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Phase-field modeling of grain growth in sintered uranium dioxide under high temperature gradients

Ben Winchester & Veena Tikare

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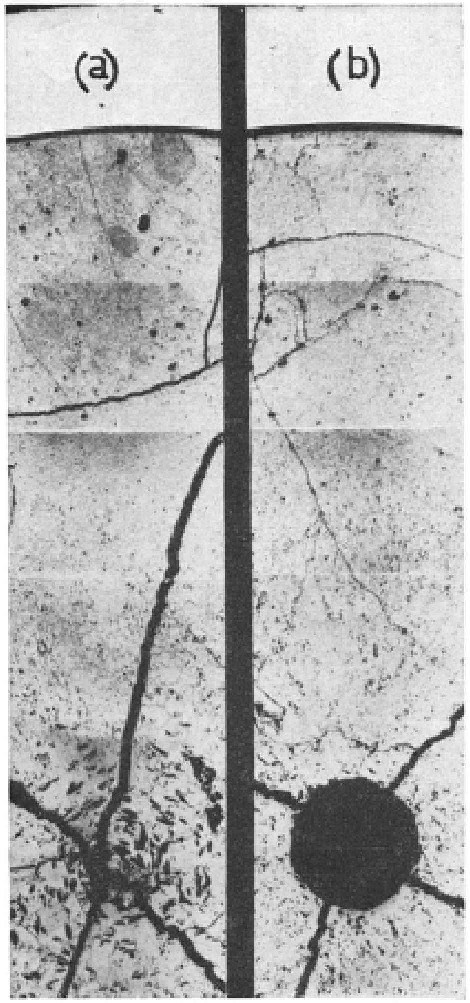
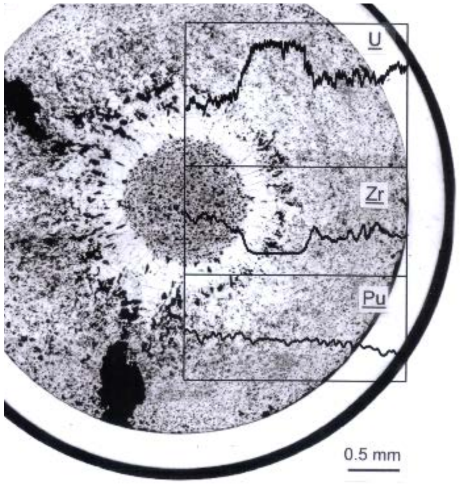
Outline

- Introduction: Problems in nuclear materials modeling
- The Approach: the phase field model
- Example cases for compositional evolution
- Adaptive meshing and microstructural evolution
- Conclusions & future work

Nuclear materials: a hot mess.

Microstructural evolution, radiation damage, extreme heat!





Lenticular void formation and growth is observed. These cause problems.

Causes are speculated and approximated:

- Vapor transport
- Soret Effect

Left and bottom-right: P.F. Sens, J. Nuc. Mat. **43**, (1972) 293-307
Top right: M. P. Anderson, *et al.*, Acta Metall., (1984), **32**, 783-791

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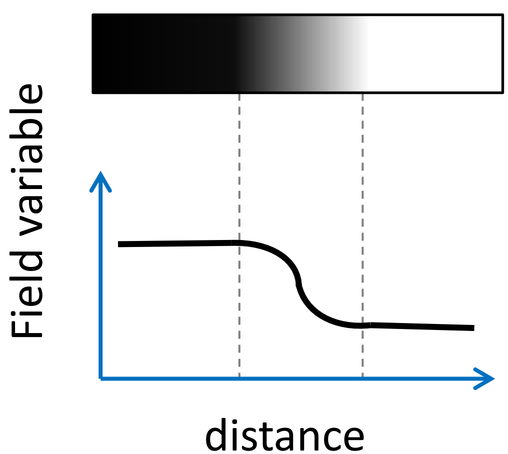
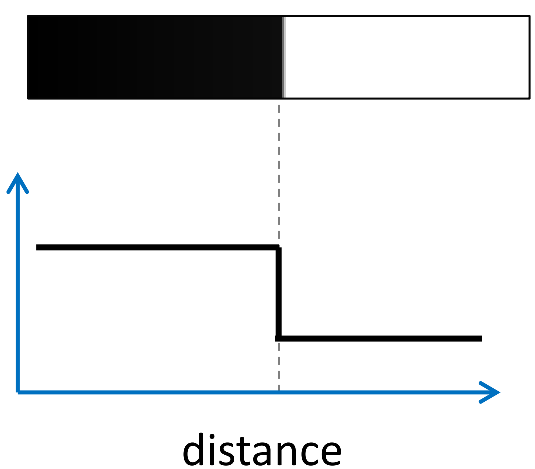
About the phase-field method

- A meso/continuum-scale method based on thermodynamics
- Takes some macro “order parameter” that varies in space (superconductivity, magnetism, etc.) and solves its evolution by a variational method.
- We treat the parameter as a continuous variable.

Phase-field model
(diffuse interface)



Sharp-interface model



The phase-field model

$$F = \int \left[h(\eta) f_{bulk,solid}(c) + j(\eta) f_{bulk,void}(c) + f_{spin}(\phi_i, \eta) + f_{gradient}(c, \eta, \phi_i)\right] dV$$

Bulk energies:

$$f_{bulk,solid}(c) = E_v^f c_v + E_i^f c_i + E_g^f c_g + k_B T\left[c_v \ln(c_v) + c_i \ln(c_i) + c_g \ln(c_g) + (1 - c_v - c_g - c_i) \ln(1 - c_v - c_g - c_i)\right]$$

$$f_{bulk,void} = (c_v - 1)^2 + {c_i}^2 + c_g\left(\mu_g^0 + k_B T\left[\ln(c_g) + \ln(k_B T)\right]\right)$$

Terms coupling phase (η) and c_α

$$h(\eta) = (\eta - 1)^2$$

$$j(\eta) = \eta^2$$

Gradient energies:

$$f_{gradient}(c, \eta) = \kappa_{c_g}(\nabla c_g)^2 + \kappa_{c_i}(\nabla c_i)^2 + \kappa_{c_v}(\nabla c_v)^2 + \kappa_\eta(\nabla \eta)^2$$

[1] P. Millett, A. El-Azab, and D. Wolf, Comp. Mat. Sci. **50** (2011) 960-970

Evolution of the order parameters

Non-conserved order parameter - Allen-Cahn equation:

$$\frac{\partial \eta}{\partial t} = -L_\eta \frac{\delta F}{\delta \eta}$$

Conserved order parameters - Cahn-Hilliard equation:

$$\frac{\partial c_\alpha}{\partial t} = \nabla \cdot \left(M_{c_\alpha} \nabla \frac{1}{N} \frac{\delta F}{\delta c_\alpha} \right) + R_\alpha + P_\alpha$$

Recombination term:

$$R_{iv} = R_r c_v c_i = \left(R_{bulk} + \eta^2 R_{surface} \right) c_v c_i$$

Production term:

$$P_v = b_{v/i} P_i = \begin{cases} 0, & if \;\; \eta > 0.8 \; or \; (rand[0,1]) > C_{prob} \\ V_G(rand[0,1]), & otherwise \end{cases}$$

What's *not* in the model? (and could be important?)

- Elastic strain response of material
- Dislocations
- Other gases, phases, or types of vacancies.
- Anisotropic effects (anisotropic stesses, grain boundary energy, mobility, etc.)

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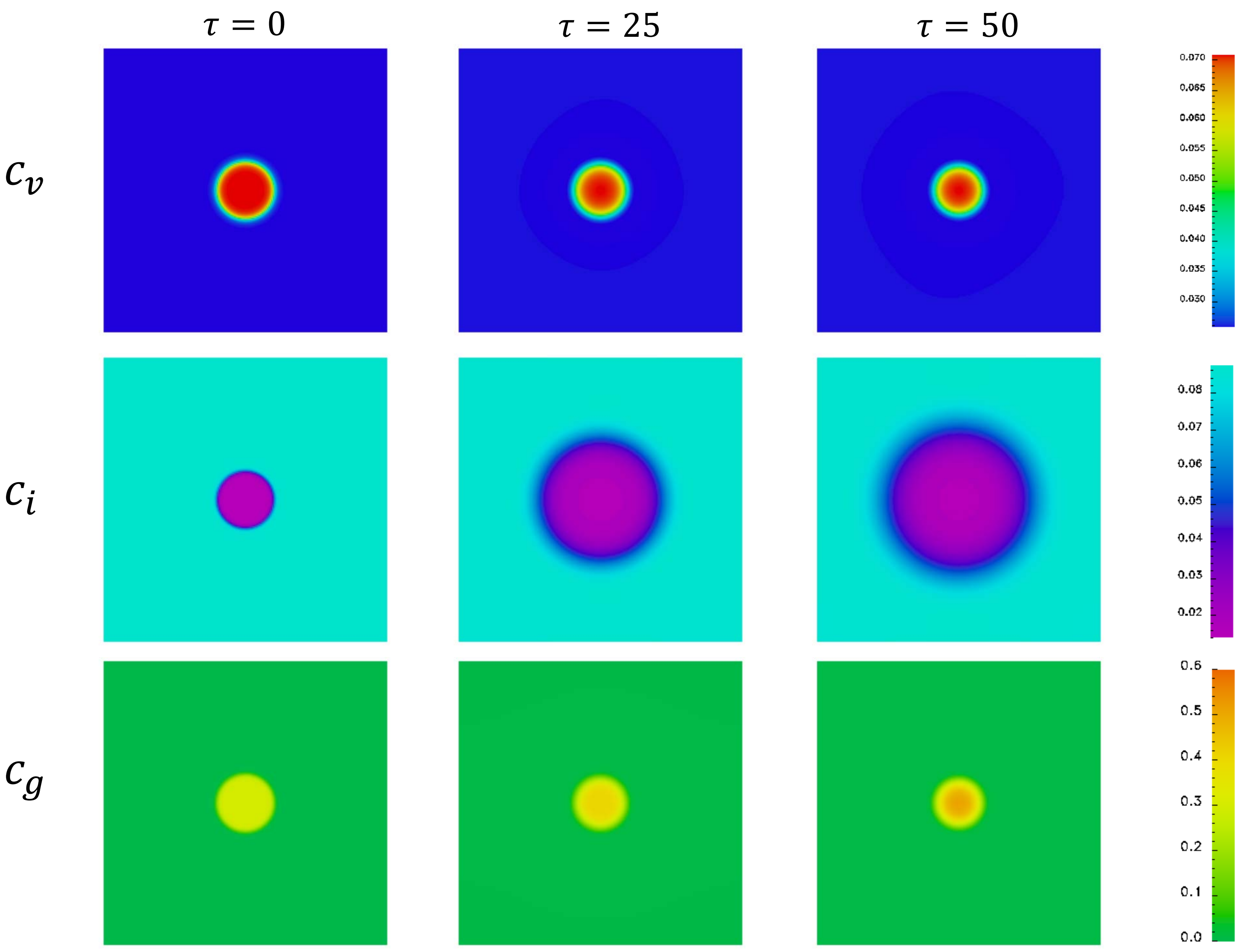
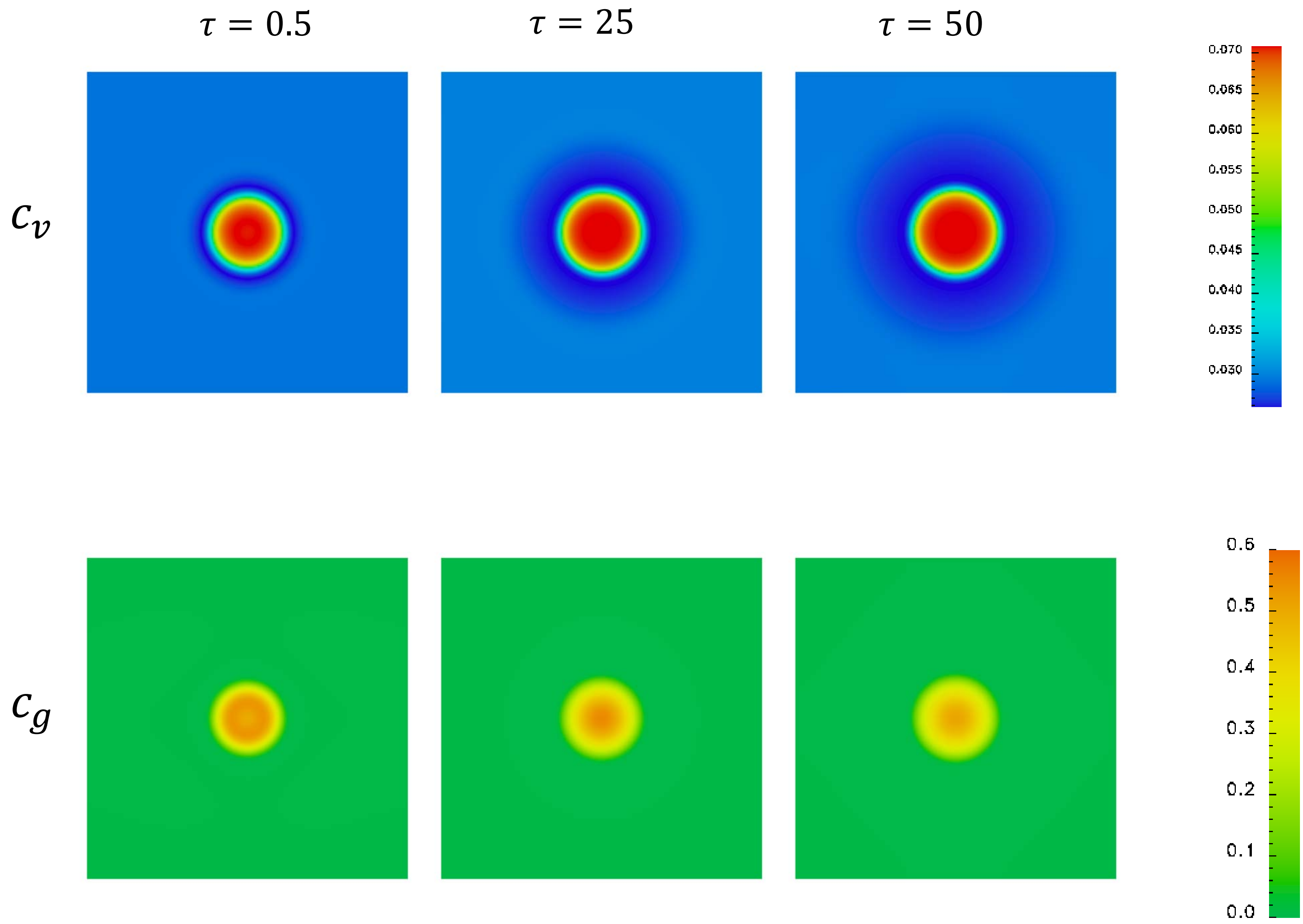
Test cases: void shrinkage, with $c_i > 0$ in the matrix



Test cases: void growing, with $c_v > c_{v,eq}$ in the matrix



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Microstructural evolution with adaptive meshing

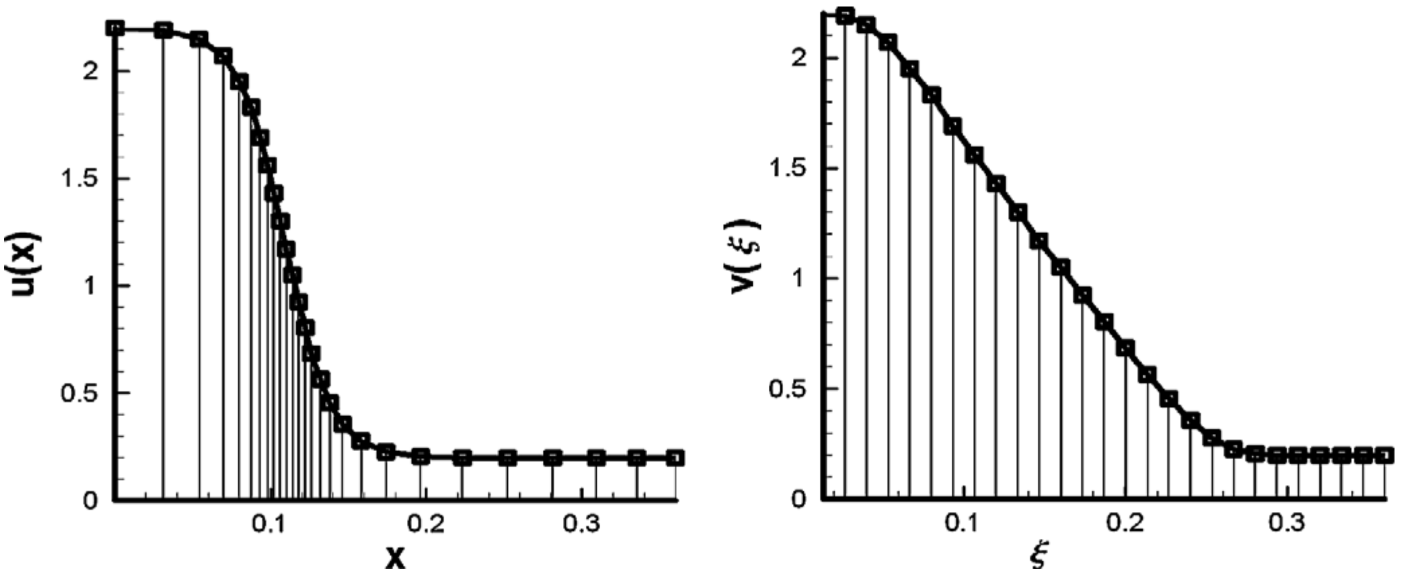
Mesh moves to where it's most needed: using a monitor function to approximate the error.

Variational eq'n

$$I[\xi] = \int \sum_{i=1}^{3} \frac{\nabla_x \xi^i \cdot \nabla_x \xi^i}{\omega} dx$$

Monitor function

$$\omega \cong \sqrt{1 + \beta^2 |\nabla_x u|^2}$$



Physical domain (left) and computational domain (right)[1].

[1] W.M. Feng *et al.*, J. Comp. Phys. **220** (2006) 498-510

Microstructural Evolution with Adaptive Meshing (cont'd)

Non-conserved order parameter: "spins",ϕ_i, for treating microstructural evolution.

System energy consists of 'bulk' and gradient terms, depending on q spins:

$$f_{spin} = f_{spin,bulk} + f_{spin,gradient}$$

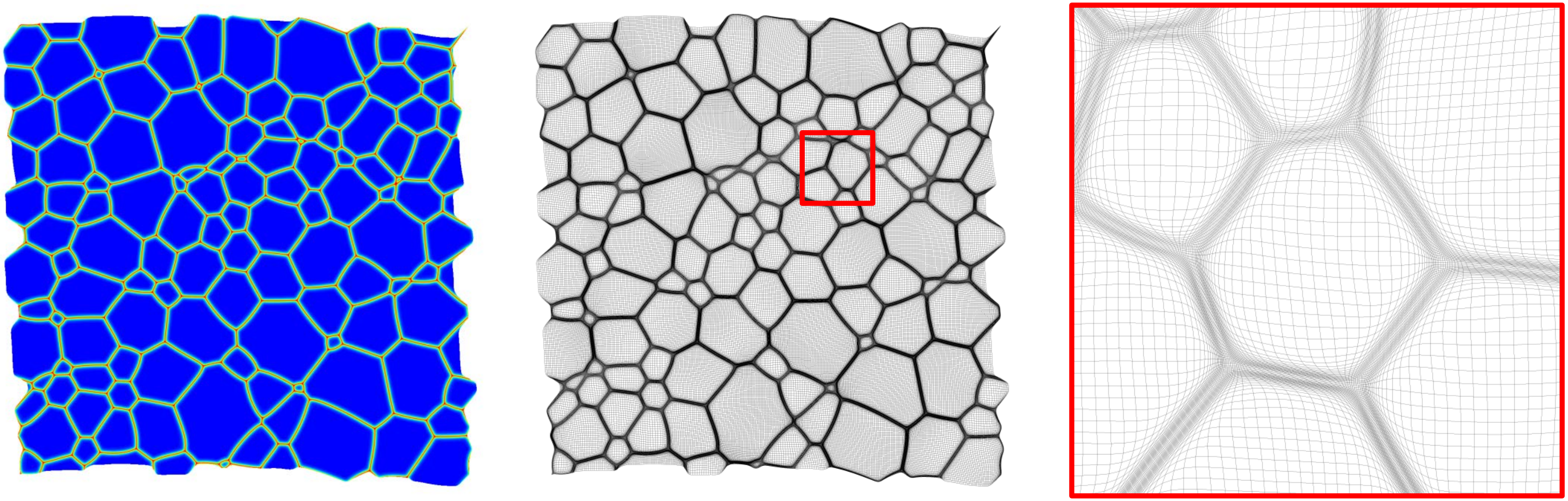
$$f_{spin,bulk} = 3\left(\sum_{i=1}^{q} {\phi_i}^2 + \frac{\eta^2}{q}\right)^2 - 4\eta^3 - 4\sum_{i=1}^{q} {\phi_i}^3$$

$$f_{spin,gradient} = \kappa_{\phi_i}(\nabla\phi_i)^2$$

Temporal evolution via Allen-Cahn equation:

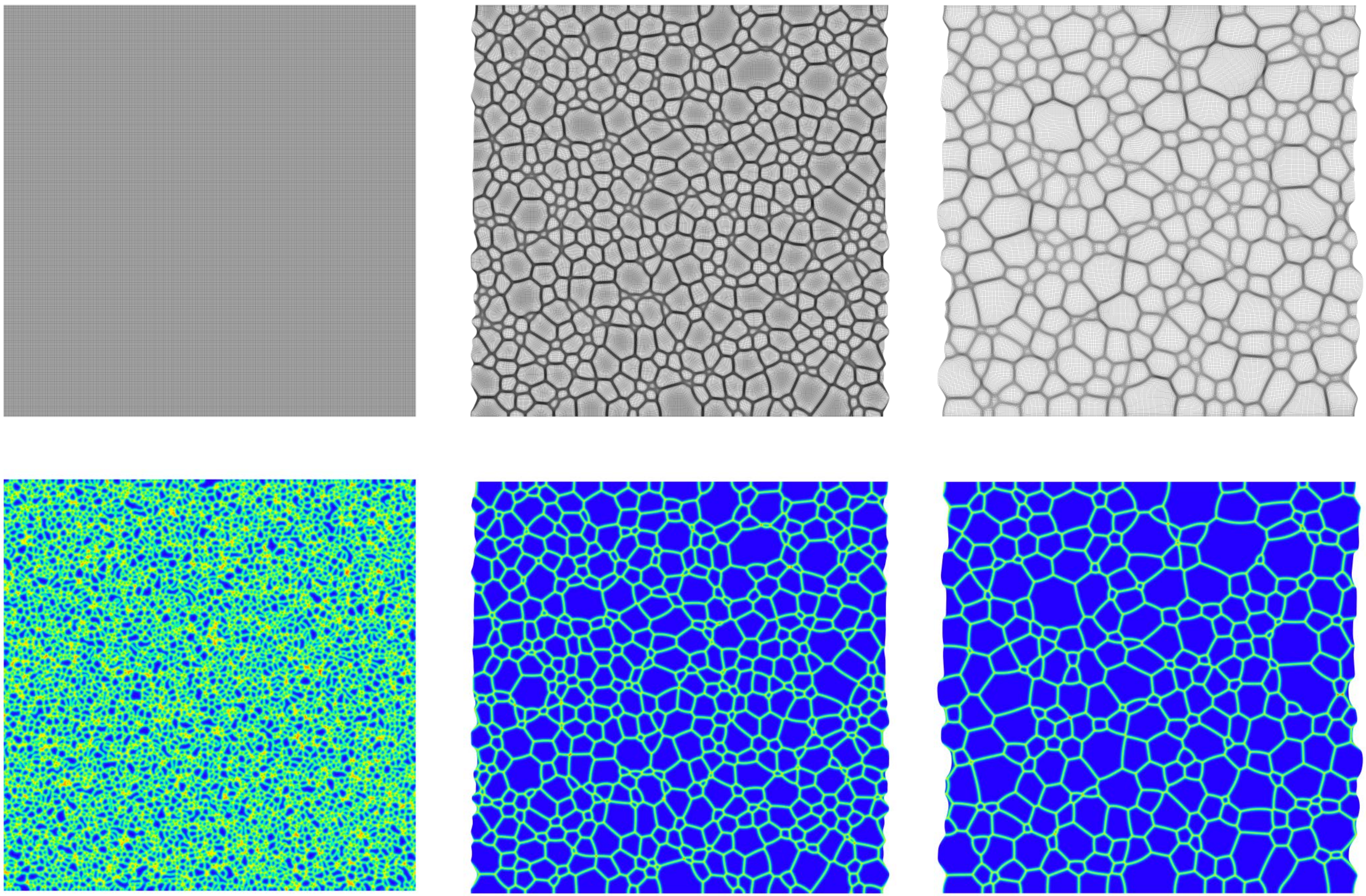
$$\frac{\partial\phi_i}{\partial t} = -L_{\phi_i}\frac{\delta F}{\delta\phi_i}$$

(512 x 512) simulation of microstructural evolution and resulting mesh



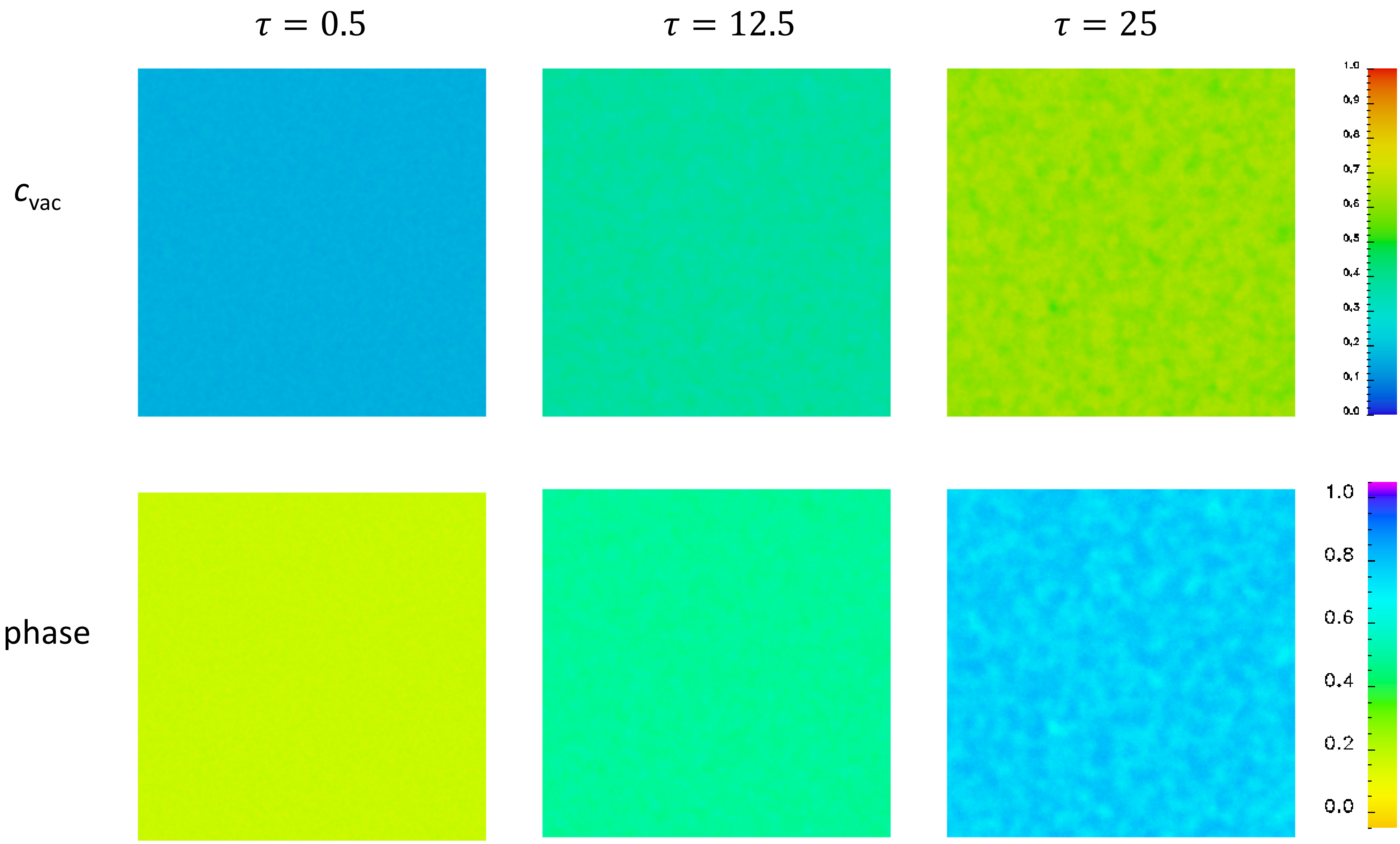
Adaptive meshing and grid coarsening

$\tau = 10$ | $\tau = 200$ | $\tau = 400$



Introducing radiation damage in a single crystal system

(Need to further examine nucleation conditions)



Conclusions

- We developed a semi-implicit moving-mesh phase field model for microstructural evolution.
- The model produced qualitatively accurate results for several simple examples and is being employed to study evolution under radiation.
- We demonstrate a moving mesh for the phase field model which greatly reduces the computational time needed for these grain + compositional evolution in phase-field models.

Future Work

- Examine kinetics of nucleation and segregation of bubbles on grain boundary vs. bulk.
- Introduce radiation into grain microstructure, and examine the effect of temperature gradients on bubble migration.
- Obtain quantitative comparison with experiments or other types of models.
- Include other important aspects of microstructural evolution: anisotropic grain properties, elastic properties, etc.

Acknowledgements

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