An Introduction to Finite Element Analysis (FEA) of Material Microstructure Properties in nanoHUB

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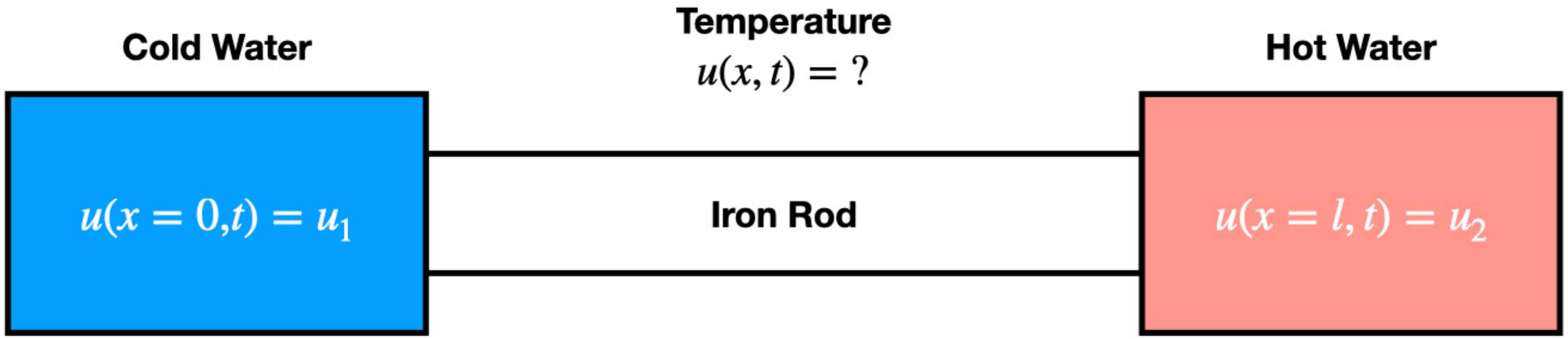
Outline

- Fundamentals of finite element analysis in OOF2
- Demonstration of OOF2 simulations

Modeling a System with Differential Equations

- Physics systems can be modeled by differential equations.
  - Ordinary or partial differential equations
  - Initial conditions and boundary conditions
- Example: heat transfer problem in an ideal iron rod
  - Heat equation: $\dfrac{\partial u(\mathbf{r}, t)}{\partial t} - \kappa \nabla^2 u(\mathbf{r}, t) = 0$
  - Fixed temperature at both ends (Dirichlet boundary condition)



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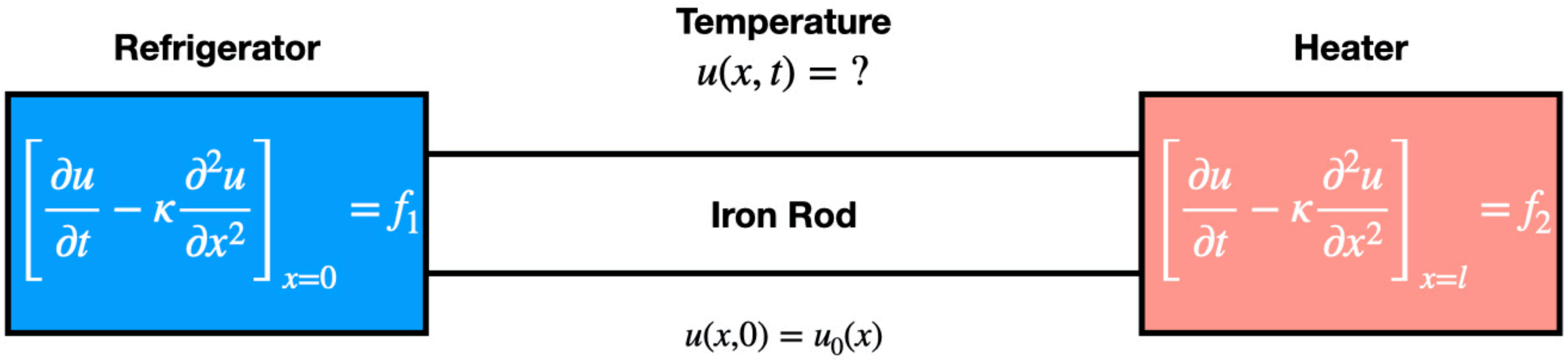
  - Heat sources at both ends (Neumann boundary condition)



Refrigerator

Temperature

$u(x,t) = ?$

Heater

$\left[\frac{\partial u}{\partial t} - \kappa \frac{\partial^2 u}{\partial x^2}\right]_{x=0} = f_1$

Iron Rod

$\left[\frac{\partial u}{\partial t} - \kappa \frac{\partial^2 u}{\partial x^2}\right]_{x=l} = f_2$

$u(x,0) = u_0(x)$

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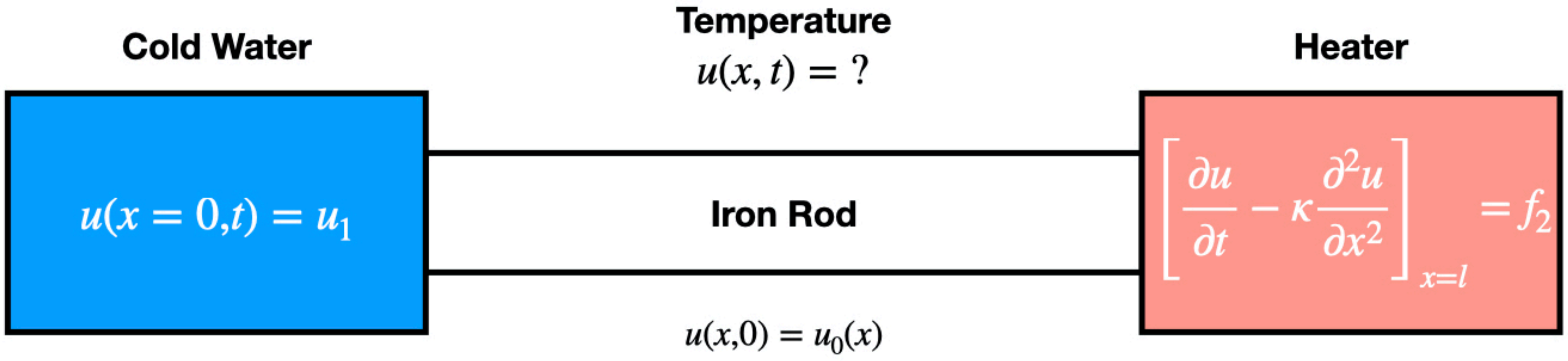

Cold Water

$u(x=0,t) = u_1$

Temperature

$u(x,t) = ?$

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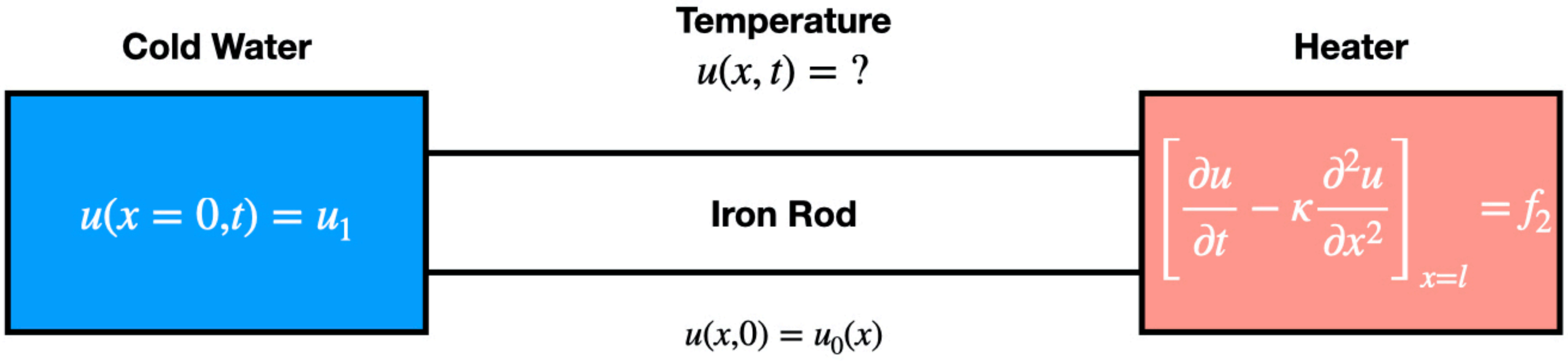
- Easy analytical solutions in these cases.
- But what happens if the system is complex?
  - non-homogeneous rod
  - irregular boundaries
  - heat exchange with changing environment



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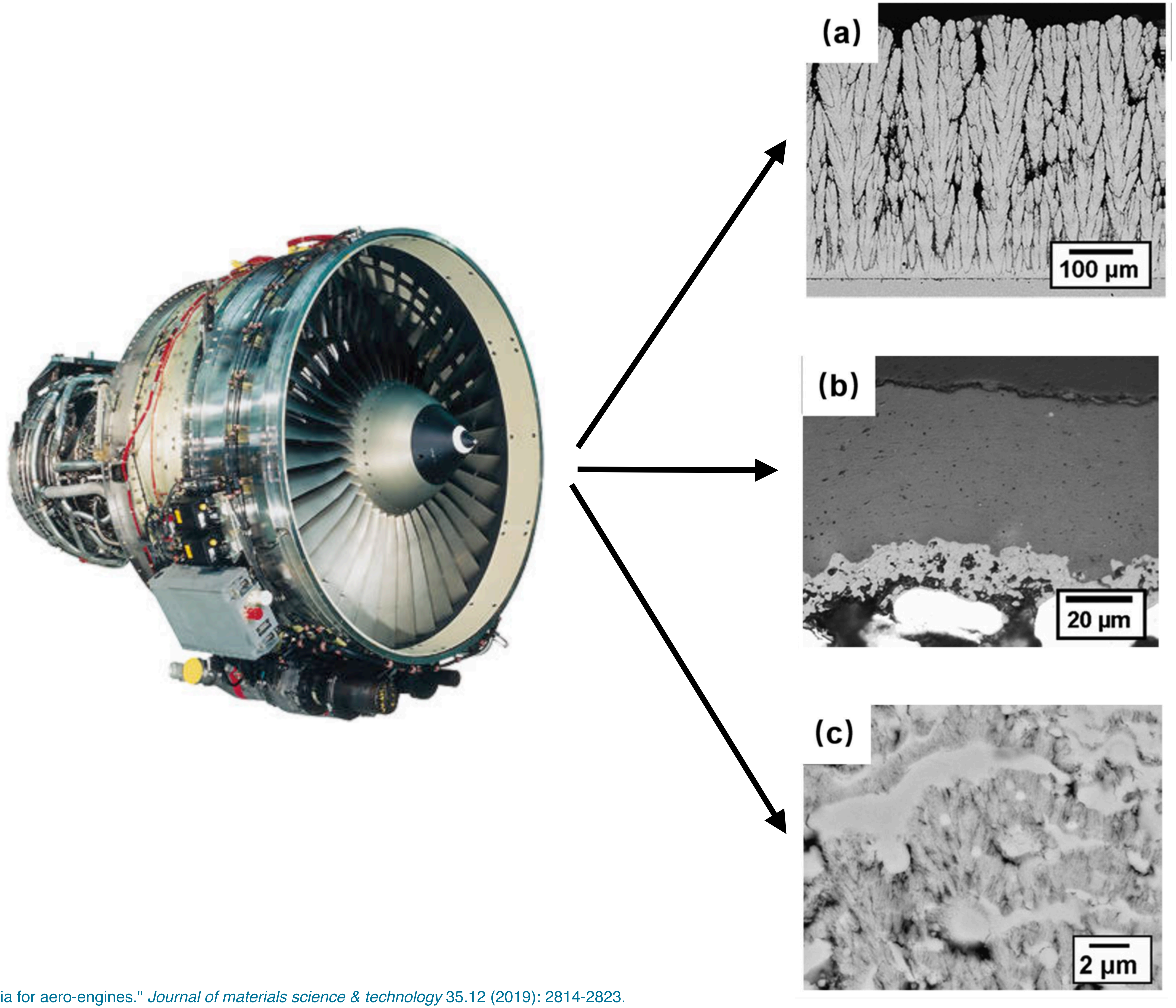
Real-world Case: Predicting Thermal Conductivity κ of Ceramic Thermal Barrier Coatings for Turbine Blades

- Thermal barrier coatings helps engines work at high temperatures.
- Measurements of κ are difficult, time consuming and expensive, hardly done in quality control process.
- How about calculation?
  - Ceramic materials have complex microstructures.



https://math.nist.gov/mcsd/Seminars/2005/2005-01-11-langer.html

Liu, Qiaomu, Shunzhou Huang, and Aijie He. "Composite ceramics thermal barrier coatings of yttria stabilized zirconia for aero-engines." *Journal of materials science & technology* 35.12 (2019): 2814-2823.

Modeling Complex Microstructures: Mean-field Method vs. Finite Element Analysis

- Mean-field method
  - Replace details with average/effective quantities
  - Computes average properties of statistically representative microstructure
  - Provides useful bounds to calculate effective properties
  - But has limitations when
    - Nonlinear relationship between macroscopic and underlying properties
    - Underlying properties not spatially uniform
    - Unclear about how to do the averaging reasonably
    - Property of interest lies in extremes conditions
- Accurately modeling the specific microstructure(s) is important -> Finite element analysis

Finite Element Analysis in OOF2: Schematic Form

- OOF2: software that computes properties of materials with complex microstructures via image-based finite element analysis.

- Schematic Form

$$\sigma(\phi, \mathbf{r}) = \sum_i k_i \nabla \phi_i$$

$$\mathbf{M}\frac{\partial^2\phi}{\partial t^2} + \mathbf{C}\frac{\partial\phi}{\partial t} - \nabla \cdot \sigma(\phi, \mathbf{r}) = f(\phi, \mathbf{r})$$

ϕ: fields

σ: fluxes

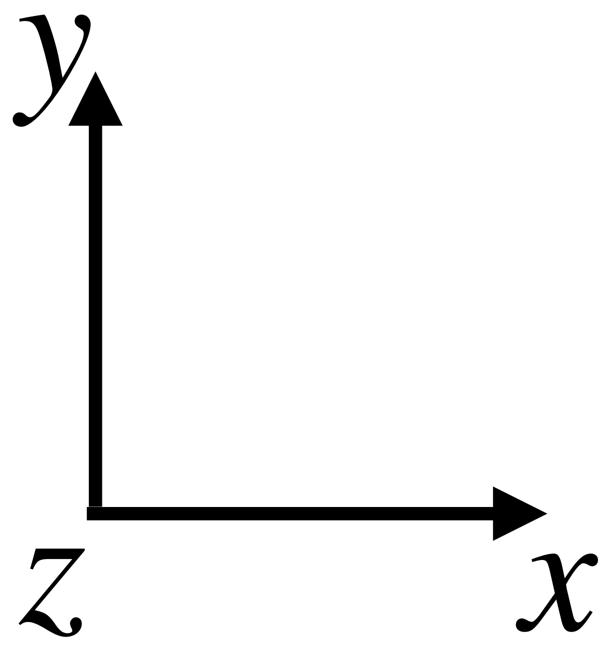
$k, \mathbf{M}, \mathbf{C}$: moduli / coupling constants

f: generalized forces

- Example
  - Heat transfer problem & thermal conductivity: $M = 0, \quad \phi = u(\mathbf{r}, t)$
  - Elasticity, thermal expansion …

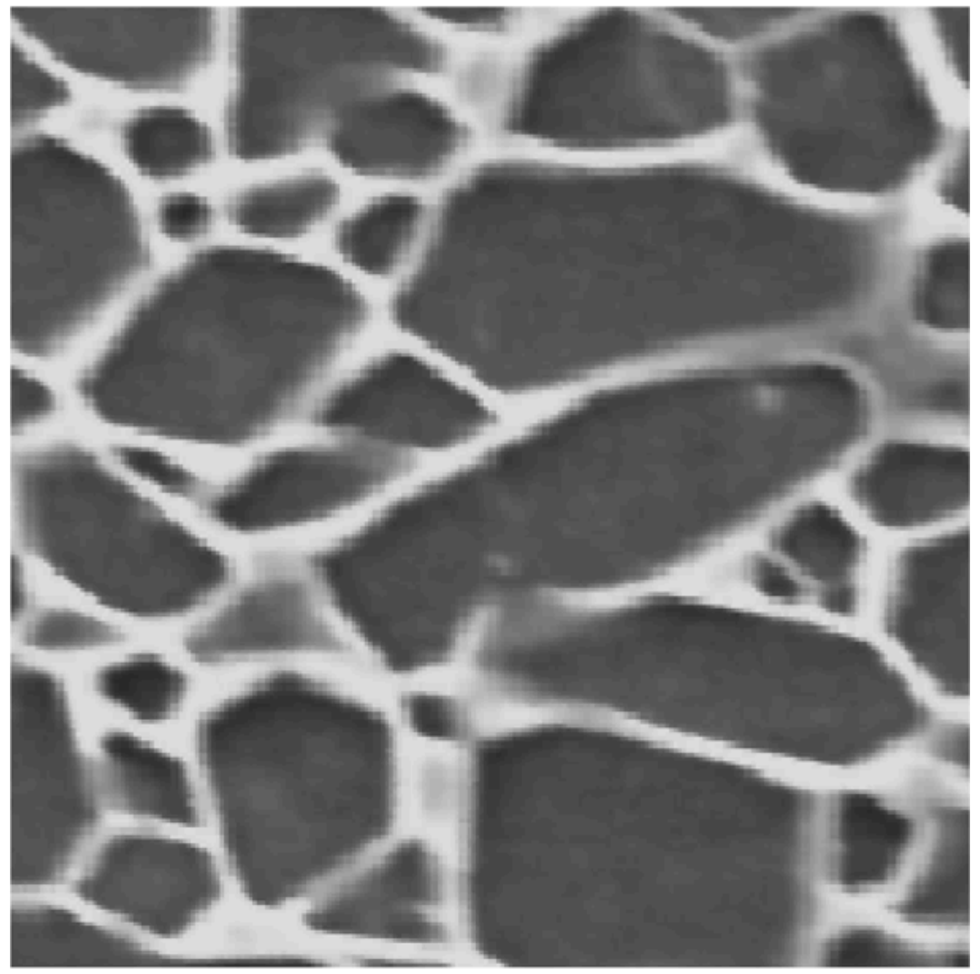
Finite Element Analysis in OOF2: Reduction to 2D

- Material properties are always specified in 3D
- Reduction to 2D when assigning material properties to image
    - plain-strain: the fields have no out-of-plane gradients (z-derivatives)
    - plain-stress: the fluxes have no out-of-plane components (z-components)
- OOF3D: handles everything in 3D



Finite Element Analysis in OOF2: Basic Concepts

- Concepts
  - Microstructure
    - Fundamental abstract entity used by OOF2
    - Formed by pixels, each pixel has local information of the material
  - Image
    - Experimental micrograph or simulation output
    - Can be read by OOF2 to create microstructure
    - A microstructure might contain multiple images
      - ◉ Images from different processing techniques that reflect different features of the microstructure

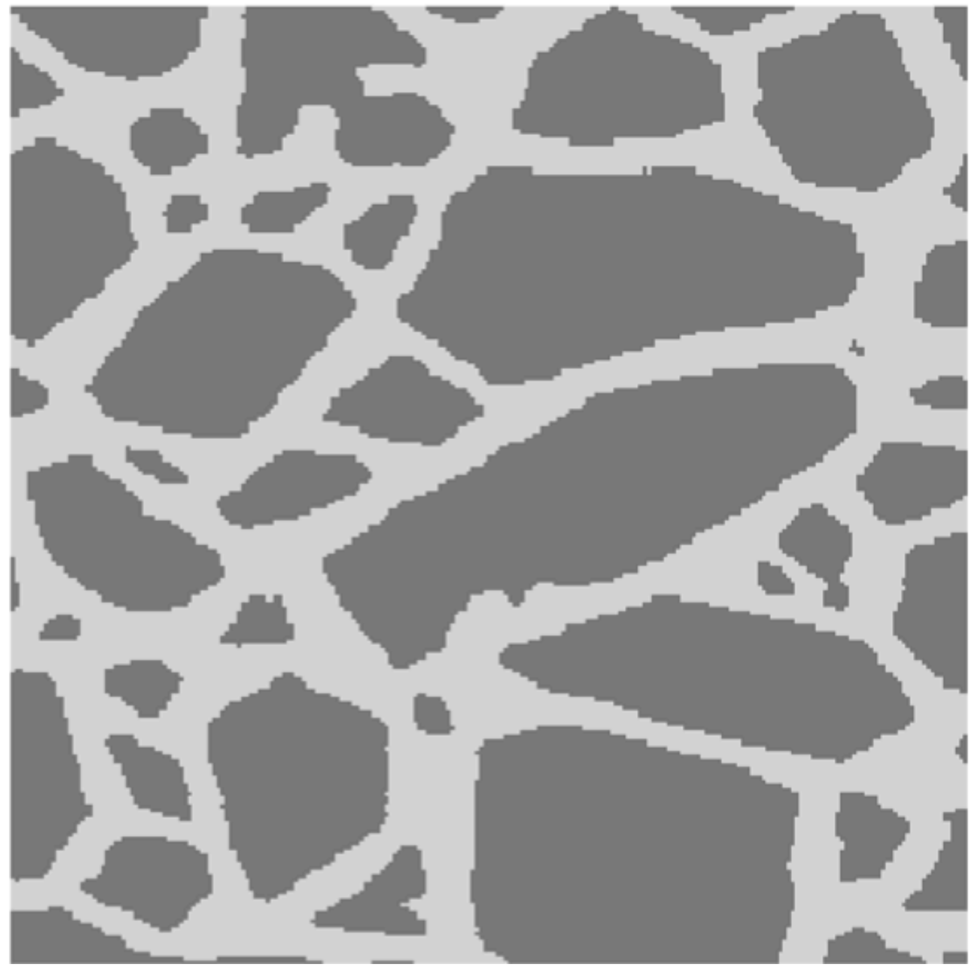


Microstructure of a Si_3N_4 ceramic

Reid, Andrew CE, et al. "Modelling microstructures with OOF2." *International Journal of Materials and Product Technology* 35.3-4 (2009): 361-373.

Finite Element Analysis in OOF2: Basic Concepts

- Concepts
  - Materials
    - Sets of properties, assigned to pixels
    - Example (right figure): color property assigned
      - Pixels thresholded and assigned into two groups
      - Dark: ‘grains’ group
      - Light: ‘matrix’ group



“Material map” of a Si_3N_4 ceramic

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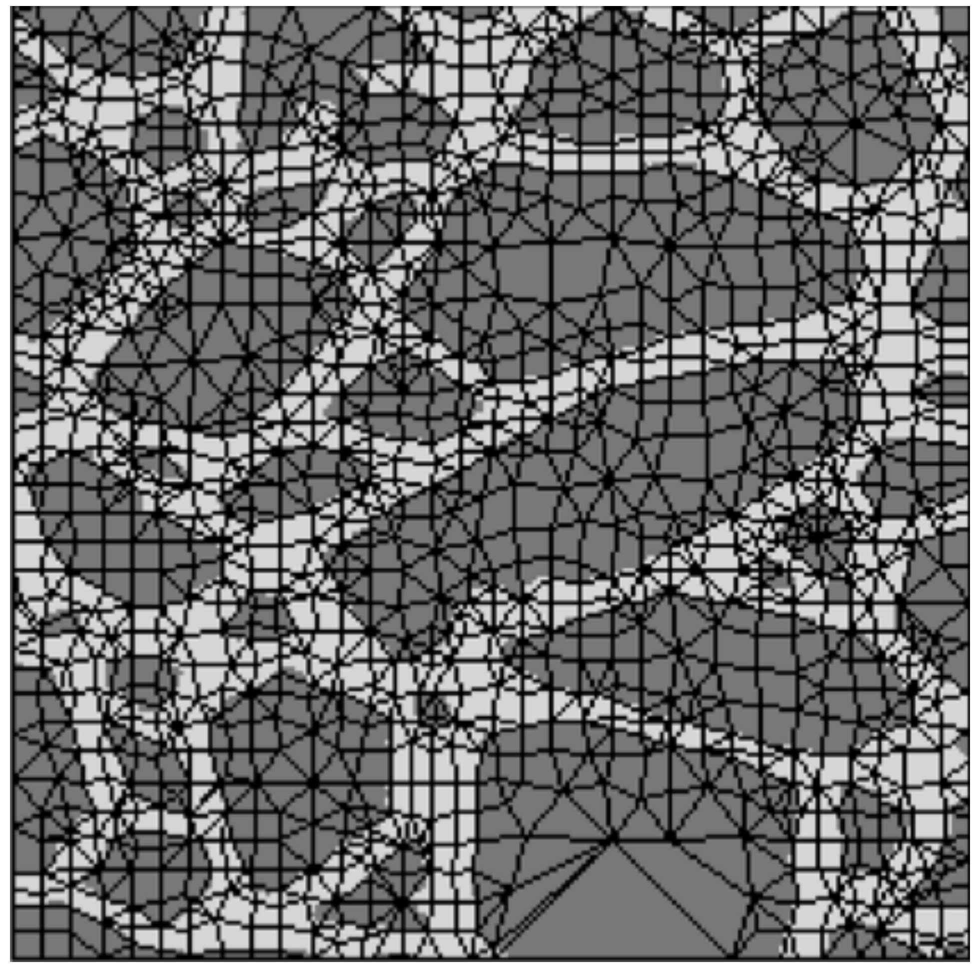
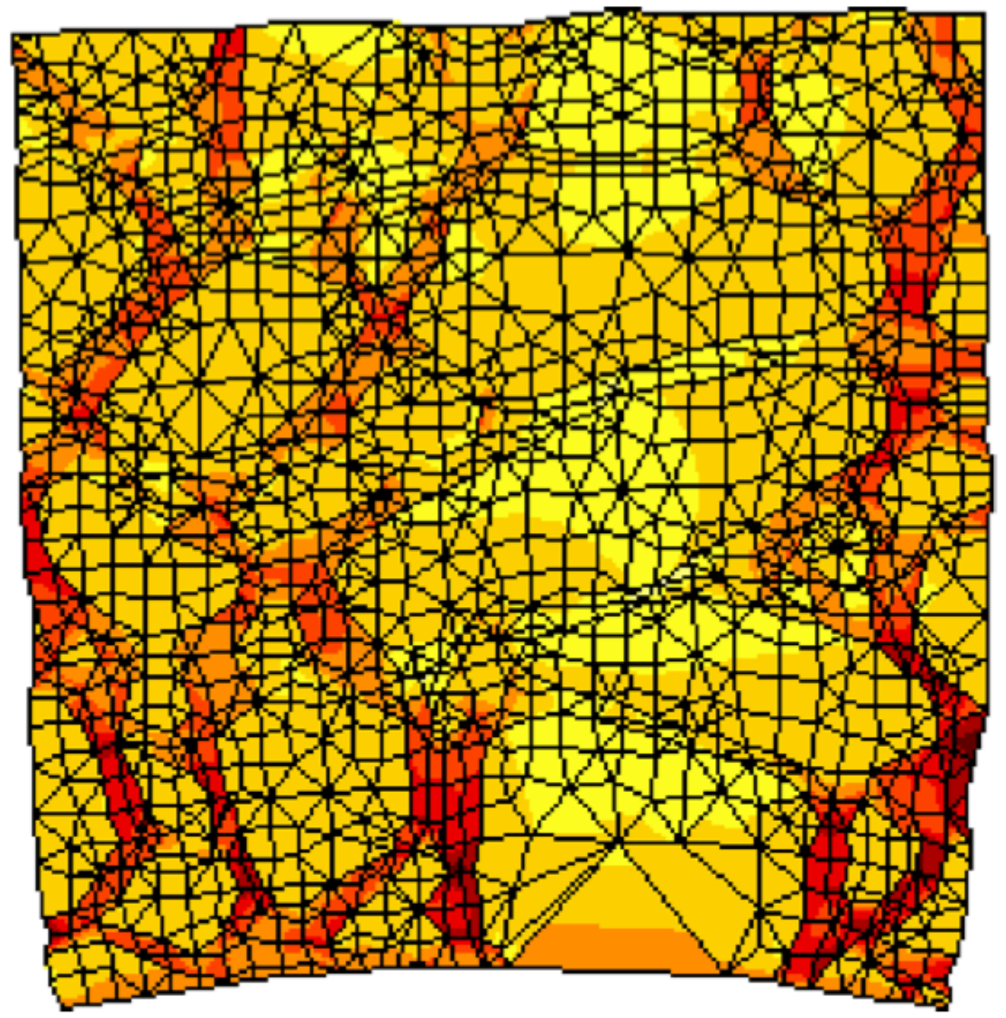
Finite Element Analysis in OOF2: Basic Concepts

- Concepts
  - Skeleton
    - mesh of finite elements; geometry only
    - A microstructure can have multiple skeletons
    - Hierarchy of approximations: actual microstructure -> image/micrograph -> material map -> skeleton
  - Mesh
    - Skeleton with the physics and math



Skeleton of the Si_3N_4 microstructure



xx strain in the Si_3N_4 microstructure, defined on mesh

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Typical Steps of Running an OOF2 Simulation

- Load an image
- Identify features in the image / (create pixel groups)
- Create materials by specifying the properties
- Assign materials to pixels or pixel groups
- Create a skeleton (mesh geometry) and adapt it to image
- Create a mesh
- Define fields and activate equations
- Solve the equations
- Visualize and analyze

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OOF2 and nanoHUB in Teaching at MatSE in UIUC

- Multiple courses incorporated OOF2 ran from nanoHUB
  - MSE 206, Mechanics for MatSE
  - MSE 404, Lab studies in MatSE
  - MSE 406, Thermal-Mech Behavior of Matls
  - MSE 440, Mechanical Behavior of Metals
- Student feedback
  - Generally reliable & easy to use
  - Increased confidence in using computational tools after training including OOF2
  - OOF2 ranked 2nd in students' most confident software, after MATLAB

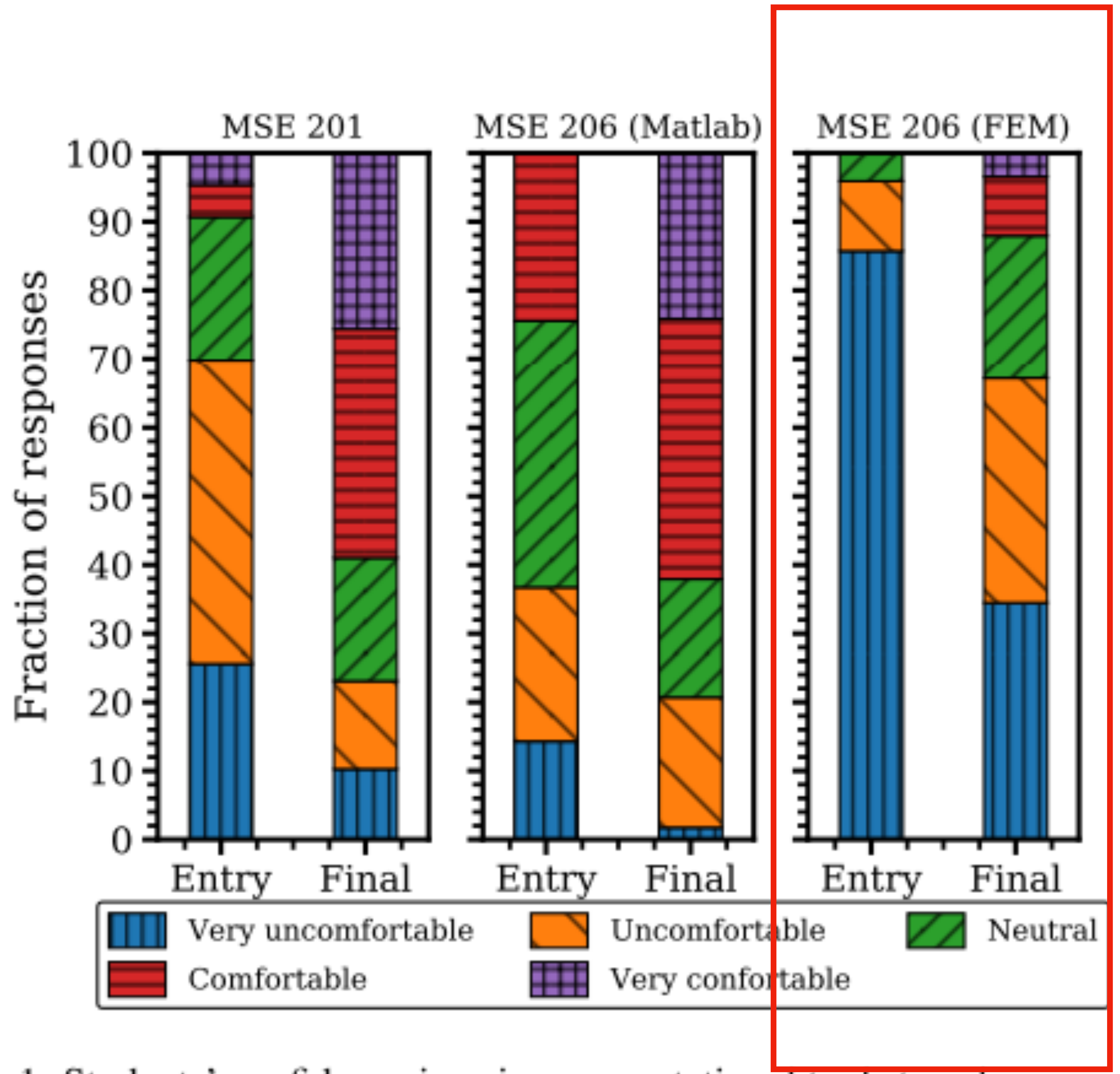

Figure 1: Students' confidence in using computational tools to solve course specific problems at entry and final surveys for MSE201 and MSE206.

Lee, Cheng-Wei, et al. "Impact of computational curricular reform on non-participating undergraduate courses: Student and faculty perspective." *2019 ASEE Annual Conference & Exposition*. 2019.

Demo 1: Stress in Front of Crack Tips in Aluminum

- Two crack tip geometries: blunt (left) and narrow (right)
- We want to calculate and visualize the stress

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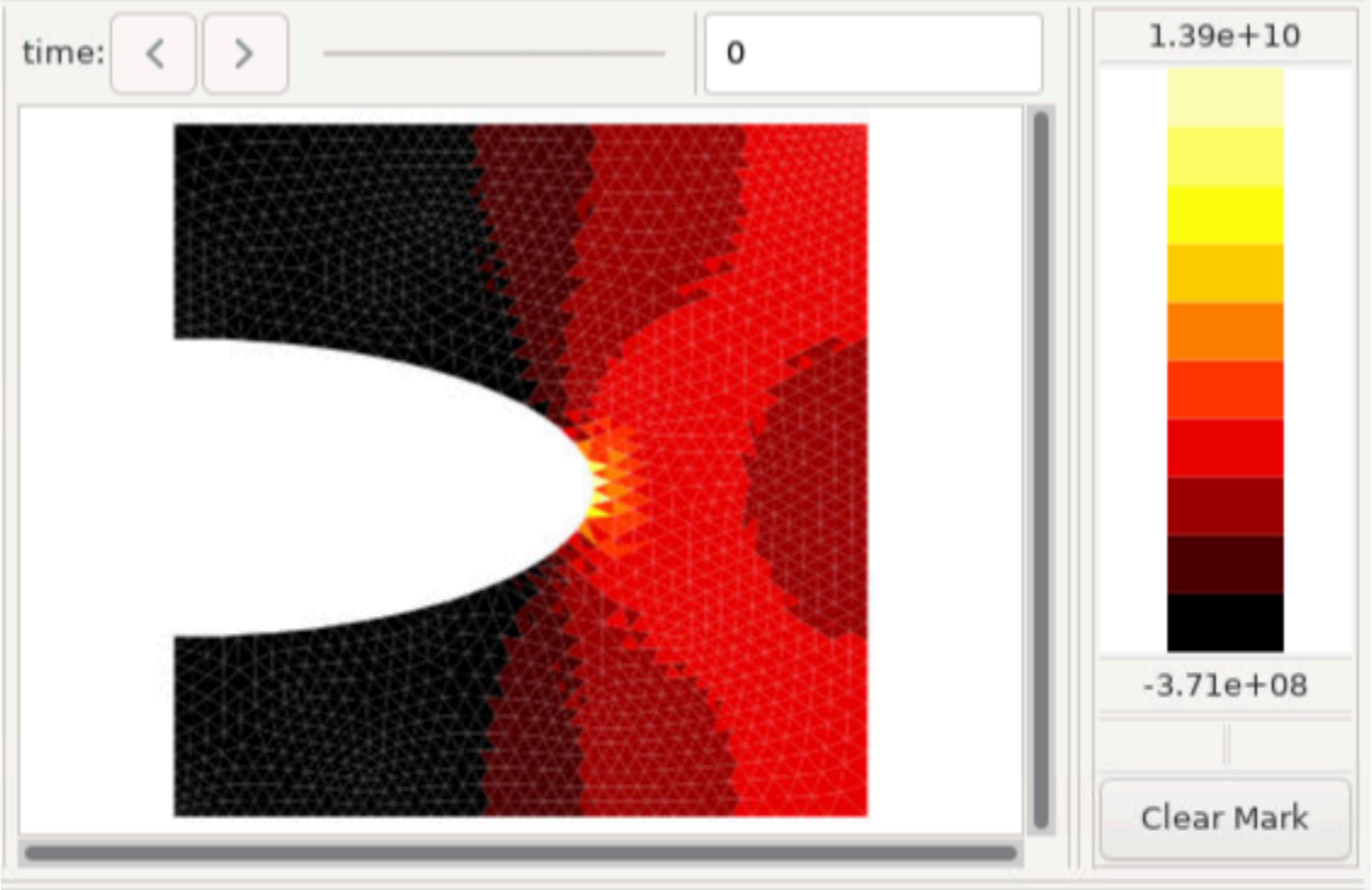
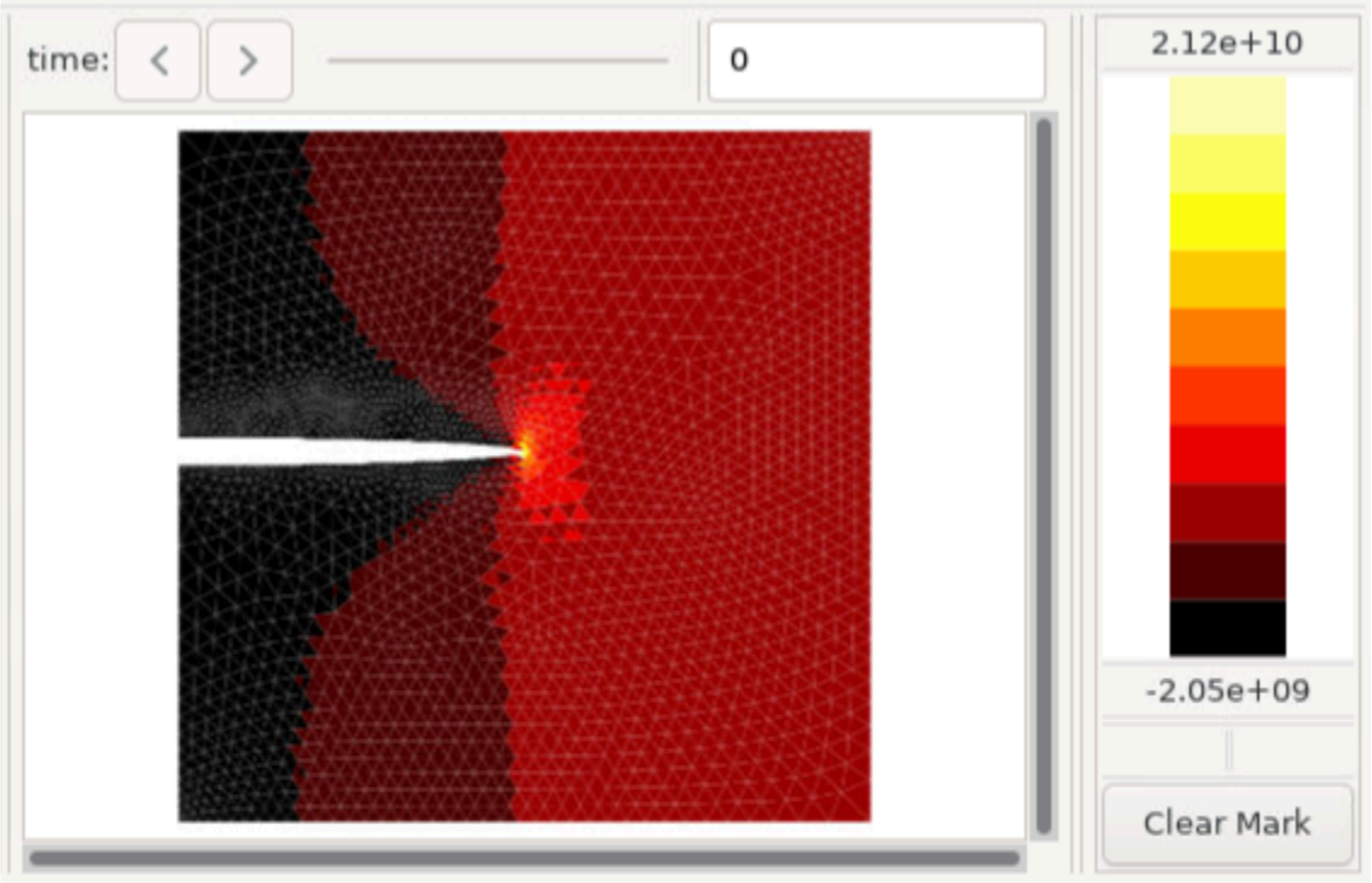


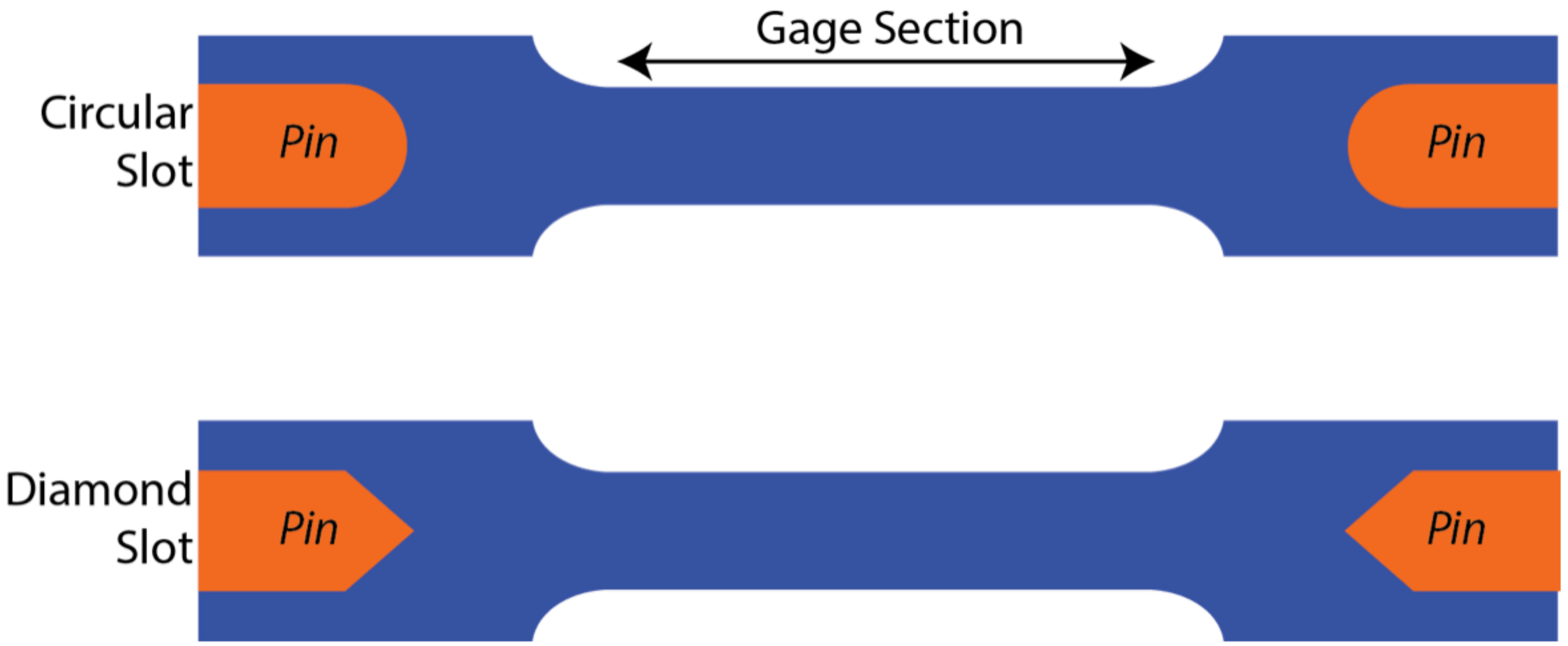


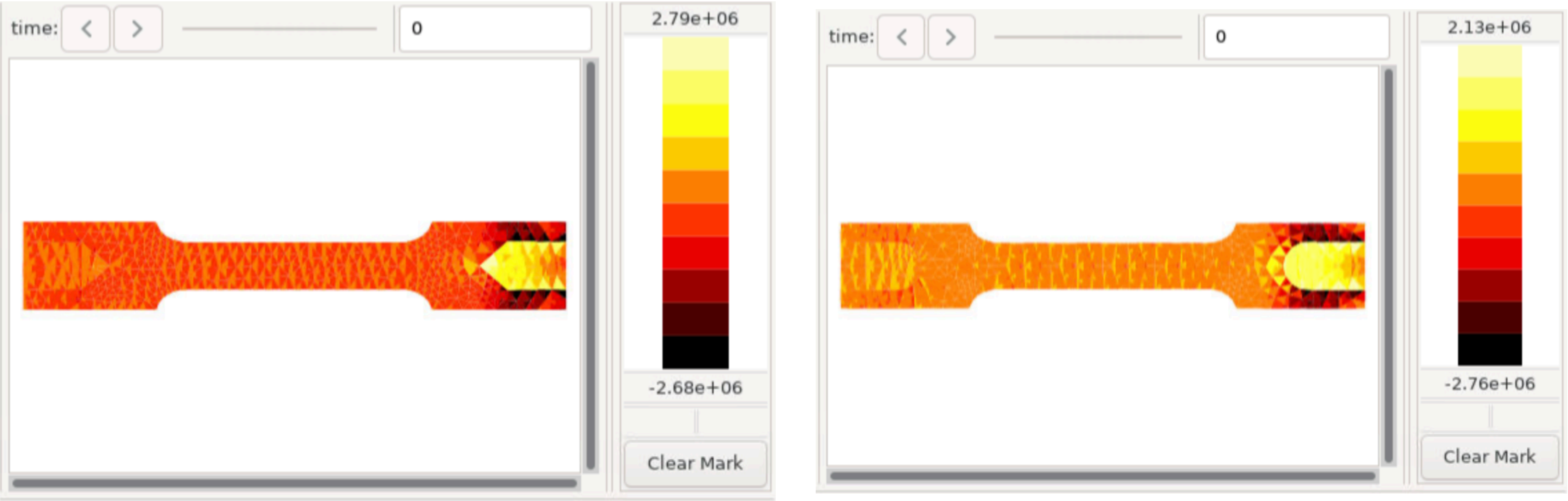
Demo 2: Thermal Stress and Stress Concentration Points in Specimens

Your lab technician has come up with a great idea to improve alignment during compression testing of “dog-bone" shaped specimens—using slots in the sample instead of traditional clamps or pins to secure the specimens. However, before you conduct any expensive, time-consuming tests, you want to make sure that the new configuration won’t impact the failure behavior of the material. You know that your compression rig tends to introduce a small thermal gradient across a sample and you need to calculate the thermal stresses of the new specimen geometry and decide which is best based on the two slots the lab technician has designed. Your specimen (in blue) is aluminum, which has a high coefficient of thermal expansion. The specimens are fixed into the test rig using steel pins (in orange)—steel has a low coefficient of thermal expansion.

Old dog-bone compression design with pins:

New possible dog-bone compression designs (using slots with pins):




time:
0
2.79e+06
-2.68e+06
Clear Mark
time:
0
2.13e+06
-2.76e+06
Clear Mark

Summary and Useful Resources

- OOF homepage (OOF2 and OOF3D): https://www.ctcms.nist.gov/oof/
- OOF2 user manual: https://www.ctcms.nist.gov/~langer/oof2man/
- Reid, Andrew CE, et al. "Modelling microstructures with OOF2." International Journal of Materials and Product Technology 35.3-4 (2009): 361-373.
- Langer, Stephen. "OOF2: Object-Oriented Finite Element Analysis of Material Microstructures." (2004).
- OOF2 user group: https://nanohub.org/groups/oof_users
- Contact information: yangdan2@illinois.edu