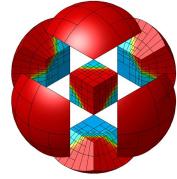




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October 26, 2023

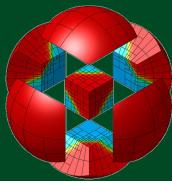


Homogenized Energy Theory for Solution of Elasticity Problems with Consideration of Higher-order Microscopic Deformations

Institute of Nuclear Engineering & Technology,
Sun Yat-Sen University
26/10/2023

Zhang Chunyu, Cao Yuheng, Wang Biao, Sang Meng Sha
(zhangchy5@mail.sysu.edu.cn)



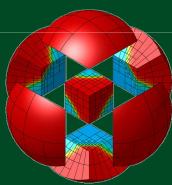


Background

Principles and Implementation

Applications

Conclusions and perspectives

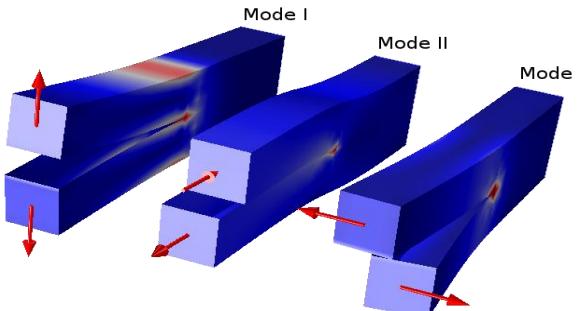


Classical solid mechanics(since 1820s, Cauchy) + Numerical solution techniques(since 1940s) → **Great Success**

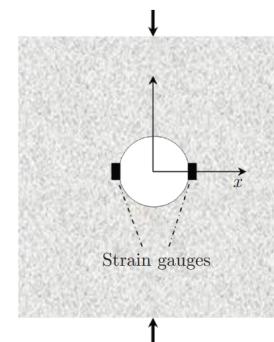
	Formulation	Source
Equilibrium equation	$\nabla \cdot \sigma + b = \rho a$	Newton's second law
Constitutive law	$\sigma = f(\epsilon, \text{state variables})$	Empirical scaling law
Geometric equation	$\epsilon = \frac{1}{2}(\nabla U + \nabla U^T + \dots)$	Continuity requirements
Boundary conditions	$U = \bar{U}, \sigma \cdot n = \bar{t}$	Operation conditions

However, many problems unresolved

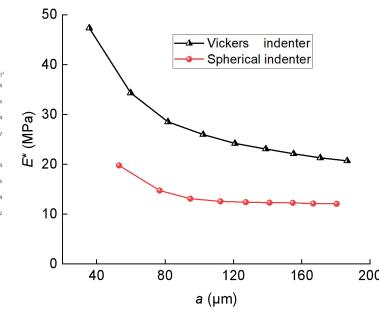
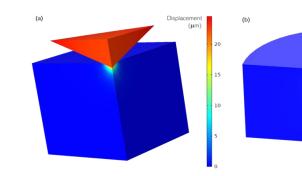
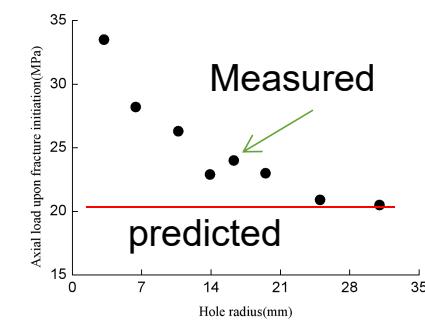
Strain/stress singularity around crack tip

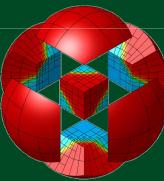


Size effect of stress/strain concentration



Size effect of constitutive parameters





Strain Gradient (Plasticity) Theory

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

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

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

.....

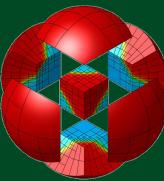
Achievements

Removal of strain/stress singularity

Interpretation of size effect

Removal of mesh-sensitivity

.....



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

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

4. Boundary conditions containing high order terms

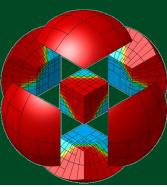
$$\int_{\Omega} \delta W \, dV = \int_{\Omega} f_i \delta u_i \, dV + \int_{\partial\Omega} t_i \delta u_i + r_i n_j \delta u_{i,j} + \boxed{s_{ik} n_k n_l \delta u_{i,kl} \, dS}$$

Principles and Implementation of Homogenized Energy theory

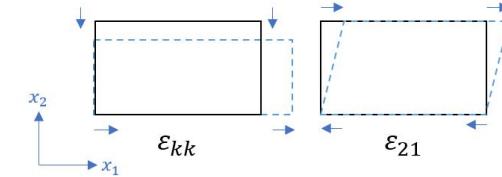
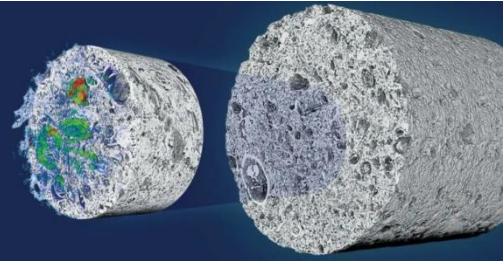
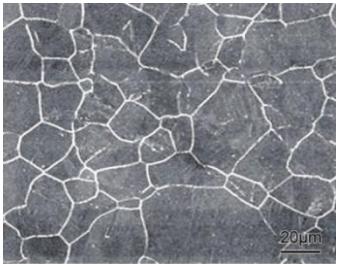
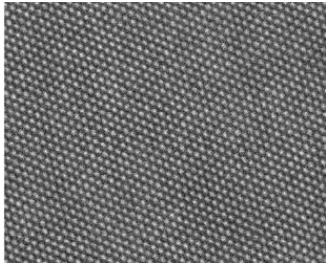


Origin of deficiency of CSM

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Real material: multiscaled and inhomogeneous

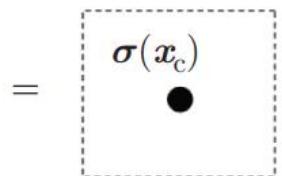
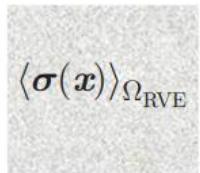


Conventional deformations



Error appears at this stage

Modeled material: ideal continuum

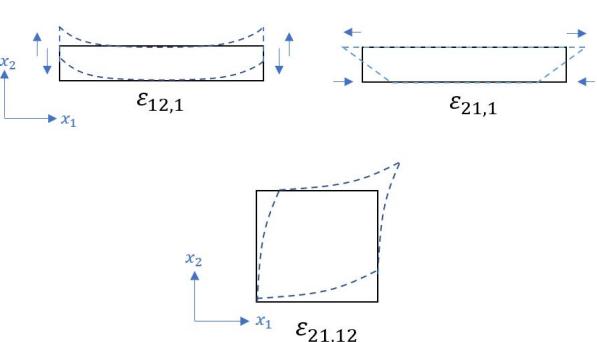


$$\langle \sigma(x) \rangle_{\Omega_{RVE}} = \sigma(x_c)$$

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

$\sigma(x_c)$: representative physical quantities at the RVE barycenter

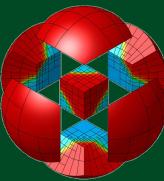
modeled material
≠
real material



High order deformations



Structural deformation



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

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

Eg. a scalar field U

$$\bar{U} \equiv \langle U \rangle_{\Omega_{RVE}} = \frac{1}{h^3} \iiint_{-\frac{h}{2}}^{\frac{h}{2}} \left(U + \vec{\nabla} U \cdot \underline{x} + \frac{1}{2} (\vec{\nabla}^2 U : \underline{x}) : \underline{x} + \dots \right) dx_1 dx_2 dx_3 = U + \frac{h^2}{24} \Delta U + \frac{h^4}{1920} \Delta^2 U + \frac{h^4}{2880} U_{,kkll(k \neq l)} \dots$$

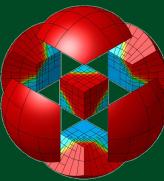
with h : RVE size

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

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Homogenized strain energy density:

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

$$\begin{aligned}\bar{U}(\underline{\varepsilon}) = & \left[\frac{\lambda}{2} \varepsilon_{ii} \varepsilon_{jj} + \mu \varepsilon_{ij}^2 \right] + \left[\frac{\lambda}{2} \left(\frac{h^2}{12} (\varepsilon_{ii} \varepsilon_{jj,kk} + \varepsilon_{ii,k} \varepsilon_{jj,k}) + \frac{h^4}{4} \left(\frac{1}{144} \varepsilon_{ii,kk} \varepsilon_{jj,ll} + \frac{1}{72} \varepsilon_{ii,kl} \varepsilon_{jj,kl} - \frac{1}{120} \varepsilon_{ii,kk} \varepsilon_{jj,kk} \right) \right) \right. \\ & \left. + \mu \left(\frac{h^2}{12} (\varepsilon_{ij,k}^2 + \varepsilon_{ij} \varepsilon_{ij,kk}) + \frac{h^4}{4} \left(\frac{1}{144} \varepsilon_{ij,kk} \varepsilon_{ij,ll} + \frac{1}{72} \varepsilon_{ij,kl} \varepsilon_{ij,kl} - \frac{1}{120} \varepsilon_{ij,kk} \varepsilon_{ij,kk} \right) \right) \right]\end{aligned}$$

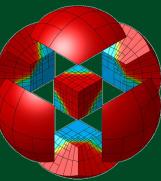
- Homogenized strain energy density = conventional strain energy density + **higher order strain energy density**
- Higher order strain energy density

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

$$U_h > 0 \text{ or } U_h < 0$$

local hardening or softening





Total potential energy functional:

$$\mathcal{J}_c(\underline{\mathbf{u}}) = \int_{\Omega} U(\underline{\boldsymbol{\varepsilon}}) + \mathbf{U}_h(\underline{\boldsymbol{\varepsilon}}) dV - \int_{\Omega} \underline{\mathbf{u}} \cdot \underline{\mathbf{f}_b} dV - \int_{\partial\Omega} \underline{\mathbf{u}} \cdot \underline{\mathbf{t}} dS$$



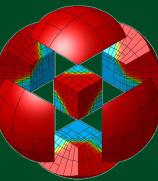
Minimization by variation

$$\int_{\Omega} \frac{\delta(U(\underline{\boldsymbol{\varepsilon}}) + \mathbf{U}_h(\underline{\boldsymbol{\varepsilon}}))}{\delta \underline{\mathbf{u}}} dV = \int_{\Omega} \underline{\mathbf{f}_b} \cdot \delta \underline{\mathbf{u}} dV + \int_{\partial\Omega} \underline{\mathbf{t}} \cdot \delta \underline{\mathbf{u}} dS$$

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

Treatment of second order gradient of strain

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

$$\begin{aligned} \forall \underline{\underline{\underline{v}}} \in \mathcal{H}^1(\Omega), \int_{\Omega} \frac{\lambda}{2} \underline{\underline{\underline{I}}}\underline{\underline{\underline{I}}} : & \left(2\underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \left(\underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \right)^T \right. \\ & + \frac{h^2}{12} \left(\underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \left(\Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \right)^T + \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \left(\Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \right)^T + 2 \left(\vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \right) \left(\vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \right)^T \right) \\ & + \frac{h^4}{4} \left(\frac{1}{72} \left(\Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \right) \left(\Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \right)^T + \frac{1}{36} \left(\left(\vec{\nabla}^2 \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \right) : \left(\vec{\nabla}^2 \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \right)^T \right) \right. \\ & \left. - \frac{1}{60} \left(\vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \underline{\underline{\nabla_d}} \right) \left(\vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \underline{\underline{\nabla_d}} \right)^T \right) \right) \\ & + \mu \left(2\underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \cdot \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} + \frac{h^2}{12} \left(\underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \cdot \Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} + \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \cdot \Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} + 2 \vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} : \vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \right) \right. \\ & + \frac{h^4}{4} \left(\frac{1}{72} \Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \cdot \Delta \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} + \frac{1}{36} \vec{\nabla}^2 \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} : \vec{\nabla}^2 \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \right. \\ & \left. \left. - \frac{1}{60} \left(\vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{u}}} \underline{\underline{\nabla_d}} \right) : \left(\vec{\nabla} \underline{\underline{\nabla_s}} \underline{\underline{\underline{v}}} \underline{\underline{\nabla_d}} \right) \right) \right) dV - \int_{\Omega} \underline{\underline{\underline{v}}} \cdot \underline{\underline{\underline{f_b}}} dV - \int_{\partial\Omega} \underline{\underline{\underline{v}}} \cdot \underline{\underline{\underline{t}}} dS = 0 \end{aligned}$$

Challenge for numerical solution:

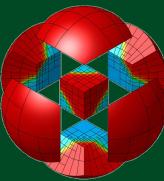
1. Evaluation of high order gradients
2. High order finite element

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

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The constraint: $\underline{\underline{\varepsilon}} = \underline{\underline{\nabla_s u}}$

$$\begin{aligned} \mathcal{J}_{ALM}(\underline{\underline{u}}, \underline{\underline{\varepsilon}}, \underline{\lambda}) &= \int_{\Omega} U(\underline{\underline{\varepsilon}}) + U_h(\underline{\underline{\varepsilon}}) dV - \int_{\Omega} \underline{\underline{u}} \cdot \underline{\underline{f_b}} dV - \int_{\partial\Omega} \underline{\underline{u}} \cdot \underline{\underline{t}} dS \\ &\quad + \int_{\Omega} \underline{\lambda} \cdot (\underline{\underline{\nabla_s u}} - \underline{\underline{\varepsilon}}) dV + \int_{\Omega} \frac{r}{2} (\underline{\underline{\nabla_s u}} - \underline{\underline{\varepsilon}}) \cdot (\underline{\underline{\nabla_s u}} - \underline{\underline{\varepsilon}}) dV \end{aligned}$$

[Fortin, Glowinski, Mercier, 1983]

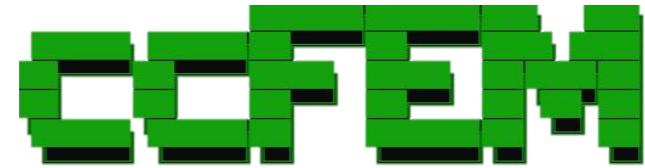
$\underline{\lambda}$: Lagrangian multiplier r : penalty parameter

Solution procedure

$$\begin{cases} \frac{\delta \mathcal{J}_{ALM}(\underline{\underline{u}}, \underline{\underline{\varepsilon}}, \underline{\lambda})}{\delta \underline{\underline{u}}} = 0 \\ \frac{\delta \mathcal{J}_{ALM}(\underline{\underline{u}}, \underline{\underline{\varepsilon}}, \underline{\lambda})}{\delta \underline{\underline{\varepsilon}}} = 0 \\ \frac{\delta \mathcal{J}_{ALM}(\underline{\underline{u}}, \underline{\underline{\varepsilon}}, \underline{\lambda})}{\delta \underline{\lambda}} = 0 \end{cases} \xrightarrow{\text{Discretization}} \begin{pmatrix} \underline{\underline{K_{uu}}} & \underline{\underline{K_{u\varepsilon}}} & \underline{\underline{K_{u\lambda}}} \\ \underline{\underline{K_{\varepsilon u}}} & \underline{\underline{K_{\varepsilon\varepsilon}}} & \underline{\underline{K_{\varepsilon\lambda}}} \\ \underline{\underline{K_{\lambda u}}} & \underline{\underline{K_{\varepsilon\lambda}}} & 0 \end{pmatrix} \begin{pmatrix} \underline{\underline{u_N}} \\ \underline{\underline{\varepsilon_N}} \\ \underline{\underline{\lambda_N}} \end{pmatrix} = \begin{pmatrix} \underline{\underline{B_{uf}}} \\ 0 \\ 0 \end{pmatrix} \xrightarrow{\text{UMF (linear solver)}} \underline{\underline{u}}, \underline{\underline{\varepsilon}}, \underline{\lambda} \xrightarrow{\text{post-processing}} \overline{U}, U_h, \frac{U_h}{\overline{U}}$$

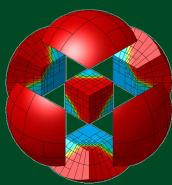
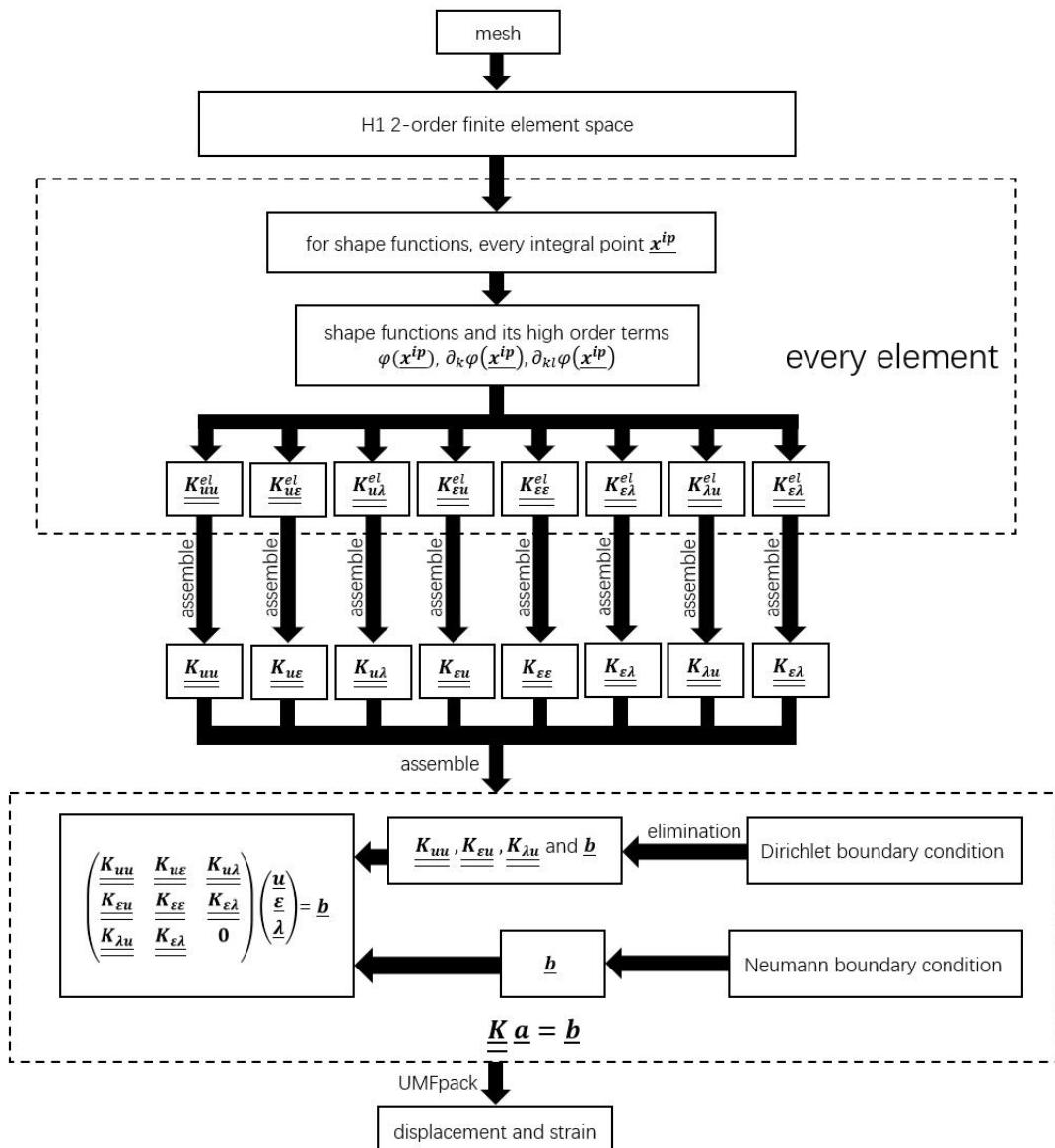
Cao Yuheng, Zhang Chunyu, Wang Biao. A New High-order Deformation Theory and Solution Procedure Based on Homogenized Strain Energy Density, International journal of engineering science, accepted, 2023.

The solver



- 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 Trilinear3DFiniteElement
fe_base	default CalcPhysHessian and CalcPhysLaplacian in fe_base are suitable only for NURBS elements. CalcPhysHessian and CalcPhysLaplacian are redefined for other types of elements
ALMElasticityIntegrator	Multiple BilinearFormIntegrator are defined for $K_{uu}, K_{ue}, K_{u\lambda}, K_{\varepsilon u}, K_{\varepsilon \lambda} \dots$

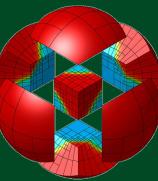


Applications



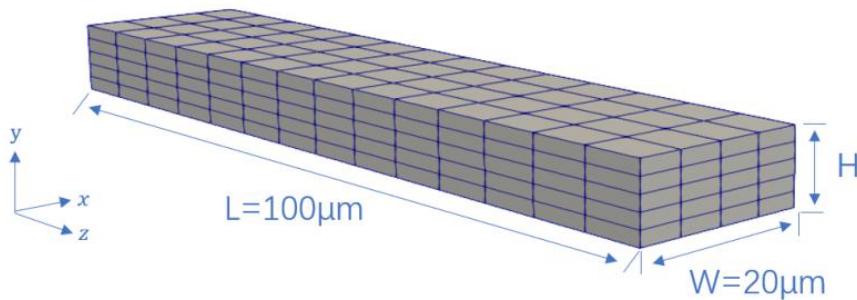
App 1: Hardening of micro-cantilever beam bending

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Experimental observation: $H \downarrow \rightarrow E^* \uparrow \rightarrow$ Hardening

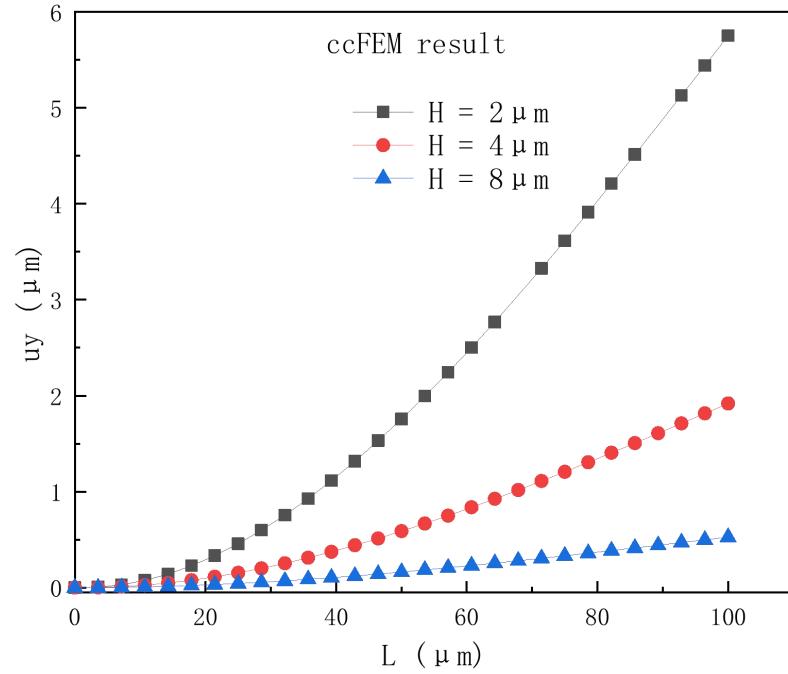
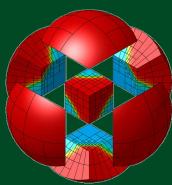
Mesh and boundary conditions of the model



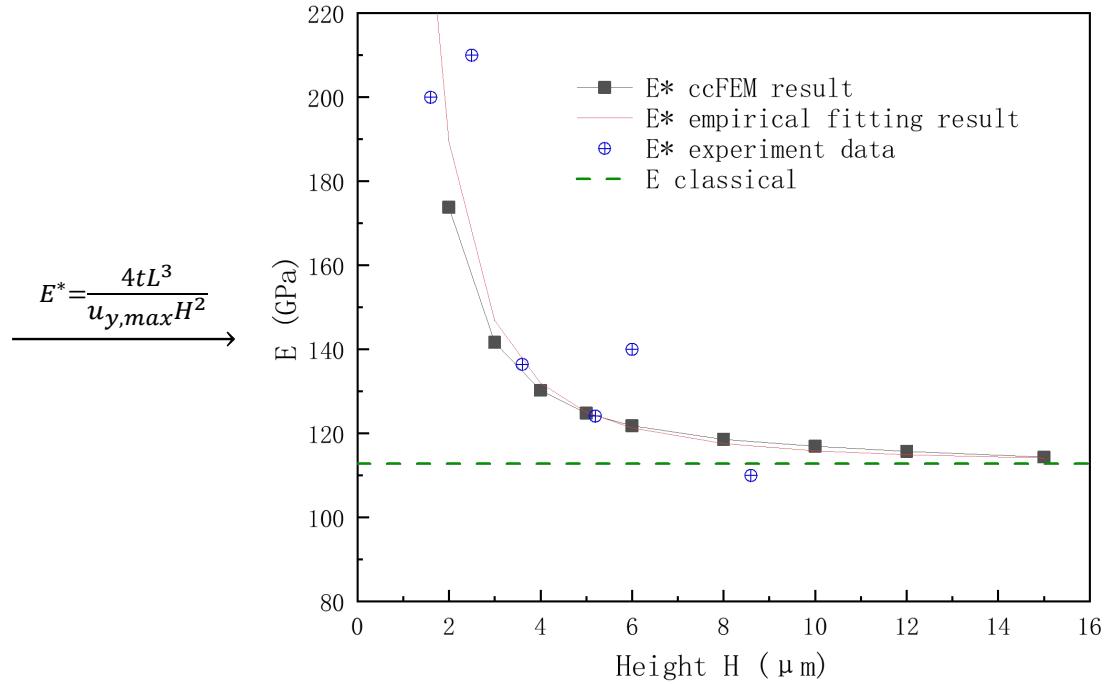
single crystal Cu : $E = 112.8 \text{ GPa}$, $\nu = 0.343$, $h = 1.4 \mu\text{m}$

App 1: Predicted results by ccFEM

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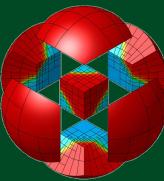
Variation of bending displacement along the length of the beam for different beam thicknesses



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

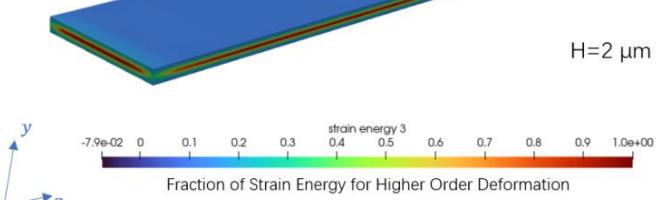
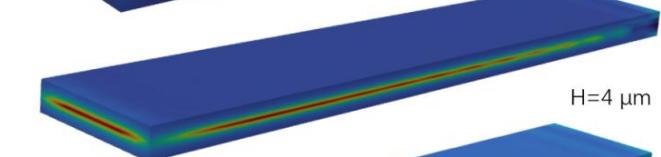
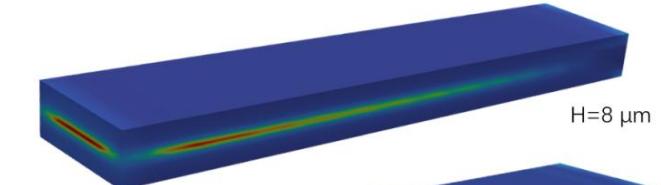
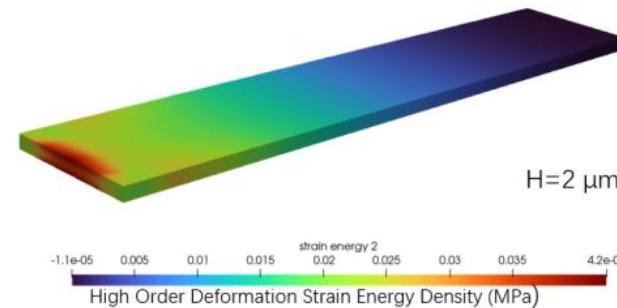
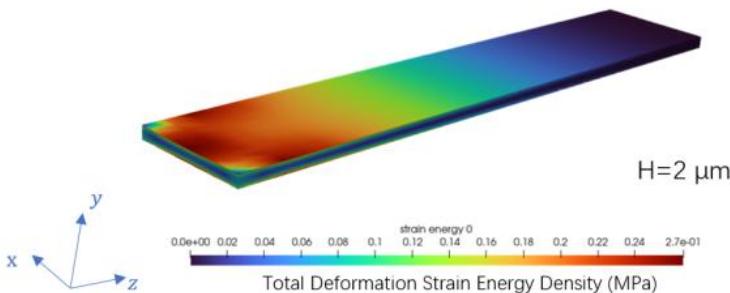
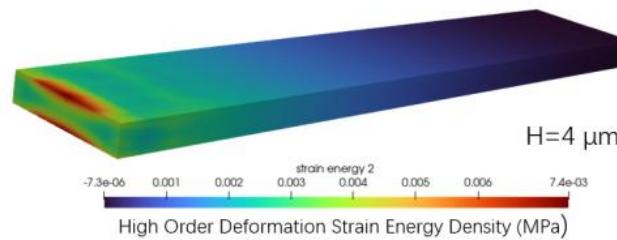
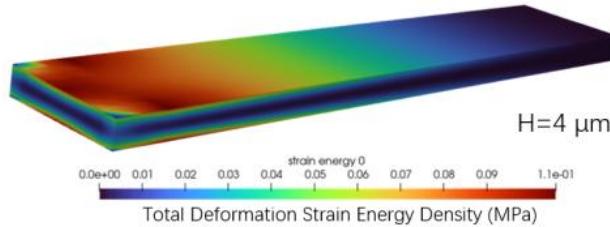
App 1: Analysis from the energy perspective

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

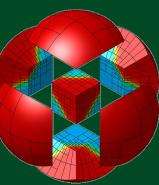
Non-uniform distribution of strain along x axis ↑ as H ↓



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

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

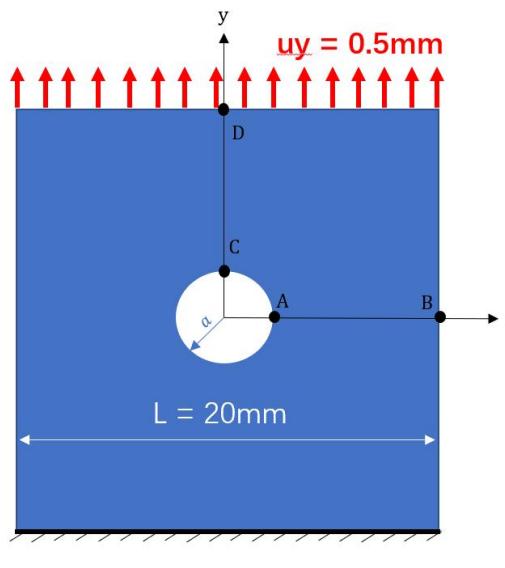
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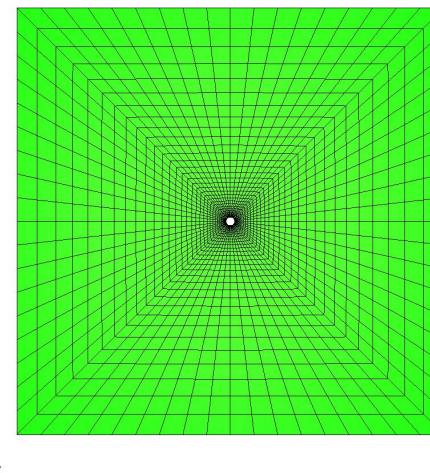
Classical solution in textbook:

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

Mesh and boundary conditions for the model:

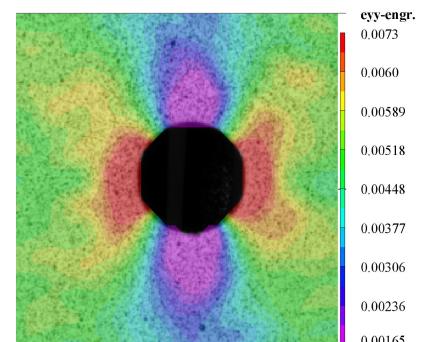
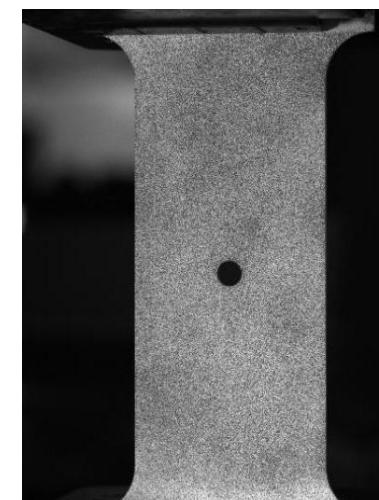


Polymethyl methacrylate (PMMA):
 $E = 3.35 \text{ GPa}$, $\nu = 0.35$, $h = 0.85 \text{ mm}$



Experimental observation: $a \downarrow \rightarrow K \downarrow$

Measurement of strain by Digital Image Correlation (DIC) technology

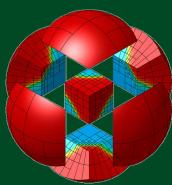


Two types of defects:



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

MFEM Community Workshop
October 26, 2023

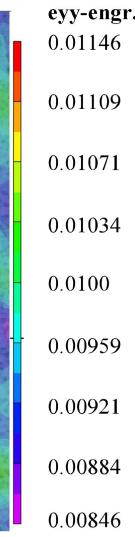
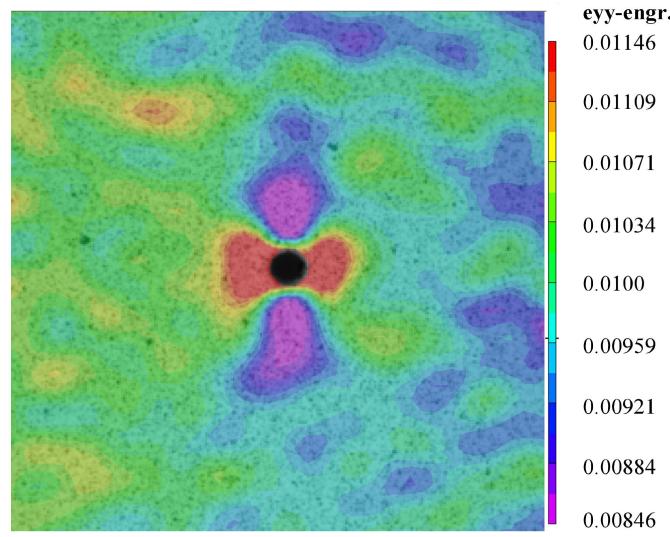


ABAQUS

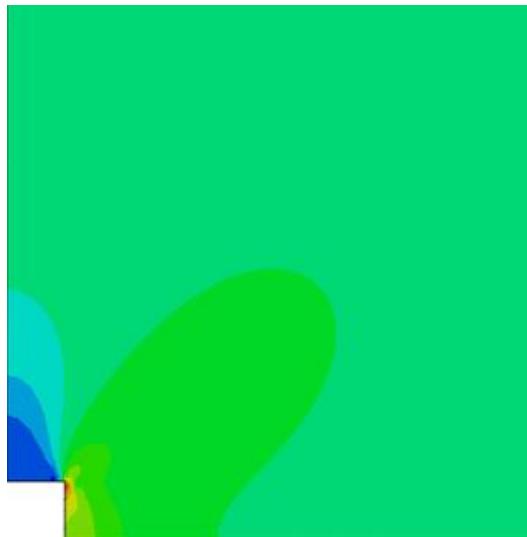
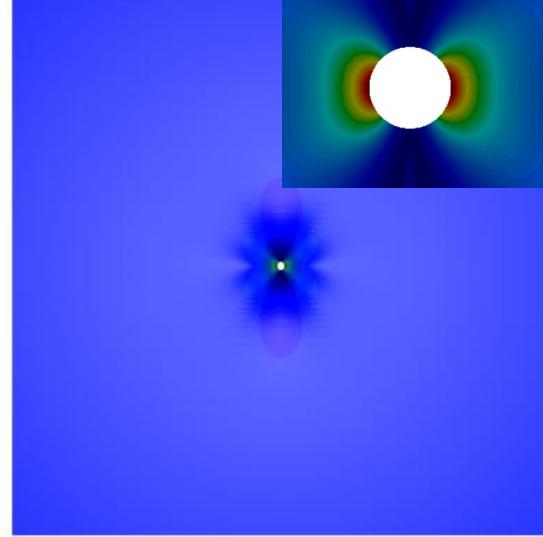


$a=0.2\text{mm}$

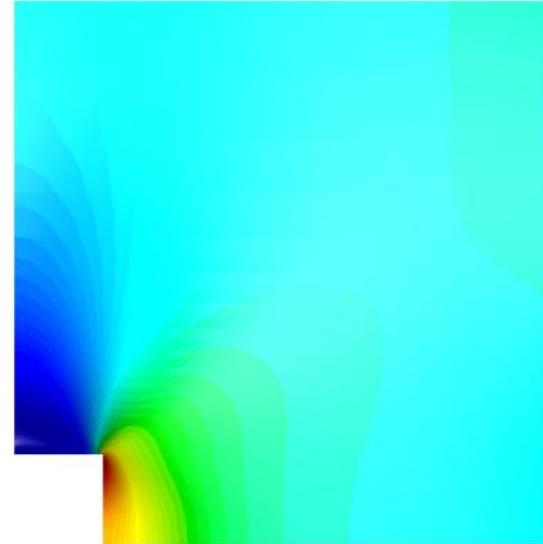
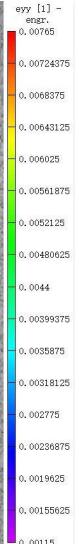
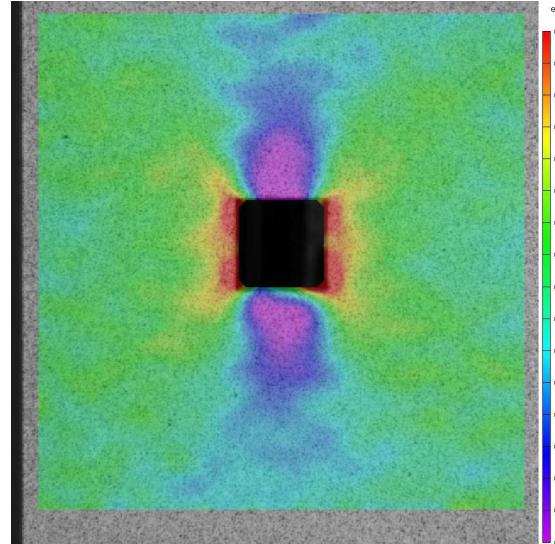
DIC



ccFEM

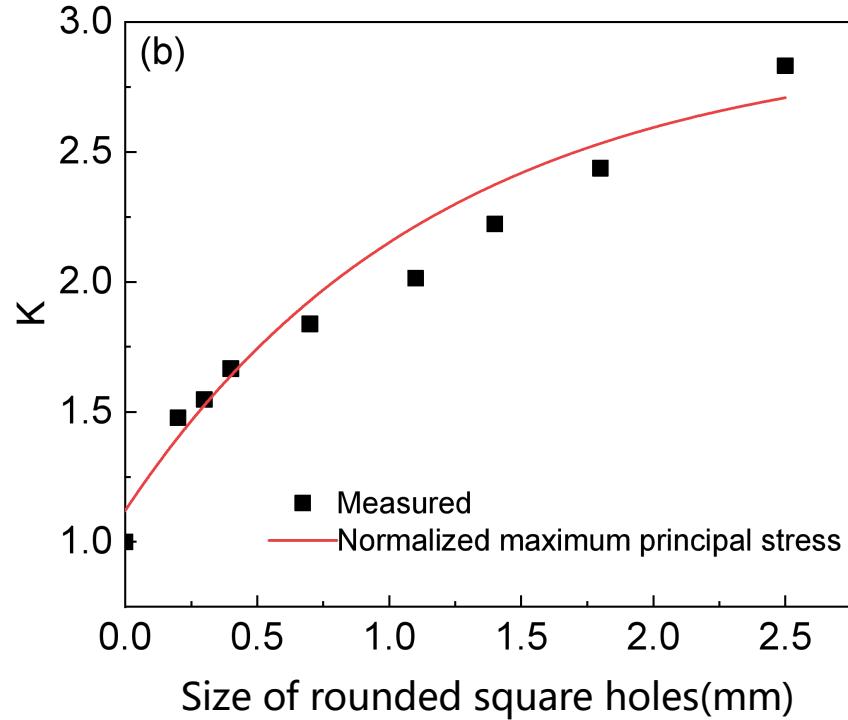
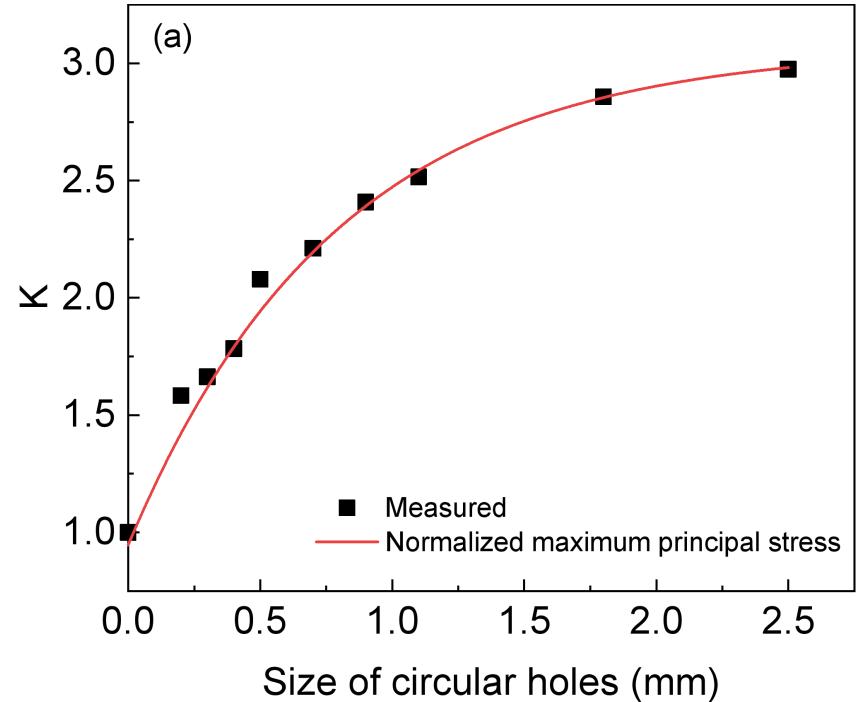
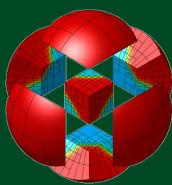


$a=2.5\text{mm}$



App 2: Predicted results by ccFEM

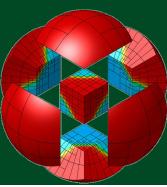
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October 26, 2023



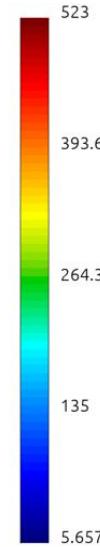
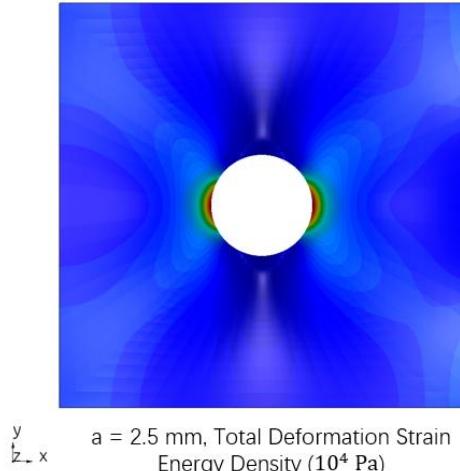
Sang Mengsha, Zhang Chunyu, Cao Yuheng, Wang Biao. Experimental and Theoretical Evaluation of Influence of Hole size on Deformation and Fracture of Elastic Perforated Plate, Mechanics of Materials, 2023, accepted

App 2: Analysis from the energy perspective

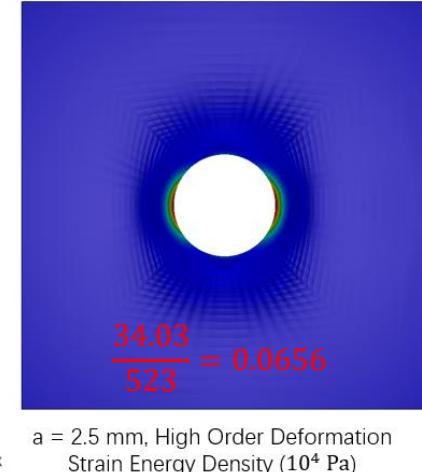
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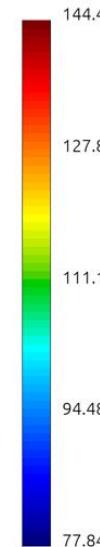
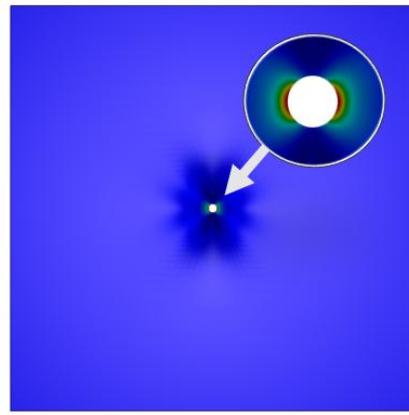
$$U(\underline{\varepsilon}) + U_h(\underline{\varepsilon})$$



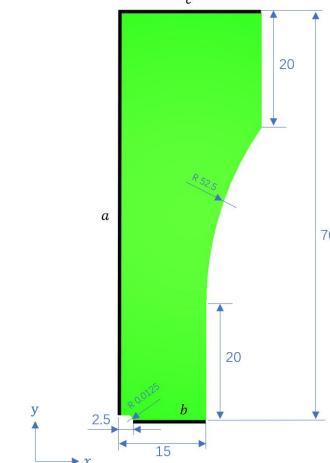
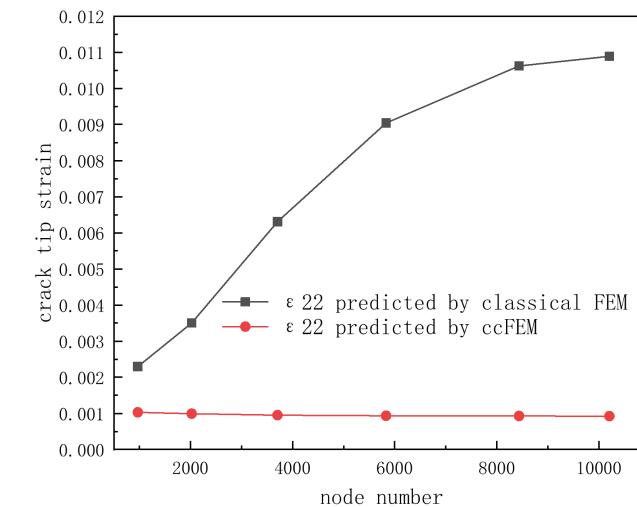
$$U_h(\underline{\varepsilon})$$



y
 z
 x

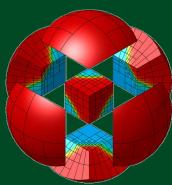


- Higher fraction of material around the hole deforms when the hole gets smaller
- Higher fraction of higher order strain energy contributes to the total strain energy density
- Singularity disappears around crack tip



App 3: Softening in indentation test

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Experimental observation:

indentation depth (contact radius) $\uparrow \rightarrow E \downarrow$,

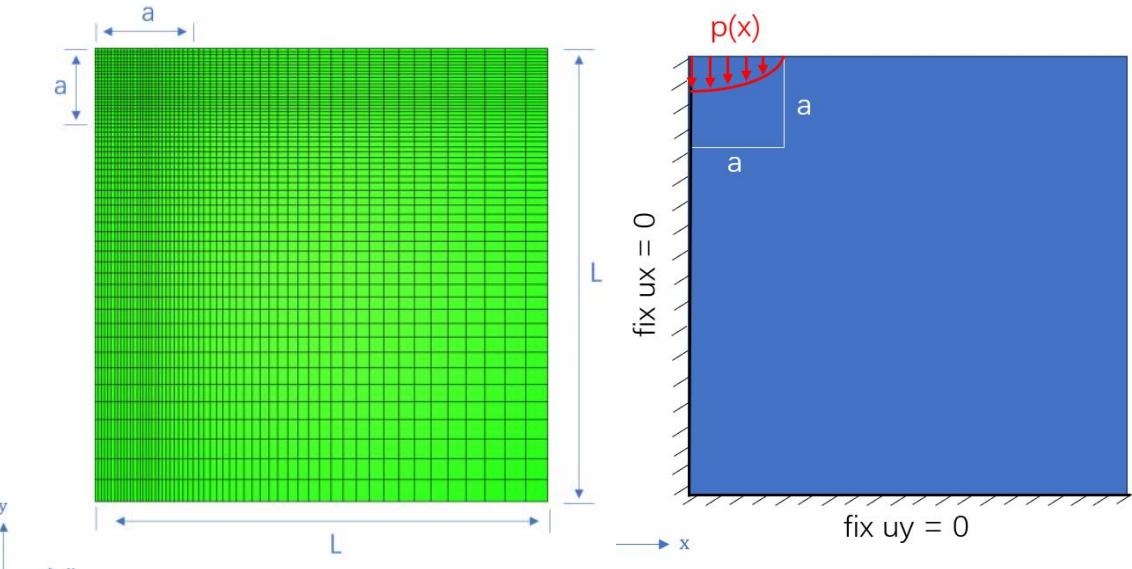
Softening

For metals: Geometrically Necessary Dislocation

For elastic material (rubber, ceramic): ?

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

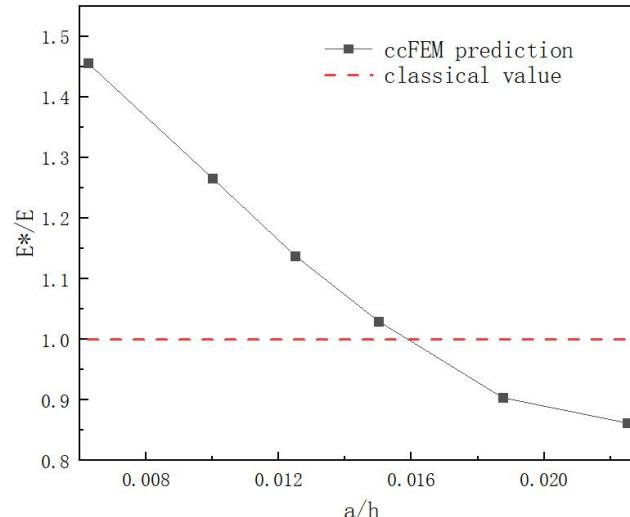
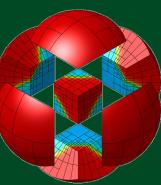
Mesh ($L=10a$) and boundary conditions



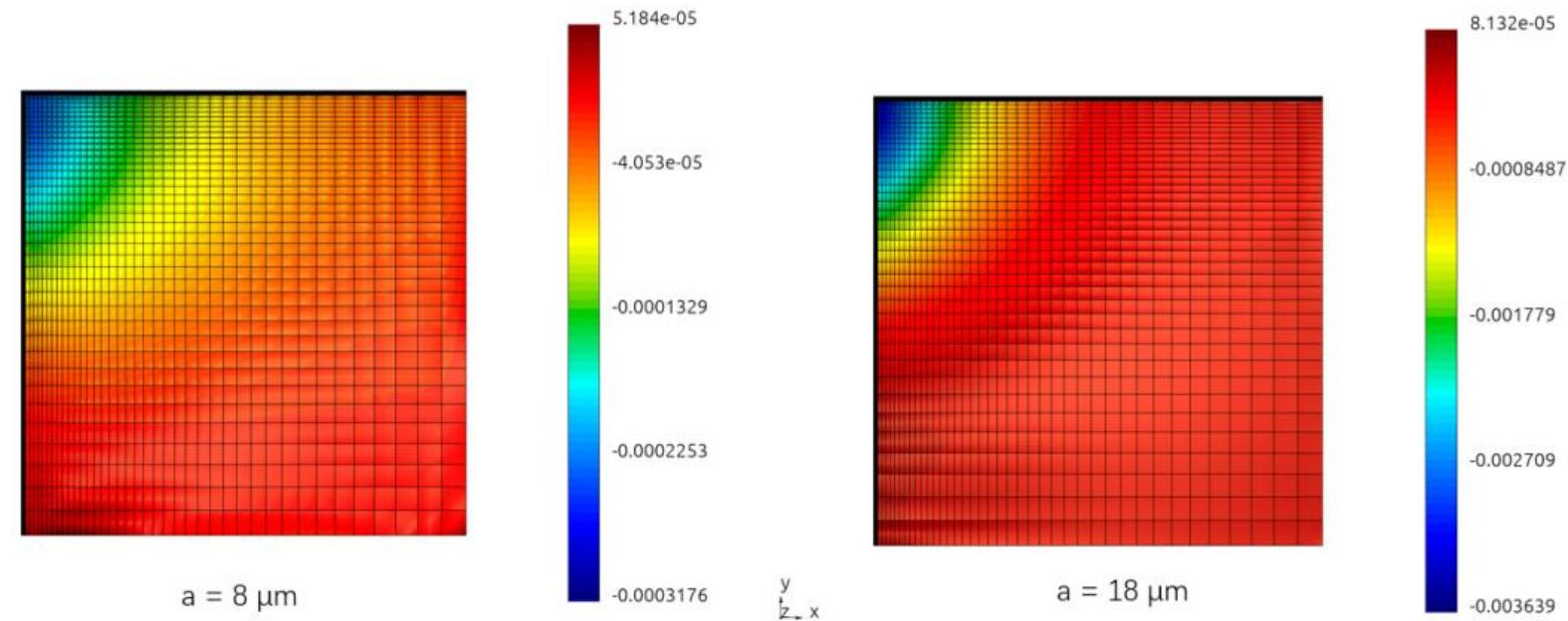
NBR: $E = 10.5$ MPa, $\nu = 0.44$, $h = 0.8$ mm

App 3: Predicted results

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October 26, 2023



Variation of the indentation modulus of the sample with contact radius



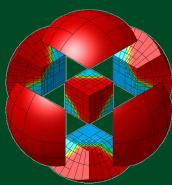
Higher-order deformation strain energy density distribution of samples at different contact radius (J/m³)

$U_h < 0$ in indented zone, contact radius $\uparrow \rightarrow$ local softening effect $\uparrow \rightarrow$ overall softening effect $\uparrow \rightarrow E \downarrow$

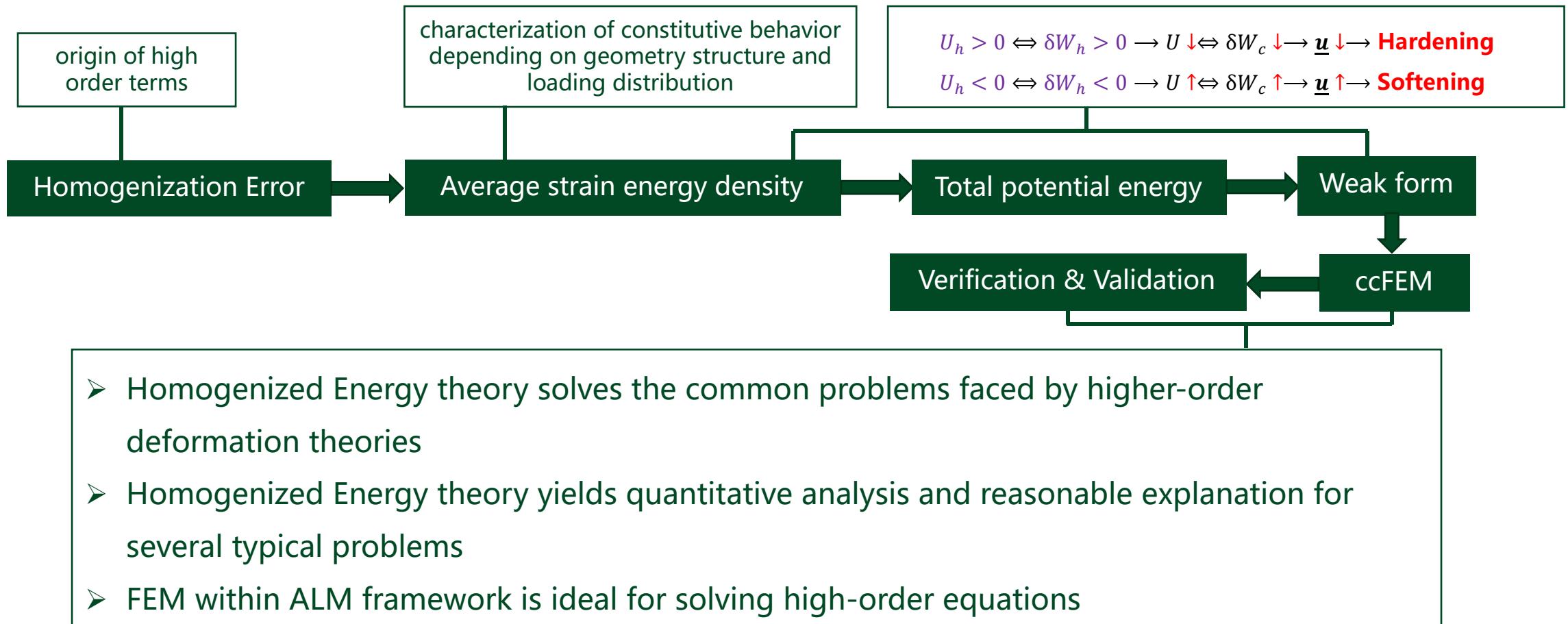
- An in-depth analysis relies on contact modeling and stability analysis
- To do next (a good solution: **Tribol**)

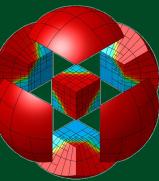
Conclusions and perspectives



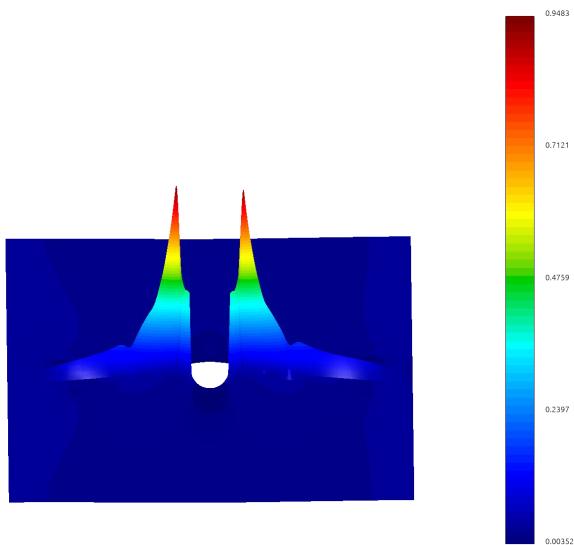


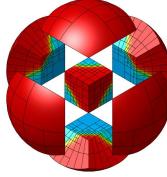
Development and implementation of Homogenized Energy theory :





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
[\(zhangchy5@mail.sysu.edu.cn\)](mailto:zhangchy5@mail.sysu.edu.cn)

