Variational phase-field models of fracture.

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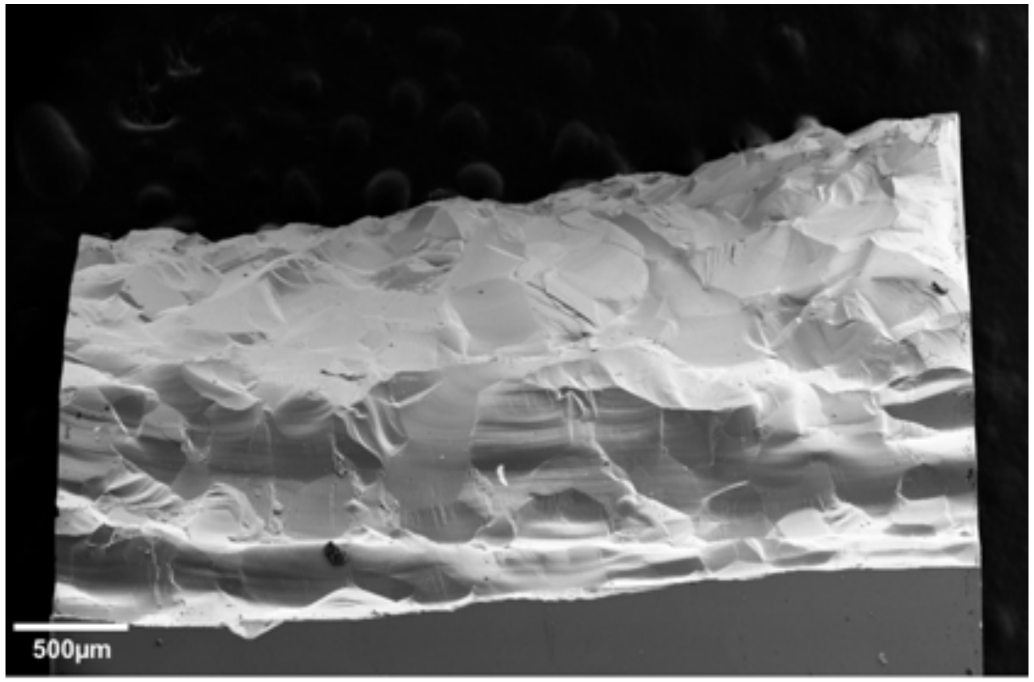
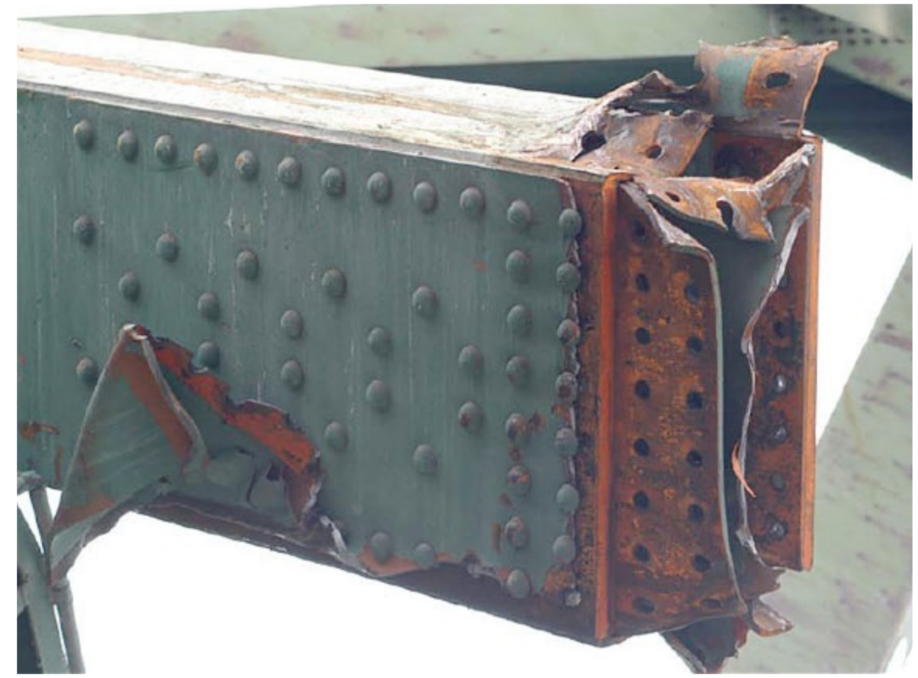
Source code: http://bitbucket.org/bourdin/mef90-sieve
dockerhub: bourdin/mef90-mpich

NSF DMS-0908267, DMS-0605320, DMS-1312739, DMS-1716763
LA Board of Regents, Chevron ETC, Corning Inc., Asahi Glass Company

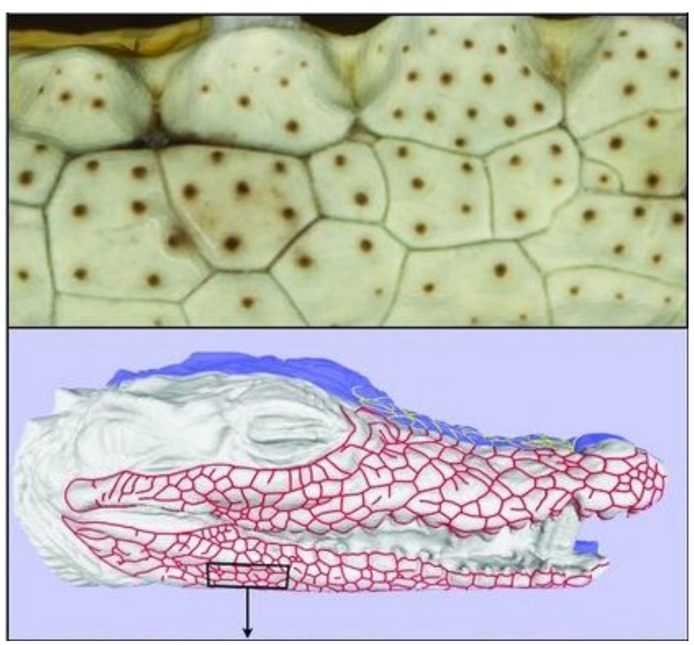
Fracture Mechanics



Fracture surface of AlON

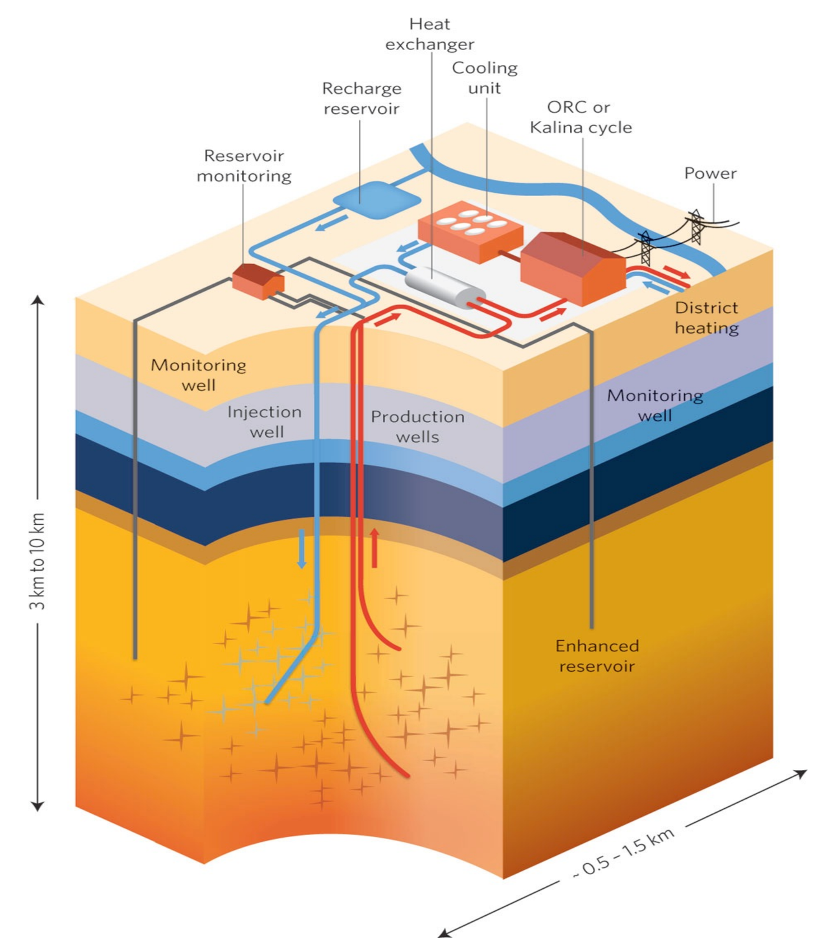


Beam of the I-35W bridge, Minneapolis



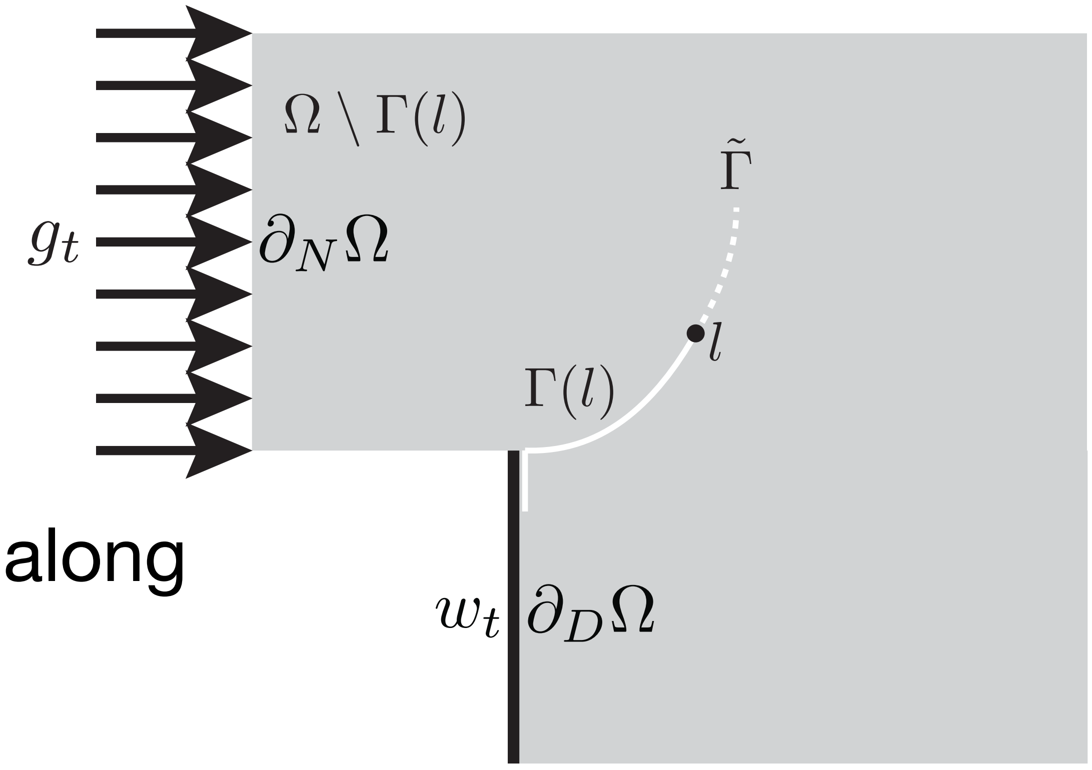
Crocodile skin

Causeway of Giants



Enhanced Geothermal Systems

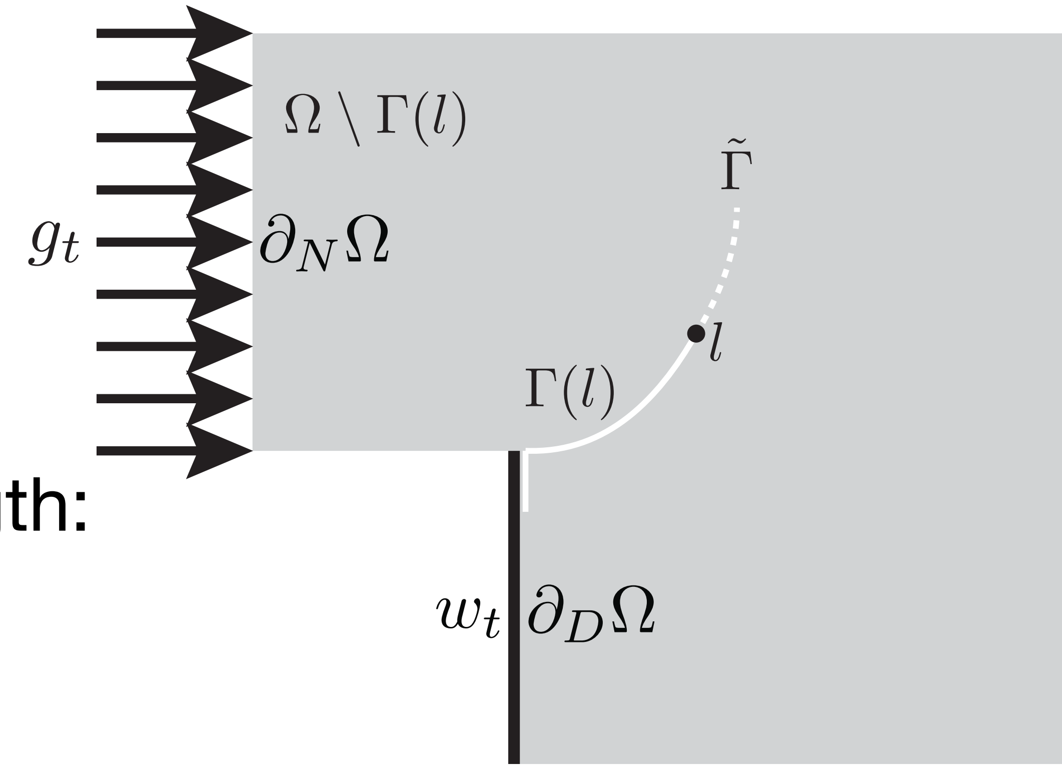
Revisiting Griffith' argument



- Quasi-static, loading parameter ("time") t
- Boundary displacement $u(t) = w_t$ on $\partial_D\Omega$
- Boundary and body forces f_t, g_t.
- Single crack $\Gamma(l)$ with length l propagating along a known path in 2D
- Equilibrium displacement $u(t,l)$
- Potential energy = mechanical energy of equilibrium displacement.

$$\mathcal{P}(t,l) := \mathcal{E}\,(t; l, u(t,l))$$

Revisiting Griffith' argument



Griffith argument:

- Crack growth hypothesis:
  $l(t)$ non-decreasing function of t
- Fracture energy proportional to crack length:
  G_c: rate of energy per unit of length (area)
- Stability principle: for any $\Delta l \geq 0$

$$\mathcal{P}(t, l(t) + \Delta l) + G_c \Delta l \geq \mathcal{P}(t, l(t))$$

$$G(t, l(t)) := -\frac{\partial \mathcal{P}}{\partial l}(t, l(t)) \leq G_c$$

- Stability principle: if $\dot{l}(t) \geq 0$, for any $\Delta l \leq 0$

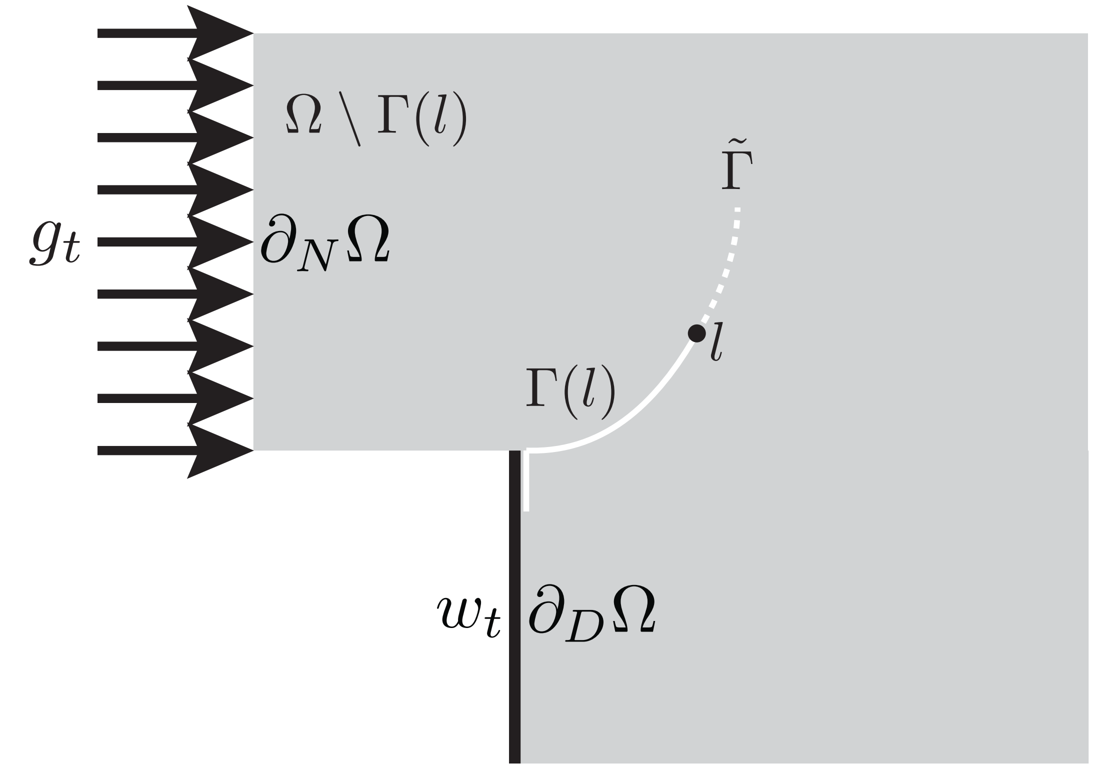
$$\mathcal{P}(t, l(t) - \Delta l) - G_c \Delta l \geq \mathcal{P}(t, l(t))$$

$$-\frac{\partial \mathcal{P}}{\partial l}(t, l(t)) \geq G_c$$

$$\begin{cases} \dot{l}(t) & \geq 0 \\ G(t, l(t)) & \leq G_c \\ (G(t, l(t)) - G_c)\, \dot{l}(t) & = 0 \end{cases}$$

A variational view of Griffith theory

$$\begin{cases} \dot{l}(t) & \geq 0 \\ G(t, l(t)) & \leq G_c \\ (G(t, l(t)) - G_c)\, \dot{l}(t) & = 0 \end{cases}$$



- Griffith solutions are minimizers of $\mathcal{P}(t, l(t)) + G_c l(t)$ under a crack growth constraint.

- Variational view of Griffith at all t, find $(u(t)$,$l(t))$ minimizing

$$\mathcal{E}(t, v, l) := \int_{\Omega \setminus \Gamma(l)} \frac{1}{2} \mathbf{A}\, \mathrm{e}(v) \cdot \mathrm{e}(v)\, dx - \mathcal{L}(t; v) + G_c l$$

amongst all l such that $l > l(s)$ for all $s < t$, v admissible.

Francfort-Marigo *JMPS* ’98, B-Francfort-Marigo *J. Elast.* ’08

Francfort-Marigo's variational model

- Griffith energy in variational form

$$\mathcal{E}(t,u,l) := \int_{\Omega\backslash\Gamma(l)} \tfrac{1}{2}\mathbf{A}\,\mathrm{e}(u)\cdot\mathrm{e}(u)\,dx - \mathcal{L}(t;u) + G_c l$$

- Generalized energy for *any* path:

$$\mathcal{E}(t,u,\Gamma) := \int_{\Omega\backslash\Gamma} \tfrac{1}{2}\mathbf{A}\mathrm{e}(u) : \mathrm{e}(u)\,dx - \mathcal{L}(u,t) + G_c\mathcal{H}^{n-1}(\Gamma)$$

- Francfort-Marigo '98: at each $t,$ find u,Γ minimizing $\mathcal{E}$ under crack growth and energy balance constraints (unilateral minimality)

"The "theorem of minimum energy" may be extended [...] if account is taken of the increase of surface energy which occurs during the formation of cracks." - Griffith 1921

Francfort-Marigo *JMPS* '98, B-Francfort-Marigo *J. Elast.* '08

Francfort and Marigo's variational approach

- Total fracture energy consistent with that of Griffith in variational form

$$\mathcal{E}(t;u,\Gamma) = \int_{\Omega\setminus\Gamma} \frac{1}{2}\mathbf{A}\,\mathrm{e}(u)\cdot\mathrm{e}(u)\,dx - \mathcal{L}(t;u) + G_c\mathcal{H}^{n-1}(\Gamma)$$

- Crack path is part of the minimization problem (Free Discontinuity problem).
- No hypotheses on crack geometry, (including connectivity, topology etc).
- Solution consistent with Griffith in variational form.
- No forces!
- Can be extended to account for:
  - Unilateral contact;
  - Non homogeneous, non-isotropic materials;
  - Non-linear elasticity;
  - …

Francfort-Marigo *JMPS* '98, B-Francfort-Marigo *J. Elast.* '08

Variational Phase-Field models

Generalized Ambrosio-Tortorelli functional:

$$\mathcal{E}_\ell(u,\alpha) := \int_\Omega a(\alpha) W(\mathrm{e}(u))\,dx + \frac{G_c}{4c_w}\int_\Omega \frac{w(\alpha)}{\ell} + \ell|\nabla\alpha|^2\,dx$$

$$a(0)=1, a(1)=0,\ w(0)=0, w(1)=1,\ c_w = \int_0^1 \sqrt{w(s)}\,dx$$

$\Gamma-$convergence to Francfort-Marigo variational energy:

- Static scalar problem: B '98, Braides '98:
- Finite element approximation if $h \ll \ell$: Bellettini-Coscia '94, B '98, Ortner-Burke-Sülli '10, '15.
- Quasi-static evolution: Giacomini '05:
- Linearized elasticity: Chambolle '04, '06, Iurlano '13,'14,'18.

MANY extensions, implementations

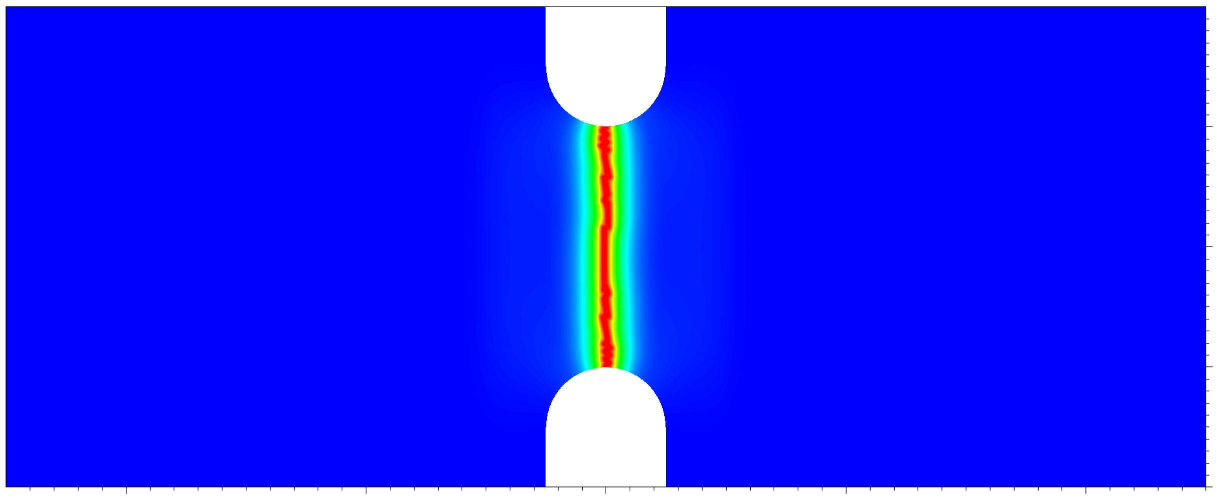
B-Francfort-Marigo *JMPS* '00, B, *IFB* 07, B-Francfort-Marigo *J. Elast.* '08

AT1 and AT2 models

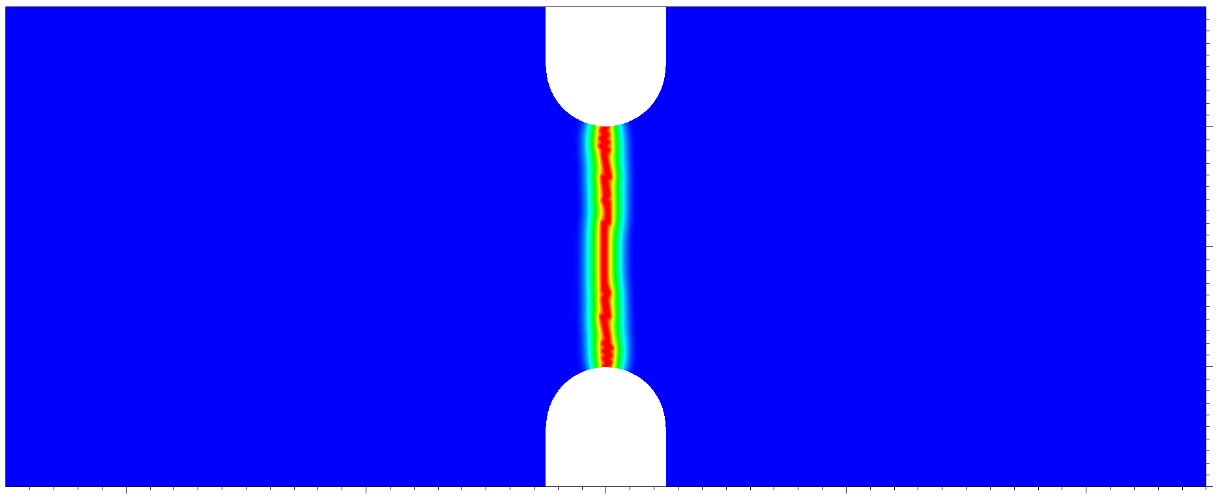
AT2: $\mathcal{E}_\ell(u,\alpha) = \int_\Omega (1-\alpha)^2 \mathrm{W}(\mathrm{e}(u))\,dx + \frac{G_c}{2}\int_\Omega \frac{\alpha^2}{\ell} + \ell|\nabla\alpha|^2\,dx$

AT1: $\mathcal{E}_\ell(u,\alpha) = \int_\Omega (1-\alpha)^2 \mathrm{W}(\mathrm{e}(u))\,dx + \frac{3G_c}{8}\int_\Omega \frac{\alpha}{\ell} + \ell|\nabla\alpha|^2\,dx$

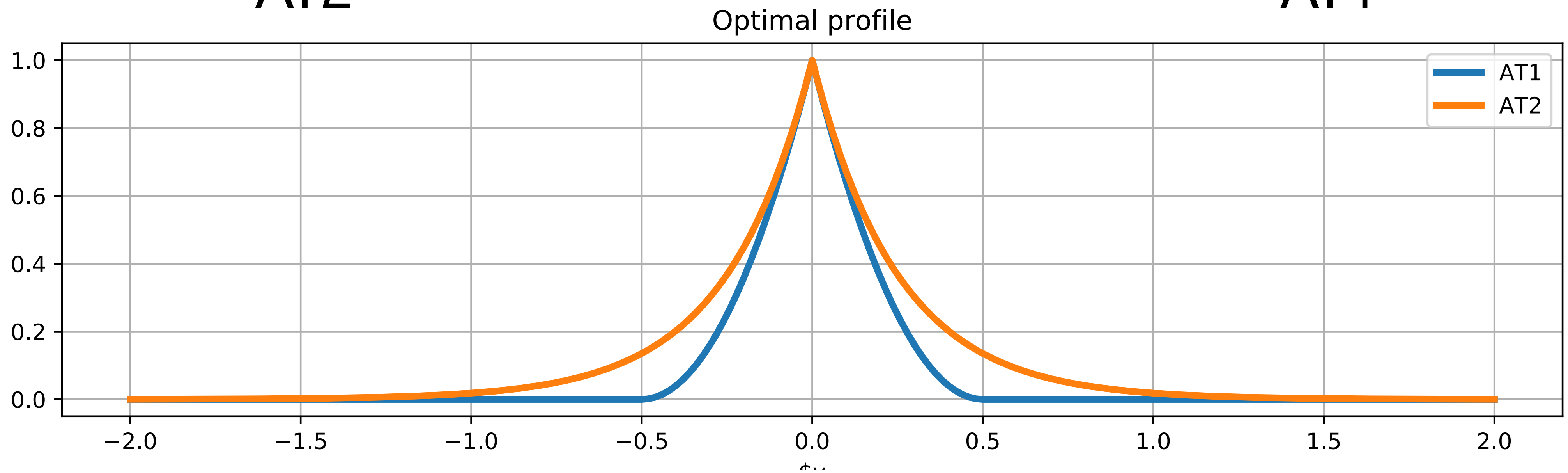
Construction of *optimal profile* as part of Γ-convergence *recovery sequence*.



AT2



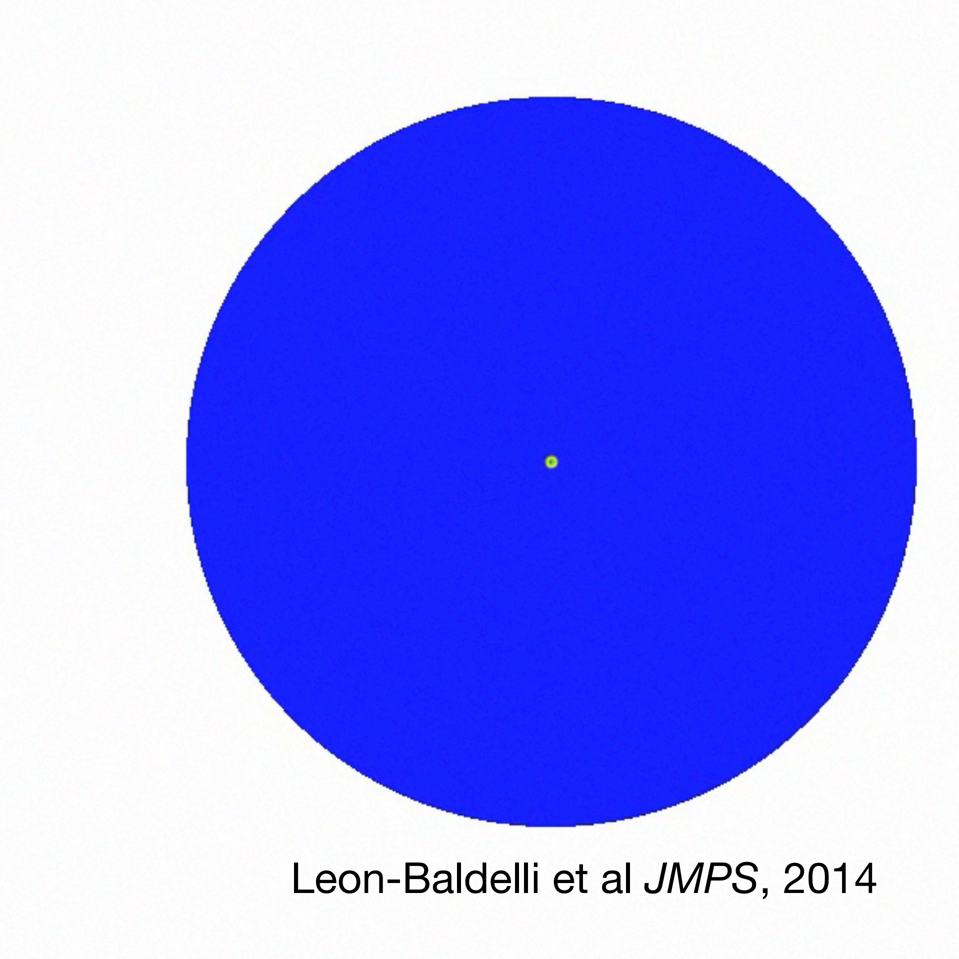
AT1



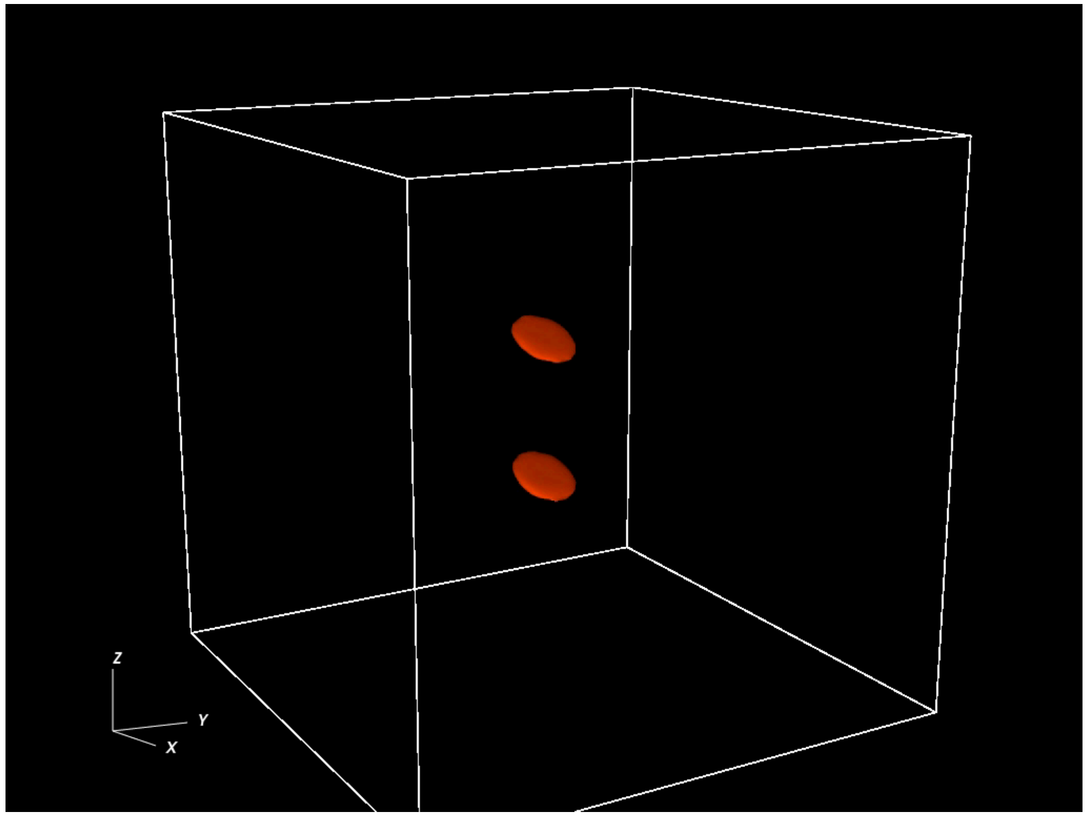
Numerical Implementation

- Time discrete alternate minimization algorithm.
    - At each time step: *iterate* until convergence
        - Minimization w.r.t u (elastic equilibrium).
        - Constrained minimization w.r.t α (variational inequality).
    - Globally stable, convergence to a critical point of the regularized energy, *monotonically decreasing energy*. B ’07, Burke-Ortner-Süli ’10, ‘13.
    - Backtracking algorithm: additional optimality conditions in trajectory space.
- mef90: unstructured parallel finite element, based on MPI + PETSc, scales up to thousands of cores. http://bitbucket.org/bourdin/mef90-sieve docker hub: bourdin/mef90-mpich
- *Coupled* minimization algorithms (Farrell-Maurini *IJNME* ’17, Gerasimov-De Lorenzis, *CMAME* ’17, Wick): fast in convex regions (stable crack propagation), unstable / unpredictable otherwise.

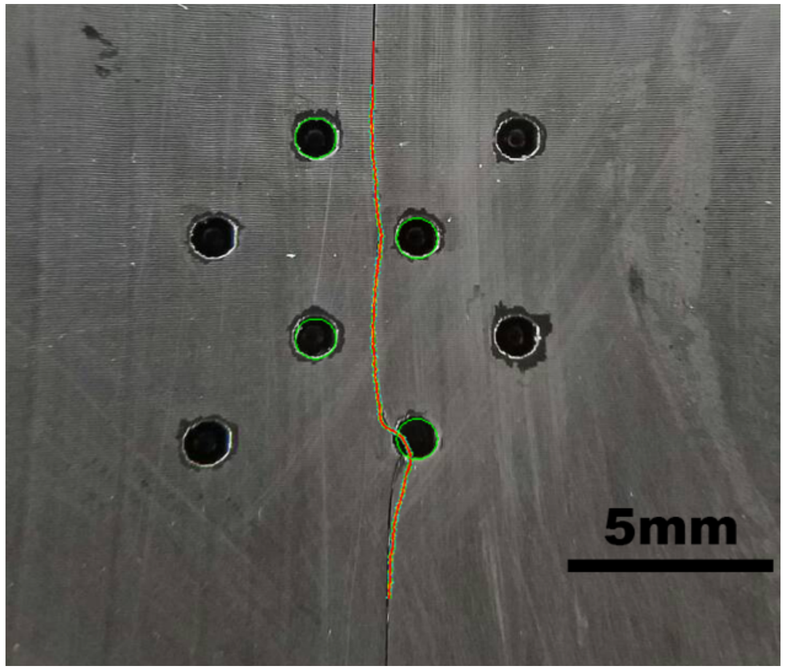
Variational Phase Field models

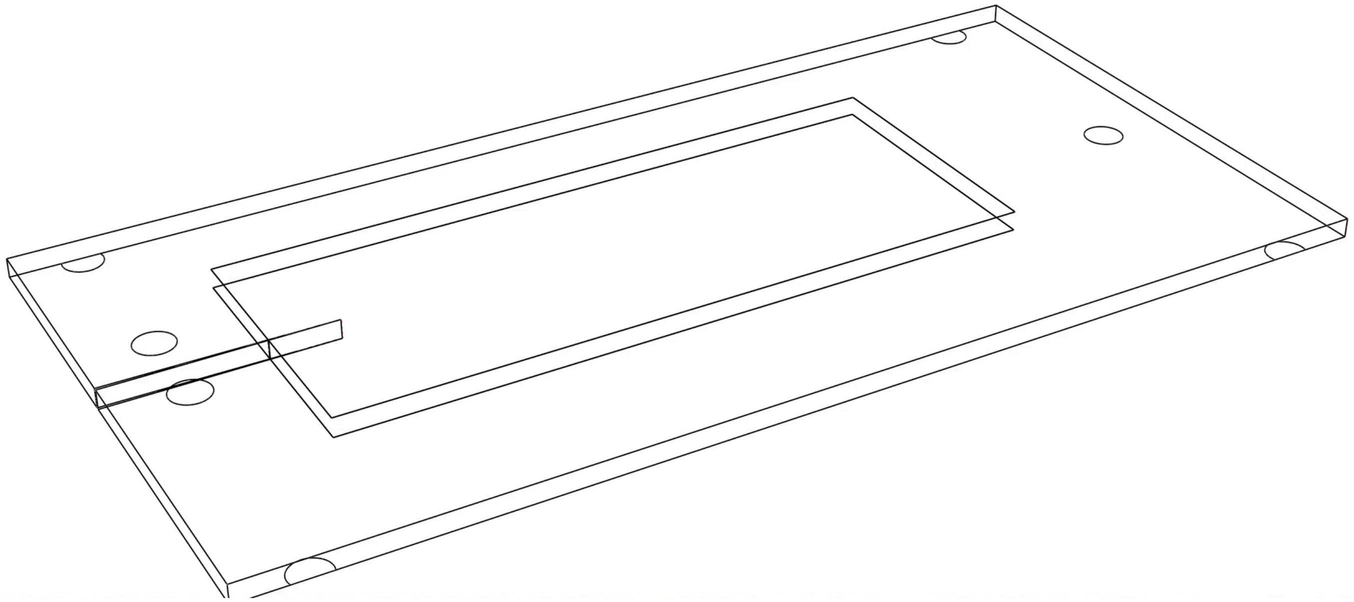


Leon-Baldelli et al *JMPS*, 2014



B-Chukwudozie-Yoshioka *SPE ATCE,* 2012





C.-J. Hsueh and N. Broadnik

“our” phase-fields vs. “your” phase-field

Modica-Mortola (rescaled GL free energy): *double well* potential.

$$\mathcal{P}_\ell(\alpha) = \frac{1}{2c_W}\int_\Omega \frac{W(\alpha)}{\ell} + \ell|\nabla\alpha|^2\,dx$$

- Free *boundary* problem, blow-up limits = surfaces with constant curvature

$$\mathcal{P}_\ell(\alpha) \xrightarrow{\Gamma} \mathcal{H}^{N-1}(\partial D)\,,\ \alpha \to \chi_D;$$

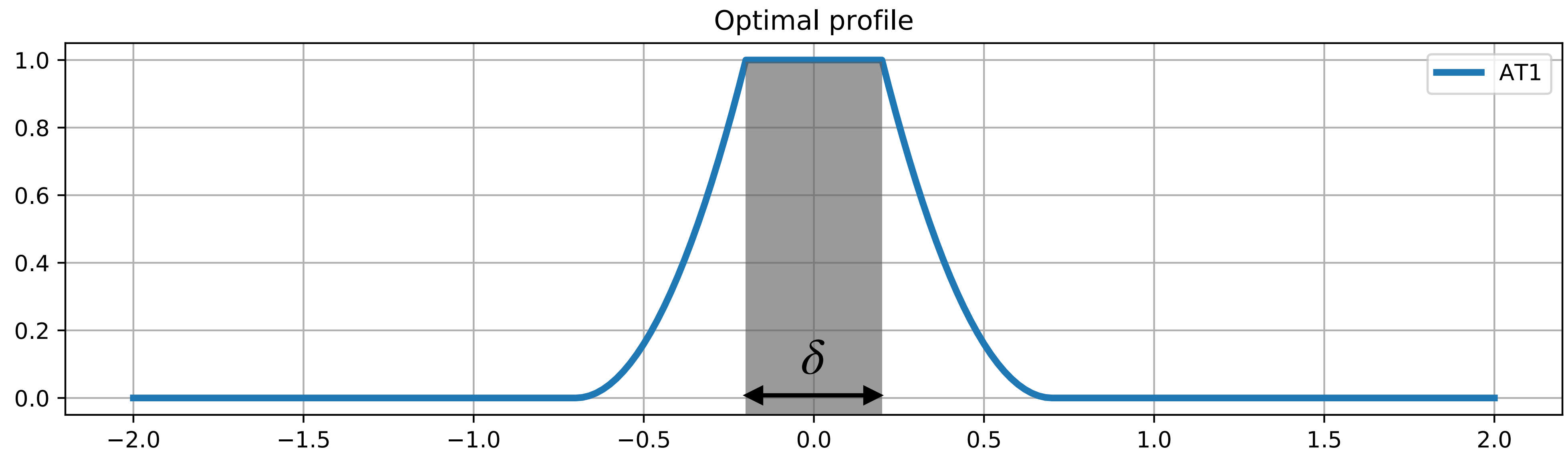
- Gradient-flow converges to mean-curvature motion;
- Cannot *localize* (nucleation requires concentrated driving forces);
- Interfaces can *(should)* move even without driving force.

“our” phase-fields vs. “your” phase-field

Ambrosio-Tortorelli: *single well* potential.

$$\mathcal{E}_\ell(u,\alpha) := \int_\Omega a(\alpha) W(\mathrm{e}(u))\, dx + \frac{G_c}{4c_w} \int_\Omega \frac{w(\alpha)}{\ell} + \ell |\nabla \alpha|^2\, dx$$

- Free *discontinuity* problem, blow up limits (2D): line, Y junction, crack tip;
- Evolution by unilateral minimization (criticality + stability). Convergence of gradient flows is an open problem;
- Interfaces cannot move under non-singular driving forces (irreversibility + energy balance), crack-tip motion requires driving force in $\mathcal{O}\left(1/r\right)$;



Surface energy: $+\mathcal{O}\left(\delta/\ell\right)$

Elastic energy: $-\mathcal{O}\left(\delta\right)$

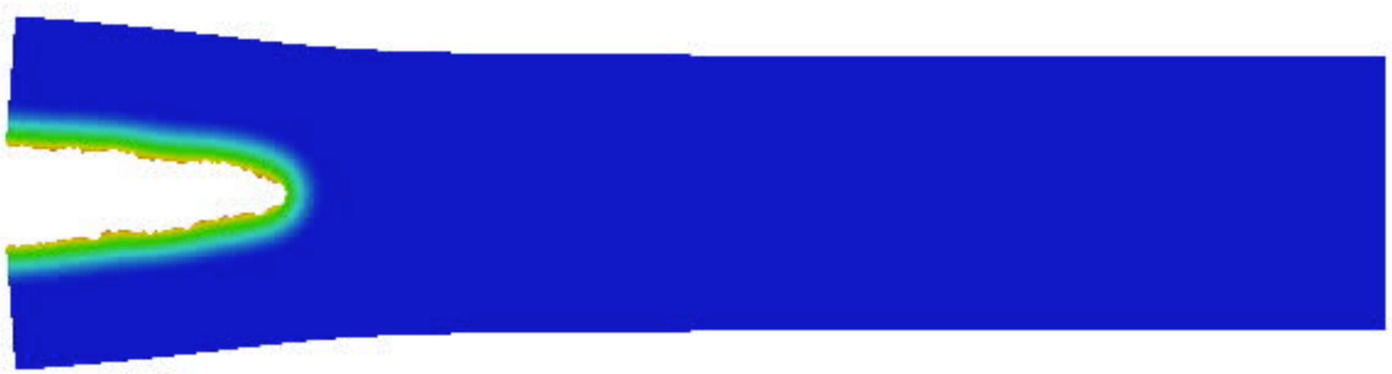
- Nucleation possible even with constant driving force.

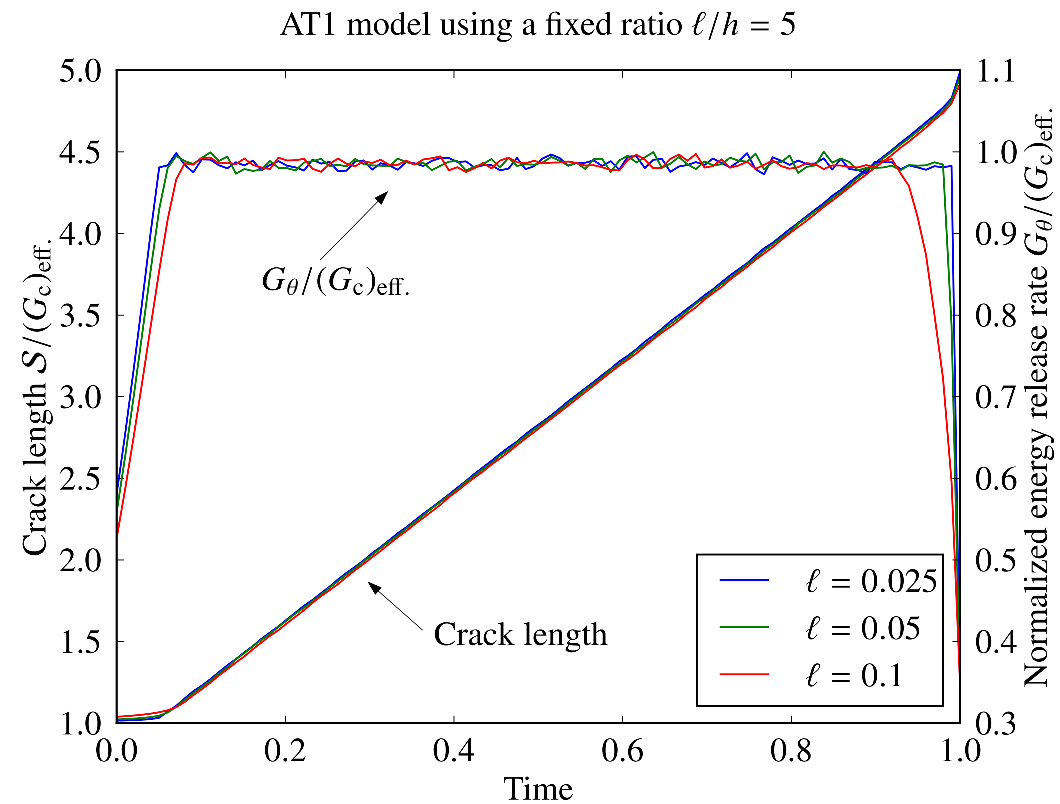
AT1 Surfing

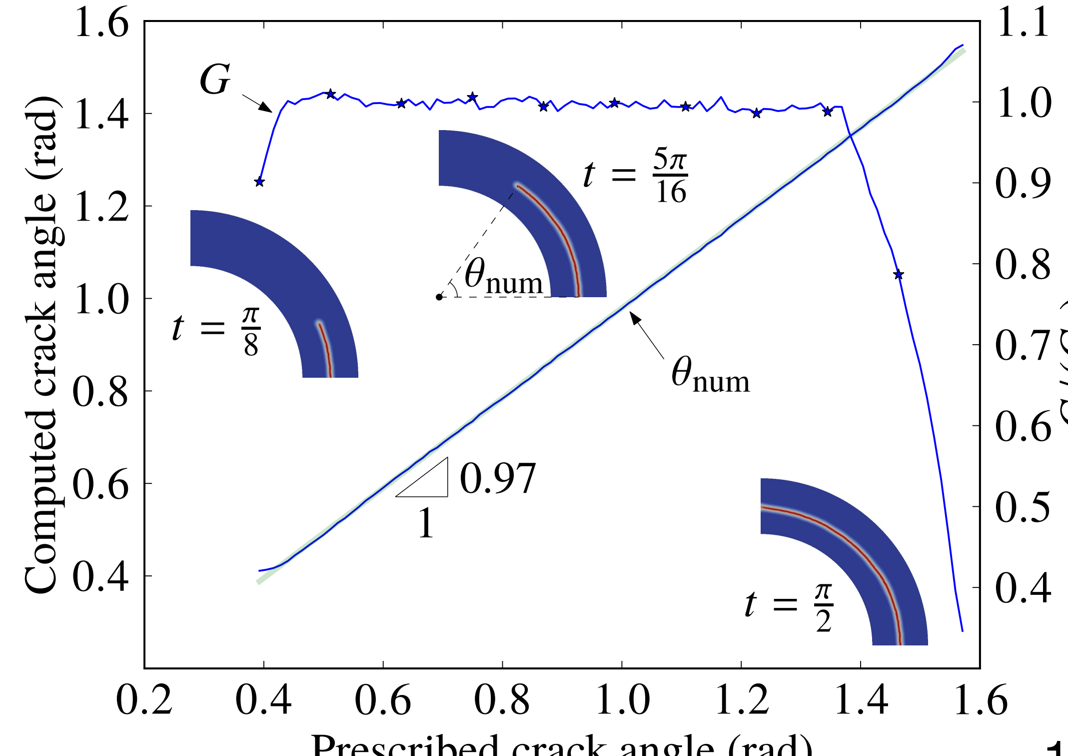
Homogeneous isotropic material with initial crack, AT1 model.

Elastic energy release rate computed with the G_θ method or J-integral

Translating boundary displacement.



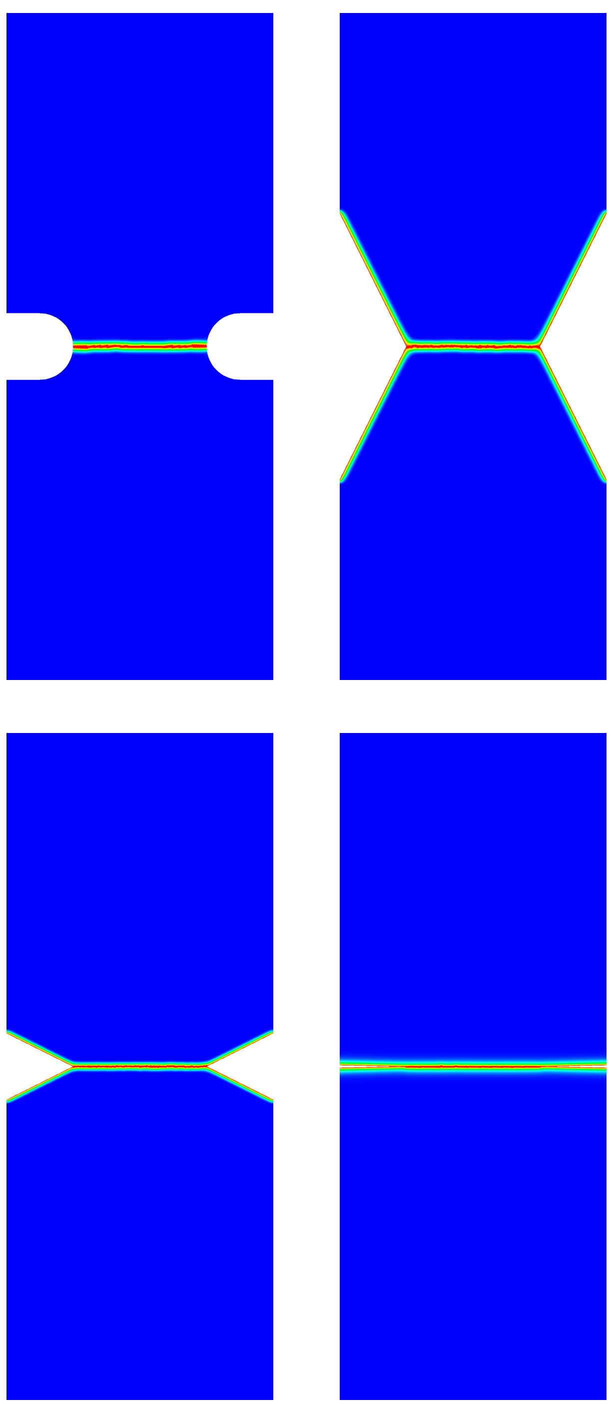


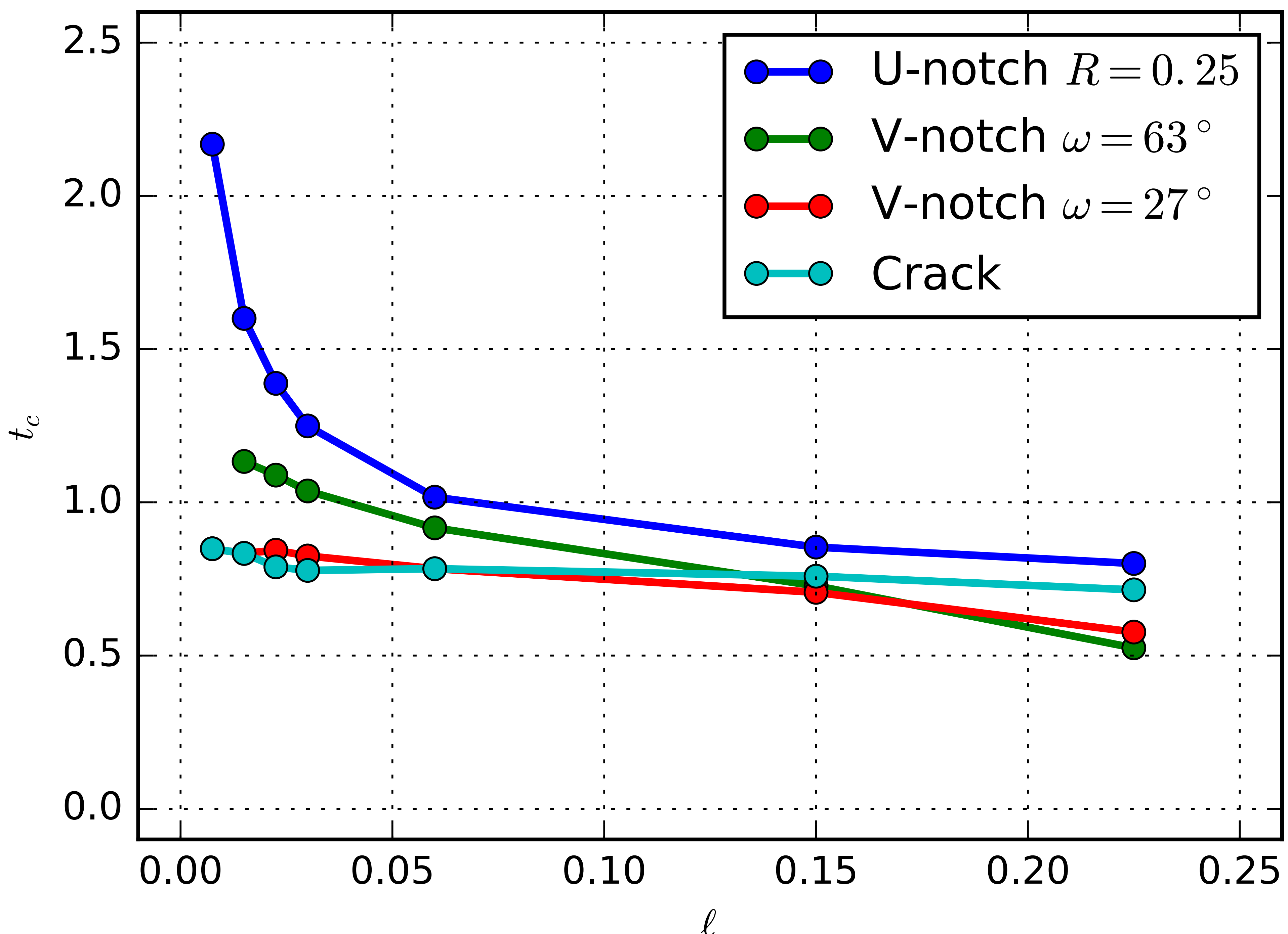


Tanné-Li-B-Marigo-Maurini JMPS ‘18

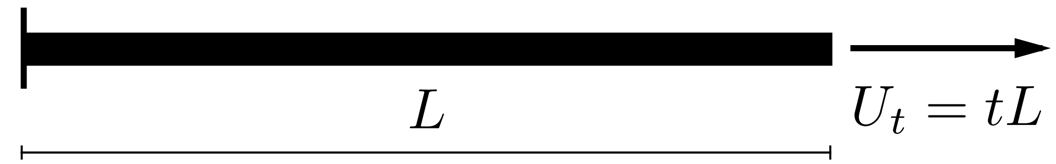
Nucleation

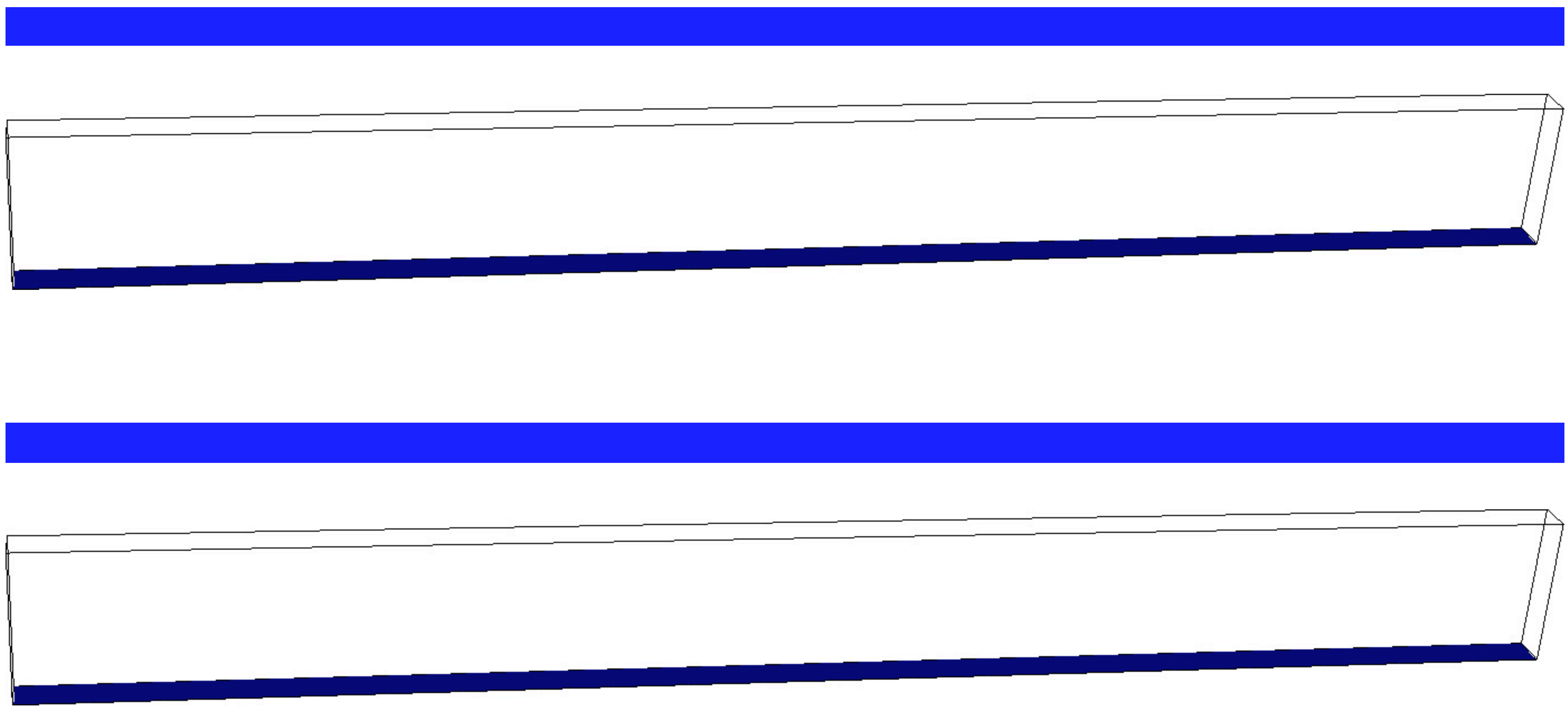
- Double Edge Notch test with 4 notch geometries, uniaxial tension
- Fixed geometry, nucleation load vs ℓ, h/ℓ constant





1D problem - AT1 vs AT2





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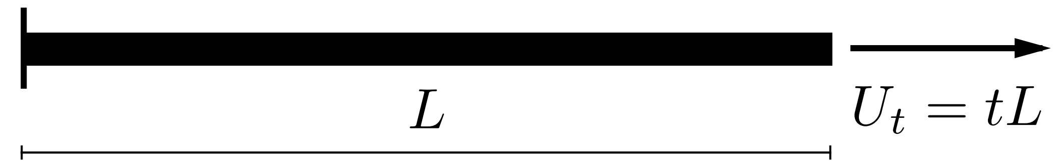
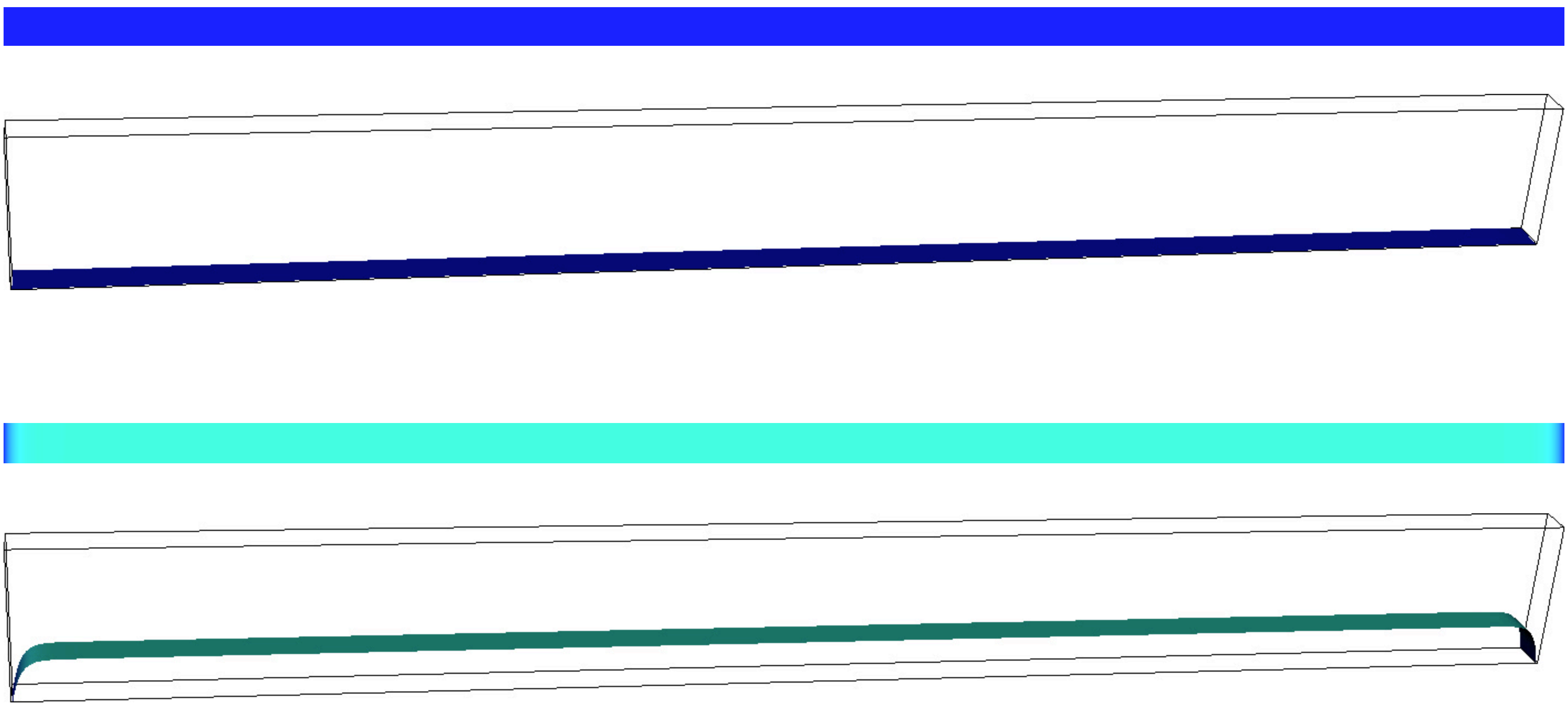
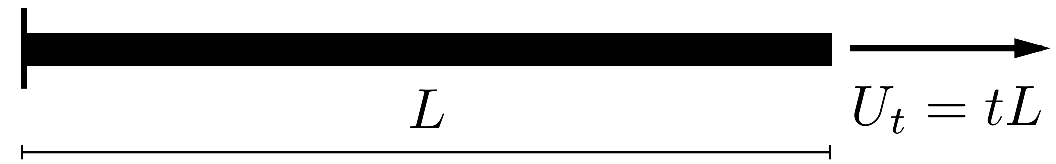




1D problem

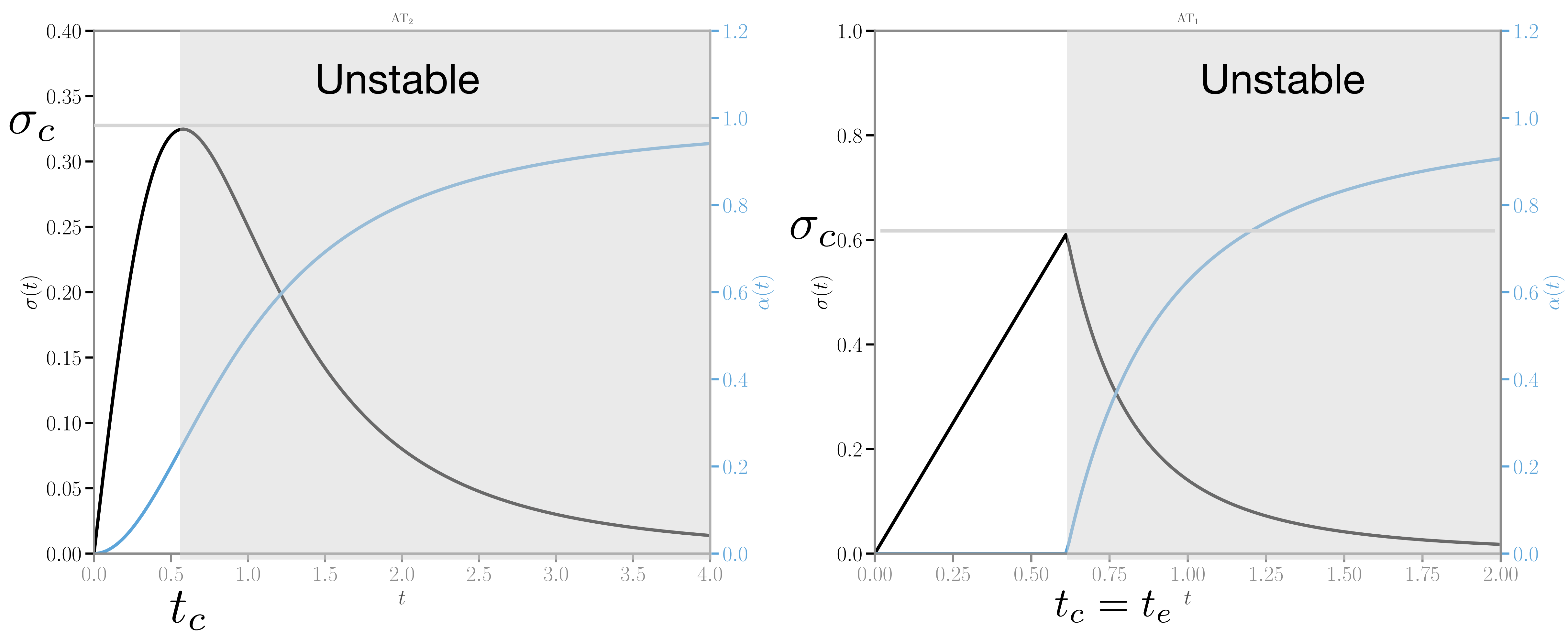


AT1 and AT2 models behave differently at *fixed* ℓ:

$$\text{AT2: } \mathcal{E}_\ell(u,\alpha) = \int_\Omega (1-\alpha)^2 \mathrm{W}(\mathrm{e}(u))\,dx + \frac{G_c}{2}\int_\Omega \frac{\alpha^2}{\ell} + \ell|\nabla\alpha|^2\,dx$$

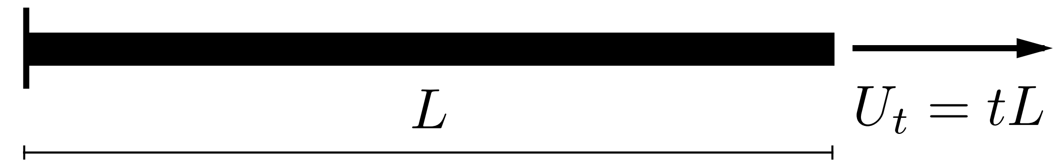
$$\text{AT1: } \mathcal{E}_\ell(u,\alpha) = \int_\Omega (1-\alpha)^2 \mathrm{W}(\mathrm{e}(u))\,dx + \frac{3G_c}{8}\int_\Omega \frac{\alpha}{\ell} + \ell|\nabla\alpha|^2\,dx$$

Construction of elastic and homogeneous states (α=cst)



Pham-Amor-Marigo-Maurini *IJDM* 2011, Pham-Marigo-Maurini *JMPS* 2011

1D problem



AT1 and AT2 models behave differently at *fixed* ℓ:

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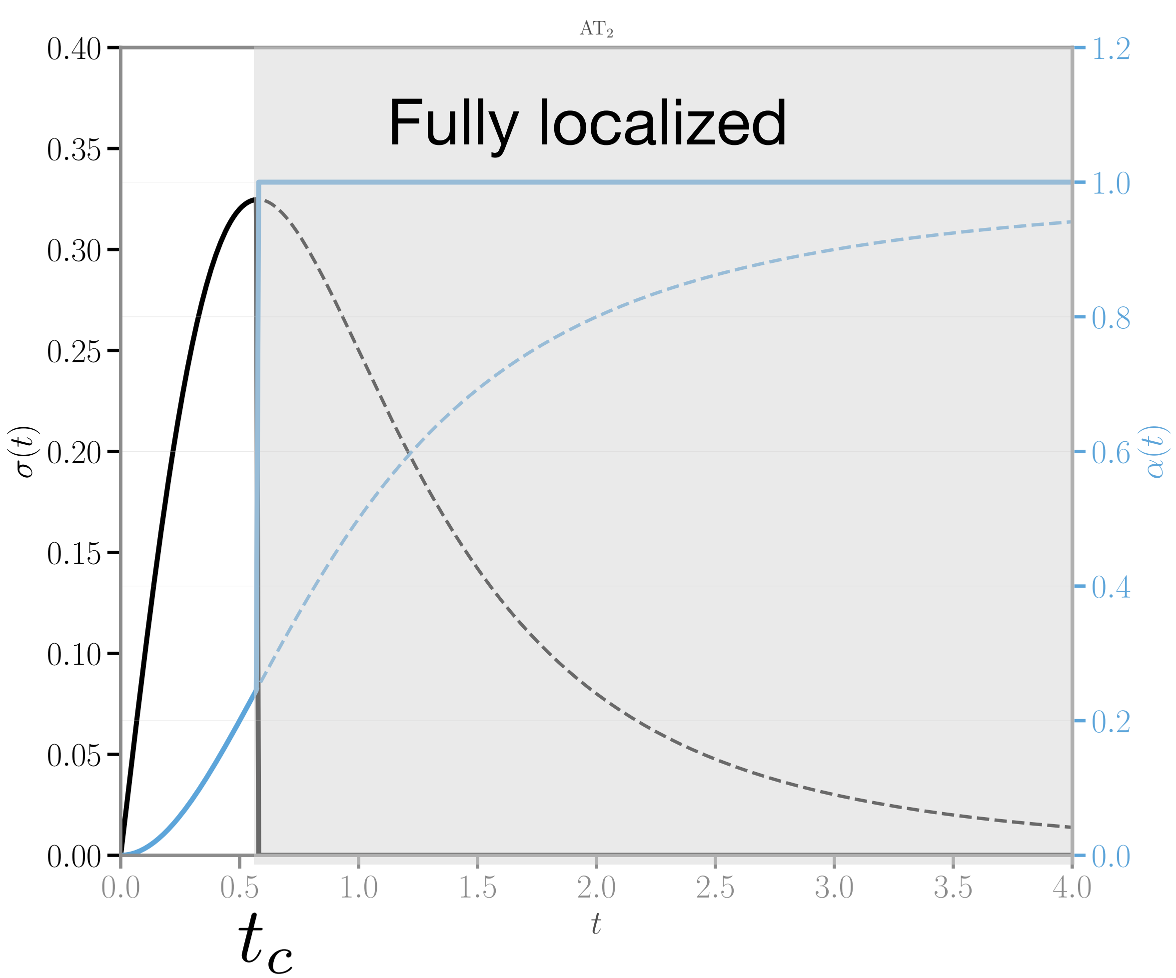
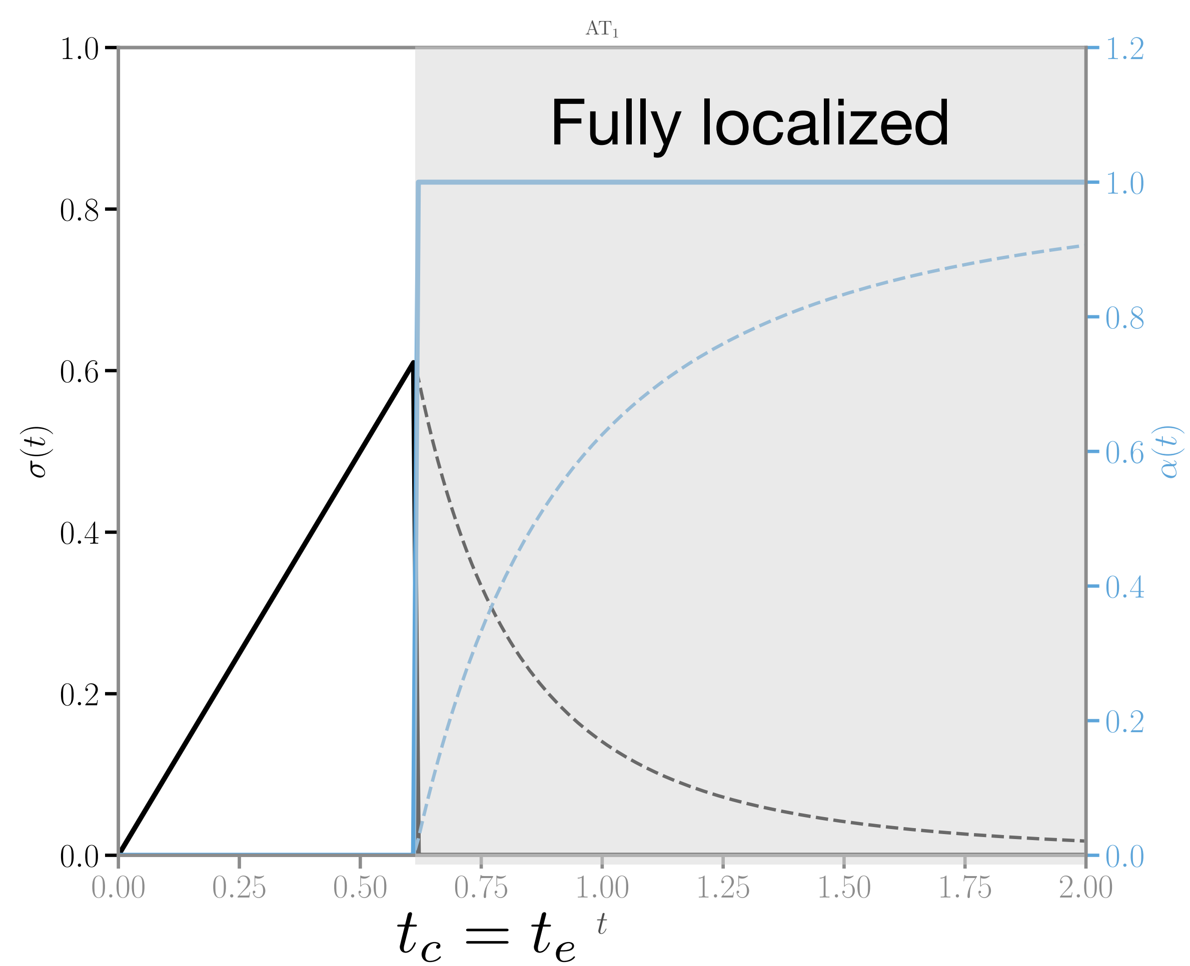
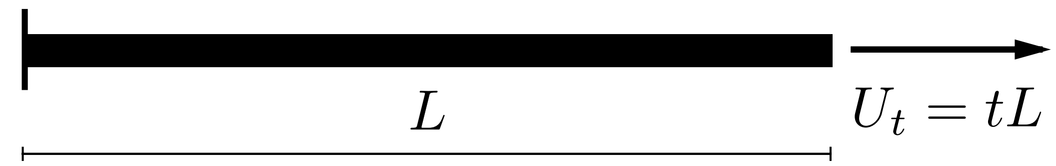
Construction of elastic, homogeneous and localized states, stability analysis





Pham-Amor-Marigo-Maurini *IJDM* 2011, Pham-Marigo-Maurini *JMPS* 2011

1D problem



AT1 and AT2 models:

model	$w(\alpha)$	$a(\alpha)$	σ_e	σ_c	D	c_w
$\mathtt{AT}_1$	α	$(1-\alpha)^2$	$\sqrt{\frac{3G_cE}{8\ell}}$	$\sqrt{\frac{3G_cE}{8\ell}}$	4ℓ	$\frac{2}{3}$
$\mathtt{AT}_2$	α^2	$(1-\alpha)^2$	0	$\frac{3}{16}\sqrt{\frac{3G_cE}{\ell}}$	∞	$\frac{1}{2}$

Regularization parameter ℓ is *not* an independent parameter.

ℓ is the material's *characteristic/internal length*, depends on σ_c, and K_{Ic}:

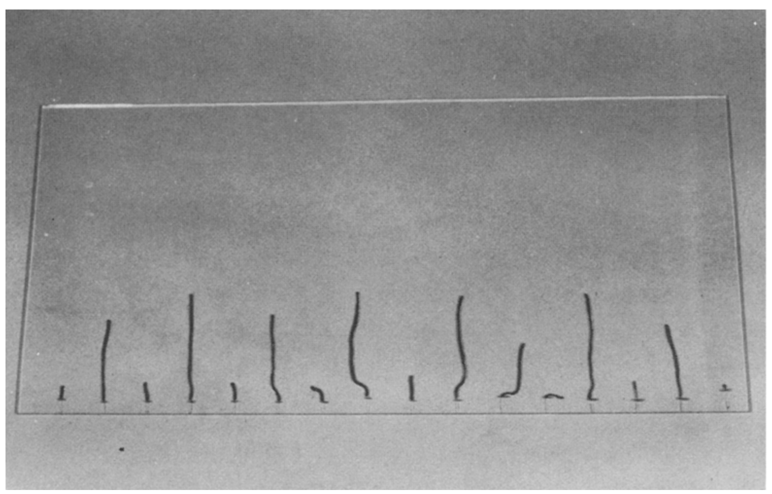
AT1: $\ell_1 := \frac{3}{8}\frac{G_cE}{\sigma_c^2} = \frac{3}{8}\frac{K_{Ic}^2}{\sigma_c^2}$

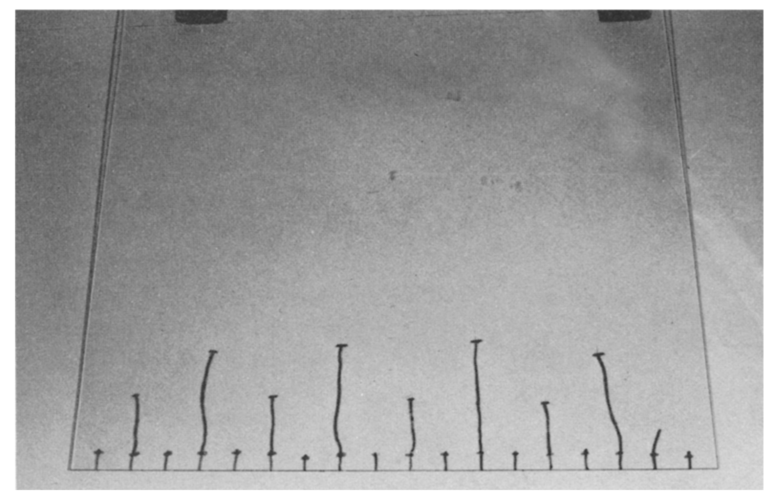
AT2: $\ell_2 := \frac{27}{256}\frac{G_cE}{\sigma_c^2} = \frac{27}{256}\frac{K_{Ic}^2}{\sigma_c^2}$

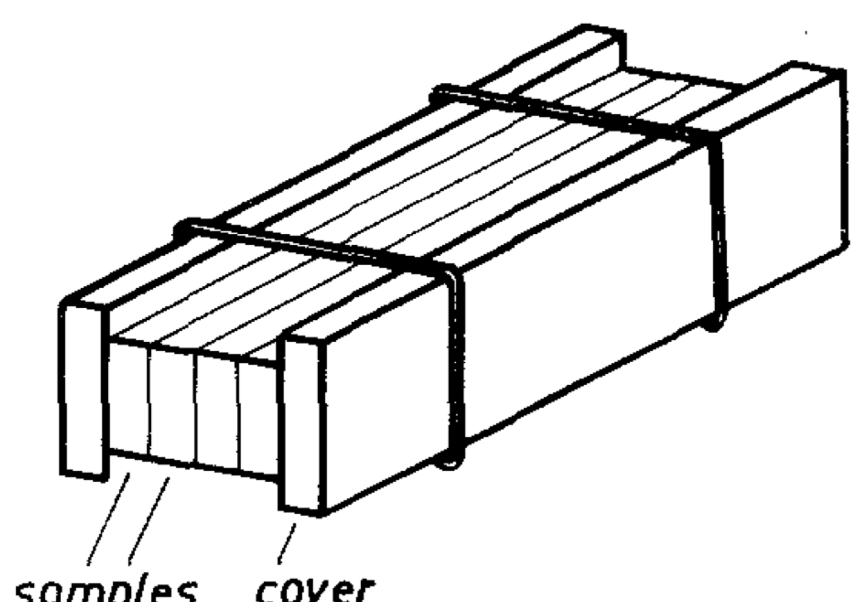
Pham-Amor-Marigo-Maurini *IJDM* '11, Pham-Marigo-Maurini *JMPS* '11

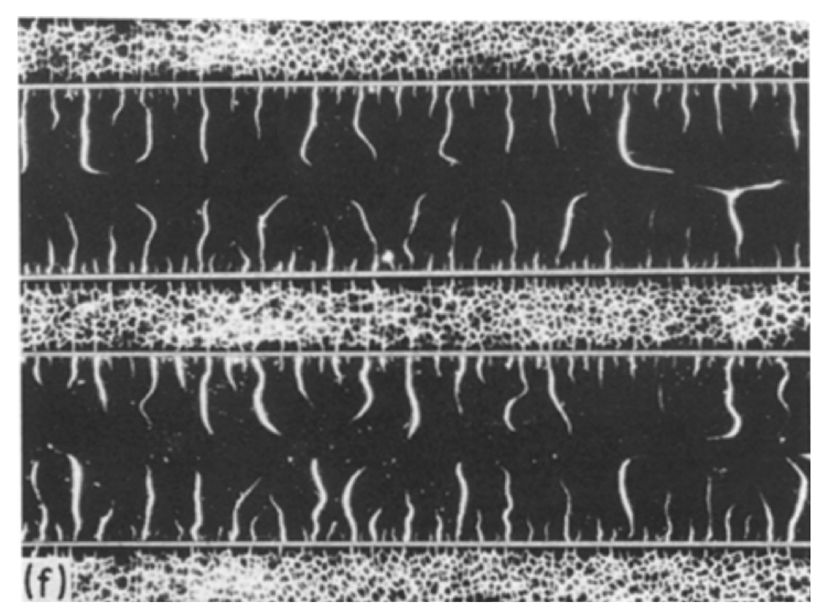
Thermal shock

- Lab experiment: thermal shock in glass, quenching of ceramic plates.
  - Original motivation: thermal reservoir stimulation.
- Uncoupled problem: effect of crack geometry on heat transfer neglected.
  - Dimensional analysis: only one parameter $\ell_0 = \dfrac{G_c}{E(\alpha \Delta T)^2}$







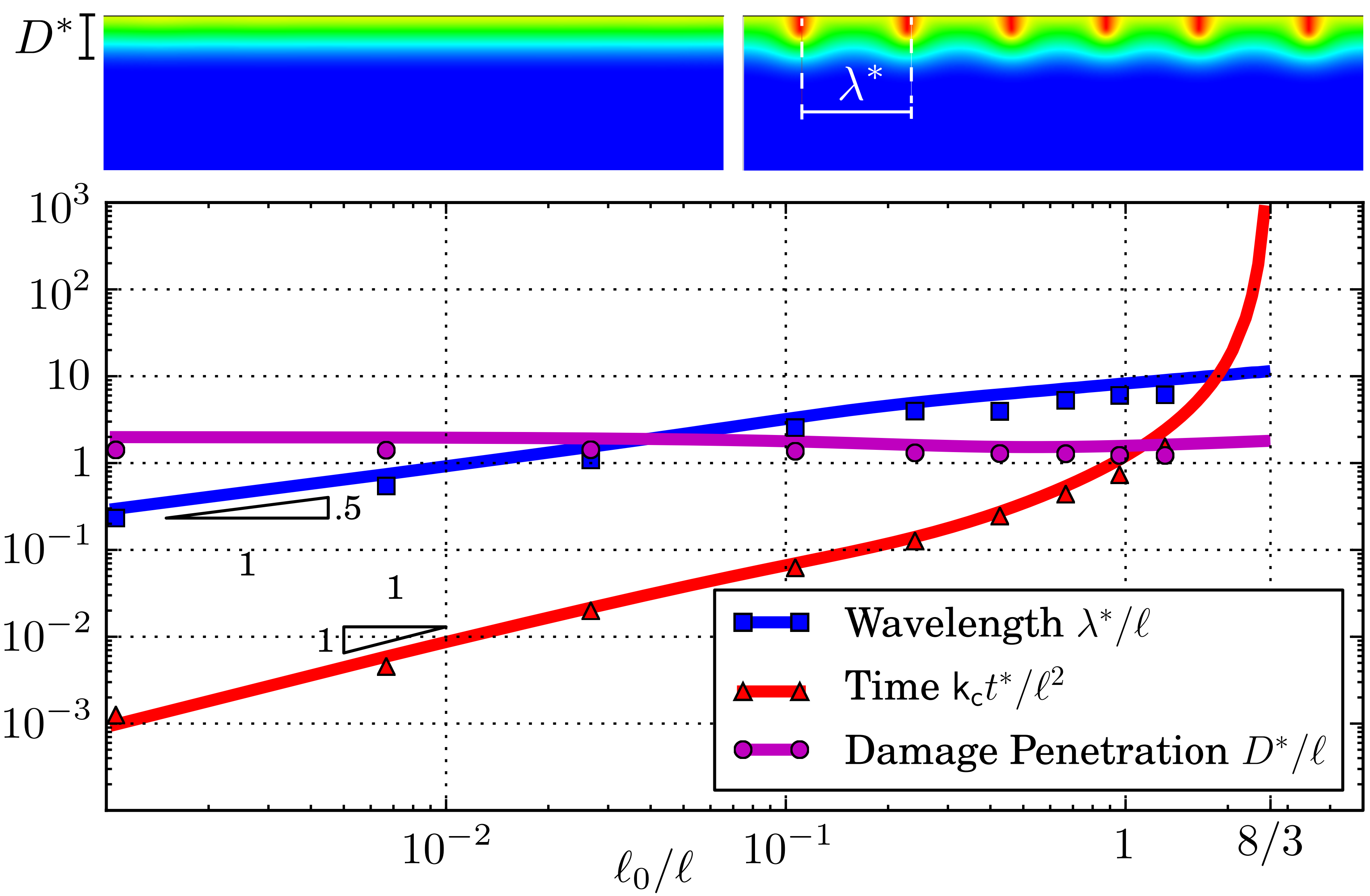


Thermal shock problem revisited

Construction of elastic and homogeneously damaged solutions

For high enough temperature contrast:

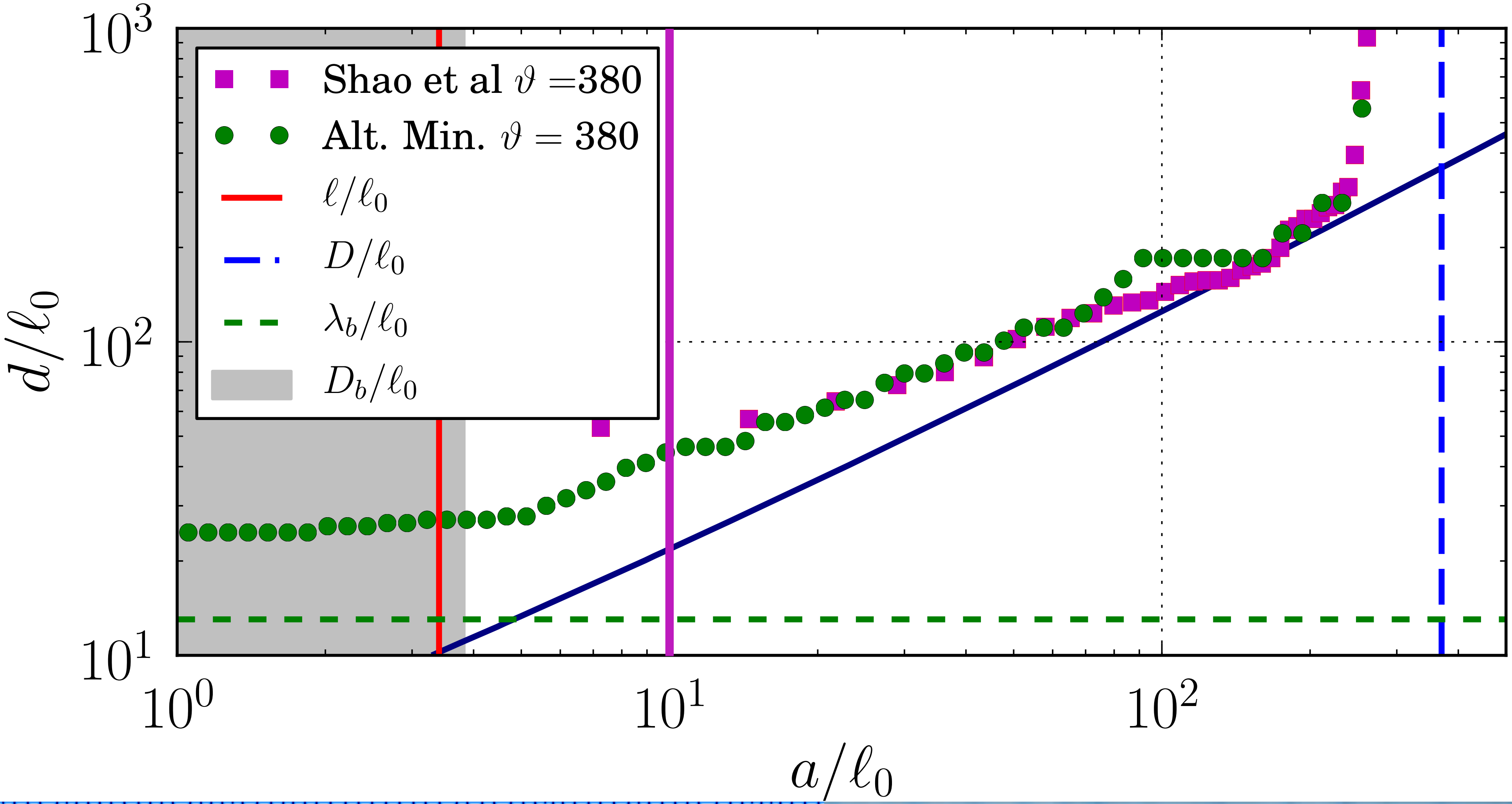
- Elastic solution
- Homogeneous damage
- Localization with spacing λ, depth D .

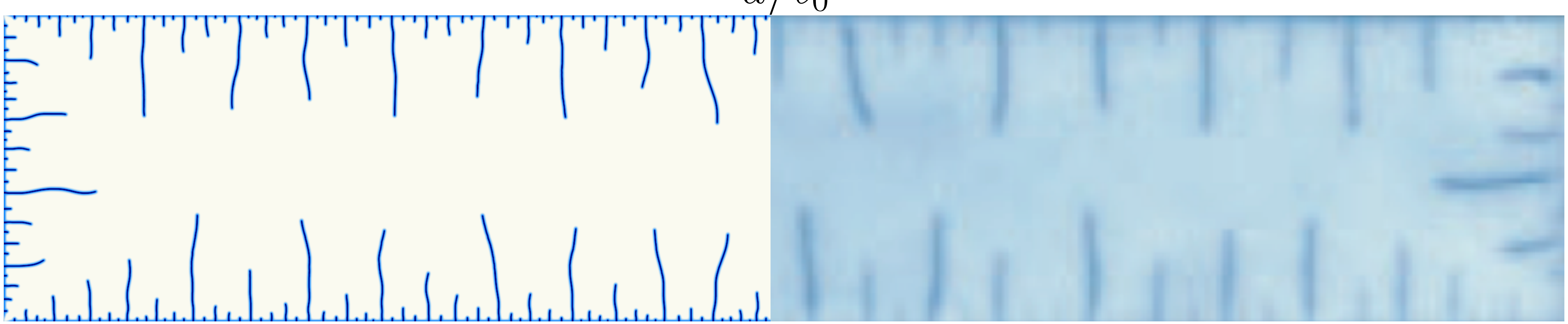


Sicsic-Marigo-Maurini, *JMPS* 2013

Validation: experiment vs. simulation

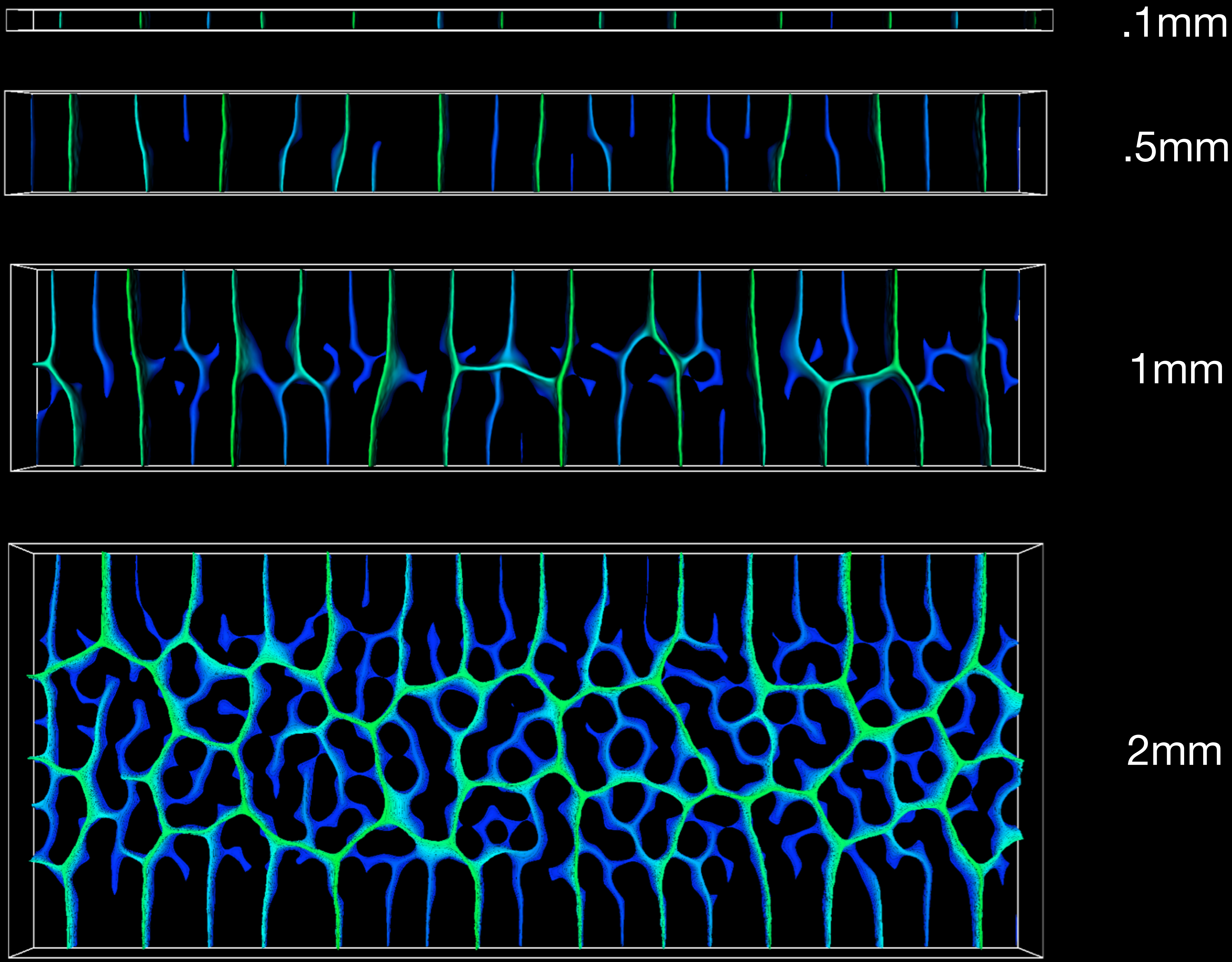
- E = 340 GPa, $\nu = 0.22$, $G_c = 42.47\ \mathrm{Jm^{-2}}$, $\sigma_c = 342.2$ MPa, $\ell = 456.24\ \mu$m
- 1 ×



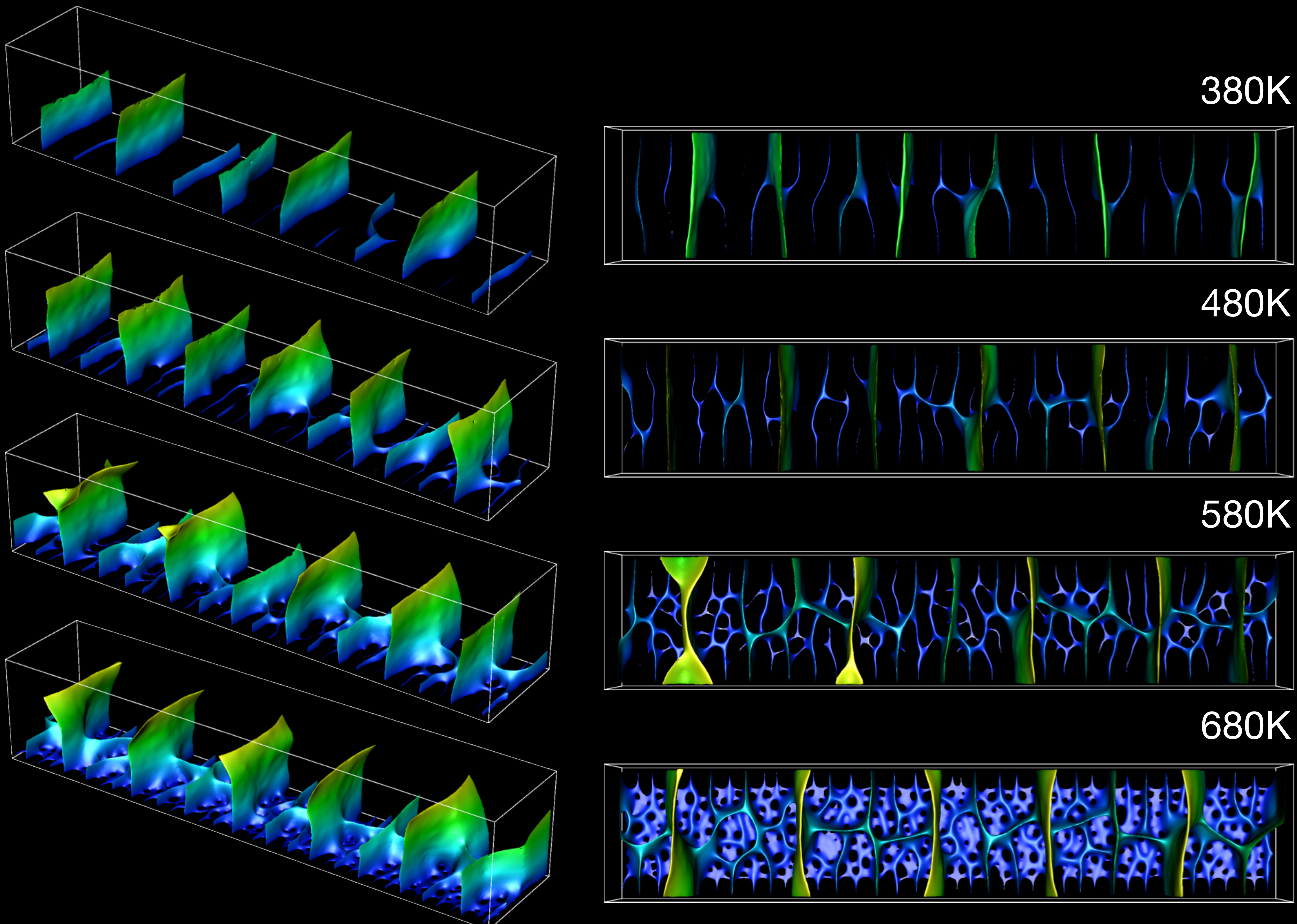


B-Marigo-Maurini-Sicsic, *PRL* 2014, Shao-Zhang-Xu-Zhou-Li-Liu, *J. AM. Ceram. Soc.* ’11.

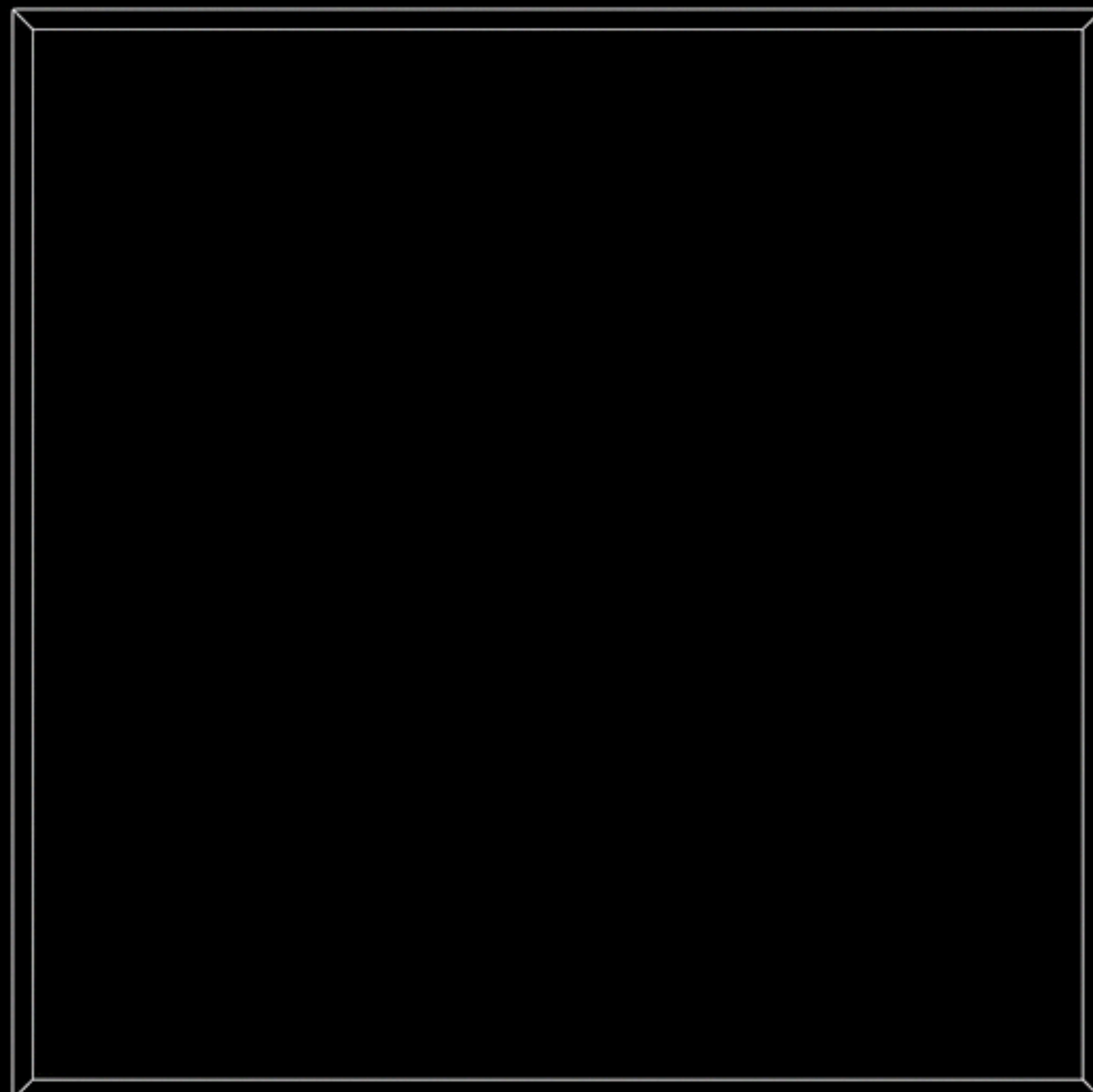
2d to 3d transition



2d to 3d transition

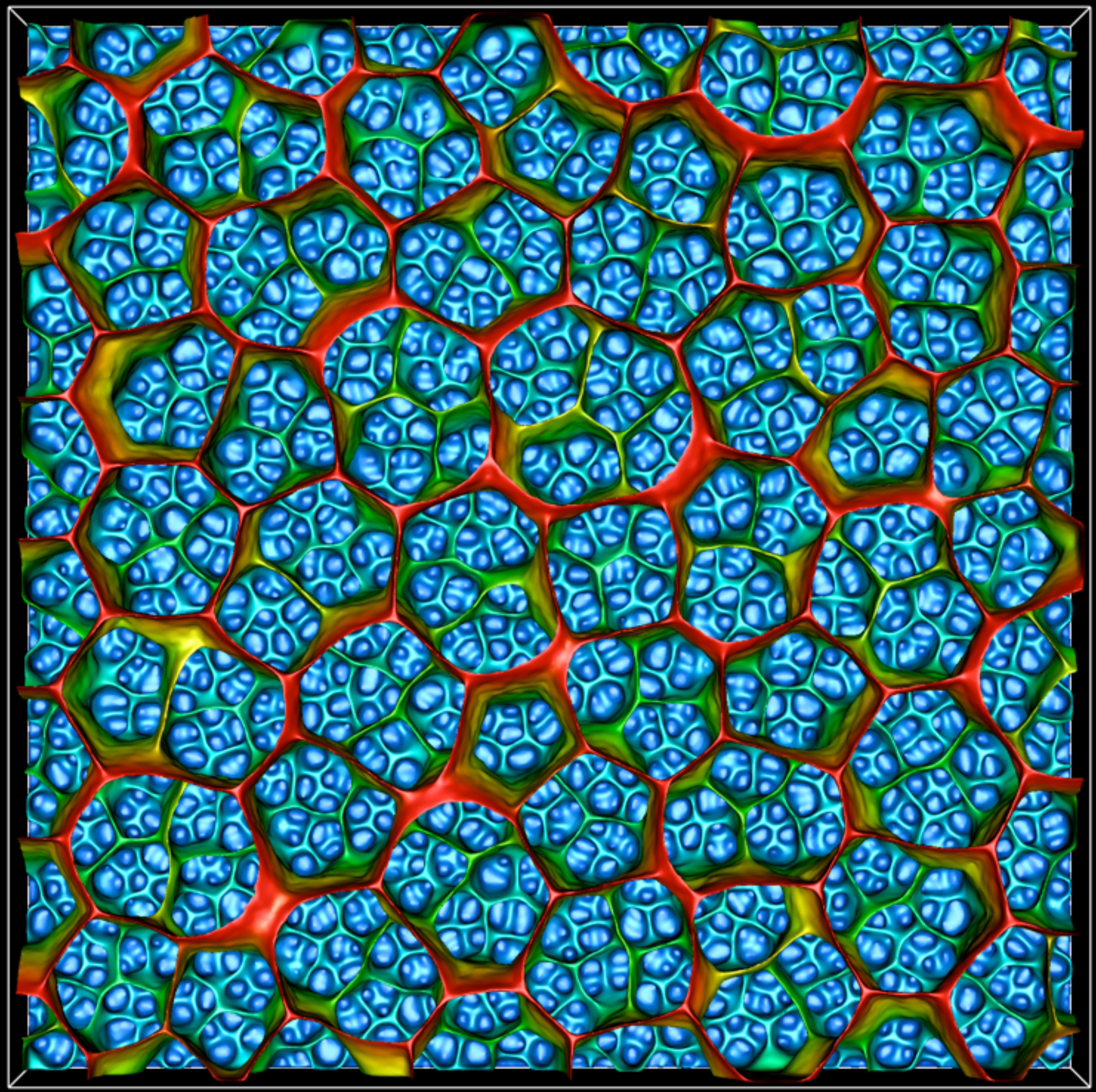


Full 3d computation



44M elements, 1536 cores (stampede, TACC), 10h.

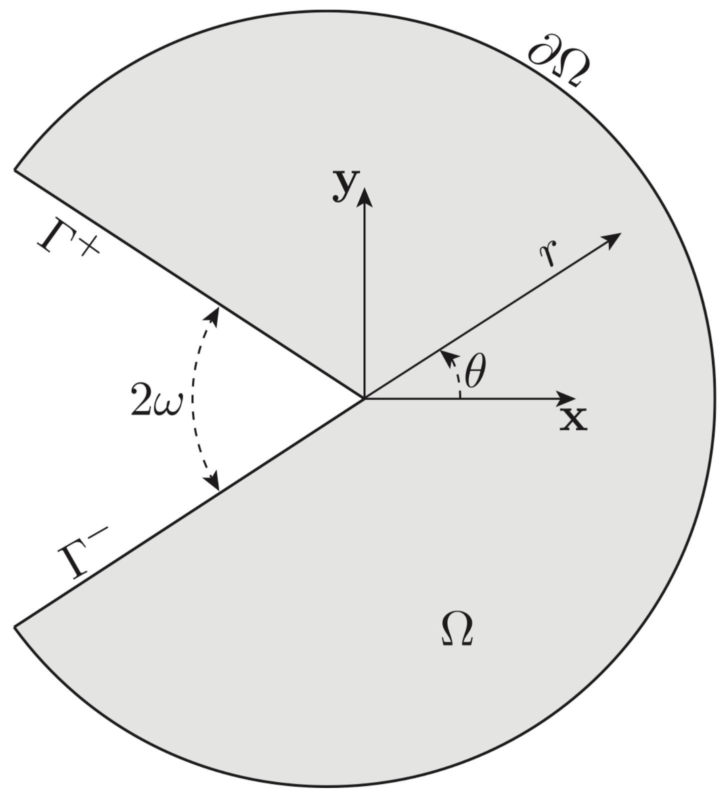
Full 3d computation

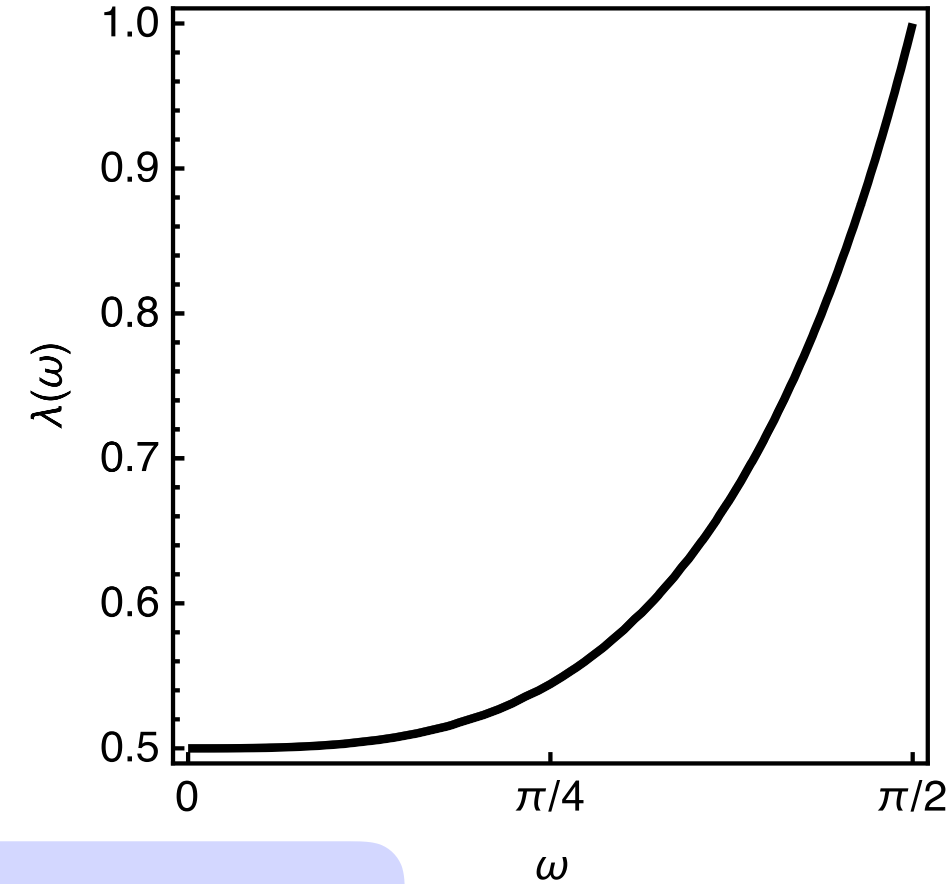


44M elements, 1536 cores (stampede, TACC), 10h.

Strength to toughness paradox

Notch angle 2ω, mode-I, singularity exponent $\lambda(\omega)$:





$$\sigma_{\theta\theta}(\theta = 0, r) = F(\theta) r^{\lambda - 1}$$

Extreme cases:

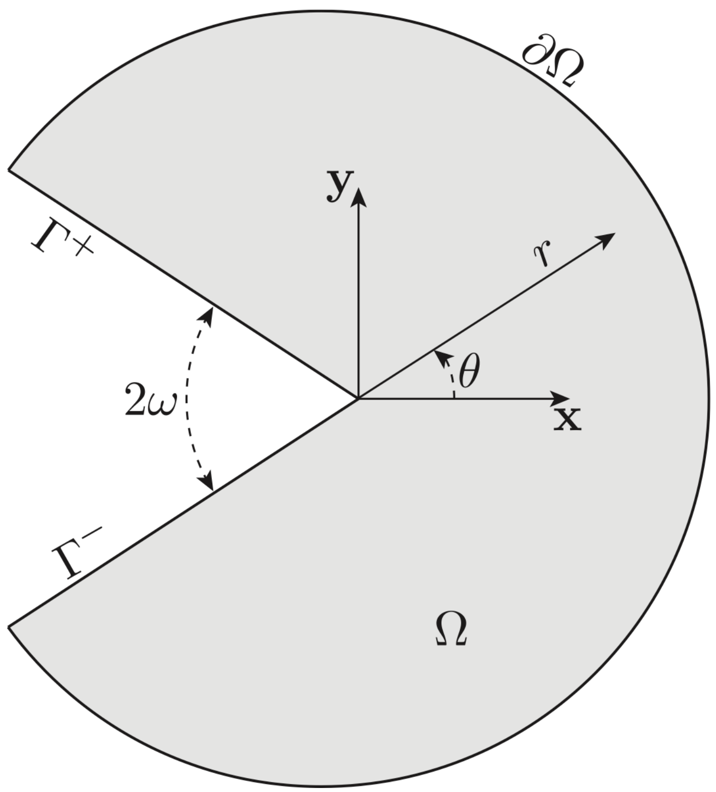
- $\omega = 0, \lambda = 1/2$: Griffith regime, progressive growth when $K_I = K_{Ic}$.
- $\omega \sim \pi/2, \ \lambda = 1$: uniaxial stress state near notch tip, nucleation at σ_c.

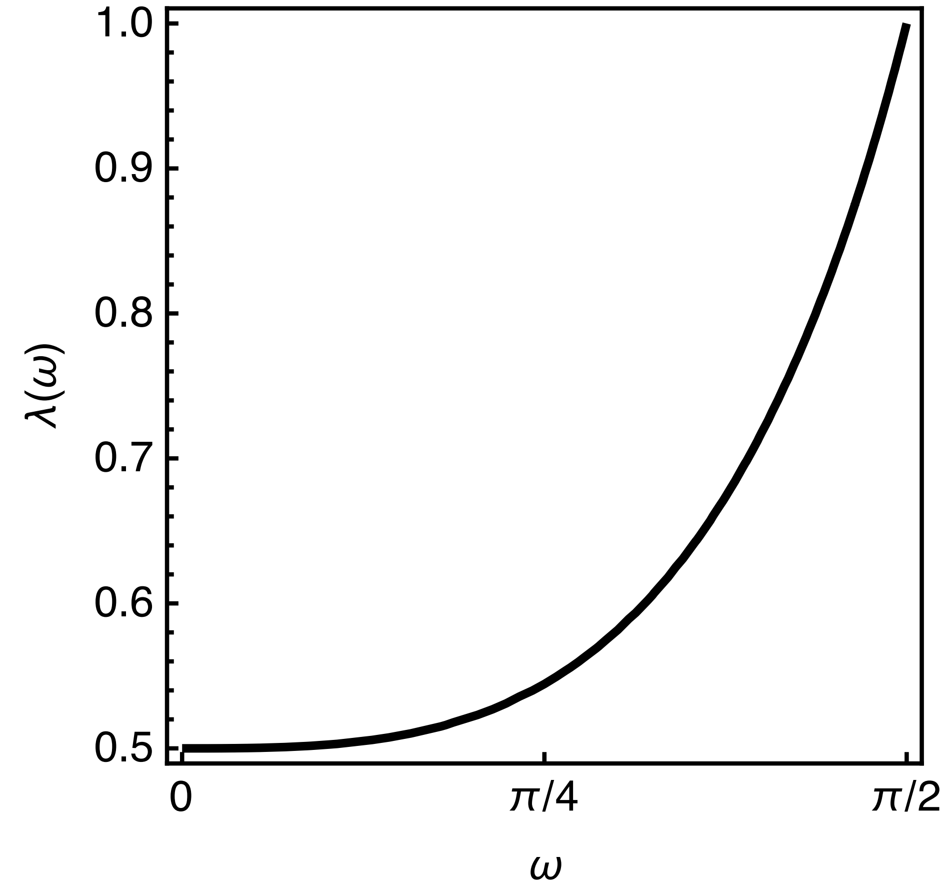
Intermediate angles:

- Nucleation impossible, according to Griffith / “local minimization”.
- Critical stress always exceeded (“weak” singularity).

Initiation at a notch

Notch angle 2ω, mode-I, singularity exponent $\lambda(\omega)$:





Generalized Stress Intensity Factor:

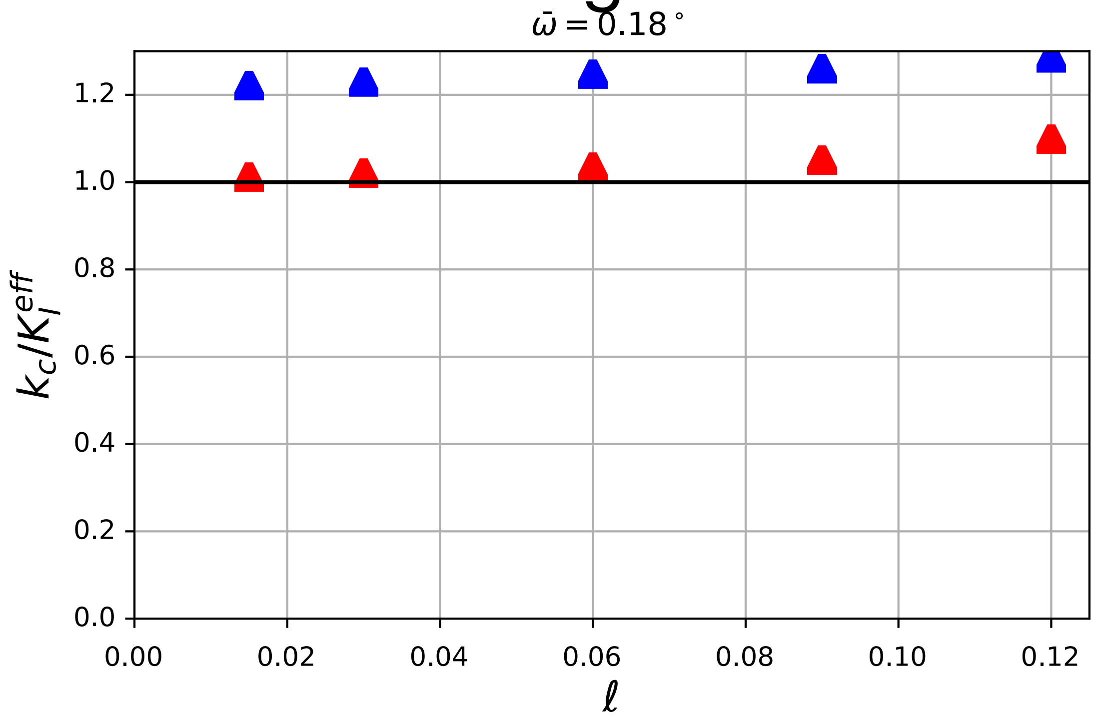
$$k = \lim_{r \to 0} \frac{\sigma_{\theta\theta}(r,0)}{(2\pi\, r)^{\lambda - 1}}$$

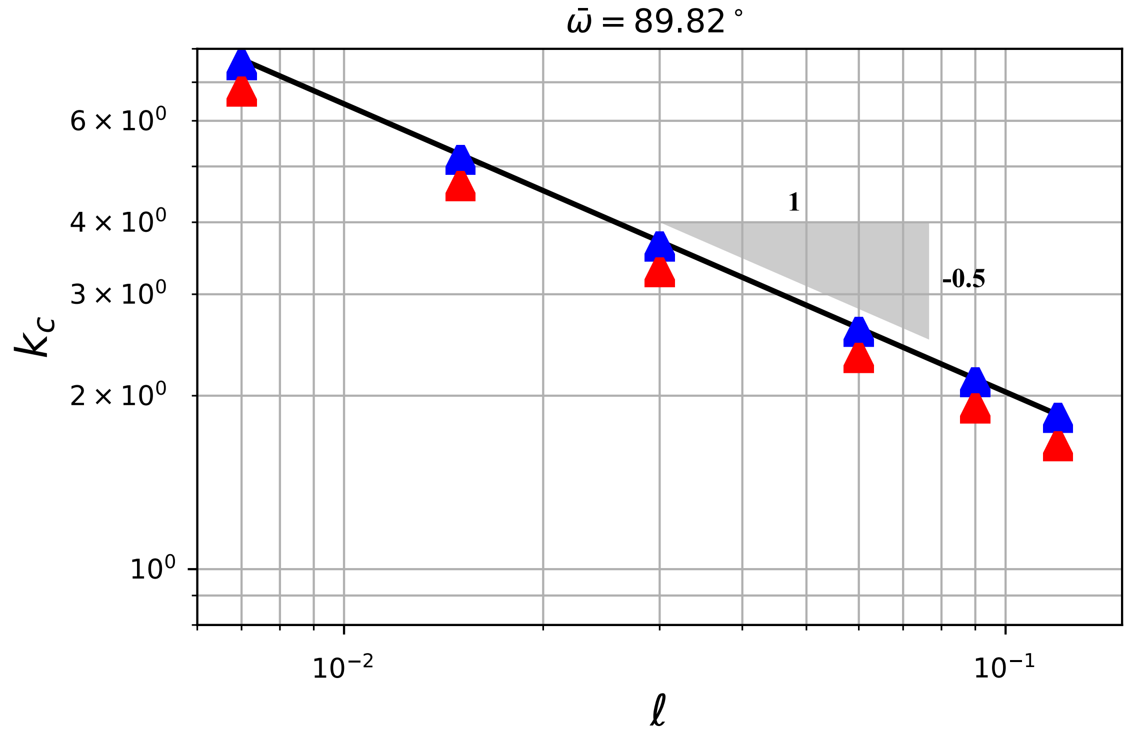
Extreme cases:

- $\omega = 0$, $k = K_I$.
- $\omega = \pi/2$, $k = \sigma_{yy}$.

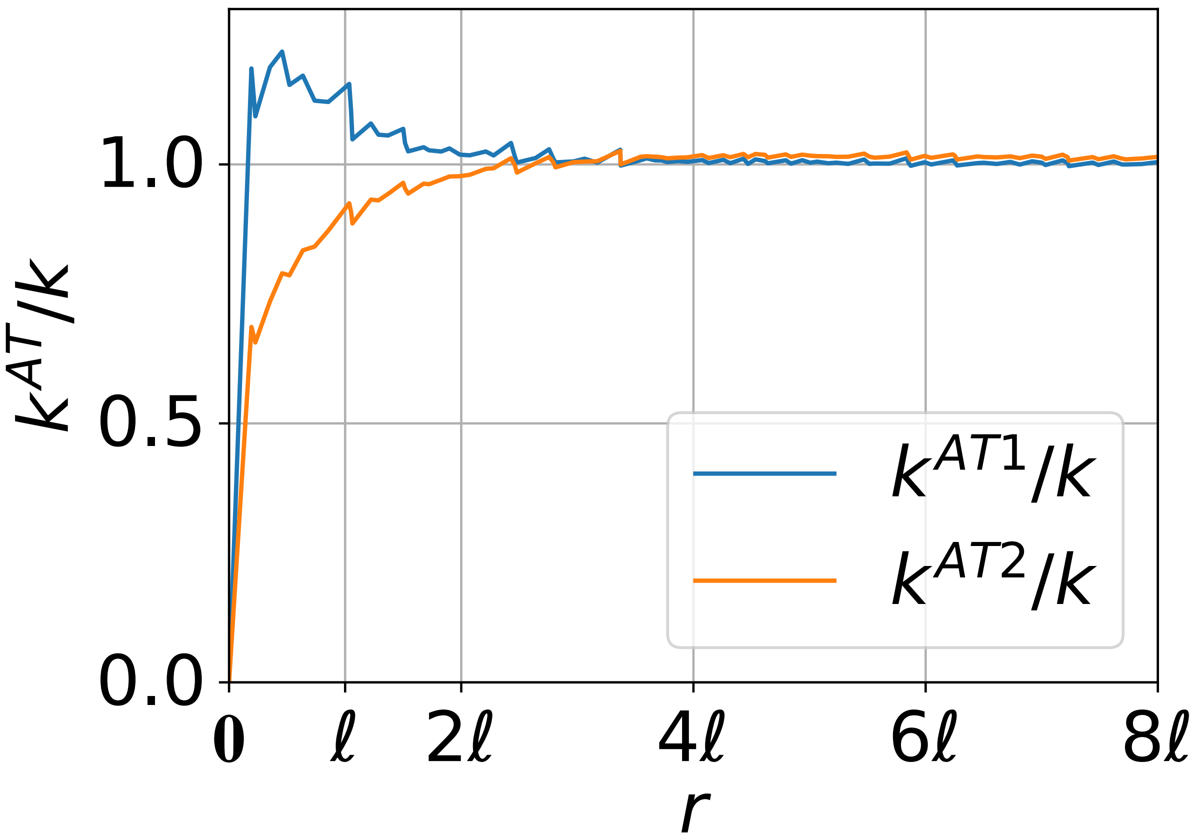
Initiation at a notch, AT1

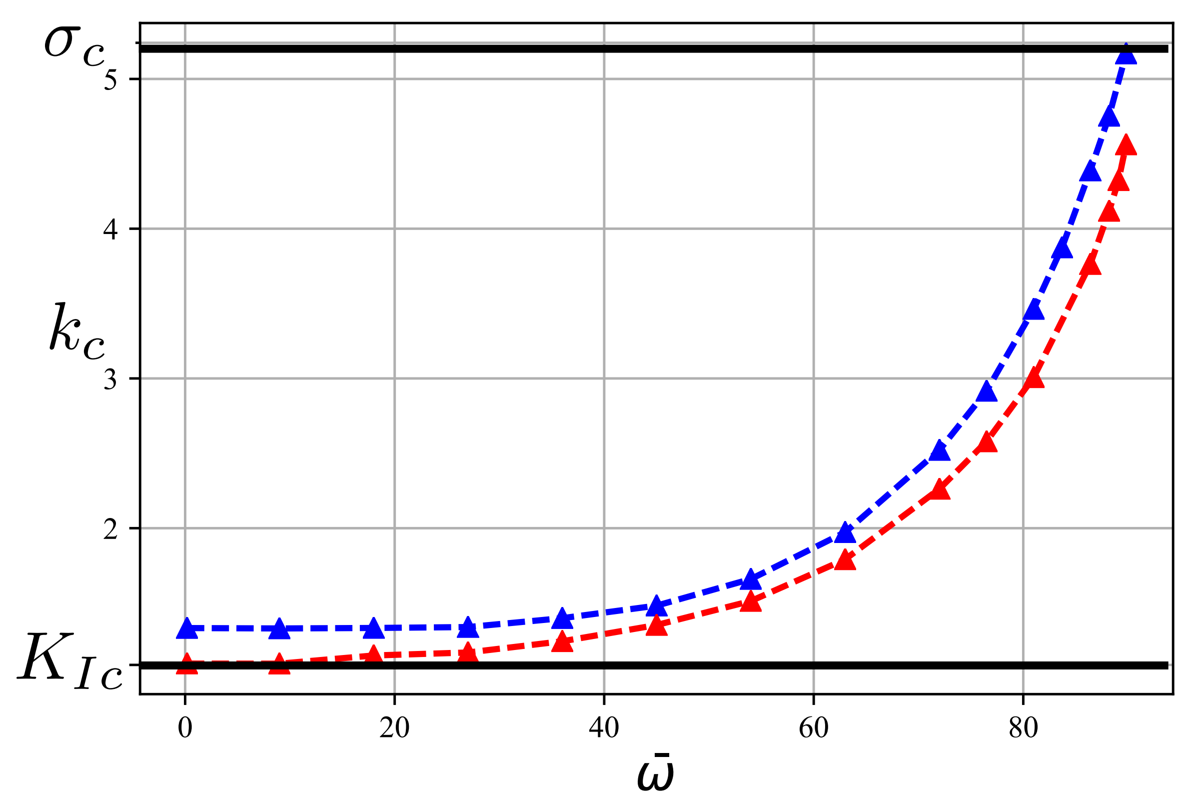
Effect of internal length:



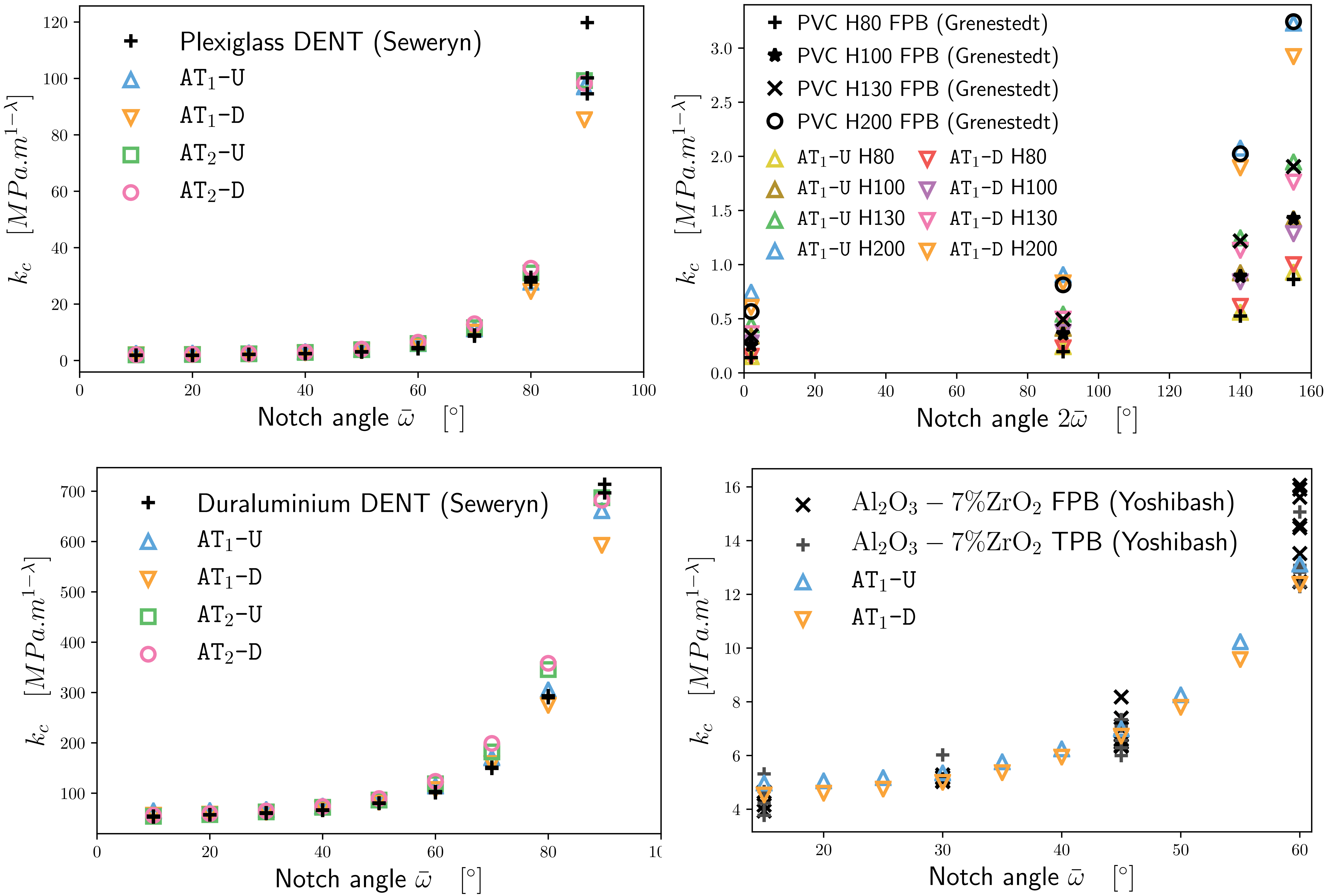


Critical generalized SIF vs notch angle $k = \sigma_{yy}/(2\pi r)^{\lambda-1}$

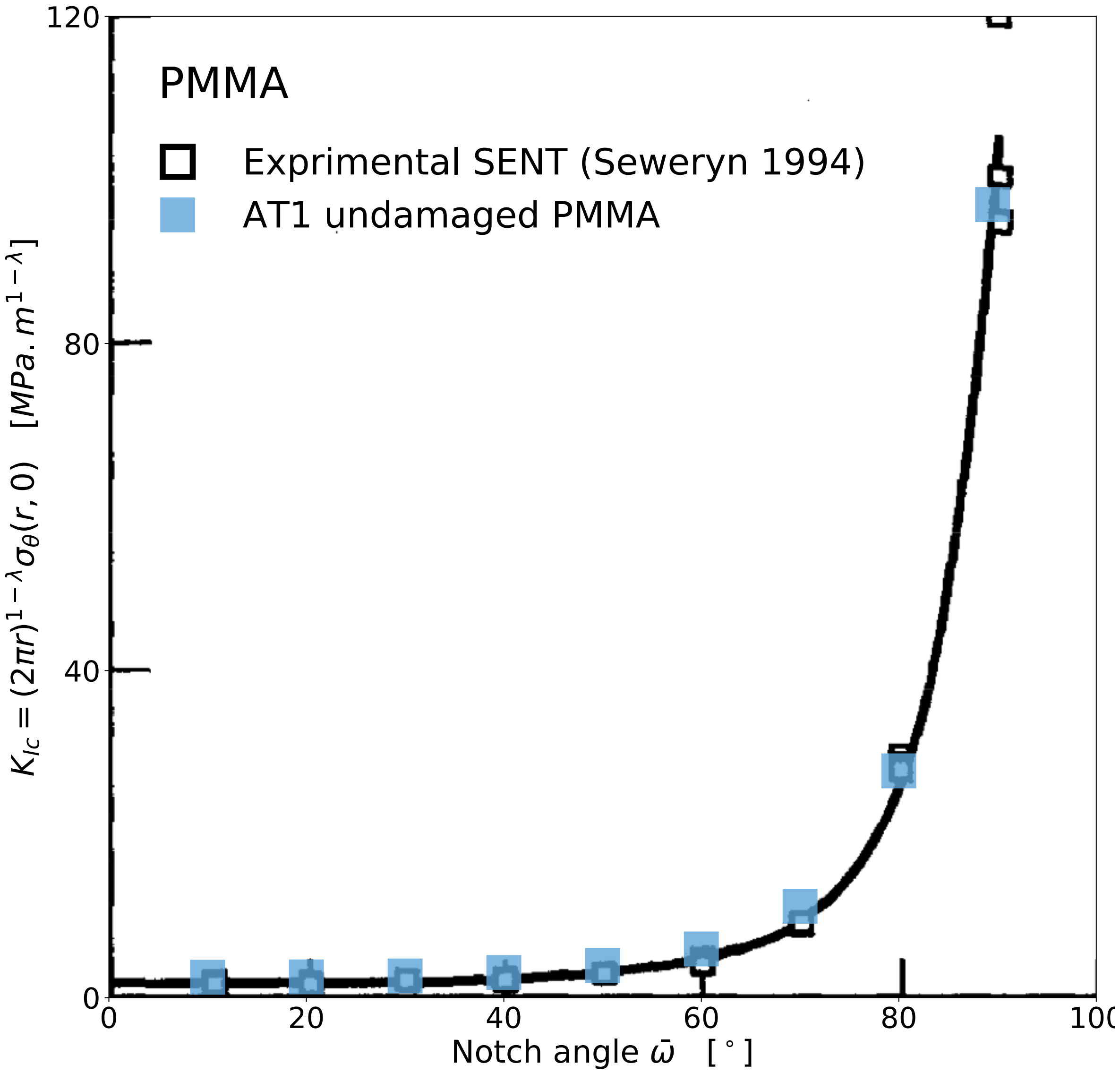


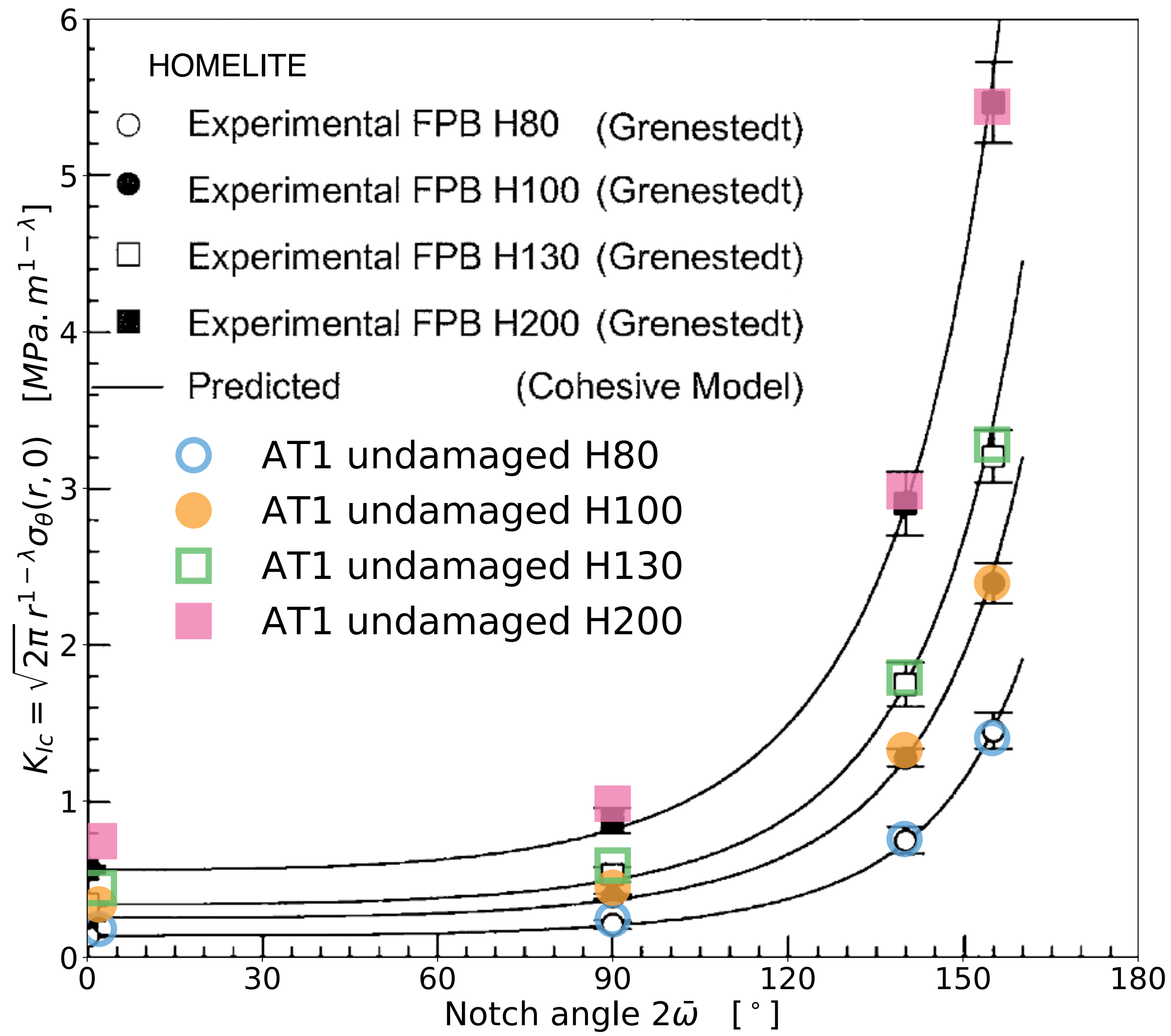


Validation: V-notch, GSIF



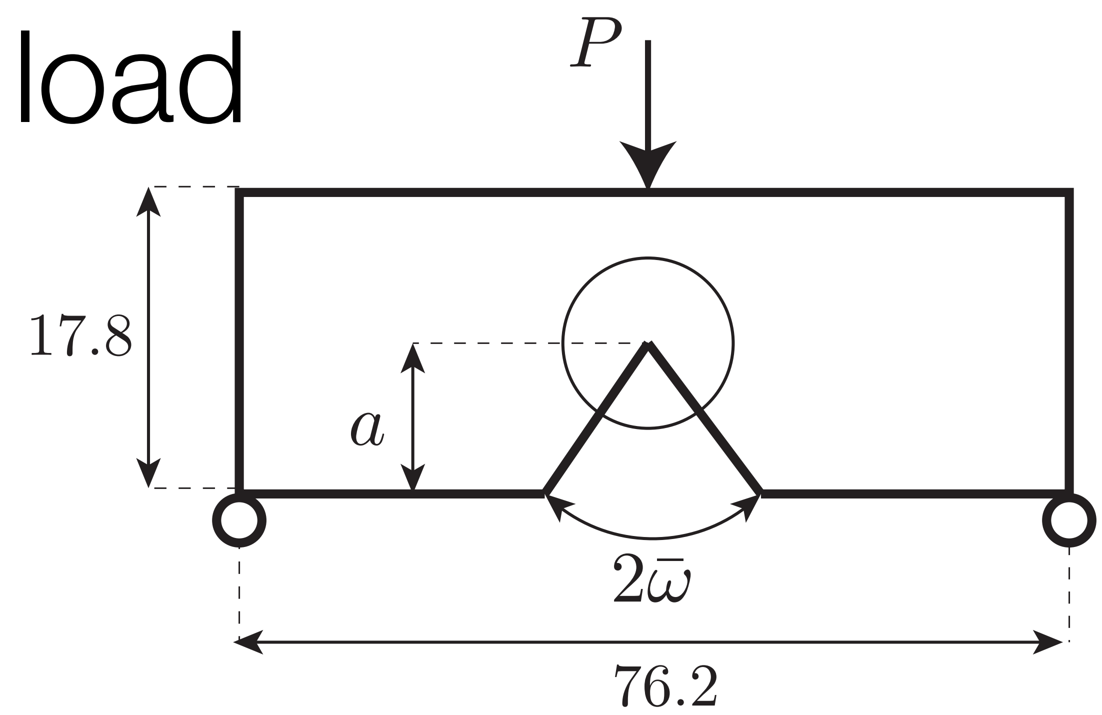
Validation: V-notch, GSIF

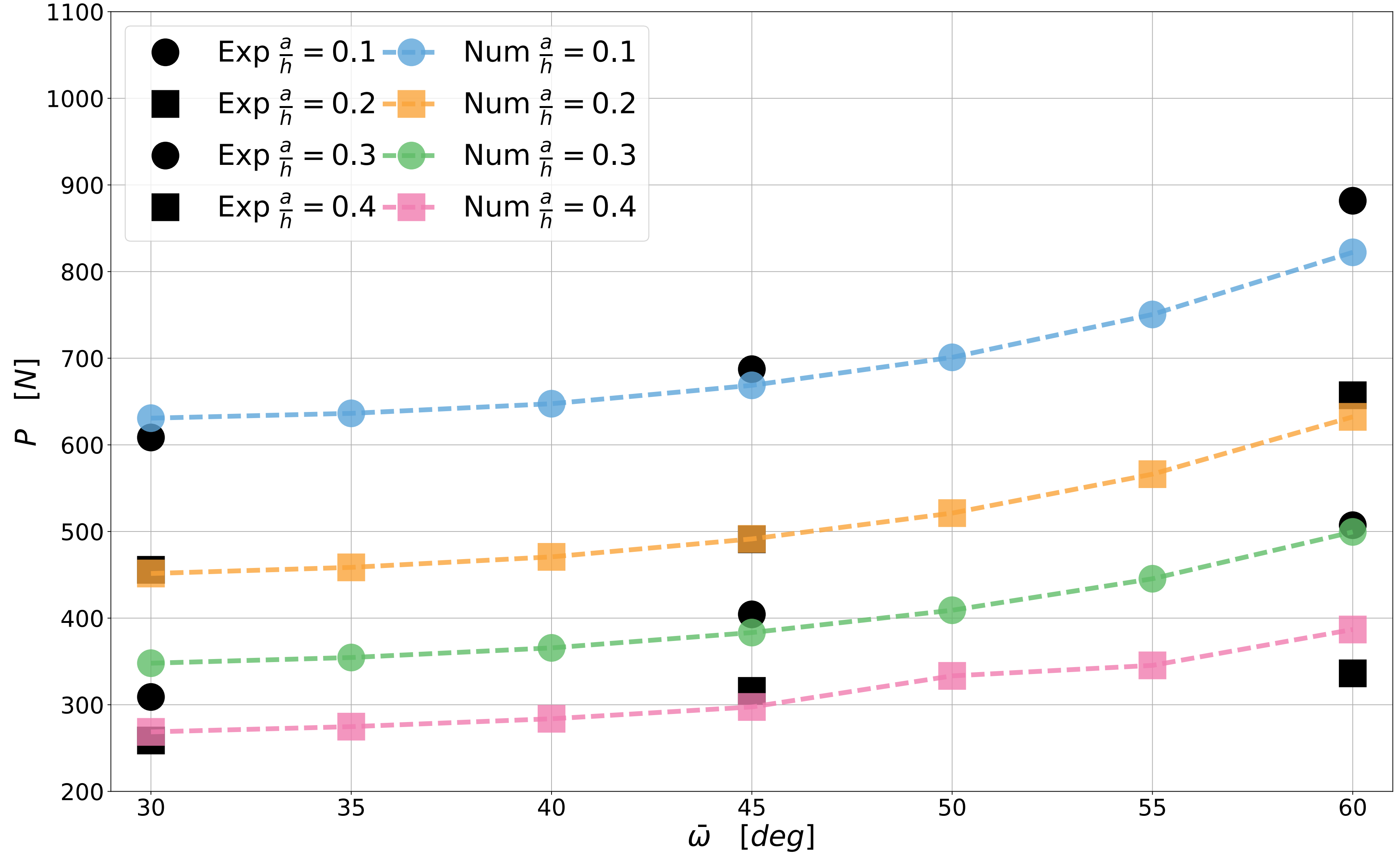




V-notch, cGSIF vs Gómez-Elices *IJF* ’06, Seweryn *EFM* ‘94

Validation: V-notch, crit. load





V-notch,TPB, PMMA. Failure load vs. Yosibash et al '04

Current state of phase-field fracture models

Dual view of Variational Phase-Field fracture models.

- Regularization method for the variational approach to fracture:
  - Crack *propagation* insensitive to a, w and *to some extend* ℓ.
  - Strong influence of a, w, ℓ on nucleation.
- Gradient-damage models with $\ell = \ell_{\mathrm{ch}} = \mathcal{O}(K_{Ic}^2 / \sigma_c^2)$
  - Effect of a, w on nucleation can be understood by stability analysis.

Predictive, validated theory for propagation *and* nucleation in brittle materials (see also Pham-Ravi-Chandar-Landis, *IJF*, ’17).

Variational phase field models of fracture provide a unified way to recover well-accepted propagation and nucleation criteria from a variational model. They involve the same characteristic length as cohesive laws while remaining faithful to Griffith’s postulates.

Toughening in the brittle regime

Commonly accepted toughening mechanisms:

- Crack path deviation, bridging;
- Dissipation by microscopic cracks;
- Plastic dissipation, ductile effects.

What is toughening, “effective toughness” of heterogeneous materials?

- Giacomini ’05: elastic and fracture properties homogenize separately, effective toughness through Γ-limit.
- Hossain-Hsueh-Bhattacharya-B *JMPS* ’14: mechanism to compute effective toughness:
  - Surfing BC at *macroscopic* scale, free path at *microstructure* scale.
  - Compute the peaks of the ERR (driving force to obtain steady state).

Hossain-Hsueh-Bhattacharya-B *JMPS* ‘14

V&V: “Bittencourt’s door”

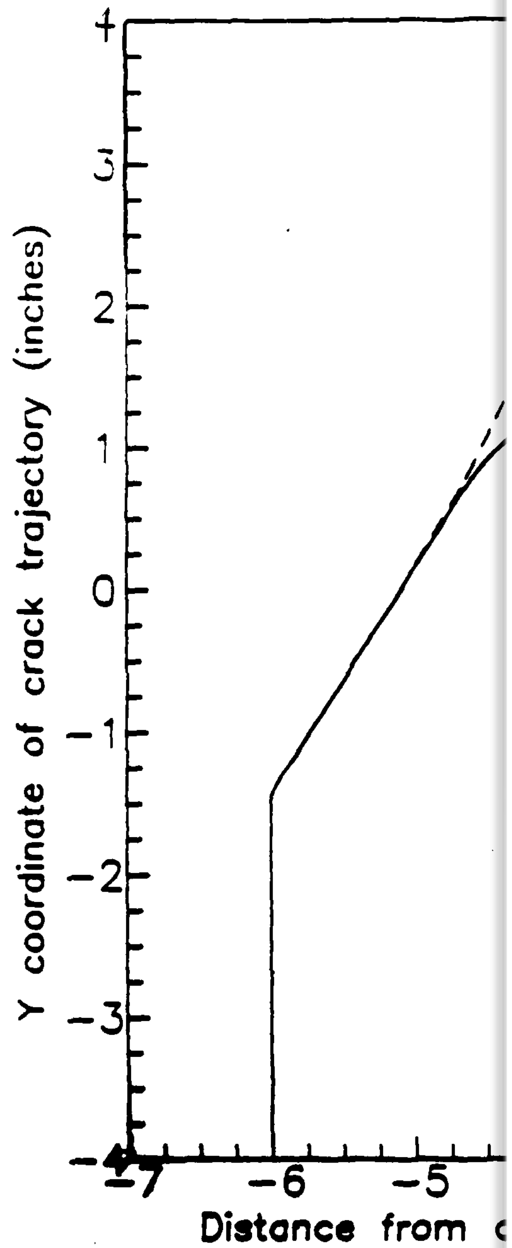
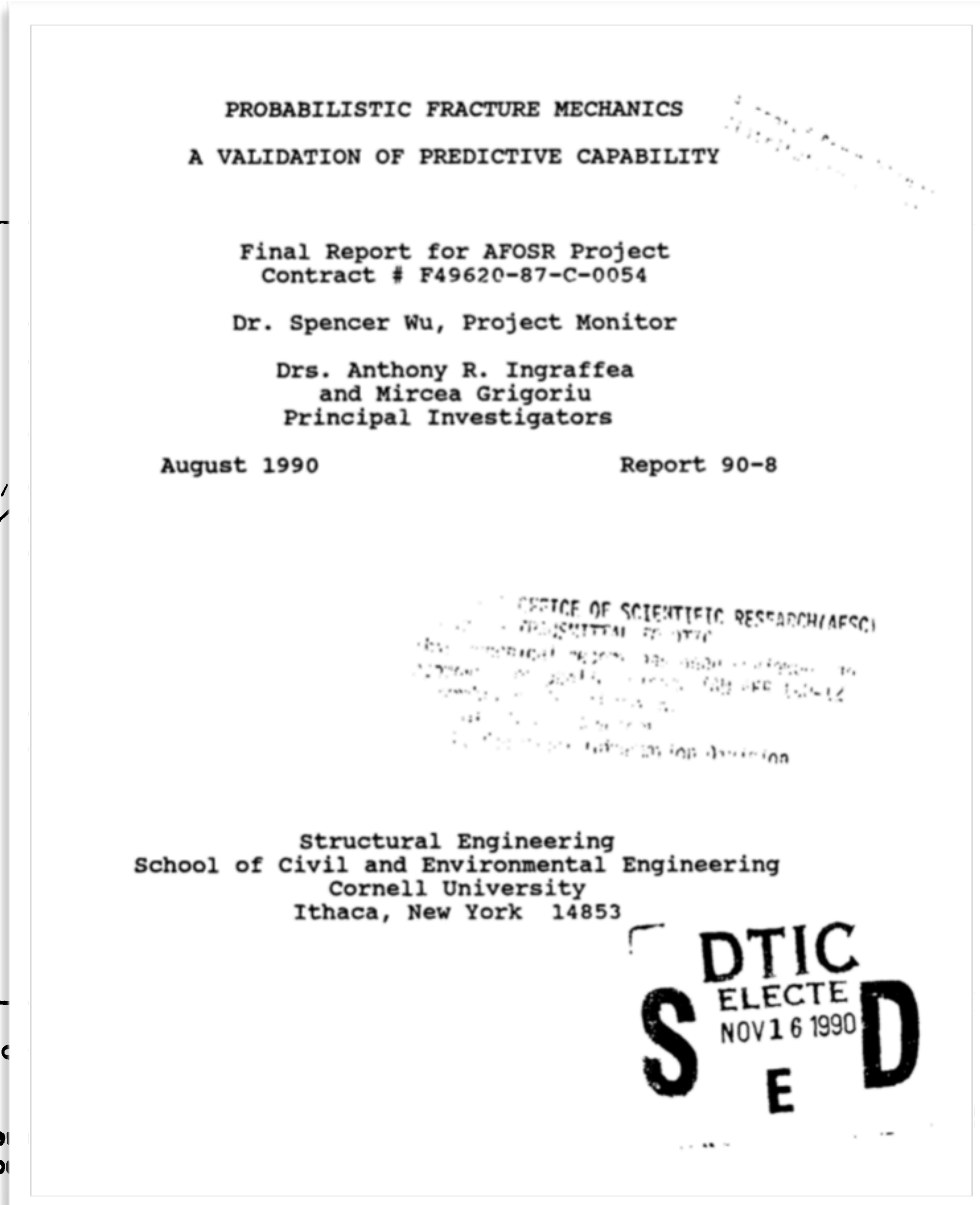


Figure 5.6 Plots of obse
with and witho



PROBABILISTIC FRACTURE MECHANICS

A VALIDATION OF PREDICTIVE CAPABILITY

Final Report for AFOSR Project
Contract # F49620-87-C-0054

Dr. Spencer Wu, Project Monitor

Drs. Anthony R. Ingraffea
and Mircea Grigoriu
Principal Investigators

August 1990 Report 90-8

Structural Engineering
School of Civil and Environmental Engineering
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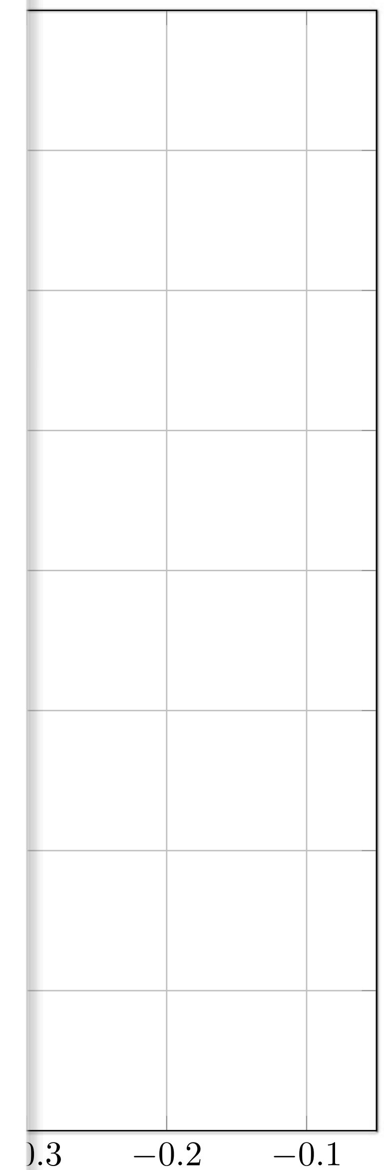
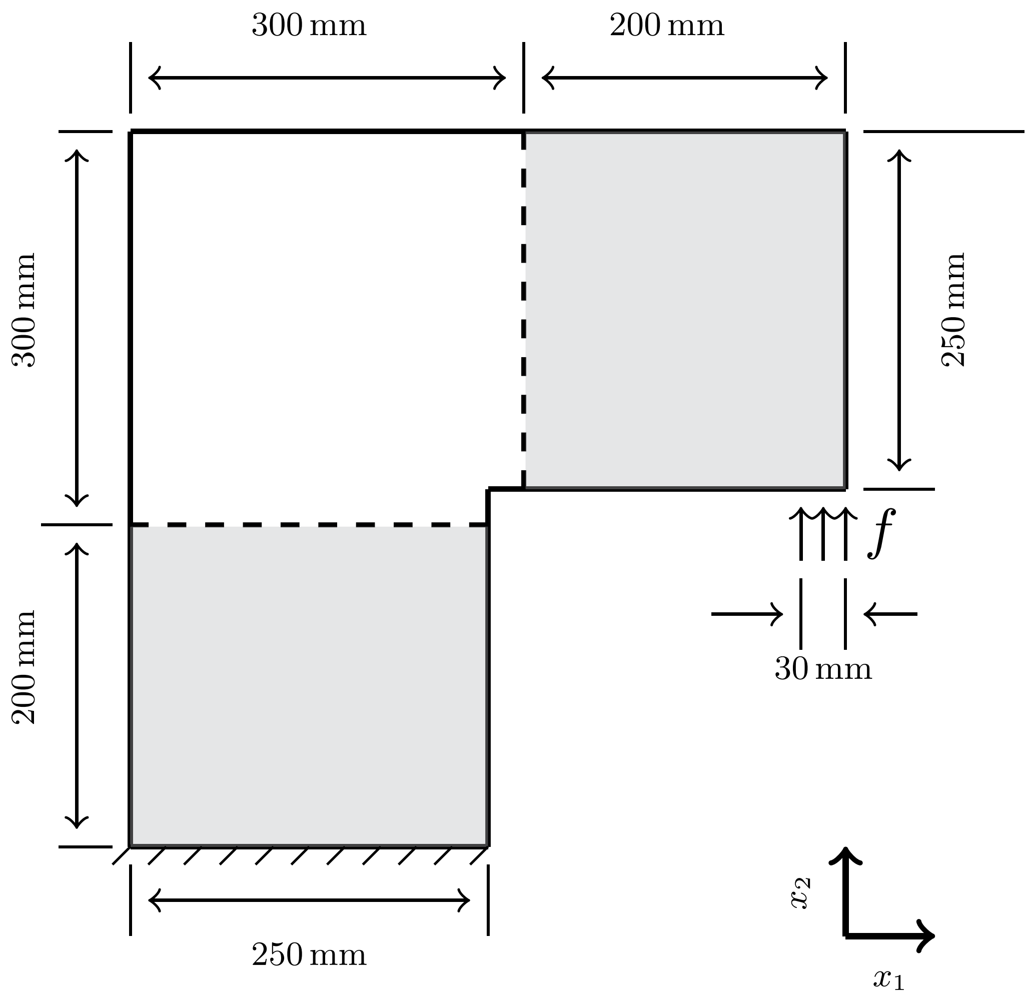
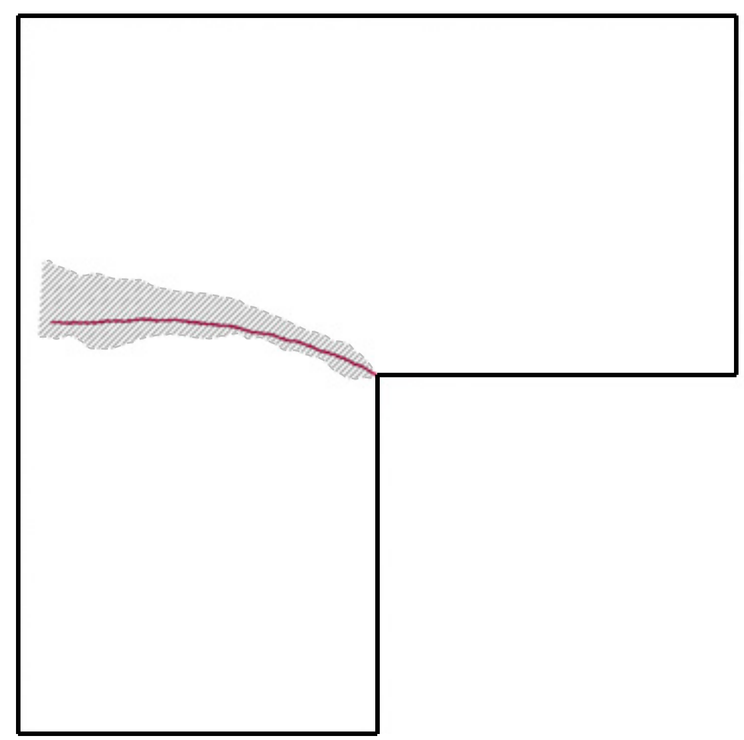
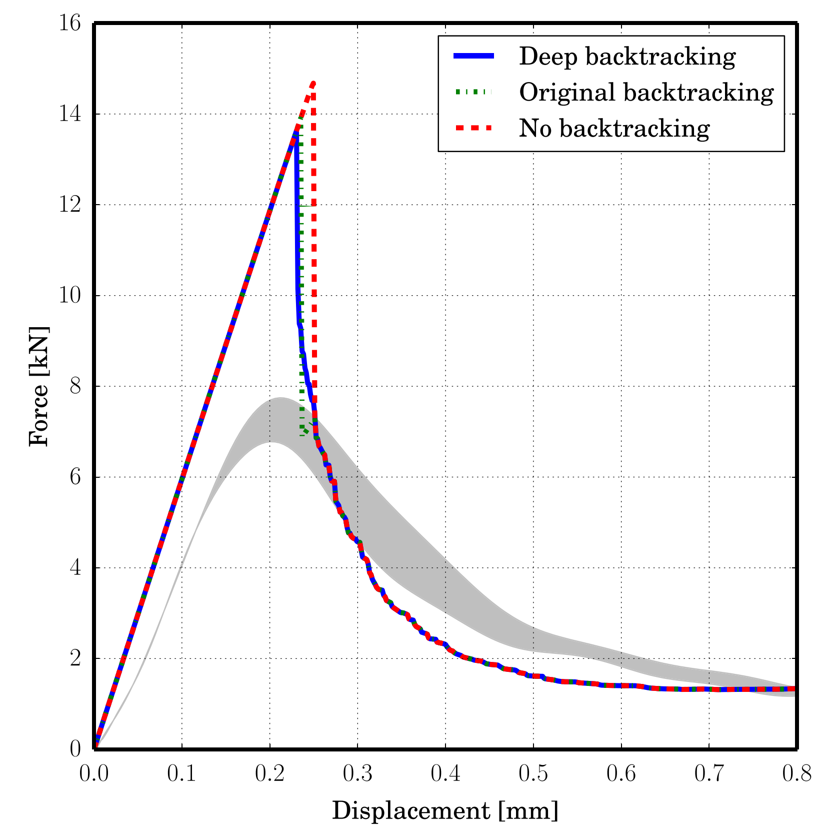


ari, *CMAME* ’15

V&V: L-shaped plate

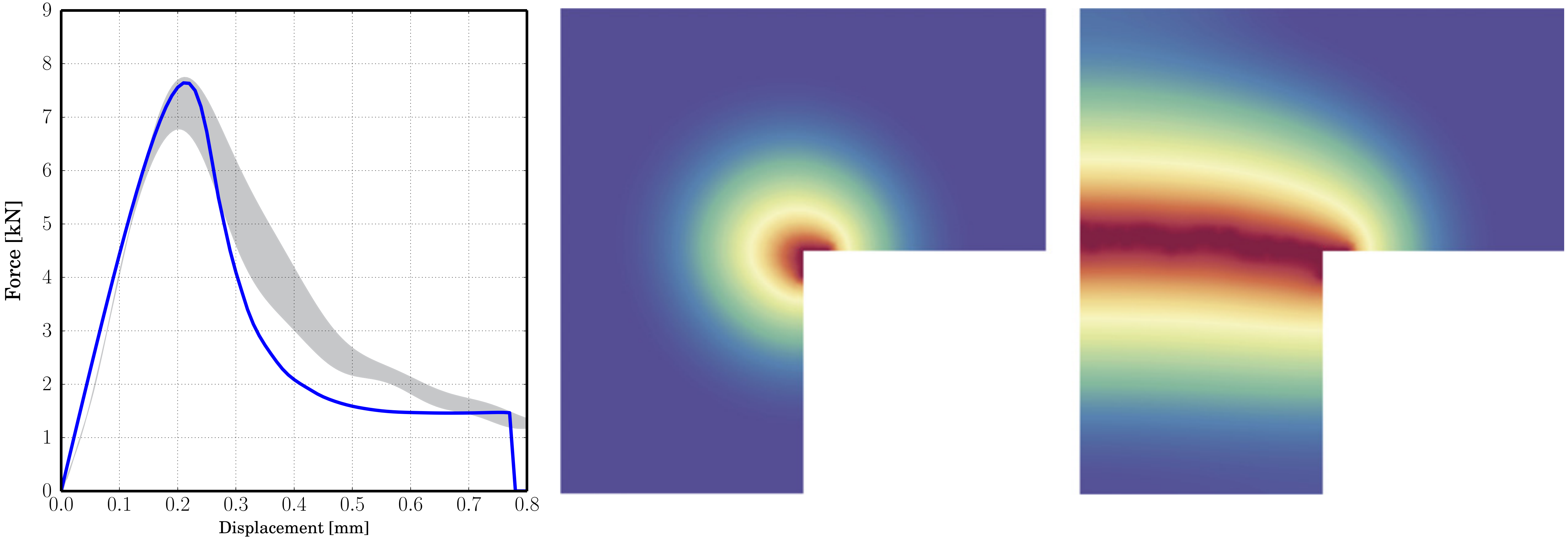






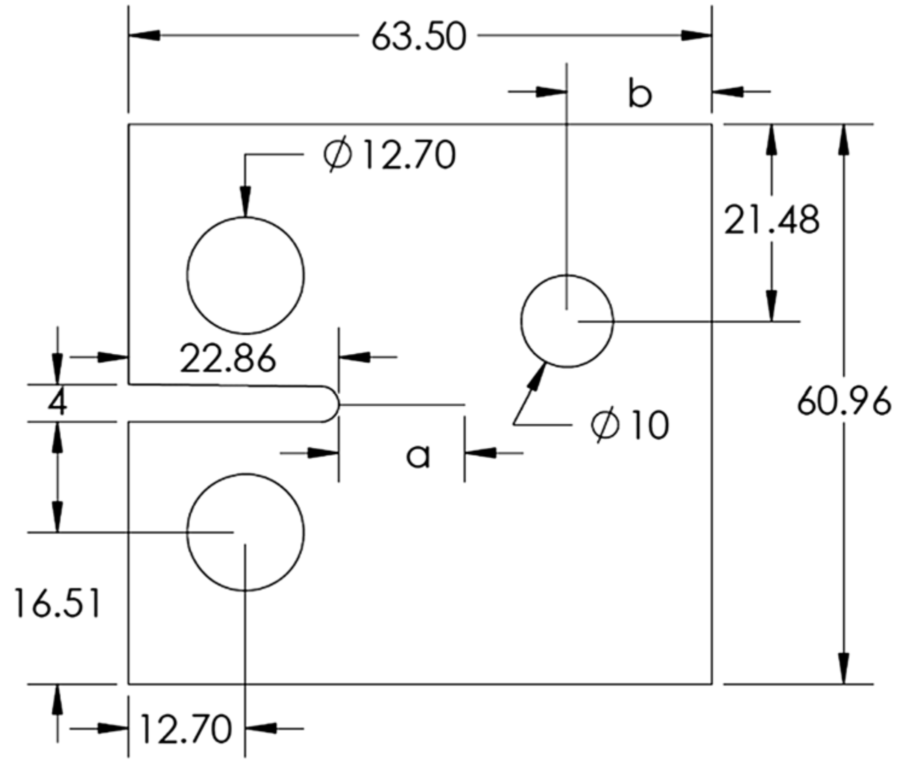
Mesgarnejad-B-Khonsari, *CMAME* '15

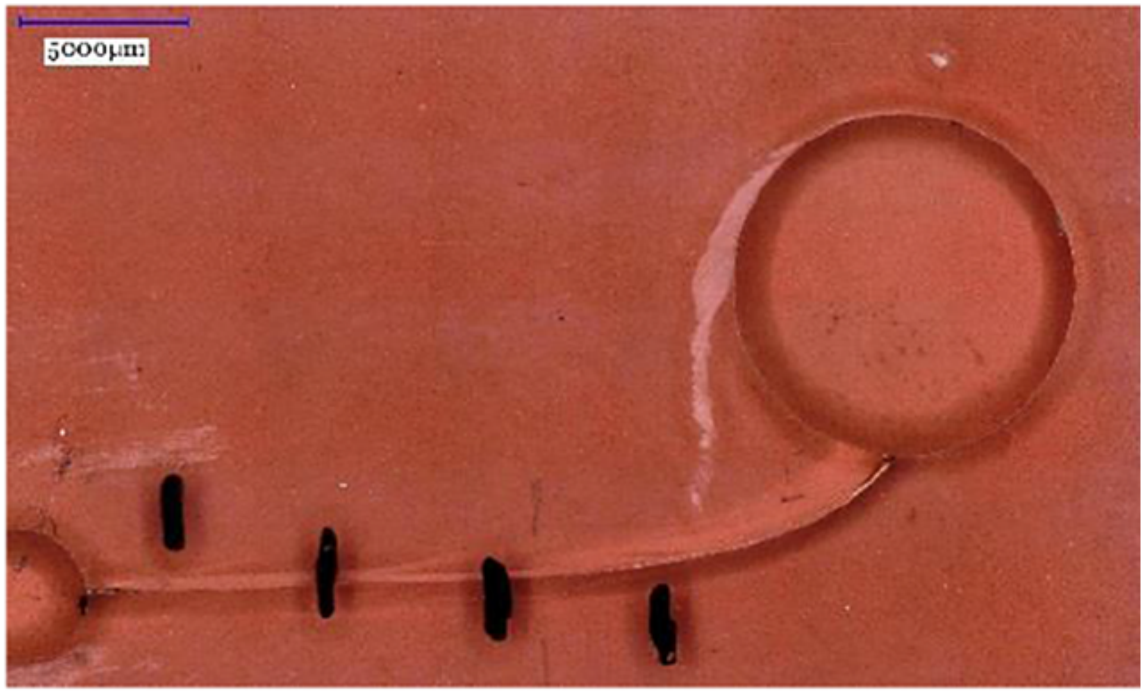
V&V: L-shaped plate

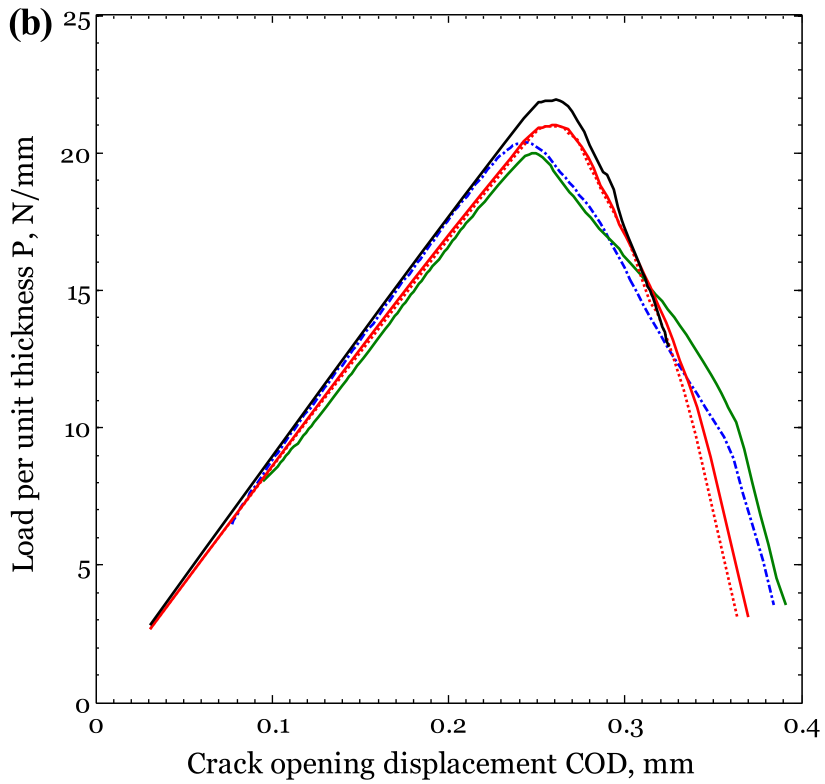


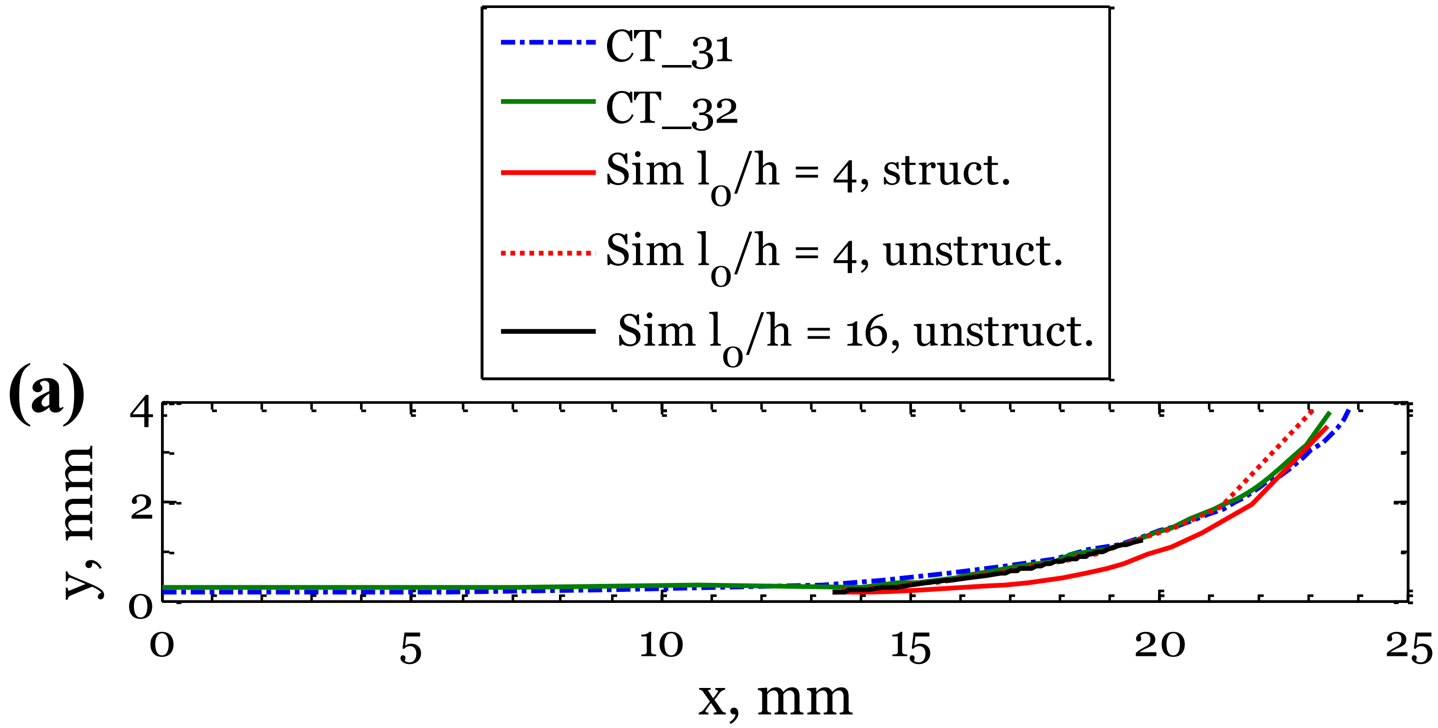
Mesgarnejad-B-Khonsari, *CMAME* '15

V&V: Mixed-mode Compact-Tension





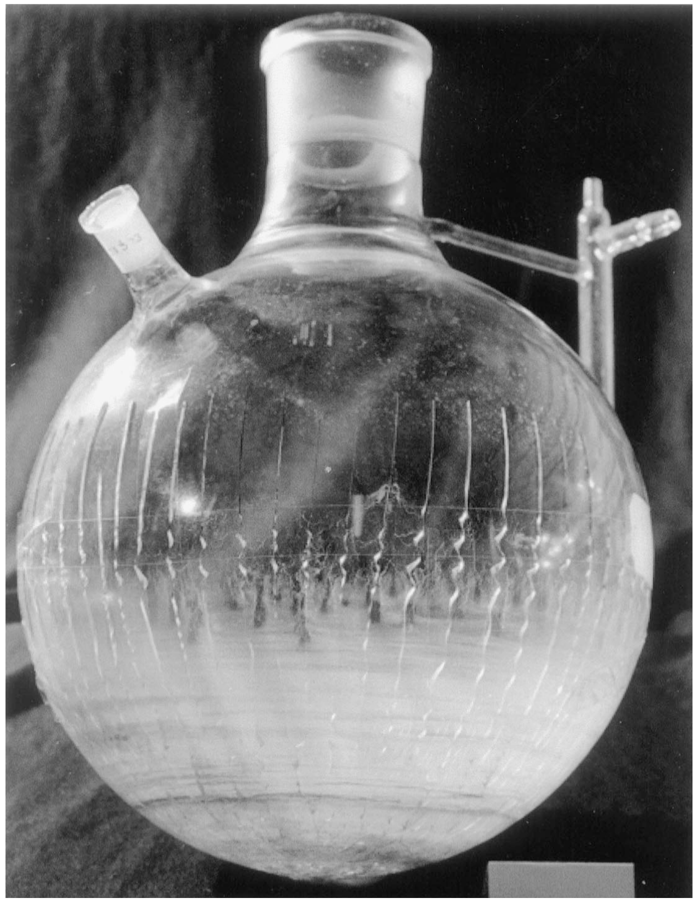


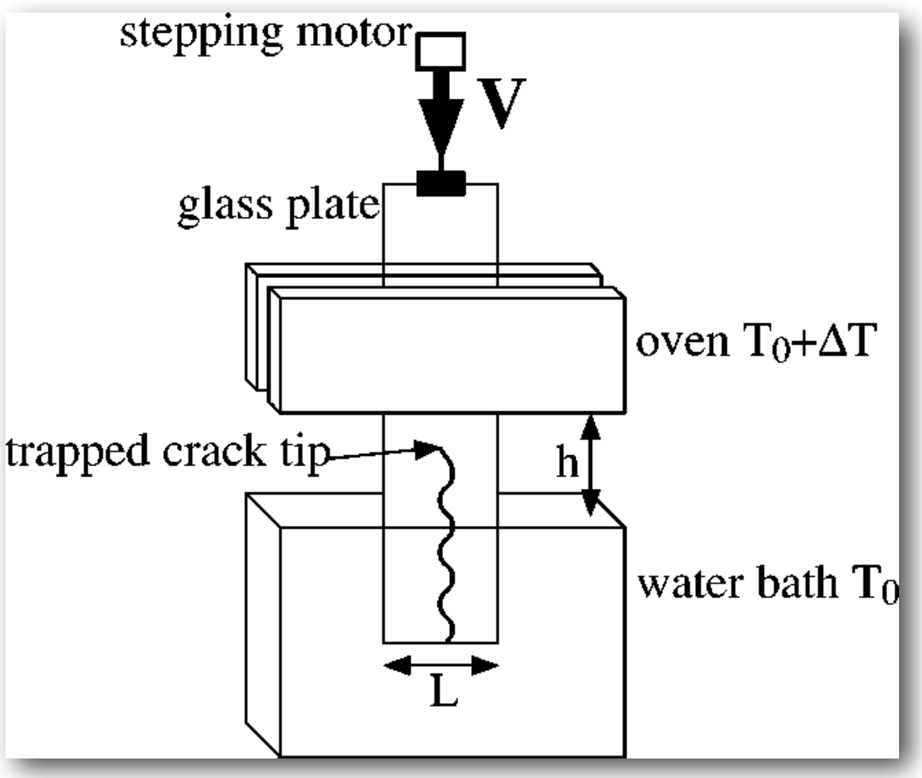


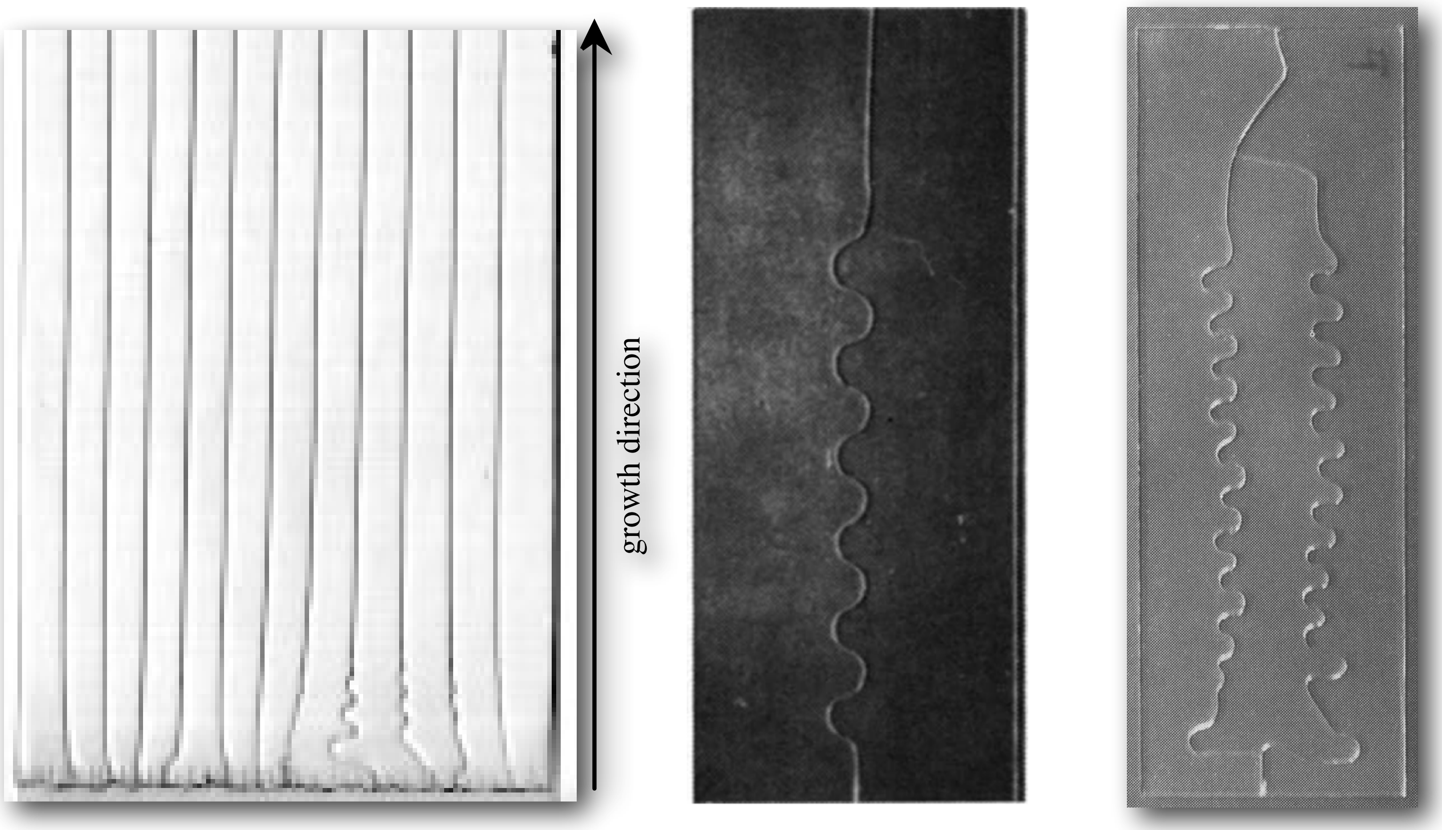
Pham Ravi-Chandar Landis, *IJF* ’17

Yuse-Sano experiment

- Glass slabs heated up then quenched in cold water.
- 2 parameters: shock intensity $\Delta\theta$, quenching speed V
- 3 regimes: straight, oscillating, erratic.
- $\textit{Limited sources of experimental data.}$

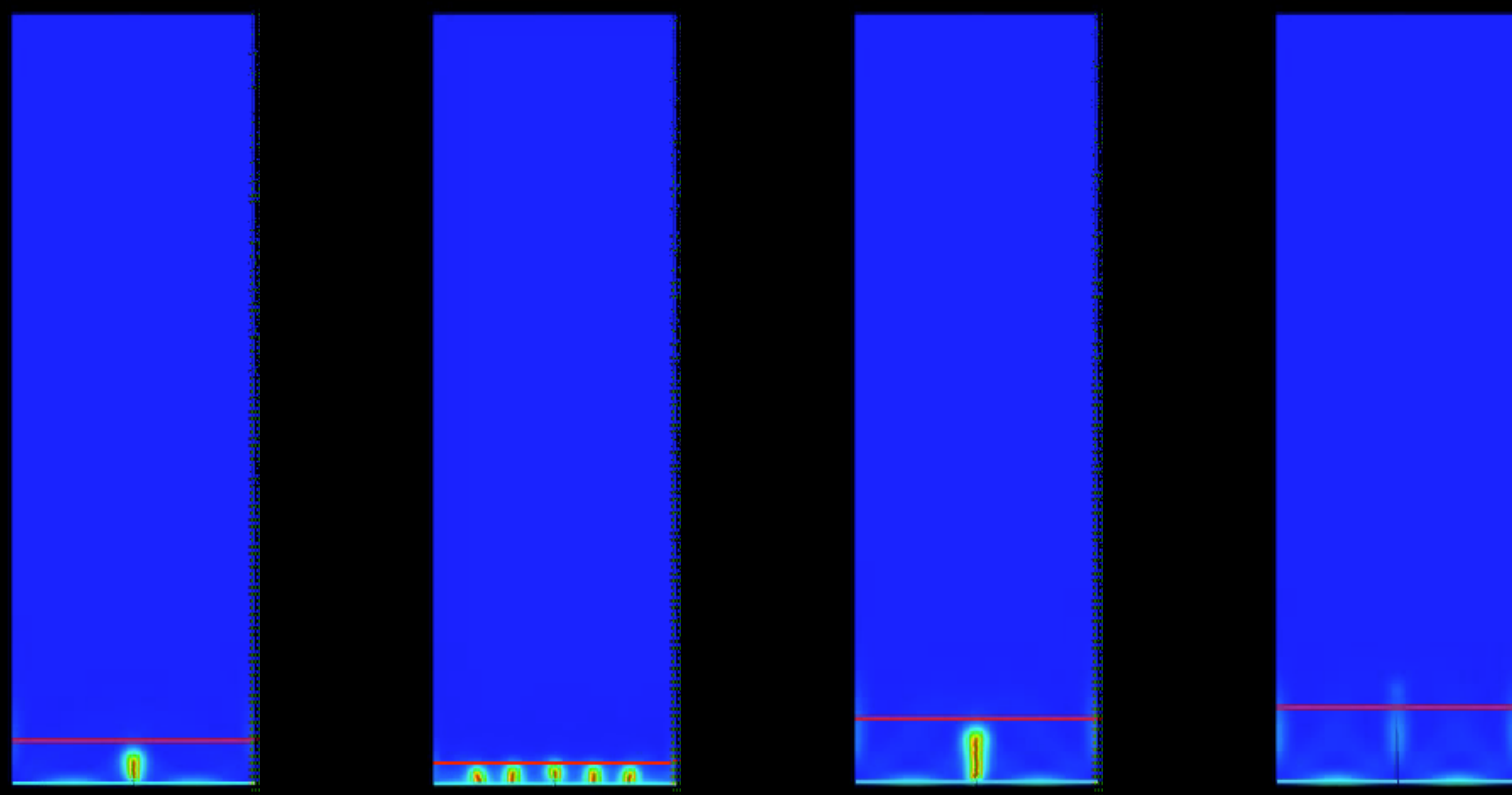






Numerical simulations

- Quantitative comparison difficult without direct access to material properties and experimental data.
- Impact of nucleation, heat transfer on simulations.
- Impact of crack geometry on heat transfer?



Issues and proposed benchmarks

- Fracture community is focused on V&V, not benchmarks
  - Verification: lots of closed form solutions, not all applicable (SIF computations near configurations that cannot be attained!)
  - Validation: good experiments are hard, experimental literature can be sloppy, materials not well quantified.
- Benchmark problems are skewed towards specific class of models (few with mixed mode, complex path, …)
  - Surfing problem (propagation, ERR, dependance on curvature)
  - Uniaxial tension (elastic domain, critical nucleation stress, closed form solution.
  - Pacman (nucleation with varying singularity), lots of experimental data.
  - Mixed mode, complex path, renucleation?
- Performance comparison: is it enough to upload benchmarks? How about VM / containers and data files?