Constitutive equations

- Scalar microstress ϖ conjugate to $\dot{\mathsf{d}}$

$$\varpi = \underbrace{\frac{\partial \hat{\psi}_{\mathsf{R}}(\mathbf{\Lambda})}{\partial \mathsf{d}}}_{\varpi_{\mathsf{en}}} + \underbrace{\alpha + \zeta \dot{\mathsf{d}}}_{\varpi_{\mathsf{diss}}},$$

with $\alpha = \hat{\alpha}(\mathbf{\Lambda})$ and $\zeta = \hat{\zeta}(\mathbf{\Lambda})$ positive-valued scalar functions.

- Vector microstress $\boldsymbol{\xi}$ conjugate to $\nabla\dot{\mathsf{d}}$

$$\boldsymbol{\xi} = \frac{\partial \hat{\psi}_{\mathsf{R}}(\mathbf{\Lambda})}{\partial \nabla \mathsf{d}}.$$

This is taken to be energetic, with no dissipative contribution.

Governing pdes

1. **Equilibrium equation**:

$$\boxed{\mathrm{Div}\,\mathbf{T}_{\mathrm{R}} + \mathbf{b}_{0\mathrm{R}} = \mathbf{0},}$$

   where $\mathbf{b}_{0\mathrm{R}}$ is a non-inertial body force.

2. **Microforce balance**:

   The microforces ϖ and $\boldsymbol{\xi}$ obey the balance,

$$\mathrm{Div}\,\boldsymbol{\xi} - \varpi = 0.$$

   This microforce balance, together with the thermodynamically consistent constitutive equations for ϖ and $\boldsymbol{\xi}$ gives the evolution equation for the damage variable d,

$$\boxed{\hat{\zeta}(\boldsymbol{\Lambda})\dot{d} = \left\langle -\frac{\partial\hat{\psi}_{\mathrm{R}}(\boldsymbol{\Lambda})}{\partial d} + \mathrm{Div}\left(\frac{\partial\hat{\psi}_{\mathrm{R}}(\boldsymbol{\Lambda})}{\partial\nabla d}\right) - \hat{\alpha}(\boldsymbol{\Lambda})\right\rangle.}$$

   Since ζ is positive-valued, the right hand side of the equation above must be positive for $\dot{\mathrm{d}}$ to be positive and the damage to increase monotonically.

Boundary and initial conditions

1. Boundary conditions for the pde governing the evolution of χ:

$$\left.\begin{aligned} \chi &= \breve{\chi} \quad \text{on } \mathcal{S}_{\chi} \times [0,T], \\ \mathrm{T}_{\mathrm{R}}\mathrm{n}_{\mathrm{R}} &= \breve{\mathrm{t}}_{\mathrm{R}} \quad \text{on } \mathcal{S}_{\mathrm{t}_{\mathrm{R}}} \times [0,T]. \end{aligned}\right\}$$

2. Boundary conditions for the pde governing the evolution of d:

$$\begin{aligned} \dot{\mathrm{d}} &= 0 \quad \text{on } \mathcal{S}_{\mathrm{d}} \times [0,T], \\ \nabla \mathrm{d} \cdot \mathrm{n}_{\mathrm{R}} &= 0 \quad \text{on } \partial \mathrm{B} \setminus \mathcal{S}_{\mathrm{d}} \times [0,T]. \end{aligned}$$

The initial data is taken as

$$\chi(\mathrm{X},0) = \mathrm{X}, \quad \text{and} \quad \mathrm{d}(\mathrm{X},0) = 0. \quad \text{in} \quad \mathrm{B}.$$

Specialization of the constitutive equations

- Replace chain stretch with distortional effective stretch and allow for slight compressibility:

$$\bar{\lambda} = \sqrt{\frac{\operatorname{tr}\bar{\mathbf{C}}}{3}}$$ distortional effective stretch $\quad$ $J = \det \mathbf{F}$ volumetric Jacobian

- Entropy density: $$\boxed{\eta_{\mathsf{R}} = \hat{\eta}_{\mathsf{R}}(\bar{\lambda}, \lambda_b) = -N k_B n \left[\left(\frac{\bar{\lambda}\lambda_b^{-1}}{\sqrt{n}} \right) \beta + \ln \left(\frac{\beta}{\sinh \beta} \right) \right] \qquad \beta = \mathcal{L}^{-1}\left(\frac{\bar{\lambda}\lambda_b^{-1}}{\sqrt{n}} \right)}$$

  - N number of chains per unit reference volume
  - n number of links in each chain

- Internal energy density: $$\boxed{\hat{\varepsilon}_{\mathsf{R}}(\lambda_b, J, d, \nabla d) = (1-d)^2 \hat{\varepsilon}_{\mathsf{R}}^0(\lambda_b, J) + \hat{\varepsilon}_{\mathsf{R,nonloc}}(\nabla d).}$$

$$\hat{\varepsilon}_{\mathsf{R}}^0(\lambda_b, J) = \frac{1}{2}\bar{E}_b(\lambda_b - 1)^2 + \frac{1}{2}K(J-1)^2,$$

$\bar{E}_b = N\, n\, E_b$ — net bond stiffness

K — bulk modulus

$$\hat{\varepsilon}_{\mathsf{R,nonloc}}(\nabla \mathrm{d}) = \frac{1}{2}\varepsilon_{\mathsf{R}}^f\, \ell^2\, |\nabla \mathrm{d}|^2\,,$$

$\varepsilon_{\mathsf{R}}^f = N n \varepsilon_b^f$ — net bond dissoc. energy

ℓ — intrinsic length scale

- Bond deformation stretch still given by local free energy minimization $$\boxed{\frac{\partial \psi_{\mathsf{R}}}{\partial \lambda_b} = 0.}$$

Evolution equation for damage variable

- Scalar microforce:

$$\varpi = 2(1-d)\varepsilon^0(\lambda_b, J) + \varepsilon_{\mathsf{R}}^f + \zeta\dot{d}$$

$\varepsilon_{\mathsf{R}}^f \overset{\text{def}}{=} Nn\varepsilon_b^f$ net dissociation energy $\quad \zeta > 0$ viscous regularization parameter

- Vector microforce: $\quad \boldsymbol{\xi} = \varepsilon_{\mathsf{R}}^f \ell^2 \nabla \mathrm{d}$

- Microforce balance, $\mathrm{Div}\,\boldsymbol{\xi} - \varpi = \mathbf{0}$: $\quad \zeta\dot{\mathrm{d}} = 2(1-d)\varepsilon^0(\lambda_b, J) - \varepsilon_{\mathsf{R}}^f + \varepsilon_{\mathsf{R}}^f \ell^2 \nabla \mathrm{d}$

- To enforce $\mathrm{d} \in [0,1]$: $\quad \zeta\dot{d} = 2(1-\mathrm{d})\left\langle \hat{\varepsilon}_{\mathsf{R}}^0(\lambda_b, J) - \varepsilon_{\mathsf{R}}^f/2 \right\rangle - \varepsilon_{\mathsf{R}}^f\left[d - \ell^2 \Delta \mathrm{d}\right],$

  and to account for the irreversible nature of chain scission $\dot{\mathrm{d}} \geq 0$, we introduce

$$\mathcal{H}(t) \overset{\text{def}}{=} \max_{s\in[0,t]} \left\langle \hat{\varepsilon}_{\mathsf{R}}^0(\lambda_b(s), J(s)) - \varepsilon_{\mathsf{R}}^f/2 \right\rangle.$$

- Then the evolution equation for d may be written as

$$\boxed{\zeta\dot{d} = \left\langle 2(1-d)\mathcal{H} - \varepsilon_{\mathsf{R}}^f\left[d - \ell^2 \Delta \mathrm{d}\right] \right\rangle.}$$

Governing pdes

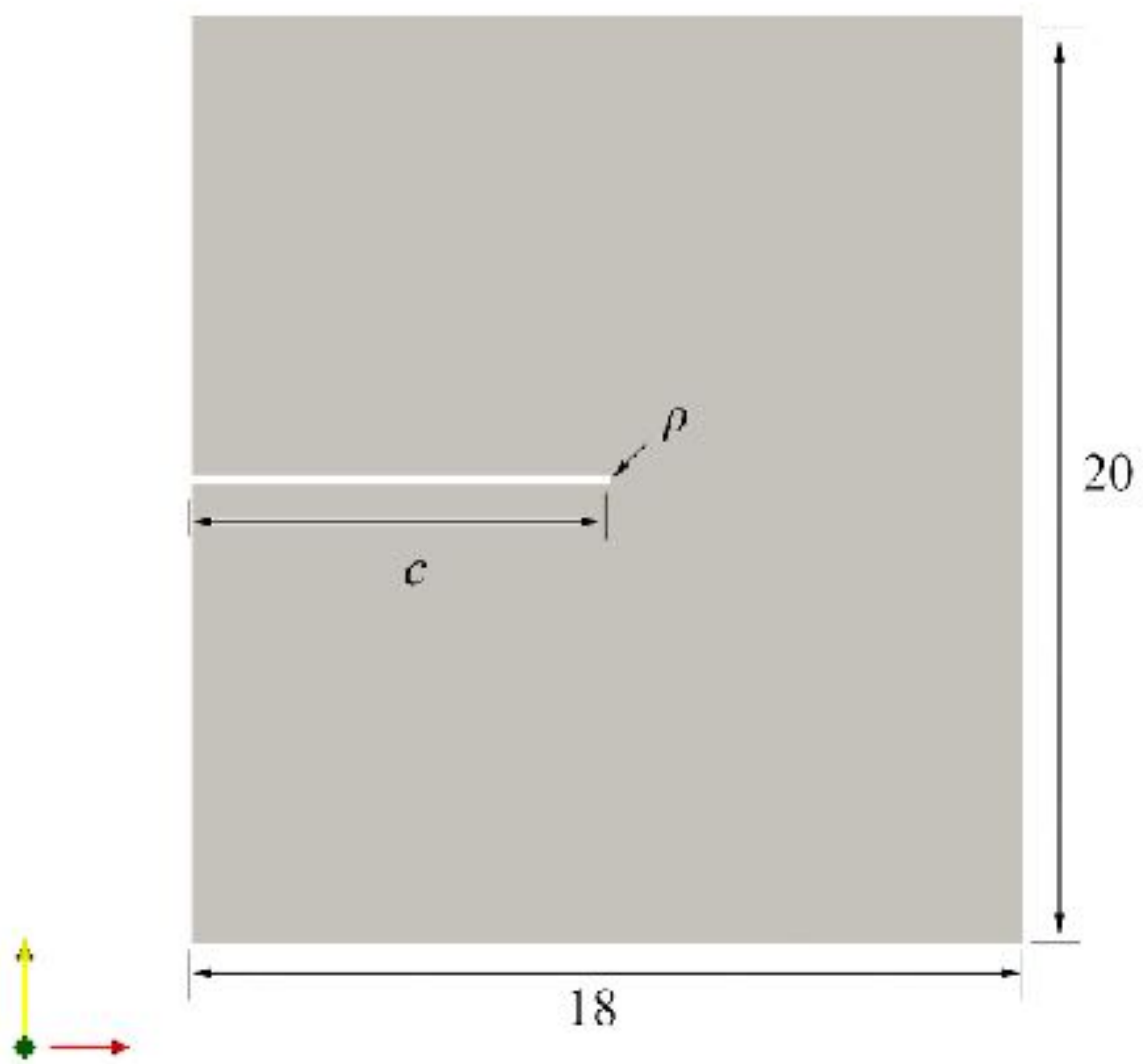
Equilibrium equation: $$\operatorname{Div}\mathbf{T}_{\mathsf{R}} + \mathbf{b}_{\mathsf{R}} = \mathbf{0}$$

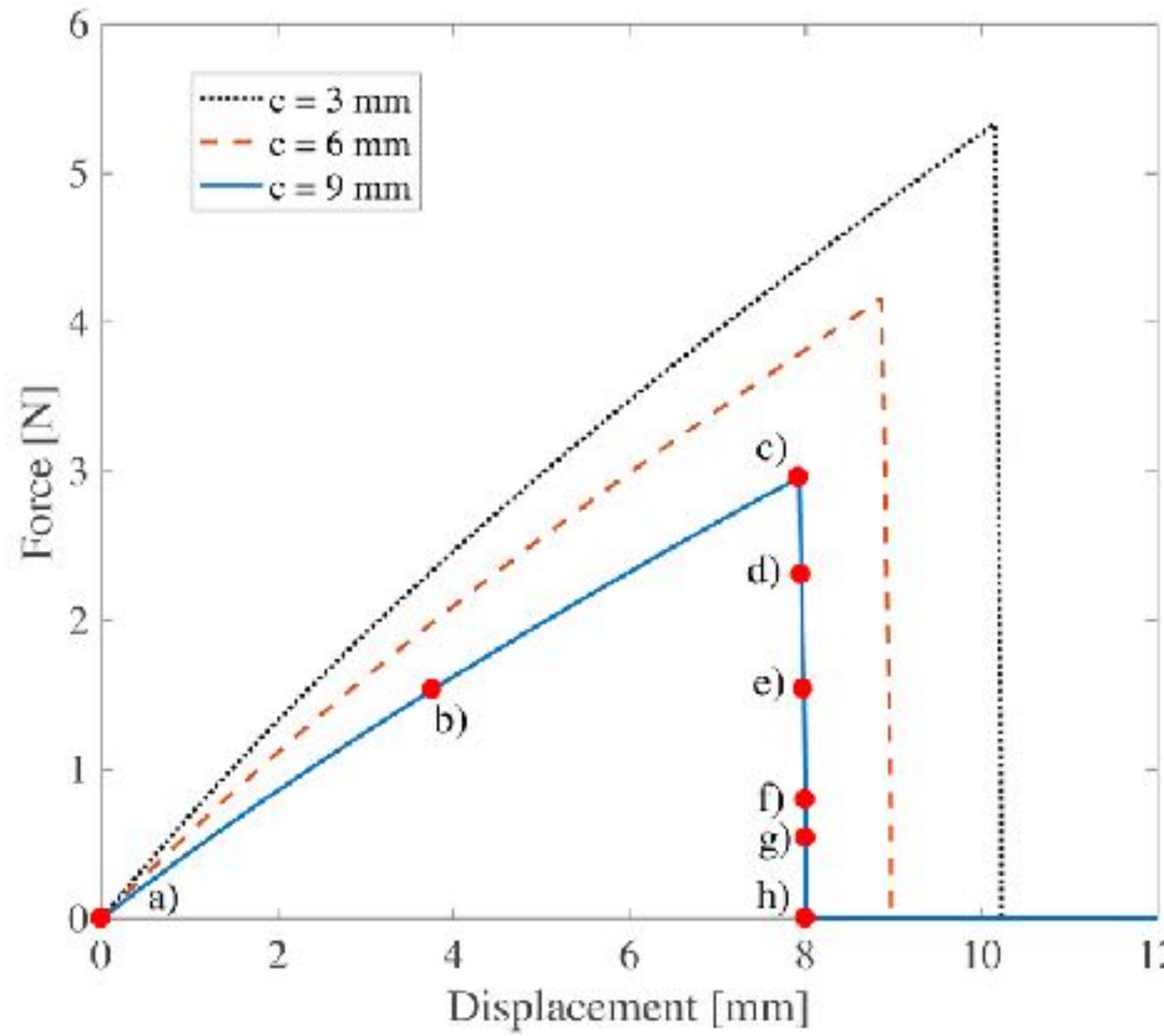
Evolution equation for d: $$\zeta \dot{d} = \left\langle 2(1-d)\mathcal{H} - \varepsilon^f_{\mathsf{R}} \left[d - \ell^2 \Delta d \right] \right\rangle$$

$$\mathcal{H}(t) \overset{\text{def}}{=} \max_{s\in[0,t]} \left\langle \hat{\varepsilon}^0_{\mathsf{R}}(\lambda_b(s), J(s)) - \varepsilon^f_{\mathsf{R}}/2 \right\rangle$$

+ BCs and ICs

Plane-stress simulation of single-edge-notch fracture of an elastomeric sheet





Dimensions in mm

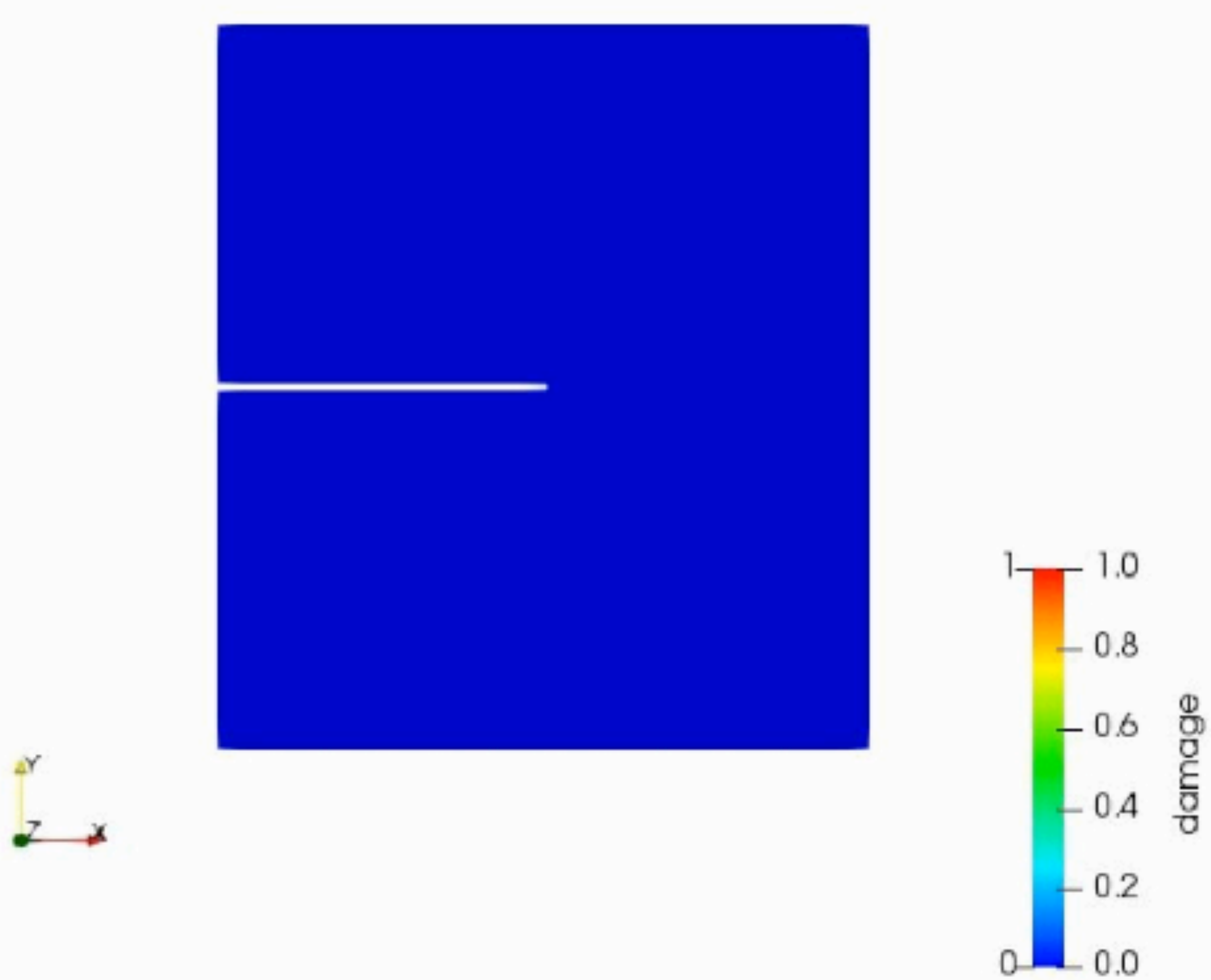
- Thickness: 1mm; $\rho = 0.1\,\mathrm{mm}$
- Stretch rate $1 \times 10^{-3}/s$

Material parameters

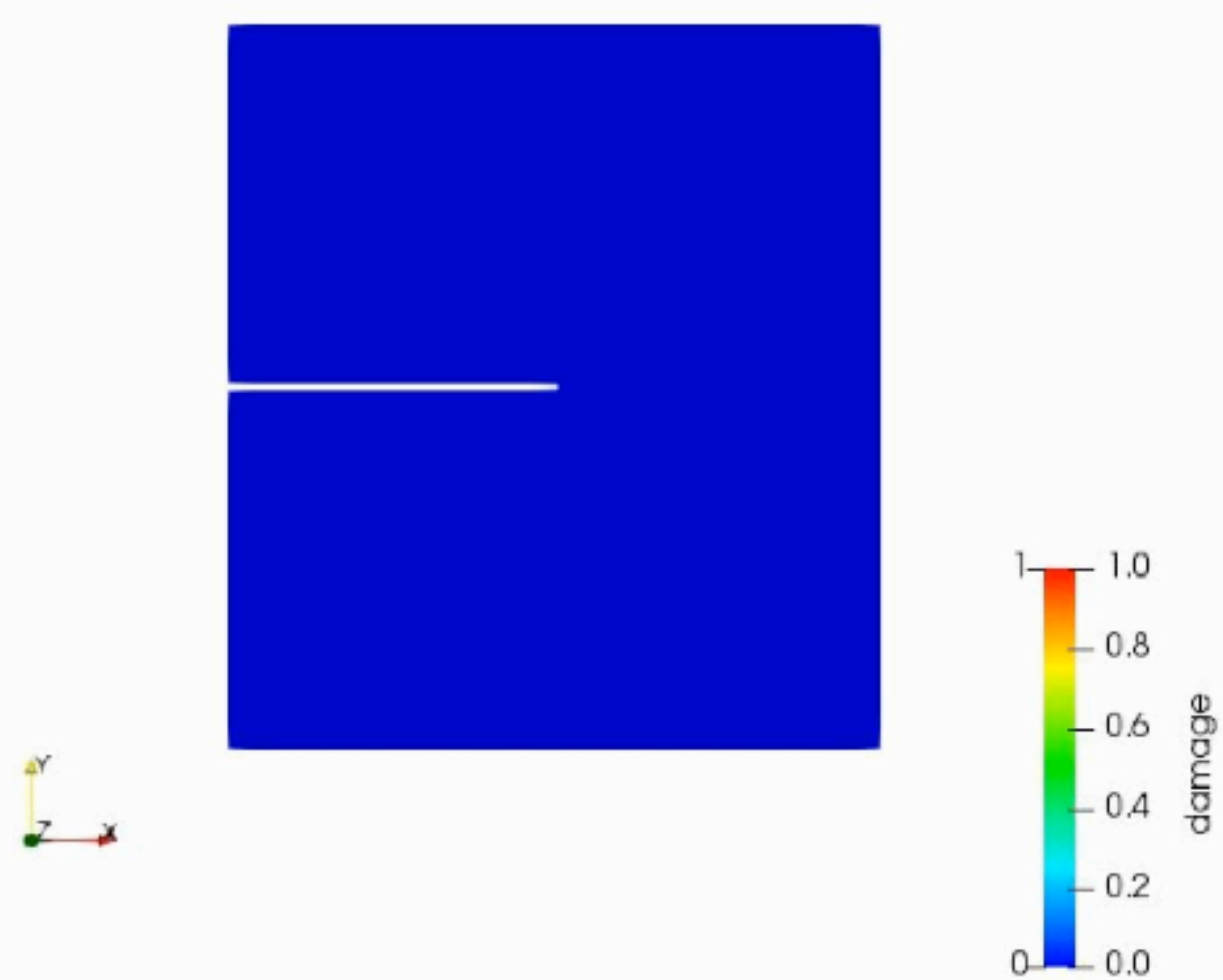
$G_0 = N k_B \vartheta$	n	$\bar{E}_b = N n E_b$	K	$\varepsilon_{\mathrm{R}}^f = N n \varepsilon_b^f$	ℓ	ζ
0.25 MPa	4	5 MPa	5 MPa	$2.5\,\mathrm{MJ/m^3}$	$100\,\mu\mathrm{m}$	20 kPa·s

Plane stress simulation of single-edge-notch fracture of an elastomeric sheet

Contours of damage
with highly damaged elements
shown

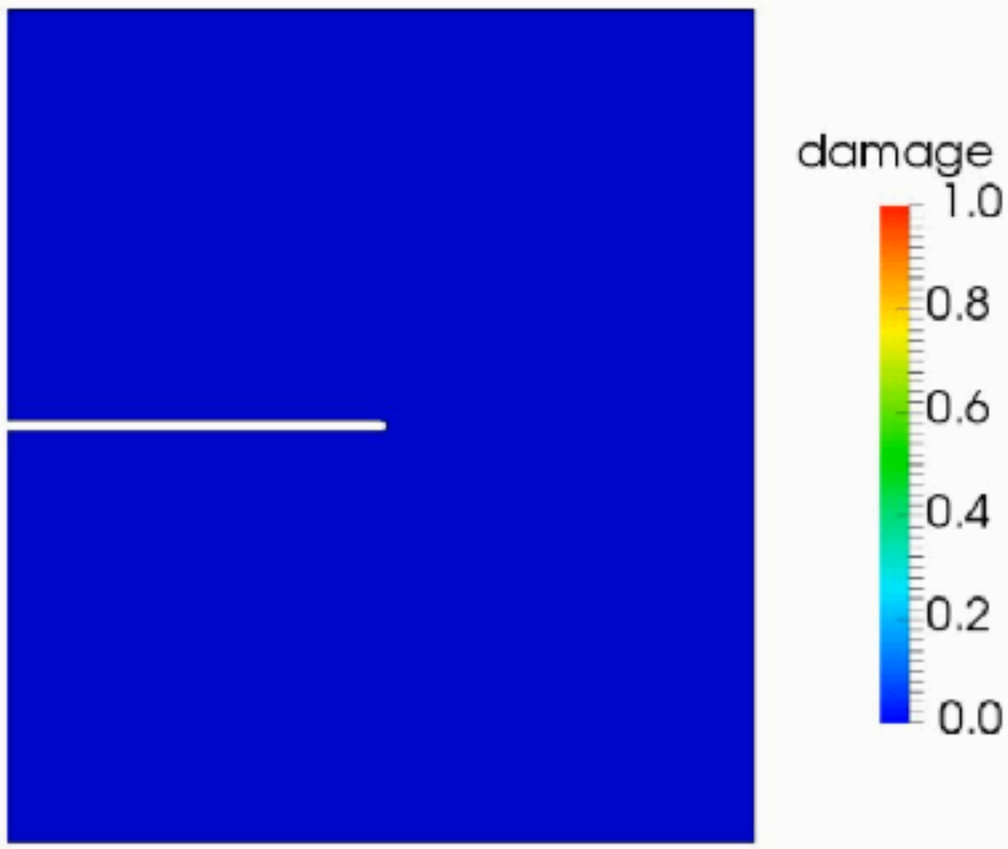


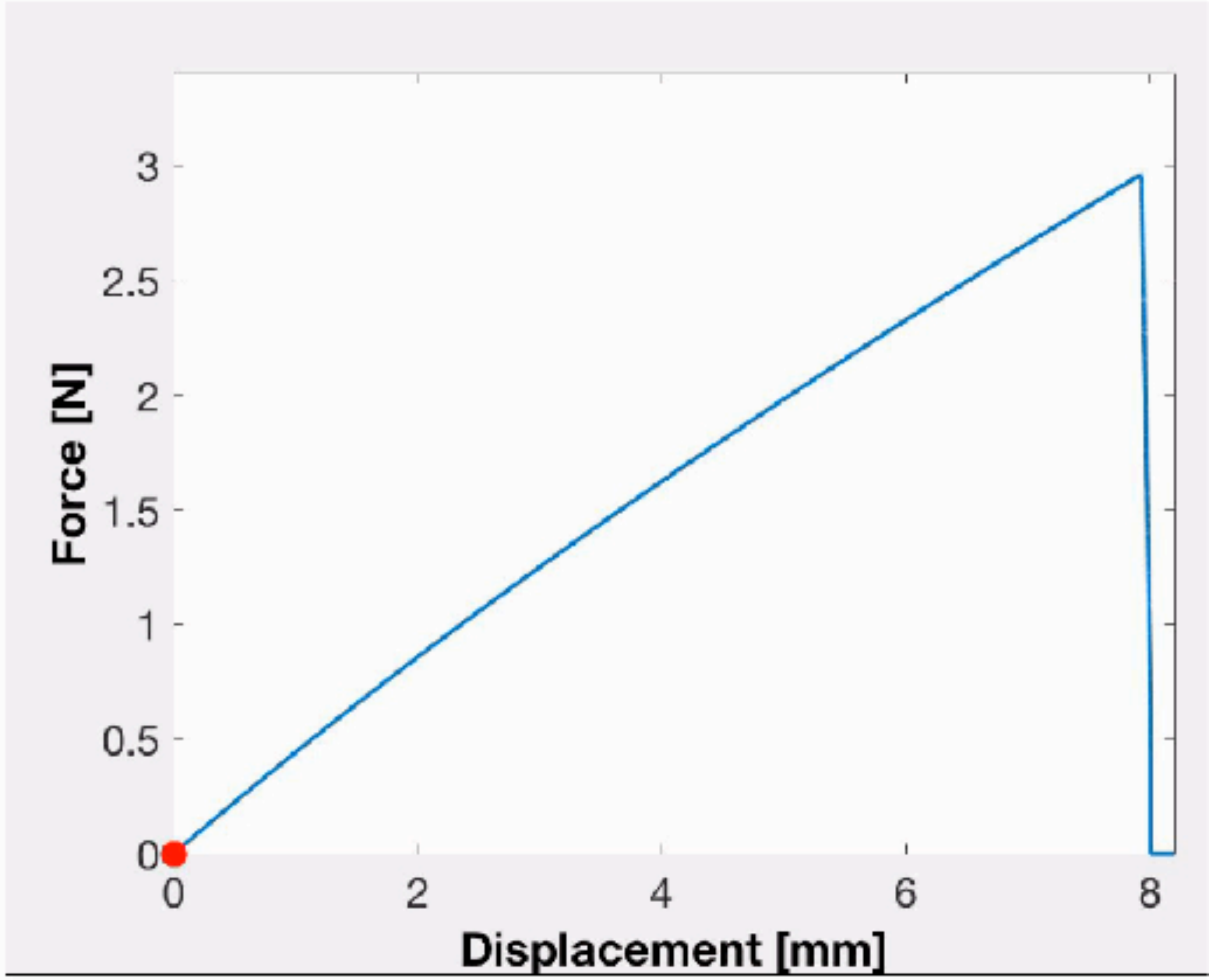
Contours of damage
without highly damaged elements



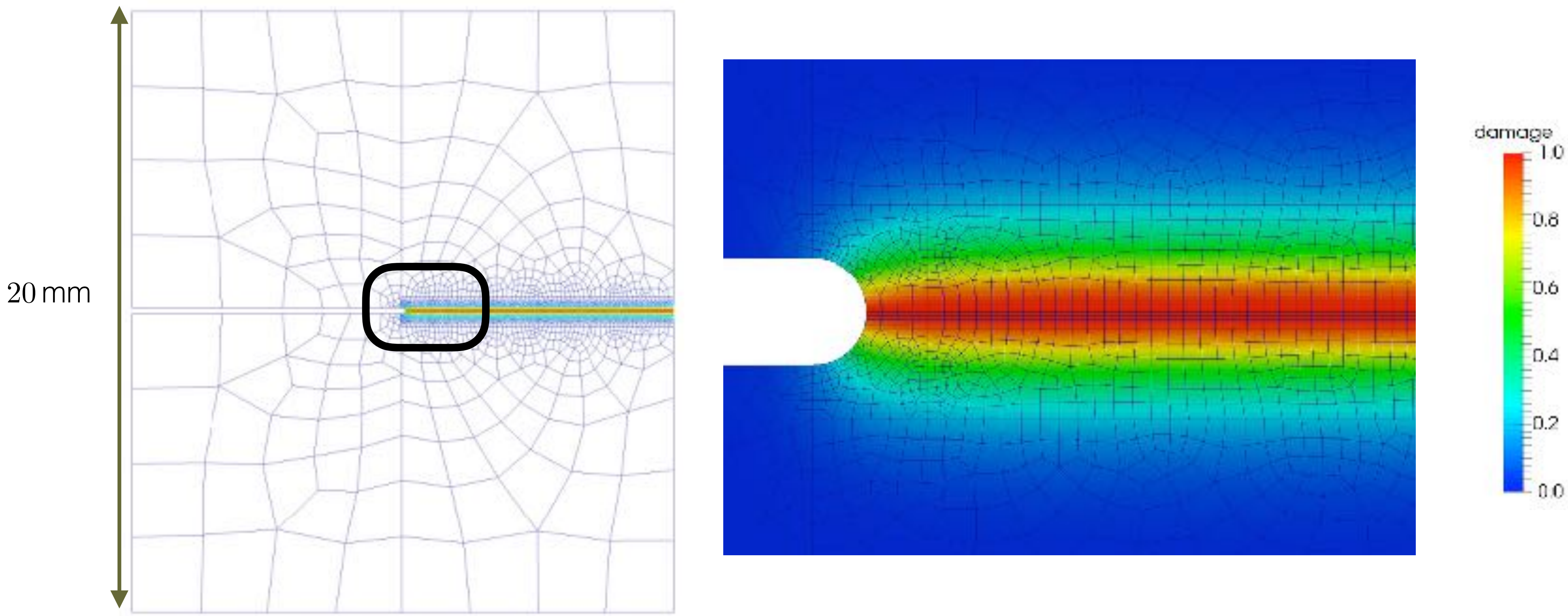
Single-edge-notch fracture of an elastomeric sheet

Contours of damage





The length scale ℓ and mesh for the single-edge-notched specimen



$h_e \lessapprox \ell/10$

- Actual values of ℓ in elastomeric materials are expected to be $\ell \lessapprox 1\mu$m. For $h_e \lessapprox \ell/10$ — so that $h_e \lessapprox 100$nm, which is ***exceedingly small***.

- For modeling macroscopic-dimensioned specimens, several mm in length, for pragmatic reasons we consider ℓ to be regularization parameter for the gradient-damage theory.

- Corresponding to a small but computationally-tractable mesh size h_e selected for macroscopic-dimensioned specimens, a suitably large value of $\ell = 100\mu$m has been chosen, and the value of $\varepsilon_{\mathrm{R}}^{f}$ suitable reduced so that

$$\varepsilon_{\mathrm{R}}^{f} \times \ell \approx G_c,$$

where G_c is the value of experimentally-measured macroscopic critical energy release rate for a given material.