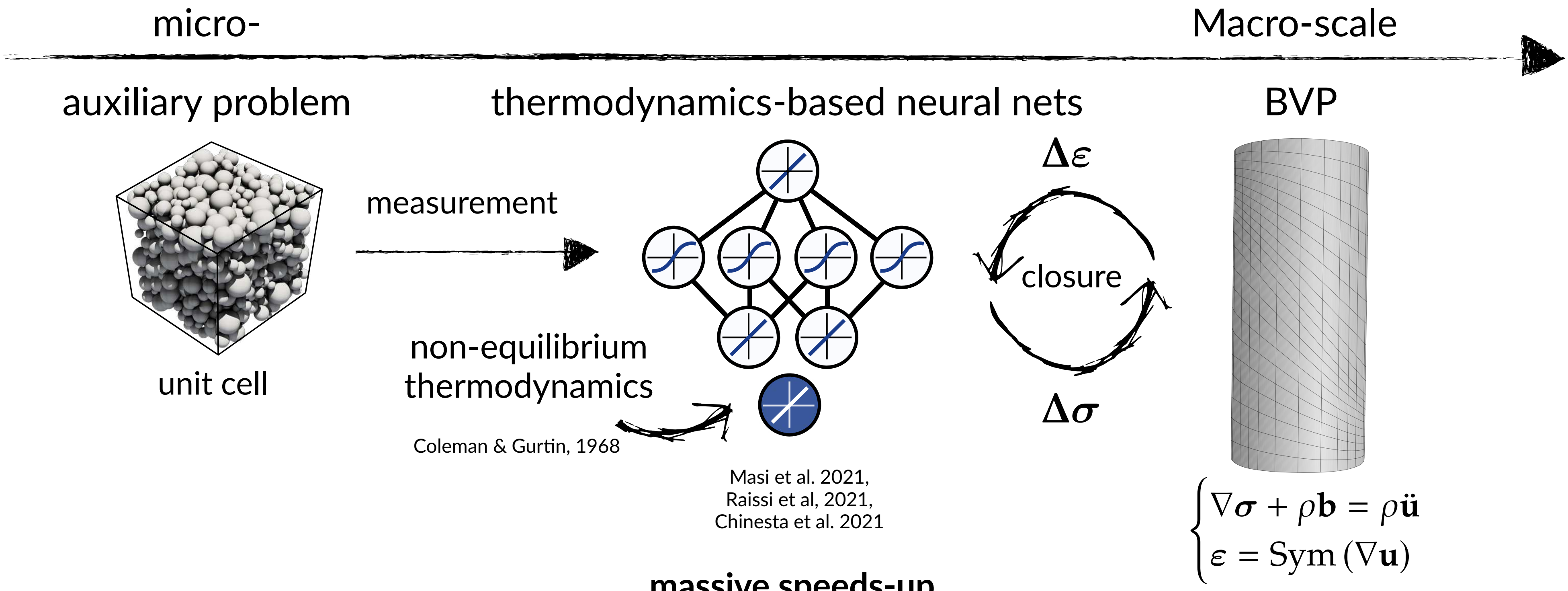

micro-

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auxiliary problem

thermodynamics-based neural nets

BVP

measurement

unit cell

non-equilibrium thermodynamics

Coleman & Gurtin, 1968

$\boldsymbol{\Delta\varepsilon}$

closure

$\boldsymbol{\Delta\sigma}$

Masi et al. 2021,
Raissi et al, 2021,
Chinesta et al. 2021

$$\begin{cases} \nabla\boldsymbol{\sigma} + \rho\mathbf{b} = \rho\ddot{\mathbf{u}} \\ \boldsymbol{\varepsilon} = \mathrm{Sym}\left(\nabla\mathbf{u}\right) \end{cases}$$

massive speeds-up,
consistent, good generalisation

Overview

I) Background setting
  a) Non-equilibrium thermodynamics

II) Thermodynamics-based artificial neural networks
  a) Methods
  b) Discovery of internal state variables
  c) Experiments

III) Multiscale computing

IV) Neural equations from small data
  a) Data scarcity and sparsity
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Non-equilibrium thermodynamics

Coleman and Gurtin, 1967

Non-equilibrium thermodynamics

Coleman and Gurtin, 1967

- Balance of energy and entropy (local)

$$\dot{e} = p^i - \nabla \cdot \mathbf{q} + r, \qquad (1) \qquad\qquad \gamma = \dot{\eta} + \nabla \cdot \left(\frac{\mathbf{q}}{T}\right) - \frac{r}{T} \geq 0 \qquad (2)$$

internal energy density e,	heat flux, source $\mathbf{q}, r$,	power of internal forces $p^i = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}$
entropy density $\dot{\eta}$,	absolute temperature T,	dissipation rate γ

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- Clausius-Duhem inequality

$$\gamma = p^i - \dot{e} + T\dot{\eta} - \mathbf{q} \cdot \frac{\nabla T}{T} = p^i - \left(\dot{\psi} + \dot{T}\eta\right) - \mathbf{q} \cdot \frac{\nabla T}{T} \geq 0 \qquad (3)$$

$$d = p^i - \left(\dot{\psi} + \dot{T}\eta\right) \geq 0 \qquad (4)$$

Helmholtz free energy $\psi = e - T\eta$, dissipation rate d

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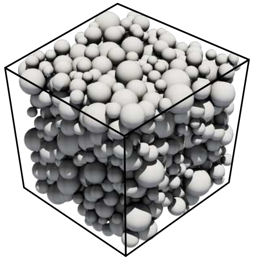
- Volume average Clausius-Duhem inequality



(periodic displ. & anti-periodic tract.)

$$\langle d \rangle = \langle p^i \rangle - \langle \dot{\psi} \rangle - \langle \dot{T}\eta \rangle \geq 0 \qquad (5)$$

$$\langle p^i \rangle = \langle \boldsymbol{\sigma} \rangle : \langle \dot{\boldsymbol{\varepsilon}} \rangle$$

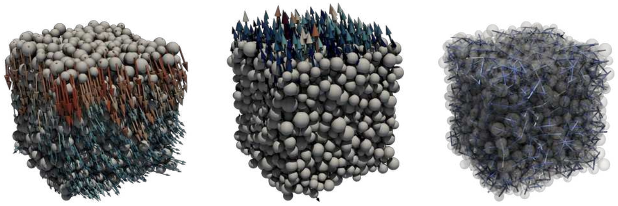
$$\langle \psi \rangle = \frac{1}{|\mathcal{V}|} \int_{\mathcal{V}} \psi \, dy$$

Non-equilibrium thermodynamics

Coleman and Gurtin, 1967

- State functions and variables $\psi = \hat{\psi}(\mathbb{X}) \qquad \{\boldsymbol{\varepsilon}, T, \mathbf{z}, \rho, \cdot\} \subset \mathbb{X}$ (6)

internal state variables $\mathbf{z} = \{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_p\}$



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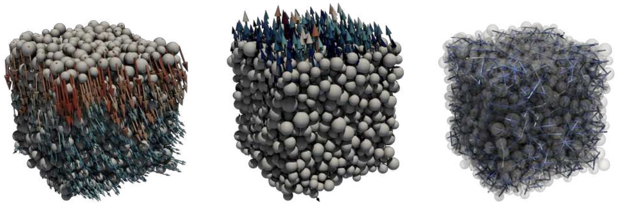

- Evolution equations for the internal variables (general) $\dot{\mathbf{z}} = \mathbf{f}\left(\mathbb{X}\right) \qquad (7)$

(special cases: Onsager-Casimir relationships, Generalised Standard Materials, etc.)

Onsager 1931, Moreau 1973, Halphen, Son Nguyen, 1975, de Saxcé 1998

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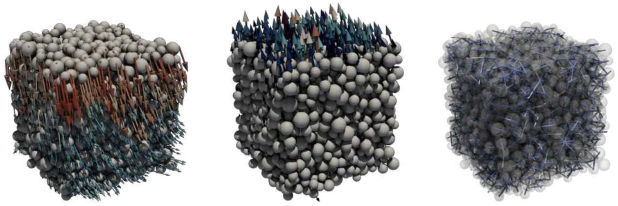

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- Substituting the time derivative of $\hat{\psi}$ into the CD inequality yields

$$\left(\boldsymbol{\sigma} - \frac{\partial \hat{\psi}}{\partial \boldsymbol{\varepsilon}}\right) : \dot{\boldsymbol{\varepsilon}} + \left(\frac{\partial \hat{\psi}}{\partial T} + \eta\right) \dot{T} + \frac{\partial \hat{\psi}}{\partial \mathbf{z}} \cdot \dot{\mathbf{z}} - d = 0 \quad \forall \dot{\boldsymbol{\varepsilon}}, \dot{T}, \dot{\mathbf{z}} \qquad (8)$$

$$d \geq 0$$

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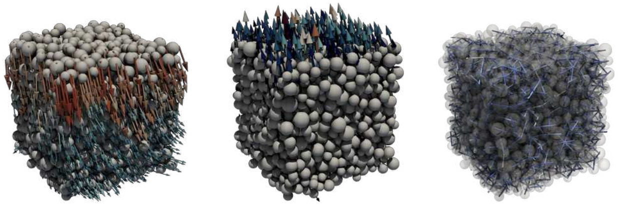

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$$d \geq 0$$

- Thermodynamics-admissible material processes

$$\boldsymbol{\sigma} = \frac{\partial\hat{\psi}}{\partial\boldsymbol{\varepsilon}}\left(\mathbb{X}\right), \qquad \eta = -\frac{\partial\hat{\psi}}{\partial T}\left(\mathbb{X}\right) \qquad d = \mathbb{Z} \cdot \dot{\mathbf{z}} \geq 0 \qquad (9)$$

$$\mathbb{Z} \equiv -\partial_{\mathbf{z}}\hat{\psi}\left(\mathbb{X}\right)$$

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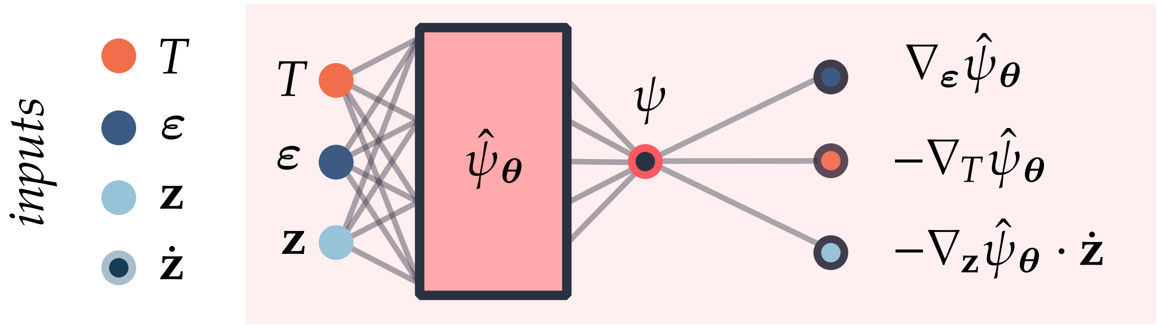
Thermodynamics-based Neural Nets

Masi et al. JMPS, 2021; Masi & Stefanou. JMPS, 2023

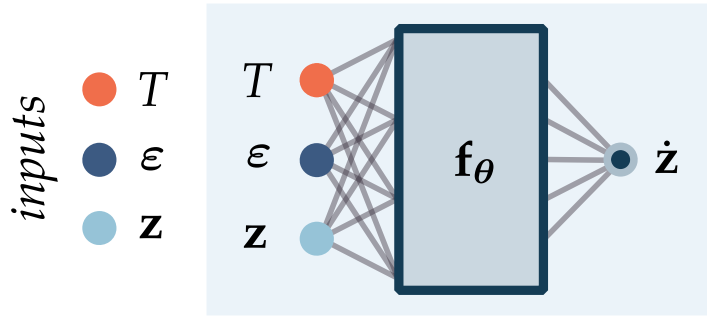
I) Free-energy density network $\hat{\psi}_{\boldsymbol{\theta}}$



$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \left(\underbrace{\ell\left(\psi, \hat{\psi}_{\boldsymbol{\theta}}\right)}_{\text{loss in } \psi} + \underbrace{\ell\left(\boldsymbol{\sigma}, \nabla_{\boldsymbol{\varepsilon}} \hat{\psi}_{\boldsymbol{\theta}}\right) + \ell\left(\eta, -\nabla_T \hat{\psi}_{\boldsymbol{\theta}}\right) + \ell\left(d, -\nabla_{\mathbf{z}} \hat{\psi}_{\boldsymbol{\theta}} \cdot \dot{\mathbf{z}}\right)}_{\text{loss in } \nabla\psi} + \underbrace{\left\langle -\nabla_{\mathbf{z}} \hat{\psi}_{\boldsymbol{\theta}} \cdot \dot{\mathbf{z}} \right\rangle}_{\text{reg.}} \right)$$

$$\langle a \rangle = \max(0, a)$$

II) Evolution equation network $\mathbf{f}_{\boldsymbol{\theta}}$

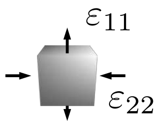


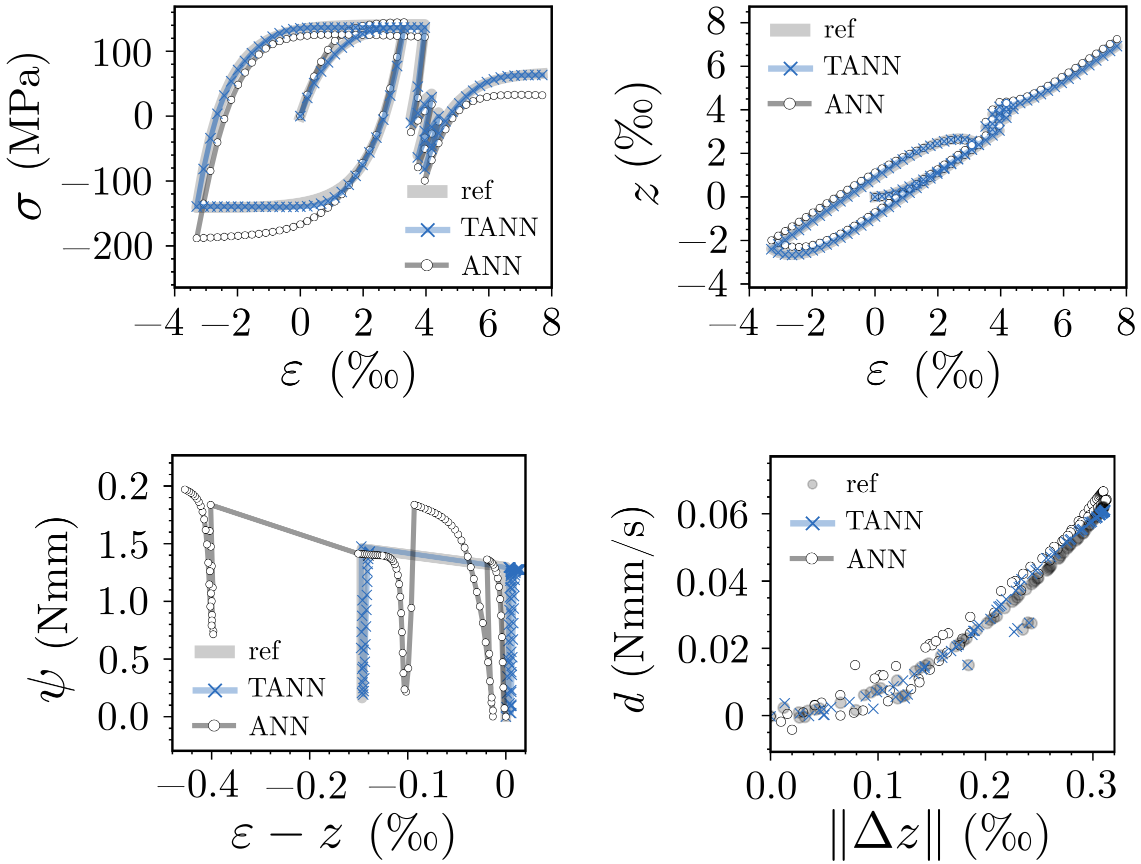
$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \left(\underbrace{\ell\left(\dot{\mathbf{z}}, \mathbf{f}_{\boldsymbol{\theta}}\right)}_{\text{loss in } \dot{\mathbf{z}}} \right)$$

Data-driven versus physics-driven

ANN versus TANN: why thermodynamics is important!

▷ Biaxial strain-driven ratcheting





▷ Data-driven (ANN)
- – Accuracy
- – Energy is not conserved
- – Dissipation rate is negative

▷ Physics-driven (TANN)
- + Accuracy
- + Energy is conserved
- + Dissipation is positive-semi def.

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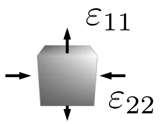

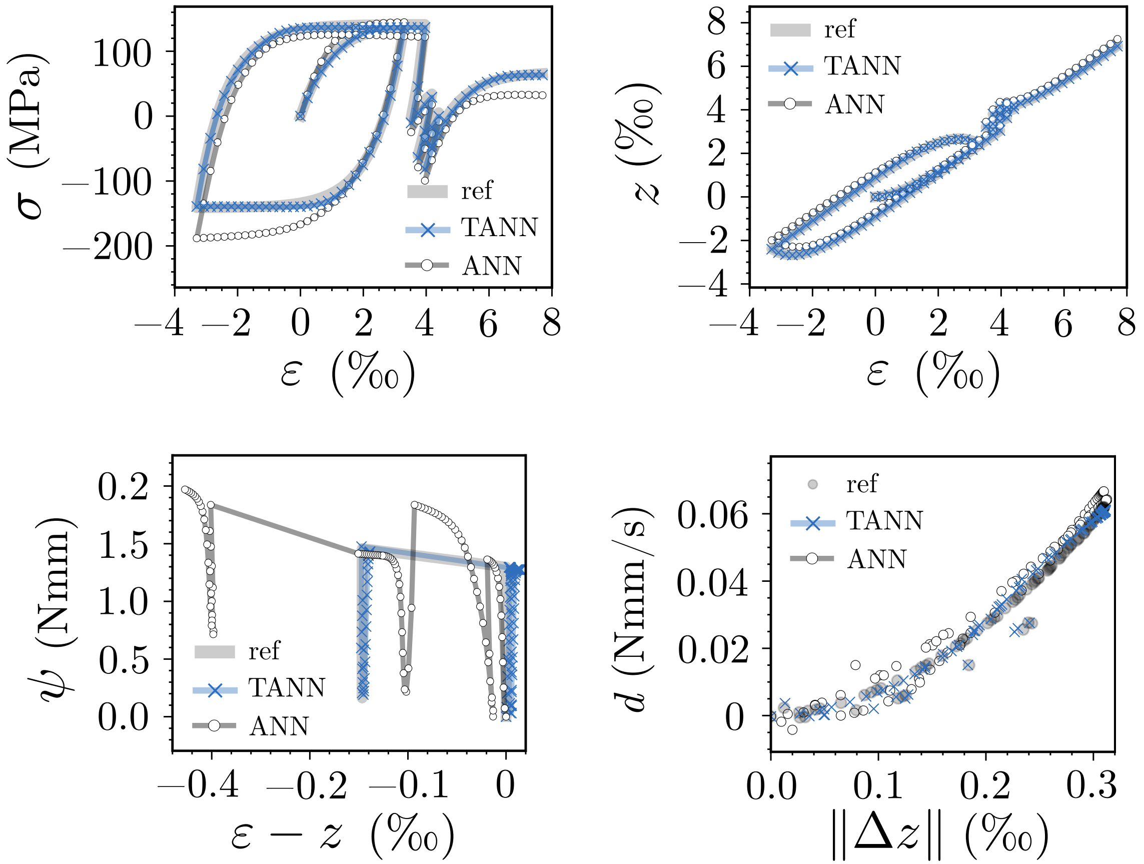

▷ Data-driven (ANN)
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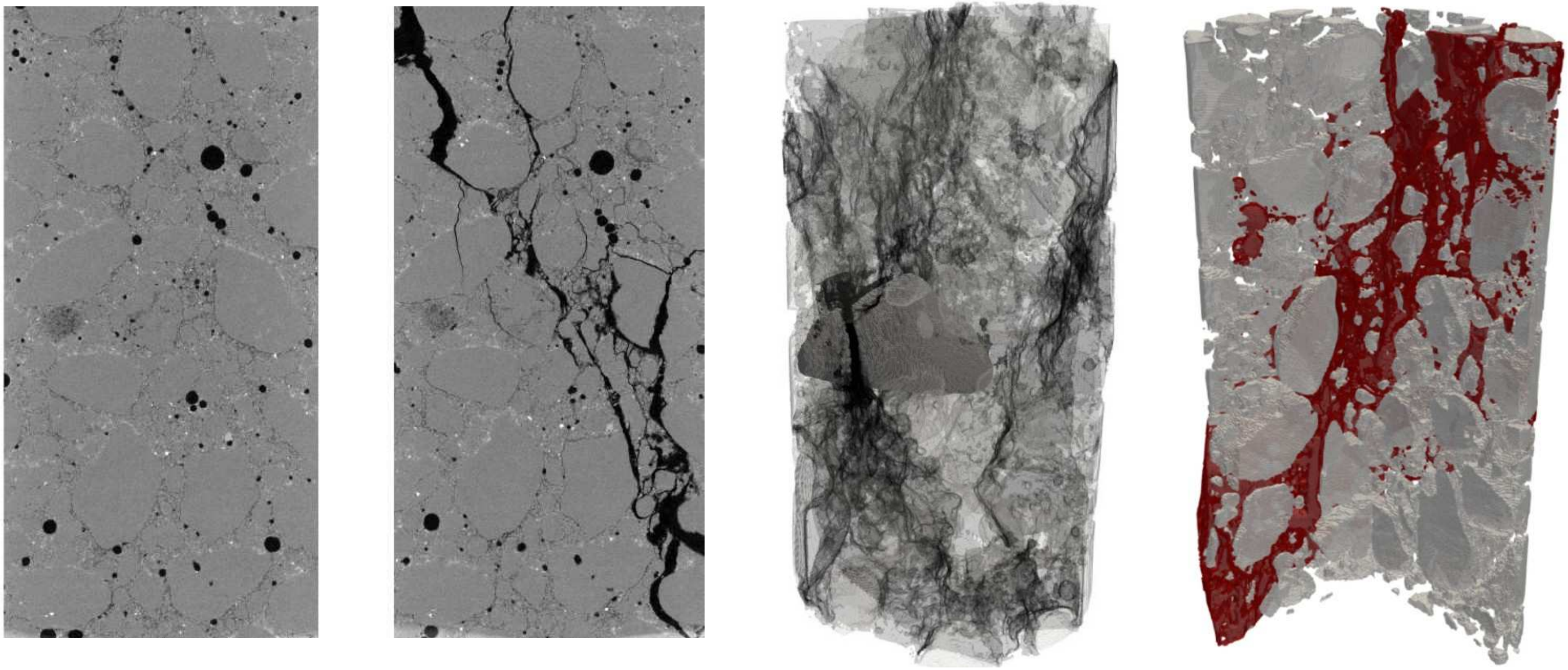
+ Energy is conserved
+ Dissipation is positive-semi def.

▷ High performances for a wide spectrum of rate-(in)dependent inelastic behaviours

Internal state variables and where to find them

Internal state variables and where to find them

Laboratory experiment: concrete under triaxial compression (x-ray tomography)



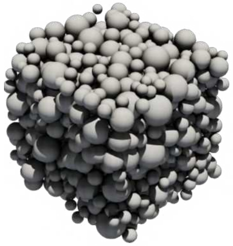
Stamati, Malecot, Roubin, 2021

Discovery of internal state variables

Masi & Stefanou. CMAME, 2022

– Internal coordinates micro-related quantities describing internal mechanisms (observable – degrees of freedom)

$\boldsymbol{\xi} \in \mathbb{M}^{\mu}$



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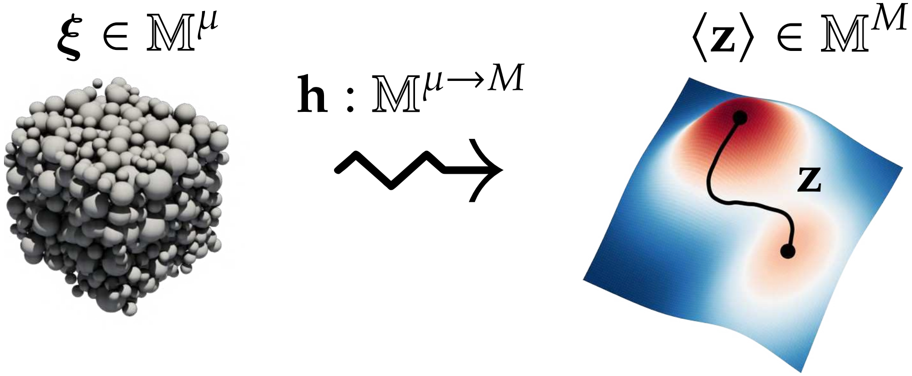

- Discovered internal variables: latent variables of the internal coordinates

$$\mathbf{z} = \mathbf{h}\left(\boldsymbol{\xi}\right) \quad \text{such that} \quad \psi = \hat{\psi}\left(\mathbb{X}\right)$$

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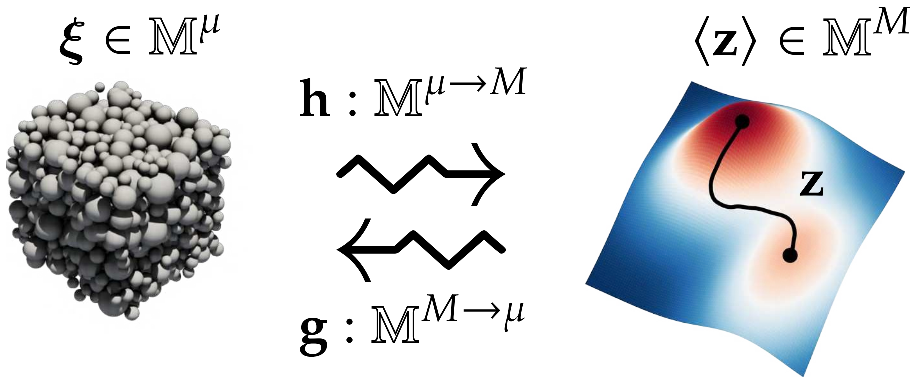

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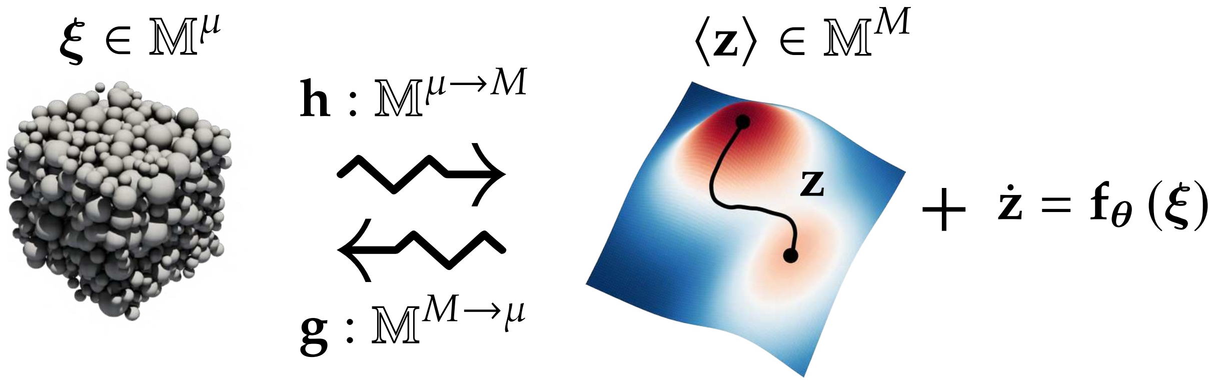
$$\tilde{\boldsymbol{\xi}} = \mathbf{g}\left(\mathbf{z}\right) \quad \text{pseudo-inverse transform}$$

Discovery of internal state variables

Masi & Stefanou. CMAME, 2022

- Internal coordinates   micro-related quantities describing internal mechanisms (observable – degrees of freedom)



- Discovered internal variables: latent variables of the internal coordinates

$$\mathbf{z} = \mathbf{h}(\boldsymbol{\xi}) \quad \text{such that} \quad \psi = \hat{\psi}(\mathbb{X})$$

$$\tilde{\boldsymbol{\xi}} = \mathbf{g}(\mathbf{z}) \quad \text{pseudo-inverse transform}$$

- Discovered evolution equations: dynamics of the internal coordinates

$$\dot{\mathbf{z}} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbb{X}) \quad \Longleftrightarrow \quad \dot{\mathbf{z}} = \frac{d\mathbf{h}}{dt}(\boldsymbol{\xi}) = \nabla_{\boldsymbol{\xi}}\mathbf{h}(\boldsymbol{\xi}) \cdot \dot{\boldsymbol{\xi}}$$

Discovery of internal state variables

Masi & Stefanou. CMAME, 2022

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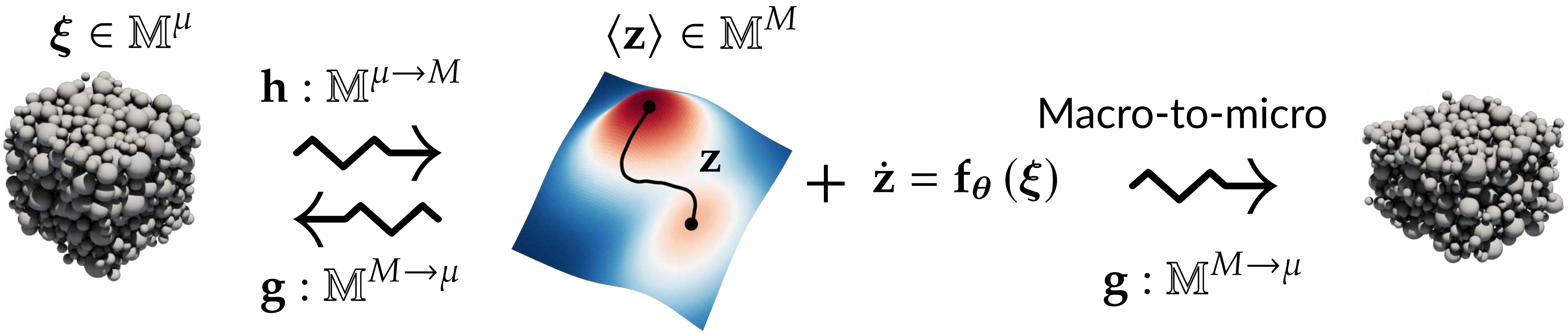

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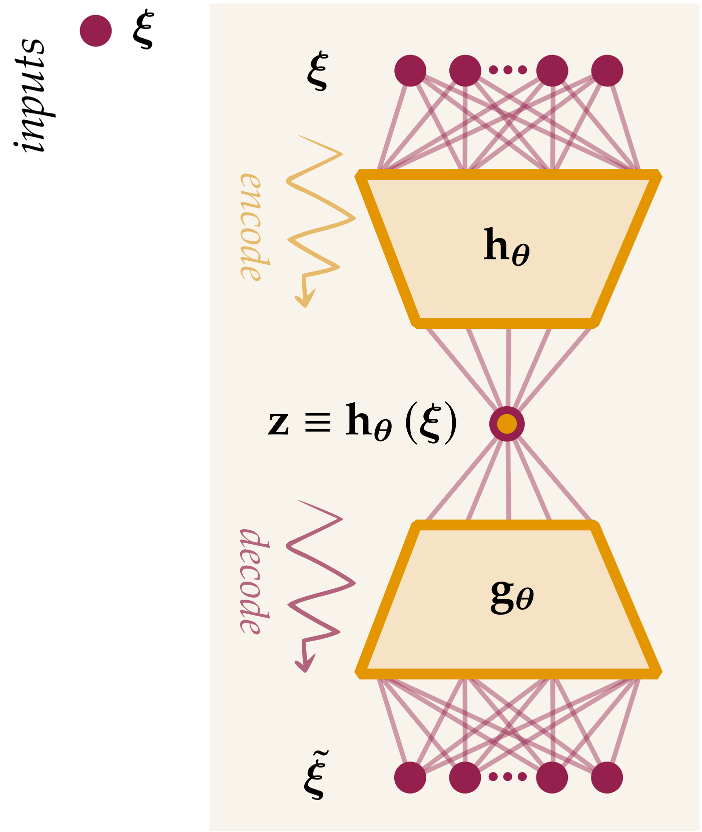
Discovery of internal state variables

Masi & Stefanou. CMAME, 2022

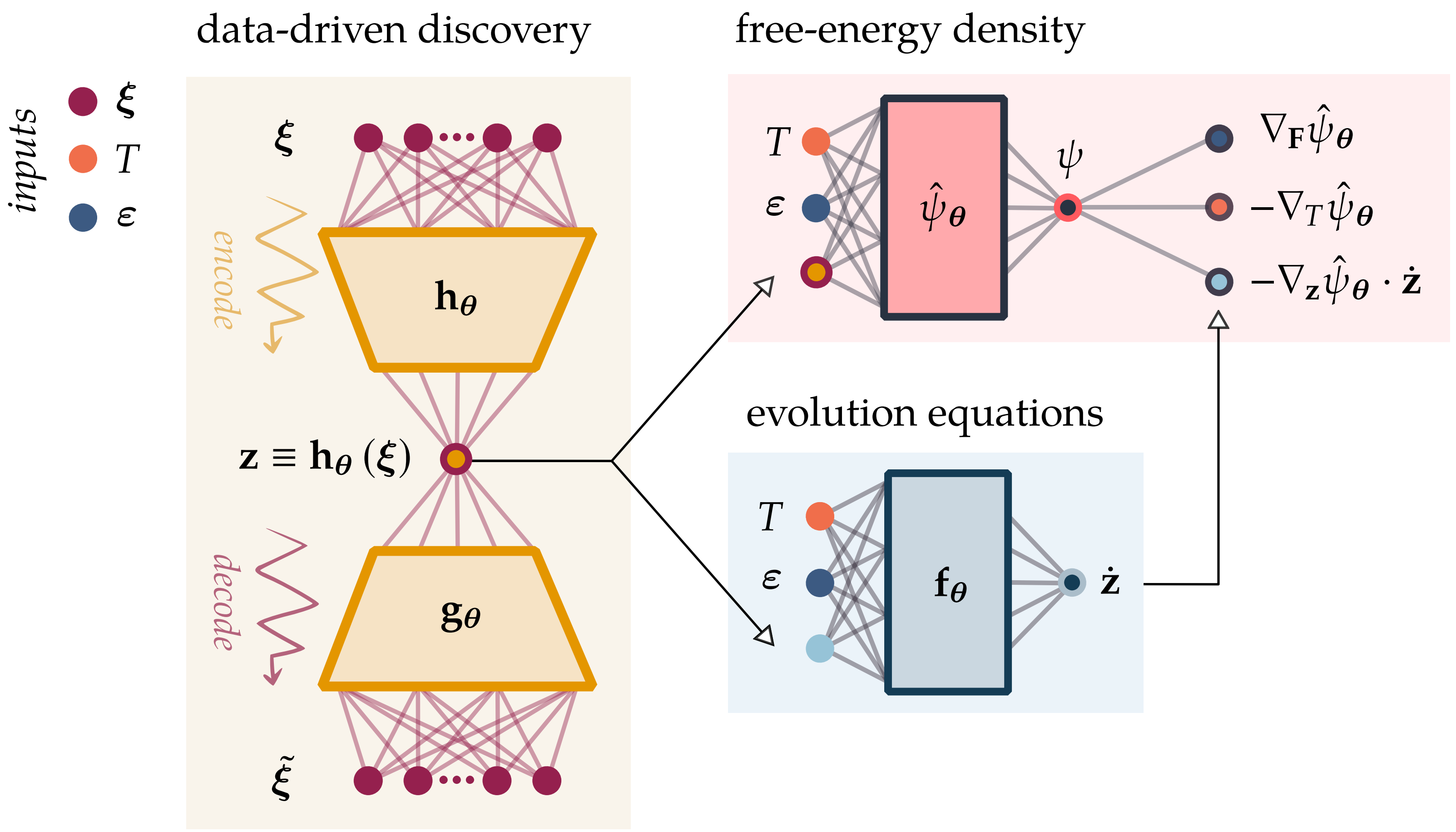
data-driven discovery



$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \left(\underbrace{\ell\left(\boldsymbol{\xi}, \mathbf{g}_{\boldsymbol{\theta}}\left(\mathbf{h}_{\boldsymbol{\theta}}(\boldsymbol{\xi})\right)\right)}_{\text{reconstruction loss}} \right)$$

Discovery of internal state variables

Masi & Stefanou. CMAME, 2022

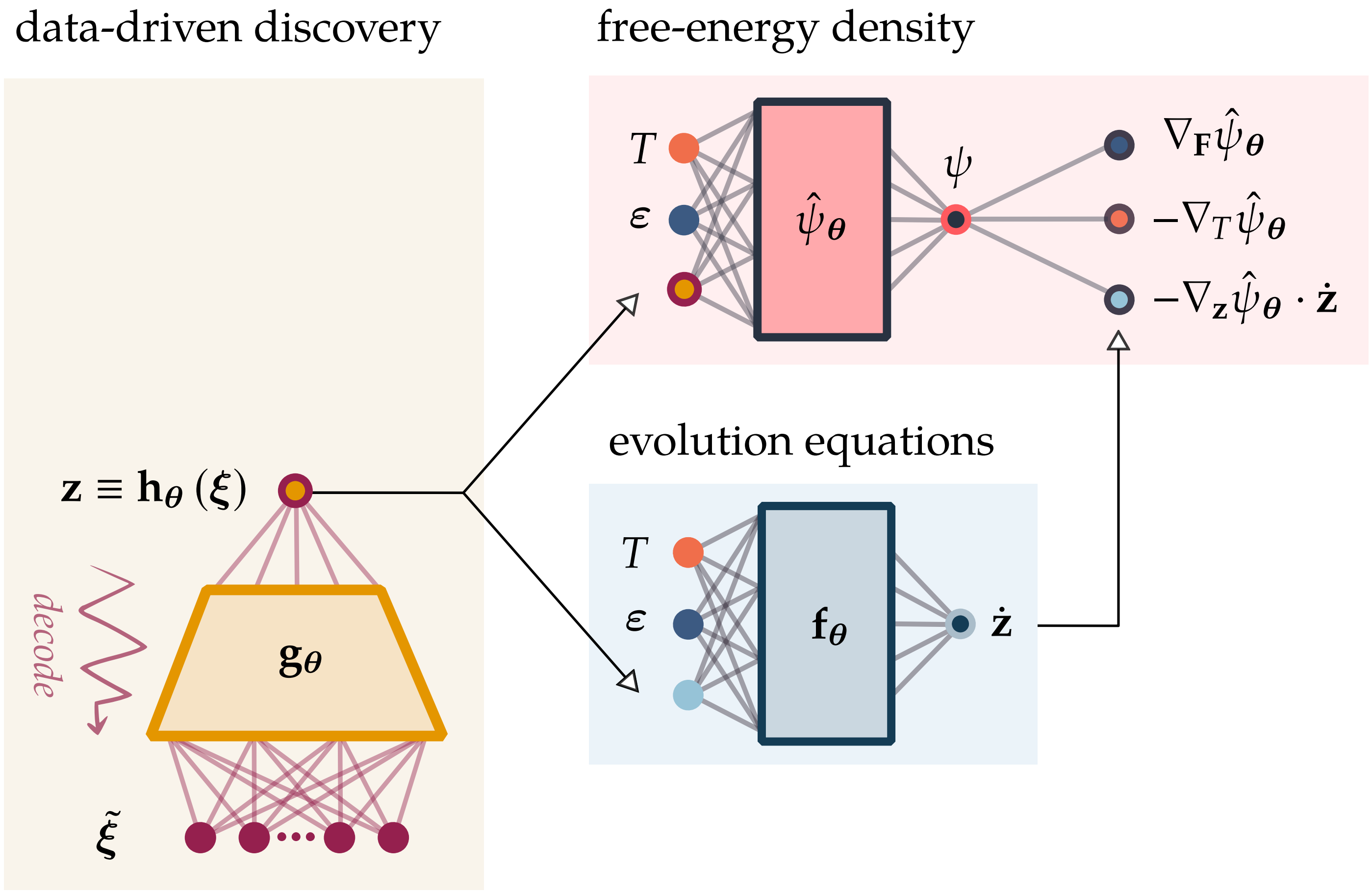


$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \Bigg(\underbrace{\ell\left(\boldsymbol{\xi}, \mathbf{g}_{\boldsymbol{\theta}}\left(\mathbf{h}_{\boldsymbol{\theta}}(\boldsymbol{\xi})\right)\right)}_{\text{reconstruction loss}} + \underbrace{\ell\left(\dot{\boldsymbol{\xi}}, \nabla_{\mathbf{z}}\mathbf{g}_{\boldsymbol{\theta}} \cdot \dot{\mathbf{z}}\right)}_{\text{loss in } \dot{\boldsymbol{\xi}}} + \underbrace{\ell\left(\psi, \hat{\psi}_{\boldsymbol{\theta}}\right)}_{\text{loss in } \psi}$$

$$+ \underbrace{\ell\left(\mathbf{P}, \nabla_{\mathbf{F}}\hat{\psi}_{\boldsymbol{\theta}}\right) + \ell\left(\eta, -\nabla_T\hat{\psi}_{\boldsymbol{\theta}}\right) + \ell\left(d, -\nabla_{\mathbf{z}}\hat{\psi}_{\boldsymbol{\theta}} \cdot \dot{\mathbf{z}}\right)}_{\text{loss in } \nabla\psi} + \underbrace{\langle -\nabla_{\mathbf{z}}\hat{\psi}_{\boldsymbol{\theta}} \cdot \dot{\mathbf{z}} \rangle}_{\text{reg.}} \Bigg)$$

Discovery of internal state variables

Masi & Stefanou. CMAME, 2022



Constitutive equations: $\dot{\mathbf{z}}(t), \boldsymbol{\sigma}(t) = \mathcal{T}_{\mathcal{ANN}}\big(T(t), \varepsilon(t), \mathbf{z}(t)\big) \quad \forall\, t$

Initial Value Problem:

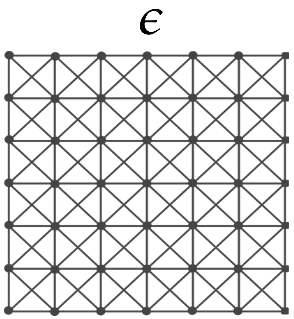
$$\mathbf{z}(t) = \int_{t_0}^{t} \mathbf{f}_{\boldsymbol{\theta}}\big(T(t), \varepsilon(t), \mathbf{z}(t)\big) + \mathbf{z}(t_0)$$

$$\mathbf{z}(t_0) = \mathbf{h}_{\boldsymbol{\theta}}\left(\boldsymbol{\xi}(t_0)\right)$$

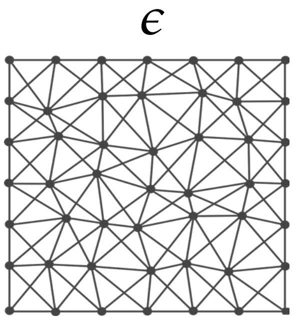
Downscaling – "*localisation*": $\boldsymbol{\xi}(t) = \mathbf{g}_{\boldsymbol{\theta}}\big(\mathbf{z}(t)\big)$

Experiments: lattice materials

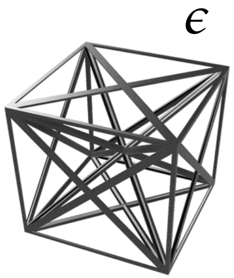
Heterogeneous lattice structures (auxiliary problem)



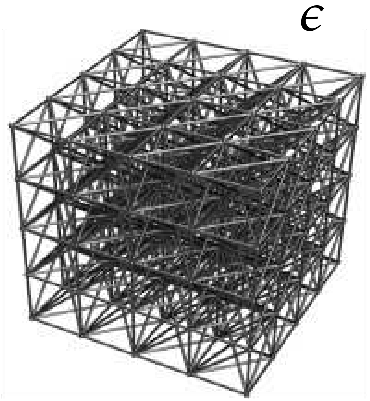
2D regular



2D irregular



3D cell



3D regular

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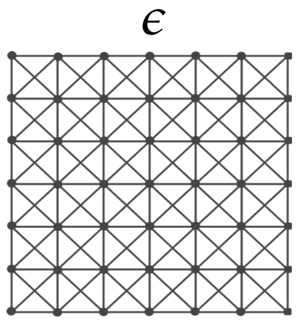

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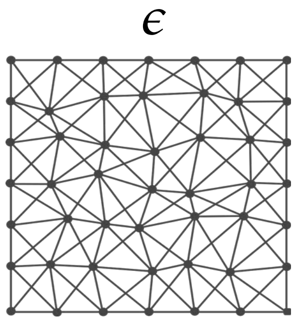
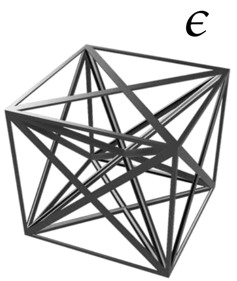
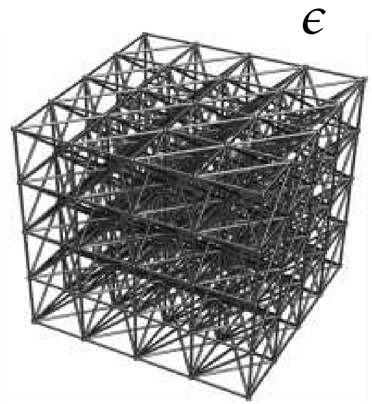


2D irregular



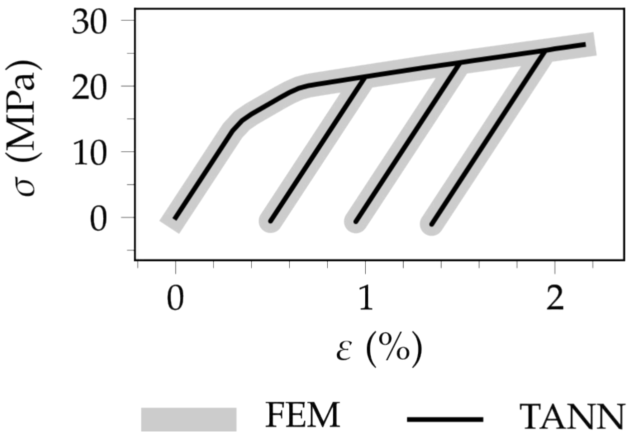
3D cell



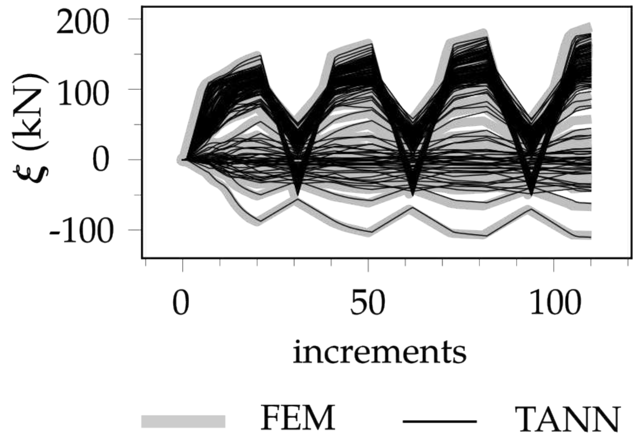
3D regular

Replacing the solution of the auxiliary problem (micromechanical FEM versus TANN)

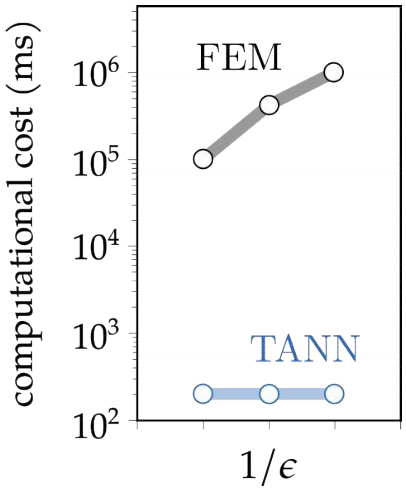
average mechanical behaviour



tracking microscopic fields



massive speeds-up

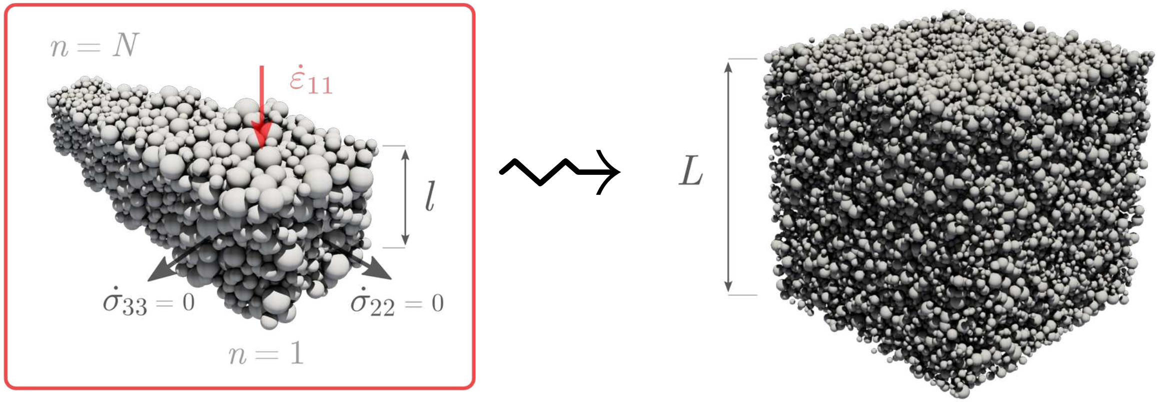


Experiments: granular matter

Experiments: granular matter

Masi & Stefanou. ML in Geomechanics, 2024

Stochastic representation (random media) – statistical ensemble approach



statistical
elementary volumes
(SEV)

representative
elementary volume
(REV)

Ostoja-Starzewski 2006
Papachristos et al. 2023
Nguyen, 2021

Experiments: granular matter

Masi & Stefanou. ML in Geomechanics, 2024

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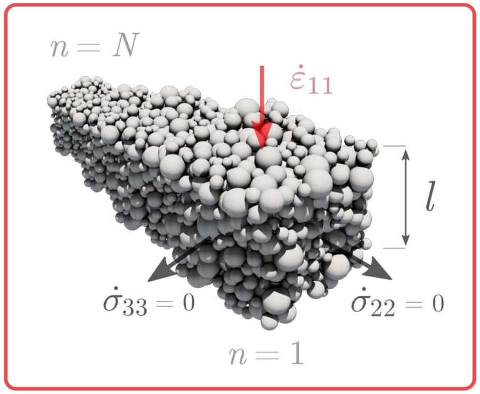

statistical
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$\rightsquigarrow$

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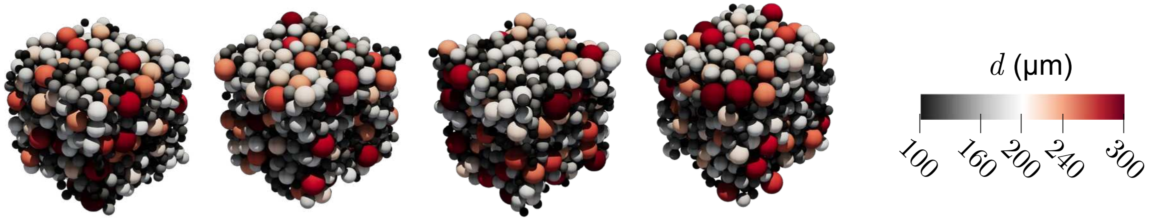
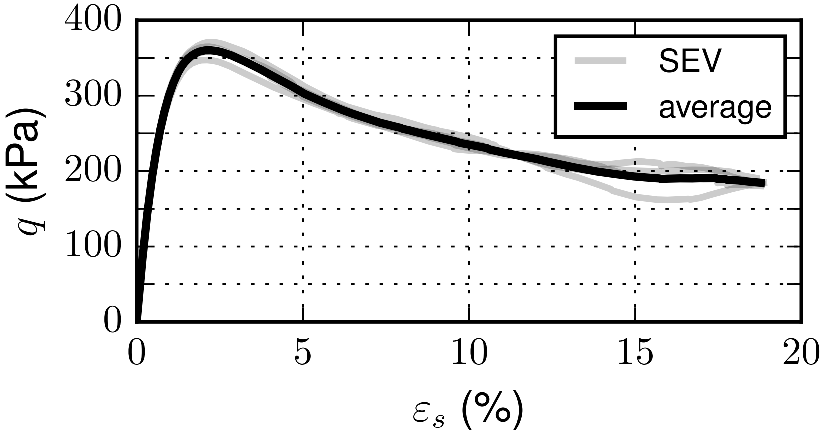
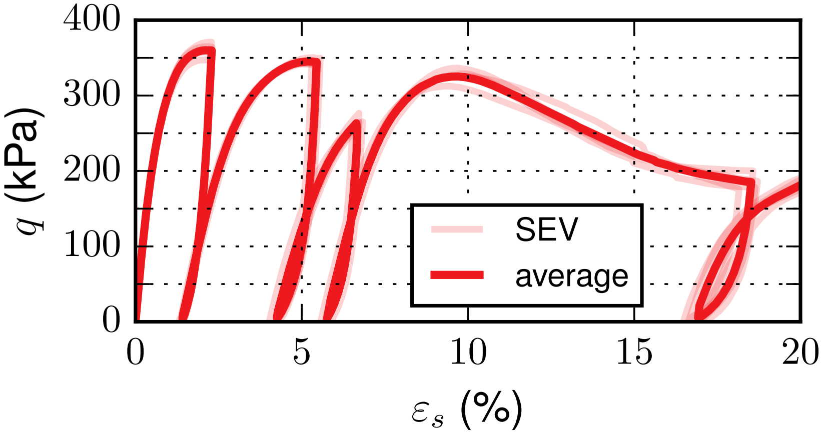
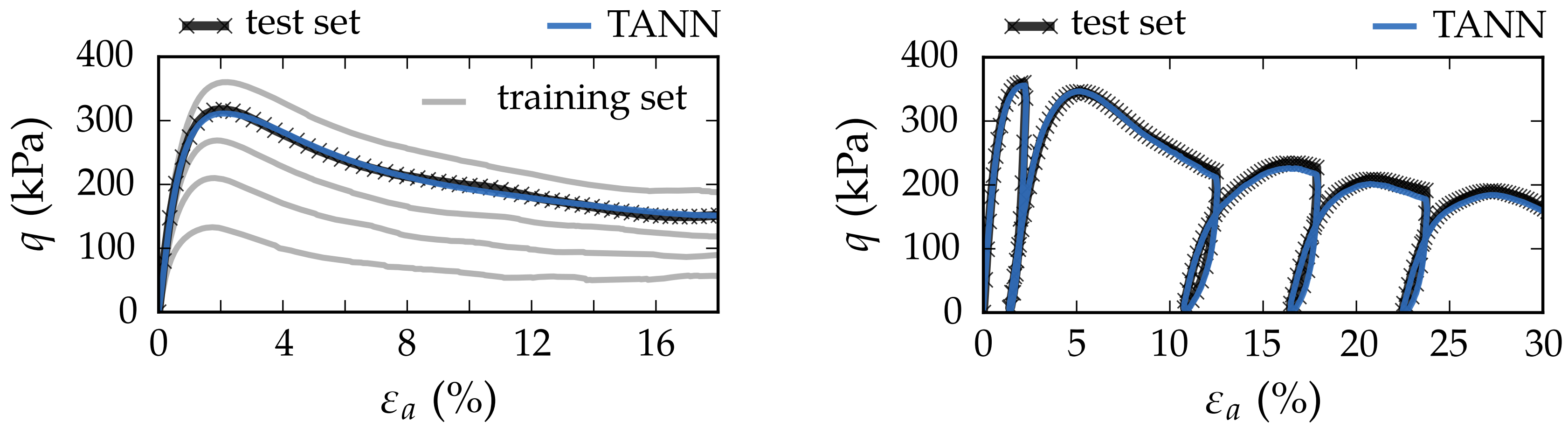






Experiments: granular matter

Predicting unobserved behaviours



Experiments: granular matter

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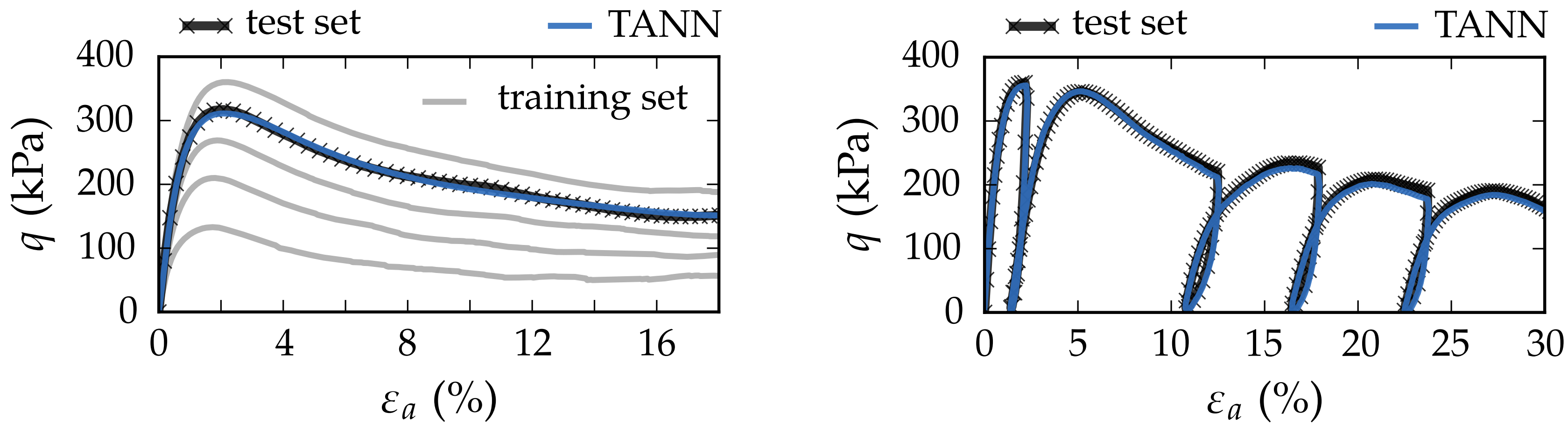
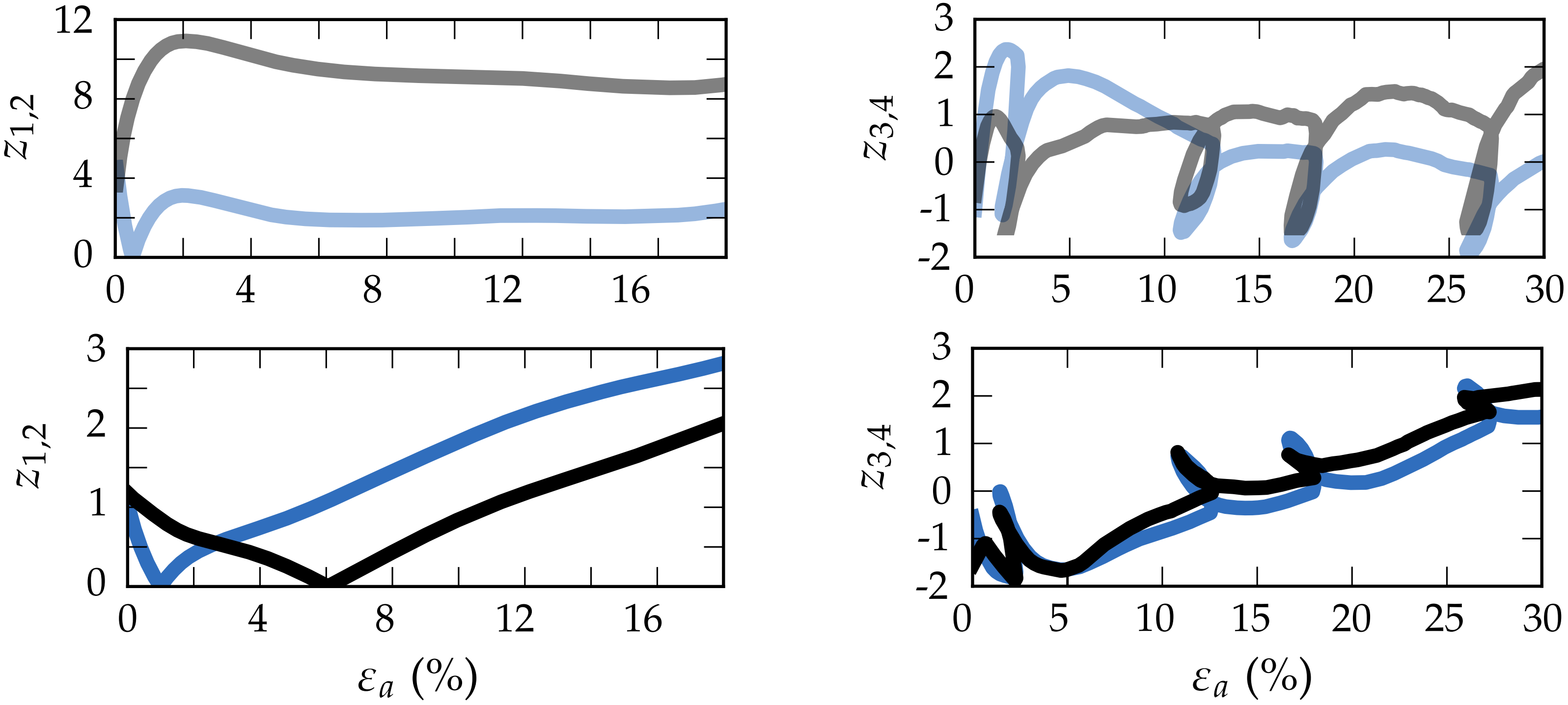


– micro-to-Macro: 4 internal state variables ~ topological descriptors



On-the-fly microstructure tracking

– Reconstructing micromechanical fields (data-driven localisation)

On-the-fly microstructure tracking

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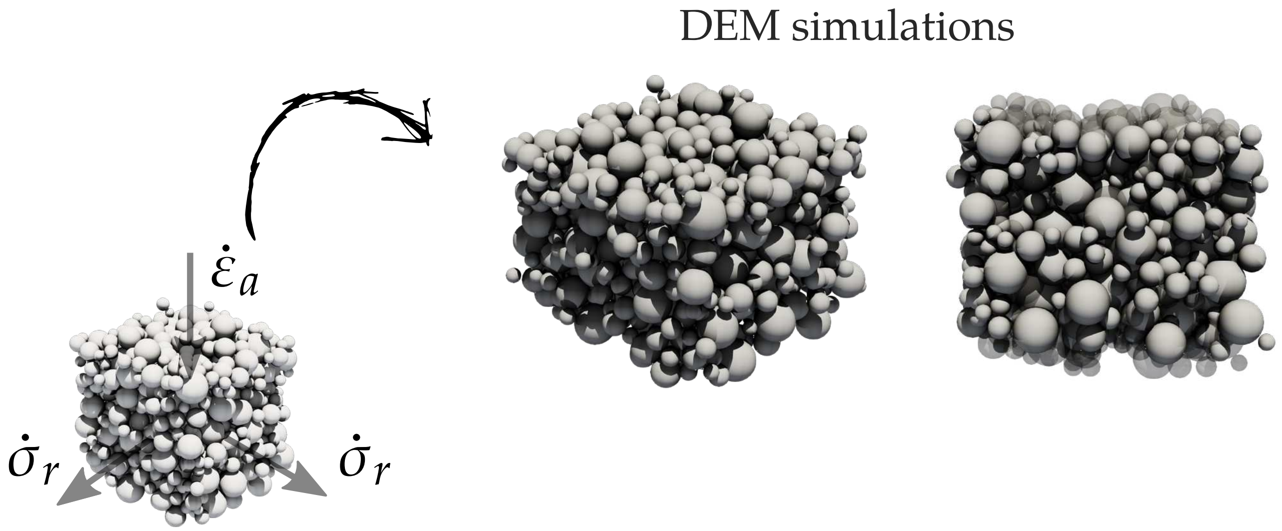

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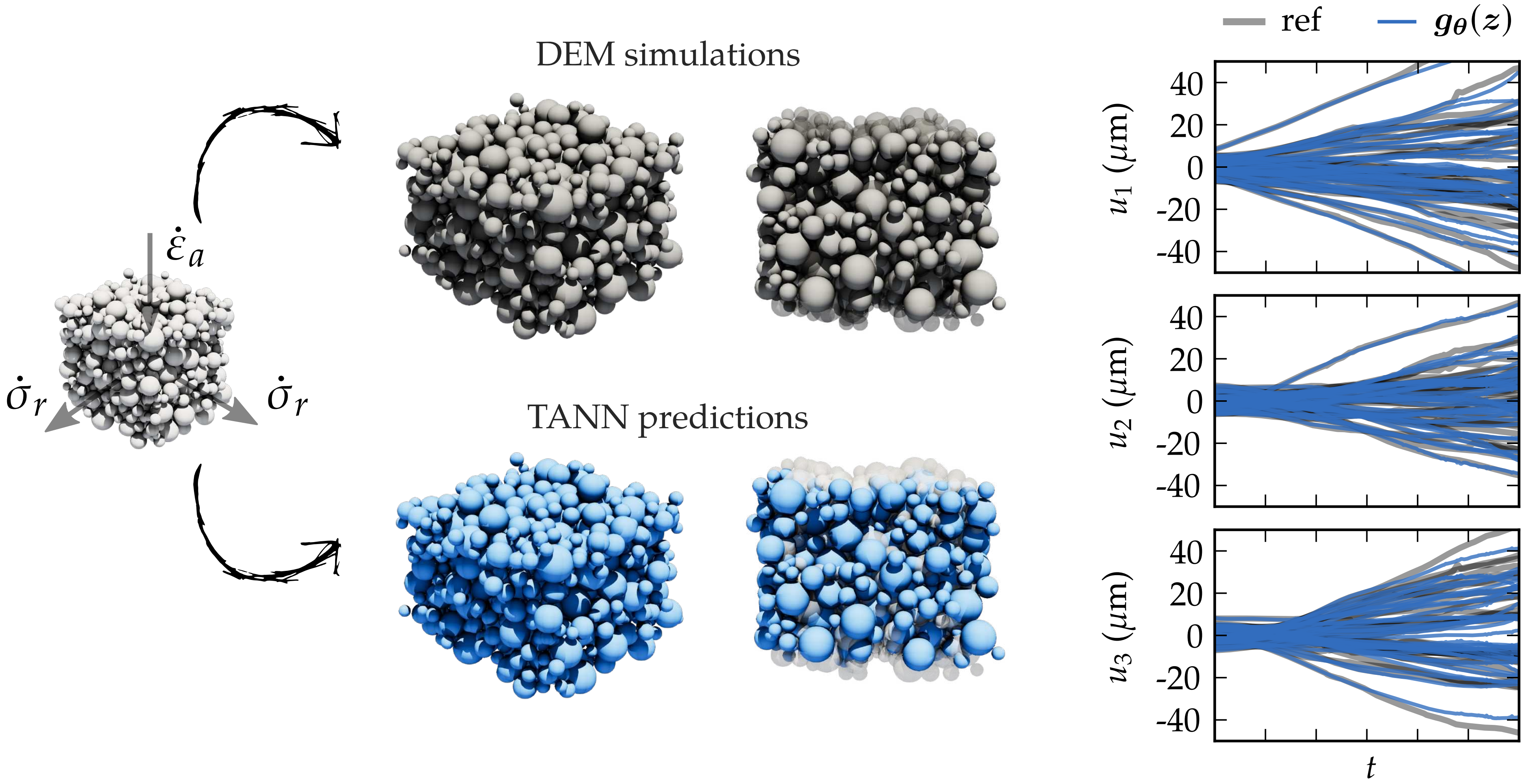

▷ Massive computational accelerations (×10^3) – DEM/TANN: 30 minutes / <0.3s

Overview

I) Background setting
  a) Non-equilibrium thermodynamics

II) Thermodynamics-based artificial neural networks
  a) Methods
  b) Discovery of internal state variables
  c) Experiments

III) Multiscale computing

IV) Neural equations from small data
  a) Data scarcity and sparsity
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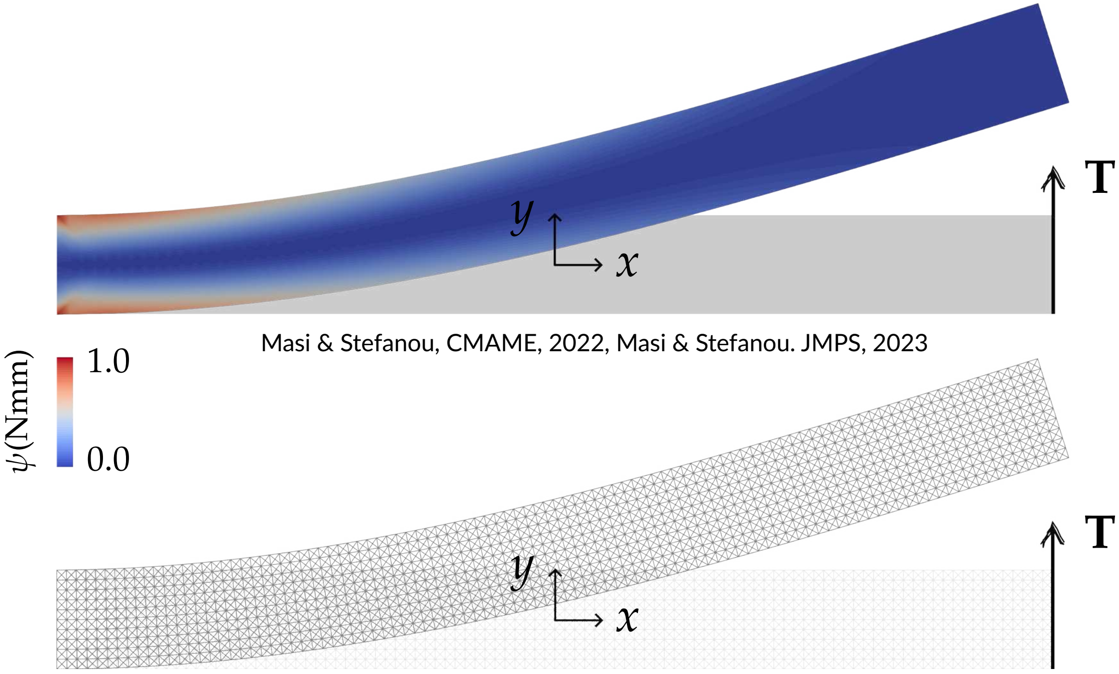
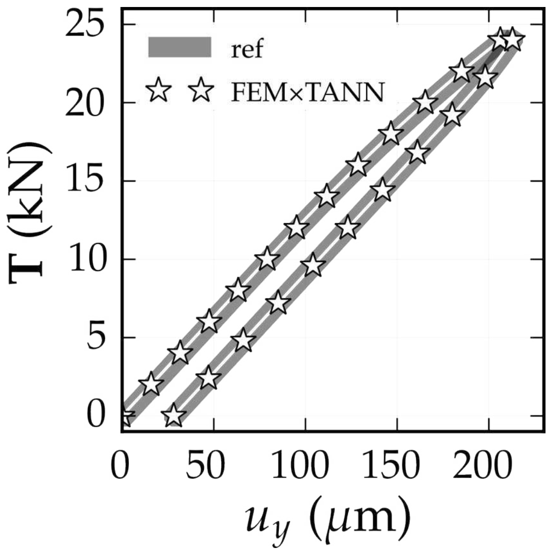
FEM×TANN and numerical homogenisation

Double-scale homogenisation scheme: rigorous (asymptotic) and fast



Masi & Stefanou, CMAME, 2022, Masi & Stefanou. JMPS, 2023



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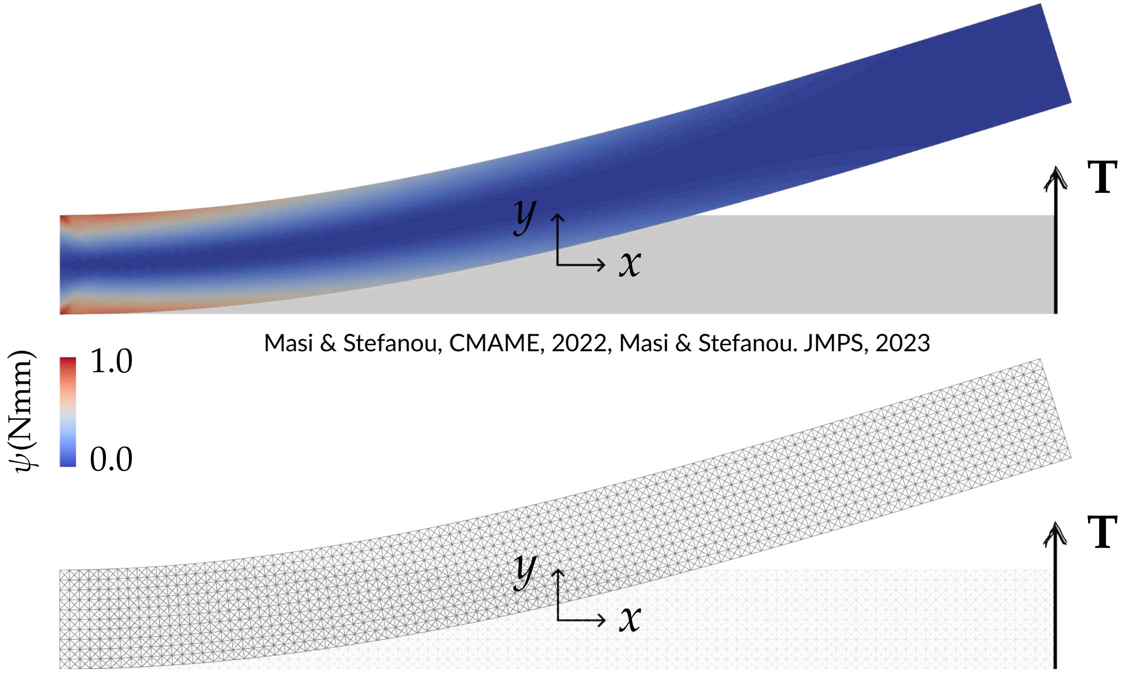

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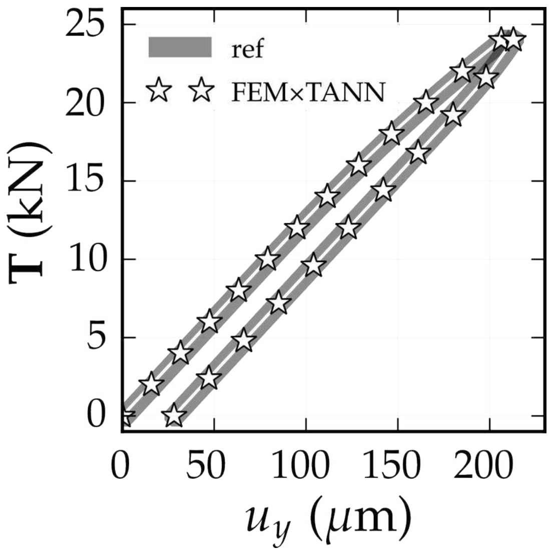
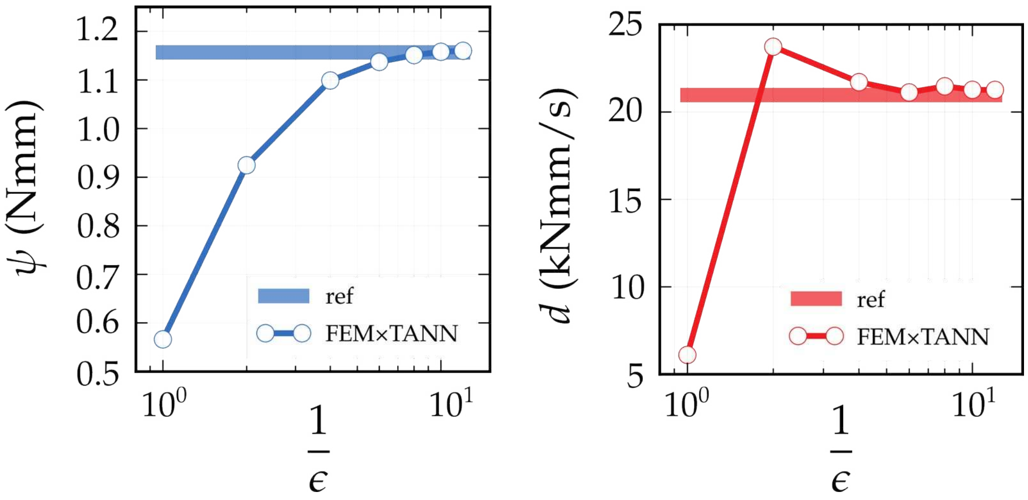


▹ Convergence (asymptotic homogenisation)



FEM×TANN and numerical homogenisation

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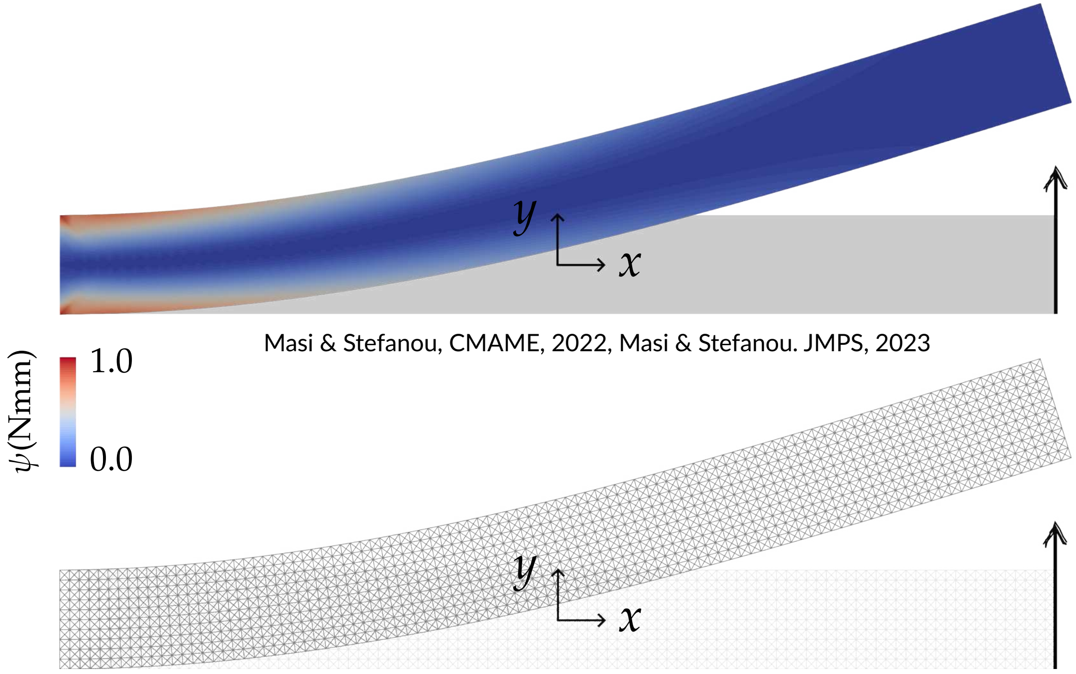

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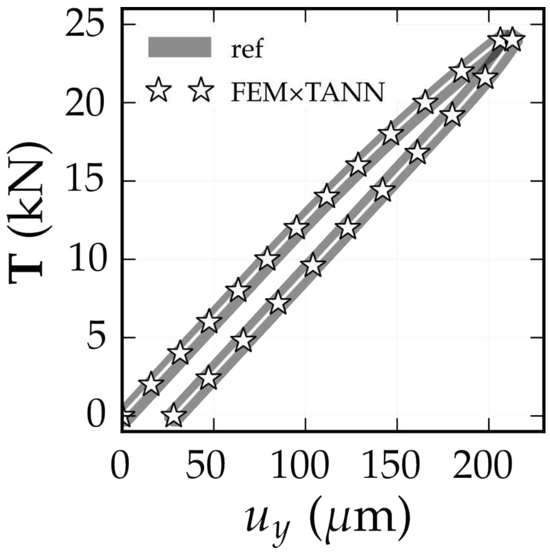

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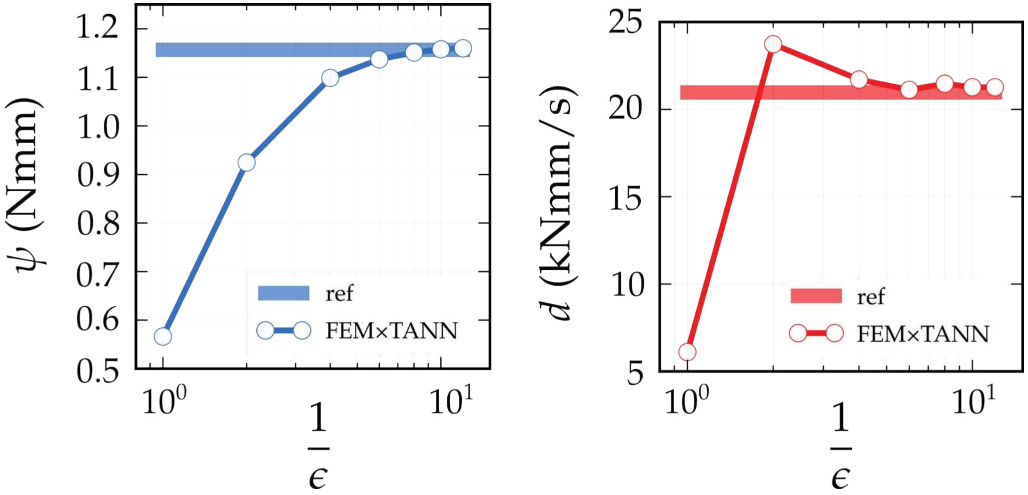
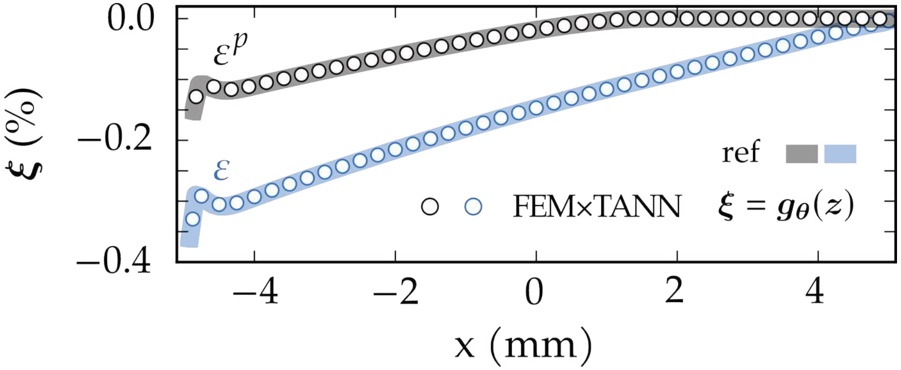


- ▹ Microstructure tracking (“localisation”)



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Data-driven identification from experiments

Masi & Einav. CMAME, 2024

Data-driven identification from experiments

Masi & Einav. CMAME, 2024

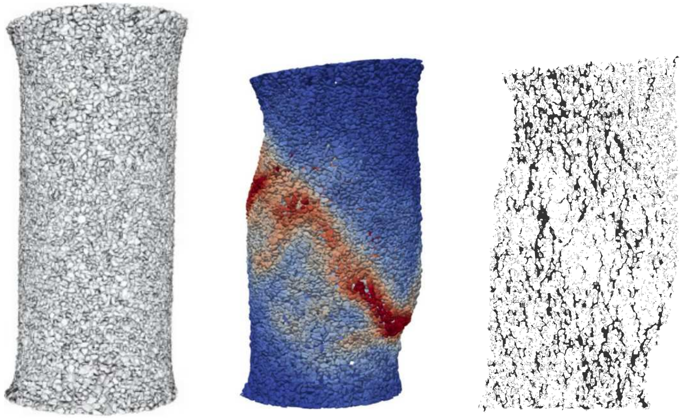
Big data (measure everything)

$$\mathcal{D} = \left\{\boldsymbol{\sigma}^{(n)}, \boldsymbol{\varepsilon}^{(n)}, \mathbb{X}^{(n)}\right\}_{n=0}^{N}$$

$$= \begin{bmatrix} \boldsymbol{\sigma}^{(0)} & \boldsymbol{\sigma}^{(1)} & \cdots & \boldsymbol{\sigma}^{(N)} \\ \boldsymbol{\varepsilon}^{(0)} & \boldsymbol{\varepsilon}^{(1)} & \cdots & \boldsymbol{\varepsilon}^{(N)} \\ \mathbb{X}^{(0)} & \mathbb{X}^{(1)} & \cdots & \mathbb{X}^{(N)} \end{bmatrix}$$

observe the entire state
(at smaller scales)

all states $\left\{\mathbb{X}^{(n)}\right\}_{n=0}^{N}$



Kawamoto et al. 2018, Karapiperis et al. 2021

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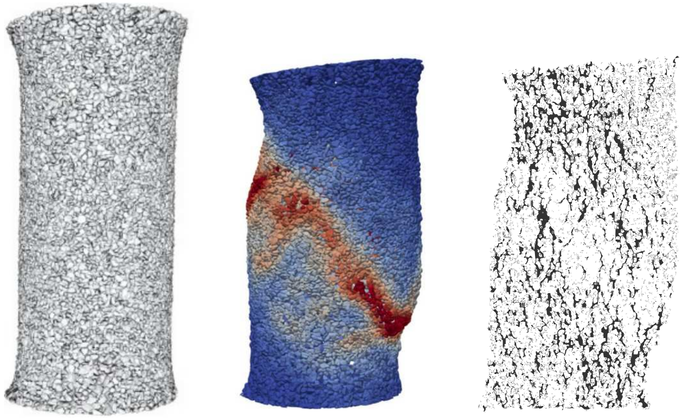


Kawamoto et al. 2018, Karapiperis et al. 2021

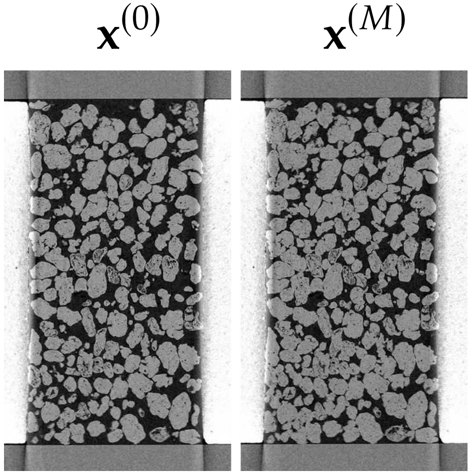
Small data (measure observable)

$$\mathcal{D} = \left\{ \boldsymbol{\sigma}^{(n)}, \boldsymbol{\varepsilon}^{(n)} \right\}_{n=0}^{N} \cup \left\{ \mathbf{x}^{(m)} \right\}_{m=0}^{M}, \; M \ll N$$

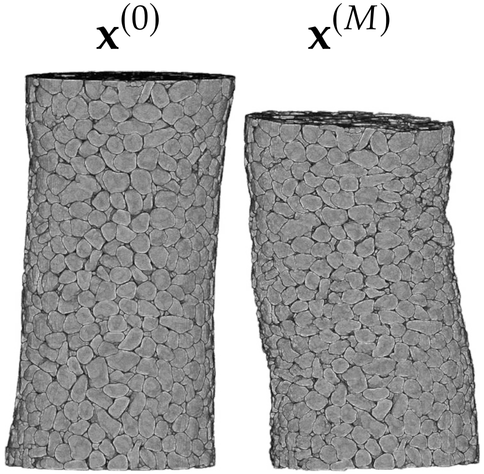
$$= \begin{bmatrix} \boldsymbol{\sigma}^{(0)} & \boldsymbol{\sigma}^{(1)} & \dots & \boldsymbol{\sigma}^{(N)} \\ \boldsymbol{\varepsilon}^{(0)} & \boldsymbol{\varepsilon}^{(1)} & \dots & \boldsymbol{\varepsilon}^{(N)} \\ \mathbf{x}^{(0)} & ? & ? & \mathbf{x}^{(M)} \end{bmatrix}$$

no observations

partial
$\mathbf{x} \subset \mathbb{X}$



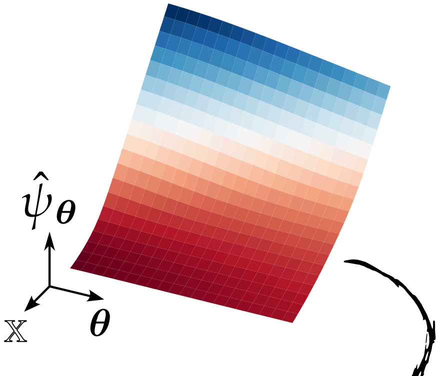
Vego, 2023

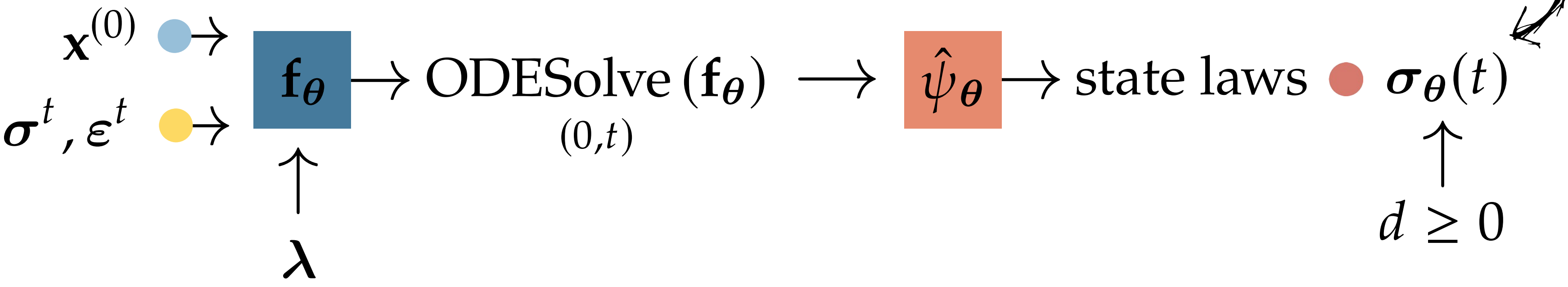


Hurley et al. 2023

Solving the big problem of small data

Neural Integration for Constitutive Equations (NICE)





$\mathbf{x}^{(0)}$ ● $\to$

$\boldsymbol{\sigma}^t, \boldsymbol{\varepsilon}^t$ ● $\to$

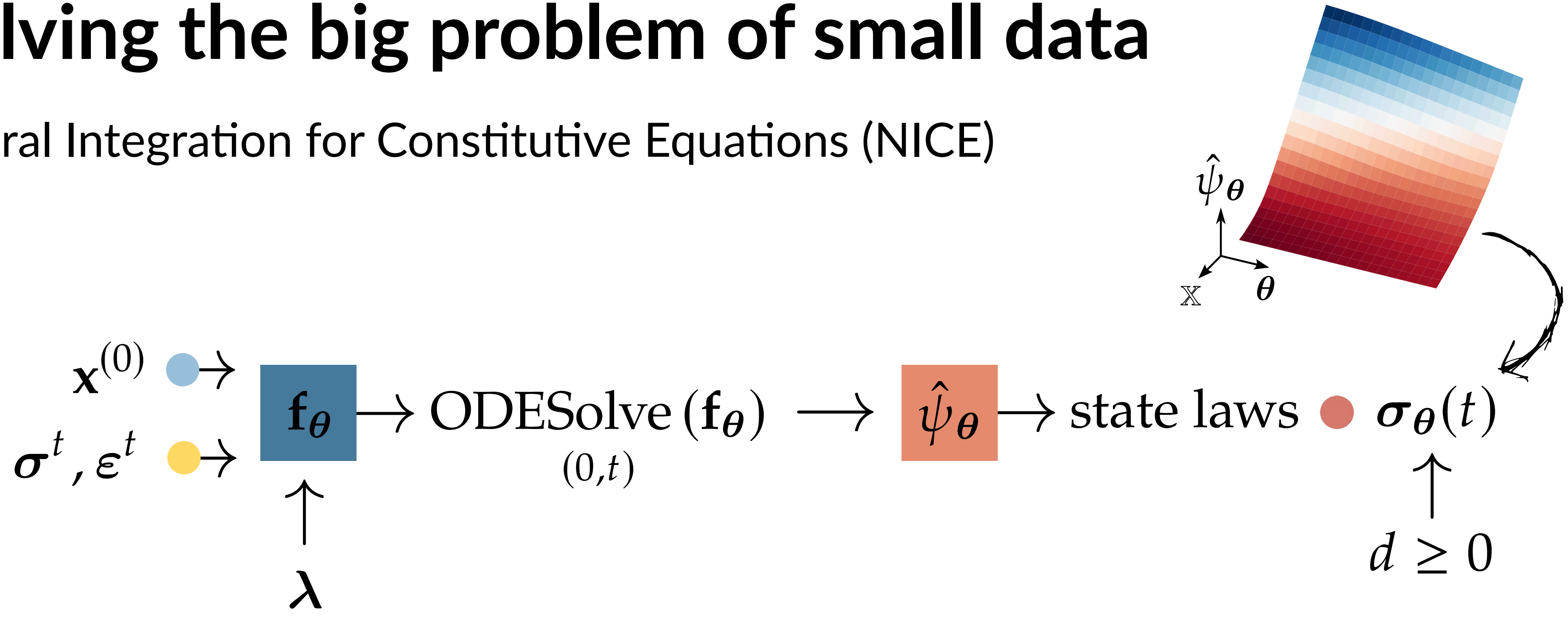
$$\boxed{\mathbf{f}_{\boldsymbol{\theta}}} \to \underset{(0,t)}{\mathrm{ODESolve}}\left(\mathbf{f}_{\boldsymbol{\theta}}\right) \longrightarrow \boxed{\hat{\psi}_{\boldsymbol{\theta}}} \to \text{state laws} \; \bullet \; \boldsymbol{\sigma}_{\boldsymbol{\theta}}(t)$$

$\uparrow$ $\boldsymbol{\lambda}$

$\uparrow$ $d \geq 0$

Solving the big problem of small data

Neural Integration for Constitutive Equations (NICE)



Optimisation problem:

$$\boldsymbol{\theta}^{*}, \boldsymbol{\lambda}^{*} = \operatorname{argmin}\left(\varrho + \mathcal{L}_{\boldsymbol{\sigma}} + \mathcal{L}_{\mathbf{x}} + \langle -d_{\boldsymbol{\theta}} \rangle + \|\boldsymbol{\theta}\|_{2}^{2}\right)$$

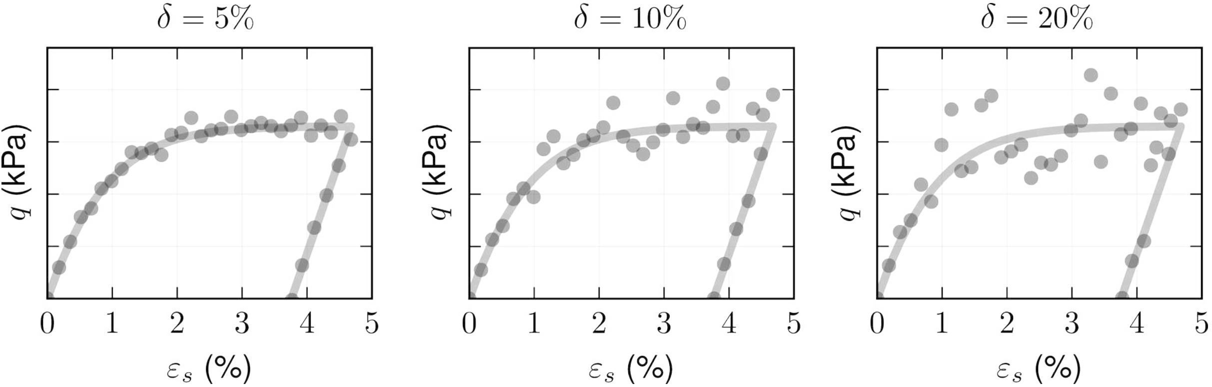
- Residual for initial conditions (elastic strain, etc.) $\varrho = \ell\left(\boldsymbol{\sigma}_{\boldsymbol{\theta}}\left(\boldsymbol{\lambda}, \mathbf{x}^{(0)}\right) - \boldsymbol{\sigma}^{(0)}\right)$
- Thermodynamics-based loss (stress) $\mathcal{L}_{\boldsymbol{\sigma}} = \ell\left(\underset{\forall n \in [0,N]}{\boldsymbol{\sigma}_{\boldsymbol{\theta}}(t^{n}), \boldsymbol{\sigma}^{(n)}}\right)$
- Thermodynamics-based loss (evolution equations) $\mathcal{L}_{\mathbf{x}} = \ell\left(\underset{\forall m \in [1,M]}{\mathrm{ODESolve}(\mathbf{f}_{\boldsymbol{\theta}} - \mathbf{x}^{(m)})}\right)$

Benchmark

Elasto-plastic material: $\mathbb{X} = \left\{ \boldsymbol{\varepsilon}^e \right\}$

$$p = \mathbf{1} : \boldsymbol{\sigma}/3$$

$$q = \sqrt{\frac{3}{2}\, \boldsymbol{\sigma}' : \boldsymbol{\sigma}'}$$



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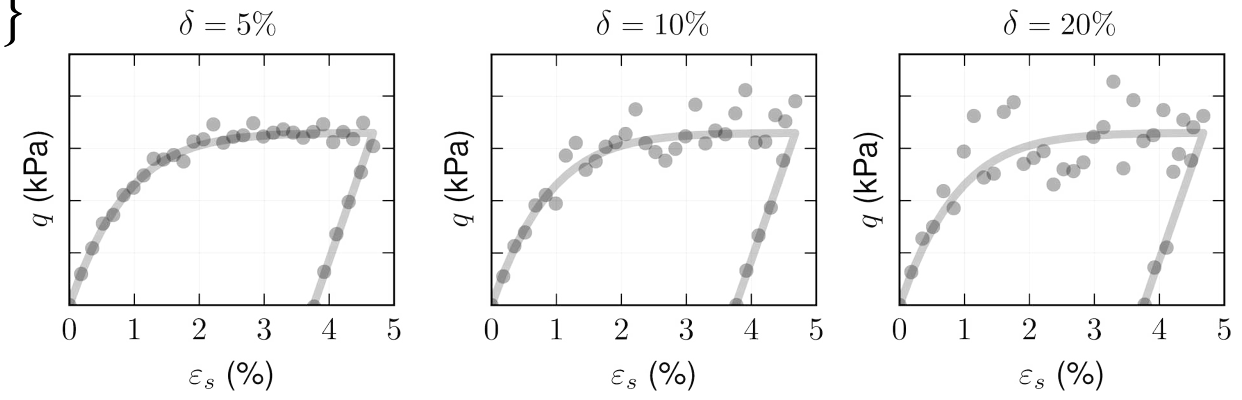
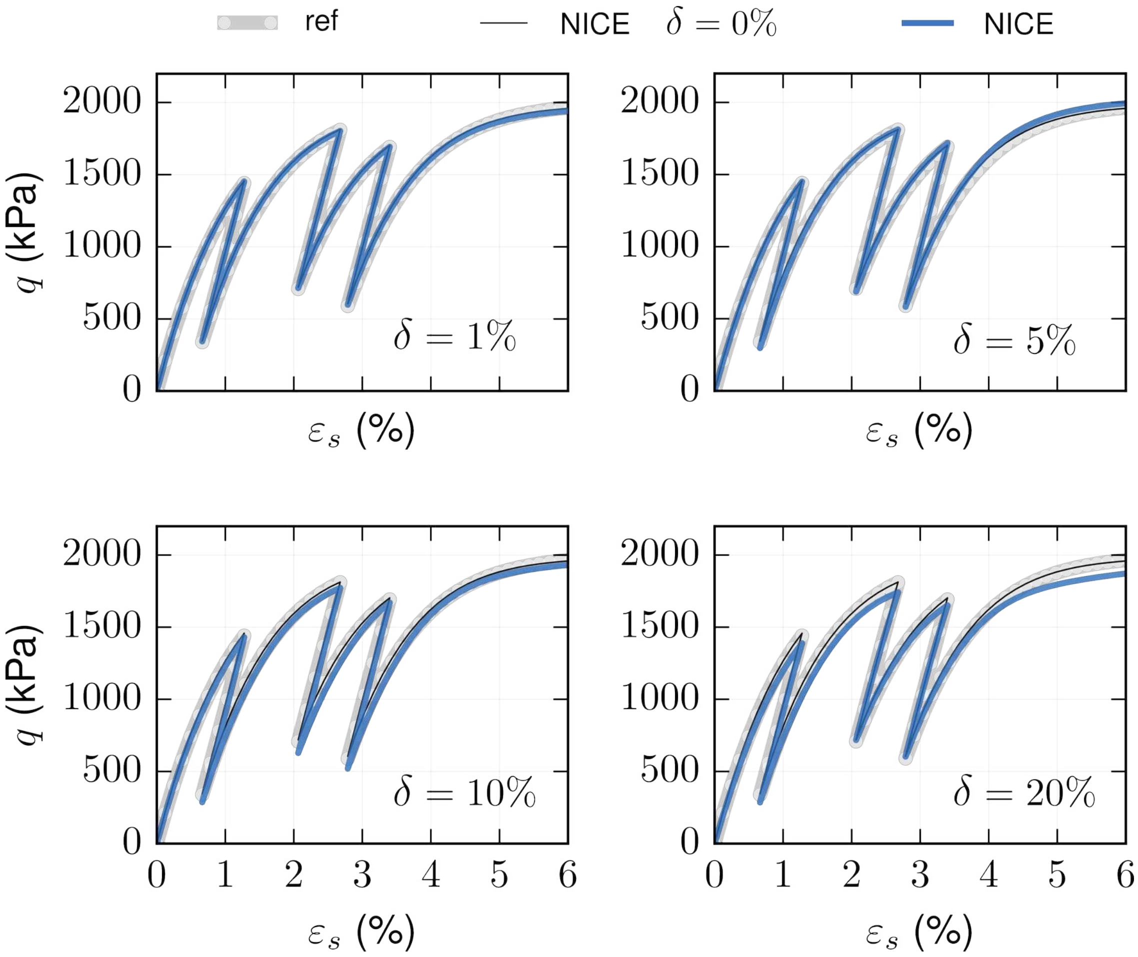
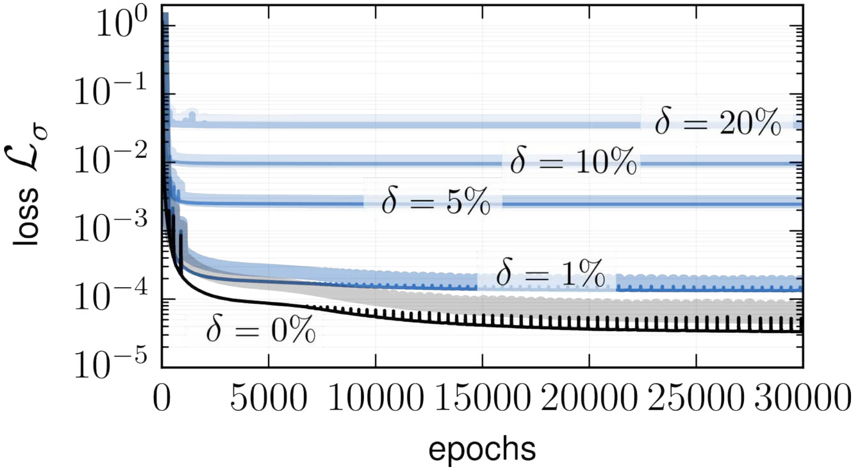


Inference:
unobserved loading path/protocol

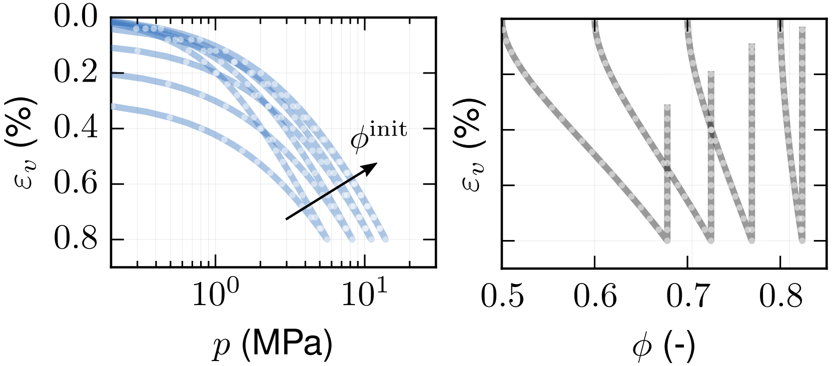




▷ High-level generalisation, robustness

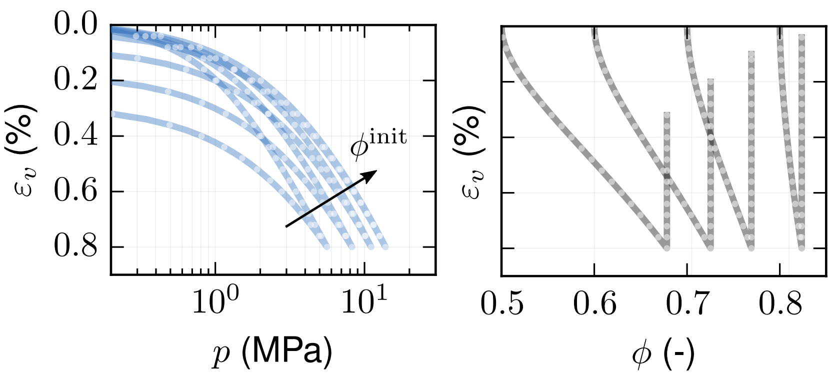
Numerical experiment

Porous elasto-plastic material: $\mathbb{X} = \left\{\rho, \boldsymbol{\varepsilon}^e, \mathbf{z}\right\}$

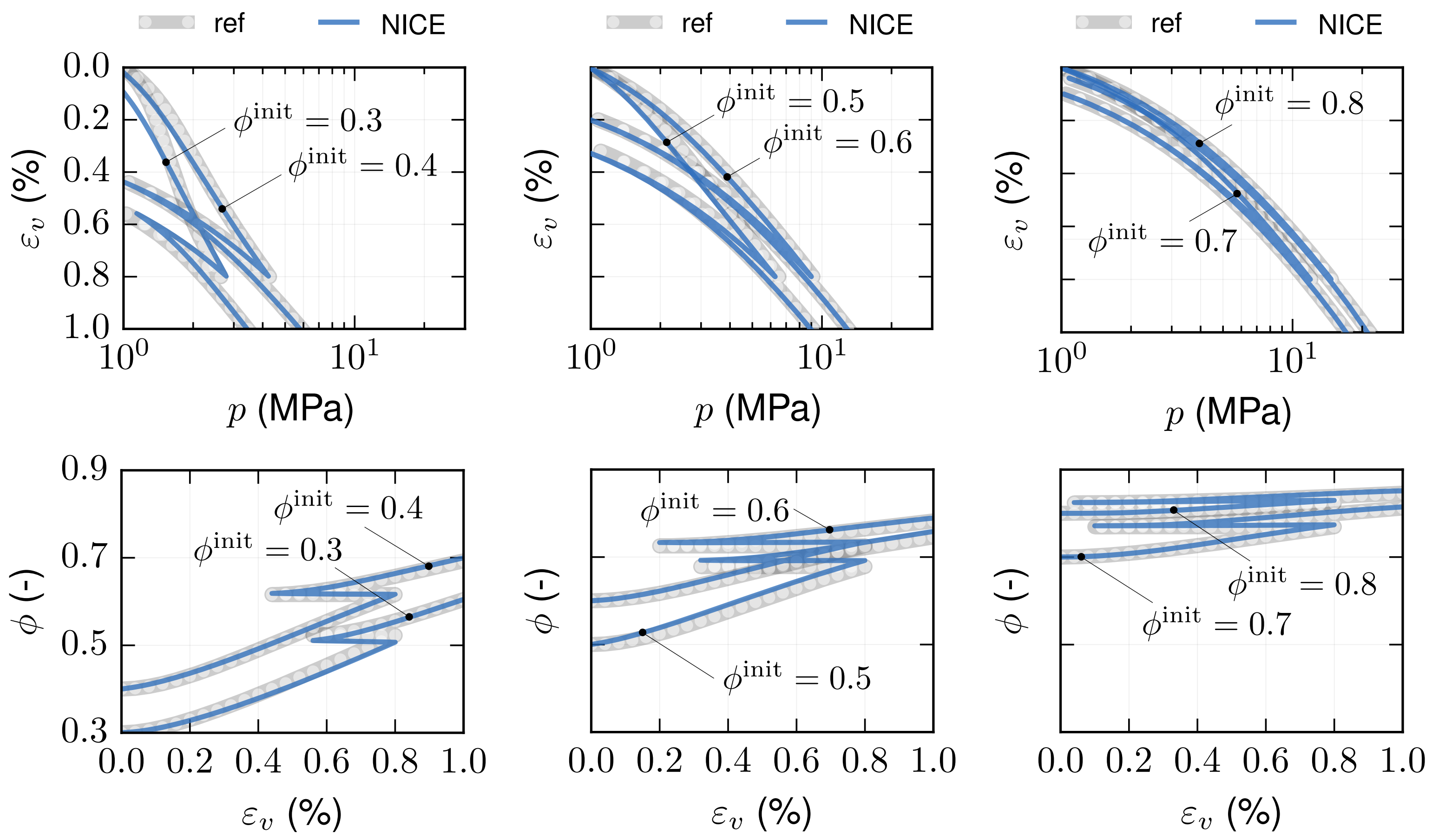


Numerical experiment

Porous elasto-plastic material: $\mathbb{X} = \{\rho, \boldsymbol{\varepsilon}^e, \mathbf{z}\}$



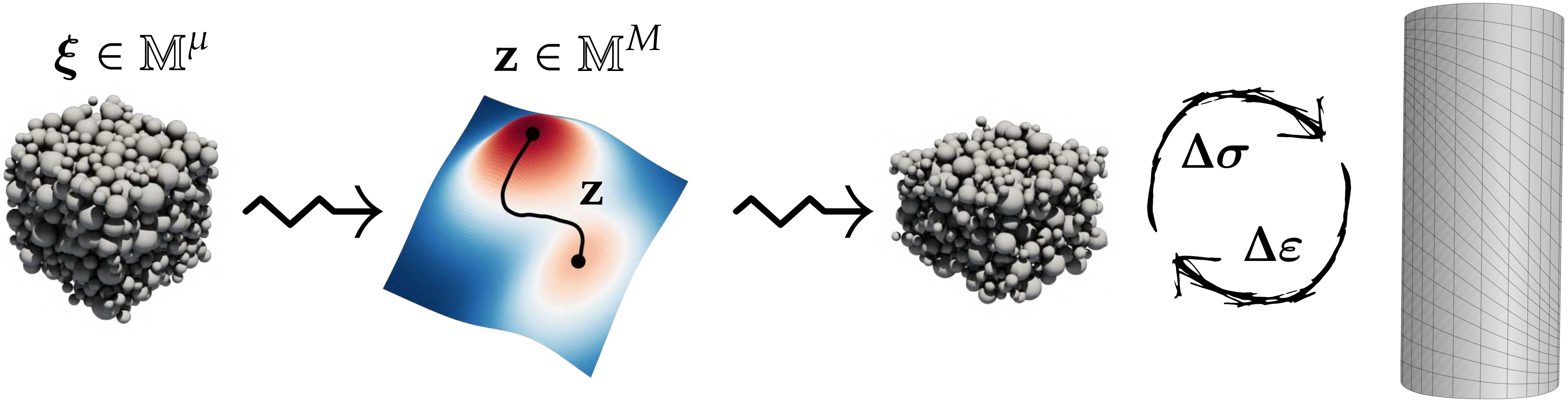
Inference:
unobserved loading path/protocol



▷ High-level generalisation, robustness: discover constitutive equations

Summary

- **Numerical homogenisation** driven by machine learning methods
- Thermodynamics- and data-driven **scale bridging**
- Data from various provenance (material-point and numerical experiments)
- **Massive speed-ups** of multiscale simulations (×10^3)
- **History dependence** (plasticity, damage, viscosity, etc.)
- **Discovery of internal descriptors**
- **Learn from small data** (sparse and scarce)



References, codes & hands-on

References

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- F. Masi (2024). Machine Learning in Geomechanics, vol I. Wiley.
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- F. Masi, I. Einav (2024). Comput Methods Appl Mech Eng 420, 116698.

Codes & hands-on

- TANN: github.com/filippo-masi/Thermodynamics-Neural-Networks
- TANN-multiscale: github.com/filippo-masi/TANN-multiscale
- Numerical GeoLab: github.com/AlexSTA1993/numerical_geolab
- NICE: github.com/filippo-masi/NICE
- Hands-on Regression: github.com/alert-geomaterials/2023-doctoral-school
- Hands-on TANN/PINN: github.com/alert-geomaterials/2023-doctoral-school

Acknowledgements

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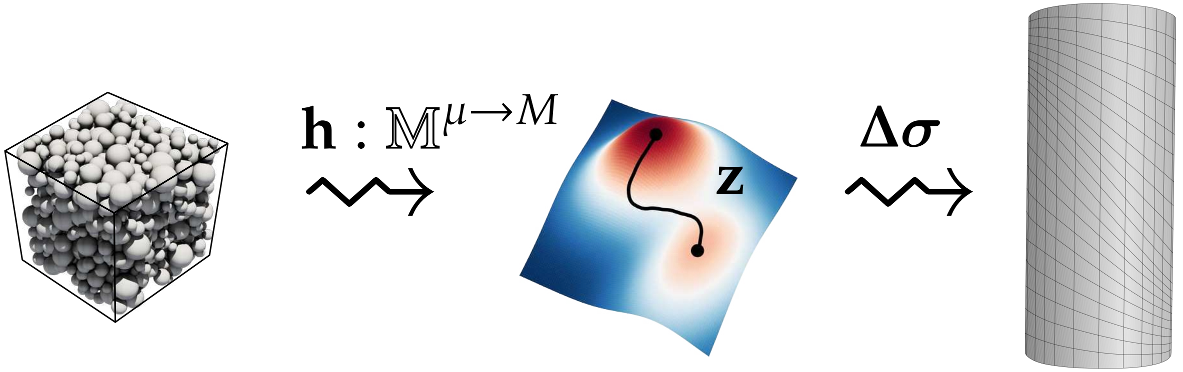
Thermodynamics- and data-driven scale bridging



Filippo Masi

Univ. Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK

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