A Coupled MPM - kMC Strategy for Modeling the Behavior of Gas Bubbles in the Microstructure of Nuclear Fuel Pins

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MPM Workshop – SLC-2008

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Outline

- **Define Problem (physics)**
- **Define our scope**
- **MPM & kMC**
- **Issues**
- **Future Work**

(SNL) Program Overview
Transient Behavior of Nuclear Fuels

Objectives:

1. **Determine margin to failure as function of**
   - **Fuel composition**
   - **Burn-up**
   - **Type of transient, …**
2. **Determine margin to design-based failure**
   - centerline or other melting
3. **Beyond Design Accidents**
   -How bad is bad?
   -Phenomena identification, fuel/clad motion

Failure is release of fission products

- **From fuel pin into reactor**
- **Due to clad breech by**
  - **Fuel swelling and FG release**
  - **Pressurization of clad**
  - **Low-T eutectic formation**
  - **Chemical corrosion of clad**
  - **Brittle fracture of clad**
  - **Creep rupture of clad**
  - **…**

Need to understand and predict fuel performance under transients to ensure safety by design.

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Characterizing Transient Behavior of Nuclear Fuels Experimental and Numerical Component

<u>Basic question</u>: How will TRU fuels perform under transients in a FBR?

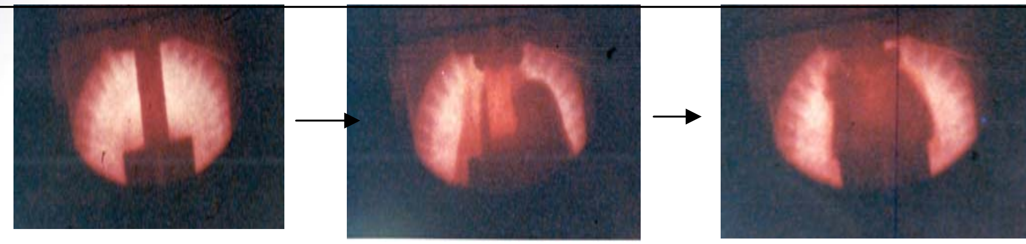
<u>Experiments will be designed to</u>
- **interrogate multiscale TRU fuel behavior and characterize difference from LWR fuels**
- **recognize and characterize conditions to failure**
- **develop models**
- **validate simulations**

<u>Simulations will be used to</u>
- **design experiments (using models developed from known behavior)**
- **incorporate understanding obtained from experiments**
- **extend predictive capability into regimes where limited or no experiments can be performed**
- **Identify critical experiments, design better fuels sysmtems**

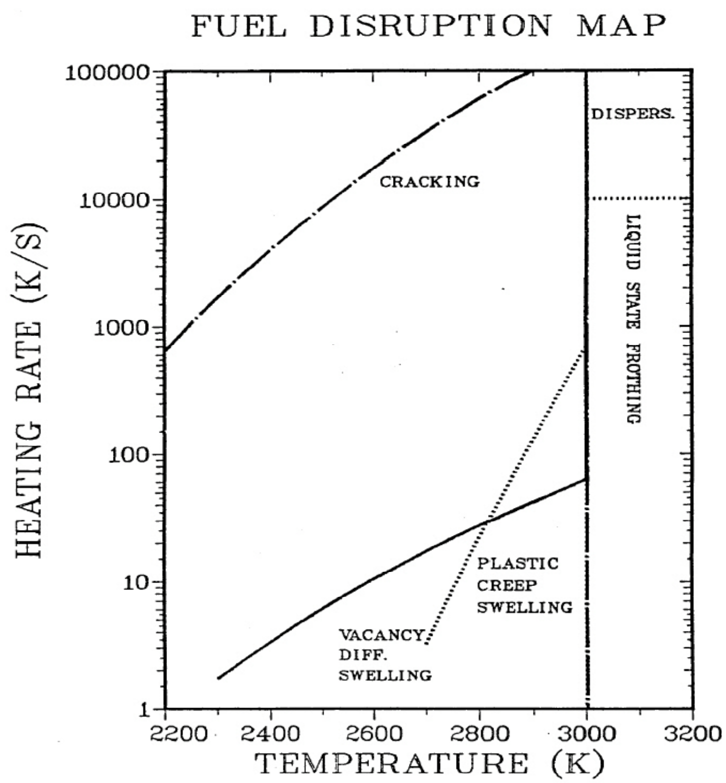
Experiments, theory, model development and simulations will be integrated tightly to develop predictive capability.

SNL – ACRR Reactor Experiments (MOX)

(Steve Wright, et. al.)

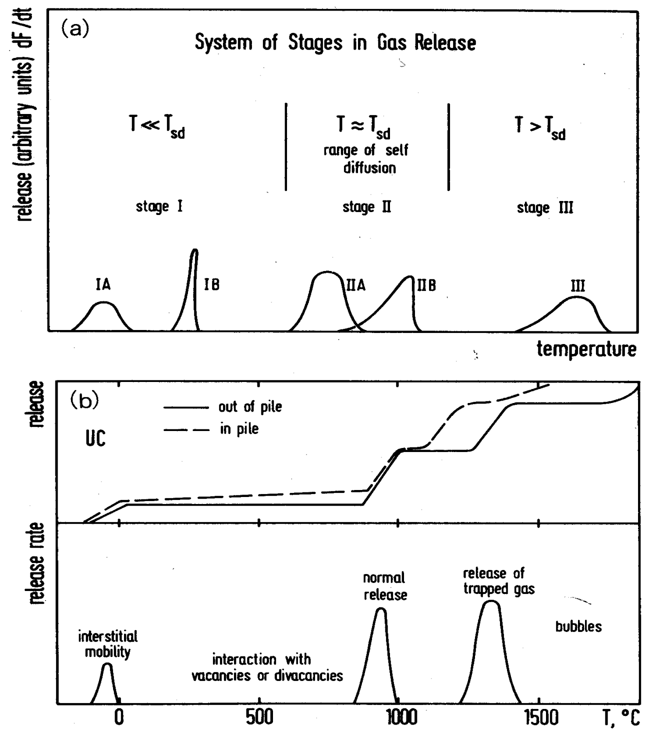


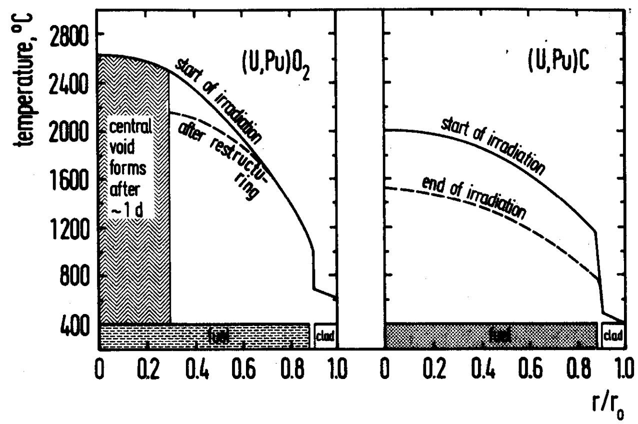
Pin heatup, clad melt and FP release, and fuel disruption sequence in LMFBR high burnup fuel pin (FD Program - PNC, UKAEA, KFK, NRC)



- Large difference between fresh and burned fuel transient response
- Why?
- Need for coupled in-pile & separate effects experiments and modeling/simulation to understand.

Hypothesis: Is the higher stored fission gas inventory for burned fuel released quickly during a temperature excursion?

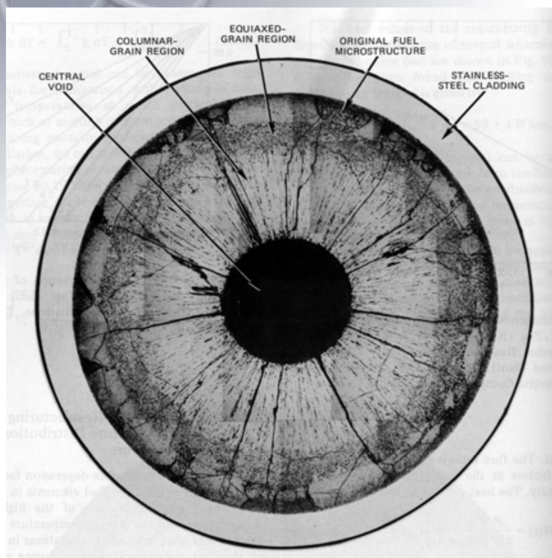




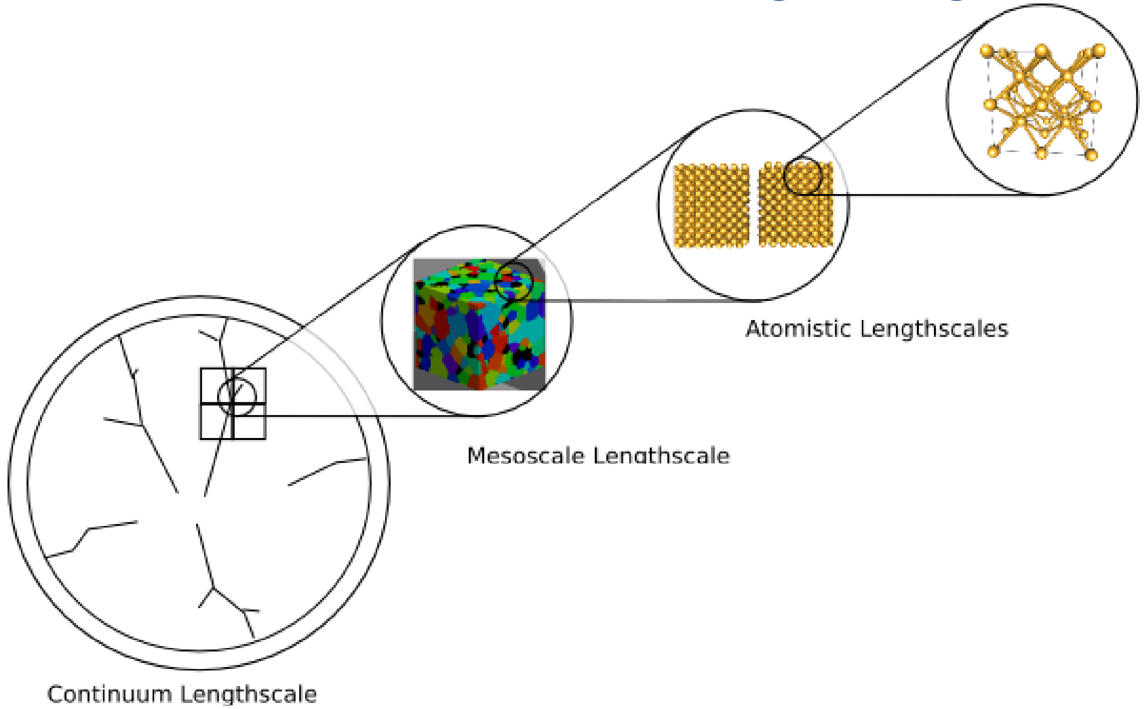
Figures from: Hj. Matzke, Science of Advanced LMFBR Fuels

- obtain equivalent results for all proposed TRU fuels (MOX and metals)?
- How to verify/disprove? (transient simulations vs fuel performance modeling)

TRU Fuels Modeling Ranges



From: D. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements

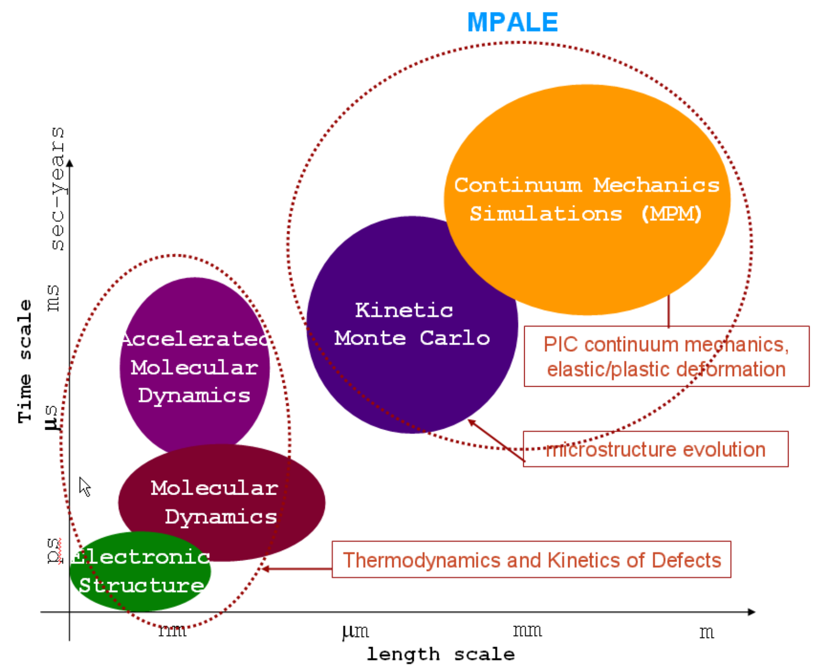


- **Fuel pins are complex coupled systems which become more complex with burnup**
- **Little data available for TRU fuels**
- **Mesoscale modeling: computational investigation of phenomena characterized by coupled interactions involving many thousands to millions of atoms**
  - **nanoseconds to microseconds time scales**
  - **bubble transport (intragrain to grain boundaries)**
  - **failure phenomena: crack and dislocation dynamics**

Current Strategy

Goal: To develop a validated, predictive capability to simulate the mechanical response, to failure, of a TRU fuel pin (i.e. fuel & clad) by fuel swelling, cracking, and creep during a transient event.

Strategy: Directly couple, using time splitting, a kMC model for microscale features and transport with a Material Point Method (MPM) continuum model for the stress fields and deformations and perform V&V using existing experimental data and/or bridging information from atomic scale simulations.



Coupled Approach

MPM

- self-consistent stress & thermal fields
- PIC approach
- quasi-static
- use velocity update instead of acceleration
  - increased damping
  - simplify implicit algorithm

kMC (kinetic Monte Carlo)

- MC grain restructuring
  - Potts – Glauber
  - single particle change/flip
  - dual 2 color approach for mpp
    - particles & cells
- MC “bubble” transport and growth
  - Potts – Kawasaki
  - pair exhange
  - mpp issues – 7 color?

$$\tau_{kMC} > \tau_{MPM} \quad \text{or} \quad \Delta t_{kMC} > \Delta t_{MPM}$$

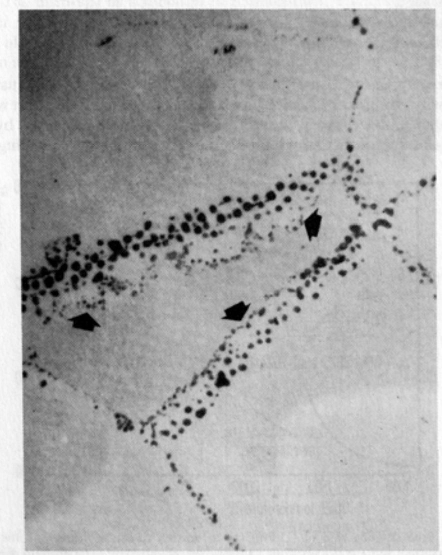


Fig. 9.40. Sweeping of bubbles in UC by moving grain boundaries [152].

§ 9.3. Fission gas diffusion and release 471

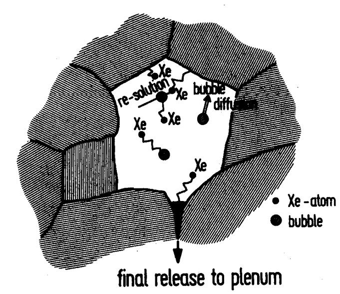


Fig. 9.4. Sequence of events in the creation of fission gas (Xe) within a grain of the MX structure and subsequent release by gas atom diffusion, precipitation in gas-filled bubbles, re-solution and/or bubble diffusion and finally venting of grain boundary bubbles along channels or cracks connected with the gap and thus with the plenum.

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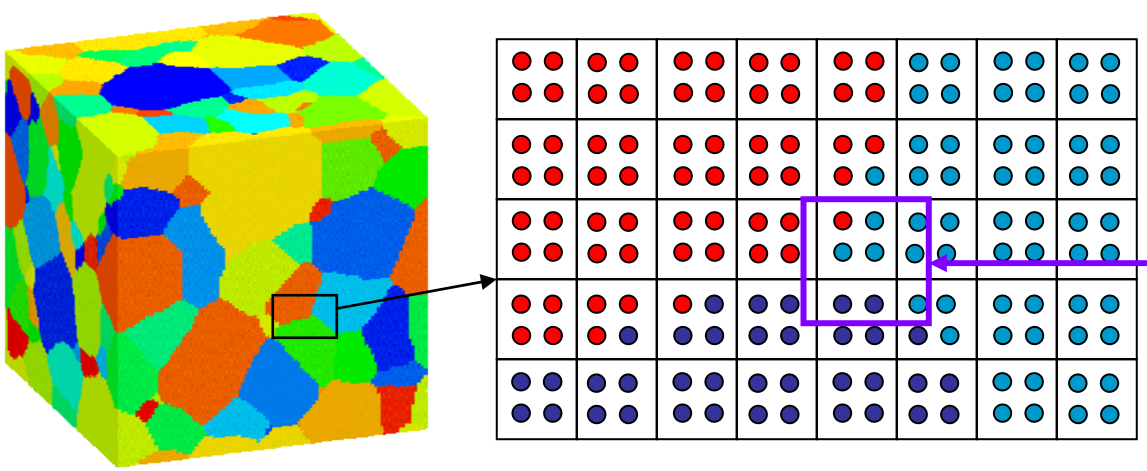
MPALE

- **Continuum Mechanics**
  - stress and temperature fields
  - modified MPM algorithm (PIC & FEM)

- **Discrete Physics (major unknowns)**
  - grain restructuring
  - pore and bubble transport
  - Potts Models (probabilistic transport)

* Particles contain information about crystallographic orientation, as well as mechanical state.



-Determine particle free energies based on elastic strain energy (at individual particle) and surface energy (from particle neighborhood)

-MC decision algorithm

MPALE: Discretize space using material points

- **material point:**
  - representative volume/mass
  - single material type (material, grain orientation, etc)
  - ‘solution’ resides at material points NOT grid
    - *mass, momentum, energy, stress tensor, etc*
- **gas bubble**
  - 0.01 to 0.1 micron radius
  - different transport issues:
    - *small bubbles: thermal diffusion dominates (Soret effect)*

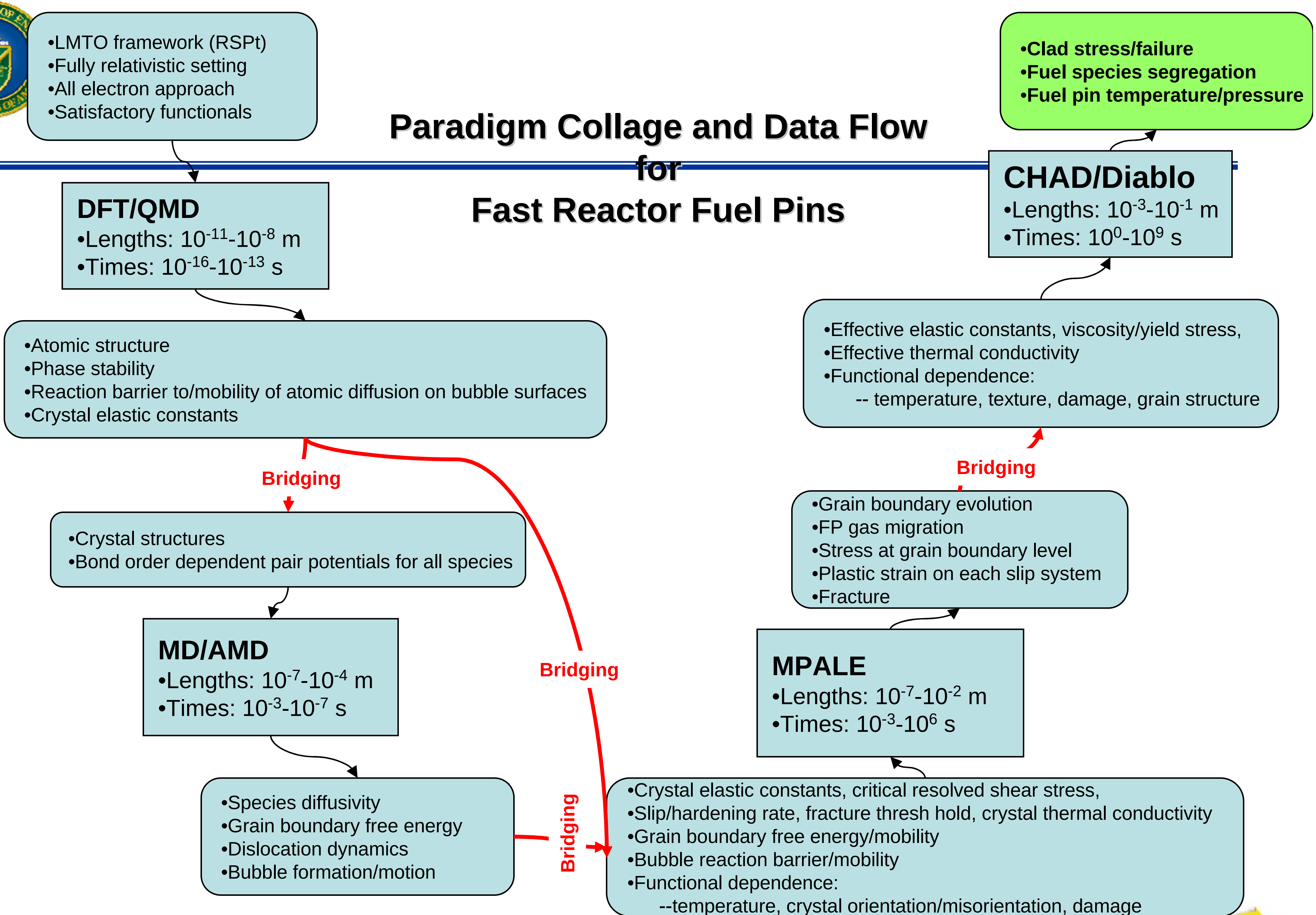
$$F_b = \left(\frac{2\pi R^3}{a_o^3}\right)\frac{Q^*}{T}\left(\frac{dT}{dx}\right)$$

    - *interaction with grain boundaries and defects (pores)*
  - limit MPM material point to micro-bubble size
    - *large bubble composed of many micro-bubbles*

kMC/MPM : MPALE

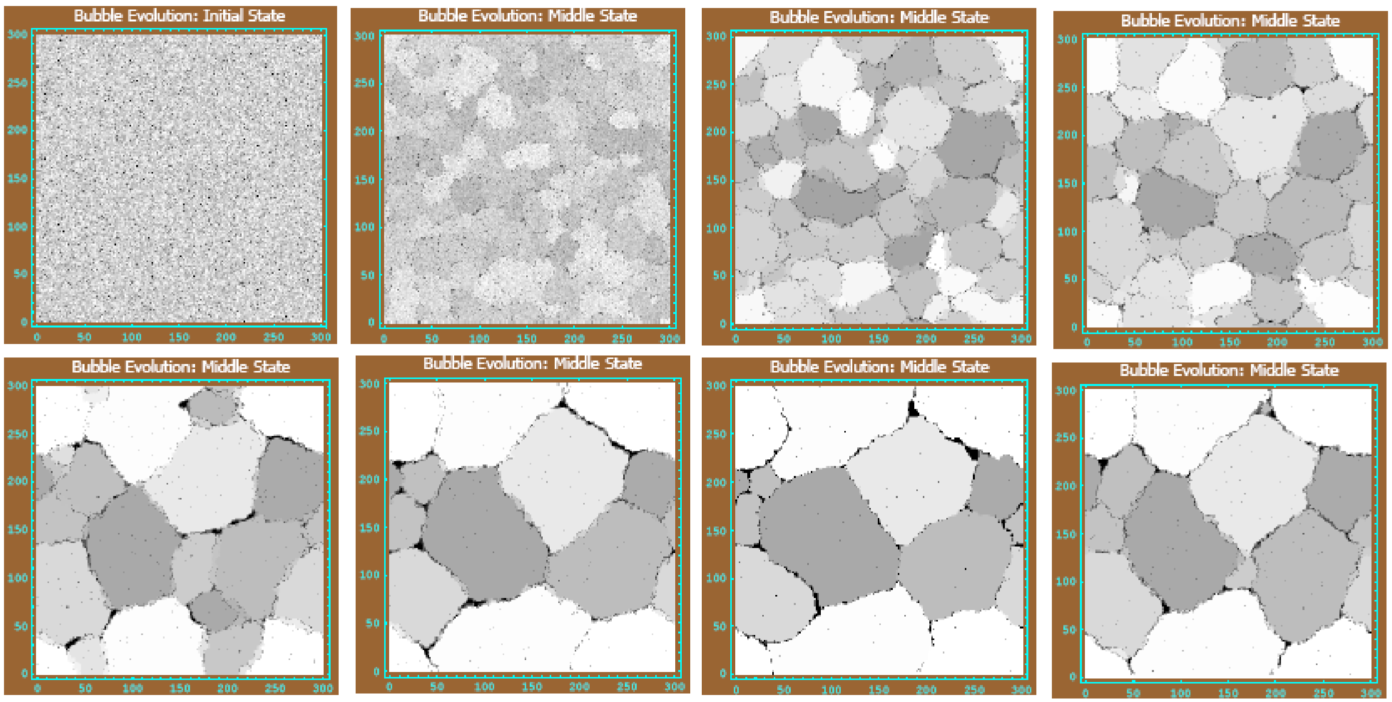
- **Direct coupling in a time split algorithm**
  - kMC: all particles are candidate kMC particles
    - multiple Potts Models
    - grain or texture evolution
    - single micro-bubble transport (‘diffusion’)
  - MPM: all particles are candidate MPM particles
    - boundary conditions
    - stress & thermal field
    - mechanical response
- **Issues:**
  - time steps
    - kMC (physical based – *reaction* rates)
      - material transport – calibration studies
    - MPM – fraction of CFL
      - wave speed (stress field)
  - current problems of interest: $\Delta t_{MPM} << \Delta t_{KMC}$

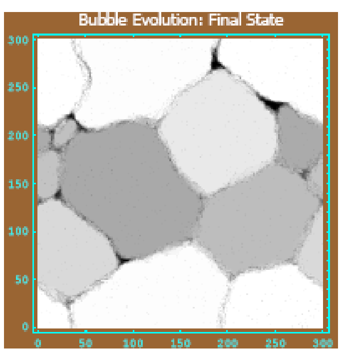
Paradigm Collage and Data Flow for Fast Reactor Fuel Pins



Bubble Transport (preliminary)

- Coupled bubble motion and grain evolution (no stress field)





10 averaged

```
!INPUT PARAMETERS FOR PLANAR EVOLUTION OF A RANDOM TEXTURE EVOLUTION: JUNE 2007
 PARAMETER (ITOT  = 300, JTOT = 300, NTOT = ITOT*JTOT)
 PARAMETER (NQMAX = 90)
 PARAMETER (B     = 0.0D0)
 PARAMETER (RJ    = 1.0)
 PARAMETER (TEMP  = 0.6)
 PARAMETER (SCALETIME = 1.0)
 PARAMETER (MTOT      = 160000)
 PARAMETER (GASFRAC   = 0.02)
 PARAMETER (GASFACTOR = 0.4)
 PARAMETER (INEUMANN  = 0)

!DATA OUTPUT PARAMETERS
 PARAMETER (NUMWRITES = 100)

MFREEZE = MTOT/4

DO 10 M = 1, MTOT

 IF(M.LT.MFREEZE) THEN
  GASFREQ = 0.25
 ELSE
  GASFREQ = 0.75
 ENDIF
```

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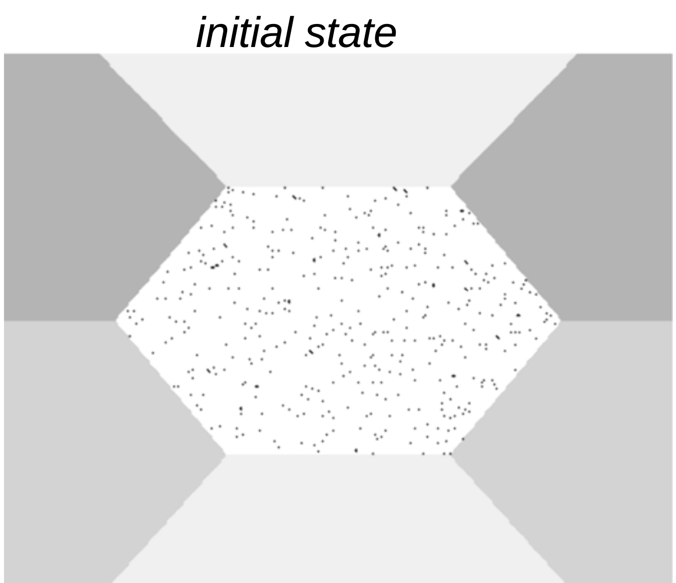
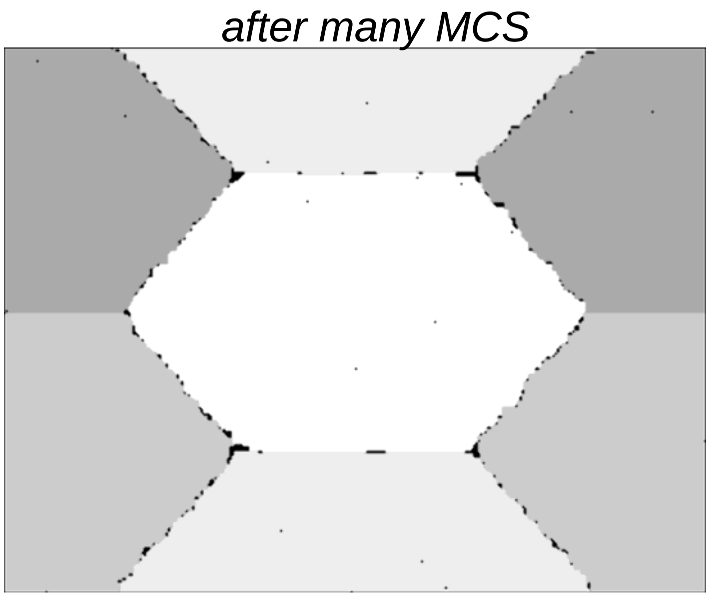
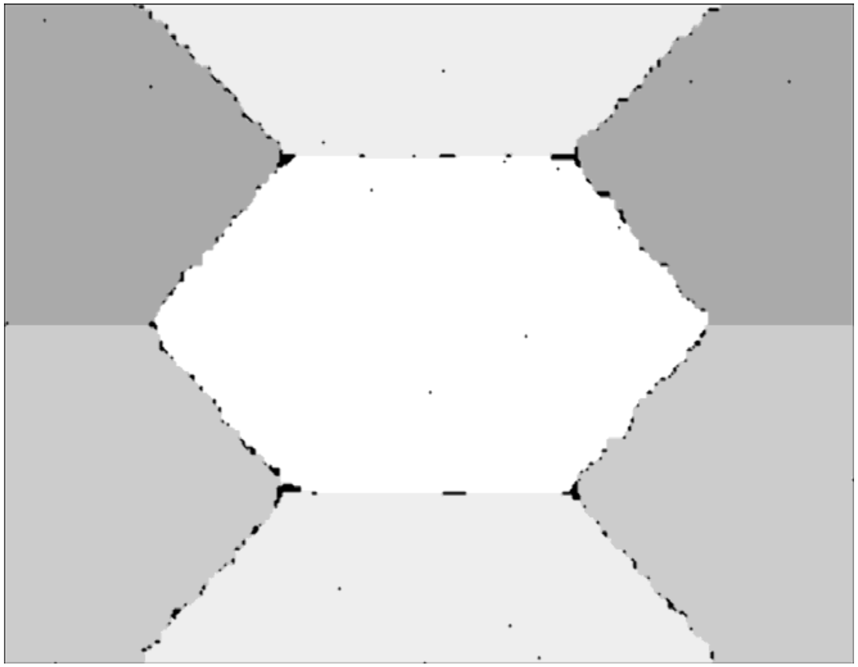
MPALE Simulation: Micro-bubble Transport (Potts)



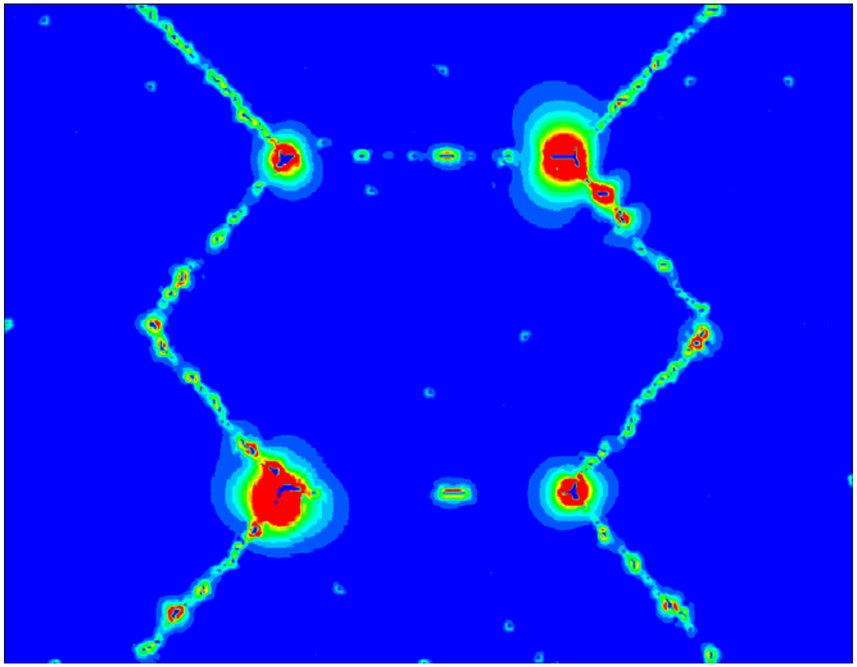


- **micro-bubble transport using Potts algorithm**
  - material point represents a micro-bubble
  - no coupled stresses or temperature gradient
- **larger bubbles formed along grain boundaries and triple junctions**

MPALE Simulation: Gas/Solid Stresses (MPM)



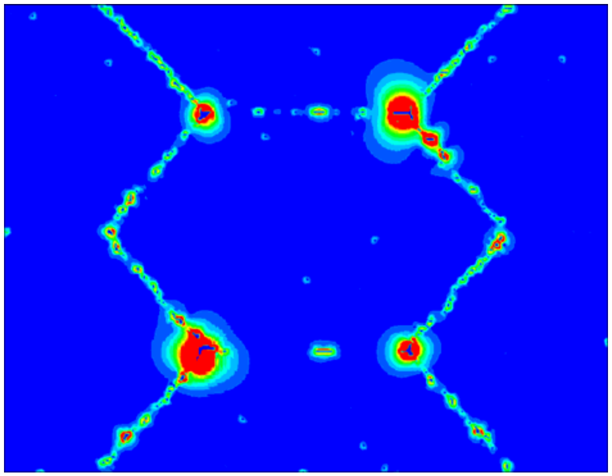
bubble distribution by kMC transport –
<u>no coupled stress field</u>

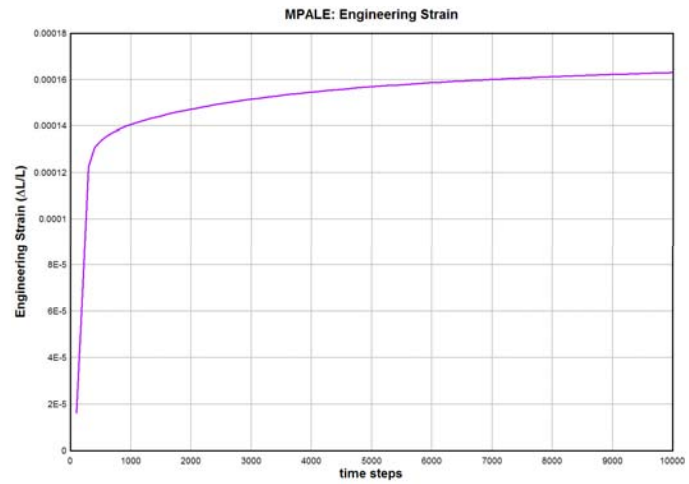


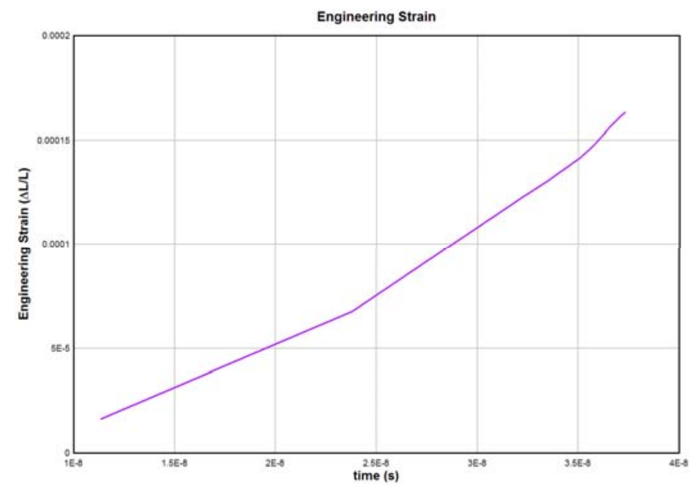
von Mises stress for rapid gas bubble pressurization (transient response) –
<u>no bubble motion</u>

direct coupling of kMC & MPM requires implicit solver

MPALE Simulation: Gas/Solid Stresses (MPM)







- **free surface boundary conditions on domain**
- **computed swelling (engineering strain)**

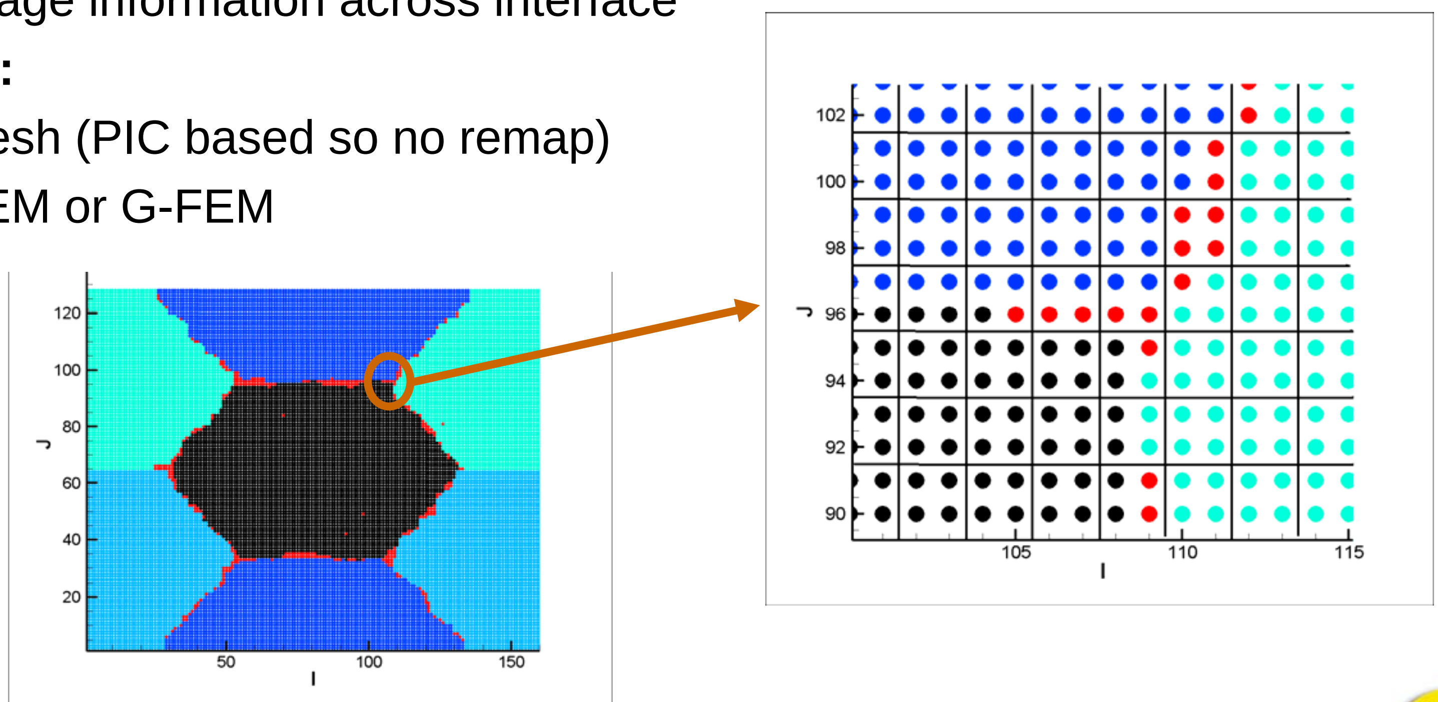
Challenges

- **Implicit Time Integration**
  - transient times 5 – 10 s
  - explicit time step ~ 10^{-7} or 10^{-8} s
  - MPALE – looks like a lagrangian FE code
    - *straightforward to make implicit (Aztec solver package)*
    - *2 state approach for MC Plasticity model*
      - multiple slip planes

- **Interface (grain boundary & bubble) resolution**
  - normal interface stress discontinuity
  - cracks
  - cracks contain fission gas (hydrostatic pressure); cannot treat simply as a stress/material discontinuity

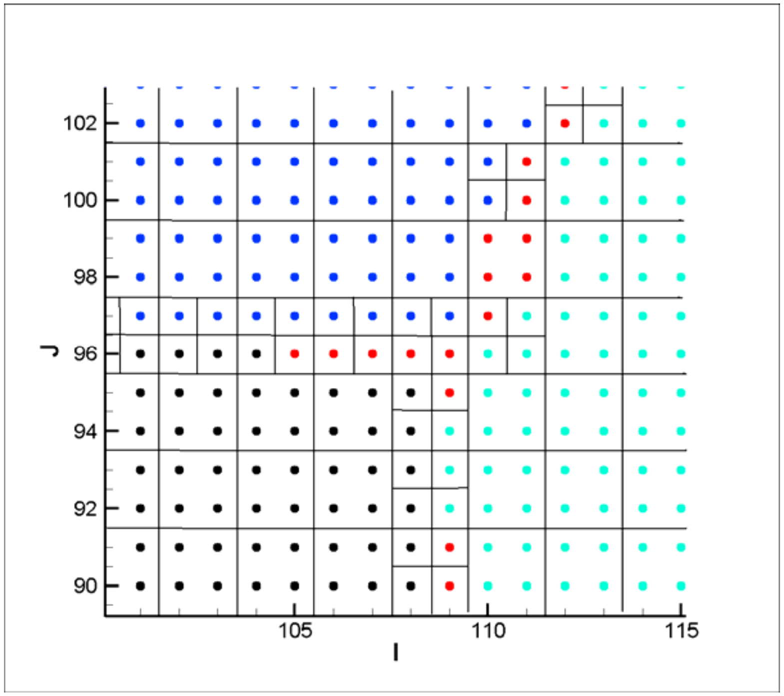
MPALE: Interface resolution issue (PIC issue)

- **Issue: need to increase intracell resolution to resolve stress jump at grain boundary or solid/bubble interface**
- **MPALE ‘naturally’ captures interface (PIC method)**
- **MPALE uses std. linear FEM shape functions**
  - average information across interface
- **Options:**
  - remesh (PIC based so no remap)
  - X-FEM or G-FEM

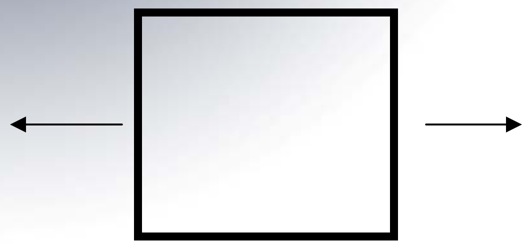


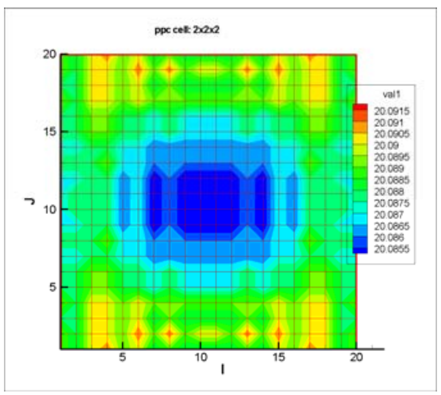
Proposed Interface Resolution Strategy: Dynamic Adaption of Uniform Mesh

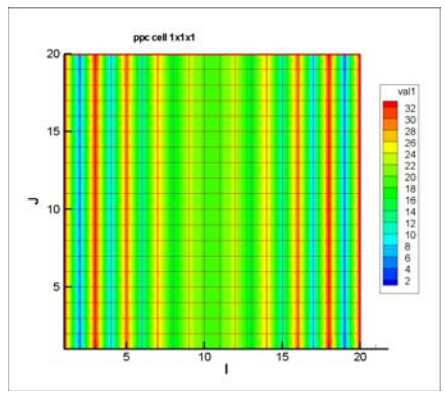
- **determine mesh cell with interface**
  - multiple material point types
- **subdivide mesh cell into a uniform sub-mesh with 1 material point per cell**
  - original material points
  - NO remap interpolation
  - maintains nodal structure for implicit scheme
  - hanging nodes require small deformations
- **tested with 1D MPM code**
  - multi-dimensional issues to address
- **enable crack propagation**
- **maintains the particle lattice connectivity of kMC algorithm**
- **MPM: meshless (arbitrary mesh) method**

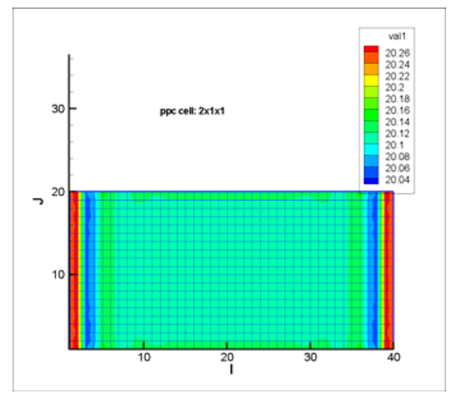


gedanken problem:
constant traction, linear elastic (γ=.15), lagrangian mesh
contours of σ_{xx} – <u>particles</u> not grid









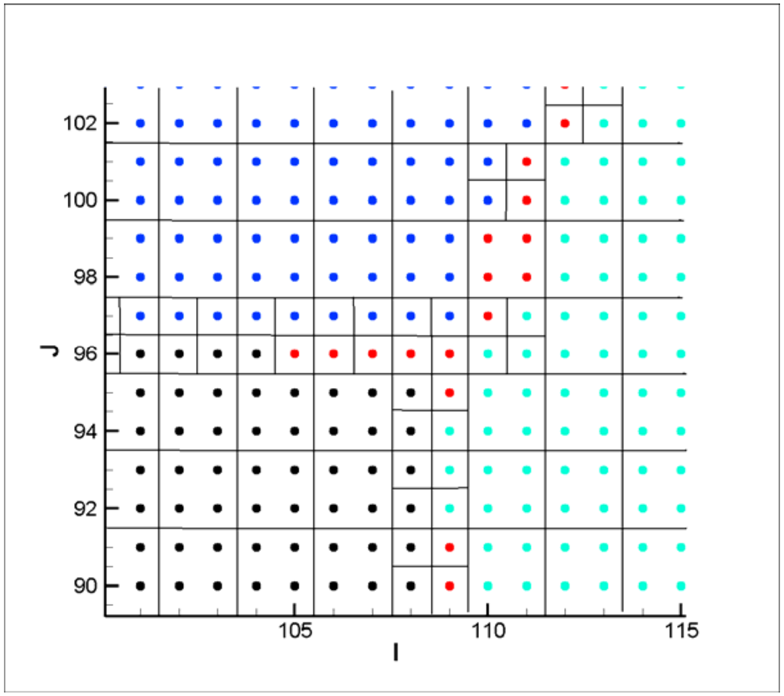
2x2x2 ppc, 10x10x10 mesh, engr. strain ~ theoretical value

1x1x1 ppc, 20x20x20 mesh

2x1x1 ppc, 20x20x20 mesh

multi-grid mesh

- map and re-map an issue with 1ppc (compare to single integration pt FEM)
- consider using lagrangian FEM for single ppc mesh ??
- V&V with body fitted FEM solution



V&V FEM Triple Junction Soln.

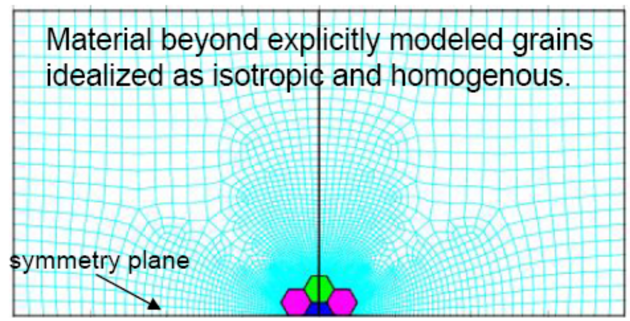
Initial FEA model being used to analyze triple junctions

- Model used to determine junction stress intensity factors and region of dominance.
- Expect stress intensities to differ at junctions A, B, C, and D (no material symmetry).
- Can uniformly scale geometry to examine size effect.
- Can perturb positions of junctions A, B, (C, D) to look at variations in crystal sizes and orientations.
- Can run calculation using polycrystalline plasticity to investigate effect of a singular junction stress state.
- Plane strain calculations.

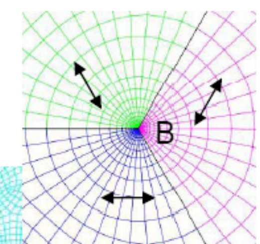
Some notable previous work:

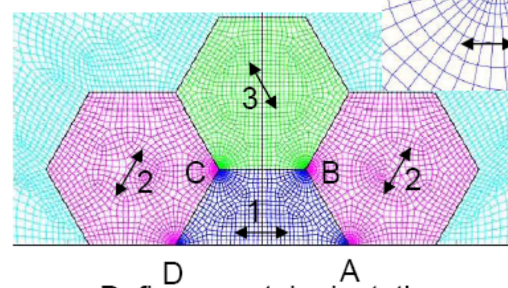
1. R. C. Picu, and V. Gupta: JAM 63, p295 (1996).
2. V. Tvergaard, and J. W. Hutchinson: J Am Ceram Soc 71, p157 (1988).

This previous work only considered certain special cases and did not determine stress intensity factors, region of dominance, alignment with slip planes, etc.



21 logarithmically spaced rings surrounding triple points A, B, C, and D (radius of adjacent rings differ by a factor of 1.33).





⟷ Defines crystal orientation (crystal orientation 3 = -crystal orientation 2, and orientation 1 = 0 degs, measured counter clockwise from horizontal)

Conclusions

- **Algorithmic issues**
  - **implicit time intergration**
  - **mesh (gradient) refinement**
    - **cracks??**
- **Material Physics**
  - **subscale physics by MD/AMD**
  - **Bubble transport in a combined thermal and stress field????**

- **Is MPM with kMC a good strategy for fuels problem?**
  - **Consider lagrangian FEM with superimposed material points**