A geometric approach to stochastically modeling fatigue crack propagation at the microstructural length scale

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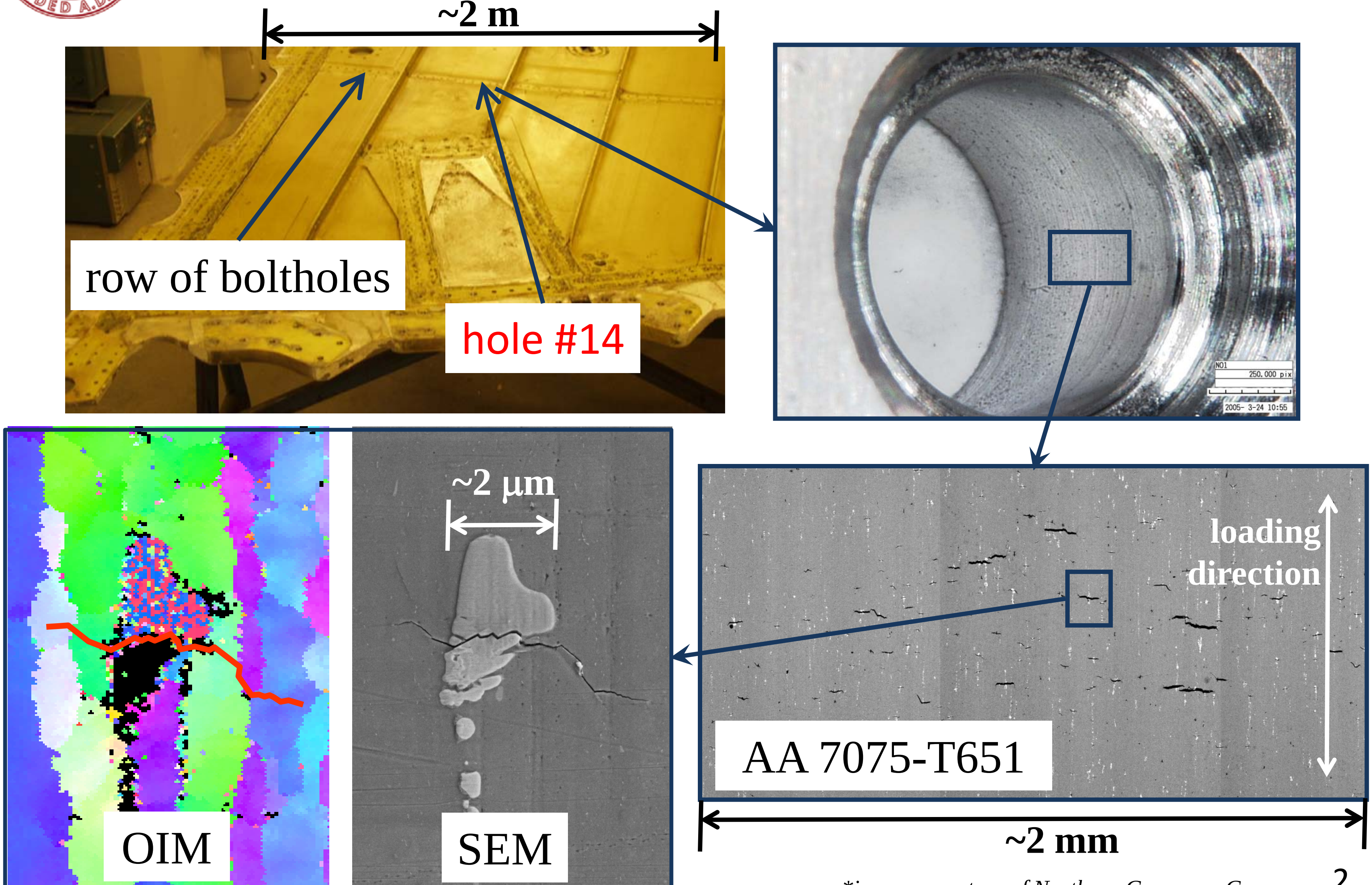
Need for probabilistic da/dN predictions accounting for inherently stochastic processes at the μscale



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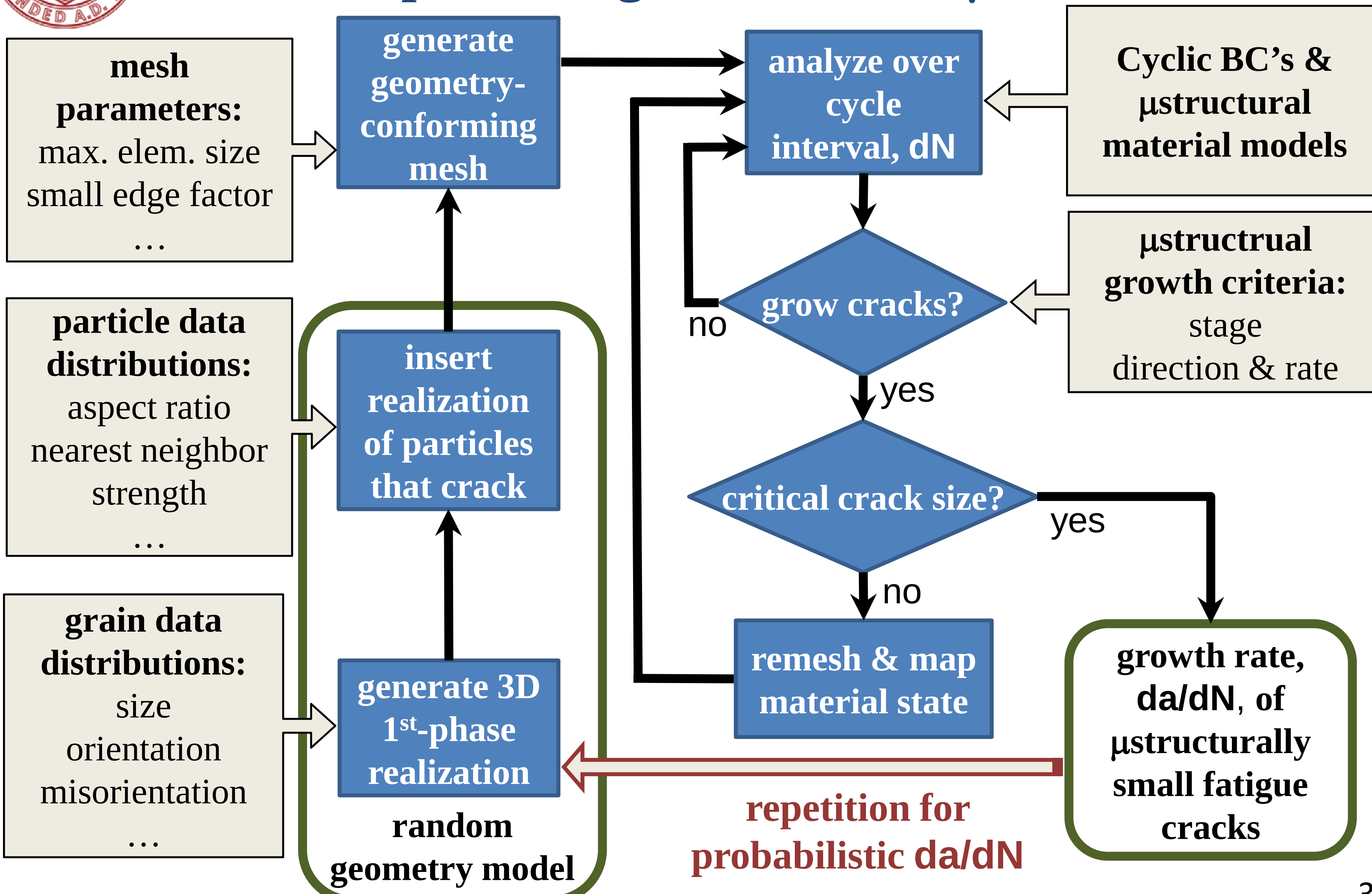
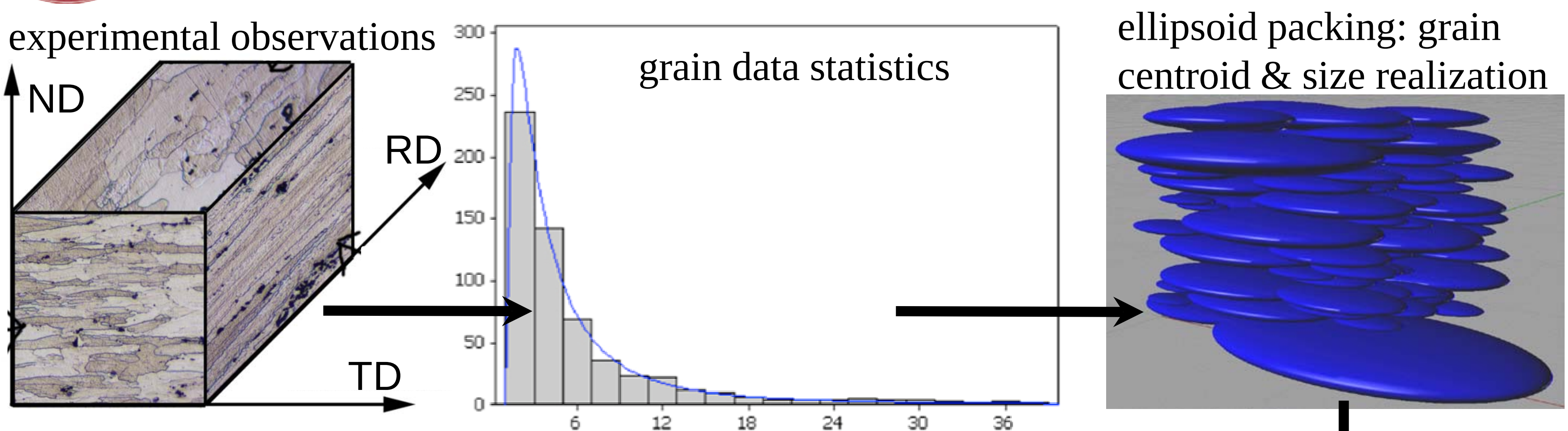
Geometric approach to probabilistically predicting da/dN at the µscale



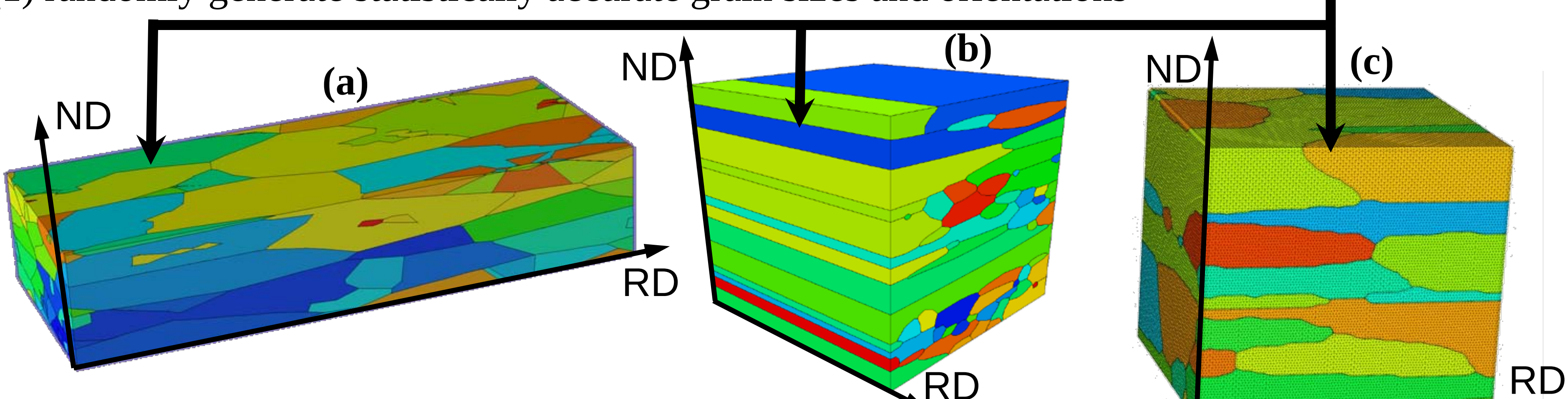
Presentation outline

I. Microstructure geometry modeling
   A. First-phase realizations
   B. Two-phase realizations
   C. Automated microstructure meshing
   D. Microstructurally small fatigue cracks (MSFC’s)
      1. Explicit geometry representation
      2. Material state mapping
II. MSFC propagation simulation
   A. MSFC propagation terminology
   B. Intragranular propagation
      1. Direction criteria: Stage I and Stage II
      2. Rate criterion
III. Ongoing work & conclusions

First-phase realizations



(1) randomly generate statistically accurate grain sizes and orientations*



(2) digitally replicate morphology*: (a) Voronoi and stretch, (b) snap-to-grid and extrusion, or (c) voxellation and marching cubes

*in collaboration with Rollett, Lee and Sintay, CMU

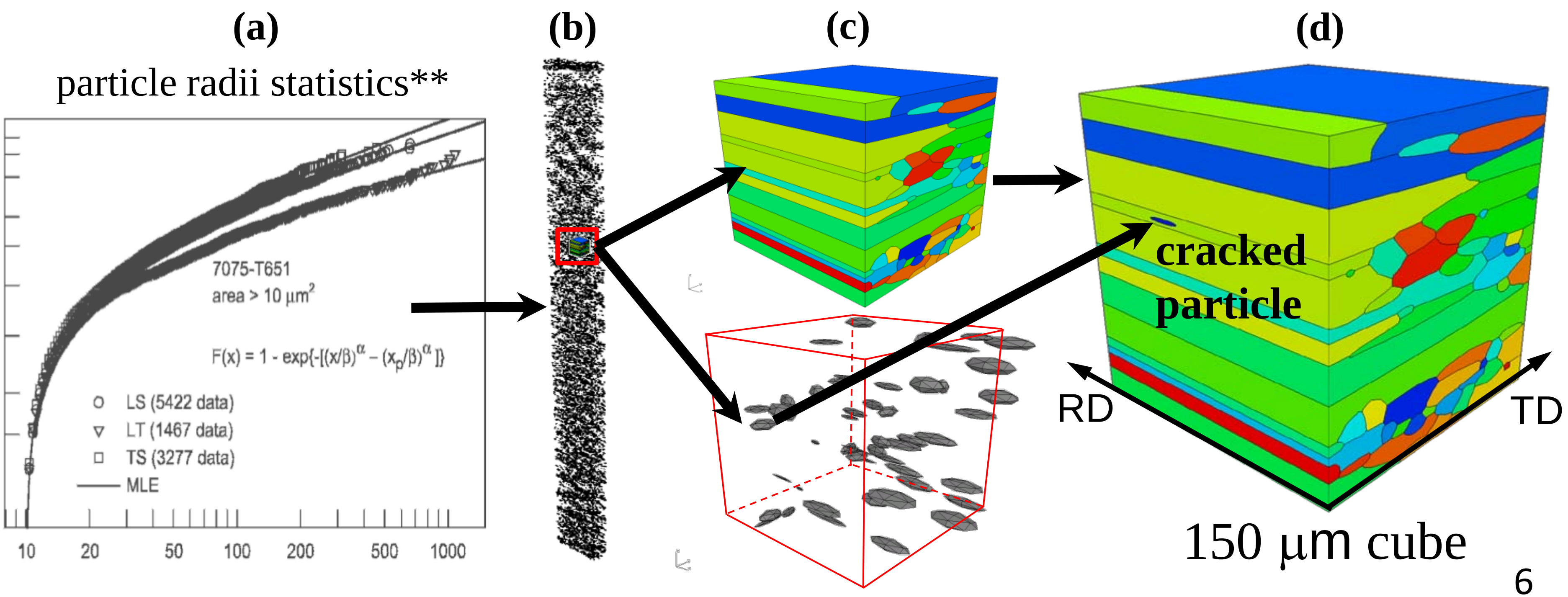
Two-phase realizations

(a) Collect particle statistical data from microstructure observations

(b) Generate particle location & size realization, ~10,000 particles/realization, and randomly place first-phase realization inside

(c) Keep only particles intersecting first-phase realization

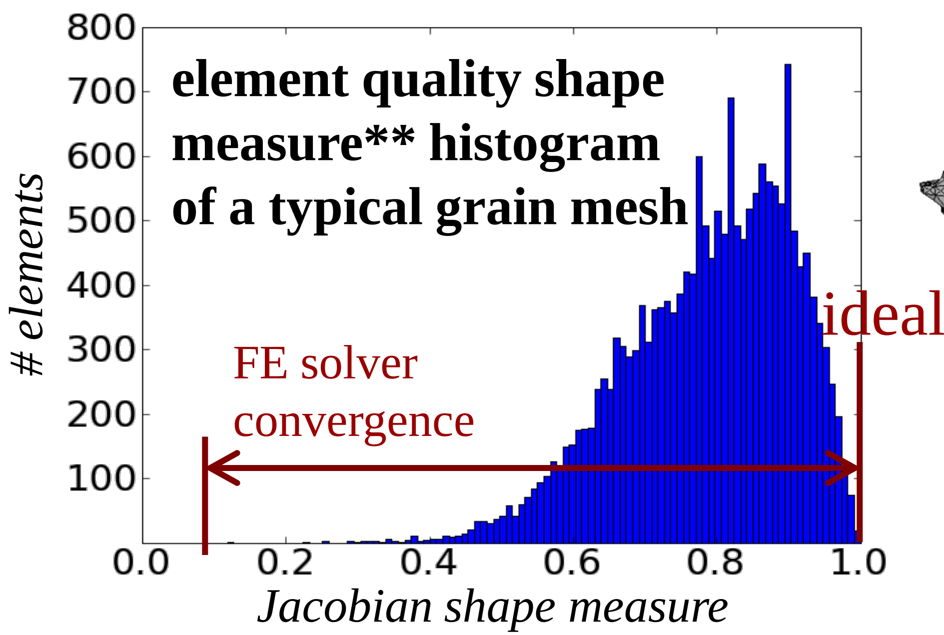
(d) Filter & insert particles that crack
- fracture mechanics-based MSFC incubation filter*
- particle inclusion algorithm for inserting particles into first-phase realization

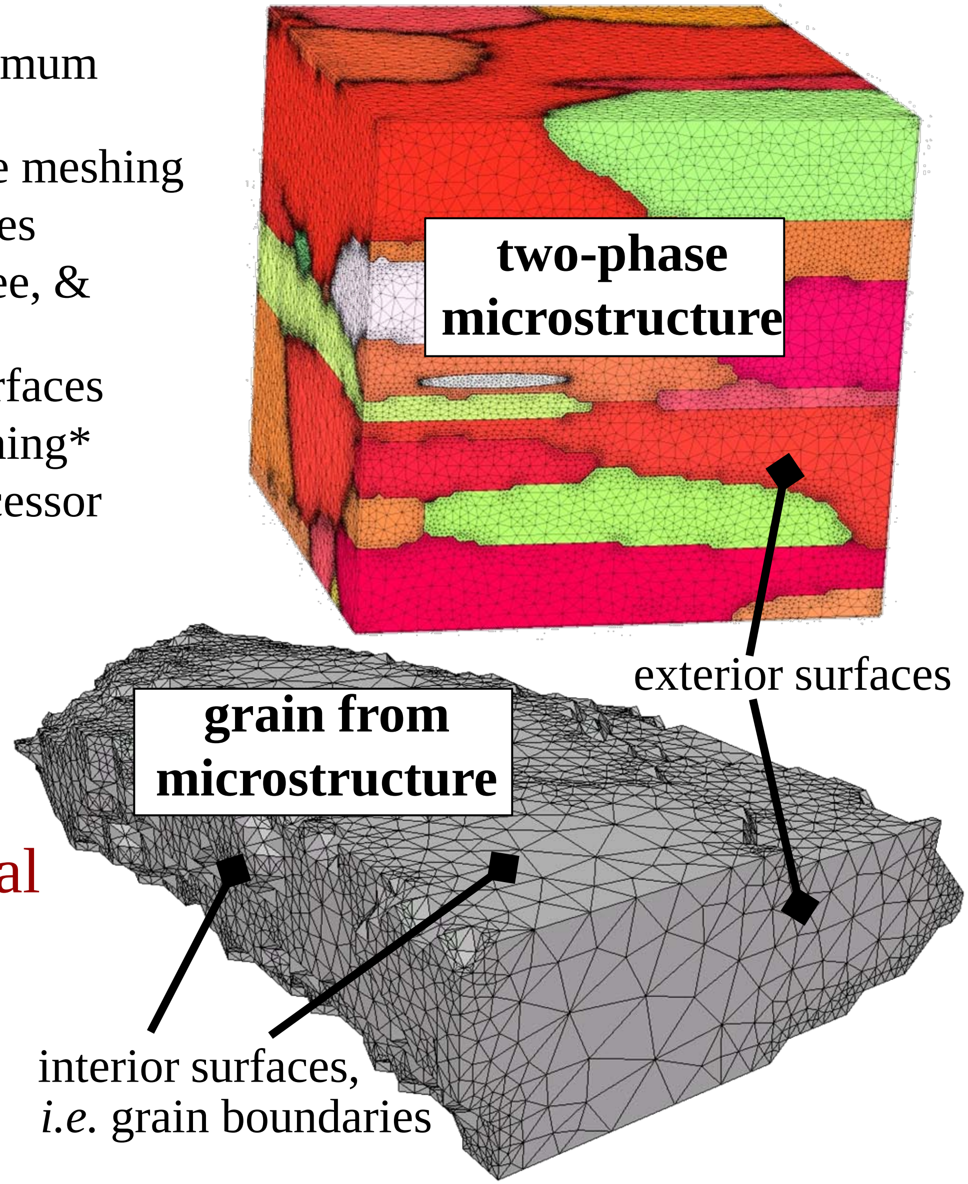


*Bozek et al., MSMSE (2008) **Harlow et al., MM Trans A (2006)

Automated microstructure meshing

- Input: 3D two-phase model, global maximum element size, & size gradation factors
- Local element size seeds assigned before meshing
  - conform to small geometrical features
  - smooth gradation via octree, quadtree, & rangetree algorithms
- Mesh conforms to exterior & interior surfaces
- Advancing front surface & volume meshing*
- Parallel volume meshing: 1+ grains/processor



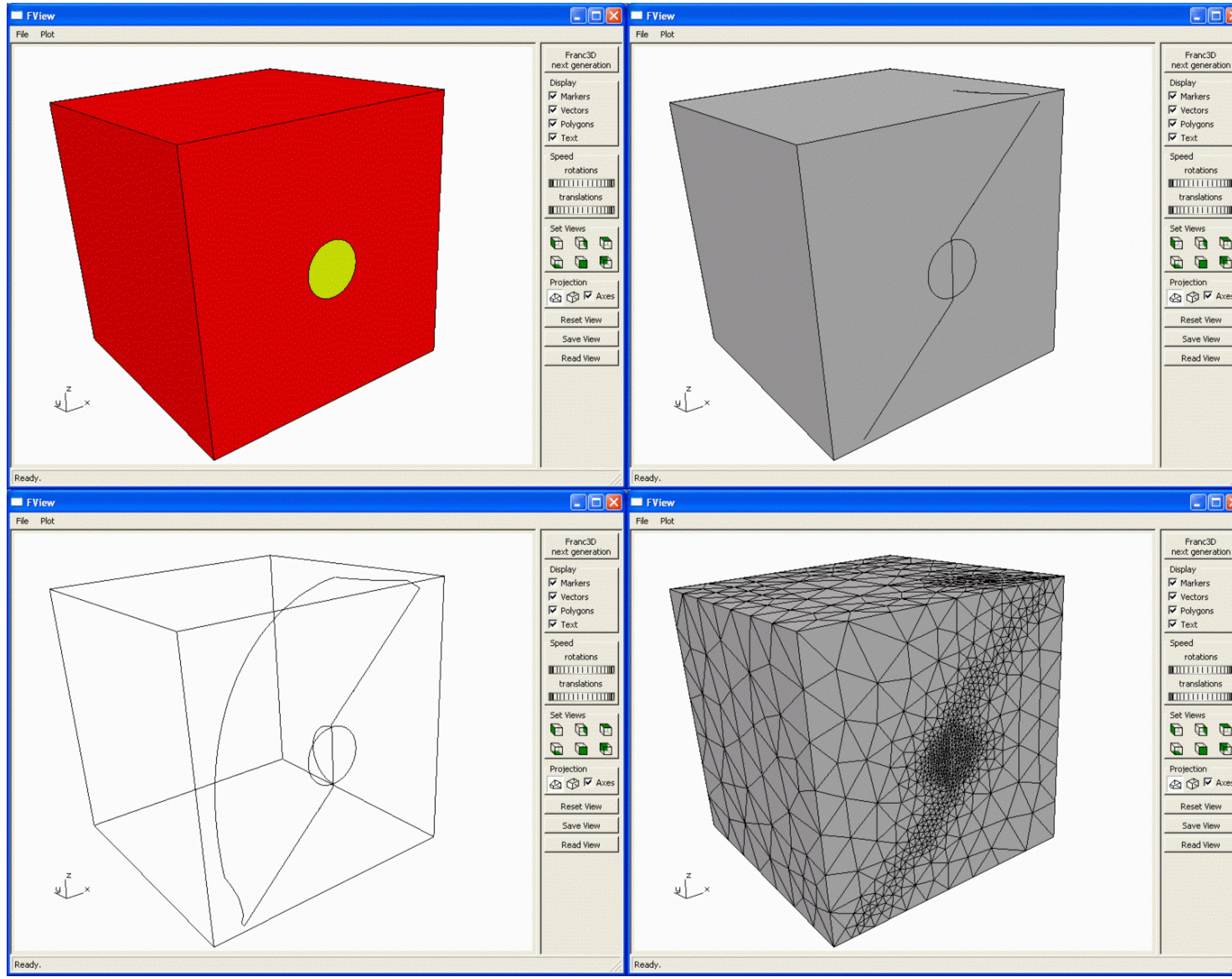


*Cavalcante-Neto et al., CNME (2005)

**Freitag and Knupp, 8th Mesh Roundtable (1999)

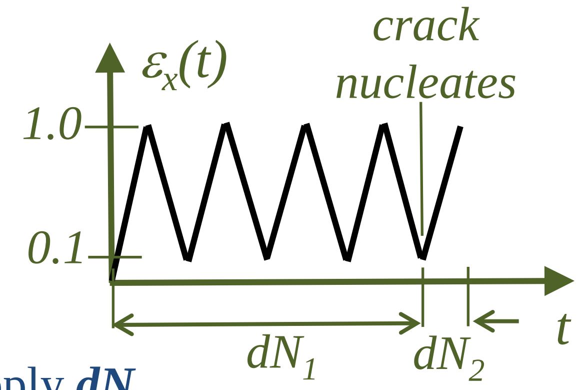
Crack insertion & propagation

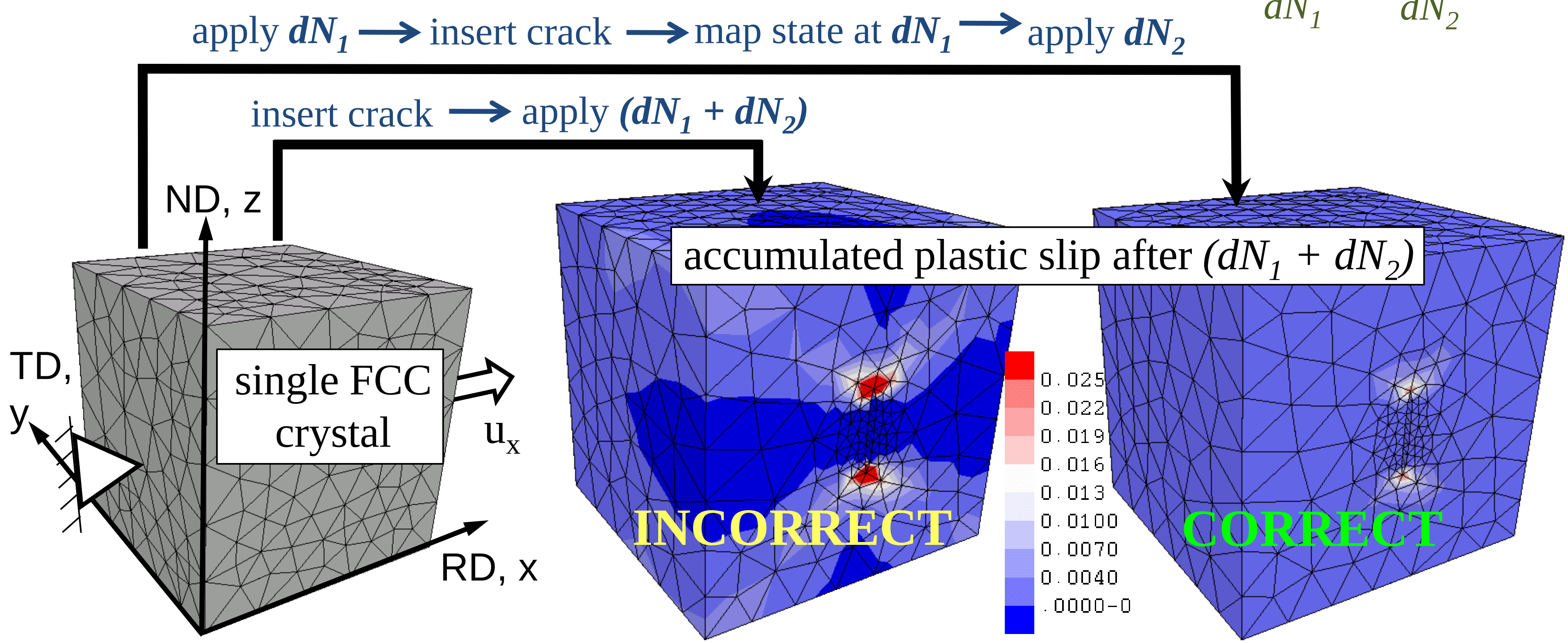
- FRANC3D/NG: arbitrarily non-planar, geometric crack representation
  - direction & rate vary along crack front
  - deflection/arrest allowed at interfaces
- Adaptive remeshing local to cracks
- Material state mapping
- Plug-compatible physics-based routines determine crack front points



Material state mapping

- Applies 3D equivalent of mapping routine from FRAN2D/L*
- Example: $u_x = 0$ on x_{min} face $u_x = L_x{*}\varepsilon_x(t)$ on x_{max} face
  $u_y = 0$ on y_{max} face $u_z = 0$ on z_{min} & z_{max} faces
  traction-free on y_{min} and crack faces





*James, KSU Ph.D. (1998)

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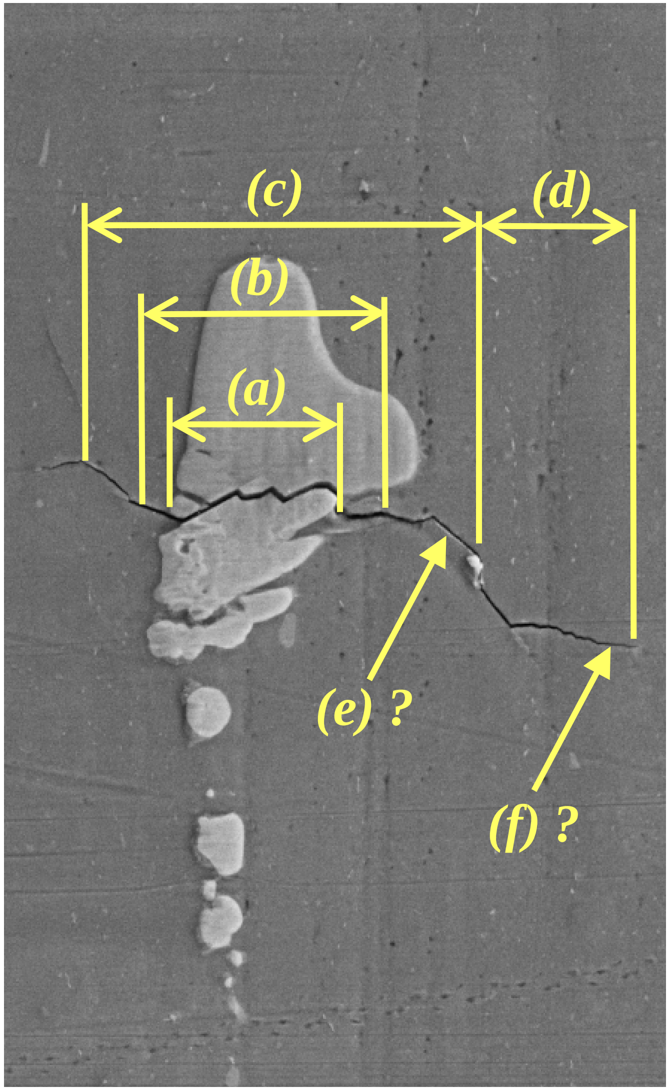
MSFC propagation terminology

- *(a) Incubation*: cracking of Fe-bearing second-phase particles
- *(b) Matrix crack nucleation*: extension from particle into neighboring grain(s)
- *(c) Intragranular propagation*: within grains, not near material interfaces
- *(d) Transgranular propagation*: near & across grain boundaries
- *(e) Stage I propagation*: slip-dominated, along crystallographic planes
- *(f) Stage II propagation*: maximum tensile stress dominated, *e.g.* mode I



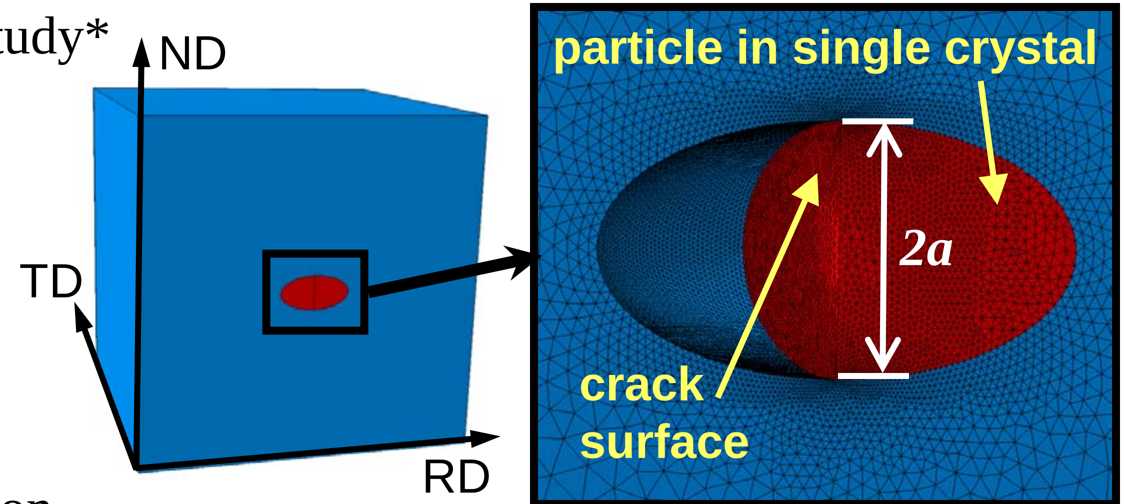
Intragranular propagation direction

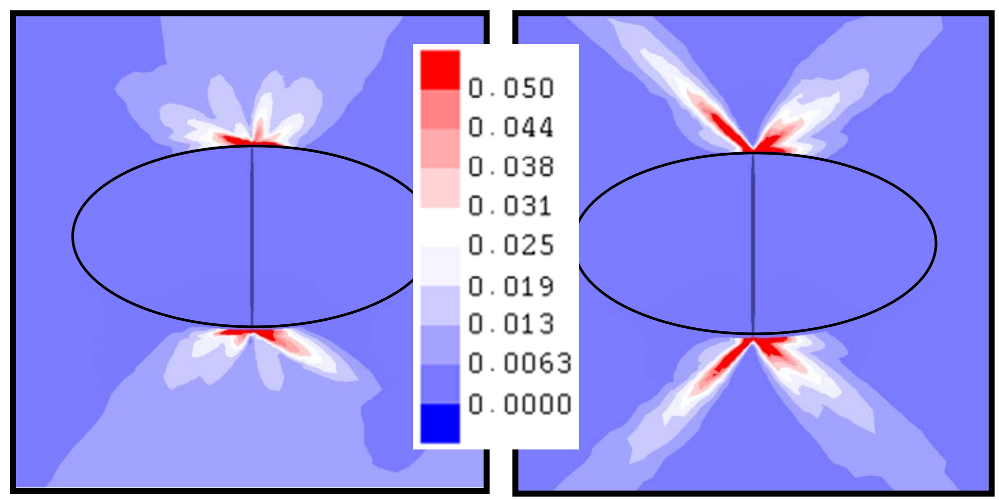
- Stage I: criteria from nucleation study*
  - direction of maximum slip-based damage, D_i, *e.g.*:

    $D_1 = max(\gamma^j)$

    where γ^j = slip on system j
    - grain orientation dependent
    - non-local D_i calculation
- Stage II: max. tensile stress criterion
- Example from nucleation study:
  - 5 cycles, $R = 0.1$, $\varepsilon_{max,RD} = 0.01$
  - convergence at $O(a/50)$ crack tip element sizes
  - orientations with 2+ high Schmid factors have higher D_i, along 2+ slip systems (right plot)

is propagation immediately Stage II?





D_1 contour plots for 2 grain orientations*

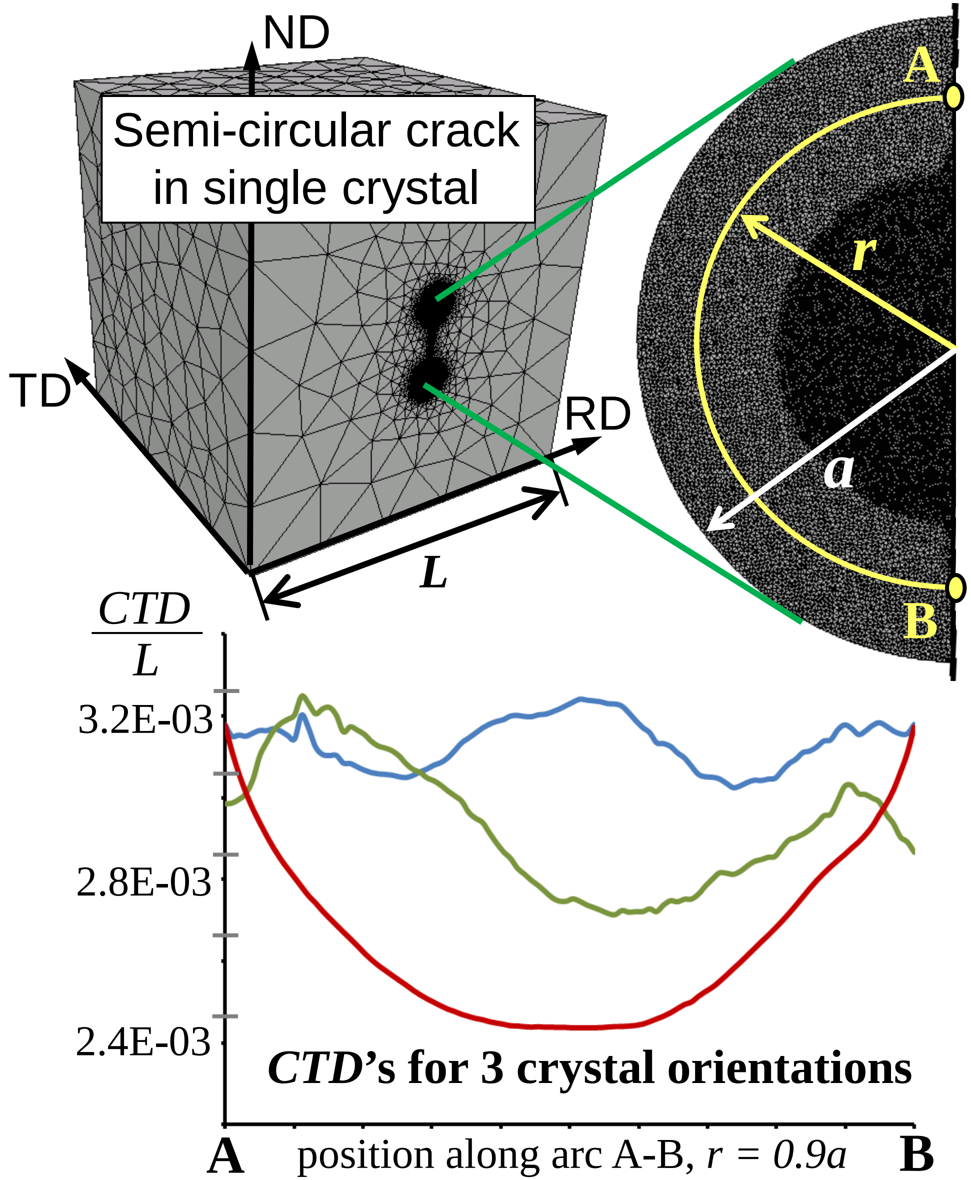
**from Hochhalter et al., MSMSE (to appear 2009)*

Intragranular propagation rate

- Crack tip displacement, *CTD*, criterion, *e.g.*:*

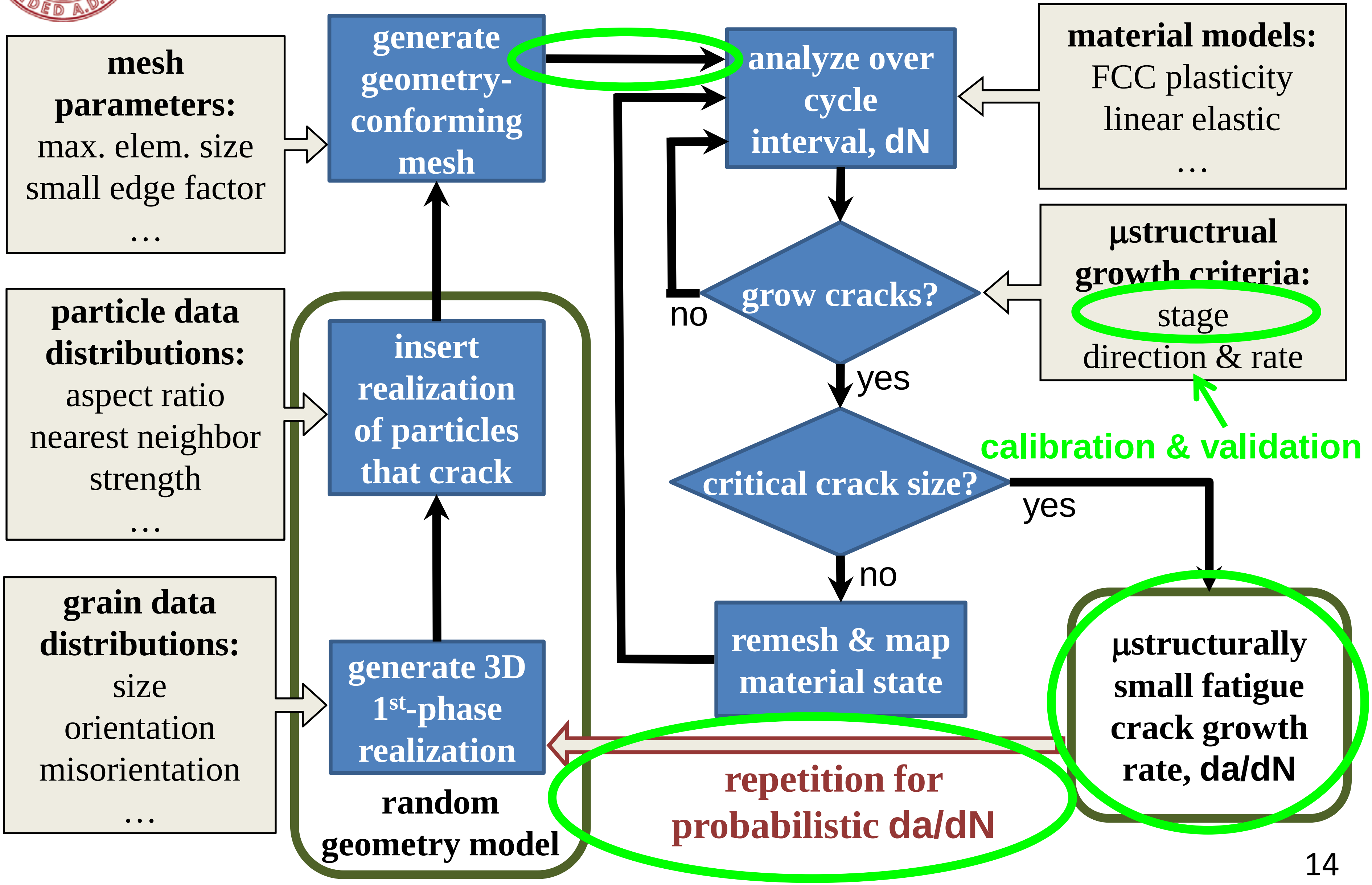
$$\frac{da}{dN} = G\left(\Delta CTD - \Delta CTD_{TH}\right)$$

  - ΔCTD_{TH} is displacement threshhold
  - *G* unknown: requires calibration
  - ΔCTD explicitly calculated
    - vector magnitude: combined opening & sliding displacements
    - measured behind crack front
- *CTD* convergence study:
  - monotonic load, $\varepsilon_{max,RD} = 0.01$
  - convergence at *O(r/50)* crack tip element sizes
  - orientation dependent
  - opening displacement $O(10^1)$ greater than sliding displacement



**Xue et al., EFM (2007)*

Ongoing work



Conclusions

Introduced and developed significant components of a geometric approach to stochastically modeling fatigue crack propagation at the microstructural length scale

- Microstructure geometry modeling
  - algorithms for generating two-phase realizations
    - statistically representative of microstructural observations
    - contain only particles predicted to crack from fracture mechanics criteria
  - fully automated procedure for generating geometry-conforming meshes
  - crack insertion/propagation w/ adaptive remeshing & material state mapping
- Simulation of microstructurally small fatigue crack propagation
  - criteria implemented for intragranular crack growth direction and rate
    - slip-based damage metrics for direction and *ΔCTD* for rate are non-locally calculated
    - FE convergence requires crack tip element sizes *O(a/50)*
    - all criteria show significant grain orientation dependence

Acknowledgements

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