SUN YAT-SEN UNIVERSITY

MFEM Community Workshop
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# Homogenized Energy Theory for Solution of Elasticity Problems with Consideration of Higher-order Microscopic Deformations

Institute of Nuclear Engineering & Technology,
Sun Yat-Sen University
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Zhang Chunyu, Cao Yuheng, Wang Biao, Sang Meng Sha
(zhangchy5@mail.sysu.edu.cn)

# Contents

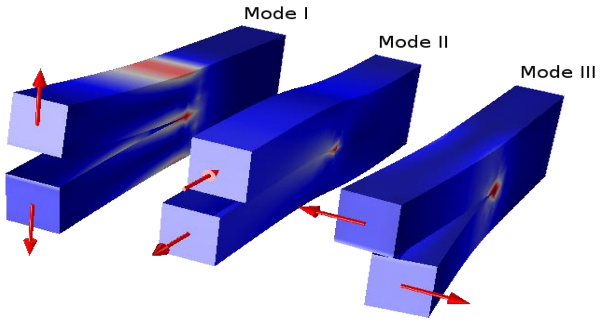
# Classical solid mechanics(CSM)

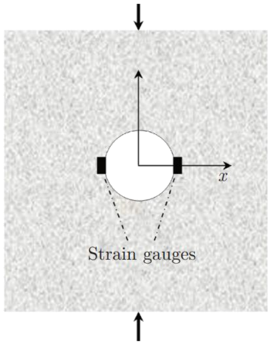
Classical solid mechanics(since 1820s, Cauchy) + Numerical solution techniques(since 1940s) ⟶ **Great Success**

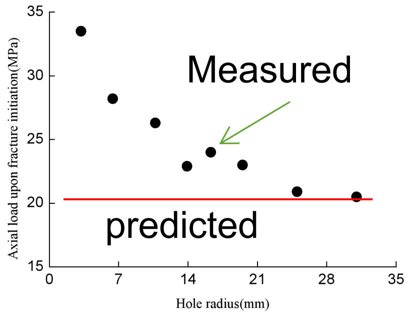
| | **Formulation** | **Source** |
|---|---|---|
| Equilibrium equation | $\nabla.\boldsymbol{\sigma} + \boldsymbol{b} = \rho\mathbf{a}$ | Newton's second law |
| Constitutive law | $\boldsymbol{\sigma} = f(\boldsymbol{\varepsilon}, \text{state variables})$ | **Emprical scaling law** |
| Geometric equation | $\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla\mathbf{U} + \nabla\mathbf{U}^T + \ldots)$ | Continuity requirements |
| Boundary conditions | $\mathbf{U} = \bar{\mathbf{U}}, \quad \boldsymbol{\sigma}.\mathbf{n} = \bar{\mathbf{t}}$ | Operation conditions |

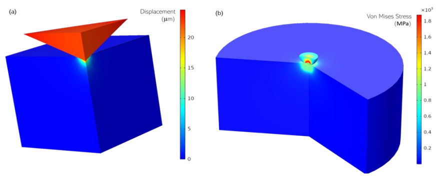
**However, many problems unresolved**

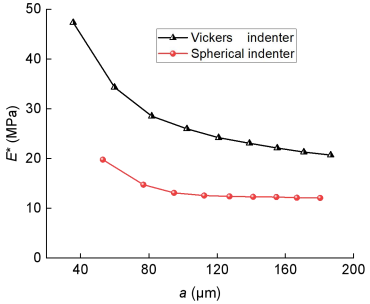
| Strain/stress singularity around crack tip | Size effect of stress/strain concentration | Size effect of constitutive parameters |
|---|---|---|





# High order deformation theories

**Strain Gradient (Plasticity) Theory**

[ Mindlin, 1964; Aifantis, 1984; Hutchinson, 1993 ]

$$U_G(\underline{\boldsymbol{\varepsilon}}) = \frac{\lambda}{2}\varepsilon_{ii}\varepsilon_{jj} + \mu\varepsilon_{ij}{}^2 + \frac{\lambda}{2}\left(l_1{}^2\varepsilon_{ii,k}\varepsilon_{jj,k} + l_2{}^4\varepsilon_{ii,kl}\varepsilon_{jj,kl}\right) + \mu\left(l_1{}^2\varepsilon_{ij,k}{}^2 + l_2{}^4\varepsilon_{ij,kl}{}^2\right),$$

**Nonlocal Continuum Theory**

[ Eringen, 1972; Engelen, 2003 ]

$$\sigma_{ij}(\vec{x}) = \int_V k(|\vec{x}-\vec{x}'|)\{\lambda\varepsilon_{kk}(\vec{x}')\delta_{ij}+2\mu\varepsilon_{ij}(\vec{x}')\}\,dv'$$

**Mircomorphic Theory**

[ Forest, 2009 ]

$$\mathcal{H}\vec{\nabla}\cdot\sigma_{ij} - f_j = 0$$

$$\mathcal{H} := 1 - l_c^2\Delta$$

**Many other theories**

......

| Achievements |
| --- |
| Removal of strain/stress singularity |
| Interpretation of size effect |
| Removal of mesh-sensitivity |
| ...... |

# Problems of high order deformation theories

1. Sources of the high order terms
2. Definition and characterization of the length scale parameters
3. a posteriori determination of hardening or softening

$$\mathcal{H}\sigma_{ij}^{C} = \sigma_{ij} \Rightarrow \sigma_{ij}^{C} = \mathcal{H}'\sigma_{ij},\ \mathcal{H}' := \begin{cases} 1 + l_1^2\Delta \ \ if\ softening \\ 1 - l_1^2\Delta \ \ else \end{cases}$$

4. Boundary conditions containing high order terms

$$\int_{\Omega} \delta W\, dV = \int_{\Omega} f_i \delta u_i\, dV + \int_{\partial\Omega} t_i \delta u_i + r_i n_j \delta u_{i,j} + \boxed{s_{ik} n_k n_l \delta u_{i,kl}\, dS}$$

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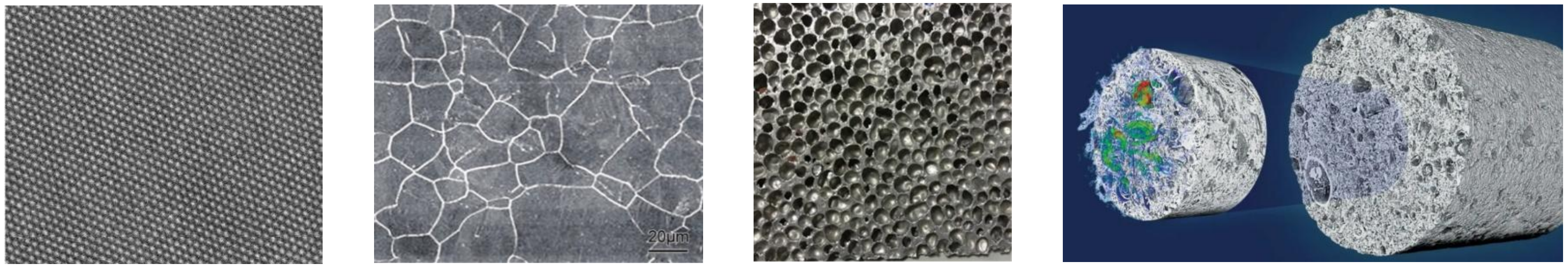
# Principles and Implementation of Homogenized Energy theory

# Origin of deficiency of CSM

## Real material: multiscaled and inhomogeneous




Error appears at this stage

## Modeled material: ideal continuum

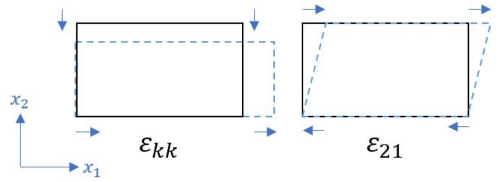
$$\langle \boldsymbol{\sigma}(\boldsymbol{x}) \rangle_{\Omega_{\mathrm{RVE}}} = \boldsymbol{\sigma}(\boldsymbol{x}_{\mathrm{c}})$$

$$\langle \boldsymbol{\sigma} \rangle_{\Omega_{RVE}} := \frac{\int_{\Omega_{RVE}} \boldsymbol{\sigma}(\mathbf{x}) d\mathbf{x}}{\int_{\Omega_{RVE}} d\mathbf{x}}$$

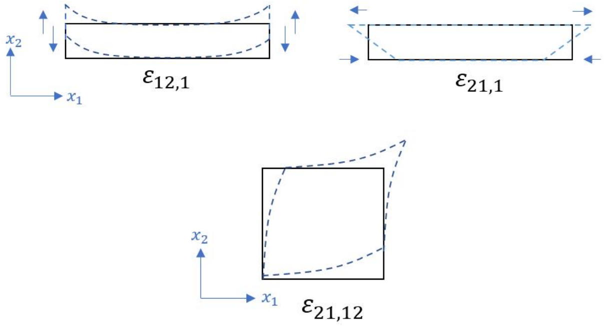
$\boldsymbol{\sigma}(\boldsymbol{x}_c)$ : representative physical quantities at the RVE barycenter

**modeled material ≠ real material**

Structural deformation




Conventional deformations




High order deformations

# Homogenization error theory

The homogenization error theory [ Zhang, Wang, 2022 ]:

- Within RVE (small but **finite** in size), average behavior≠ behavior of representative point
- Source of higher order terms: homogenization error $:= \left|\langle \mathbf{p}\rangle_{\Omega_{RVE}} - \mathbf{p}\left(\underline{x_c}\right)\right|$
- Homogenization error can be effectively alleviated or removed by including high order gradients

Eg. a scalar field $U$

$$\overline{U} \equiv \langle U\rangle_{\Omega_{RVE}} = \frac{1}{h^3}\iiint_{-\frac{h}{2}}^{\frac{h}{2}}\left(U + \vec{\nabla}U\cdot \underline{\boldsymbol{x}} + \frac{1}{2}\left(\vec{\nabla}^2 U:\underline{\boldsymbol{x}}\right):\underline{\boldsymbol{x}} + \dots\right)dx_1dx_2dx_3 = U + \frac{h^2}{24}\Delta U + \frac{h^4}{1920}\Delta^2 U + \frac{h^4}{2880}U_{,kkll(k\neq l)}\dots$$

with $h$: RVE size

**The only scale parameter $h$ has a clear physical meaning**

Zhang C.Y., Wang B.: Influence of nonlinear spatial distribution of stress and strain on solving problems of solid mechanics,Appl. Math. Mech. -Engl. Ed., 43(9), 1355–1366 (2022)

# Homogenized strain energy density

Homogenized strain energy density:

**nonlinear strain distribution within RVE yields the average strain energy density**,

$$\overline{U}(\boldsymbol{\varepsilon}) = \frac{\lambda}{2}\varepsilon_{ii}\varepsilon_{jj} + \mu\varepsilon_{ij}{}^{2} + \frac{\lambda}{2}\left(\frac{h^2}{12}\left(\varepsilon_{ii}\varepsilon_{jj,kk} + \varepsilon_{ii,k}\varepsilon_{jj,k}\right) + \frac{h^4}{4}\left(\frac{1}{144}\varepsilon_{ii,kk}\varepsilon_{jj,ll} + \frac{1}{72}\varepsilon_{ii,kl}\varepsilon_{jj,kl} - \frac{1}{120}\varepsilon_{ii,kk}\varepsilon_{jj,kk}\right)\right)$$

$$+\mu\left(\frac{h^2}{12}\left(\varepsilon_{ij,k}{}^{2} + \varepsilon_{ij}\varepsilon_{ij,kk}\right) + \frac{h^4}{4}\left(\frac{1}{144}\varepsilon_{ij,kk}\varepsilon_{ij,ll} + \frac{1}{72}\varepsilon_{ij,kl}\varepsilon_{ij,kl} - \frac{1}{120}\varepsilon_{ij,kk}\varepsilon_{ij,kk}\right)\right)$$

- Homogenized strain energy density = conventional strain energy density + **higher order strain energy density**
- Higher order strain energy density

Positive or negative cross-terms $\varepsilon_{ii}\varepsilon_{jj,kk}$, $\varepsilon_{ij}\varepsilon_{ij,kk}$

$$U_h > 0 \ or \ U_h < 0$$

local hardening or softening

# Computation of structural deformation

## Total potential energy functional:

$$\mathcal{J}_c(\underline{\boldsymbol{u}}) = \int_\Omega U(\underline{\boldsymbol{\varepsilon}}) + U_h(\underline{\boldsymbol{\varepsilon}})\, dV - \int_\Omega \underline{\boldsymbol{u}} \cdot \underline{\boldsymbol{f_b}}\, dV - \int_{\partial\Omega} \underline{\boldsymbol{u}} \cdot \underline{\boldsymbol{t}}\, dS$$

Minimization by variation

$$\int_\Omega \frac{\delta\left(U(\underline{\boldsymbol{\varepsilon}}) + U_h(\underline{\boldsymbol{\varepsilon}})\right)}{\delta \underline{\boldsymbol{u}}} dV = \int_\Omega \underline{\boldsymbol{f_b}} \cdot \delta\underline{\boldsymbol{u}}\, dV + \int_{\partial\Omega} \underline{\boldsymbol{t}} \cdot \delta\underline{\boldsymbol{u}}\, dS$$

Do **NOT** perform integration by parts: no higher order terms in boundary conditions

# Treament of second order gradient of strain

$$\frac{\delta \mathcal{J}_C(\underline{\boldsymbol{u}})}{\delta \underline{\boldsymbol{u}}} = 0$$

$$\begin{aligned}
\forall \underline{\boldsymbol{v}} \in \mathcal{H}^1(\Omega), \int_\Omega \frac{\lambda}{2} \underline{\underline{\boldsymbol{II_d}}} : \Bigg( & 2 \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \left( \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \right)^T \\
& + \frac{h^2}{12} \left( \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \left( \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \right)^T + \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \left( \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \right)^T + 2 \left( \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \right) \left( \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \right)^T \right) \\
& + \frac{h^4}{4} \Bigg( \frac{1}{72} \left( \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \right) \left( \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \right)^T + \frac{1}{36} \left( \left( \vec{\nabla}^2 \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \right) : \left( \vec{\nabla}^2 \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \right)^T \right) \\
& - \frac{1}{60} \left( \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}}\, \underline{\underline{\boldsymbol{\nabla}_d}} \right) \left( \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}}\, \underline{\underline{\boldsymbol{\nabla}_d}} \right)^T \Bigg) \Bigg) \\
& + \mu \Bigg( 2 \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \cdot \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} + \frac{h^2}{12} \left( \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \cdot \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} + \underline{\underline{\boldsymbol{\nabla}_s}} \underline{\boldsymbol{v}} \cdot \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} + 2 \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \vdots \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \right) \\
& + \frac{h^4}{4} \Bigg( \frac{1}{72} \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \cdot \Delta \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} + \frac{1}{36} \vec{\nabla}^2 \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}} \vdots \vec{\nabla}^2 \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}} \\
& - \frac{1}{60} \left( \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{u}}\, \underline{\underline{\boldsymbol{\nabla}_d}} \right) : \left( \vec{\nabla} \underline{\underline{\boldsymbol{\nabla}_s}}\, \underline{\boldsymbol{v}}\, \underline{\underline{\boldsymbol{\nabla}_d}} \right) \Bigg) \Bigg) dV - \int_\Omega \underline{\boldsymbol{v}} \cdot \underline{\boldsymbol{f}_b}\, dV - \int_{\partial\Omega} \underline{\boldsymbol{v}} \cdot \underline{\boldsymbol{t}}\, dS = 0
\end{aligned}$$

Challenge for numerical solution:

1. Evaluation of high order gradients
2. High order finite element

Alternatives:

1. Define strain as supplementary variable
2. Solve displacement and strain simultaneously
3. Order of gradient no more than 2

# Augmented Lagrangian Method to impose the constraint

The constraint: $\underline{\boldsymbol{\varepsilon}} = \underline{\underline{\boldsymbol{\nabla}_s}}\underline{\boldsymbol{u}}$

$$\mathcal{J}_{ALM}(\underline{\boldsymbol{u}}, \underline{\boldsymbol{\varepsilon}}, \underline{\boldsymbol{\lambda}}) = \int_\Omega U(\underline{\boldsymbol{\varepsilon}}) + U_h(\underline{\boldsymbol{\varepsilon}})\, dV - \int_\Omega \underline{\boldsymbol{u}} \cdot \underline{\boldsymbol{f_b}}\, dV - \int_{\partial\Omega} \underline{\boldsymbol{u}} \cdot \underline{\boldsymbol{t}}\, dS$$

$$+ \int_\Omega \underline{\boldsymbol{\lambda}} \cdot \left(\underline{\underline{\nabla_s}}\, \underline{\boldsymbol{u}} - \underline{\boldsymbol{\varepsilon}}\right) dV + \int_\Omega \frac{r}{2} \left(\underline{\underline{\nabla_s}}\, \underline{\boldsymbol{u}} - \underline{\boldsymbol{\varepsilon}}\right) \cdot \left(\underline{\underline{\nabla_s}}\, \underline{\boldsymbol{u}} - \underline{\boldsymbol{\varepsilon}}\right) dV$$

[ Fortin, Glowinski, Mercier, 1983 ]

$\underline{\boldsymbol{\lambda}}$: Lagrangian multiplier  $r$: penalty parameter

Solution procedure

$$\begin{cases} \dfrac{\delta \mathcal{J}_{ALM}(\underline{\boldsymbol{u}}, \underline{\boldsymbol{\varepsilon}}, \underline{\boldsymbol{\lambda}})}{\delta \underline{\boldsymbol{u}}} = 0 \\ \dfrac{\delta \mathcal{J}_{ALM}(\underline{\boldsymbol{u}}, \underline{\boldsymbol{\varepsilon}}, \underline{\boldsymbol{\lambda}})}{\delta \underline{\boldsymbol{\varepsilon}}} = 0 \\ \dfrac{\delta \mathcal{J}_{ALM}(\underline{\boldsymbol{u}}, \underline{\boldsymbol{\varepsilon}}, \underline{\boldsymbol{\lambda}})}{\delta \underline{\boldsymbol{\lambda}}} = 0 \end{cases} \xrightarrow{\text{Discretization}} \begin{pmatrix} \underline{\underline{\boldsymbol{K}_{uu}}} & \underline{\underline{\boldsymbol{K}_{u\varepsilon}}} & \underline{\underline{\boldsymbol{K}_{u\lambda}}} \\ \underline{\underline{\boldsymbol{K}_{\varepsilon u}}} & \underline{\underline{\boldsymbol{K}_{\varepsilon\varepsilon}}} & \underline{\underline{\boldsymbol{K}_{\varepsilon\lambda}}} \\ \underline{\underline{\boldsymbol{K}_{\lambda u}}} & \underline{\underline{\boldsymbol{K}_{\varepsilon\lambda}}} & 0 \end{pmatrix} \begin{pmatrix} \underline{\boldsymbol{u}_N} \\ \underline{\boldsymbol{\varepsilon}_N} \\ \underline{\boldsymbol{\lambda}_N} \end{pmatrix} = \begin{pmatrix} \underline{\boldsymbol{B}_{uf}} \\ 0 \\ 0 \end{pmatrix} \xrightarrow{\text{UMF (linear solver)}} \underline{\boldsymbol{u}}, \underline{\boldsymbol{\varepsilon}}, \underline{\boldsymbol{\lambda}} \xrightarrow{\text{post-processing}} \overline{U},\ U_h, \frac{U_h}{\overline{U}}$$

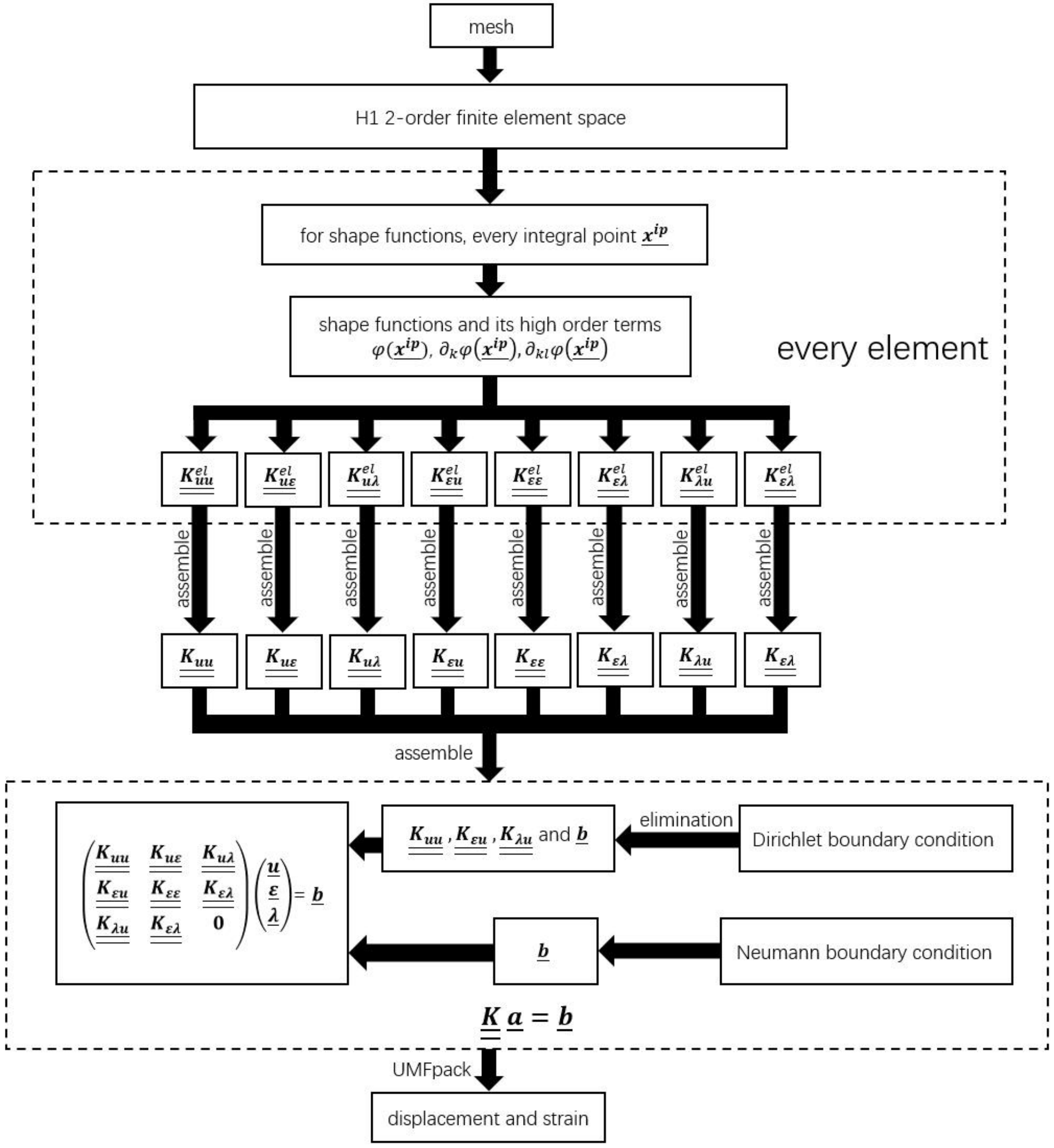
Cao Yuheng, Zhang Chunyu, Wang Biao. A New High-order Deformation Theory and Solution Procedure Based on Homogenized Strain Energy Density, Internaltional journal of engineering science, accepted, 2023.

# The solver

ccFEM

- ccFEM: curvature-corrected FEM
- Developed with the framework of **MFEM**
- Methods supplemented/redefined

| Class | Supplemented methods |
|---|---|
| fe_fixed_order | CalcPhysHessian and CalcPhyLaplacian for Linear2DFiniteElement， Linear3DFiniteElement and Trilinear3DFiniteElemen |
| fe_base | default CalcPhysHessian and CalcPhysLaplacian in fe_base are suitable only for NUBRS elements. CalcPhysHessian and CalcPhysLaplacian are redefined for other types of elements |
| ALMElasticityIntegrator | Multiple BilinearFormIntegrator are definded for $K_{uu}, K_{u\varepsilon}, K_{u\lambda}, K_{\varepsilon\varepsilon}, K_{\varepsilon\lambda}...$ |

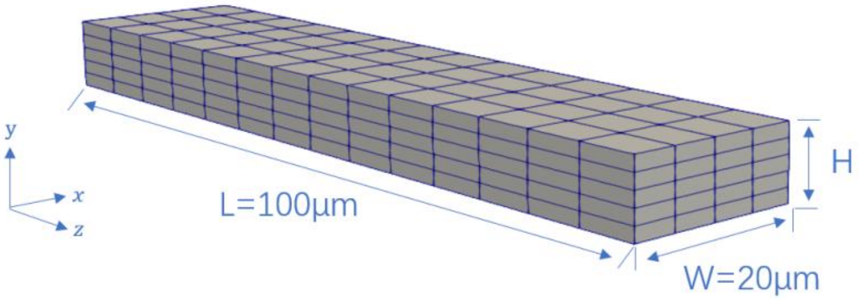


# Applications

# App 1: Hardening of micro-cantilever beam bending

**Experimental observation:** H↓ → $E^*$↑ → Hardening

Mesh and boundary conditions of the model

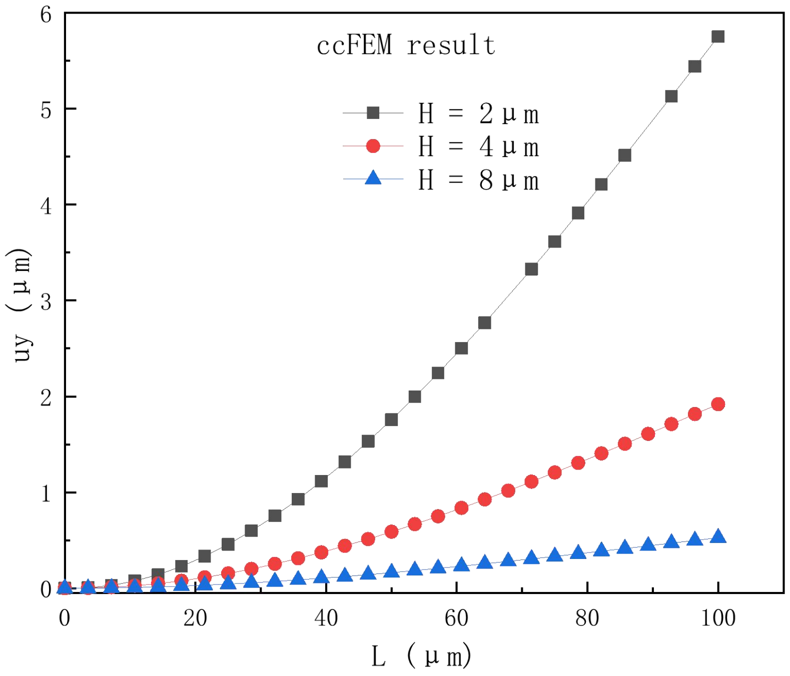




single crystal Cu : $E = 112.8\ \text{GPa}$, $v = 0.343$, $h = 1.4\ \mu\text{m}$

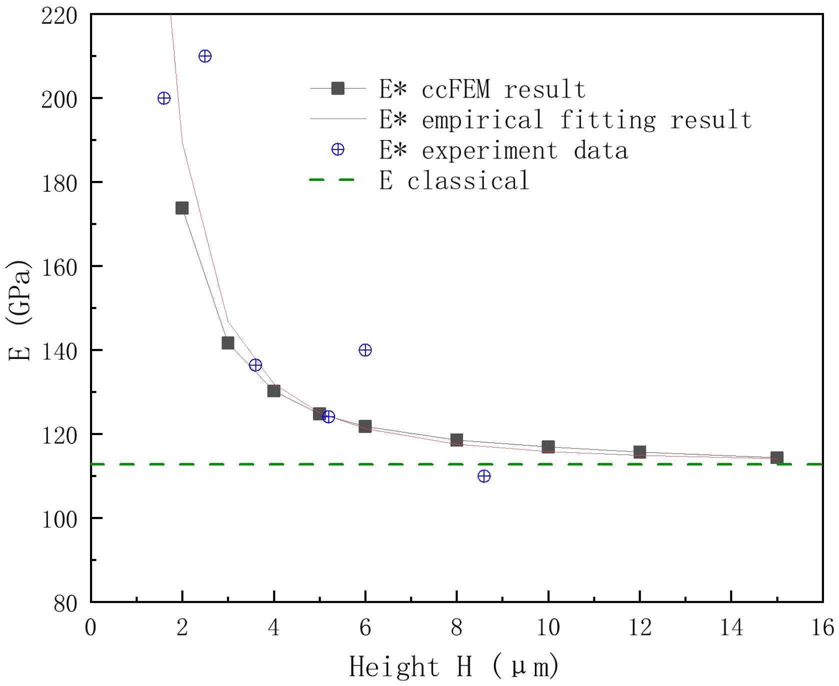
# App 1: Predicted results by ccFEM






Variation of bending displacement along the length of the beam for different beam thicknesses

$$E^* = \frac{4tL^3}{u_{y,max}H^2}$$

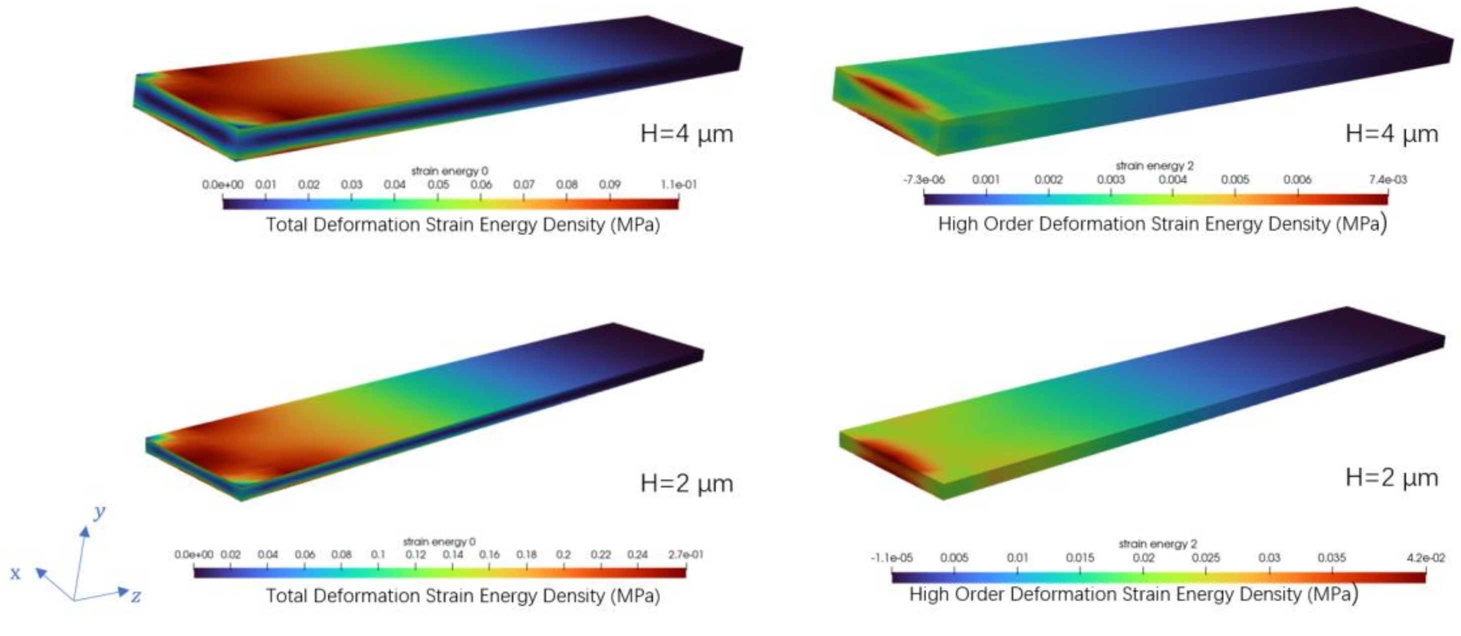


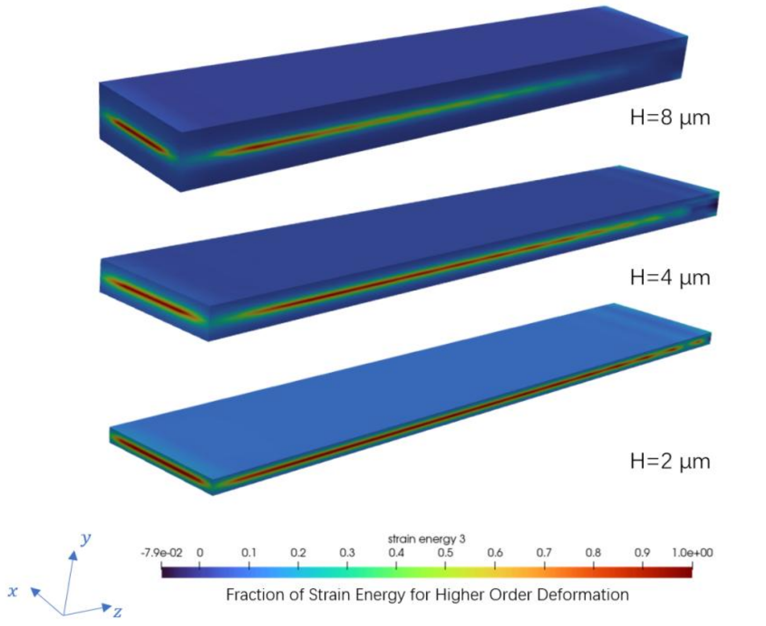

Variation of Young's modulus with beam thickness
(experimental data from [ Choi, 2022 ])

# App 1: Analysis from the energy perspective

Strain energy density and higher order strain energy density distribution predicted by ccFEM

**Non-uniform distribution of strain along x axis ↑ as H ↓**



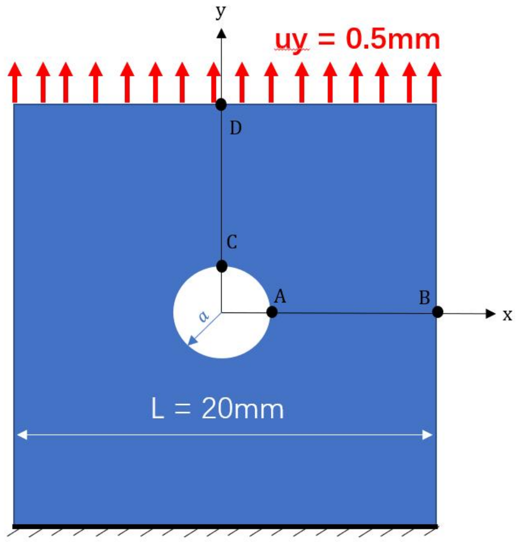

$H\downarrow \longrightarrow$ influence of $U_h$ on the overall deformation $\uparrow \longrightarrow$ **hardening** of the whole structure

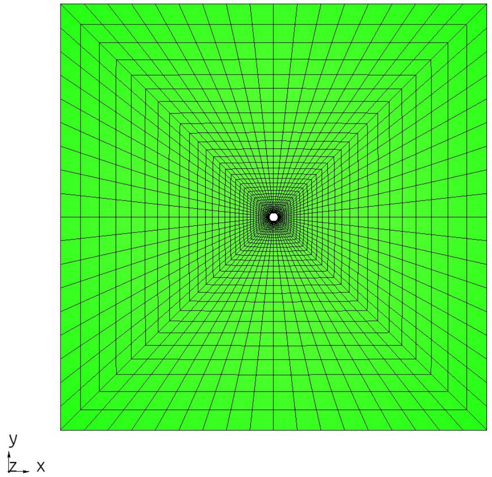
# App 2: Hole size-dependence of stress/strain concentration of perforated plates

Classical solution in textbook:

$$K := \frac{\sigma_{22}^{A}}{\sigma_{22}^{D}} = \frac{\varepsilon_{22}^{A}}{\varepsilon_{22}^{B}} = 3$$

Mesh and boundary conditions for the model:

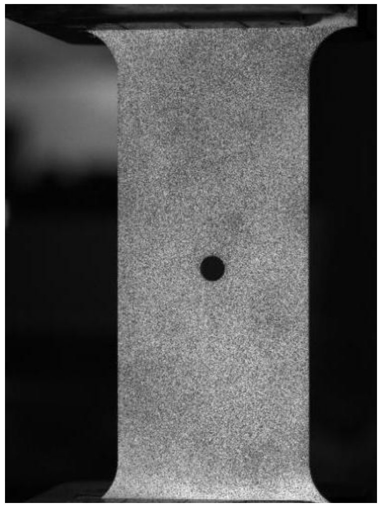


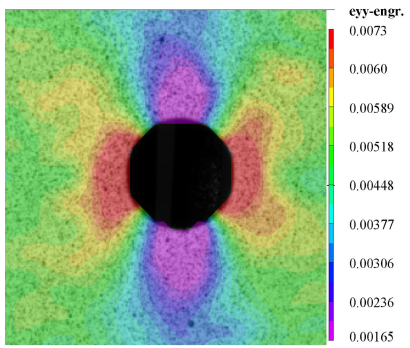



Polymethyl methacrylate (PMMA):
$E = 3.35$ GPa, $v = 0.35$, $h = 0.85$ mm

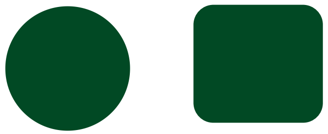
Experimental observation: a↓ → K↓

Measurment of strain by Digital Image Correlation (DIC) technology






Two types of defects:

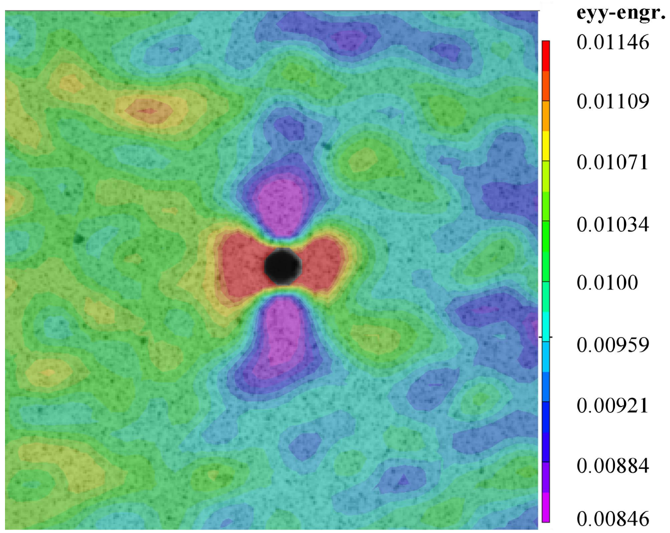


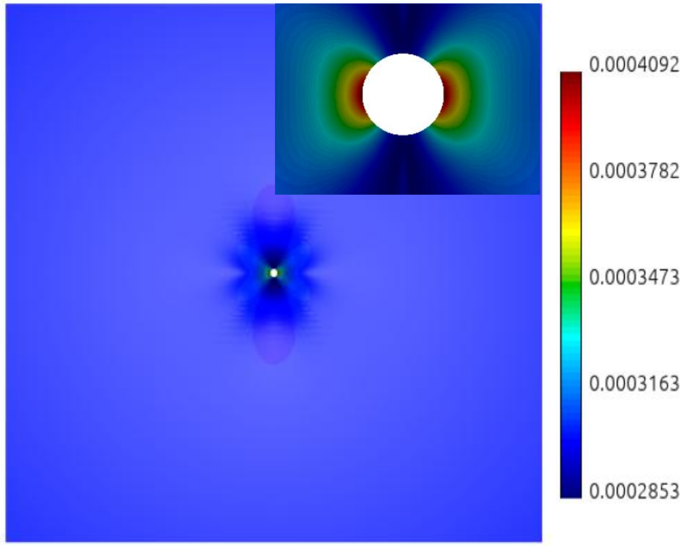
# App 2: Hole size-dependence of stress/strain concentration of perforated plates



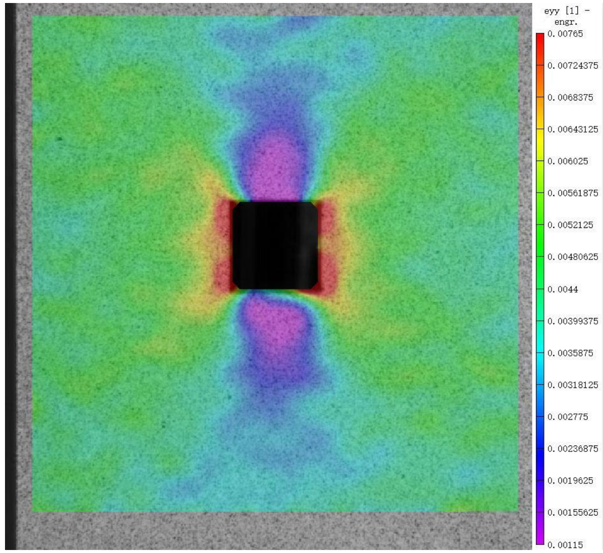
ABAQUS | DIC | ccFEM

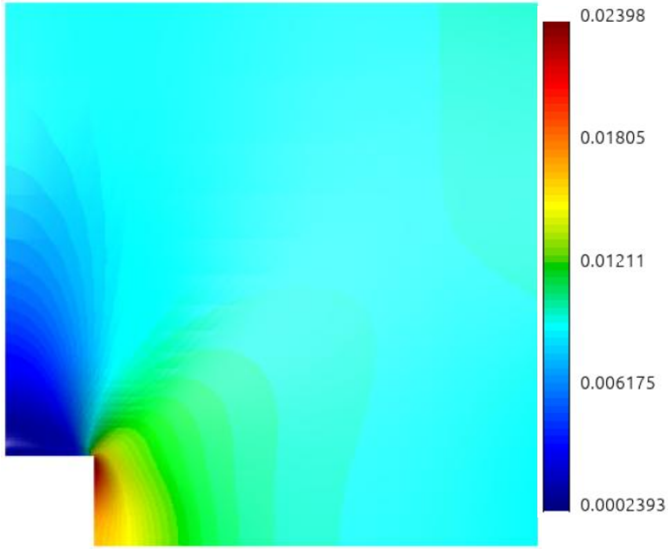
a=0.2mm



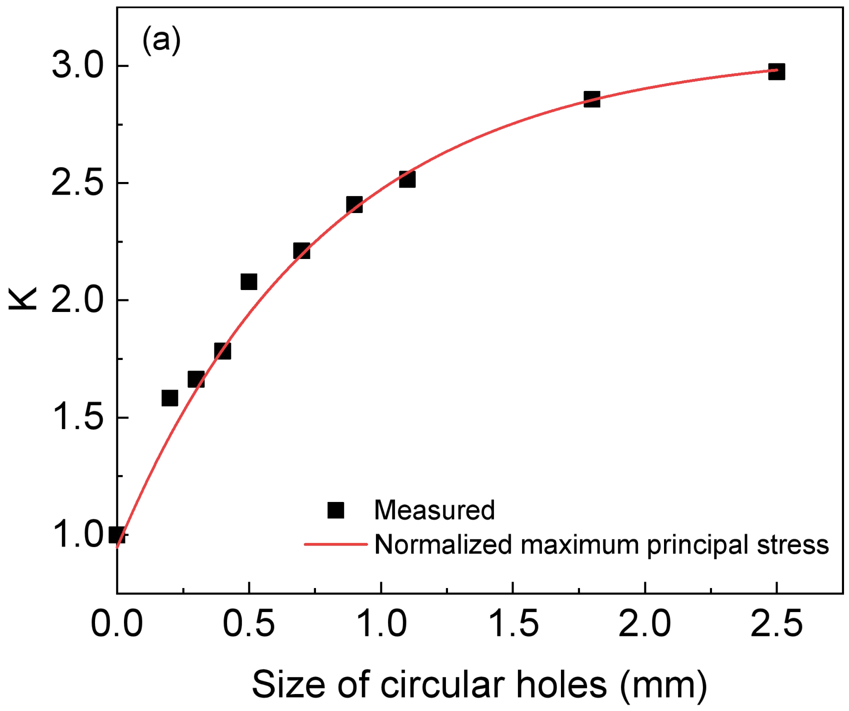



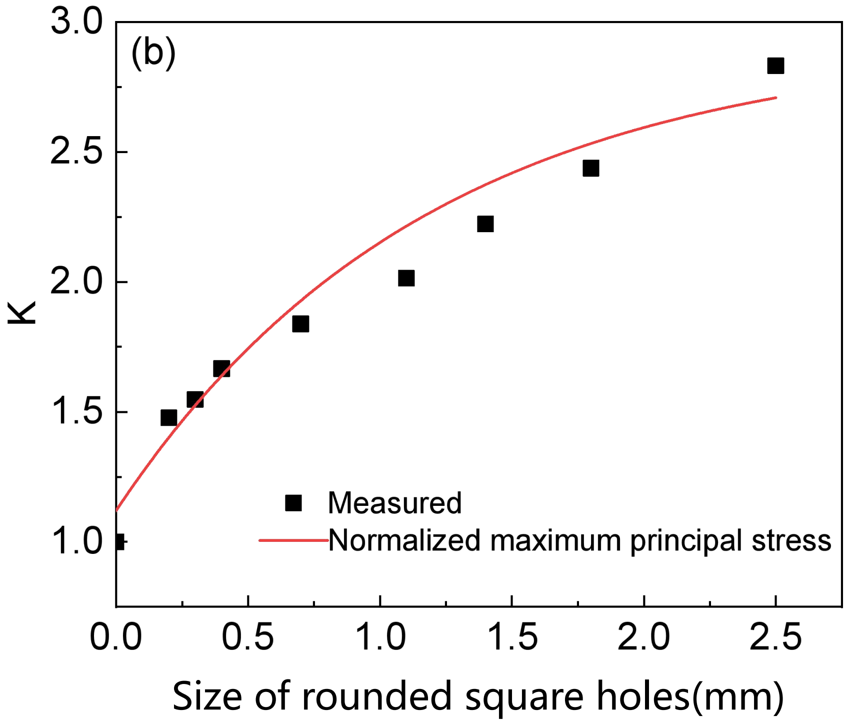

a=2.5mm



# App 2: Predicted results by ccFEM



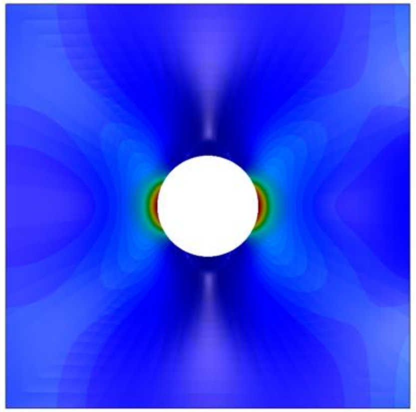



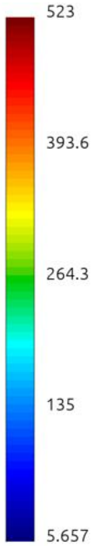

Sang Mengsha, Zhang Chunyu, Cao Yuheng, Wang Biao. Experimental and Theoretical Evaluation of Influence of Hole size on Deformation and Fracture of Elastic Perforated Plate, Mechanics of Materials, 2023, accepted

# App 2: Analysis from the energy perspective



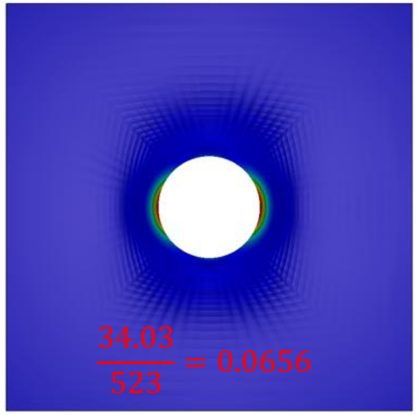
$U(\underline{\boldsymbol{\varepsilon}}) + U_h(\underline{\boldsymbol{\varepsilon}})$

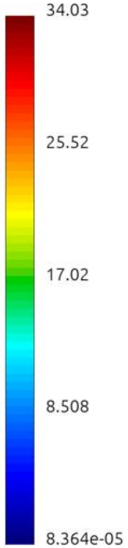




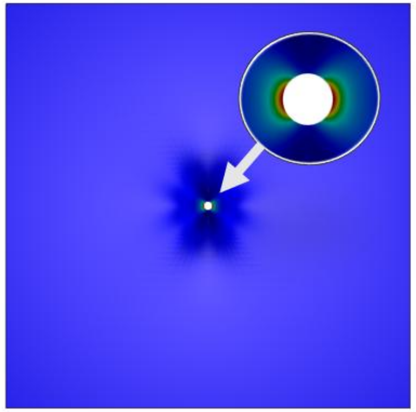

a = 2.5 mm, Total Deformation Strain Energy Density ($10^4$ Pa)

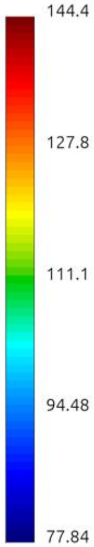
$U_h(\underline{\boldsymbol{\varepsilon}})$



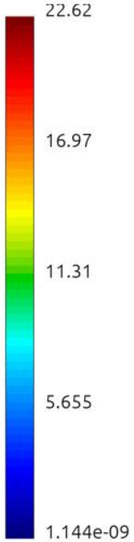




a = 2.5 mm, High Order Deformation Strain Energy Density ($10^4$ Pa)



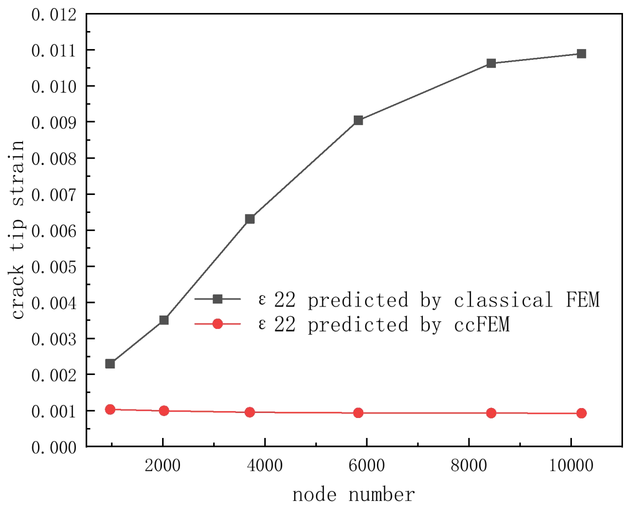


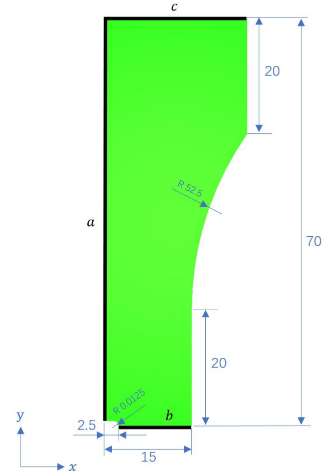

a = 0.2 mm, Total Deformation Strain Energy Density ($10^4$ Pa)


a = 0.2 mm, High Order Deformation Strain Energy Density ($10^4$ Pa)

- Higher fraction of material around the hole deforms when the hole gets smaller
- Higher fraction of higher order strain energy contributes to the total strain energy density
- Singularity dissappears around crack tip



# App 3: Softening in indentation test

Experimental observation:

indentation depth (contact radius) ↑ → E ↓ ,

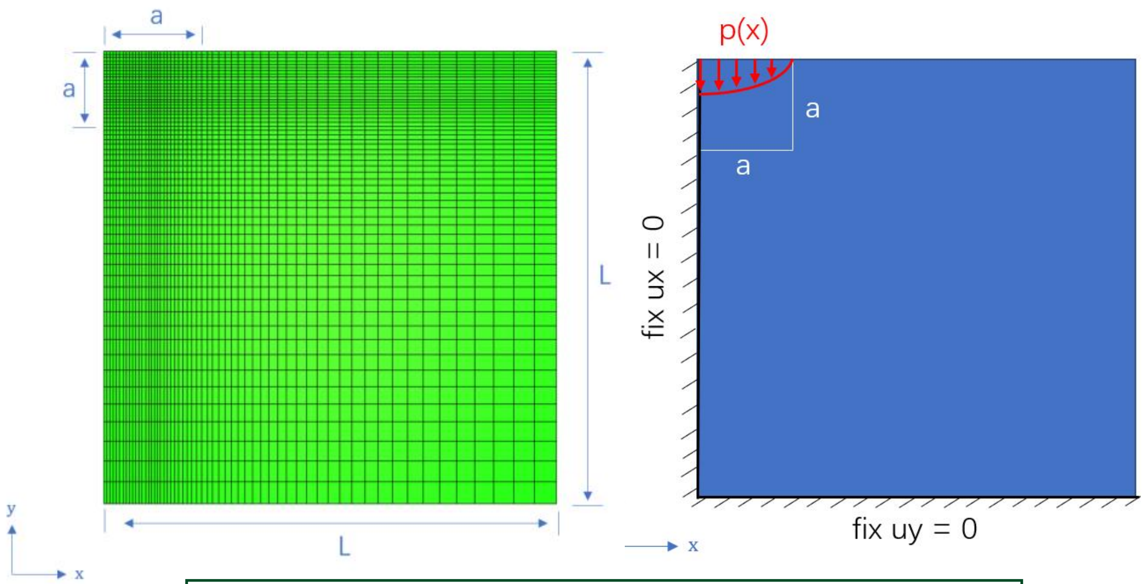
**Softening**

For metals: Geometrically Necessary Dislocation

For elastic material (rubber, ceramic): **?**

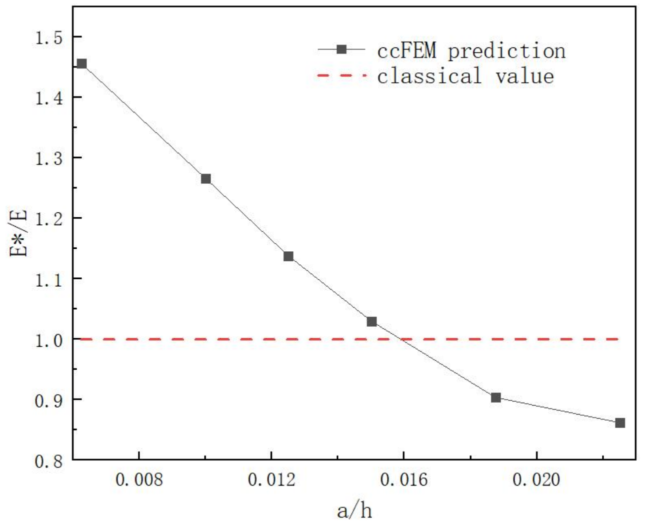
Equivalent contact pressure $p(x)$→ indentation depth $\delta_h$ predicted by ccFEM → Modulus E

Mesh (L=10a) and boundary conditions

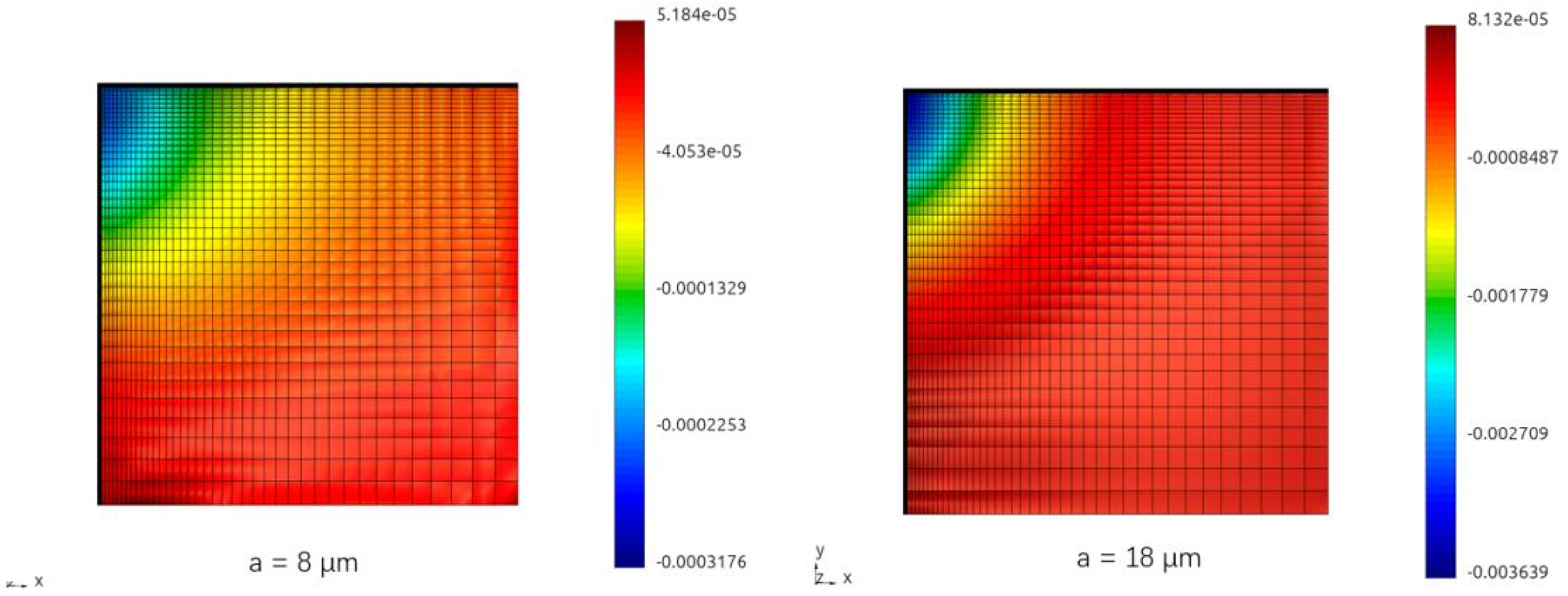



NBR: $E = 10.5$ MPa, $v = 0.44$, $h = 0.8$ mm

# App 3: Predicted results




Variation of the indentation modulus of the sample with contact radius




Higher-order deformation strain energy density distribution of samples at different contact radius ( J/m3)

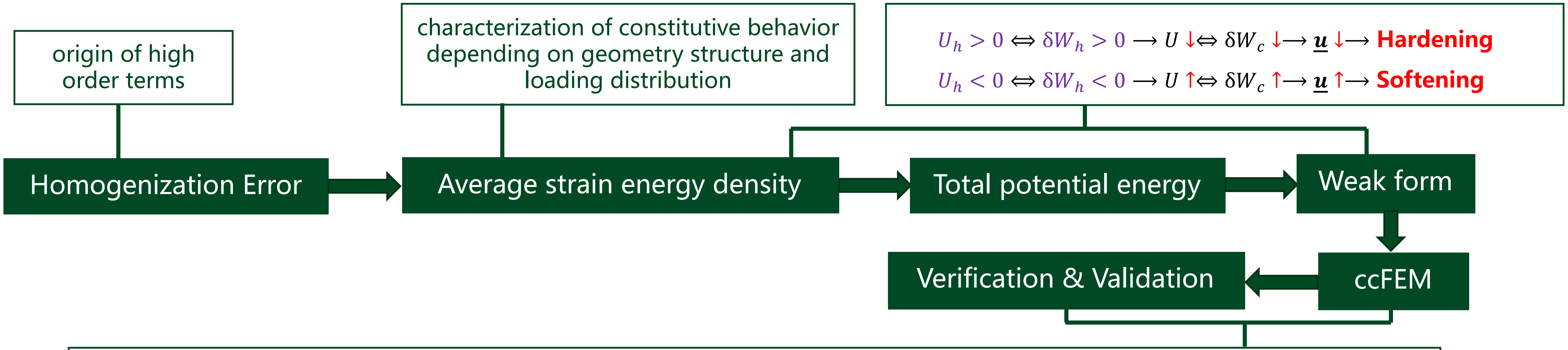
$U_h < 0$ in indented zone, contact radius ↑ → local softening effect ↑ → overall softening effect ↑ → E ↓

- An in-depth analysis relies on contact modeling and stability analysis
- To do next (a good solution: **Tribol**)

# Conclusions and perspectives

# Conclusions

## Development and implementation of Homogenized Energy theory :




- Homogenized Energy theory solves the common problems faced by higher-order deformation theories
- Homogenized Energy theory yields quantitative analysis and reasonable explanation for several typical problems
- FEM within ALM framework is ideal for solving high-order equations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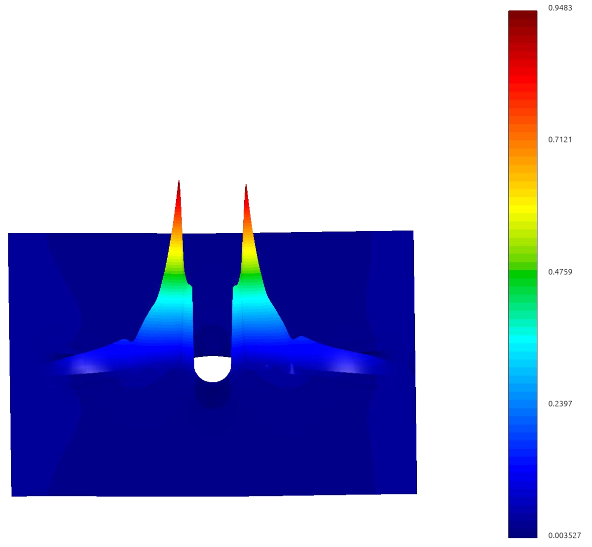
# Perspectives

1. More V&V work for classical problems such as Eshelby inclusion and deformation around the crack tip
2. Combination of phase field fracture theory to achieve accurate prediction of brittle fracture (in progress)
3. Based on the principle of minimum potential energy and maximum dissipation criterion to solve elasto-plastic problems



# Thanks

Collaboration and discussion are welcome

(zhangchy5@mail.sysu.edu.cn)