5th workshop CSMA Junior

Mai 14th-16th 2022

Île de Porquerolles

Deep learning, real-time simulation and model-order reduction

Unraveling the mechanics of materials

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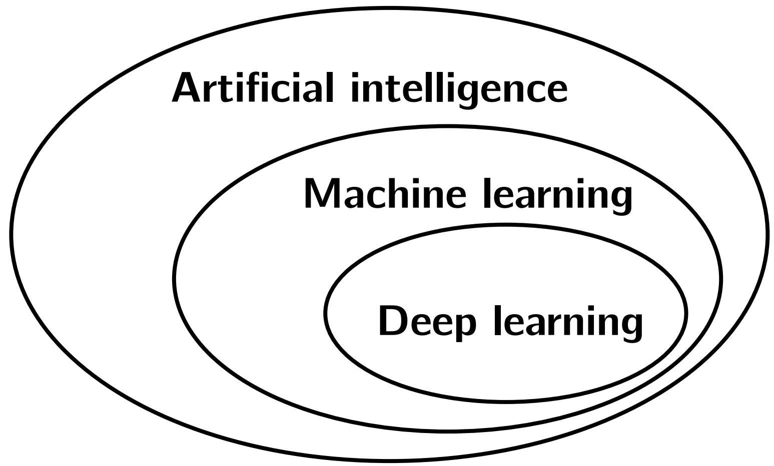
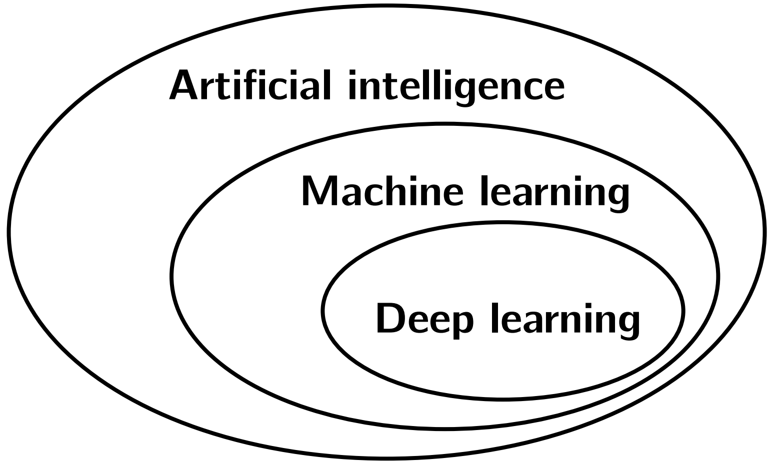
Artificial intelligence, machine learning, and deep learning

Neural Networks in a nutshell

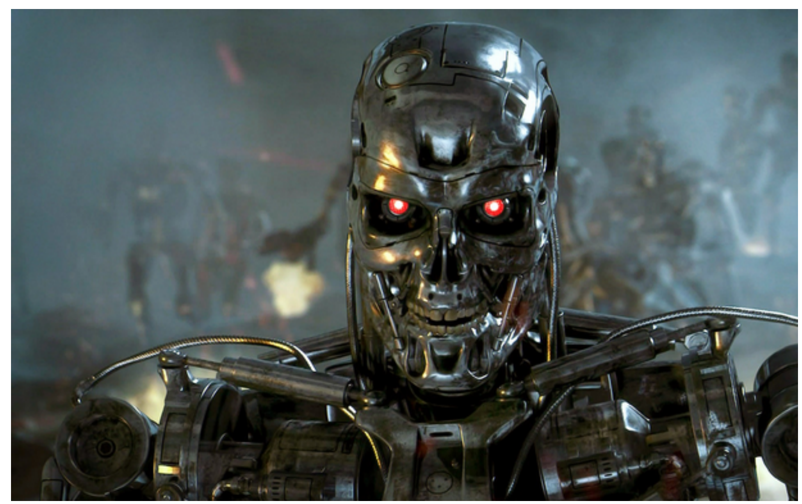


Neural Networks in a nutshell



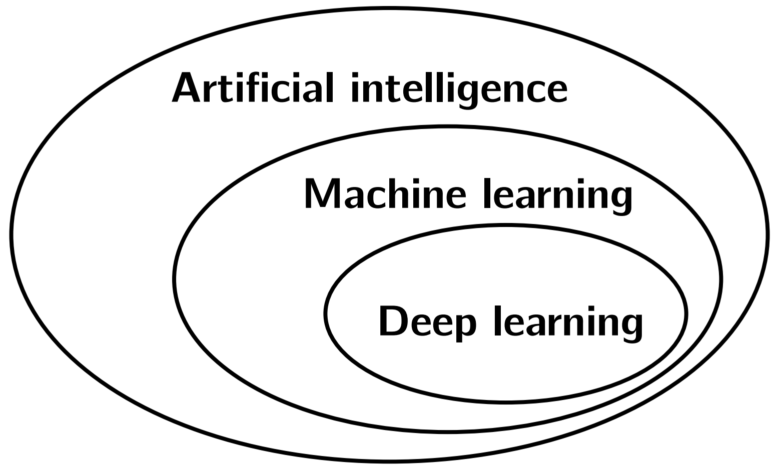
Artificial intelligence

automate intellectual tasks normally performed by humans



Terminator – Skynet

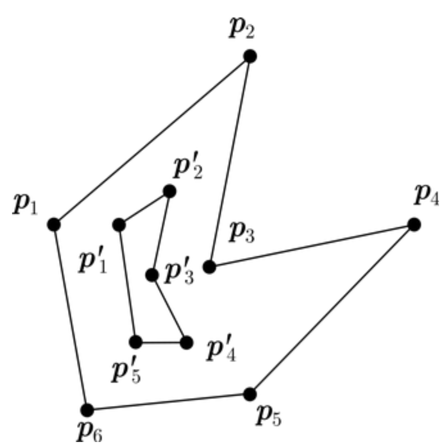
Neural Networks in a nutshell



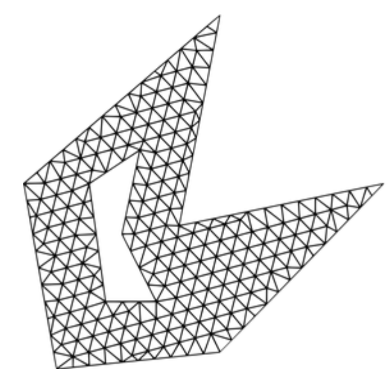
Machine learning

searching for useful representations and rules over some data

rules → *classical programming* → *answers*
data →



\+ ***rules*** →



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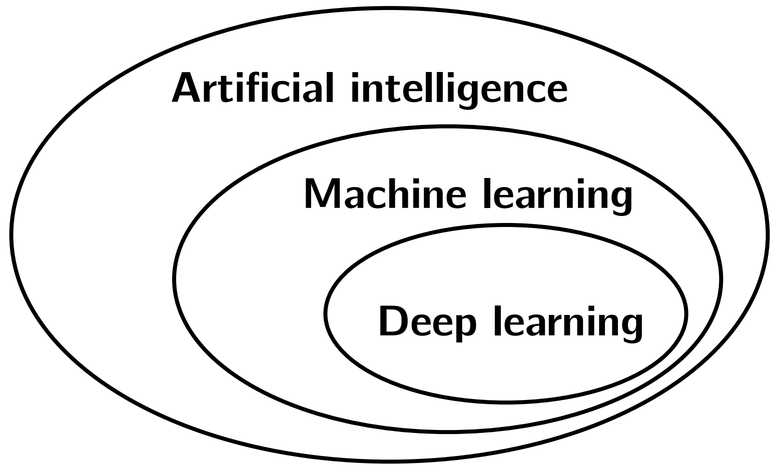

Machine learning

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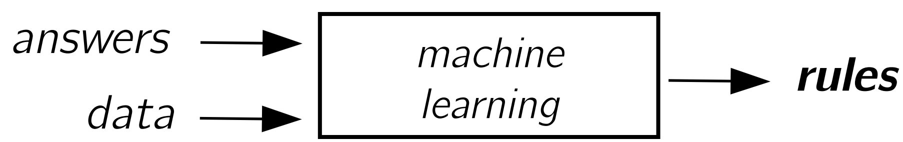
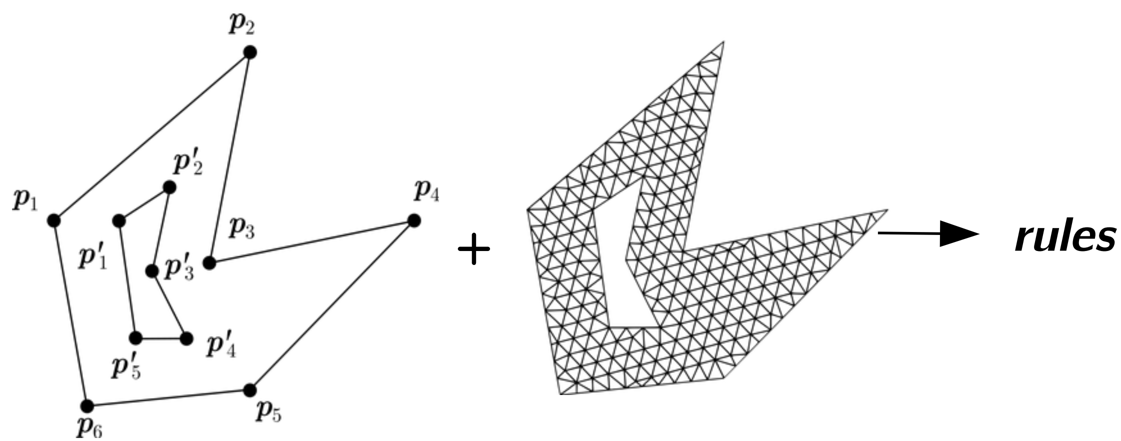
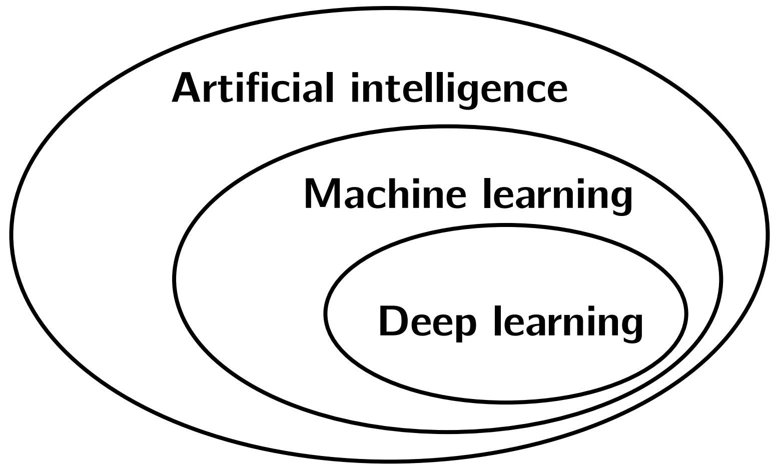


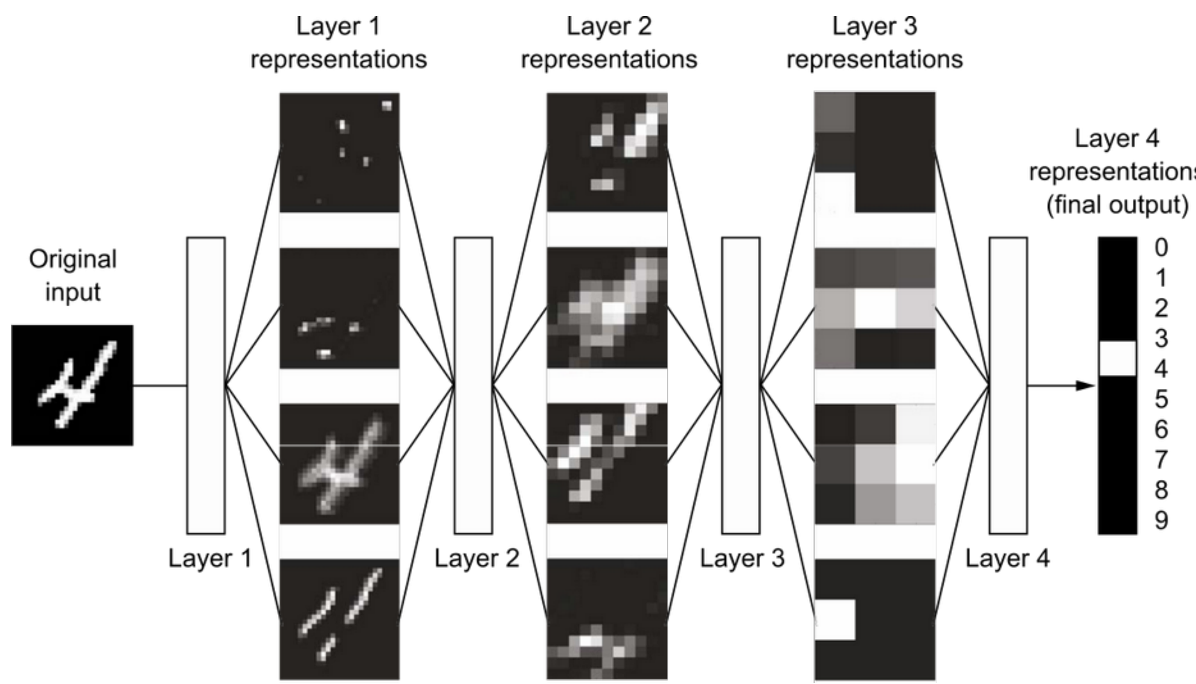


Neural Networks in a nutshell

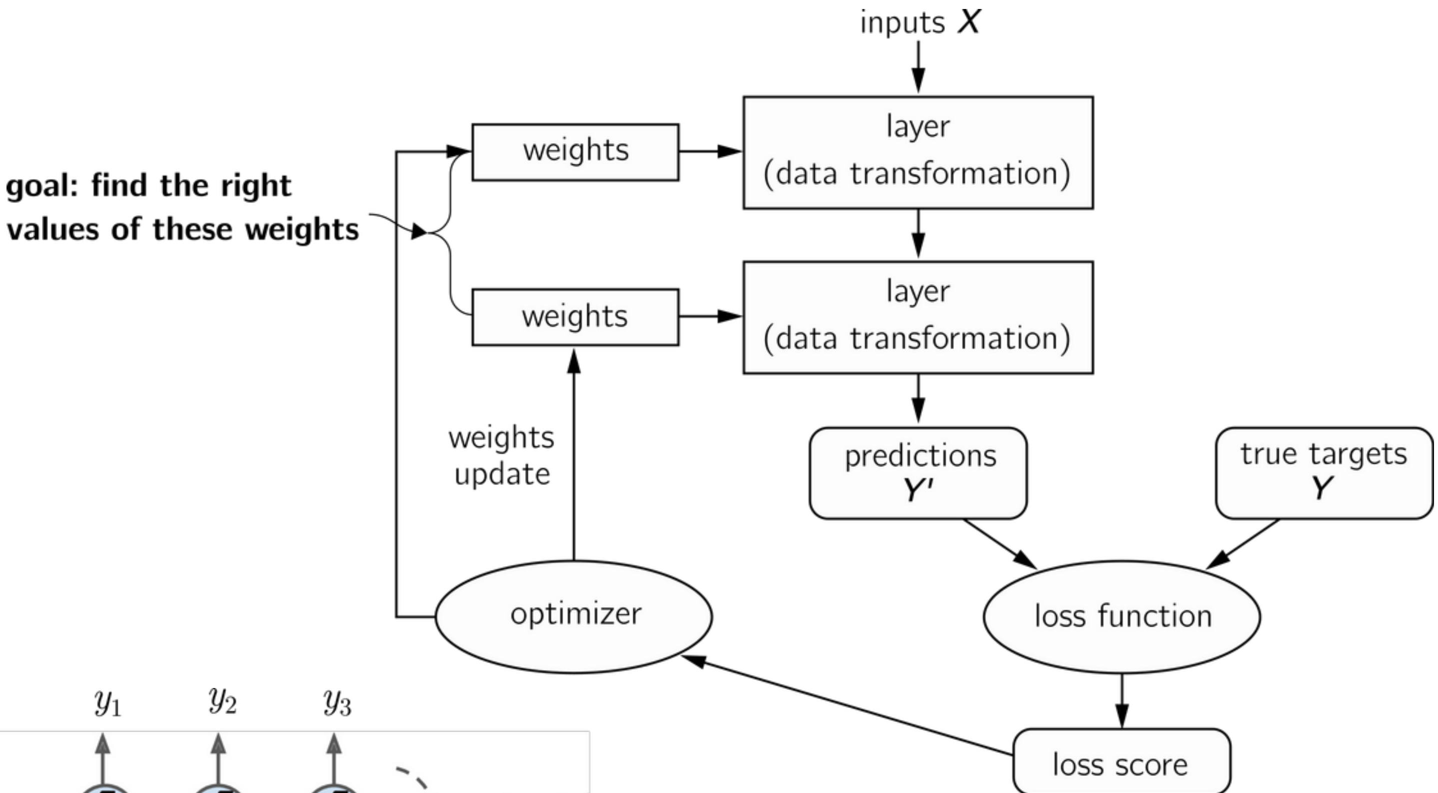


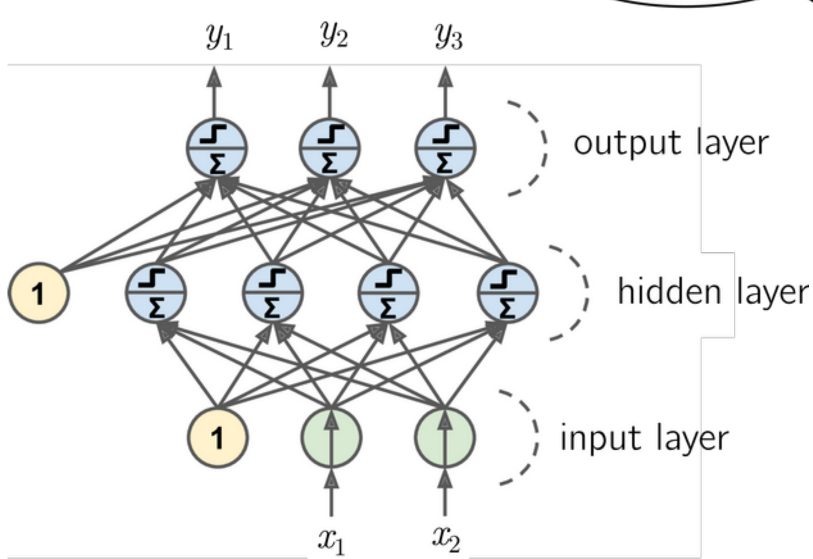
Deep learning

learning representations from data by learning successive layers of increasingly meaningful representations



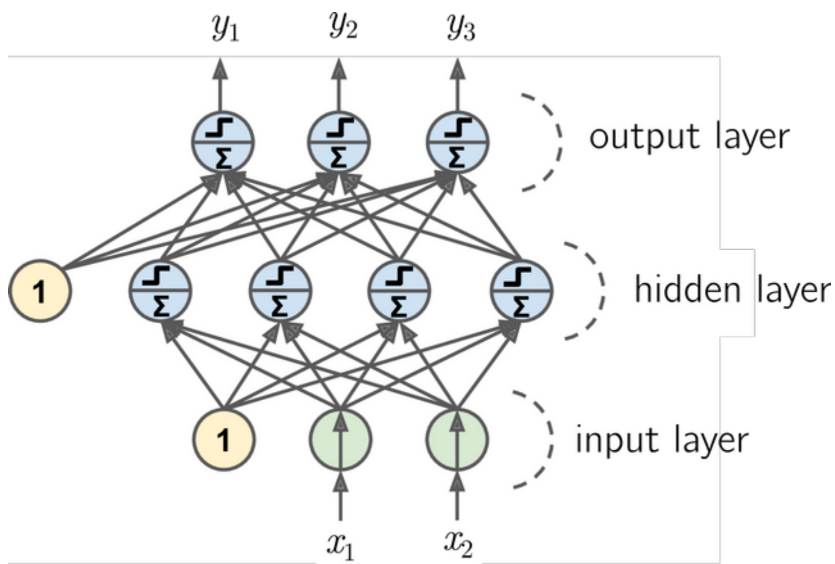
Neural Networks in a nutshell





Neural Networks in a nutshell

Multilayer perceptrons aka feed-forward neural networks



$$\underbrace{\boldsymbol{y}^{(k)}}_{\in\mathbb{R}^n} = \underbrace{\mathcal{A}^{(k)}}_{\text{activation}} \left(\underbrace{\boldsymbol{y}^{(k-1)^{\mathrm{T}}}}_{\in\mathbb{R}^m} \underbrace{\boldsymbol{W}^{(k)}}_{\in\mathbb{R}^{m\times n}} + \underbrace{\boldsymbol{b}^{(k)}}_{\in\mathbb{R}^n} \right)$$

inputs $\boldsymbol{x} \equiv \boldsymbol{y}^{(0)}$

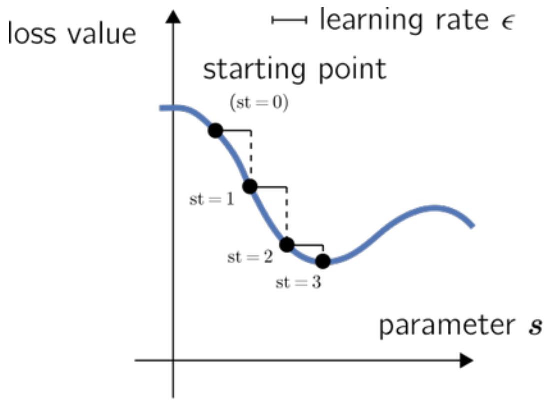
hyper-parameters

$$\boldsymbol{s} = \{\boldsymbol{W}^{(k)}, \boldsymbol{b}^{(k)}\} \quad \forall\, k \in [0, n]$$

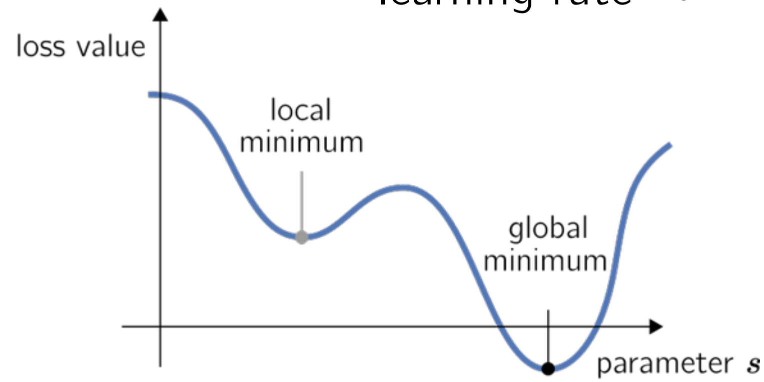
Neural Networks in a nutshell

Gradient descent

$$\boldsymbol{s}^{(\text{next step})} = \boldsymbol{s} - \epsilon \frac{\partial}{\partial \boldsymbol{s}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{s})$$

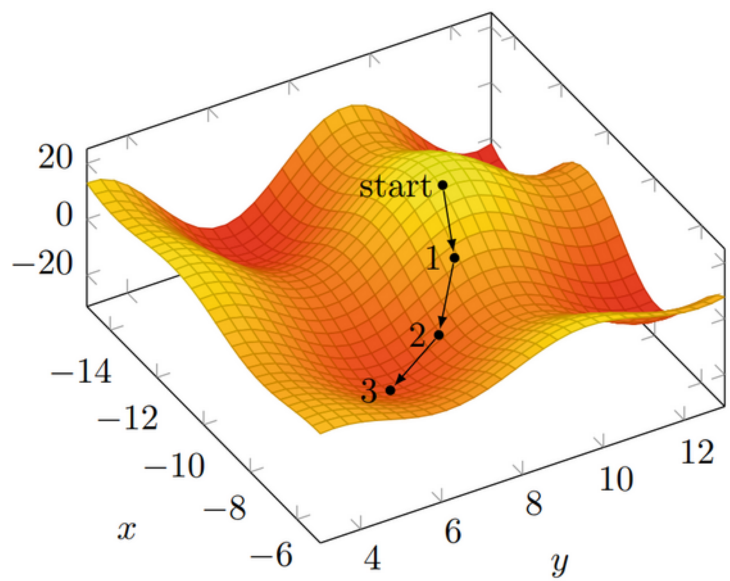


learning rate ϵ



loss function

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{s}) = \tfrac{1}{N} \sum_{i=1}^{M} \ell(\boldsymbol{o}^i, \bar{\boldsymbol{o}}^i)$$



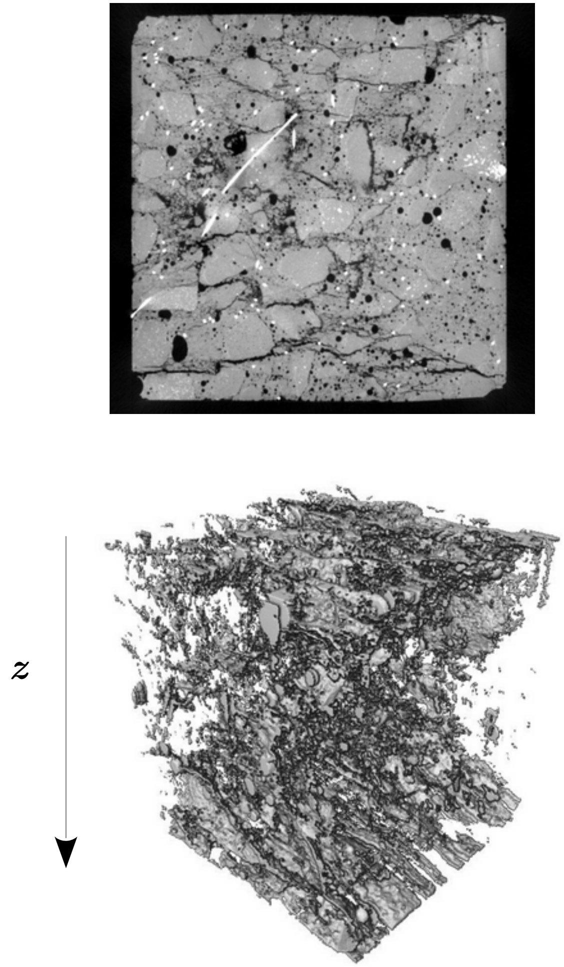
hyper-parameters

$$\arg\min_{\boldsymbol{s}} \left(\mathcal{L}(\boldsymbol{x}, \boldsymbol{s})\right)$$

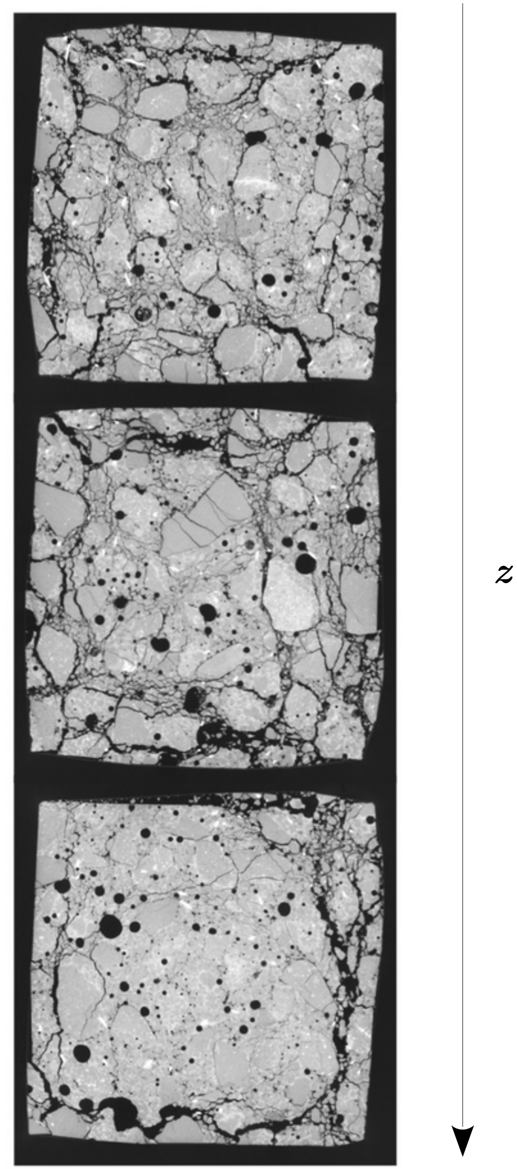
Deep learning

in mechanics of solids and structures

Complex materials



Fiber-reinforced concrete
CT and reconstruction

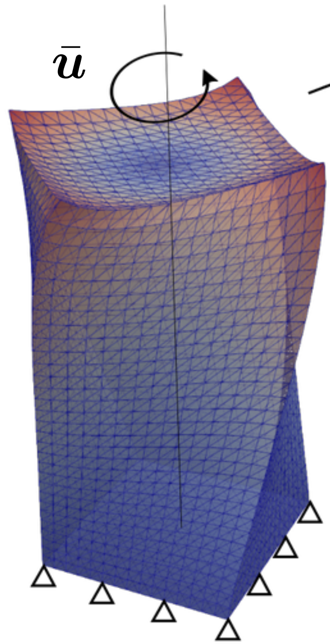


Vicente, et al, 2018

Bridging across the scales

Macro-scale

Boundary Value Problem (BVP)



$\boldsymbol{E}$

strain

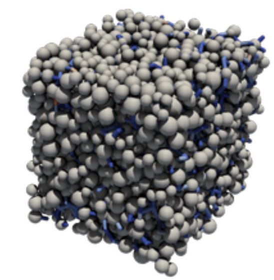
FE²
FEM×DEM
FEM×...

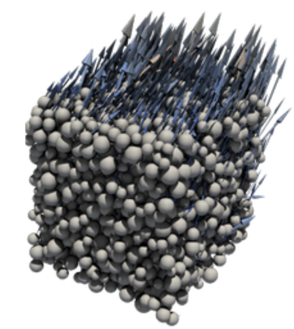
stress

$\boldsymbol{\Sigma}$

micro-scale

auxiliary problem





unit cell

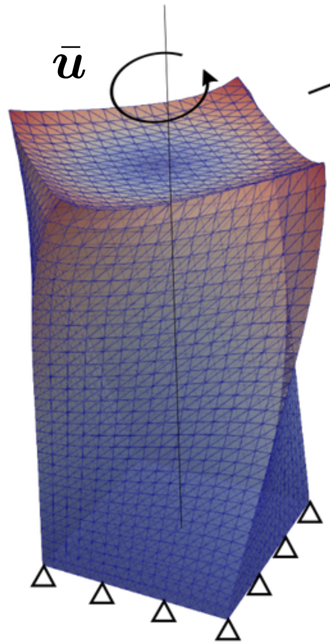
$$
\begin{cases}
\operatorname{div}\boldsymbol{\Sigma} + \boldsymbol{f} = 0 \quad \text{in } \mathcal{V} \\
\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \partial\mathcal{V}_u \\
\boldsymbol{\Sigma} \cdot n = \bar{\boldsymbol{t}} \quad \text{on } \partial\mathcal{V}_t \\
\boldsymbol{\Sigma} = \mathbb{C} : \boldsymbol{E}
\end{cases}
$$

Pinho-da Cruz et al, 2009
Geers et al, 2010
Lloberas Valls et al., 2019

Bridging across the scales

Macro-scale

Boundary Value
Problem (BVP)



$\boldsymbol{E}$

strain

FE²
FEM×DEM
FEM×...

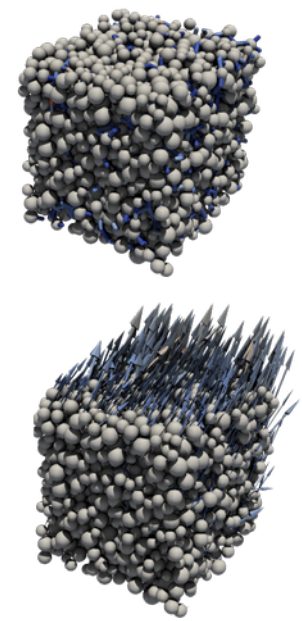
stress

$\boldsymbol{\Sigma}$

micro-scale

auxiliary problem

bottleneck
∀ point, time

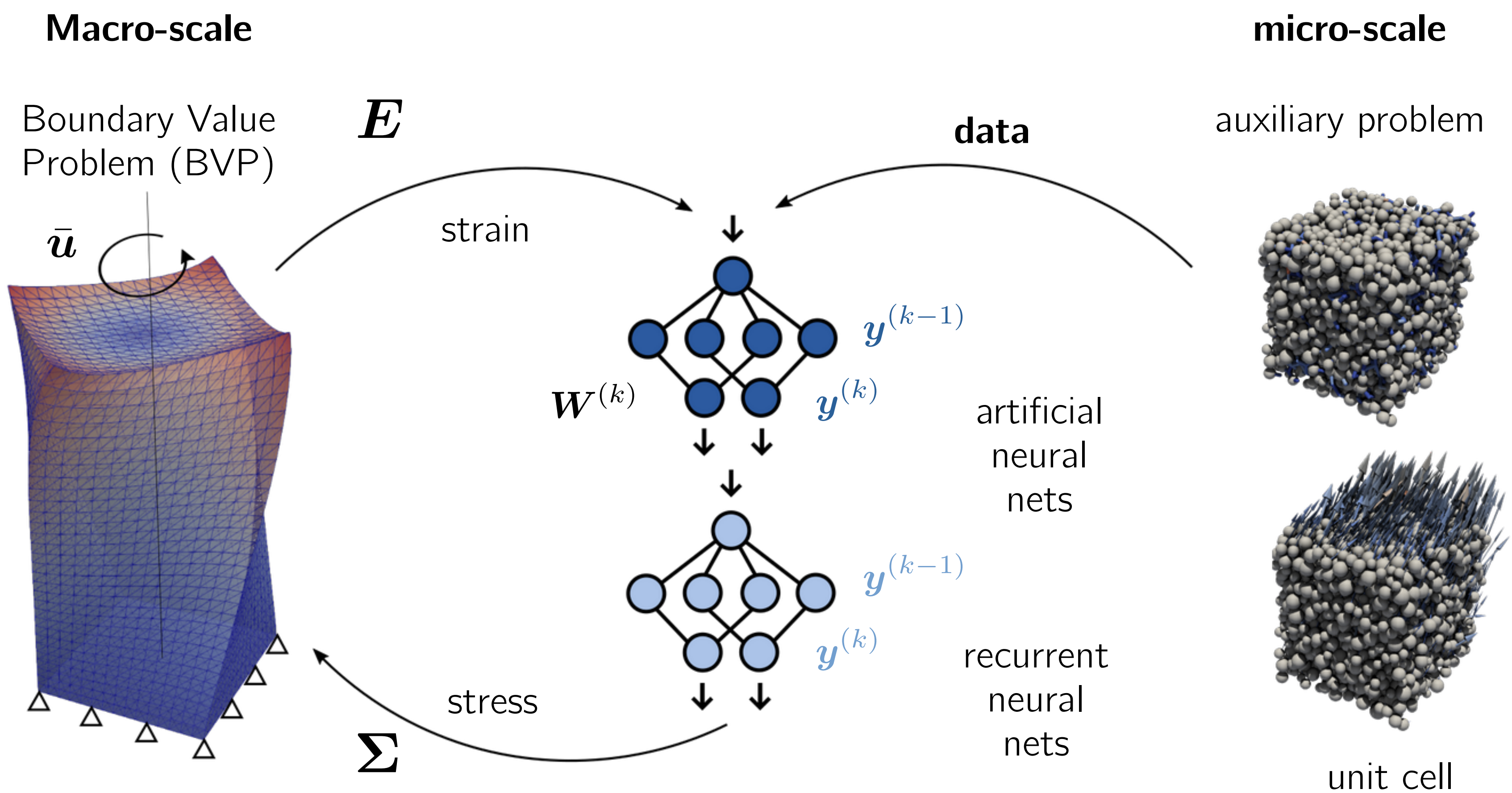


unit cell

$$\begin{cases} \operatorname{div} \boldsymbol{\Sigma} + \boldsymbol{f} = 0 \quad \text{in } \mathcal{V} \\ \boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \partial\mathcal{V}_u \\ \boldsymbol{\Sigma} \cdot n = \bar{\boldsymbol{t}} \quad \text{on } \partial\mathcal{V}_t \\ \boldsymbol{\Sigma} = \mathbb{C} : \boldsymbol{E} \end{cases}$$

Pinho-da Cruz et al, 2009
Geers et al, 2010
Lloberas Valls et al., 2019

Bridging across the scales



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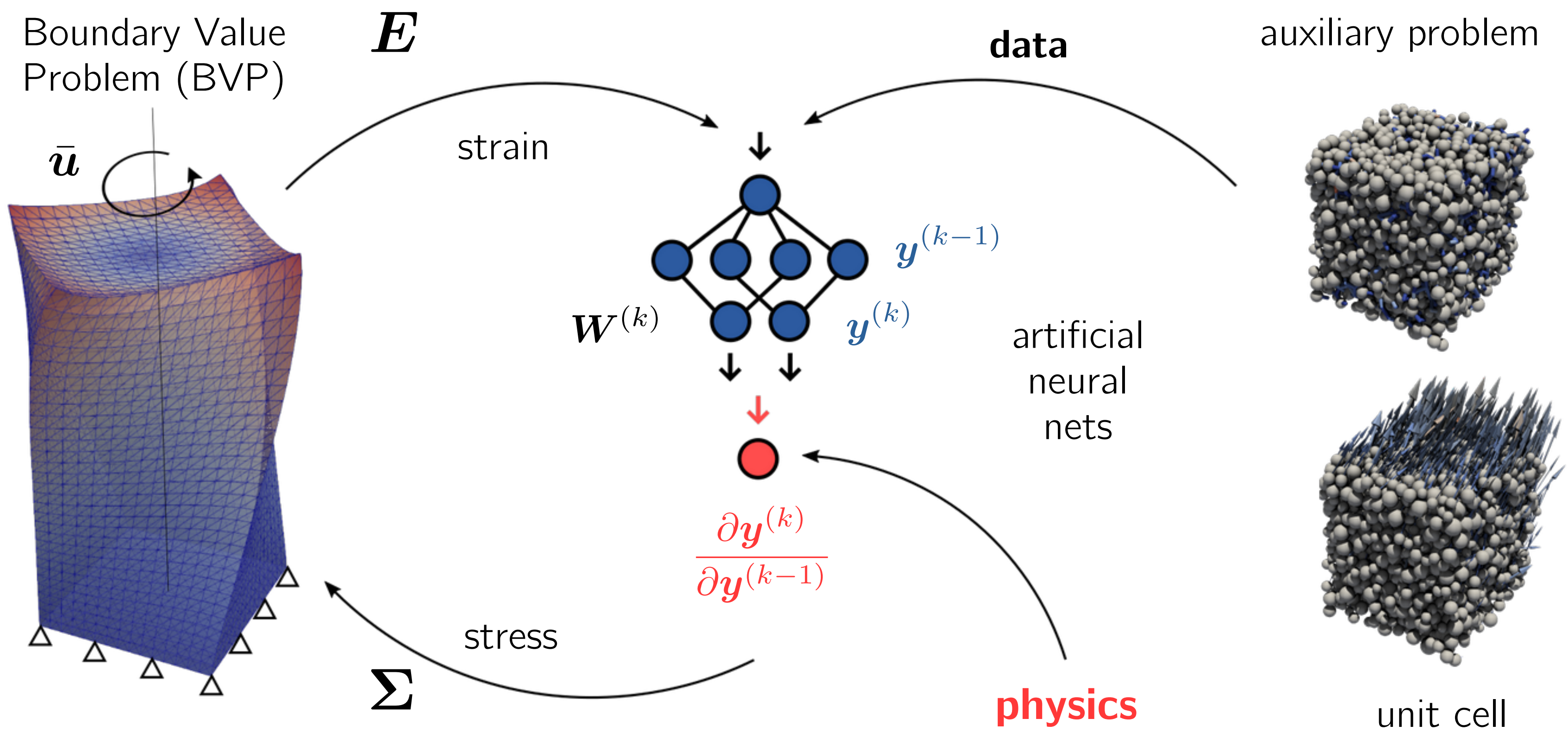
Ghaboussi et al, 1991
Lefik and Schrefler, 2003
Mozaffar et al, 2019
Mianroodi et al, 2021

Bridging across the scales

Macro-scale **micro-scale**



$$\begin{cases} \operatorname{div} \boldsymbol{\Sigma} + \boldsymbol{f} = 0 \quad \text{in } \mathcal{V} \\ \boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \partial\mathcal{V}_u \\ \boldsymbol{\Sigma} \cdot n = \bar{\boldsymbol{t}} \quad \text{on } \partial\mathcal{V}_t \\ \boldsymbol{\Sigma} = \mathbb{C} : \boldsymbol{E} \end{cases}$$

PINN Karniadakis et al, 2019
SPNN Hernandez et al, 2021

Thermodynamics-based ANN (TANN) Masi et al, 2021

Theoretical setting

Thermodynamics

Thermodynamics

Consider a solid with reference configuration $\mathcal{B}$

$$\underbrace{\dot{e}}_{\substack{\text{int. energy}\\ \text{rate}}} = \underbrace{\boldsymbol{P}}_{\substack{\text{1st Piola-}\\ \text{Kirchoff stress}}} : \underbrace{\dot{\boldsymbol{F}}}_{\substack{\text{def. grad.}\\ \text{rate}}} - \nabla \cdot \underbrace{\boldsymbol{q}}_{\substack{\text{heat}\\ \text{flux}}} + \underbrace{r}_{\substack{\text{heat}\\ \text{source}}}$$

$$\underbrace{\gamma}_{\substack{\text{entropy}\\ \text{product. rate}}} = \underbrace{\dot{\eta}}_{\substack{\text{entropy}\\ \text{rate}}} - \nabla \cdot \left(\frac{\boldsymbol{q}}{\theta}\right) - \frac{r}{\theta} \geq 0$$

Coleman and Gurtin, 1967

Thermodynamics

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Coleman and Gurtin, 1967

Clausius-Duhem inequality $\quad \gamma = \boldsymbol{P} : \dot{\boldsymbol{F}} - \left(\dot{\psi} + \eta\dot{\theta}\right) - \boldsymbol{q} \cdot \frac{\nabla\theta}{\theta} \geq 0$

Thermodynamics

Consider a solid with reference configuration $\mathcal{B}$

$$\underbrace{\dot{e}}_{\substack{\text{int. energy}\\ \text{rate}}} = \underbrace{\boldsymbol{P}}_{\substack{\text{1st Piola-}\\ \text{Kirchoff stress}}} : \underbrace{\dot{\boldsymbol{F}}}_{\substack{\text{def. grad.}\\ \text{rate}}} - \nabla \cdot \underbrace{\boldsymbol{q}}_{\substack{\text{heat}\\ \text{flux}}} + \underbrace{r}_{\substack{\text{heat}\\ \text{source}}}$$

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$$d = \boldsymbol{P} : \dot{\boldsymbol{F}} - \left(\dot{\psi} + \eta\dot{\theta}\right) \geq 0$$

Thermodynamics

Consider a solid with reference configuration $\mathcal{B}$

$$\underbrace{\dot{e}}_{\text{int. energy rate}} = \underbrace{\boldsymbol{P}}_{\text{1st Piola-Kirchoff stress}} : \underbrace{\dot{\boldsymbol{F}}}_{\text{def. grad. rate}} - \nabla \cdot \underbrace{\boldsymbol{q}}_{\text{heat flux}} + \underbrace{r}_{\text{heat source}}$$

$$\underbrace{\gamma}_{\text{entropy product. rate}} = \underbrace{\dot{\eta}}_{\text{entropy rate}} - \nabla \cdot \left(\frac{\boldsymbol{q}}{\theta}\right) - \frac{r}{\theta} \geq 0$$

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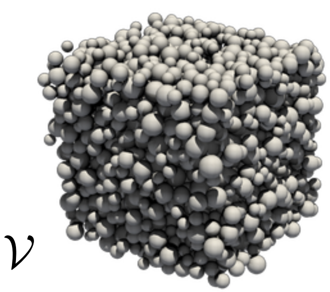
$$d = \boldsymbol{P} : \dot{\boldsymbol{F}} - \left(\dot{\psi} + \eta\dot{\theta}\right) \geq 0$$

Volume average

$$d^{(Y)} = \boldsymbol{P}^{(Y)} : \dot{\boldsymbol{F}}^{(Y)} - \left(\dot{\psi}^{(Y)} + \eta^{(Y)}\dot{\theta}^{(Y)}\right) \geq 0$$

volume average operator: $\quad \psi^{(Y)} = \langle\, \psi \,\rangle = \frac{1}{|\mathcal{V}|}\int_{\mathcal{V}} \psi \, dy$



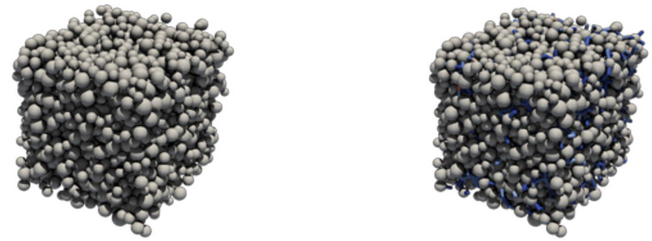
$\mathcal{V}$

unit cell

Thermodynamics

State functions and variables

$$\psi = \hat{\psi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$$



$\boldsymbol{z}$ **internal state variables**
internal material structure and mechanisms

evolution equations

$$\dot{\boldsymbol{z}} = f\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$$

Coleman and Gurtin, 1967

Thermodynamics

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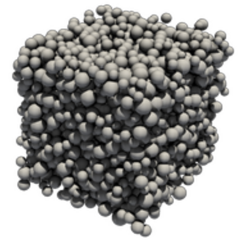

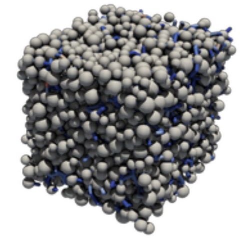

$\boldsymbol{z}$ internal state variables
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$$\dot{\boldsymbol{z}} = f\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$$

Coleman and Gurtin, 1967

Time differentiation

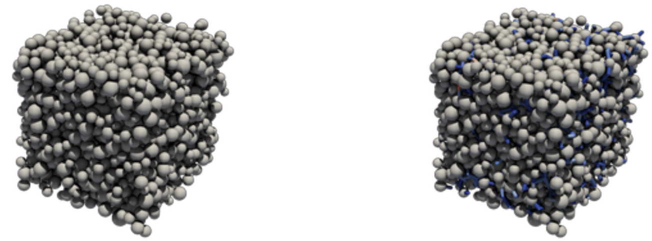
$$\dot{\psi} = \left(\partial_{\boldsymbol{F}}\hat{\psi}\right) \cdot \dot{\boldsymbol{F}} + \left(\partial_{\theta}\hat{\psi}\right)\dot{\theta} + \left(\partial_{\boldsymbol{z}}\hat{\psi}\right) \cdot \dot{\boldsymbol{z}}$$

$$\partial_{\boldsymbol{z}}\hat{\psi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right) = \frac{\partial\hat{\psi}}{\partial\boldsymbol{z}}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$$

Thermodynamics

State functions and variables

$$\psi = \hat{\psi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$$



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$$\partial_{\boldsymbol{z}}\hat{\psi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right) = \frac{\partial\hat{\psi}}{\partial\boldsymbol{z}}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$$

Thermodynamic admissible processes

stress function $\quad \boldsymbol{P} = \partial_{\boldsymbol{F}}\hat{\psi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$

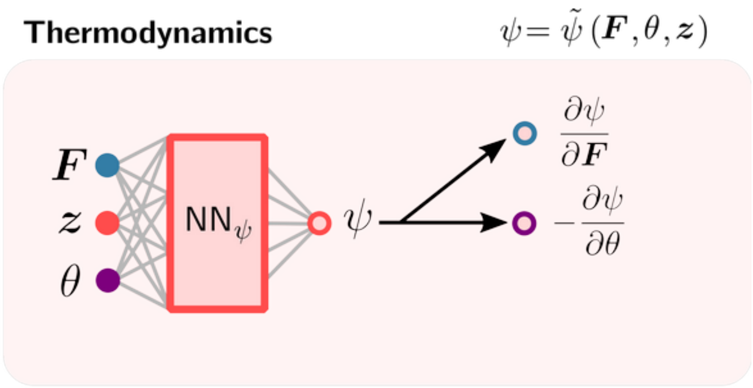
entropy function $\quad \eta = -\partial_{\theta}\hat{\psi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$

internal dissipation rate $\quad d = \boldsymbol{\Pi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)\cdot\dot{\boldsymbol{z}} \geq 0$

$$\boldsymbol{\Pi} \equiv -\partial_{\boldsymbol{z}}\hat{\psi}\left(\boldsymbol{F}, \theta, \boldsymbol{z}\right)$$

Thermodynamics-based Artificial Neural Networks

Thermodynamics-based Artificial Neural Nets



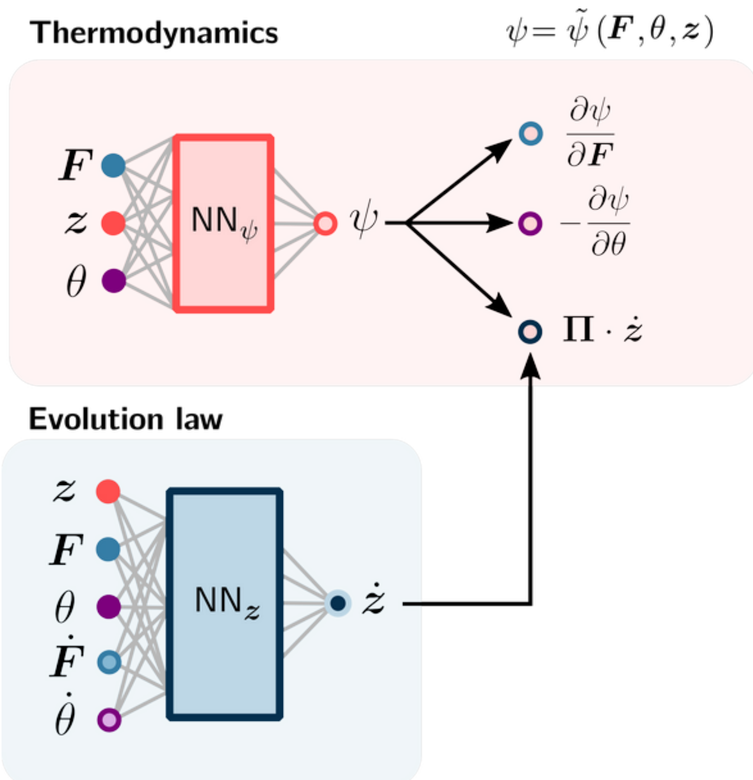
Masi et al, 2021. Thermodynamics-based artificial neural networks for constitutive modeling. JMPS

Minimize

$$\underbrace{\underbrace{\|\psi - \mathsf{NN}_\psi\|}_{\text{loss in } \psi} + \underbrace{\|\boldsymbol{P} - \partial_{\boldsymbol{F}} \mathsf{NN}_\psi\|}_{\text{loss in } \boldsymbol{P}} + \underbrace{\|\eta + \partial_\theta \mathsf{NN}_\psi\|}_{\text{loss in } \eta}}_{1^{\text{st}} \text{ principle}}$$

Thermodynamics-based Artificial Neural Nets

Masi et al, 2021. Thermodynamics-based artificial neural networks for constitutive modeling. JMPS



$\dot{\boldsymbol{z}} = f(\boldsymbol{F}, \theta, \boldsymbol{z})$

negative ramp function $[x]^- = \min(x, 0)$

Minimize

$$\underbrace{\underbrace{\|\psi - \mathsf{NN}_\psi\|}_{\text{loss in } \psi} + \underbrace{\|\boldsymbol{P} - \partial_{\boldsymbol{F}} \mathsf{NN}_\psi\|}_{\text{loss in } \boldsymbol{P}} + \underbrace{\|\eta + \partial_\theta \mathsf{NN}_\psi\|}_{\text{loss in } \eta} + \underbrace{\|d + \partial_{\boldsymbol{z}} \mathsf{NN}_\psi \cdot \dot{\boldsymbol{z}}\|}_{\text{loss in } D}}_{1^{\text{st}} \text{ principle}} + \underbrace{\left\| [-\nabla_{\boldsymbol{z}} \mathsf{NN}_\psi \cdot \dot{\boldsymbol{z}})]^- \right\|}_{2^{\text{nd}} \text{ principle}}$$

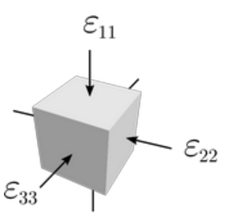
TANN – Application to homogeneous materials

TANN – Application to homogeneous materials

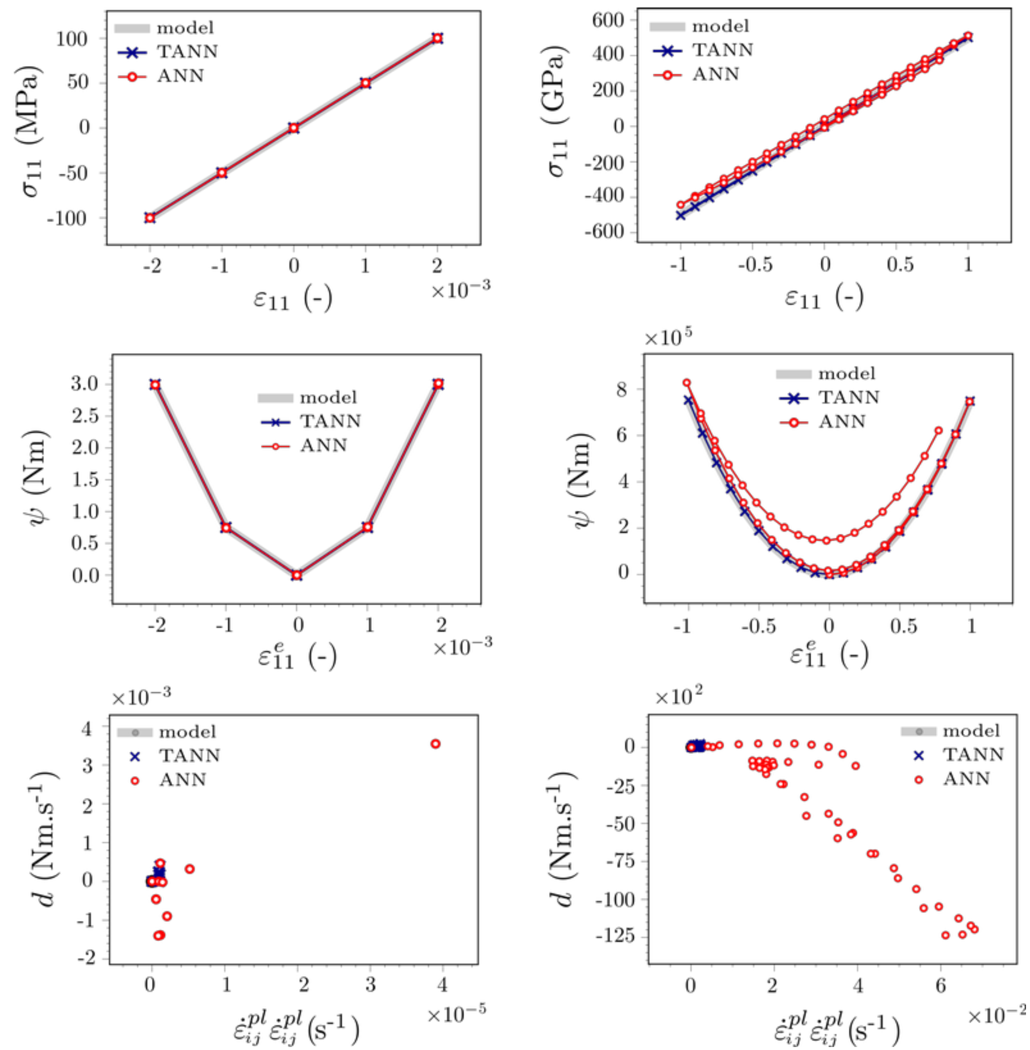
Hyperplasticity

close to the training domain | far from the training domain

Isotropic
(von Mises)

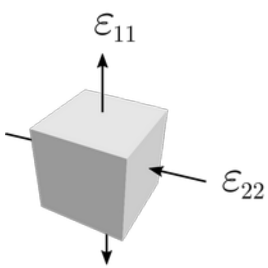


PRACTICAL SESSION



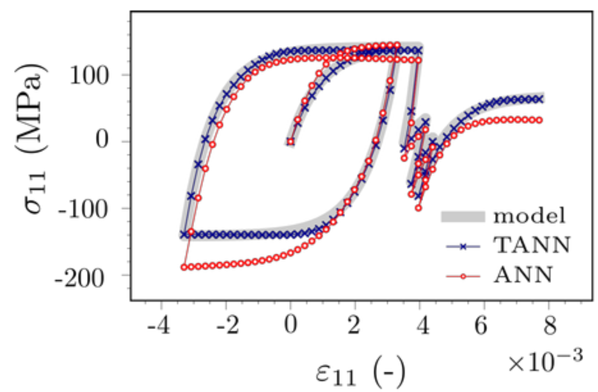
TANN – Application to homogeneous materials

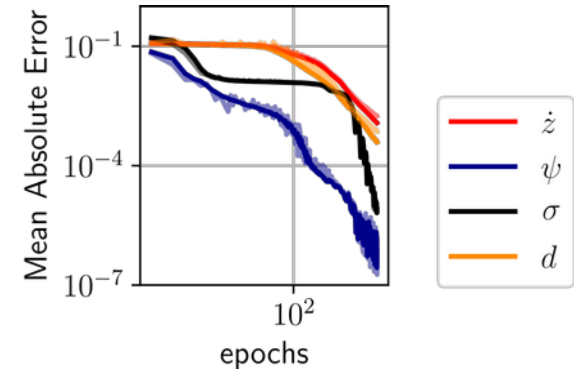
Hypoplasticity

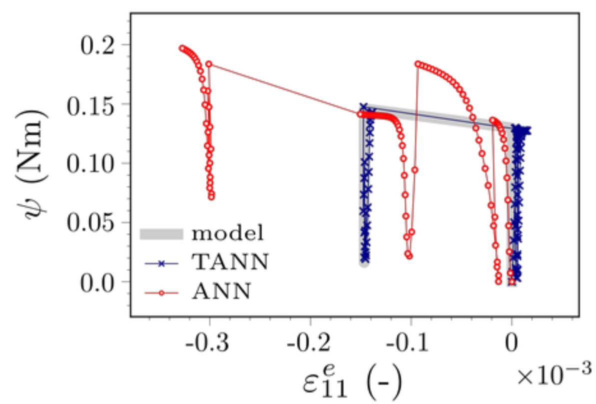


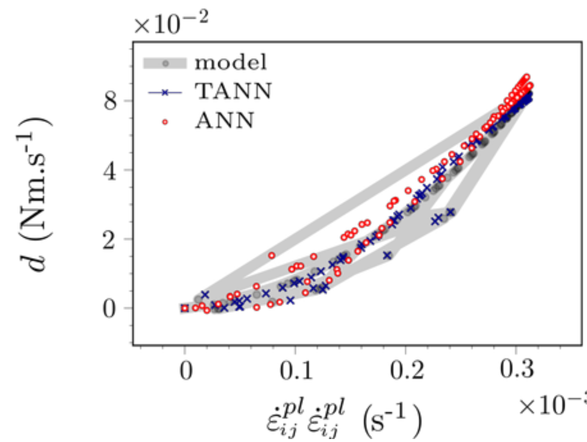
biaxial
strain-ratcheting
(von Mises)

PRACTICAL SESSION



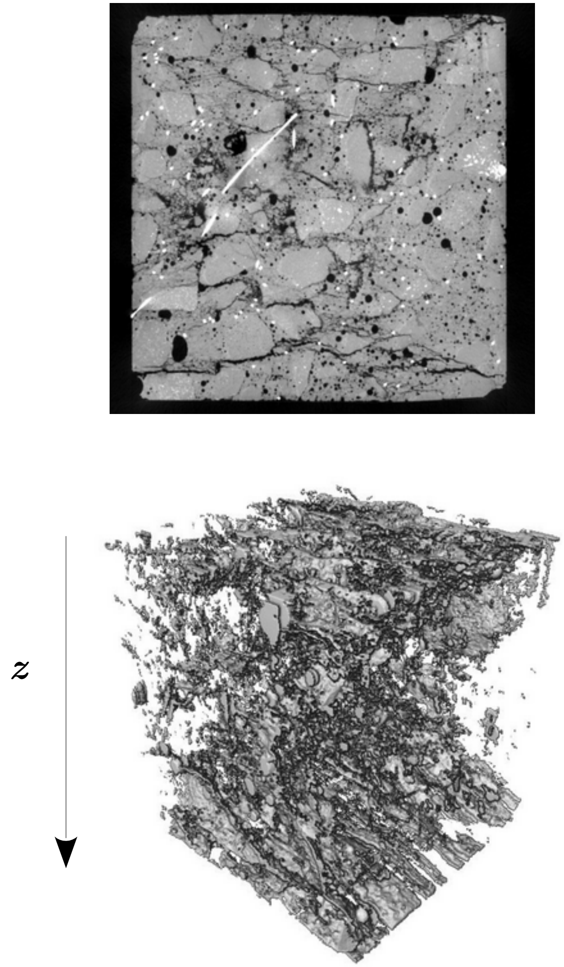




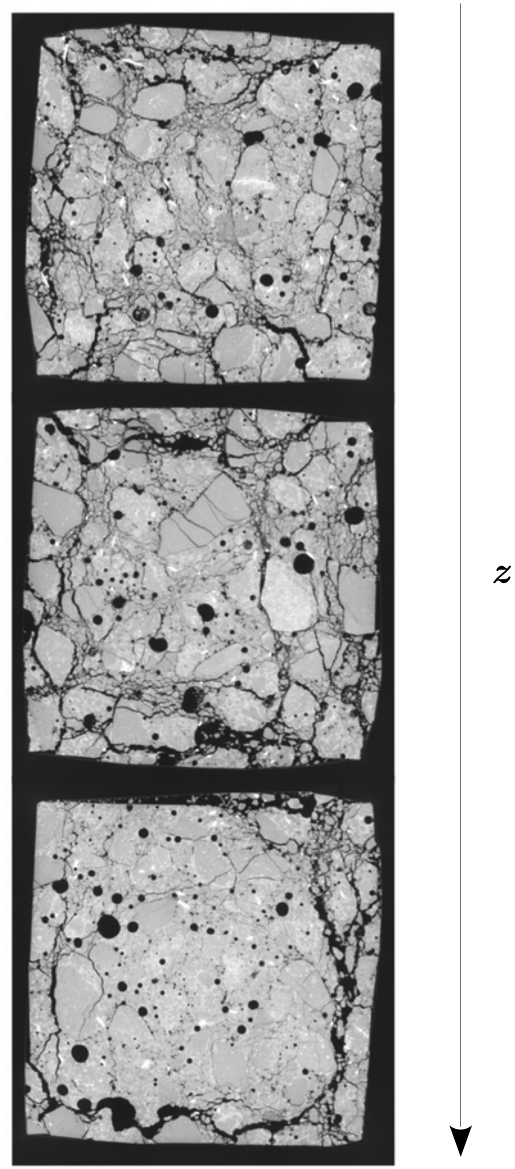


Internal variables discovery

The quest for internal variables



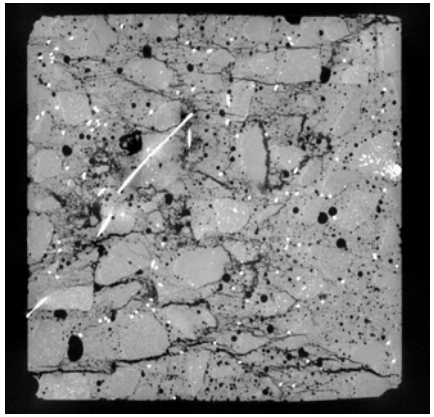
Fiber-reinforced concrete
CT and reconstruction



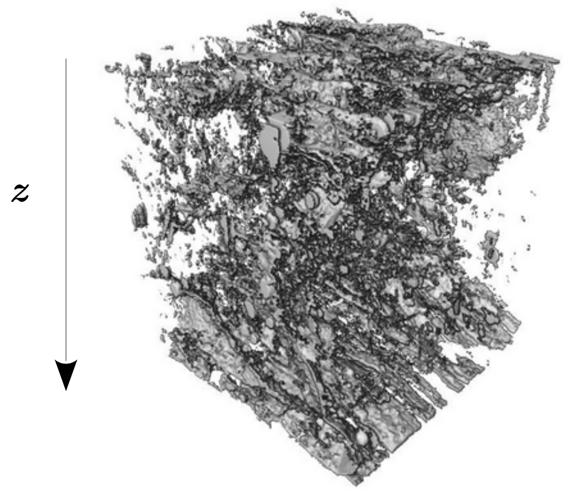
Vicente, et al, 2018

The quest for internal variables

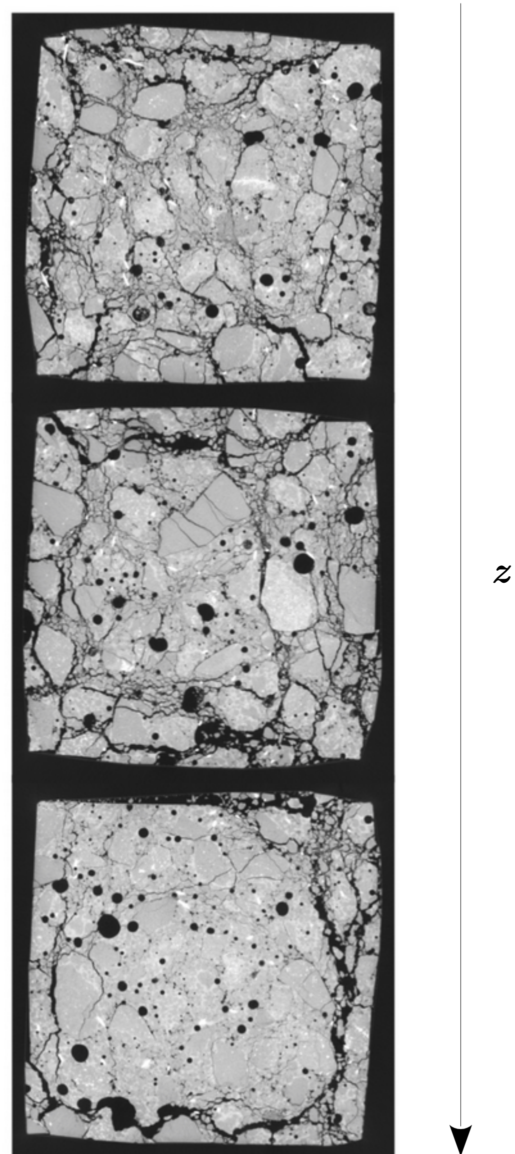
porosity?



damage?



Fiber-reinforced concrete
CT and reconstruction



grain size distribution?

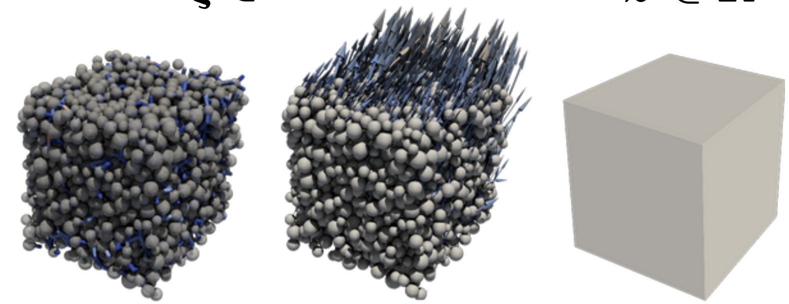
Vicente, et al, 2018

From internal coordinates

Def. **Internal coordinates**

all those microscopic quantities describing internal mechanisms

$\boldsymbol{\xi} \in \mathbb{R}^m$ $\quad$ $\boldsymbol{z} \in \mathbb{R}^M$



$m \gg M$

micro $\quad$ macro

Masi et al, 2021. TANN for multiscale modeling of materials with inelastic microstructure

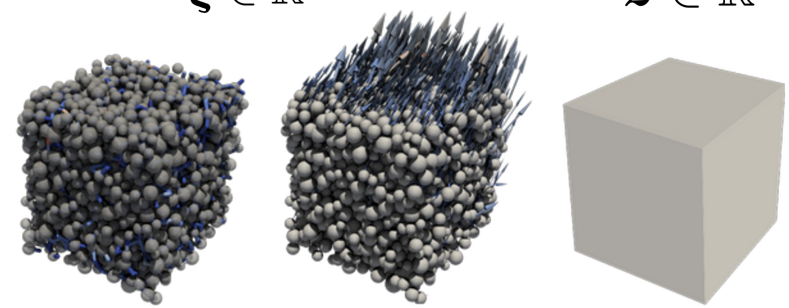
From internal coordinates ... to internal variables

Def. **Internal coordinates**

all those microscopic quantities describing internal mechanisms

Masi et al, 2021. TANN for multiscale modeling of materials with inelastic microstructure

$\boldsymbol{\xi} \in \mathbb{R}^m$ $\qquad$ $\boldsymbol{z} \in \mathbb{R}^M$

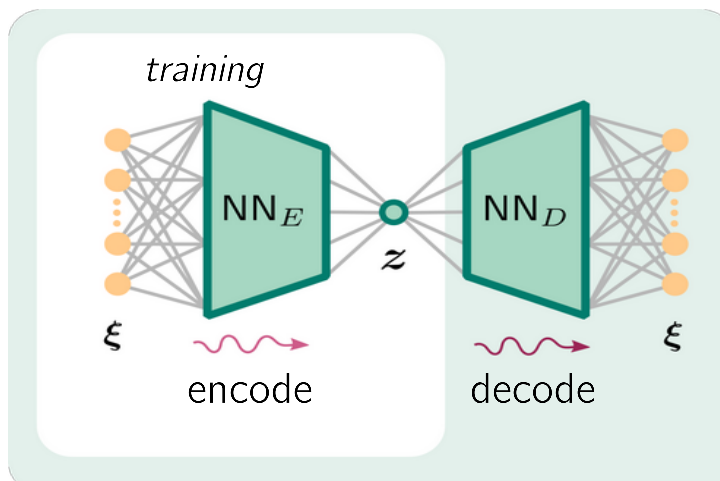


$m \gg M$

micro $\qquad$ macro

Reduced order models

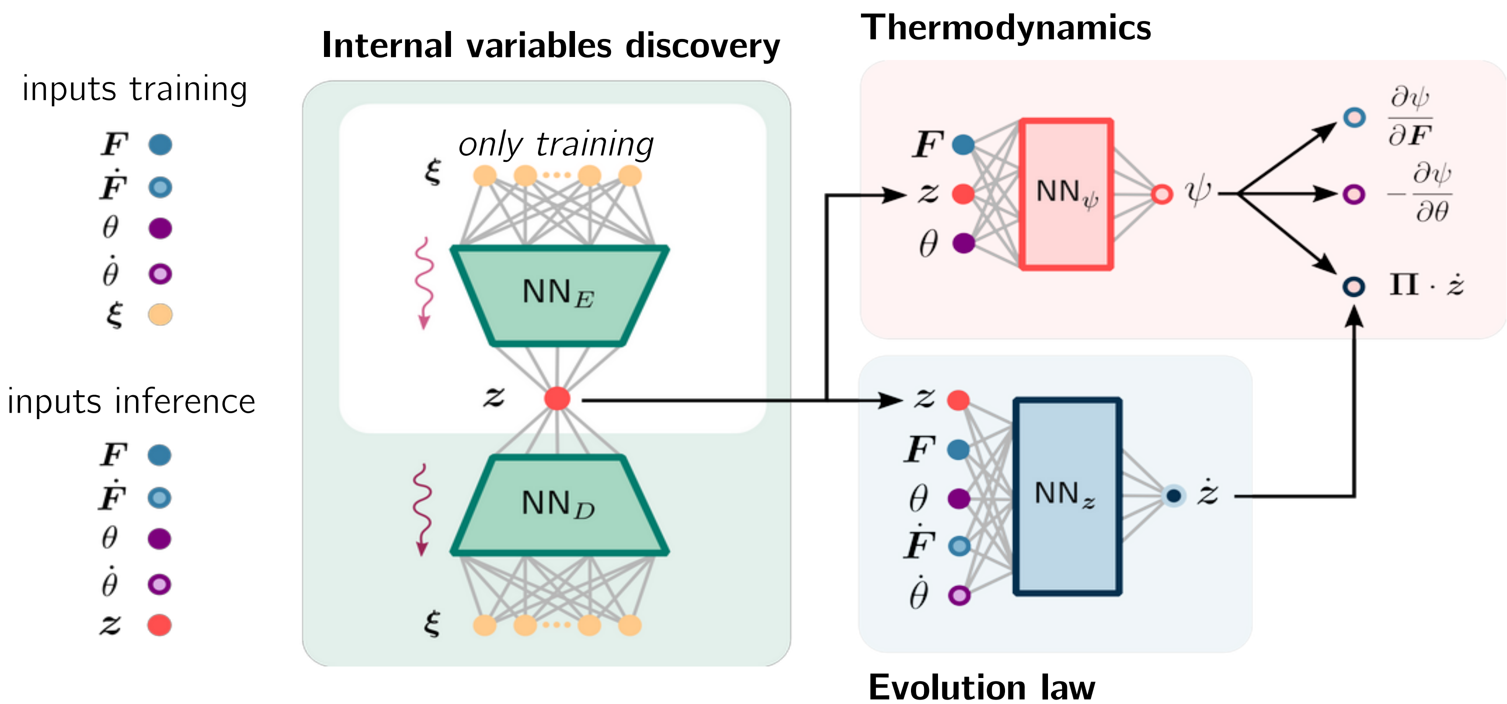
- Principal component analysis
- Proper orthogonal decomposition
- Auto-encoders



Minimize

$$\underbrace{\|\boldsymbol{\xi} - \mathsf{NN}_D(\boldsymbol{z})\|}_{\text{reconstruction loss}}$$

TANN and internal variables



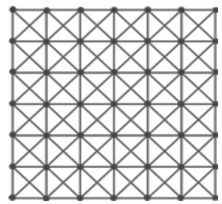
Minimize

$$\underbrace{\|\boldsymbol{\xi} - \mathsf{NN}_D(\boldsymbol{z})\|}_{\text{reconstruction loss}} + \underbrace{\underbrace{\|\psi - \mathsf{NN}_\psi\|}_{\text{loss in } \psi} + \underbrace{\|\boldsymbol{P} - \partial_{\boldsymbol{F}} \mathsf{NN}_\psi\|}_{\text{loss in } \boldsymbol{P}} + \underbrace{\|\eta + \partial_\theta \mathsf{NN}_\psi\|}_{\text{loss in } \eta} + \underbrace{\|d + \partial_{\boldsymbol{z}} \mathsf{NN}_\psi \cdot \dot{\boldsymbol{z}}\|}_{\text{loss in } D}}_{1^{\text{st}} \text{ principle}} + \underbrace{\left\| [-\nabla_{\boldsymbol{z}} \mathsf{NN}_\psi \cdot \dot{\boldsymbol{z}})]^- \right\|}_{2^{\text{nd}} \text{ principle}}$$

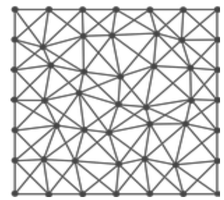
Applications at the material point level

Lattice structures

Masi et al, 2021. TANN for multiscale modeling of materials with inelastic microstructure

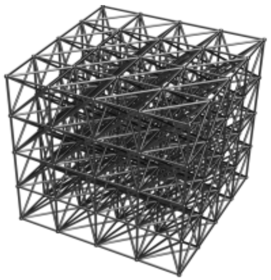


2D regular



2D irregular

3D cell

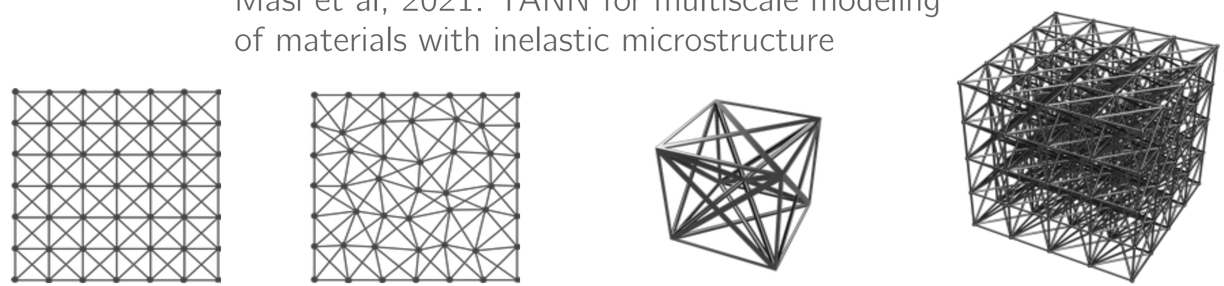


3D regular

Applications at the material point level

Lattice structures

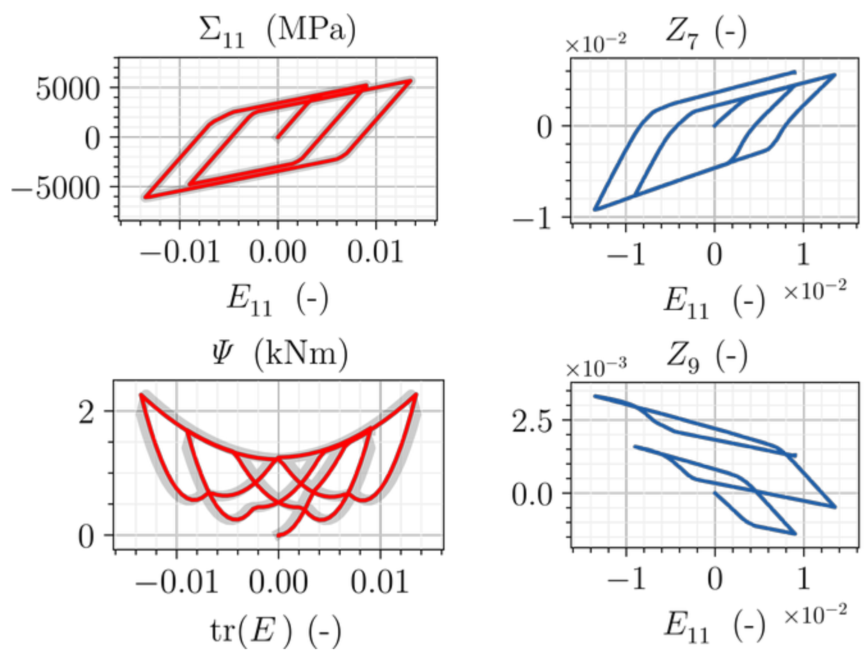
Masi et al, 2021. TANN for multiscale modeling of materials with inelastic microstructure



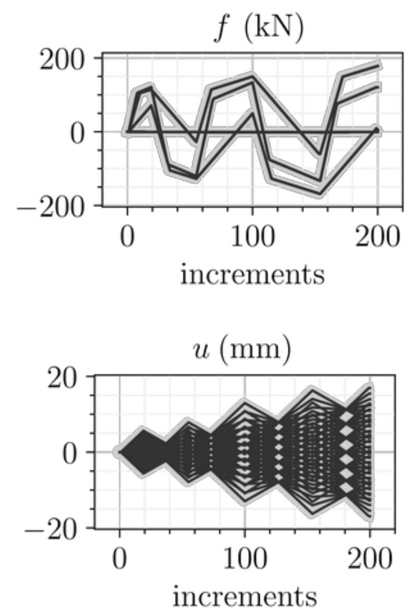
2D regular 2D irregular 3D cell 3D regular

Inference

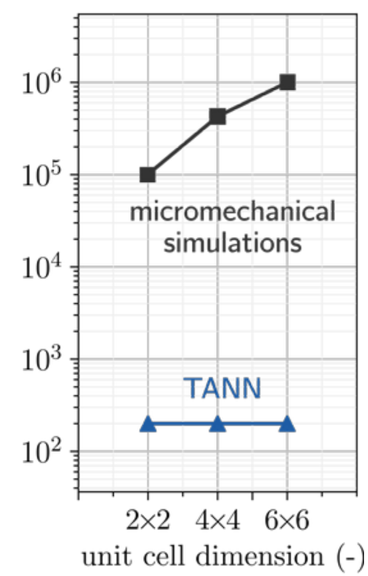
average response



microscopic state



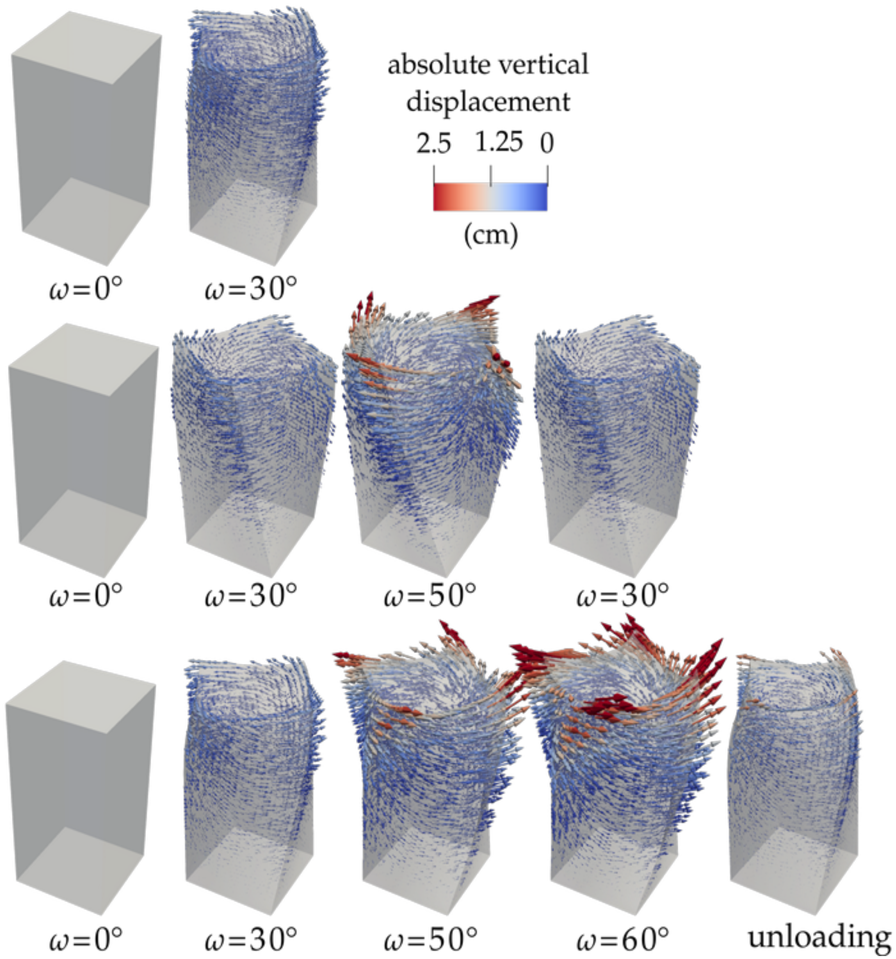
acceleration $\times10^3$



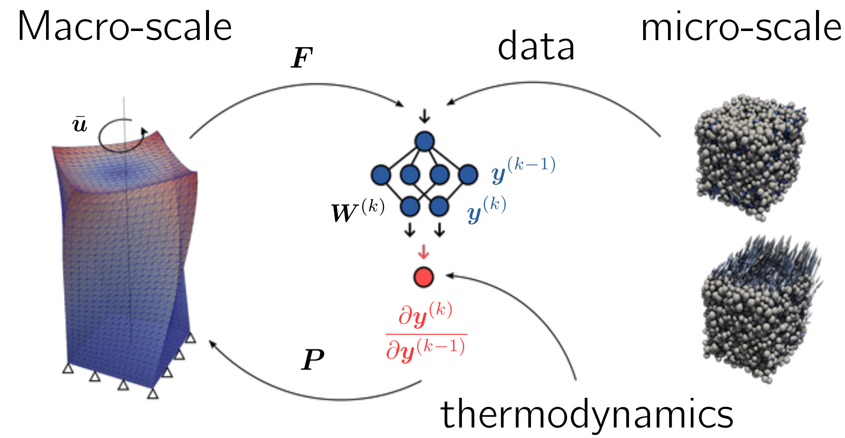
Multiscale simulations – FEM×TANN

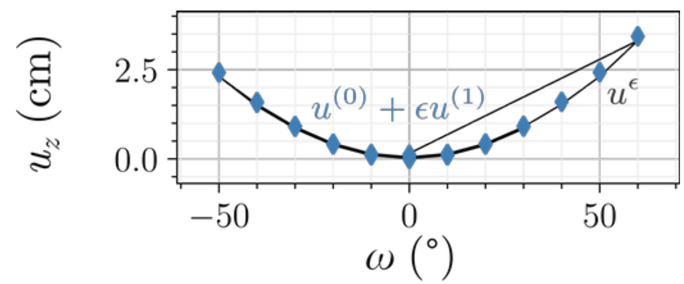
Applications to multiscale simulations

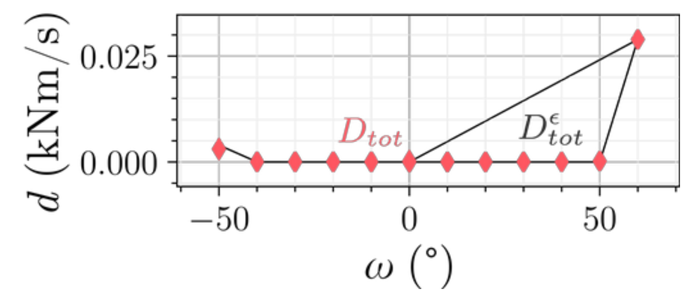
- accelerations $\times 10^3$



FEM×TANN

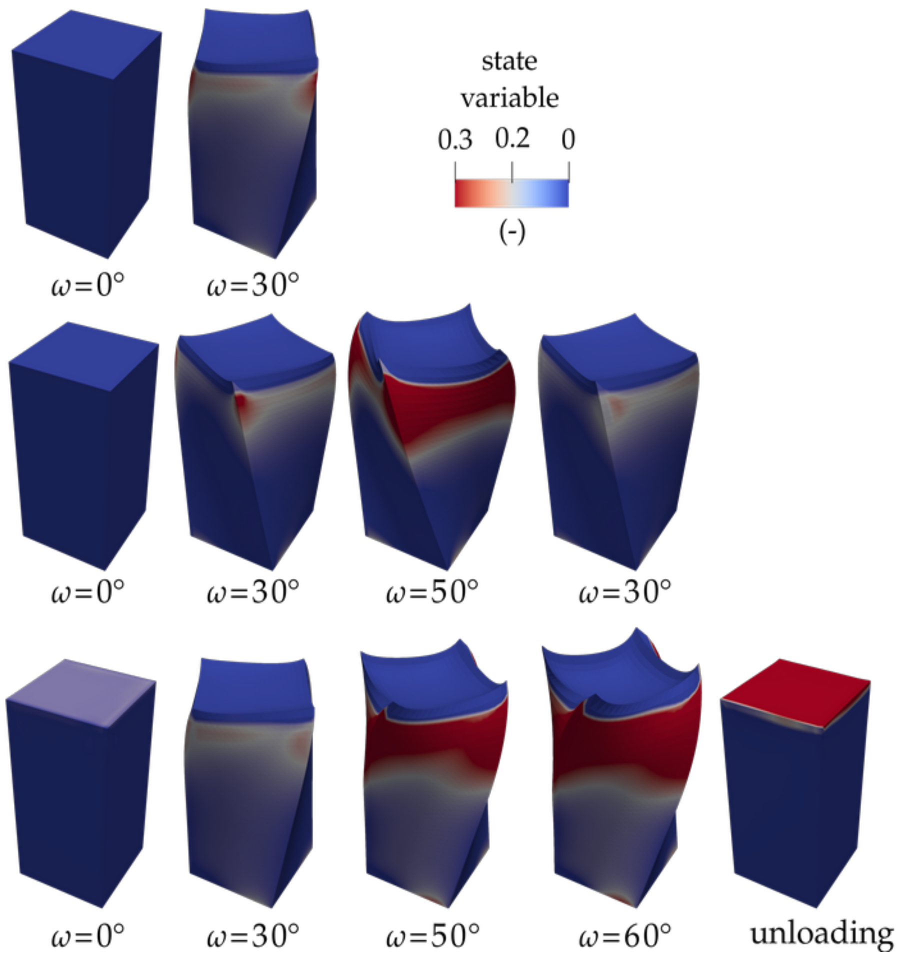




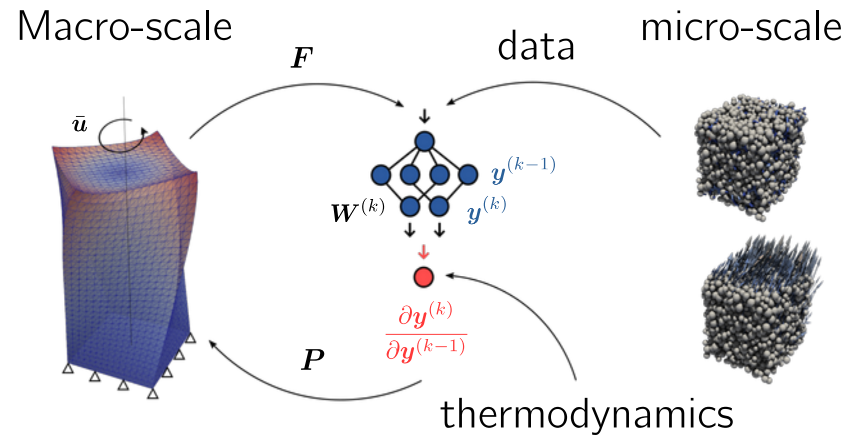


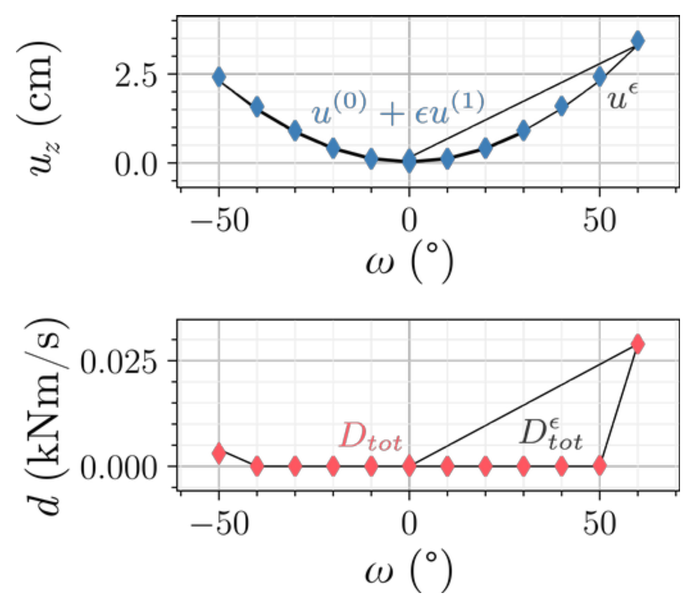
Applications to multiscale simulations

- accelerations $\times 10^3$

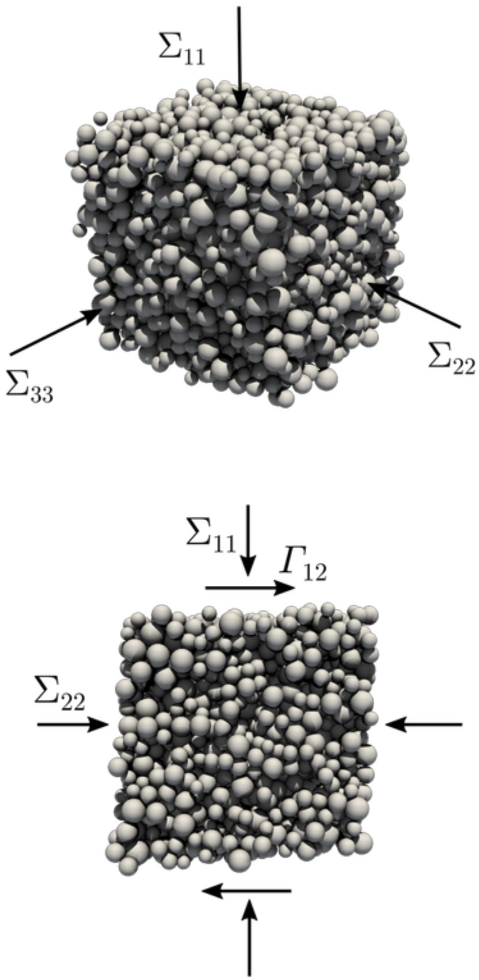


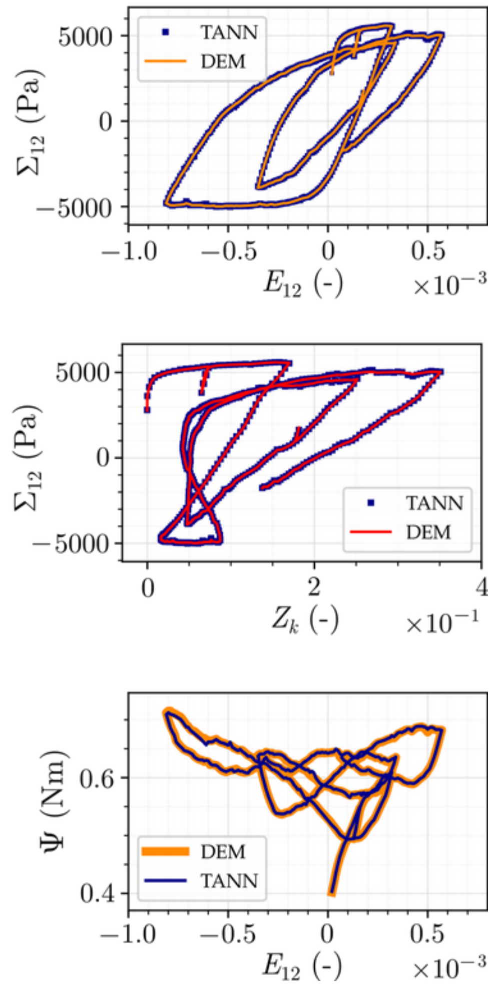
FEM×TANN





Applications to granular media





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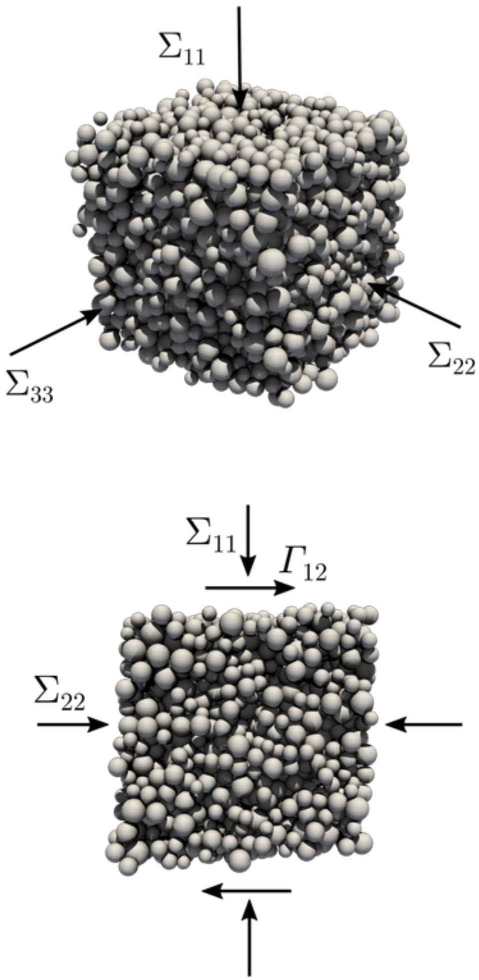
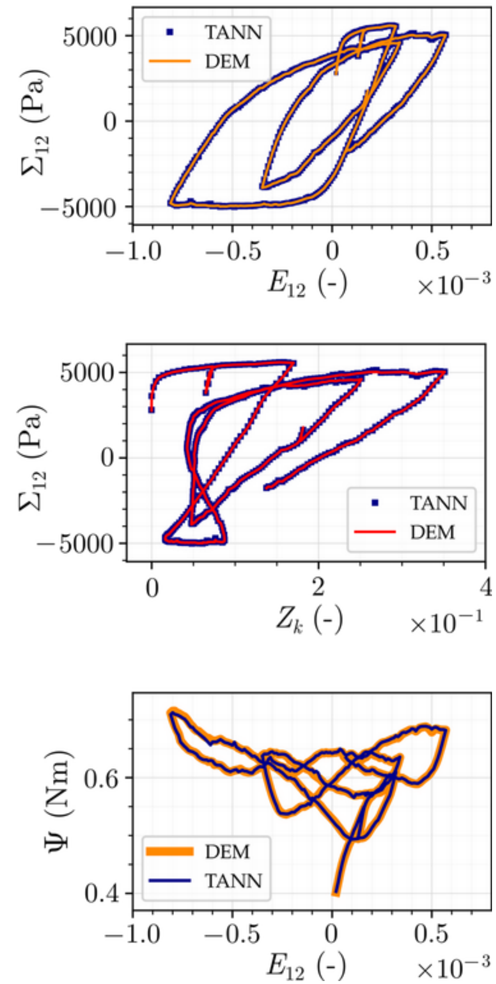
Applications to granular media





Thermodynamics – **reliable**

FEM×TANN – **fast**

internal variables – **scalable**

Masi Stefanou, 2021. TANN for multiscale computational mechanics

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5th workshop CSMA Junior

Mai 14th-16th 2022

Île de Porquerolles

Deep learning, real-time simulation and model-order reduction

Application to the constitutive modeling of materials

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