Rebuilding mef90

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PETSc

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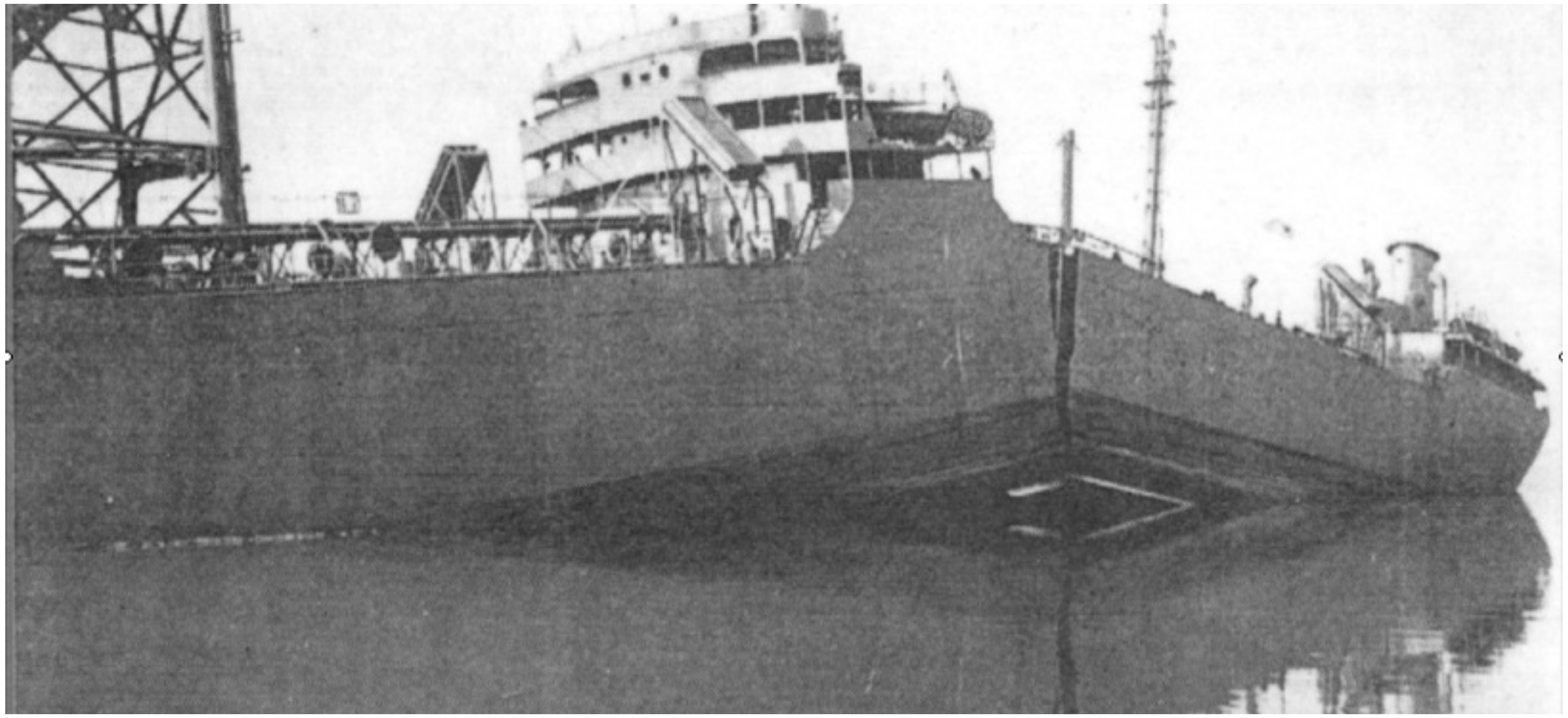
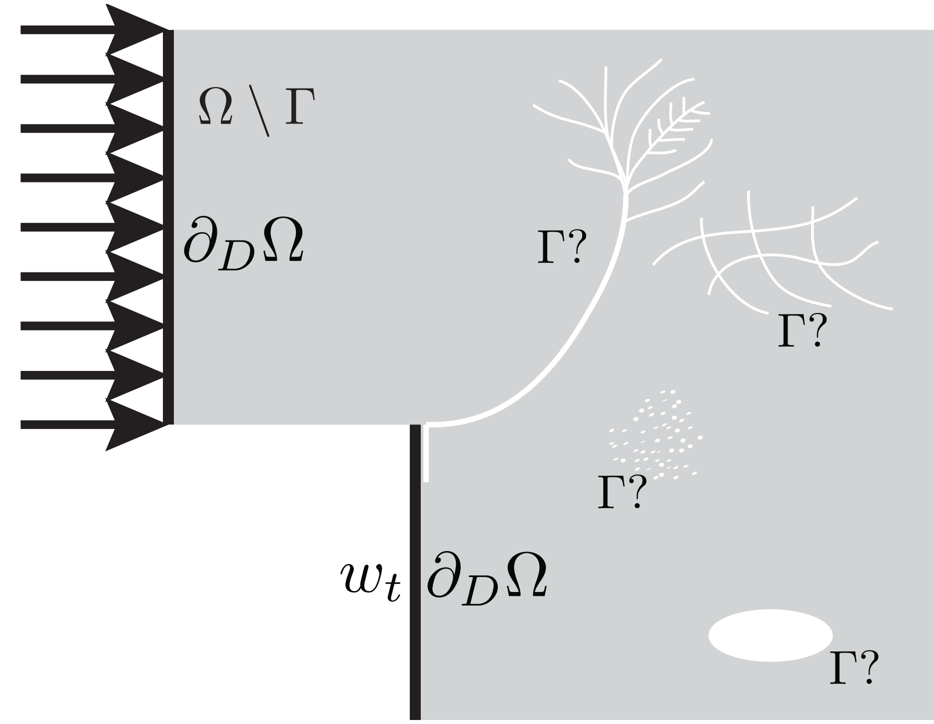
Phase-field fracture



Variational Approach to Brittle Fracture



Hypotheses:

Quasi-static (“rate independent”).

Linear brittle/elastic material, domain $\Omega \subset \mathbb{R}^n$.
Hooke’s law $\mathbf{A}$, fracture toughness G_c.

Prescribed boundary displacement w_t on $\partial_D\Omega$.

Loading parameter (“time”) t, discrete time steps $t_0 < \ldots < t_N$.

Goal:

Find the equilibrium displacement u and crack geometry Γ *without any a priori hypotheses* for all $0 \le t \le T$.

Francfort and Marigo Variational model:

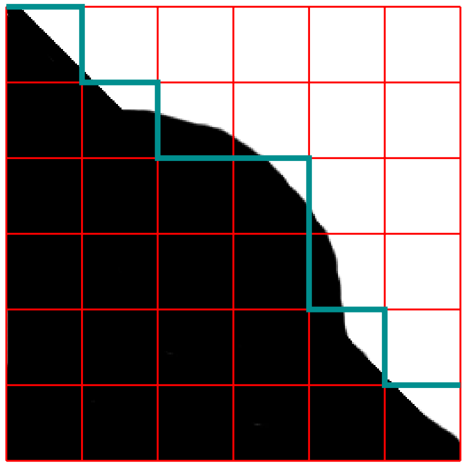
$$\mathscr{E}(u,\Gamma) := \int_{\Omega\setminus\Gamma} \frac{1}{2}\mathbf{A}\mathrm{e}(u)\cdot\mathrm{e}(u)\,dx + G_c\mathscr{H}^{n-1}(\Gamma)$$

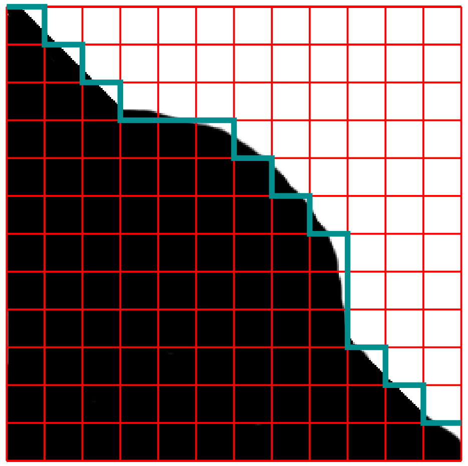
At each t_i, find (u_i, Γ_i) global minimizers of $\mathscr{E}$ subject to $\Gamma_i \supset \Gamma_{i-1}$.

Numerical Implementation

Free discontinuity problem:

- Deal with discontinuous fields along unknown lines / surfaces,
- Recover position and length / surface of cracks (mesh independent).
- Optimization friendly (do not introduce spurious local minimizers).
- Work in 2D and 3D.





Approaches:

- Adaptive FE: B-Chambolle ’00, Fraternali ‘07
- Discontinuous FE: Giacomini-Ponsiglione ’03,’06.
- Eigendeformations: Schmidt-Fraternali-Ortiz ’07
- Level sets: Larsen-Richardson-Sarkis '08, Moës etAl ’11, Allaire-Jouve-Van Goethem ’10,
- **Phase-field:** B ’98, B-Francfort-Marigo ’01, B-Francfort-Marigo ’08, …

Variational phase-field approximation

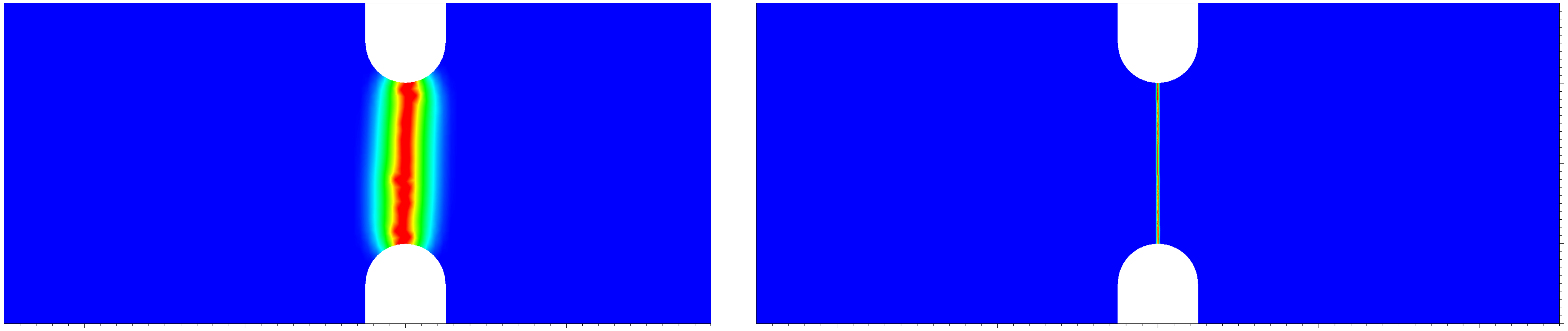
Francfort and Marigo's variational view of Griffith's criterion:

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

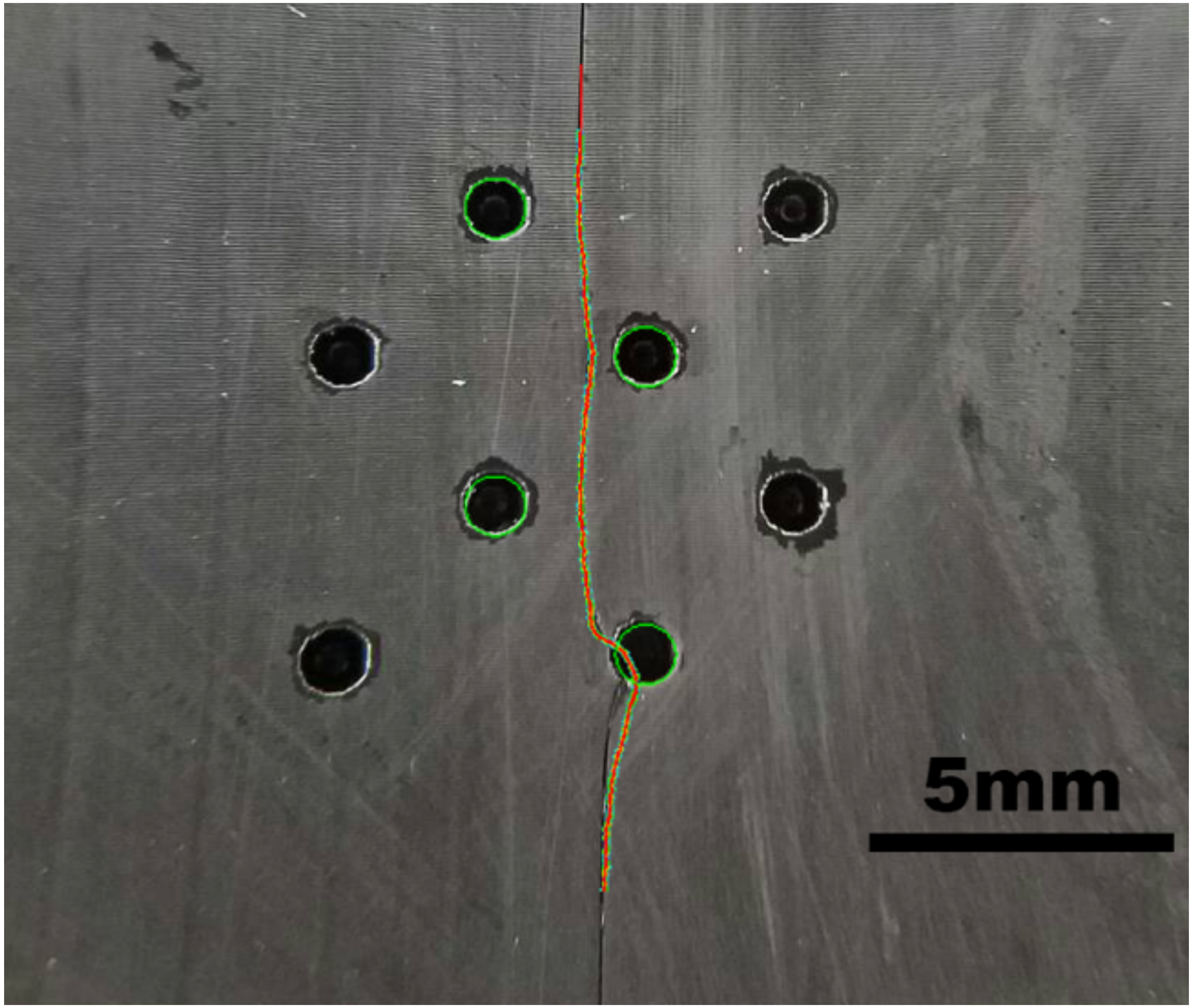
Phase-field approximation (AT_1): $\ell > 0$, $0 \leq \alpha \leq 1$:

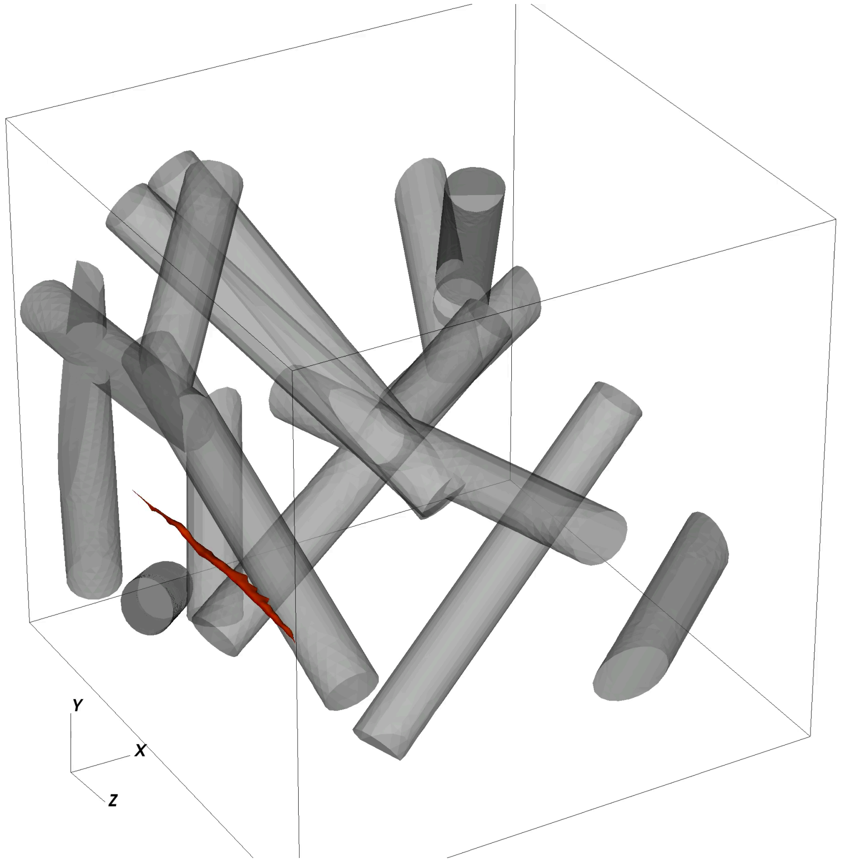
$$\mathcal{E}_\ell(u,\alpha) := \int_\Omega (1-\alpha)^2 W(\mathrm{e}(u))\,dx + \frac{3G_c}{8}\int_\Omega \frac{\alpha}{\ell} + \ell\,|\nabla\alpha|^2\,dx$$

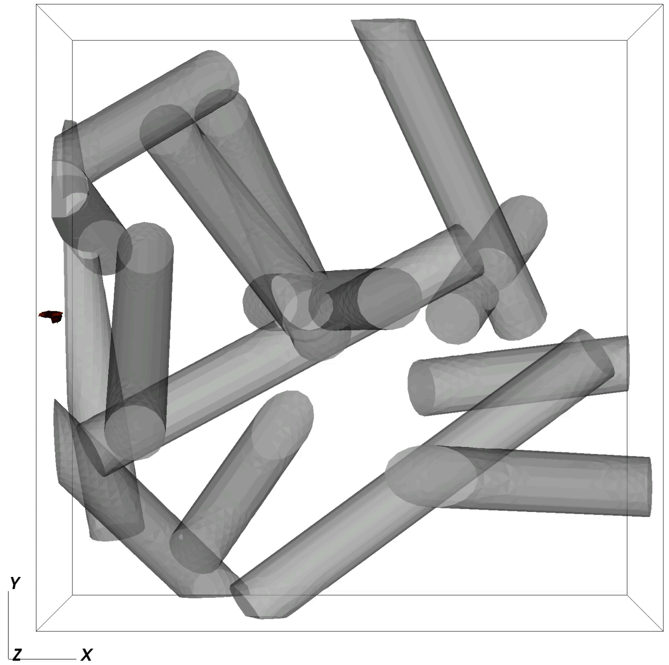
Γ-convergence of $\mathcal{E}_\ell$ to $\mathcal{E}$ + compactness of $\mathcal{E}_\ell \Longrightarrow$ convergence of minimizers.



Variational Phase-Field fracture



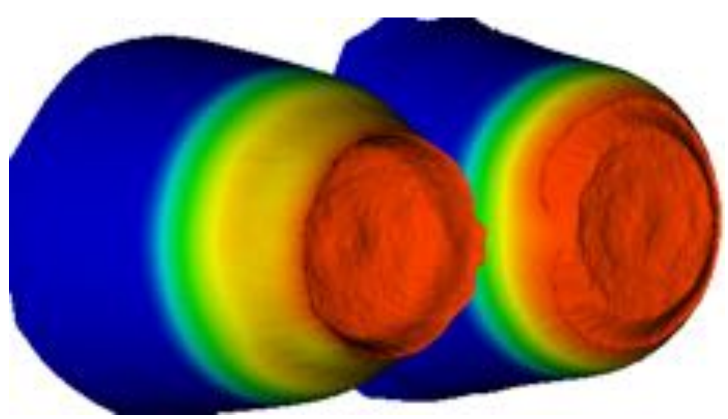


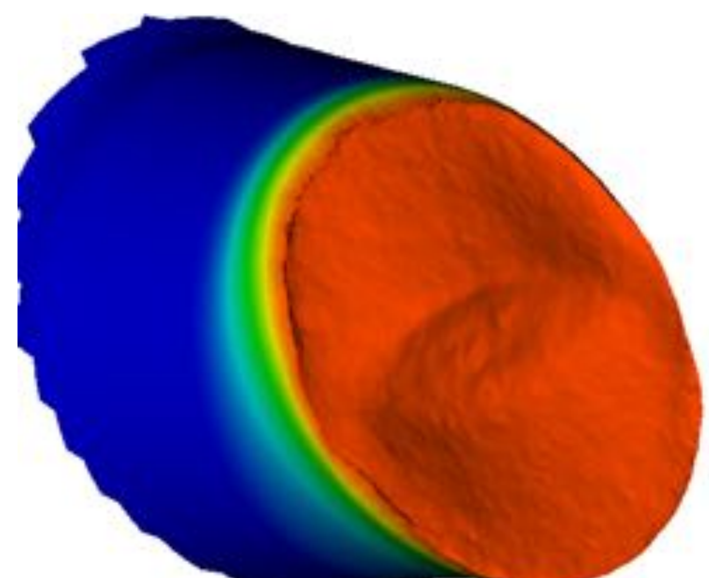


Fully coupled multi-physics problem

Ductile fracture, fracture + associated plasticity.

$$\inf_{u,p,\Gamma} \int_{\Omega\backslash\Gamma} W\left(\mathrm{e}(u) - p\right)\, dx + G_c \mathscr{H}^{N-1}(\Gamma) + \int_0^T \int_{\Omega\backslash\Gamma} H(\dot{p})\, dx\, dt$$





Multi-physics problems: one-way coupling

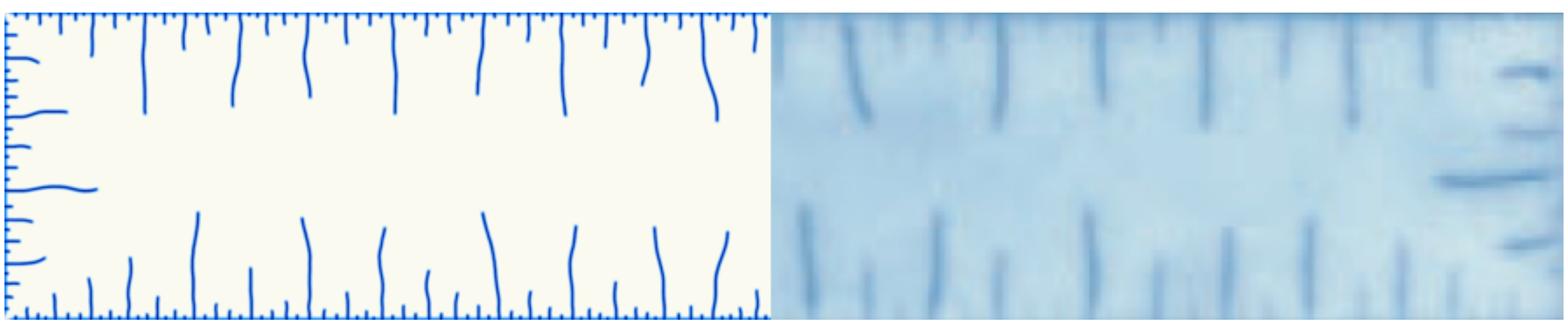
Thermal cracks, drying cracks.

- Heat transfer / diffusion on reference (un-cracked) domain).

$$\inf_{u,\Gamma} \int_{\Omega\setminus\Gamma} W\left(\mathrm{e}(u) - \beta T \mathrm{I}\right)\, dx + G_c \mathscr{H}^{N-1}(\Gamma)$$

subject to $\dot{T} - \nabla \cdot k \nabla T = 0$ in Ω,

$T(x,0) = \Delta T,\ T(0,t) = 0.$



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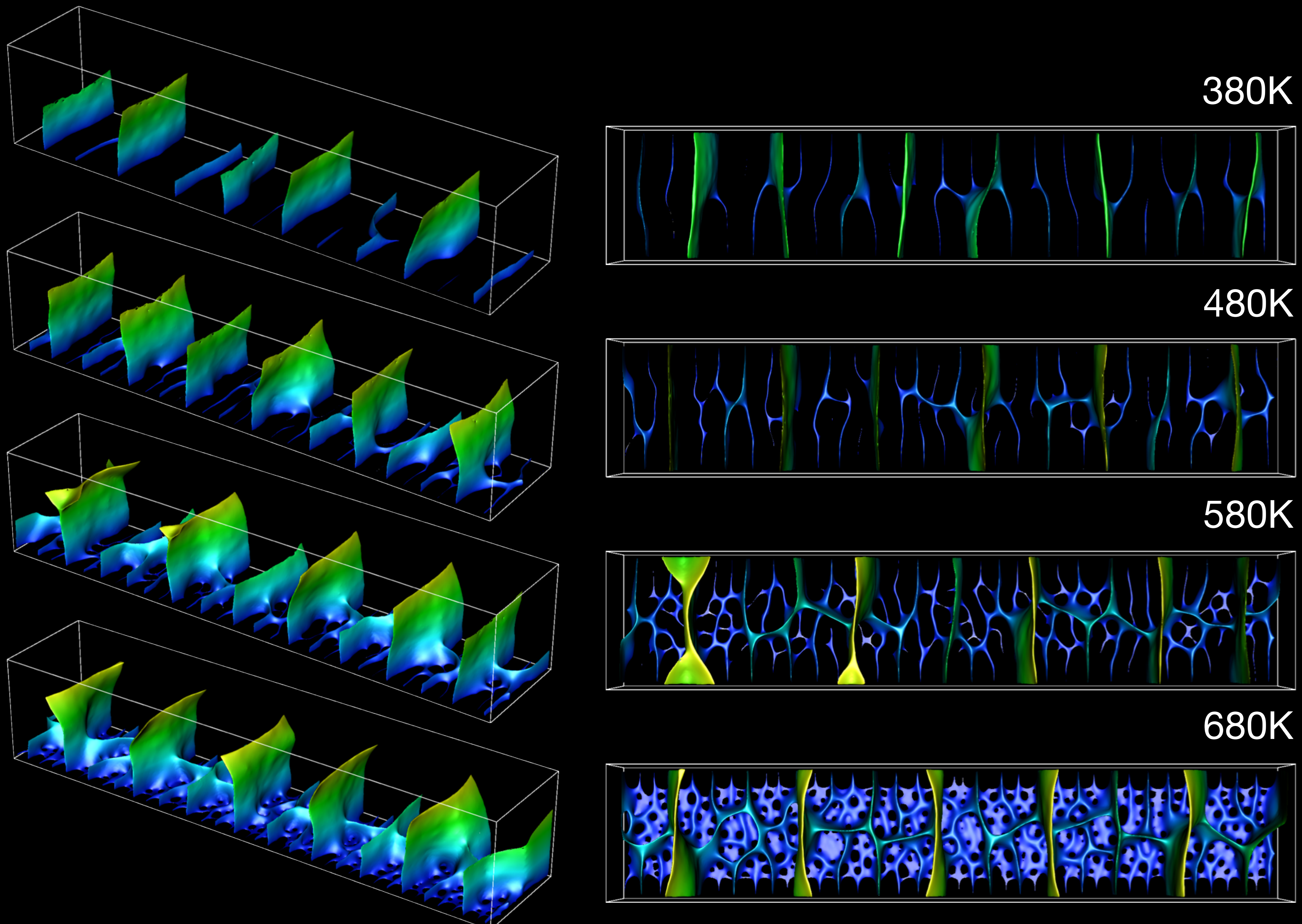
2d to 3d transition



Fully coupled multi-physics problem

Hydraulic fracturing.

Mass balance (reservoir part)

$$\frac{1}{M}\frac{\partial p_r}{\partial t} + \alpha\frac{\partial \epsilon_{vol}}{\partial t} + \nabla \cdot \vec{q}_r = q_{rs},$$

Darcy law

$$\vec{q}_r = -\frac{K}{\mu}\left(\nabla p_r - \rho\vec{g}\right).$$

Boundary conditions: $p_r = \bar{p}$ on $\partial_D\Omega$, $\vec{q}_r \cdot \vec{n} = q_n$ on $\partial_N\Omega$

Continuity: $p_r = p_f$, $q_l = -[\![\vec{q}_r]\!] \cdot \vec{n}_\Gamma$ on Γ

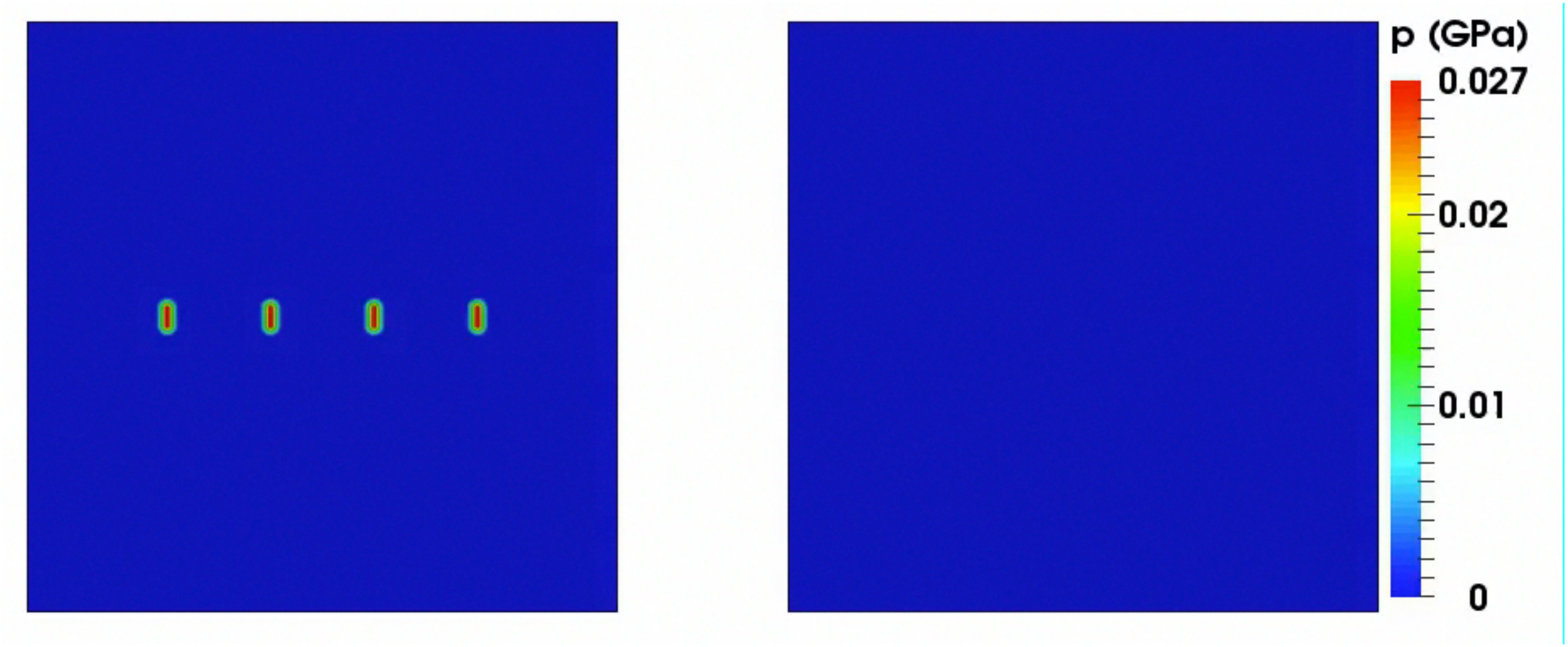
Mass balance (crack part)

$$\frac{\partial w}{\partial t} + \nabla_\Gamma \cdot (w\vec{q}_f) + q_l = q_{fs},$$

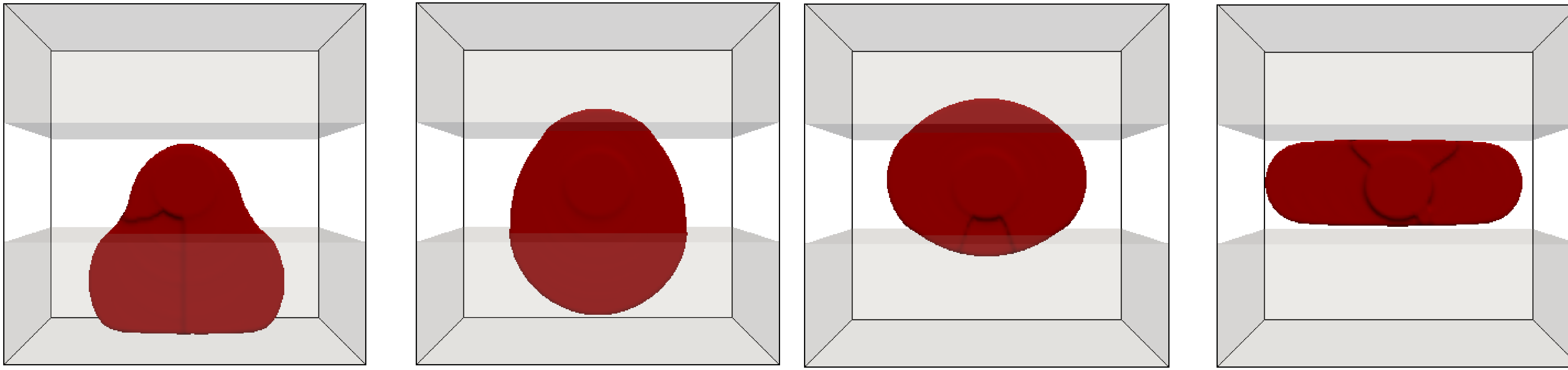
Poiseuille law

$$\vec{q}_f = -\frac{w^2}{12\mu}\nabla_\Gamma p_f,\ w = -[\![u]\!] \cdot \vec{n}_\Gamma\,.$$

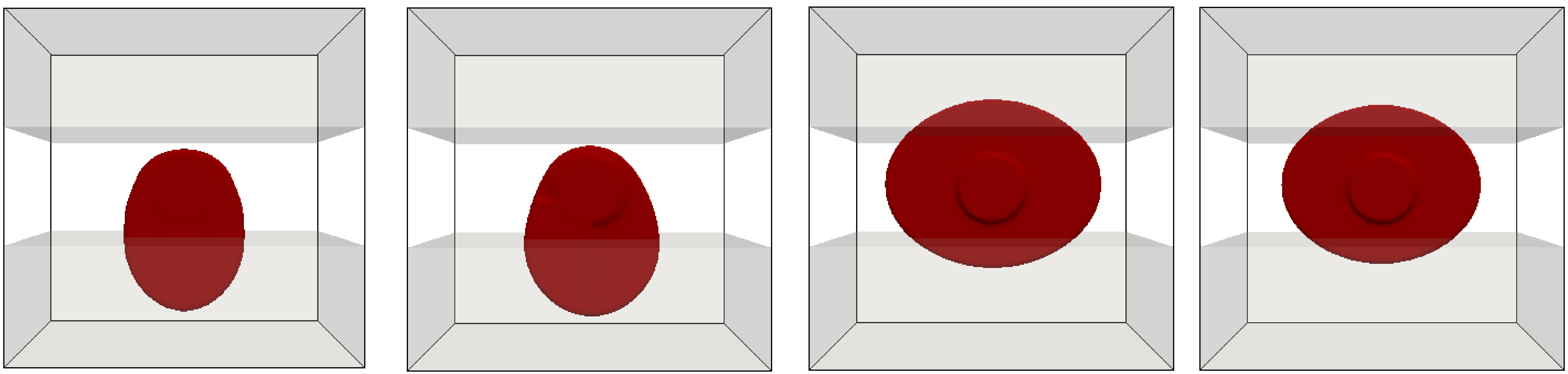
Interacting hydraulic cracks



Hydraulic fracturing in layered reservoir



$G_c^{ext}/G_c^{mid} = .7$ | $G_c^{ext}/G_c^{mid} = .9$ | $G_c^{ext}/G_c^{mid} = 1.2$ | $G_c^{ext}/G_c^{mid} = 10$



$k^{ext} = 10^{-15}\ m^2$, $k^{mid} = 10^{-13}\ m^2$

$k^{ext} = 10^{-15}\ m^2$, $k^{mid} = 6\ 10^{-14}\ m^2$

$k^{ext} = 8\ 10^{-14}\ m^2$, $k^{mid} = 10^{-15}\ m^2$

$k^{ext} = 10^{-13}\ m^2$, $k^{mid} = 10^{-15}\ m^2$

Rate independent processes

General form (discrete in time)

$$(u_i, \alpha_i) = \arg \min_{\alpha_i \geq \alpha_{i-1},\ \dot{p}_i = G(p_i, u_i, \alpha_i) = 0,} E(t_i, u_i, \alpha_i, p_i)$$

Generalization of quasi-static problems in variational form

- Solid mechanics (elasticity, plasticity, damage, fracture, …)
- Image processing (DIC, restoration, denoting, …)

R.I.P. vs standard formalism

- Time-dependent problems but not ODE (TS)
- Constrained optimization but not time-dependent (PetscAdjoint)
- PDE / VI-constrained or multi-level optimization (TAO/SNESVI)
- Non-convex but usually separately convex energies

mef90 / vDef

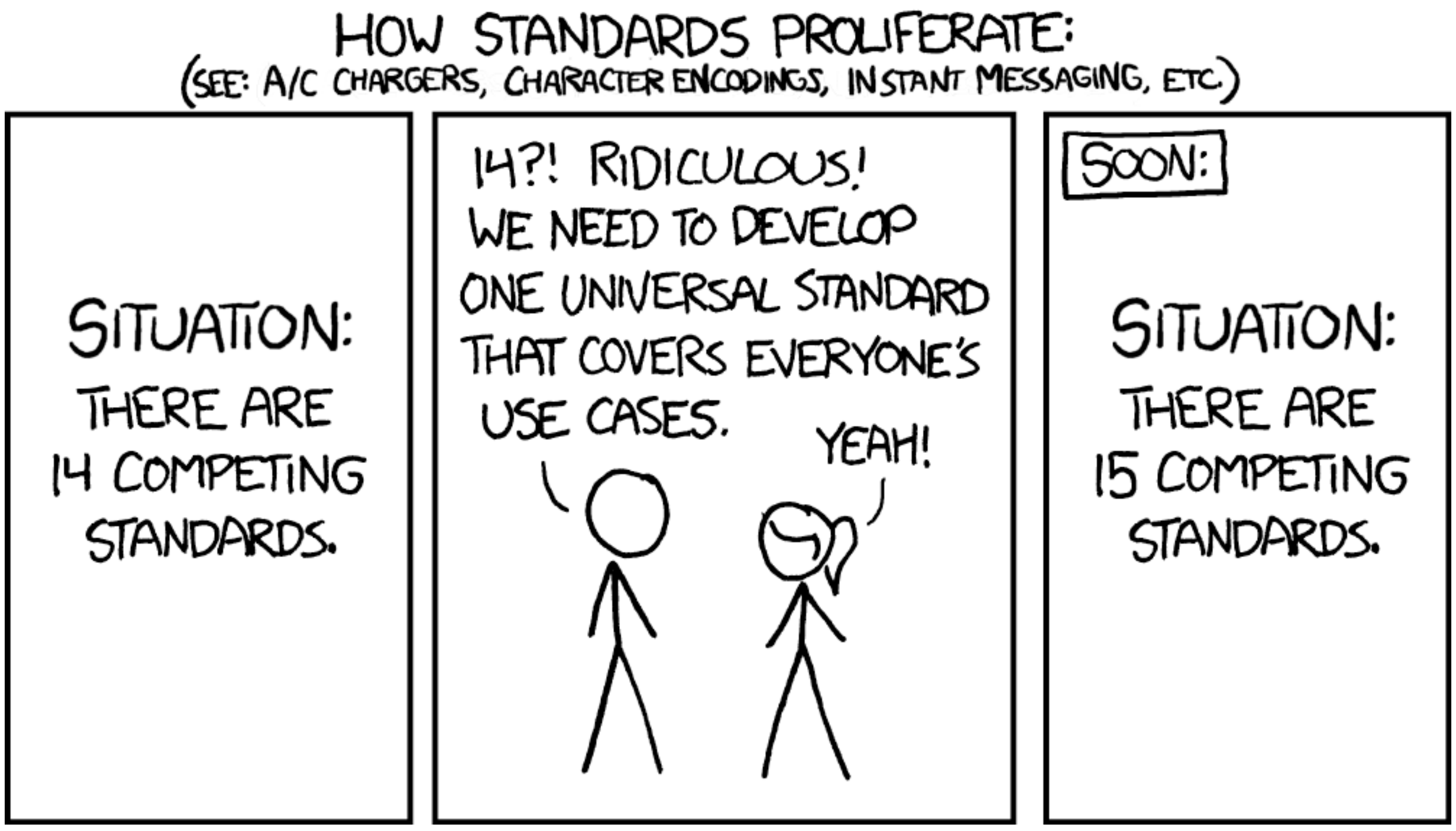
- Parallel unstructured 2D/3D finite elements.
  - P1/P2 Lagrange Finite Elements.
  - Many phase-field variants, plasticity laws, material symmetries, unilateral contact.
  - Steady state and transient heat transfer (one-way coupling only).
- Staggered solver (block Gauss-Seidel)
  - At each time step t_i: iterate until convergence
    - Minimization w.r.t u (elastic equilibrium).
    - Constrained minimization (or variational inequality) w.r.t α.
    - Solve for the state variable (transient or steady state from t_{i-1} to t_i)
  - Globally stable, convergence to a critical point of the regularized energy, monotonically decreasing energy. B ’07, Burke-Ortner-Süli ’10, ’13.
- Backtracking algorithm (optimality condition in trajectory state).

- BSD license since 2014.
  - https://github.com/bourdin/mef90
  - docker: bourdin/mef90ubuntumpicho

mef90 timeline

- Mid-90’s: “Méthode d’Eléments Finis en Fortran 90”
  - Started as a project to investigate new fortran features (derived types, overloading, dynamic allocation) for image processing, fracture mechanics, optical design. IBM RS6000, DEC alpha, Solaris.
- 2003, PETSc 2.1:
  - Switch to Vec, Mat, KSP. Still sequential.
  - First parallelization using AO, IS. Painful, unmaintainable…
- 2006: PETSc 2.3:
  - Rewrite using LocalToGlobalMapping, TAO.
  - Could never figure out how to handle the L2G for vector-valued elements…
- 2008-2010: PETSc 3.1–3.3:
  - Rewrite using Sieve, SNES / SNESVI.
  - Lots of help from Matt Knepley.
  - Sieve gets deprecated just as the port is finished…
- 2022-2023: PETSc 3.17 —
  - Rewrite using dmplex.

mef90 and PETSc



https://xkcd.com/927/

From sieve to dmplex

Little paradigm changes:

- Major simplification to section creation, local assembly routines.

- Many creeping “small” changes:
  - dmplex cells must have the same topological dimension, sieve didn’t.
  - Locality (or not) of labels.

- Main issue was not technical but the lack of documentation of ~~dmplex~~, PetscSF, PetscSection, PetscLayout.

- Fortran bindings, handling of PETSC_NULL objects.

- I/O was a pain…

Unstructured mesh I/O

Requirement:

- Well-documented, supported binary format. NOT A NEW FORMAT!
- Compatibility with modern *and* legacy visualization (TecPlot, …)
- Support for blocks of cells, faces, vertices, “high” order elements.

Strong preference:

- Compatibility with mesh generators including industry standard (ABAQUS, hypermesh, MSC-Marc, …) if possible.
- Capable of handling checkpointing *and* output.
- MPI-IO support.

exodusII format.

Limitations:

- Cell sets (element blocks) are non-overlapping, consists of sequentially numbered cells. Edge sets are #$%^*&^%
- Standard only *partially* implemented in VisIt, Paraview, meshio, cubit,…

exodusII I/O *in natural ordering*

Why?

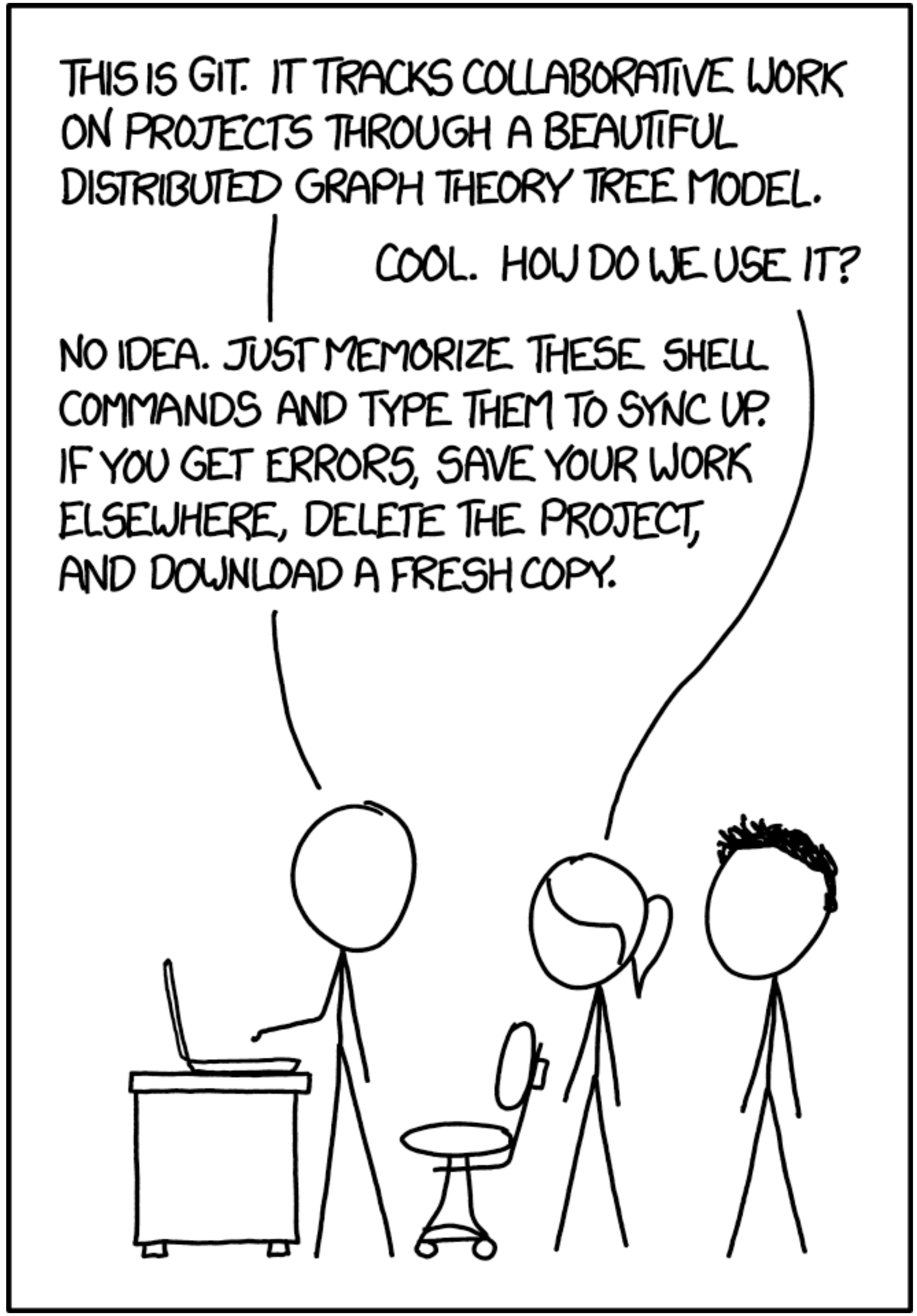
- Multiple physics / materials in cell blocks, must be made available to visualization / post processing.
- “Serialized” distributed dm may not be compatible with exodusII.
- vDef wants to be a good citizen and be *part* of an analysis chain.

“Layouts” of a Vec:

- local: Petsc local vector with constraints (non-collective)
- global: Petsc global vector without constraints (collective)
- cglobal: Petsc global vector with constraints (collective)
- natural: cglobal reordered in the initial DM ordering (collective, all values on processor 0 due to limitations of the exodusII format and reader).
- IO: natural load-balanced for MPI-IO (collective)

IO2local/local2IO,… PetscSF obtained by composition.

Thoughts

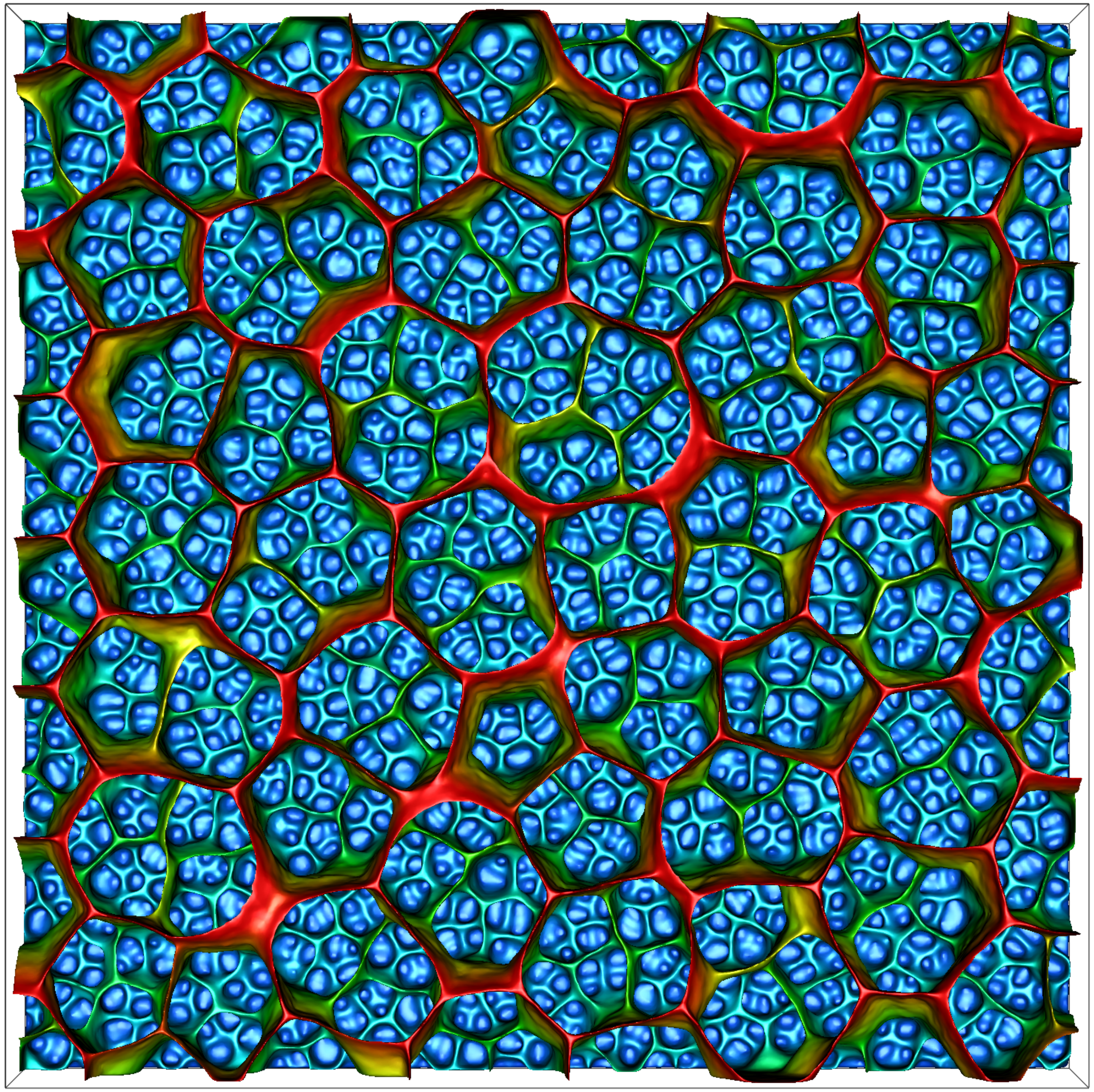


https://xkcd.com/1597/

Thoughts

- Is PETSc developed for end-users or framework developers?
- Other valuable parts of the PETSc eco-system:
  test system, makefile system
- Should there be a mechanism to indicate that a PETSc object is still evolving / will become obsolete?
- How to leverage the PETSc community for low-level labour intensive work (documentation, tests, bindings / interfaces)?
- How to incite users to contribute code to PETSc?
  - Have students contribute code early.
    - Contributing to PETSc is a fantastic educational tool.
    - Use PETSc code as reading material.
    - Contributing to PETSc leads to writing better code.

Acknowledgements



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