几何微结构的高效仿真与设计优化
Efficient Homogenization and Design for Microstructures

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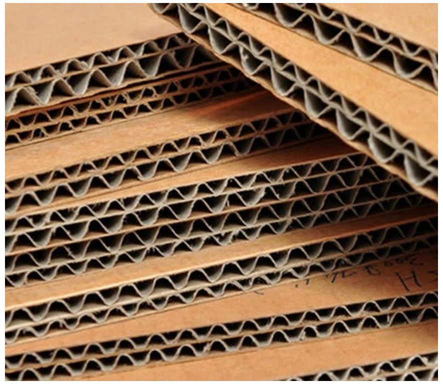
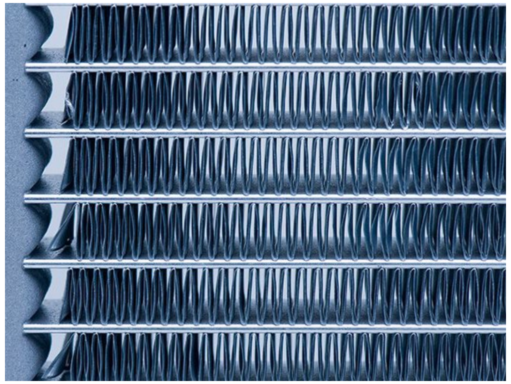
Fine structures in industry


Corrugated board


Heat exchanger
[Hydro]


Sound-absorbing panels

Aluminum foam sandwich


Porous ceramics

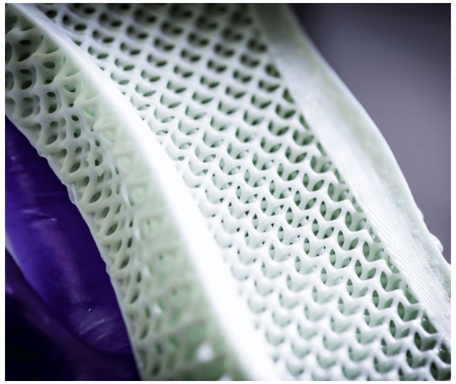
Additive Manufacturing


Heat exchanger
[NASA]

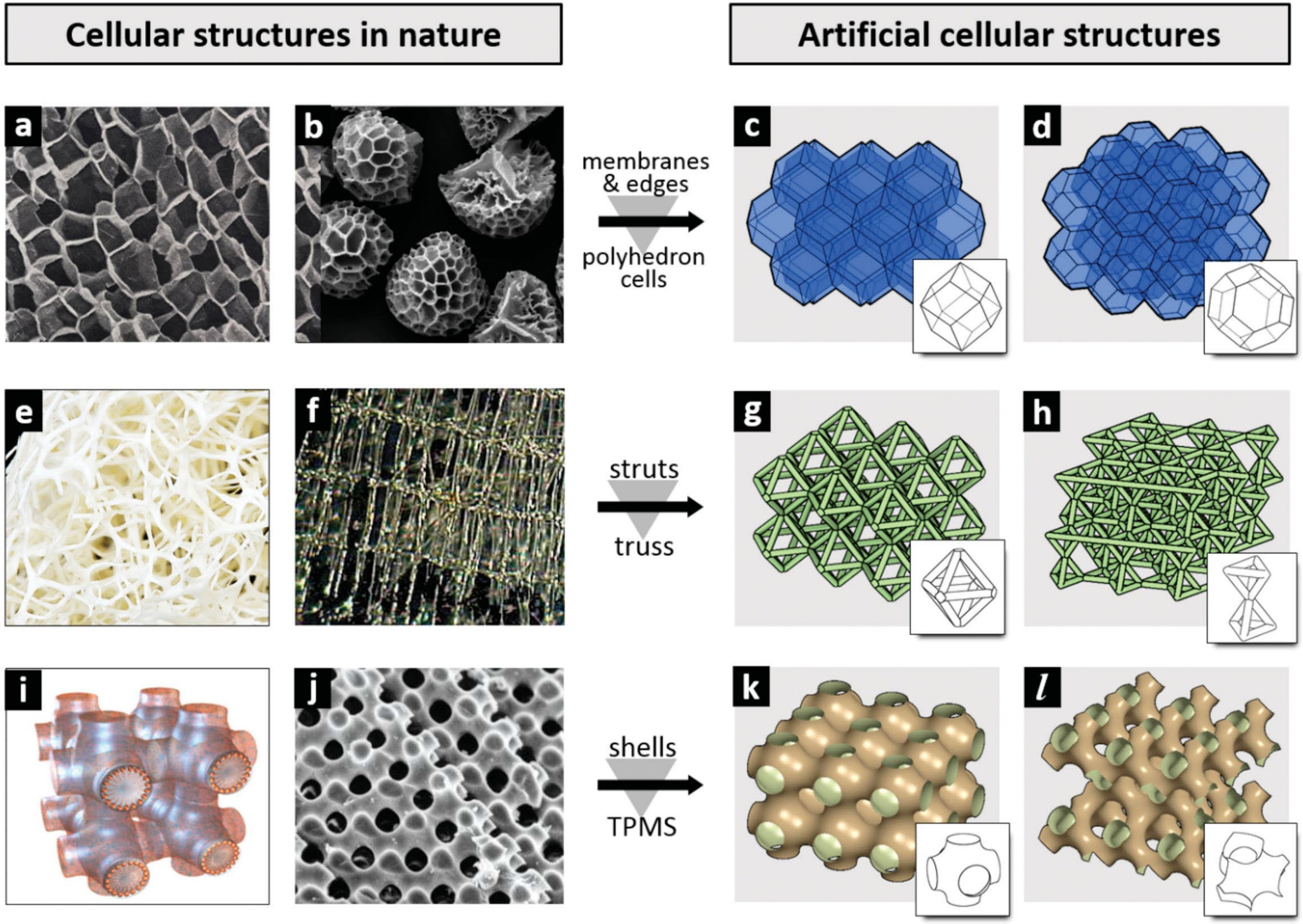

Plunger
[Oerlikon]


Medical implant
[KLS Martin]


Football helmet
[Riddell &Carbon]

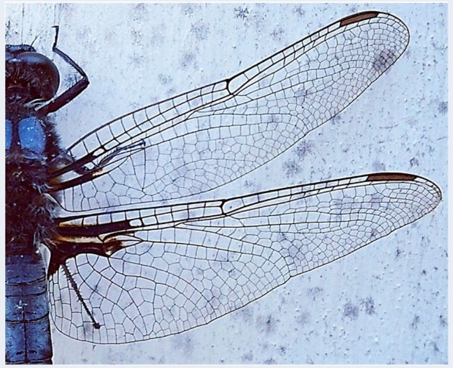
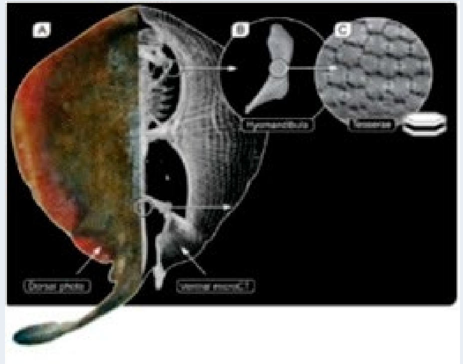
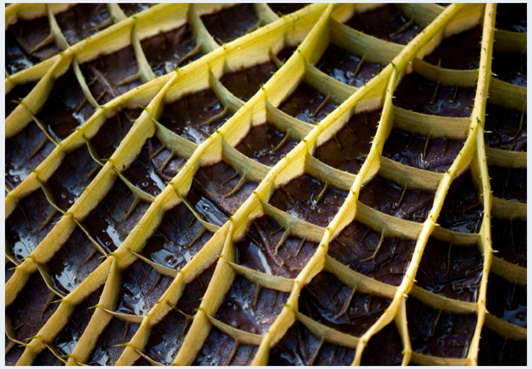

Sneaker insole
[Adidas]

Fine structures in nature



[Han et al. 2015]

Fine structures in nature

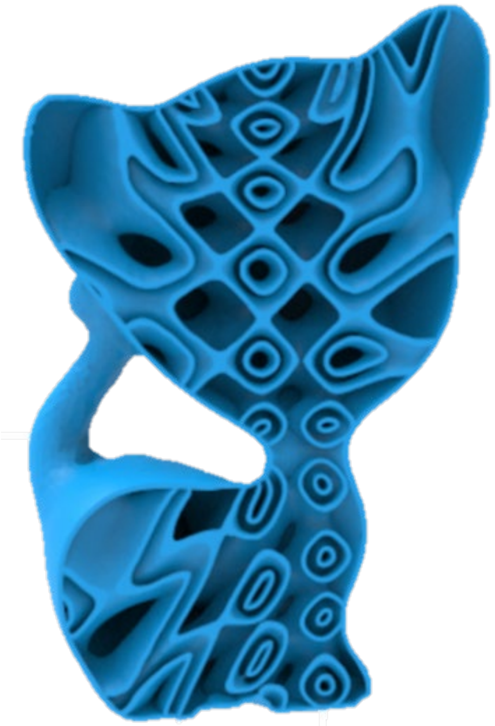
Periodic	Stochastic	Hierarchical
Honeybee Nest	Trabecular Bone	Dragonfly Wing Venation
		
Ray	Veiled Lady Mushroom	Amazon Waterlily Leaf
		

[Bhate et al. 2019]

面向目标物理属性的结构优化

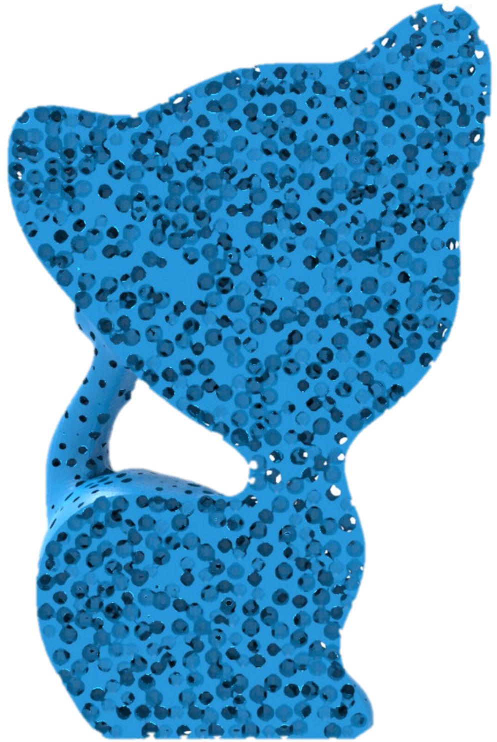
[Lu et al. TOG, 2014]

Parametric Kernel driven	
Anisotropy	×
High Stiffness	√
Double Connectivity	×



[Yan et al. TVCG, 2020]

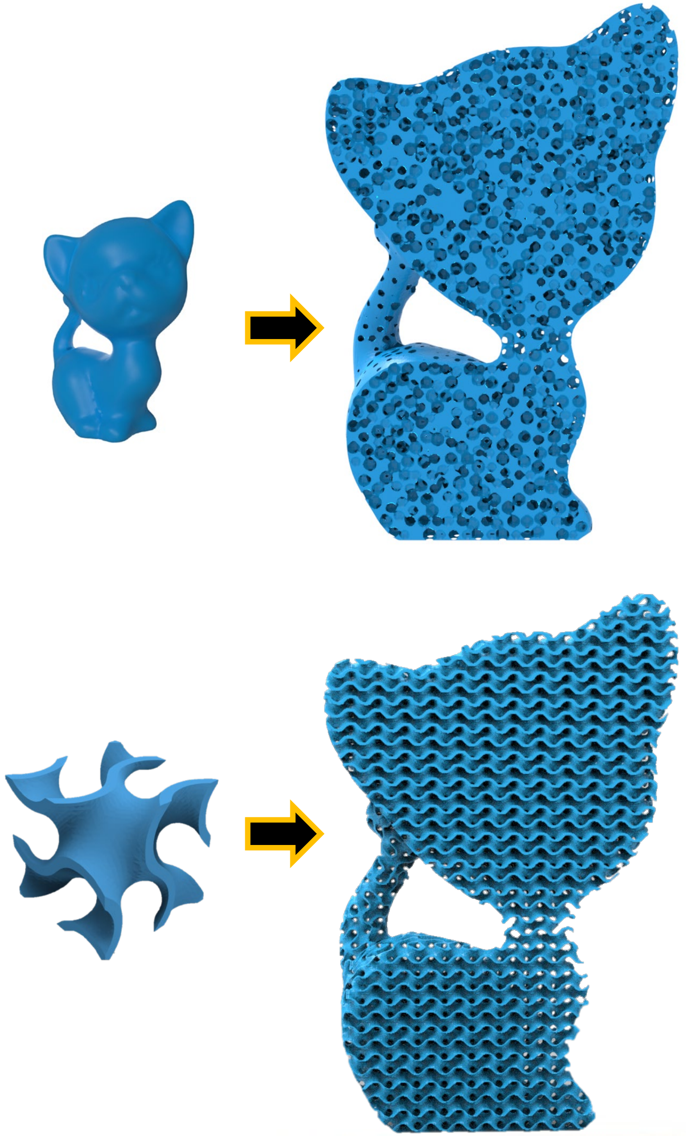
Implicit Function driven	
Anisotropy	×
High Stiffness	√
Double Connectivity	√



[Tian et al. SCF, 2020]

Parametric Kernel driven	
Anisotropy	√
High Stiffness	√
Double Connectivity	√

面向目标物理属性的结构优化



Top-down Approaches

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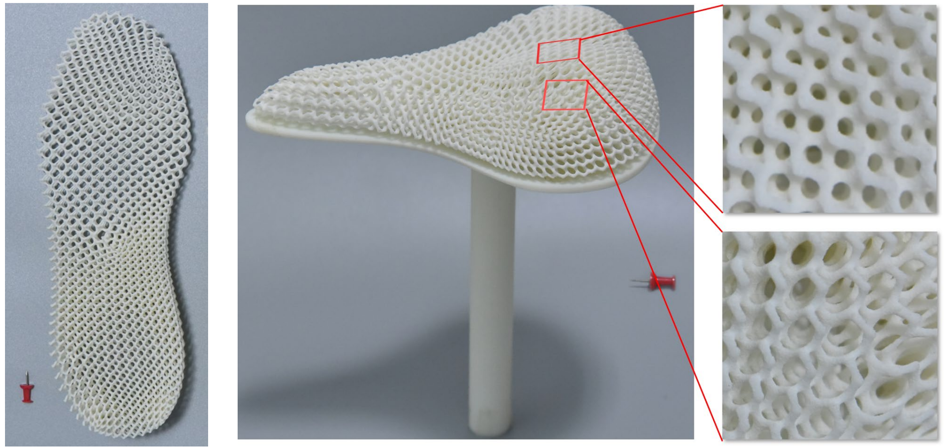
Bottom-up Approaches
(microstructures)

⇩

Two-scale Approaches

- – Coupled optimization of geometric structures and physical properties
- ✓ Modelling in a global design space
- X High computational cost

- – Decoupled optimization
- ✓ Feasible for high-resolution structures
- ✓ Efficient simulation (Homogenization)
- ✓ Efficient microstructure design (Metamaterials)

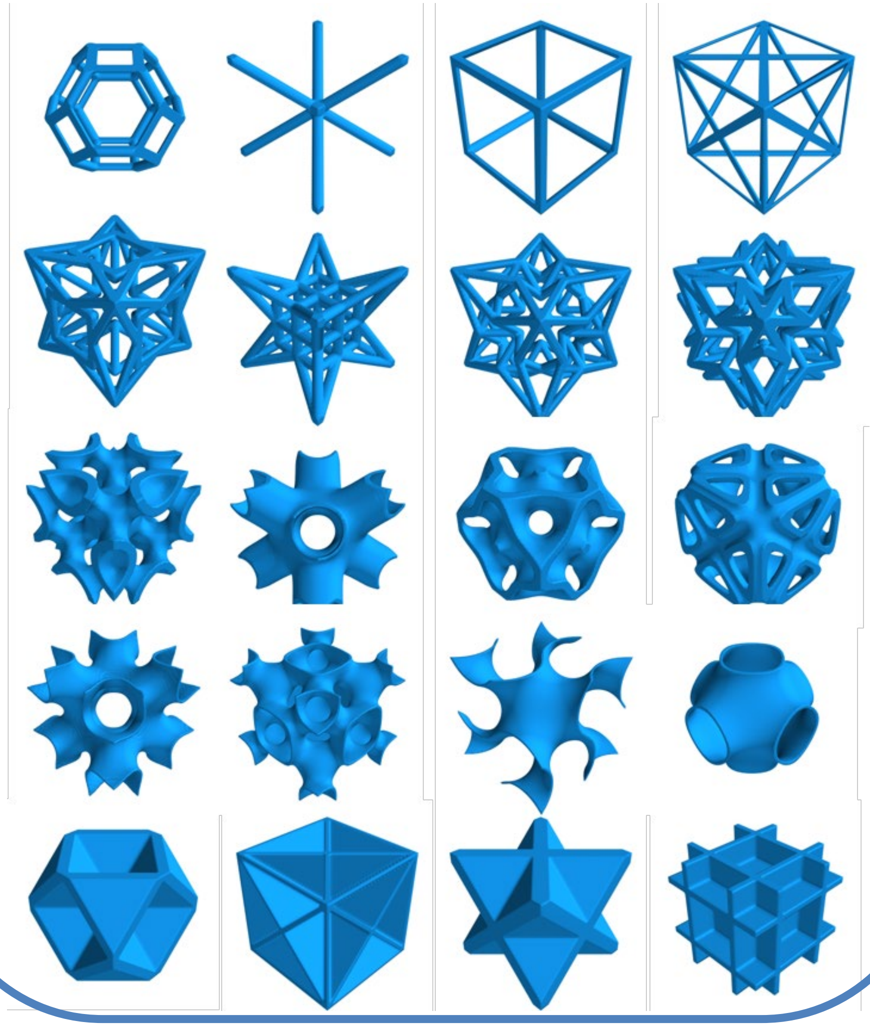


Geometric Microstructures (Metamaterials)

- 几何微结构 — 具体指相对于模型整体而言尺寸非常小的几何结构，通常可以在小范围的几何空间内充分定义其形状，并采用周期性密铺等方式填充整体模型。

- Small-scale architectures that modify the macro-scale behavior of an object.
- Separation of scales. The mechanical behavior of microstructures is the average behavior of a sufficiently large volume filled with those microstructures.

Microstructures



实验与仿真

设计与优化

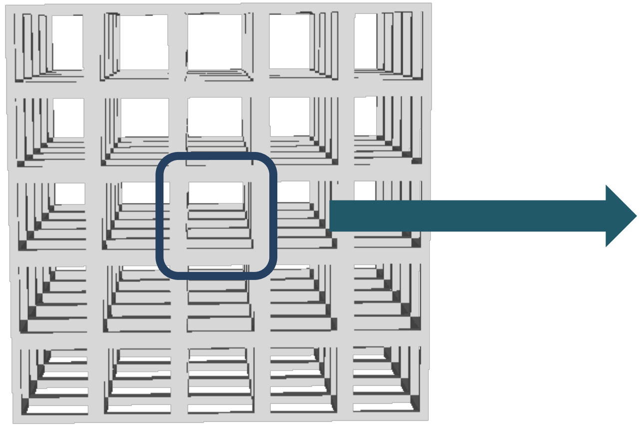
Properties

杨氏模量	孔隙率
剪切模量	扩散率
体积模量	比表面积
泊松比	相对密度
Zener ratio	表面曲率
杨氏模量面	雷诺数
应力分布	介电常数
压缩屈服强度	折射率
剪切强度	磁导率
热膨胀系数	……

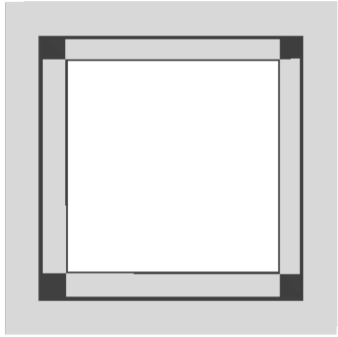
- ✓ Metamaterials derive their properties not from the properties of the base materials, but from their newly designed structures.
- ✓ The precise shape, geometry, size, orientation and arrangement gives metamaterials smart properties that go beyond what is possible with conventional materials.

微结构的仿真计算

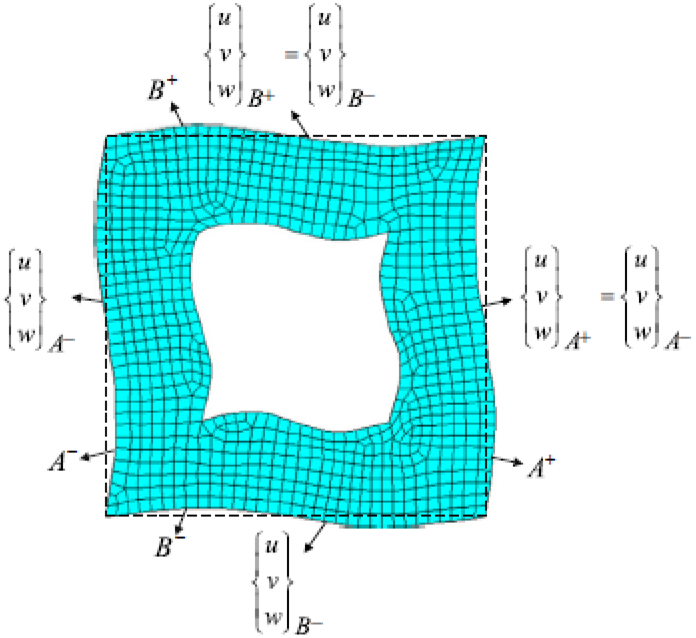
均质化理论（Homogenization）：通过分析代表性体积单元（RVE）获取微结构的等效材料性质。



微结构阵列

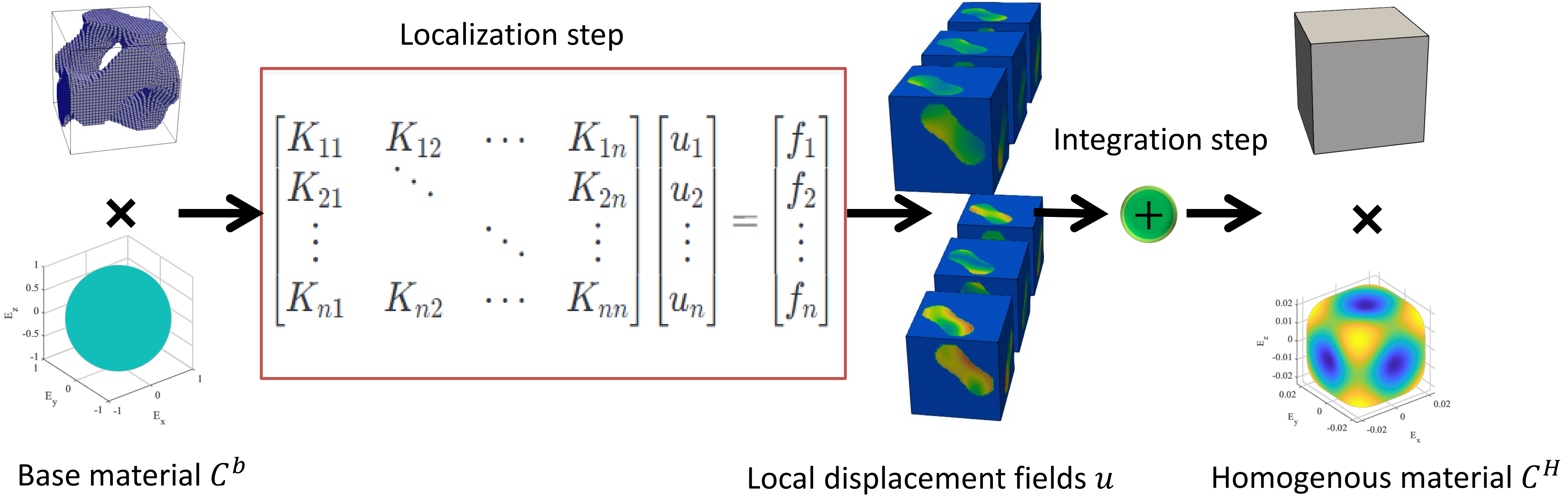


代表性体积单元（RVE）



周期性边界条件

微结构的仿真计算—均质化 (Homogenization)



Localization step: $\int_\Omega C^b_{ijkl}\varepsilon_{ij}(v)\varepsilon_{kl}(u)\mathrm{d}\Omega = \int_\Omega C^b_{ijkl}\varepsilon_{ij}(v)\bar{\varepsilon}_{kl}\mathrm{d}\Omega,$ $\Leftrightarrow$ Solving linear equation system $u = K^{-1}f$

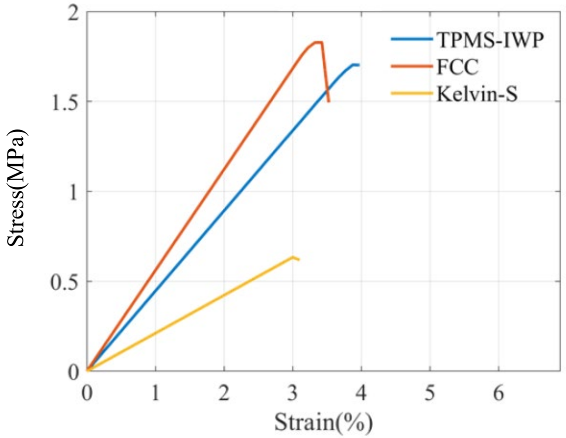
Integration step: $C^H = \frac{1}{|\Omega|}\sum_{e\in\Omega}\left(\varepsilon_0 - \varepsilon_e(u_e)\right)^T C^b \left(\varepsilon_0 - \varepsilon_e(u_e)\right) d\Omega$

微结构的仿真计算

- 屈服强度计算
- 应力-应变曲线

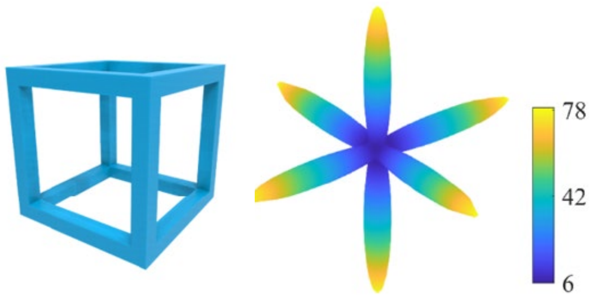
$$\bar{\varepsilon} = \bar{\varepsilon}_0 + \Delta\bar{\varepsilon},$$

$$\bar{\sigma} = \frac{1}{|\Omega^y|}\int_{\Omega^y} \sigma \, d\Omega^y.$$



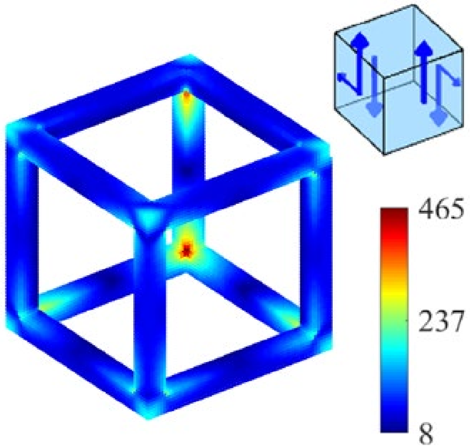
- 杨氏模量面
- 展示杨氏模量各向异性

$$\frac{1}{E_{ijk}} = S_{11}^H - 2(S_{11}^H - S_{12}^H - \frac{1}{2}S_{44}^H) \times (\ell_{i1}^2\ell_{j1}^2 + \ell_{j2}^2\ell_{k3}^2 + \ell_{i1}^2\ell_{k3}^2),$$



- 冯·米塞斯应力分布
- 展示结构内应力集中

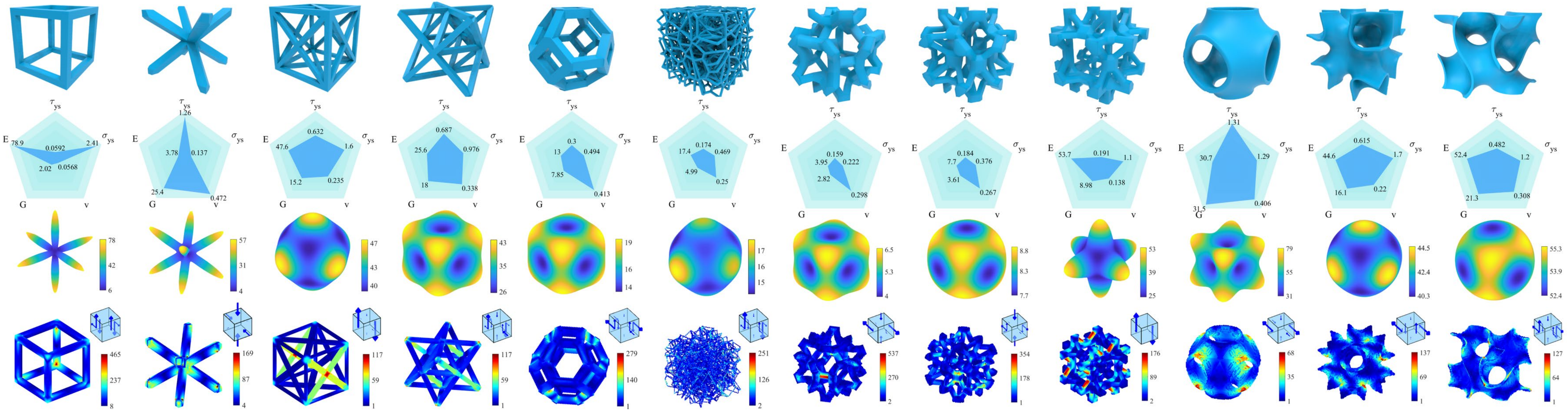
$$\sigma = C : (\bar{\varepsilon} - \varepsilon(u))$$



Physical properties of microstructures

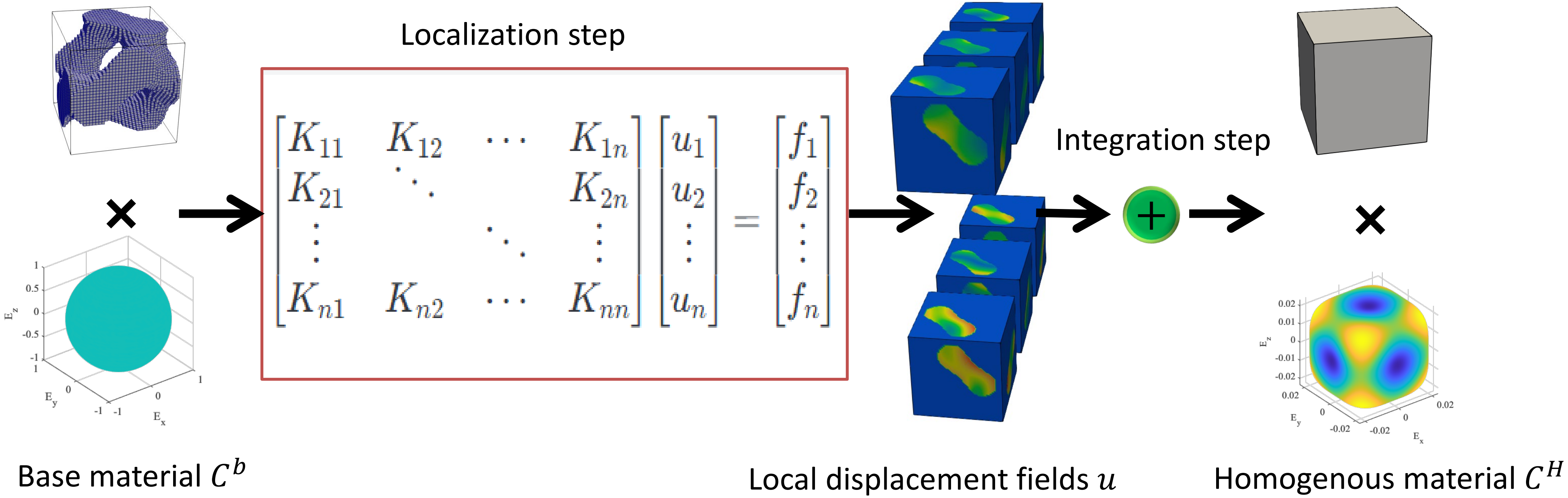
微结构力学性能画像(Mechanical Property Profiles, MPP)

杨氏模量 E, 剪切模量 G, 泊松比 v, 压缩强度σ_{ys}, 剪切强度τ_{ys}, 杨氏模量面，冯米塞斯应力分布



(a) Simple cubic (b) BCC (c) FCC (d) Octet truss (e) Kelvin truss (f) Voronoi foam (g) Elastic texture-1 (h) Elastic texture-2 (i) Elastic texture-3 (j) TPMS-P (k) TPMS-IWP (l) TPMS-G

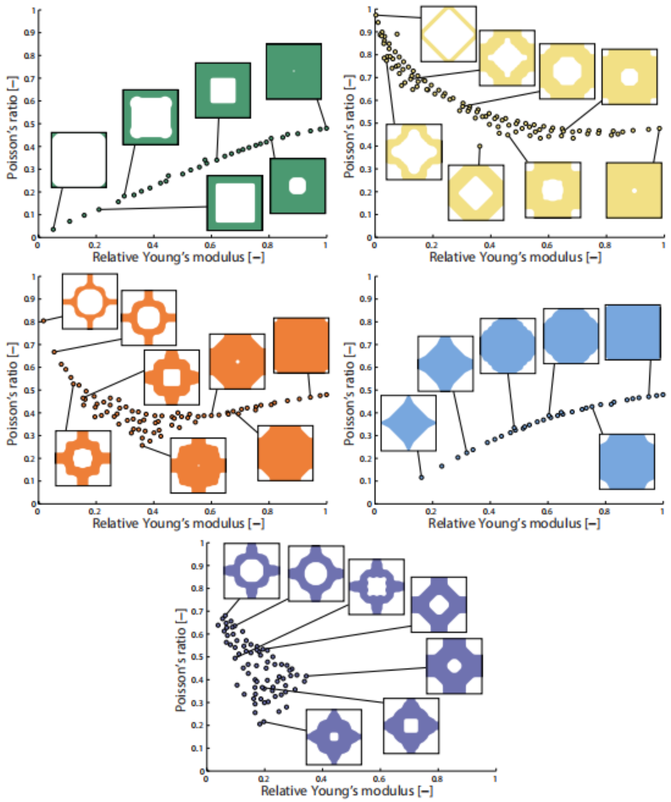
微结构的仿真计算—均质化 (Homogenization)



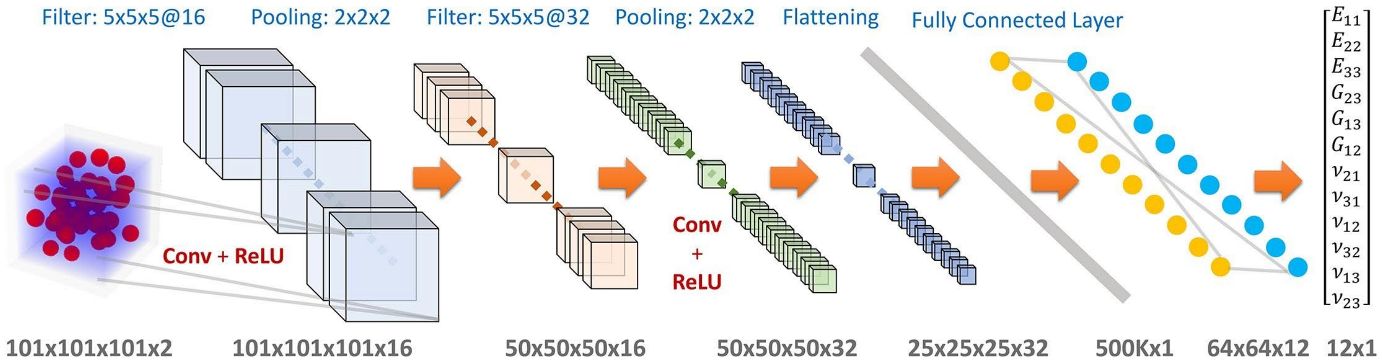
Localization step: FEM⟺Solving linear equation system $u = K^{-1}f$ is quite time-consuming!

Integration step: $C^H = \frac{1}{|\Omega|}\sum_{e\in\Omega}\left(\varepsilon_0 - \varepsilon_e(u_e)\right)^T C^b \left(\varepsilon_0 - \varepsilon_e(u_e)\right) d\Omega$

微结构的仿真计算—数据驱动均质化

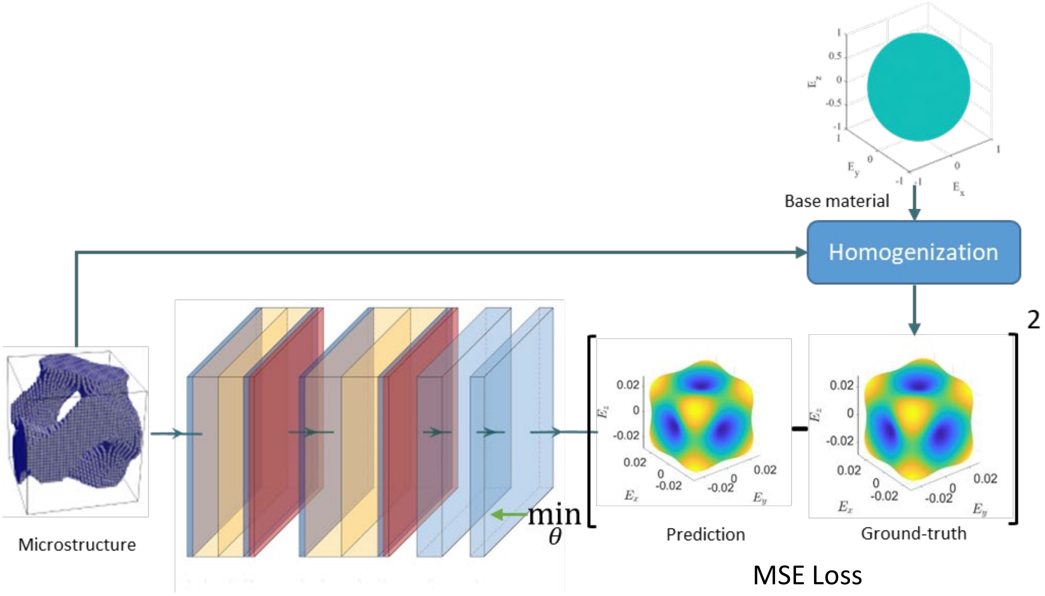


Explicit microstructure-to-material map
[Schumacher et al. 2015]

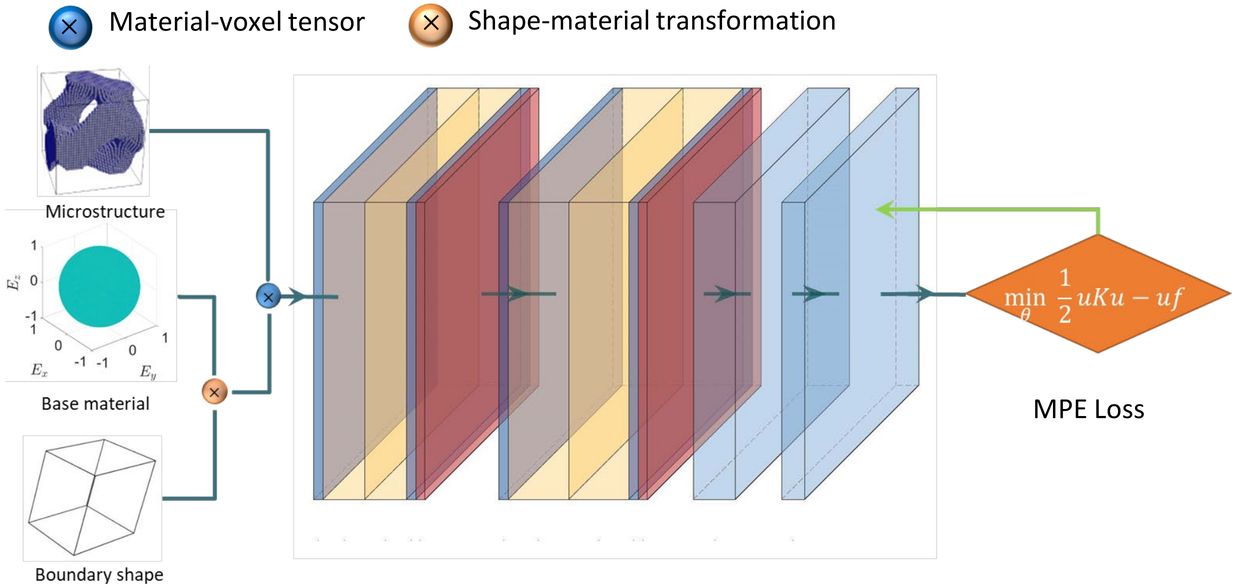


Implicit homogenization predictor via CNN
[Rao et al. 2020]

PH-Net (Parallelpiped microstructure Homogenization)

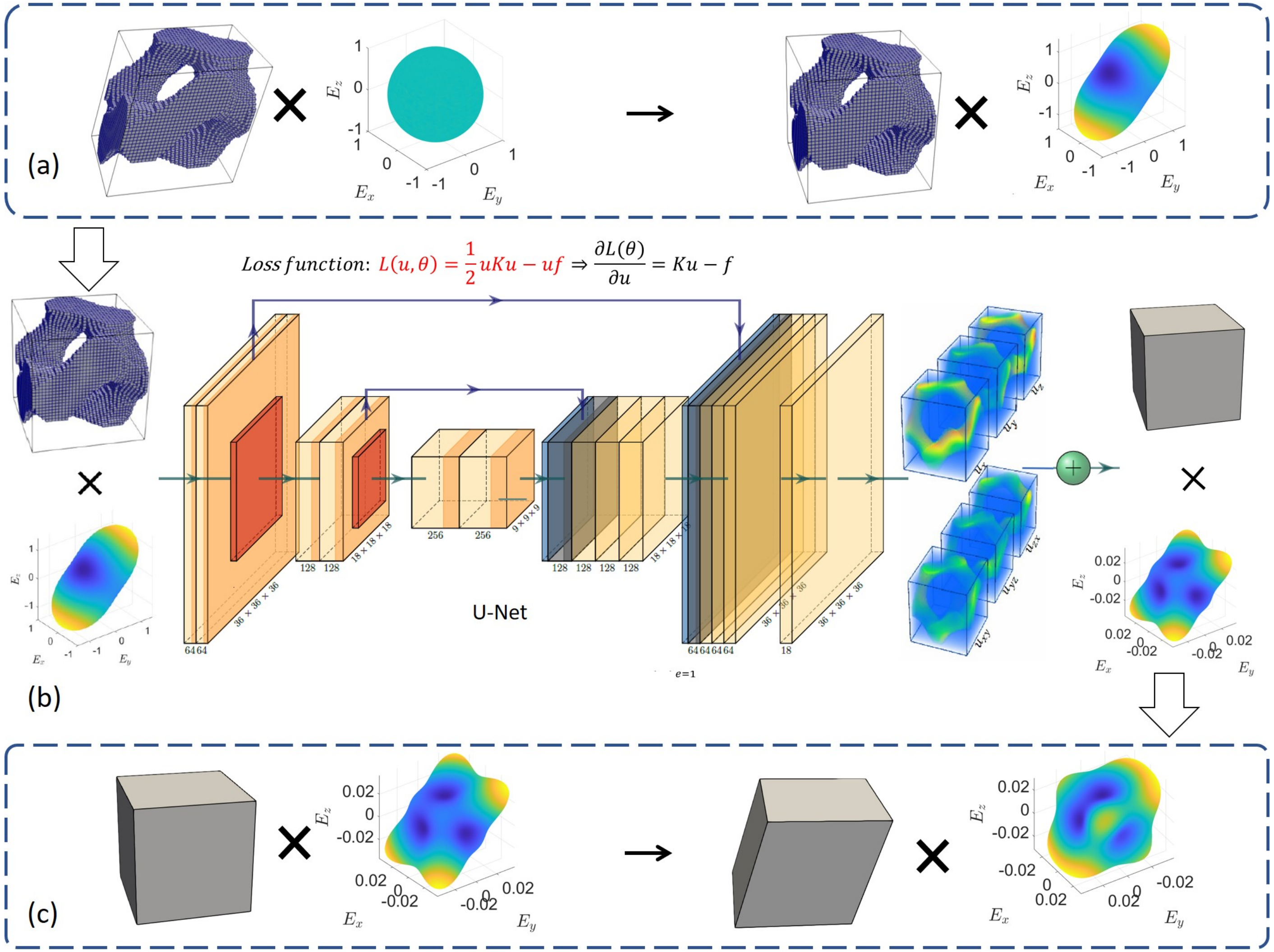


Current ML/DL methods



PH-Net

PH-Net (Parallelpiped microstructure Homogenization)

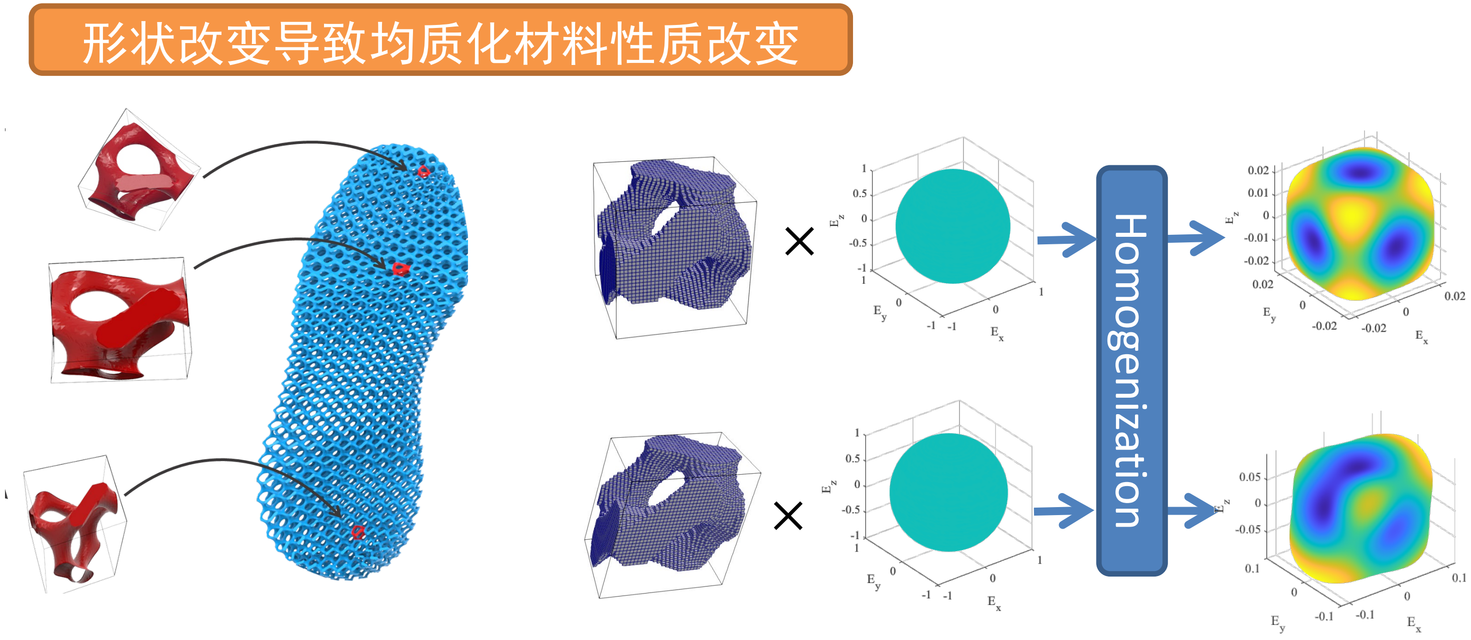


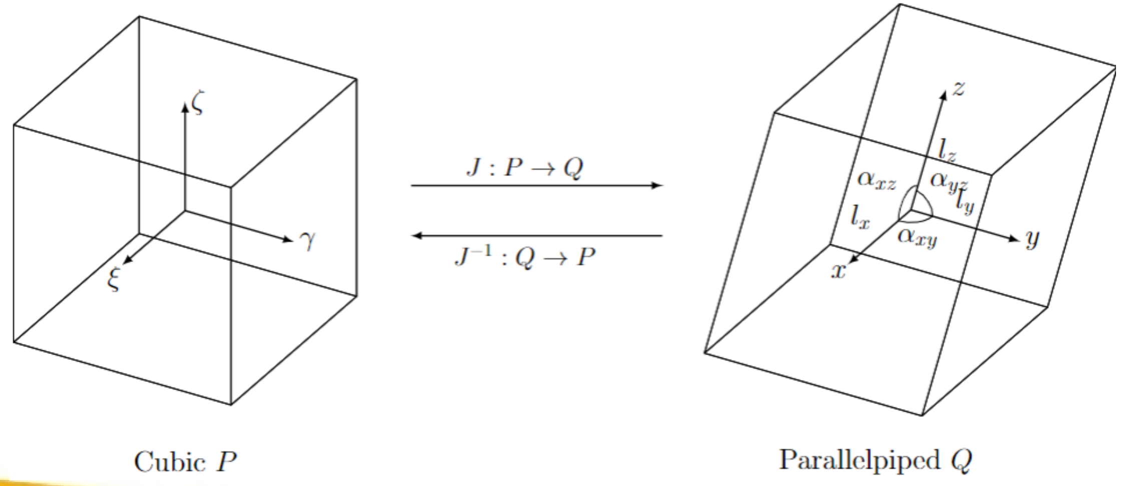
Pros:

- Material-voxel tensor and shape-material transformation make the input of PH-Net more generalize w.r.t microstructure type, base material and boundary shape
- Label-free and high efficient CNN framework
- Not only for predict homogeneous properties but also for microscopic properties, e.g., strain and stress distribution and yield strength, etc.

Parameters of PH-Net

- Microstructure $\boldsymbol{\Omega}$
- Base material
  - Hard base material $\boldsymbol{C}^{bh}$
  - Soft base material $\boldsymbol{C}^{bs}$
- Boundary shape
  - Angle $\boldsymbol{\alpha}_{xy}, \boldsymbol{\alpha}_{yz}, \boldsymbol{\alpha}_{xz}$
  - Scale $\boldsymbol{l}_x, \boldsymbol{l}_y, \boldsymbol{l}_z$



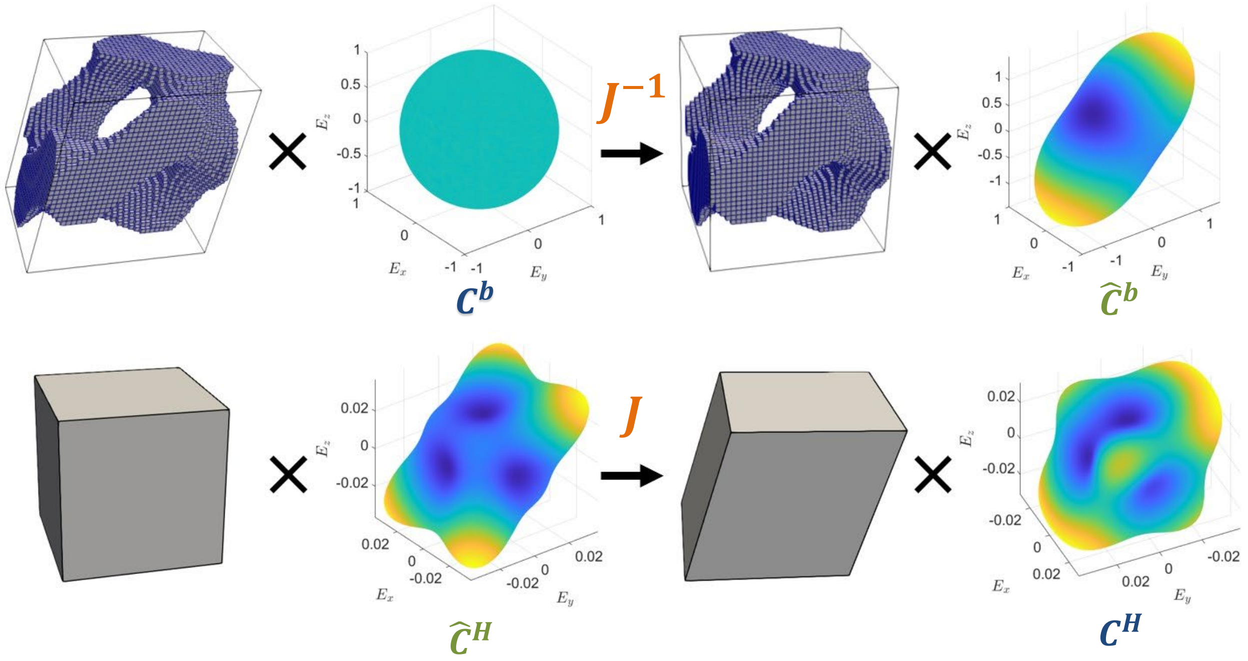


Shear matrix $\boldsymbol{S}(\boldsymbol{\alpha}_{xy}, \boldsymbol{\alpha}_{yz}, \boldsymbol{\alpha}_{xz})$
Scale matrix $\boldsymbol{T}(\boldsymbol{l}_x, \boldsymbol{l}_y, \boldsymbol{l}_z)$
Shape transformation $\boldsymbol{J} = \boldsymbol{ST}$

The generalization of PH-Net

- **Material-voxel tensor $C^{bh} \times \Omega + C^{bs} \times (1 - \Omega)$ as Input**
  - C^{bh}: hard base material
  - C^{bs}: soft base material
  - Ω: voxel-based microstructure

- **Shape-material transformation [Limited to parallelpiped boundary shape]**

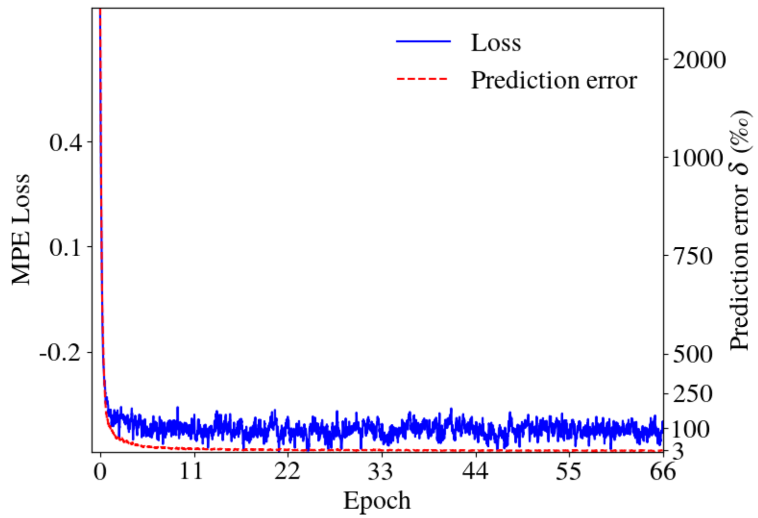


$$\hat{C}^b_{ijkl} = J^{-1}_{ip} J^{-1}_{jq} J^{-1}_{kr} J^{-1}_{ls} C^b_{pqrs}$$

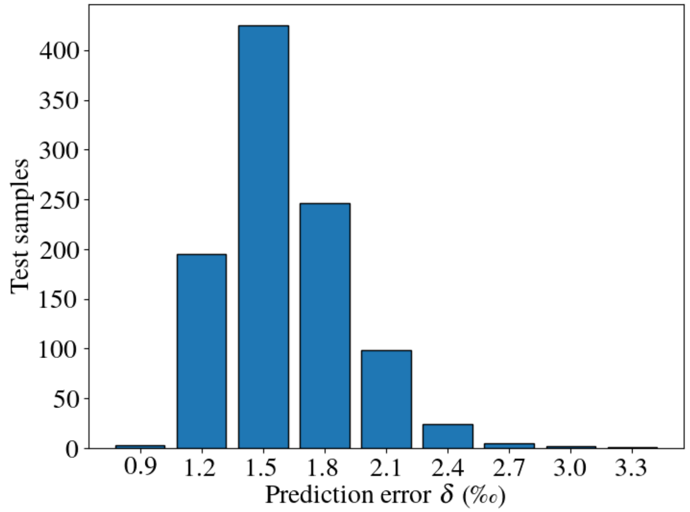
$$C^H_{ijkl} = J_{ip} J_{jq} J_{kr} J_{ls} \hat{C}^H_{pqrs}$$

Results of PH-Net

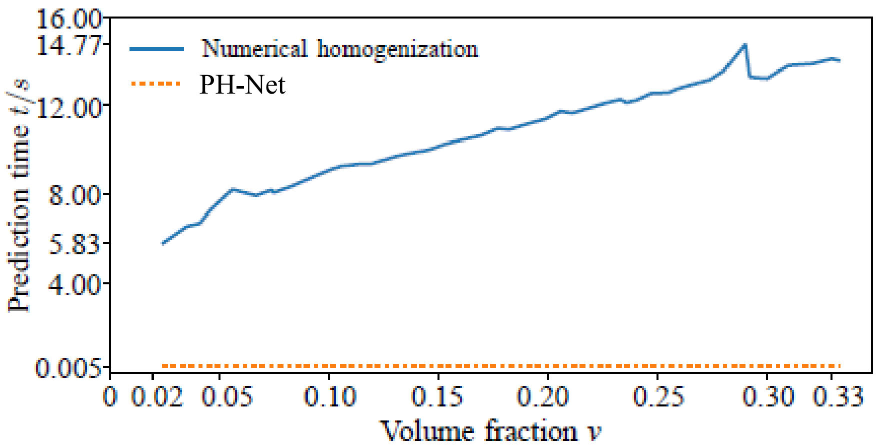
Label-free and high efficient



Training set: loss and error



Testing set: prediction error distribution



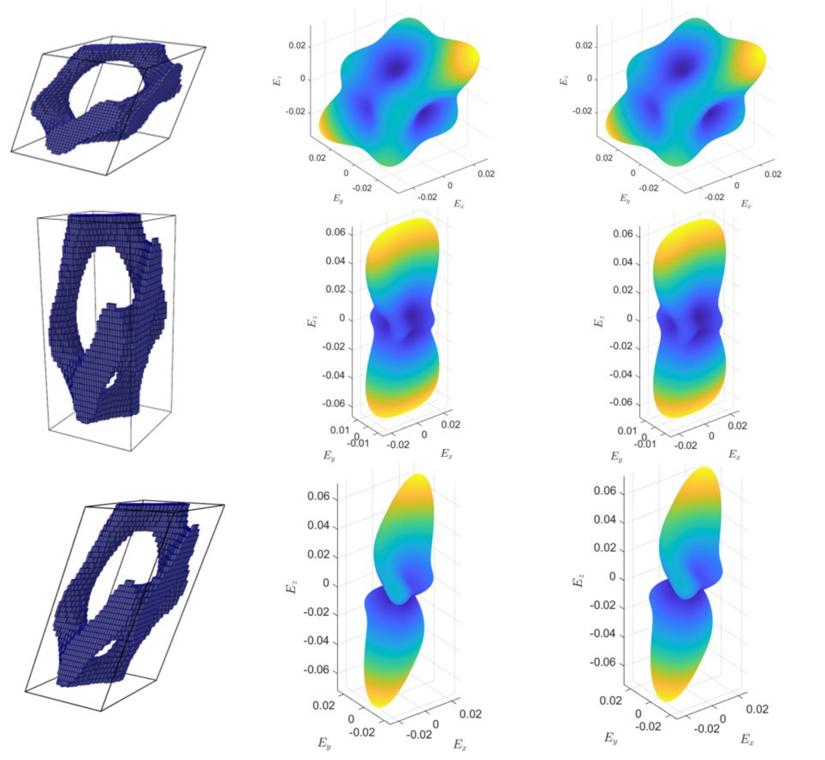
Prediction time: numerical homo. v.s. PH-Net

- Training time: PH-Net 20 hrs. (66 epochs) with 50K inputs
- Magnitude of prediction error: PH-Net $\mathbf{10^{-3}}$, Numerical homogenization $\mathbf{10^{-6}}$
- **P**rediction time: PH-Net 5ms, numerical homogenization [6*s*, 14*s*] along with the increase of volume fraction

Results of PH-Net

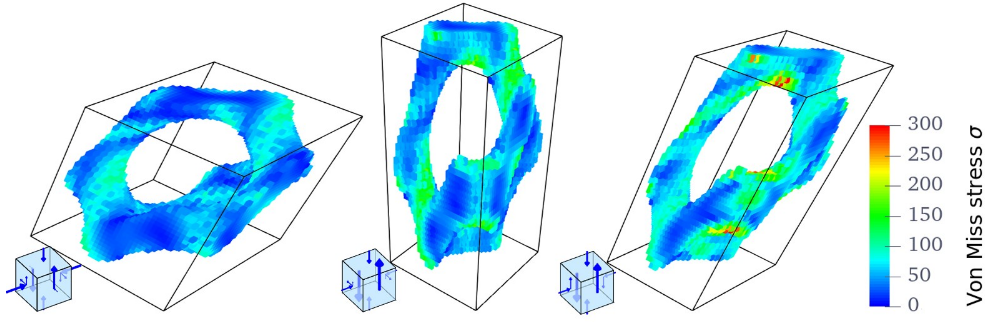
Not only for predicting homogeneous material, but also for microscopic properties

Young's modulus surface visualization

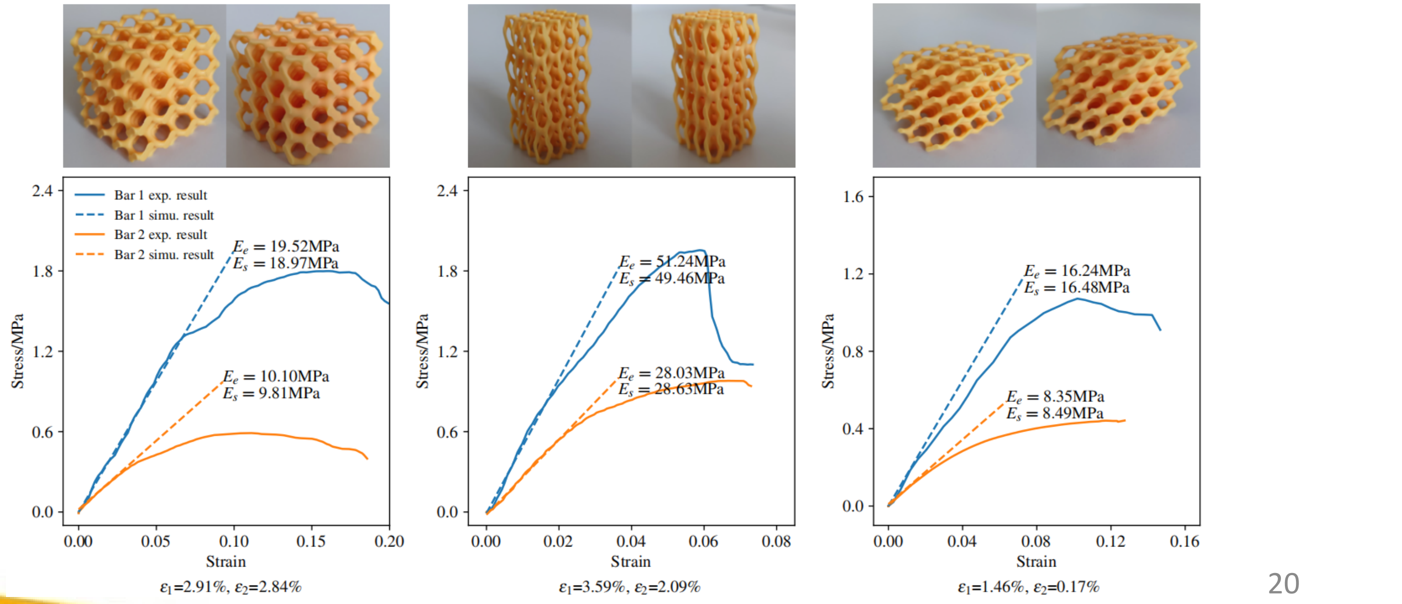


Boundary shape | Numerical Homogenization | PH-Net

Worst-case stress distribution field



$\sigma_{\max} = 146.5$ $\sigma_{\max} = 276.6$ $\sigma_{\max} = 412.2$

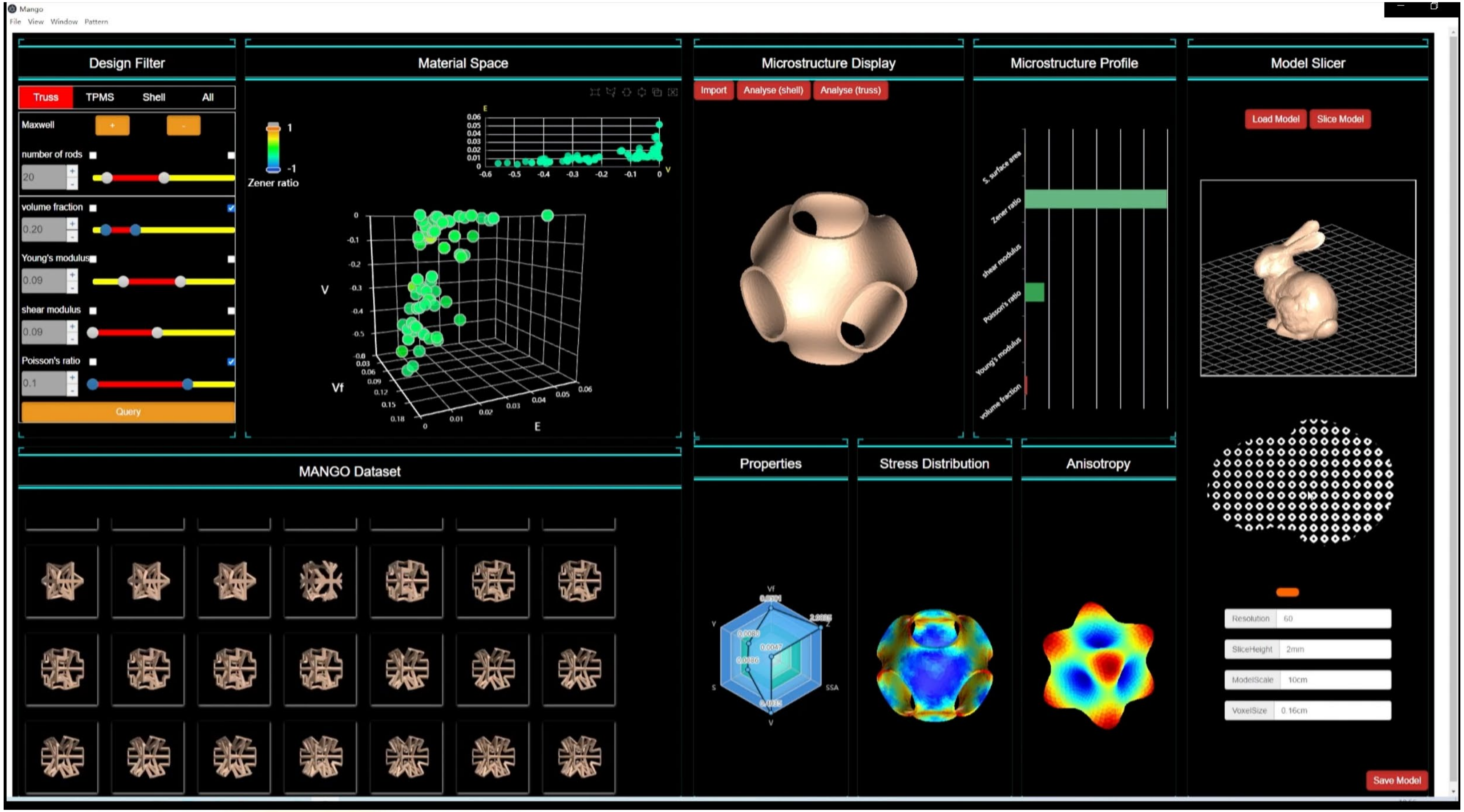


Physical experiments

Conclusion

Method	On-the-fly	Microstructure type	Base material	Boundary shape	Microscopic properties	Label-free
Numerical Homogenization	×	√	√	√	√	–
Microstructure-to-material map	√	×	×	×	×	×
Current ML/DL methods	√	√	×	×	×	×
PH-Net	√	√	√	√	√	√

MANGO: Microstructures ANalyzer, Generator and Optimizer



Live demo

Thank you!

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