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Modeling Nuclear Fuels with a Combined Potts-Phase Field Model

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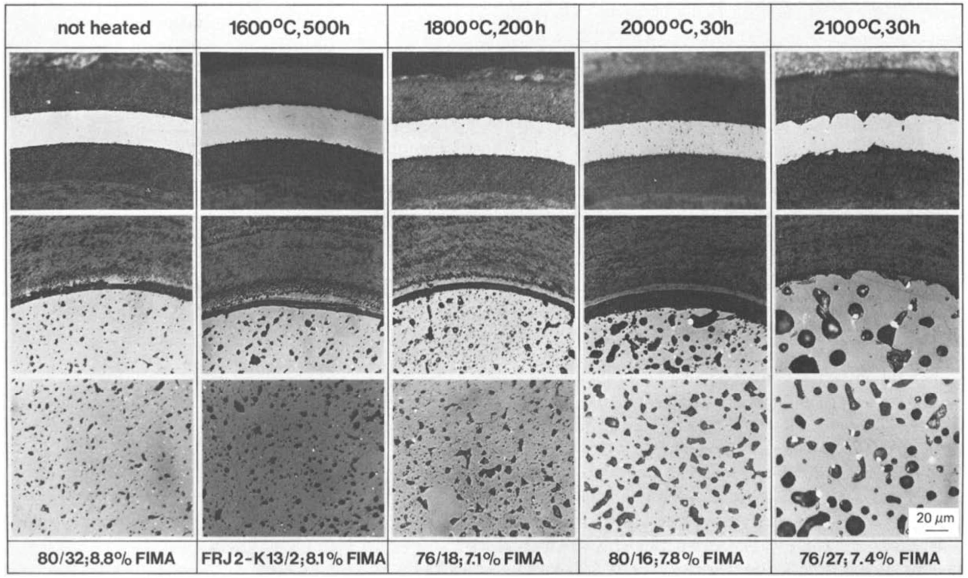
Extreme Environments of Nuclear Reactors

Irradiation & Thermal Effects

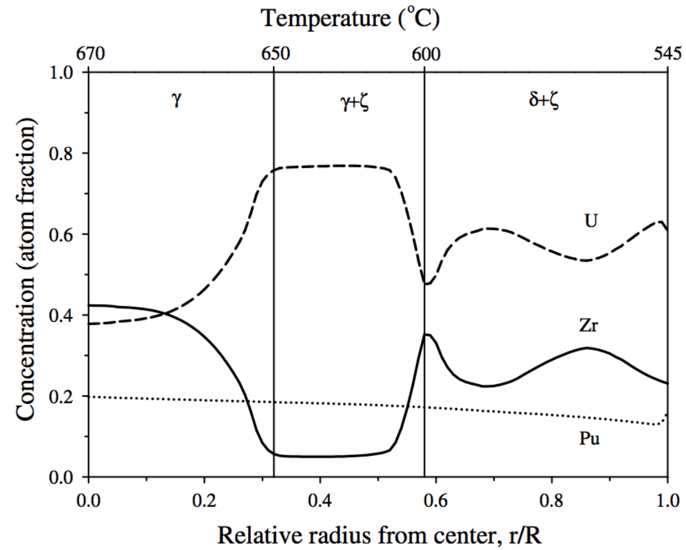
- Fission Gas Generation
- Damage / Plasticity
- Impurity Fission Bi-Products
- Diffusion
- Creep
- Chemical attack between cladding and fuel

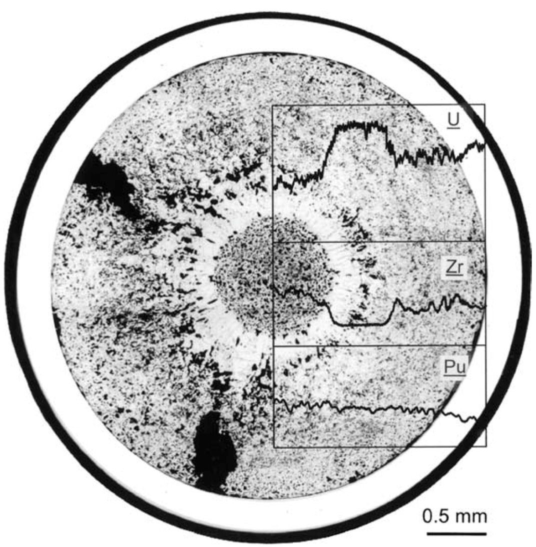


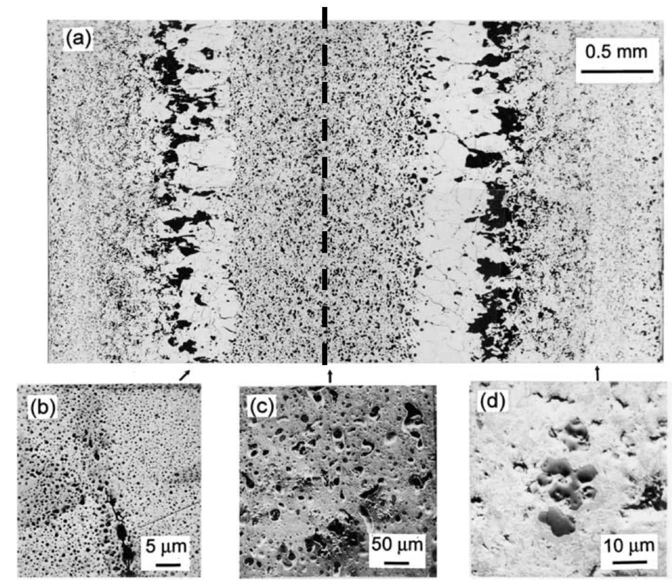
Nabielek, et al. Nucl. Eng. & Des. 1990.

Coupling microstructure and concentration

- U-Pu-Zr metallic alloy
- Exp. Breeder Reactor II
- Temperature-induced phase changes



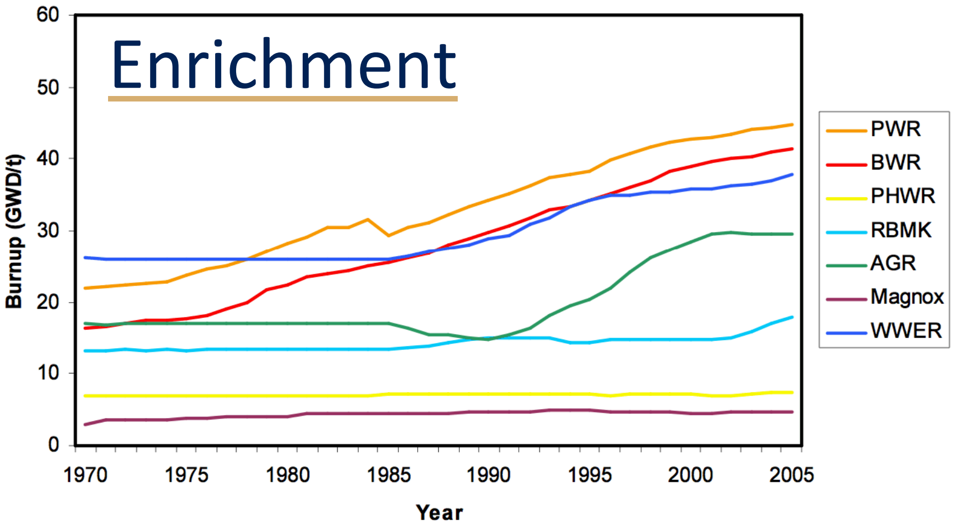




Kim, et al. J. Nucl. Mat. 2004.

Value of improving nuclear fuels

Enrichment



IAEA 51st Conference, 2007.

Materials Models

- Improved
  - Performance
  - Fuels cycles
  - Waste / Recycling

Required Materials Model

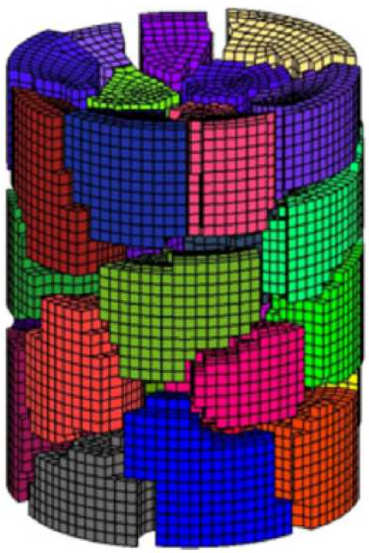
- Material
  - Microstructure
  - Phase
  - Composition
  - Temperature
  - Void
- Framework
  - Efficient
  - Scalable

Modeling techniques for microstructure evolution

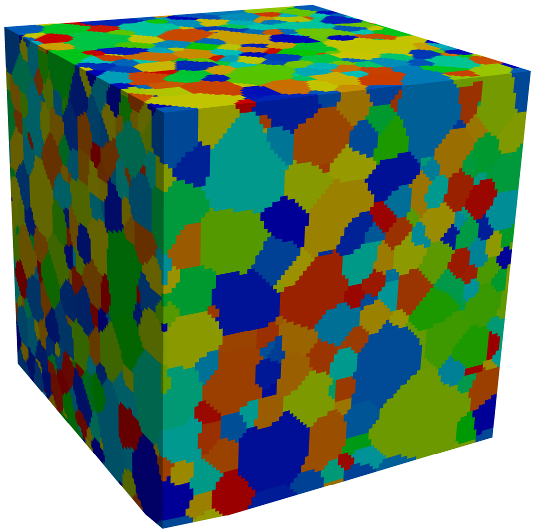
Finite Element Analysis

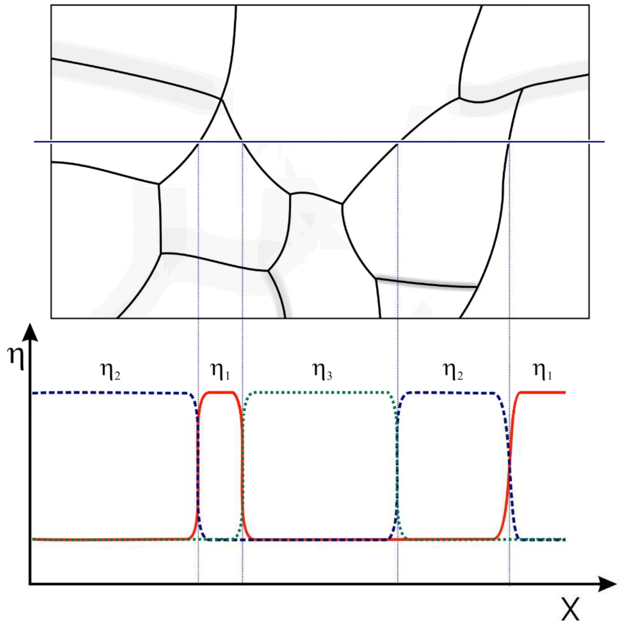
Potts Monte Carlo

Phase Field



Gaston, et al. Nucl. Eng. & Des. 2009.

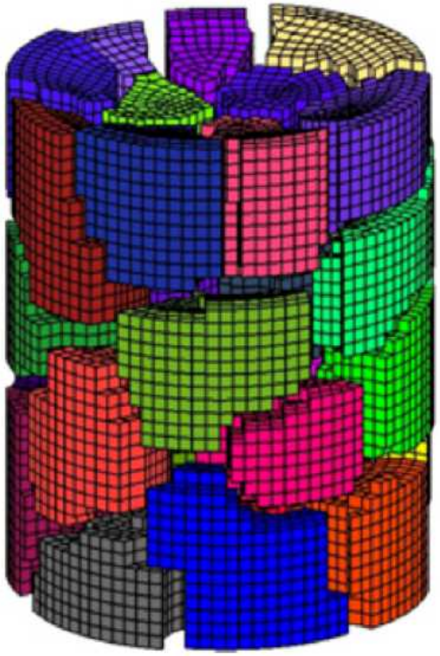




Phase field models. Wikipedia 2011.

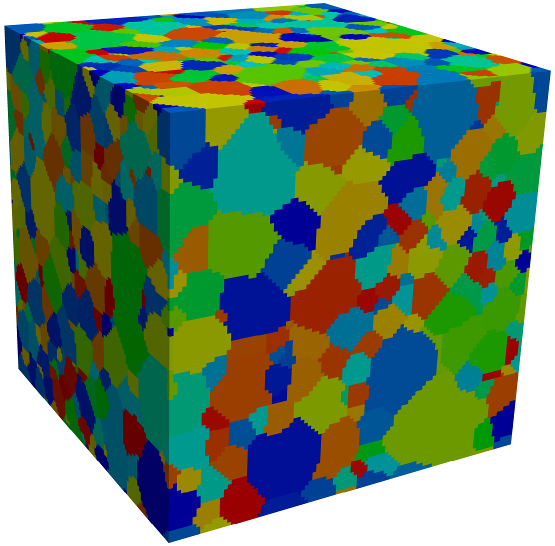
Finite Element Models

- Material
  - Continuum
- Physical evolution
  - Governed by constitutive-based materials models
- Solution
  - Solve system of equations – implicit/explicit
- Examples
  - OOF – NIST
  - MOOSE – INL/FSU



Potts Monte Carlo Model

- Material
  - Individual particles form an ensemble
- Physical evolution
  - Governed by statistical mechanics of state energetics
- Solution
  - Monte Carlo methods
- Examples
  - SPPARKS – SNL
  - MMSP – CMU



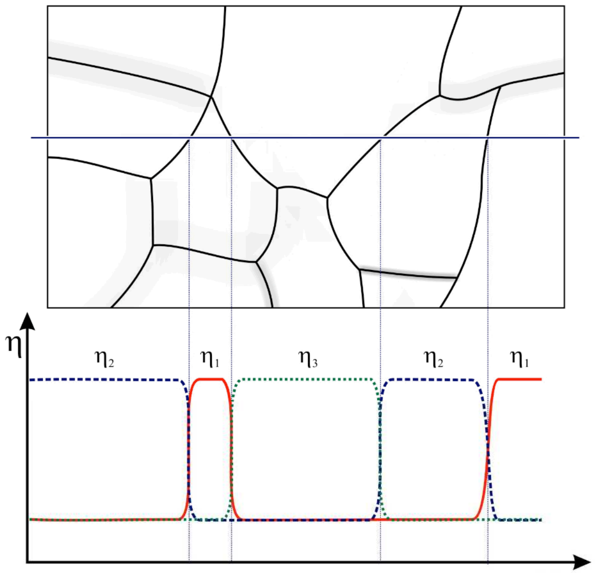
$$E = E_{vol} + E_{\text{int}}$$

$$E = \sum_{i=1}^{N}\left(E_{vol}(q_i) + \frac{1}{2}\sum_{j=1}^{n} J\left(1-\delta_{ij}\right)\right)$$

$$P = \begin{cases} 1 & for \quad E \le 0 \\ \exp\left(\dfrac{-\Delta E}{kT}\right) & for \quad E > 0 \end{cases}$$

Phase Field Model

- Material
  - Phases fields
- Physical evolution
  - Cahn-Hilliard
  - Ginzburg-Landau
- Solution
  - Implicit/explicit solution of PDEs
- Examples
  - CH-muSE/CA-muSE



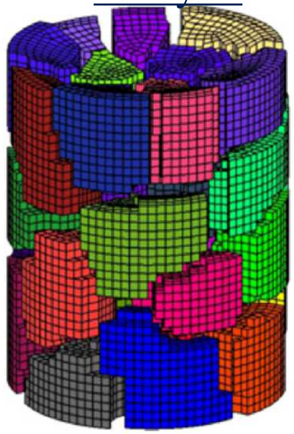
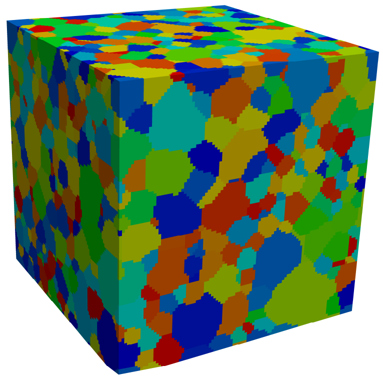
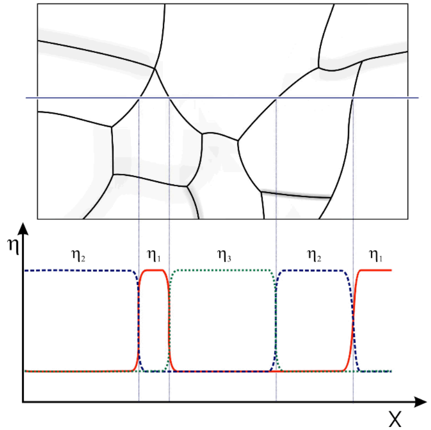
Phase field models. Wikipedia 2011.

$$E = E_{vol} + E_{\text{int}}$$

$$E = \int \left(f_o + 2\sum_{i=1}^{Q} \kappa_{\eta i} (\nabla \eta_i)^2 \right) dV$$

$$\frac{\partial C}{\partial t} = -M_c \left(\nabla^2 \frac{\partial E_{vol}}{\partial C} - \kappa_c \nabla^4 C \right)$$

Advantages / Disadvantages of modeling techniques

	Finite Element Analysis	Potts Monte Carlo	Phase Field
			
	Gaston, et al. Nucl. Eng. & Des. 2009.		Phase field models. Wikipedia 2011.
+	Geometrically / Physically Versatile	Statistical microstructures, Computationally efficient	Continuum fields, Thermodynamic model
–	Constitutive development, Solution of PDEs Rule-based	On-lattice, Discrete valued	On-lattice, Model development Computationally intensive

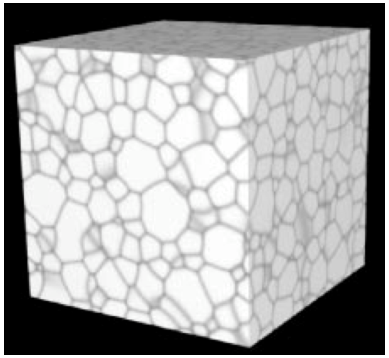
Combined approach of modeling techniques

Phase-Field

- Deterministic Continuum Model
- Smoothly varying fields
- Diffuse Interfaces

Potts Monte Carlo

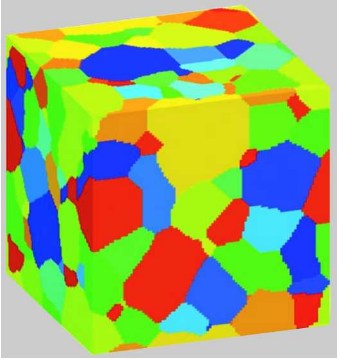
- Statistical-Mechanical Model
- Discrete Particles
- Sharp Interfaces



Chen. Annu Rev. Mat. Res. 2002.

Combined Model

- Potts: Grain evolution
- PF: Concentration evolution
- Balance resolution / efficiency



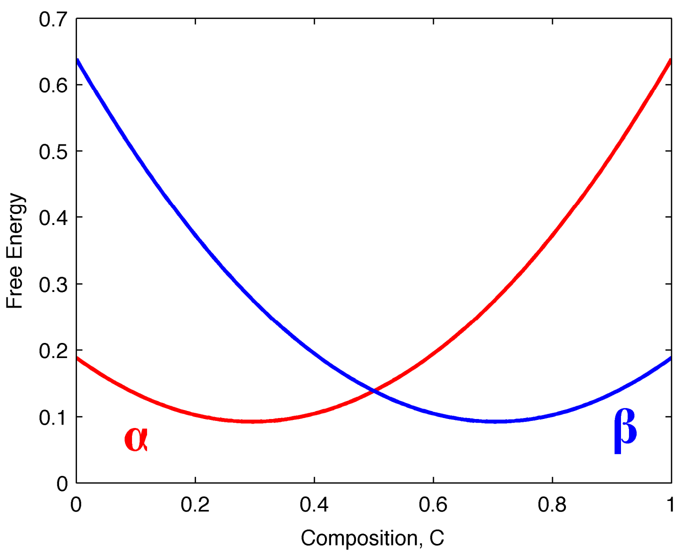
Holm. et al. JOM. 2001.

Details of the Combined Model

Combined Model Energetics

$$E_{hyb} = \sum_{i=1}^{N}\left(E_v(q_i, C) + \frac{1}{2}\sum_{j=1}^{n} J(q_i, q_j)\right) + \int \kappa_c (\nabla C)^2 dV$$

$$E_v = \gamma\left[\left(C - C_1\right)^2 + \left(C_2 - C\right)^2\right] + a_1\left(C - C_3\right)^2 q_\alpha + a_2\left(C_4 - C\right)^2 q_\beta$$



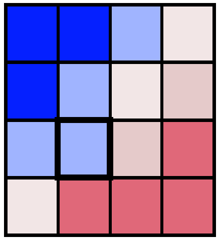
Potts Evolution

$$P = \begin{cases} \exp\left(-\dfrac{\Delta E}{k_B T}\right) & \text{for } \Delta E > 0 \\ 1 & \text{for } \Delta E \le 0 \end{cases}$$

A	A	A	B
A	A	B	B
A	A	B	B
C	C	C	C

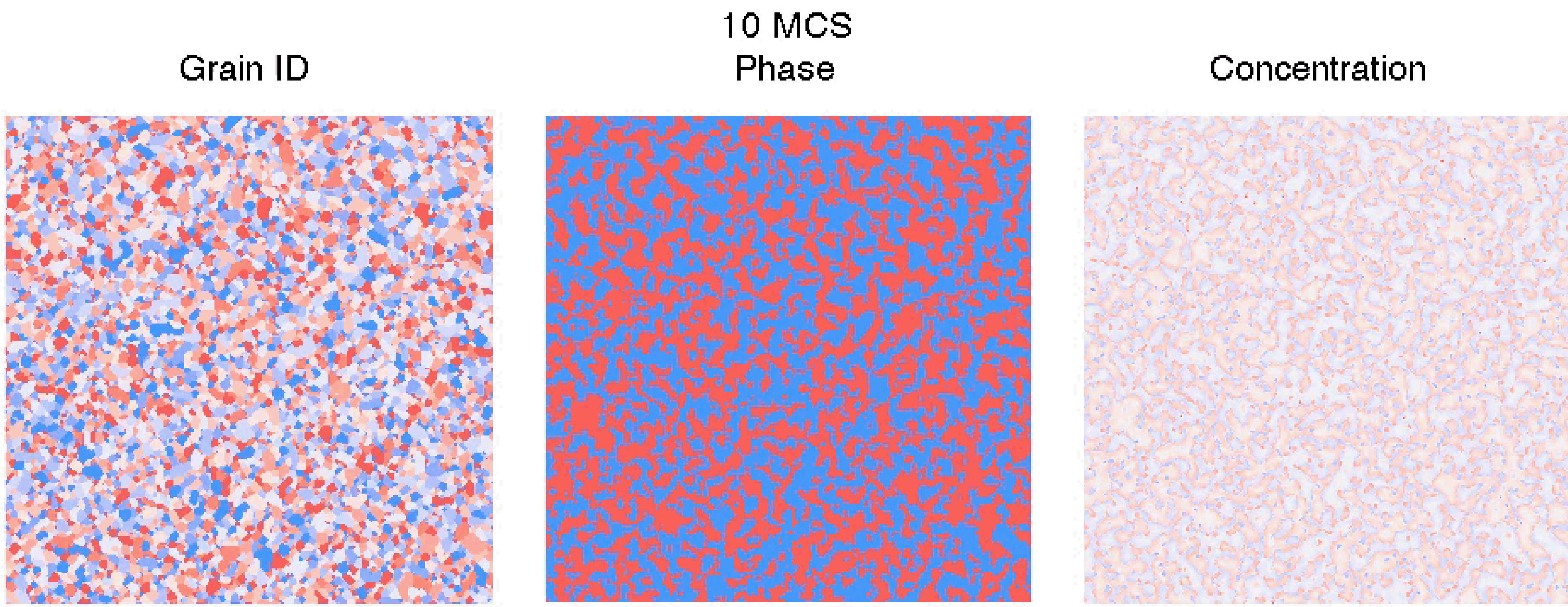
Phase-Field Evolution

$$\frac{\partial C}{\partial t} = M_c\left(\nabla^2 \frac{\partial E_v}{\partial C} - \kappa_c \nabla^4 C\right)$$



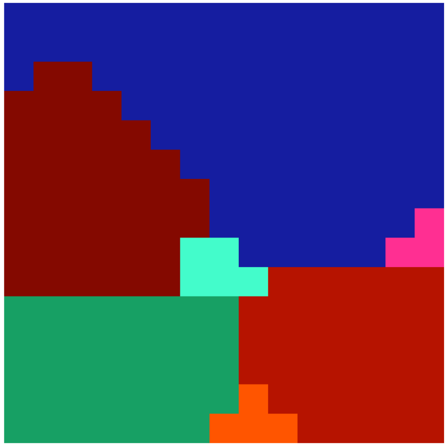
Coupled Potts – Phase Field Simulations

2-Phase 2-Component System

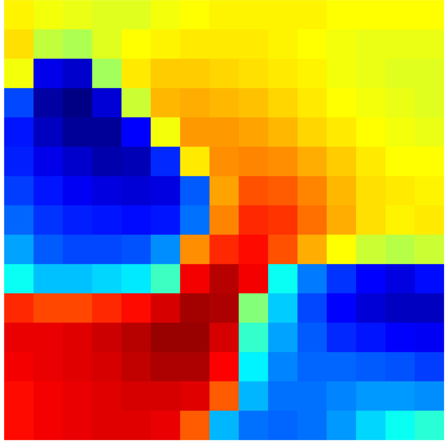


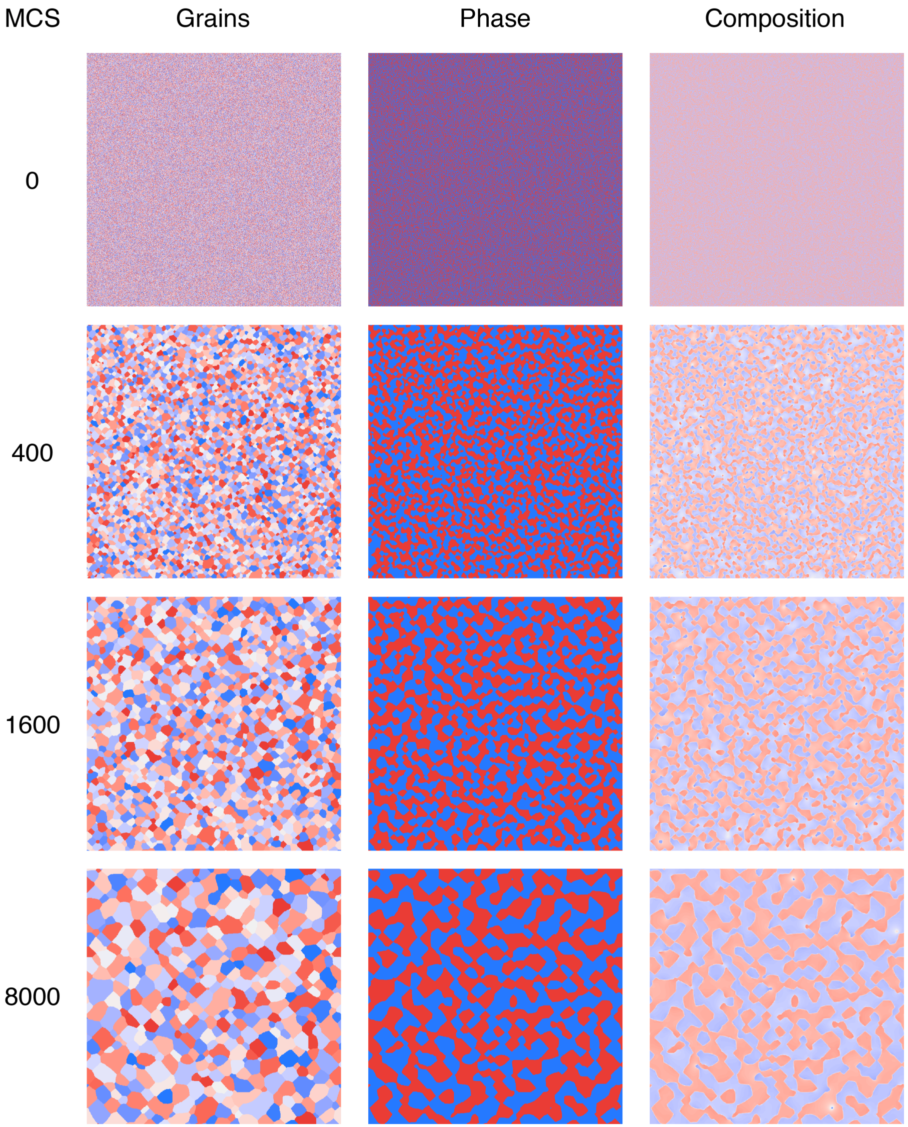
Model evolution

Microstructure



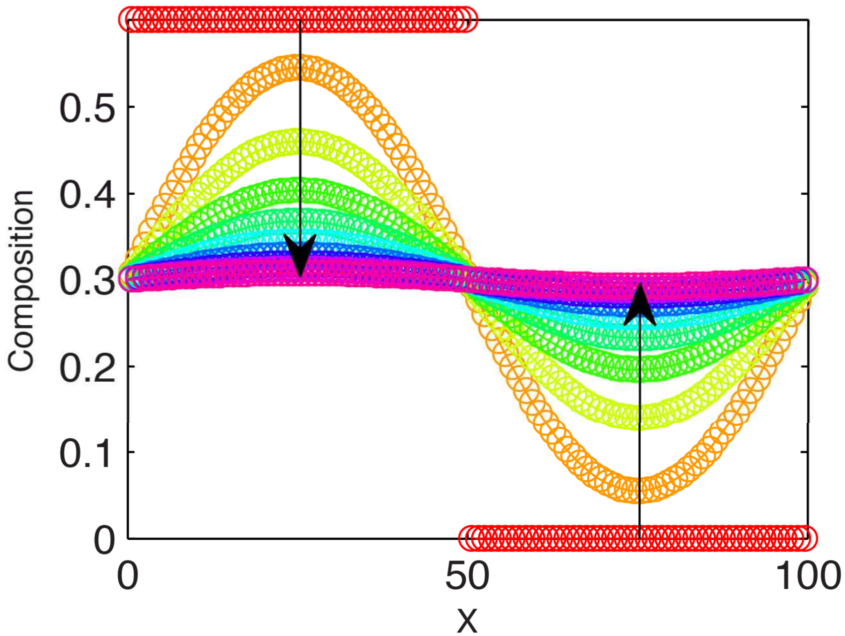
Composition





Diffusion & Effective Diffusivity

Single-Phase Step Concentration



Concentration Evolution

$$\frac{\partial C}{\partial t} = M_c\left(\nabla^2 \frac{\partial E_v}{\partial C} - \kappa_c \nabla^4 C\right)$$

$$E_v = \gamma\left[\left(C - C_1\right)^2 + \left(C_2 - C\right)^2\right] + a_1\left(C - C_3\right)^2 q_\alpha + a_2\left(C_4 - C\right)^2 q_\beta$$

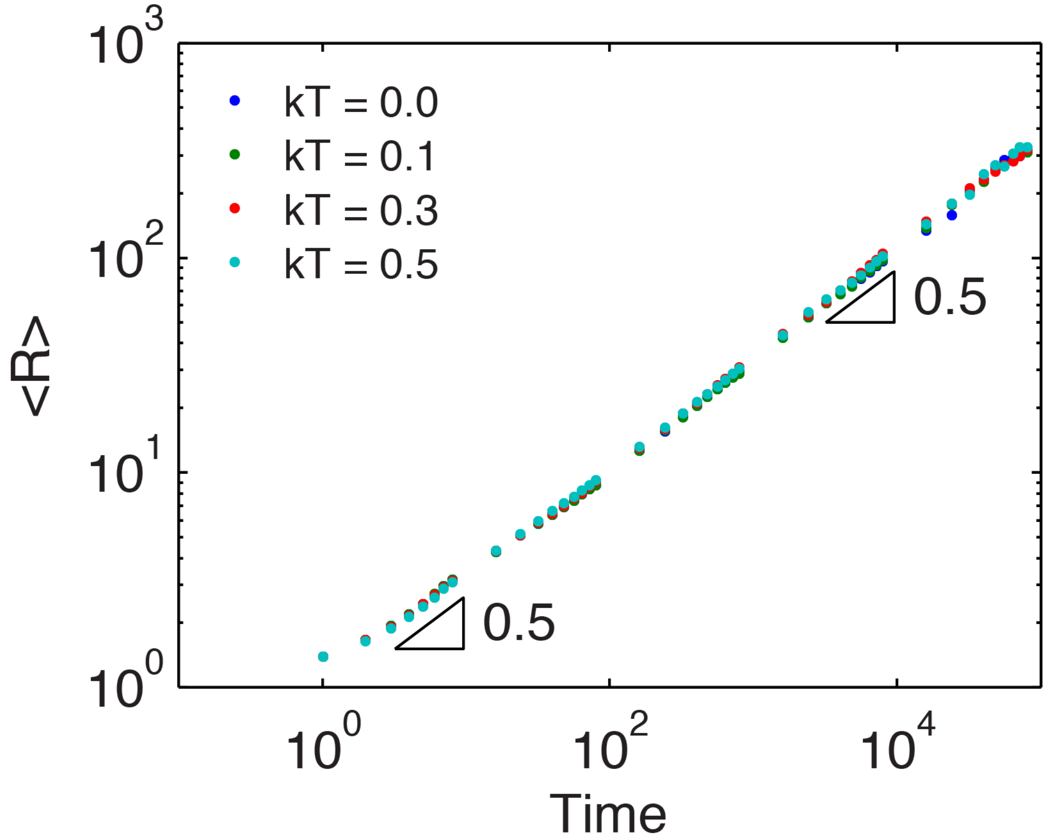
Fickian Diffusion

$$\frac{\partial C}{\partial t} = D\nabla^2 C$$

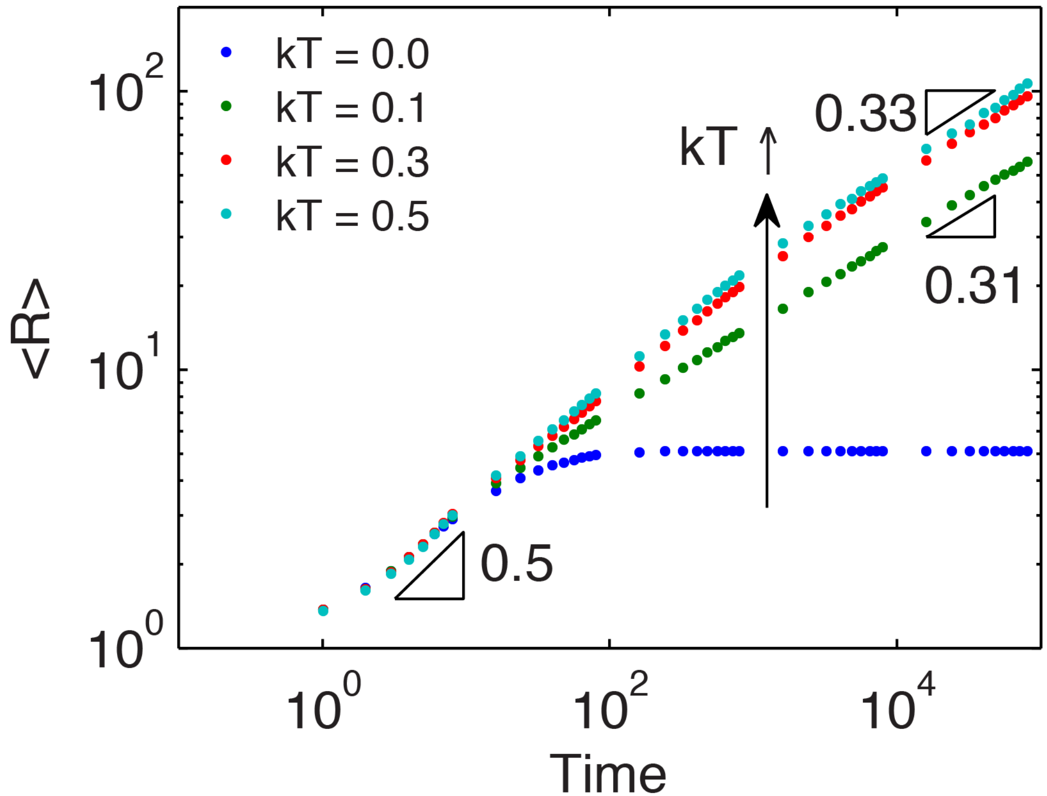
$$C(x,t) = \bar{C} + \frac{\Delta C}{2} erf\left(\frac{x}{\sqrt{4Dt}}\right)$$

Fit Effective Diffusivity

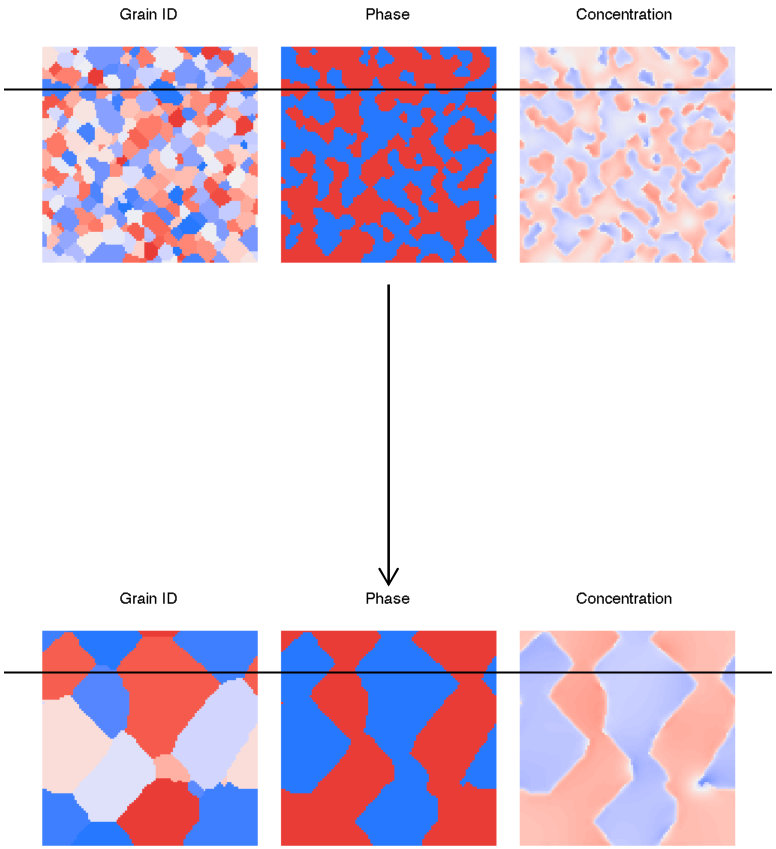
Single-phase grain growth

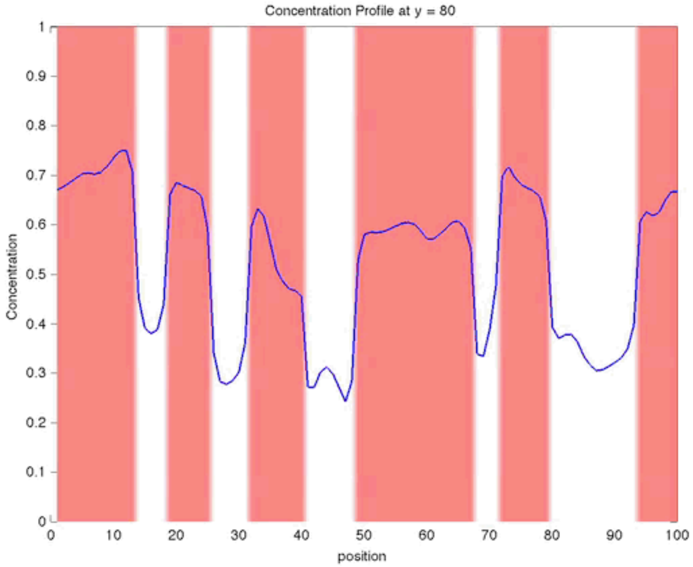


Dual-phase grain growth



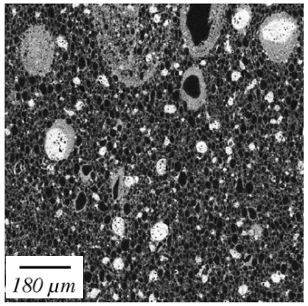
Concentration tracks phase boundaries

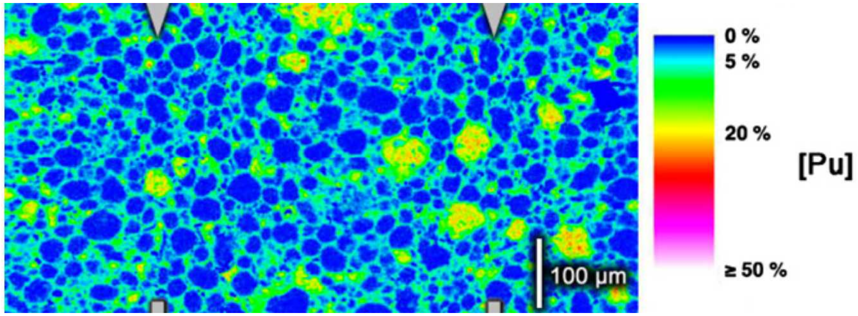




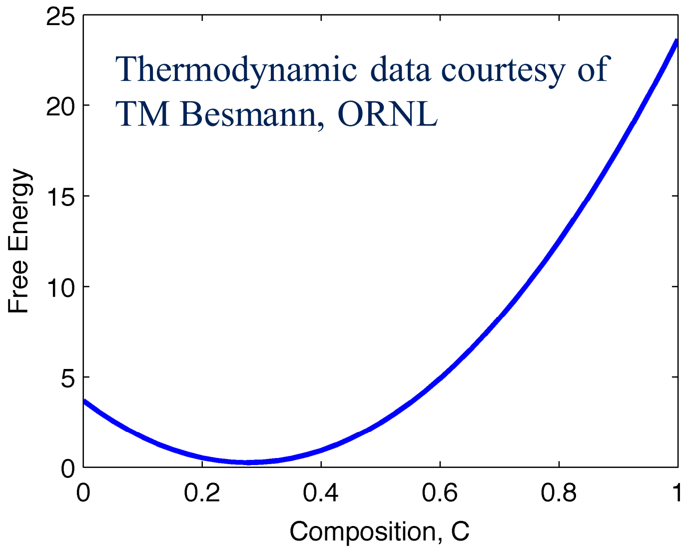
MIcronized MASterblend (MIMAS) Fuel

- $PuO_2 - UO_2$

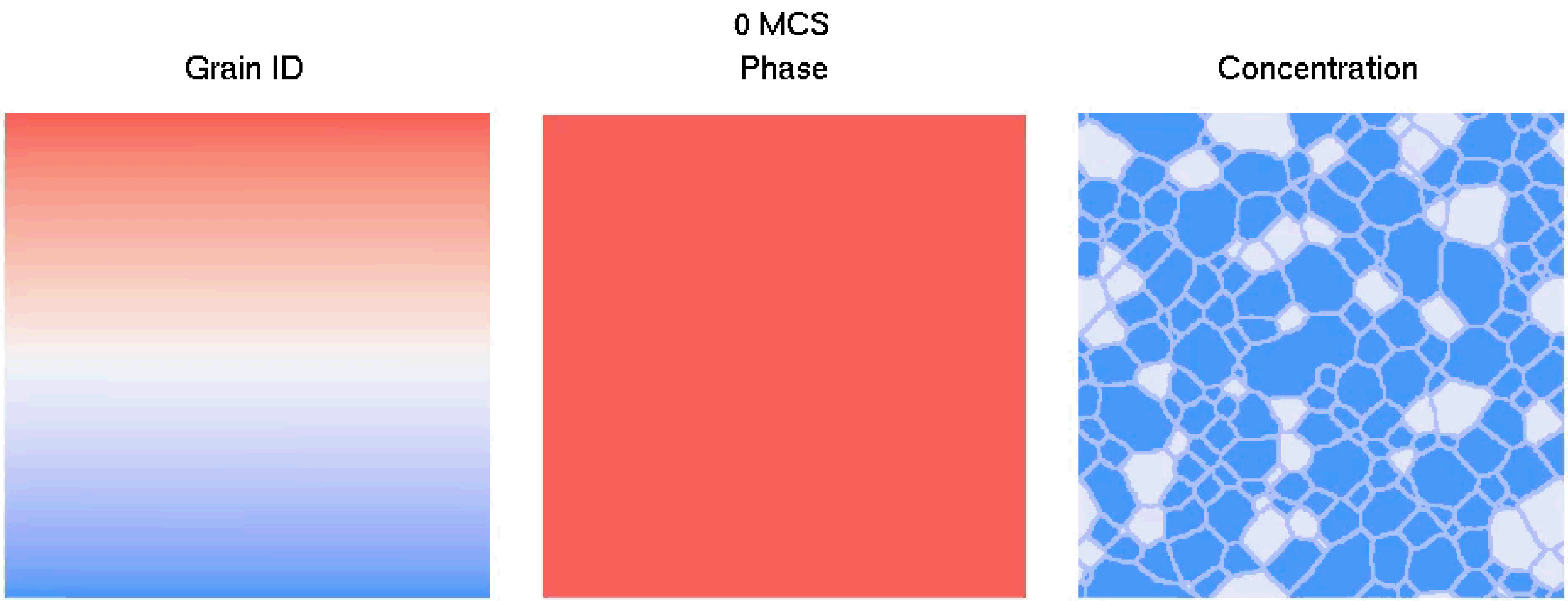




Oudinet. et. al. J. Nucl. Mat. 2008.



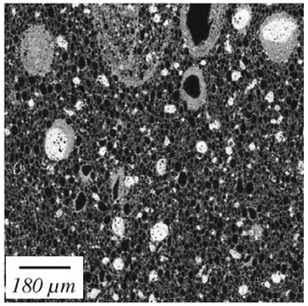
MIMAS Evolution



Future Nuclear Fuels Research

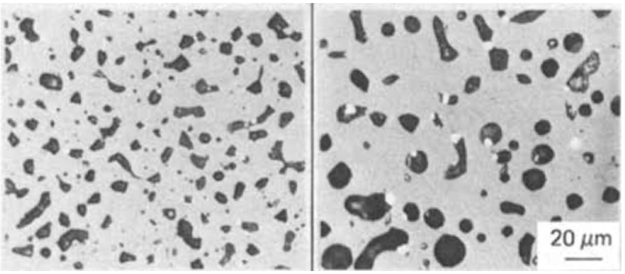
Potts – Phase Field

2-Phase Nuclear Fuel

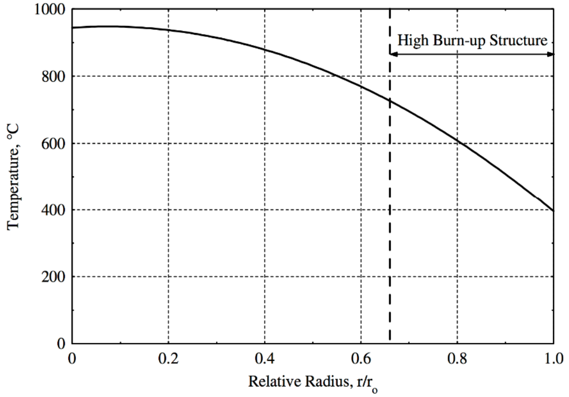


Oudinet. et. al. J. Nucl. Mat. 2008.

Void & Thermal Effects



Nabielek, et al. Nucl. Eng. & Des. 1990.



Walker. et al. J. Nucl. Mat. 2006.