Towards mechanism-based simulation of impact damage using exascale computing

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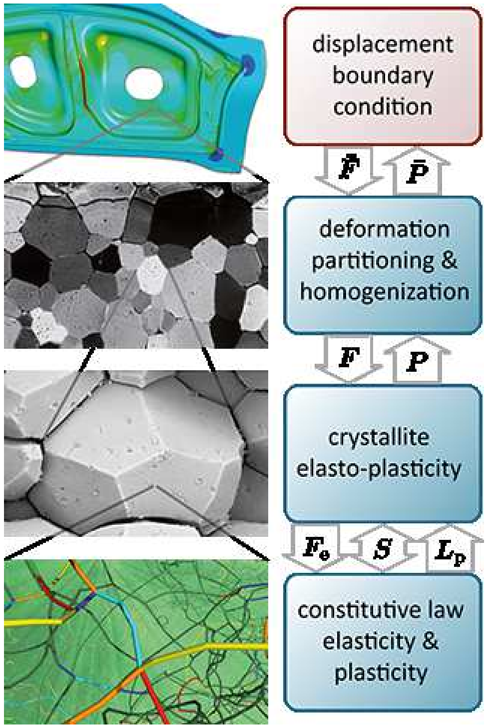
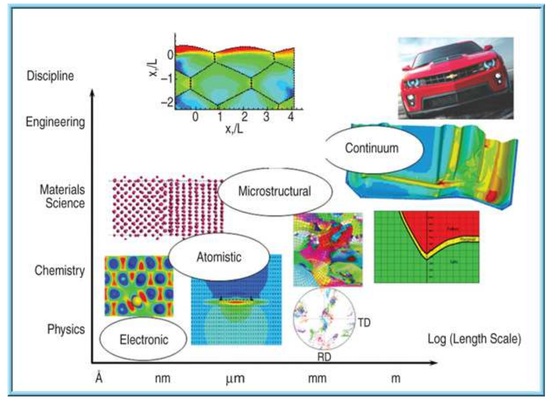
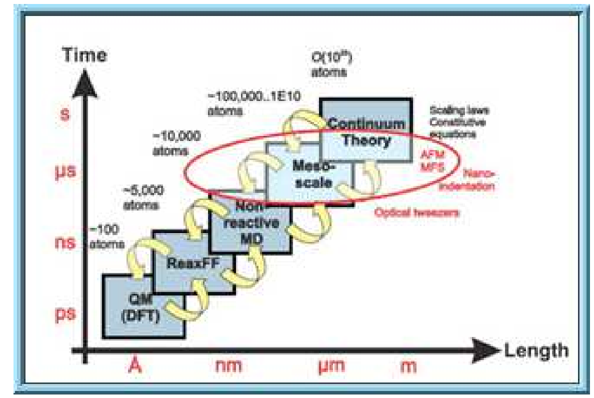
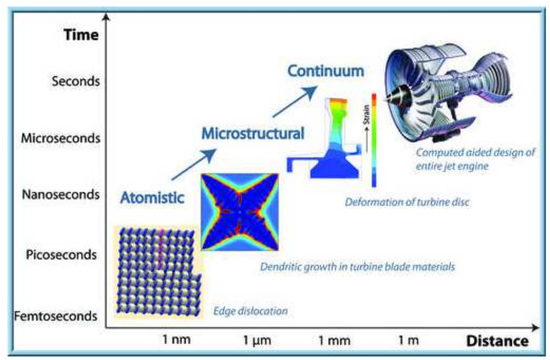
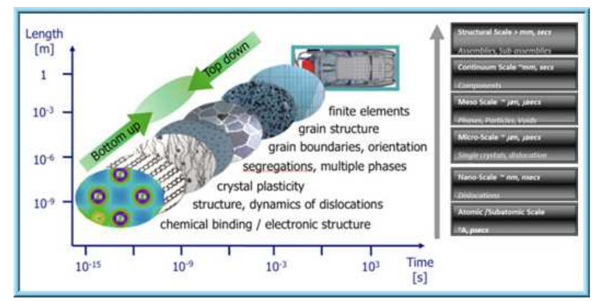
1. Multi-scale framework

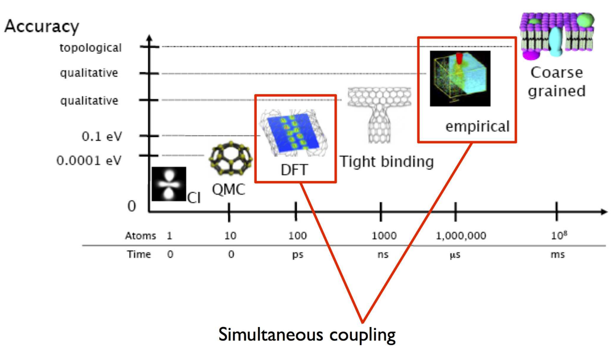


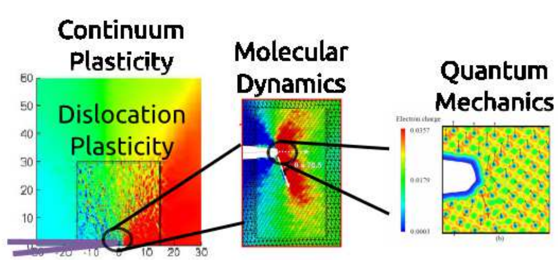


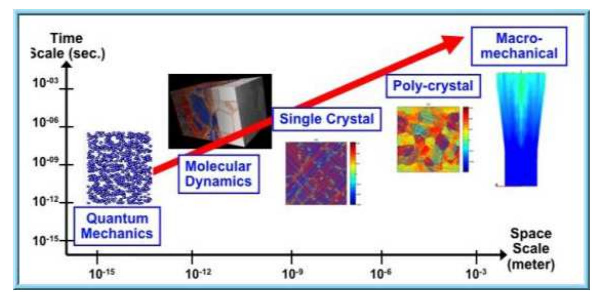












2. Trans-granular cleavage

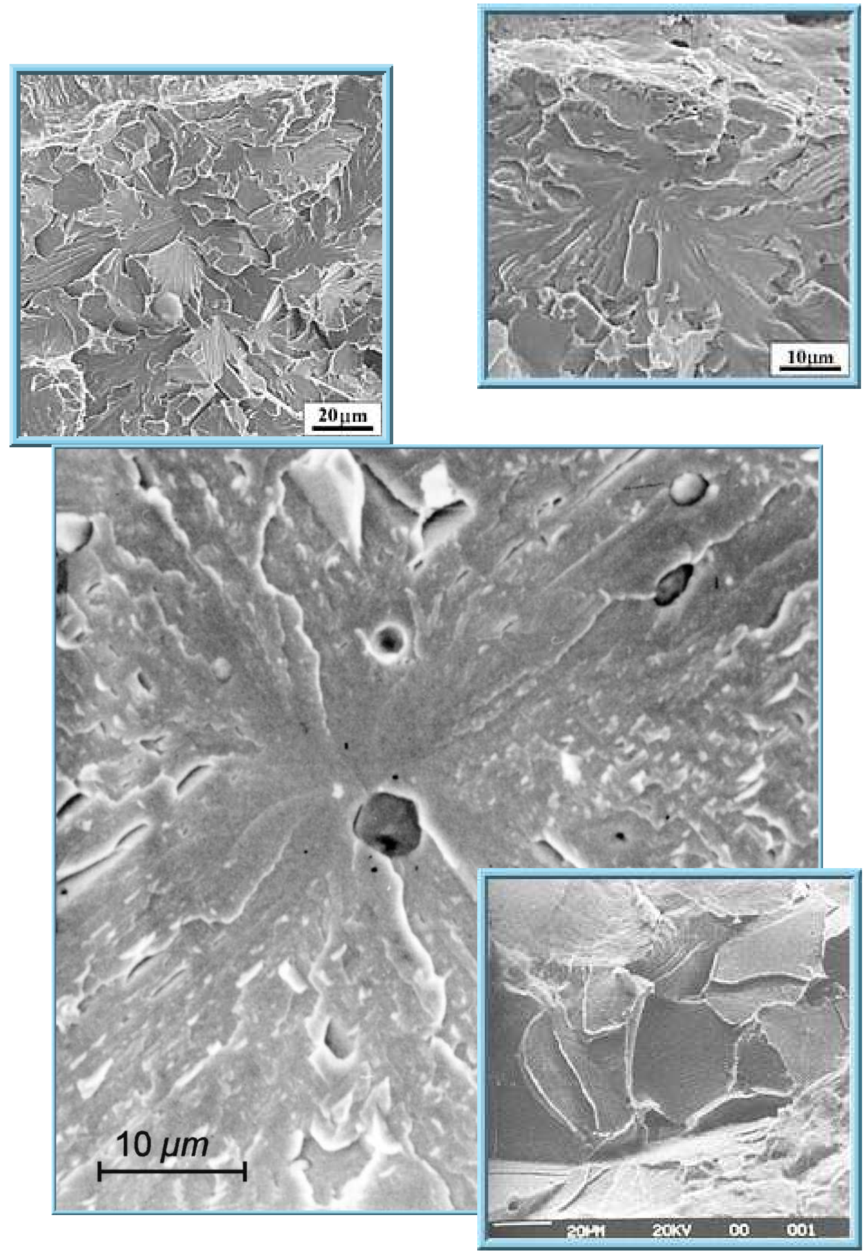
- **t** - Macro stress tensor
- t - Resolved normal stress on crystal planes
- bcc crystals: {100}, {110} planes cleave, normals $\mathbf{n}_{100}$, $\mathbf{n}_{110}$
- 24 planes of each family
- $t_{100}^{\max} = \max_{i=1\ldots24}(\mathbf{n}_{100}^{i} \cdot \mathbf{t} \cdot \mathbf{n}_{100}^{i})$
  $t_{110}^{\max} = \max_{i=1\ldots24}(\mathbf{n}_{110}^{i} \cdot \mathbf{t} \cdot \mathbf{n}_{110}^{i})$

Two parameters

- σ_F - critical stress, linked to γ, surface energy
- L - characteristic length, linked to wave speed, c.

Cleavage criterion

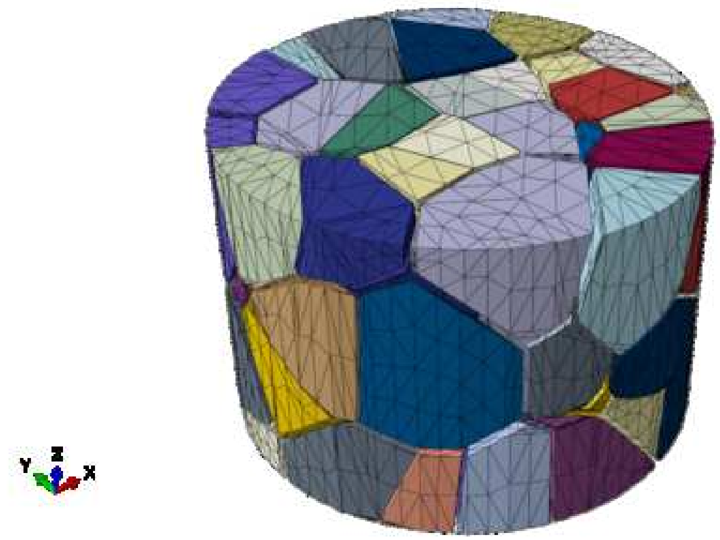
If $t_{100}^{\max} \geq \sigma_F$ or $t_{110}^{\max} \geq \sigma_F \rightarrow$ cleavage propagation over L per unit of time.

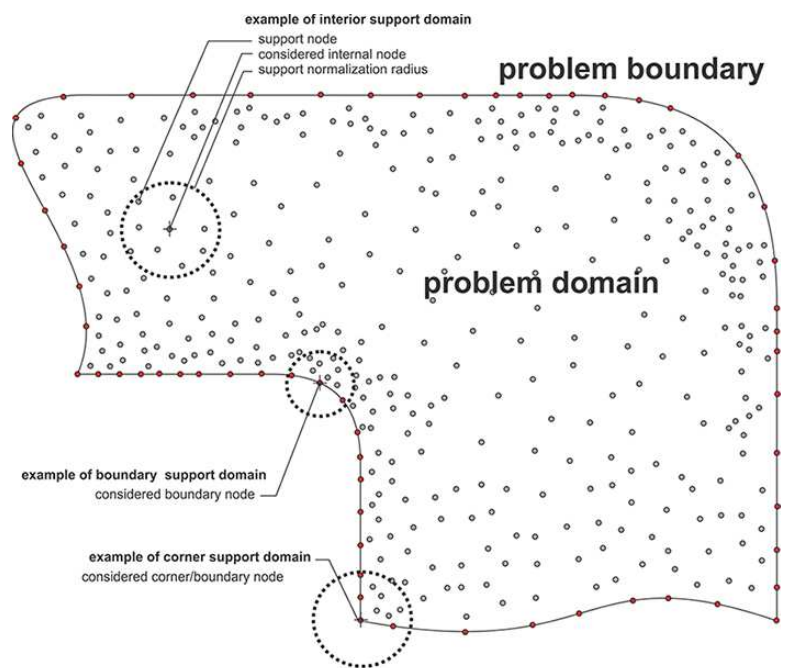


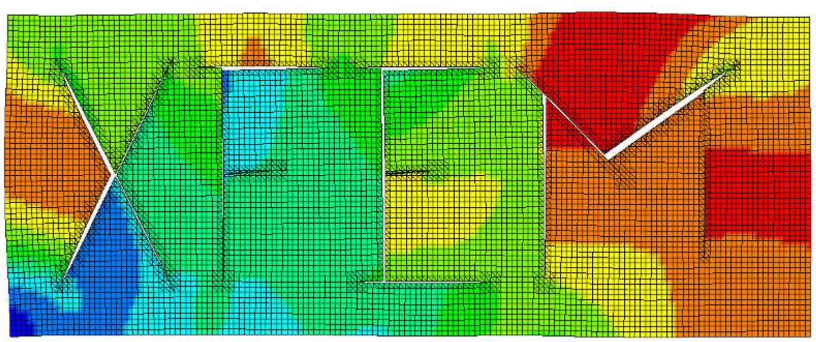
(Source: Internet)

3. Multi-scale methods

- Coupled discrete dislocation and continuum plasticity[1]
- Voronoi polyhedra FE[2]
- X-FEM[3]
- Element-free Galerkin (reproducing kernel particle)[4]
- Finite point[5]
- Free mesh[6]
- Meshless FE[7]
- Atomistic/continuum mech.[8]
- MD/continuum mechanics[9]

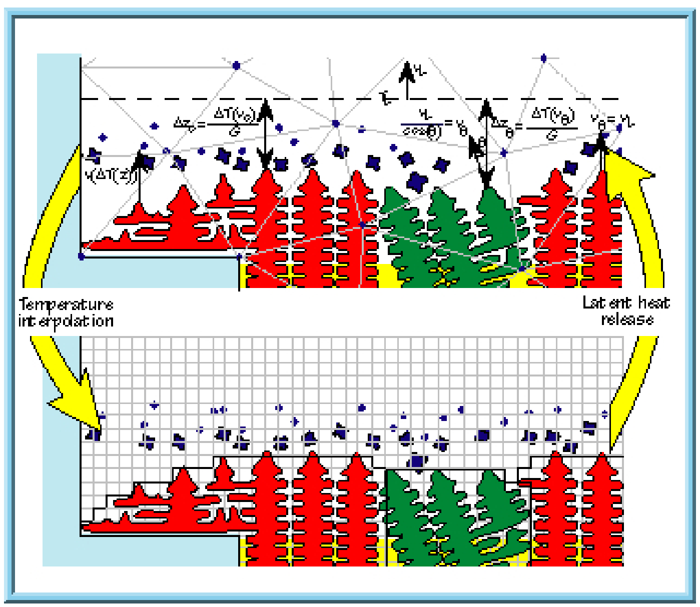


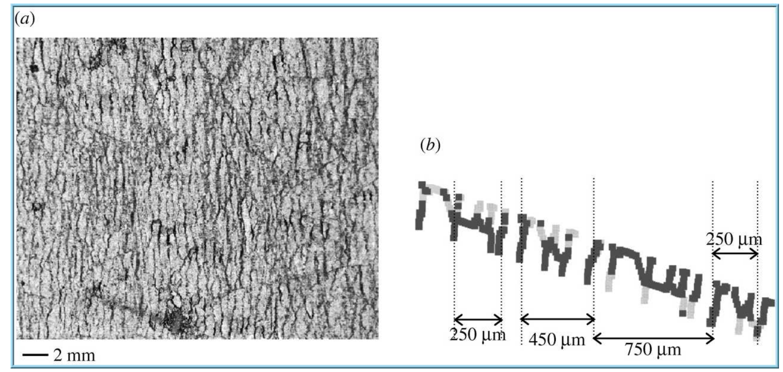


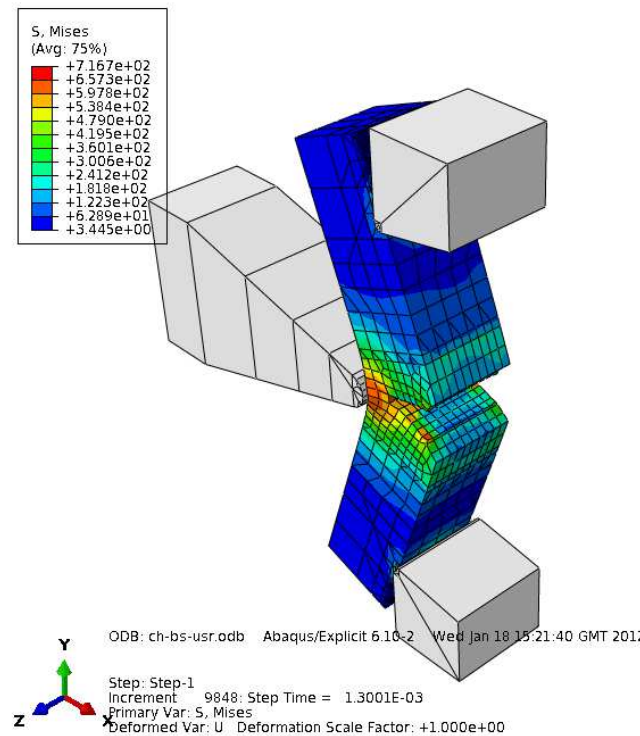


4. Cellular Automata Finite Element (CAFE)

- Used for solidification,[10] recrystallisation[11] and fracture[12, 13]
- FE - continuum mechanics - stress, strain, etc.
- CA - crystals, crystal boundaries, cleavage, grain boundary fracture
- FE $\rightarrow$ CA - stress, strain
- CA $\rightarrow$ FE - damage variables







5. Open source FE

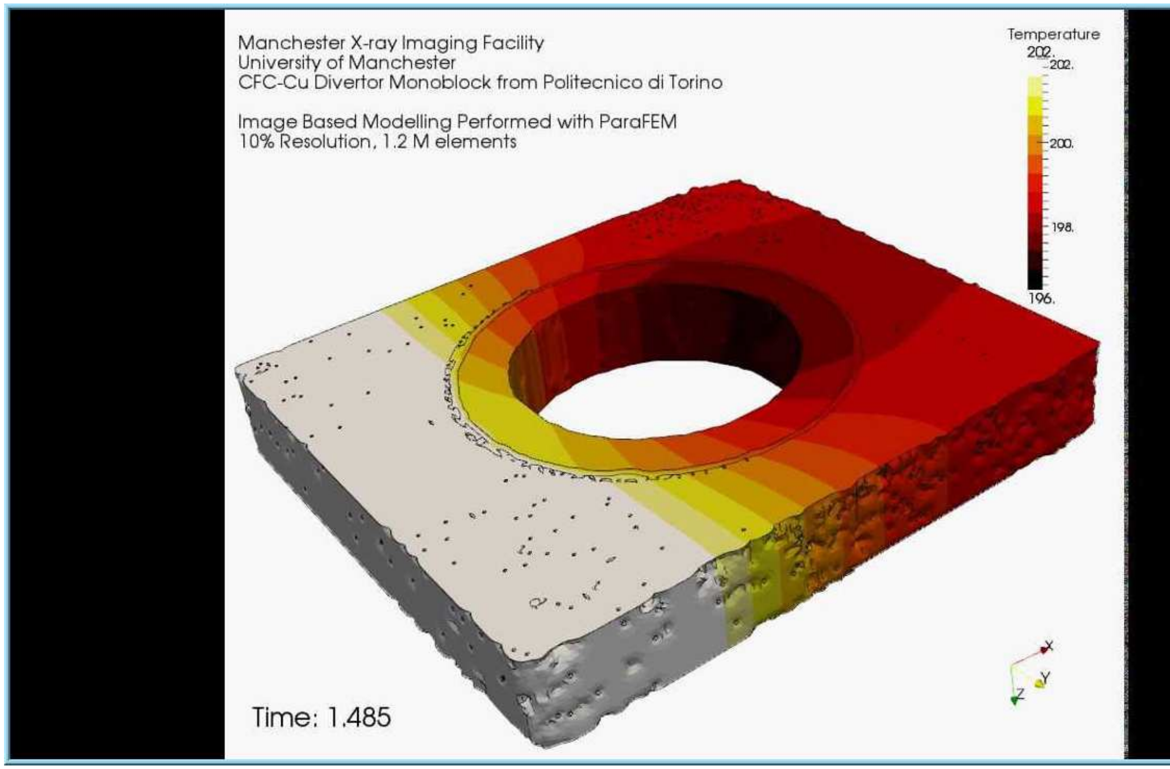
ADVENTURE
Aladdin
ALBERTA
CalculiX
CMISS
Code_Aster
deal.II
DOUG
DUNE
Elmer
FEA(S)T
FENICS
FELIB
FElt
FELYX
FEMLISP
FEM_Object
FEMOCTAVE
FEMSET
FFEP
freeFEM
Getfem++ HMD
Impact
IMS
kaskade
KFEM
LUGR
MiniFEM
MODFE
MODULEF
NASTRAN
NLFET
OLEFI
OOFEM
Open FEM
Open FEM (INRIA)
OpenSees
Padfem2
ParaFEM
Rheolef
SLFFEA
Sundance
TOCHNOG
VAPAS
VECFEM3
WARP3D
Z88

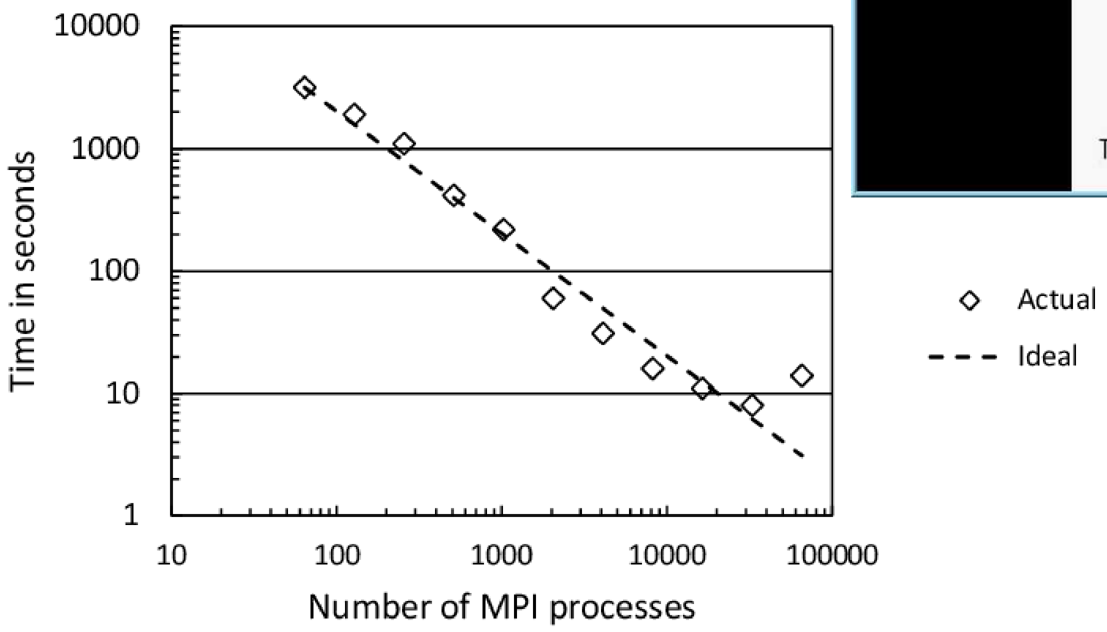
Problems

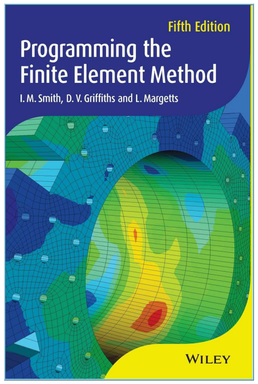
- Scaling
- Portability
- Documentation
- Flexibility
- Continuing development and future proofing
- Standard libraries
- Algorithms

6. ParaFEM[14]

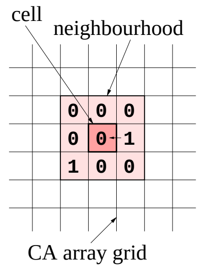
- MPI FE library
- Solids, fluids, heat transfer, dynamics, modal
- Highly scalable, >50k cores
- >125M elements
- `parafem.org.uk`

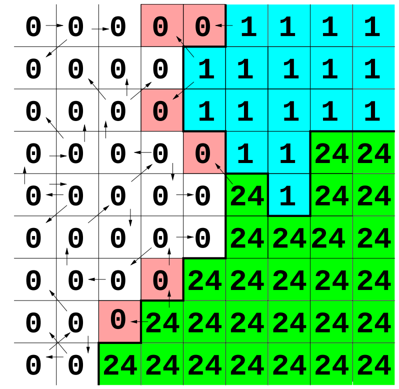


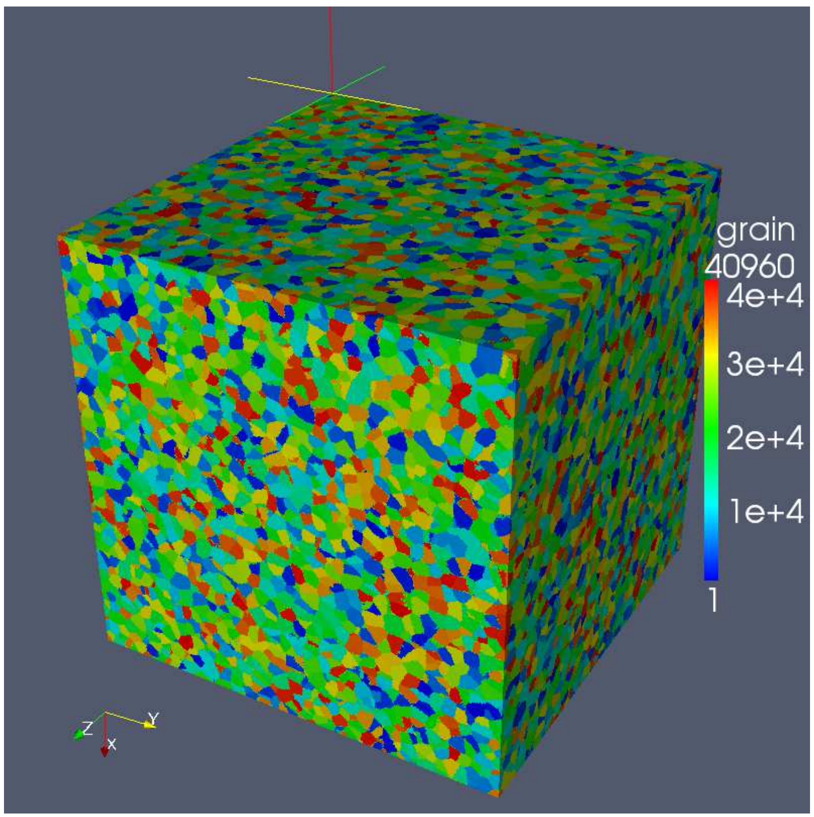


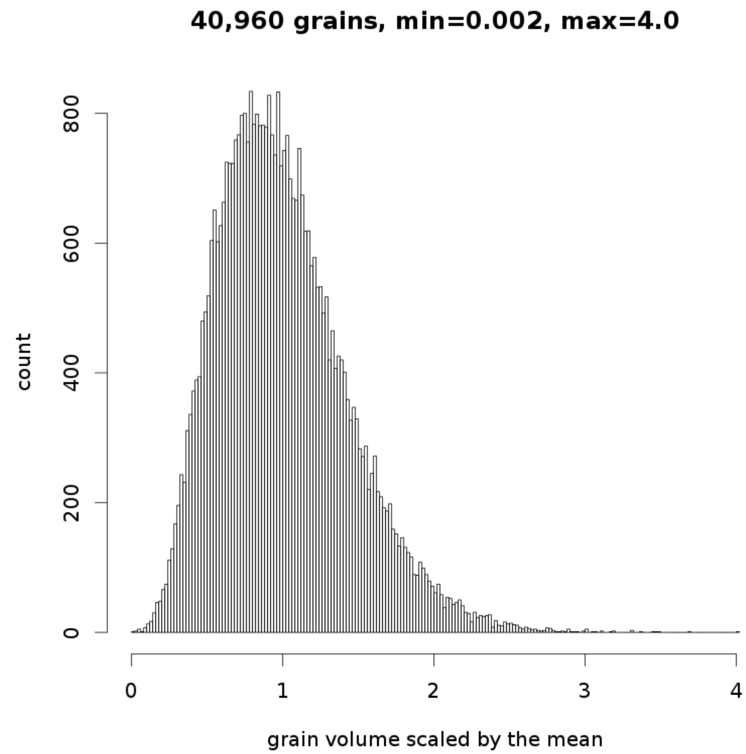


7. CGPACK[15, 16, 17] - Cellular automata for polycrystals

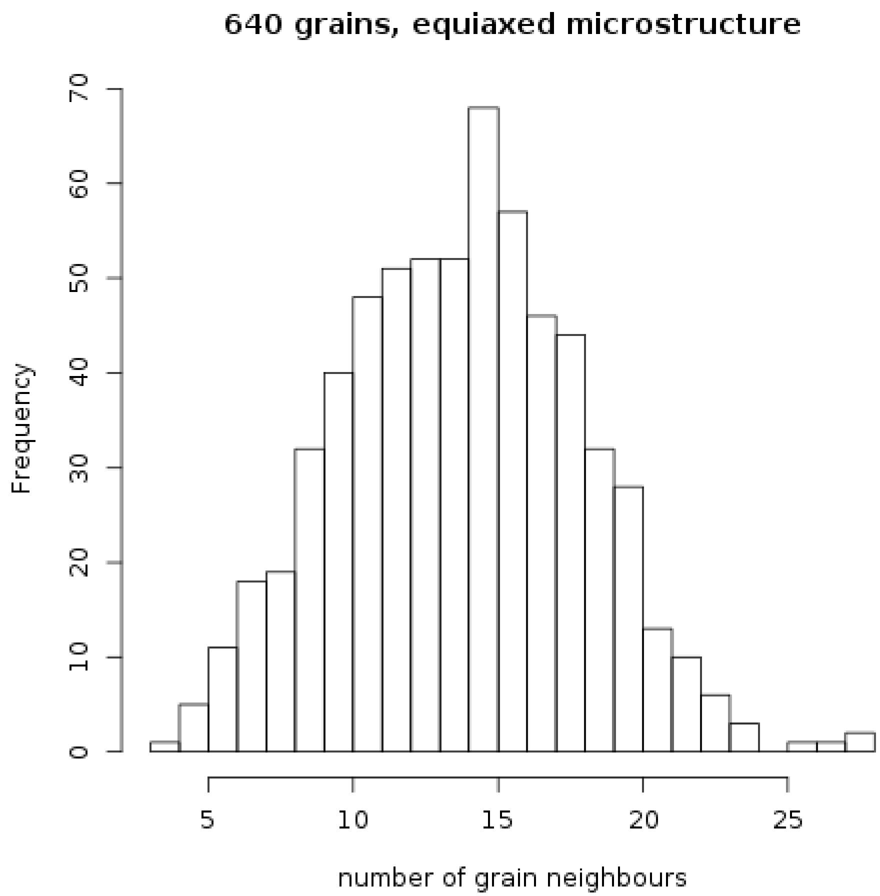


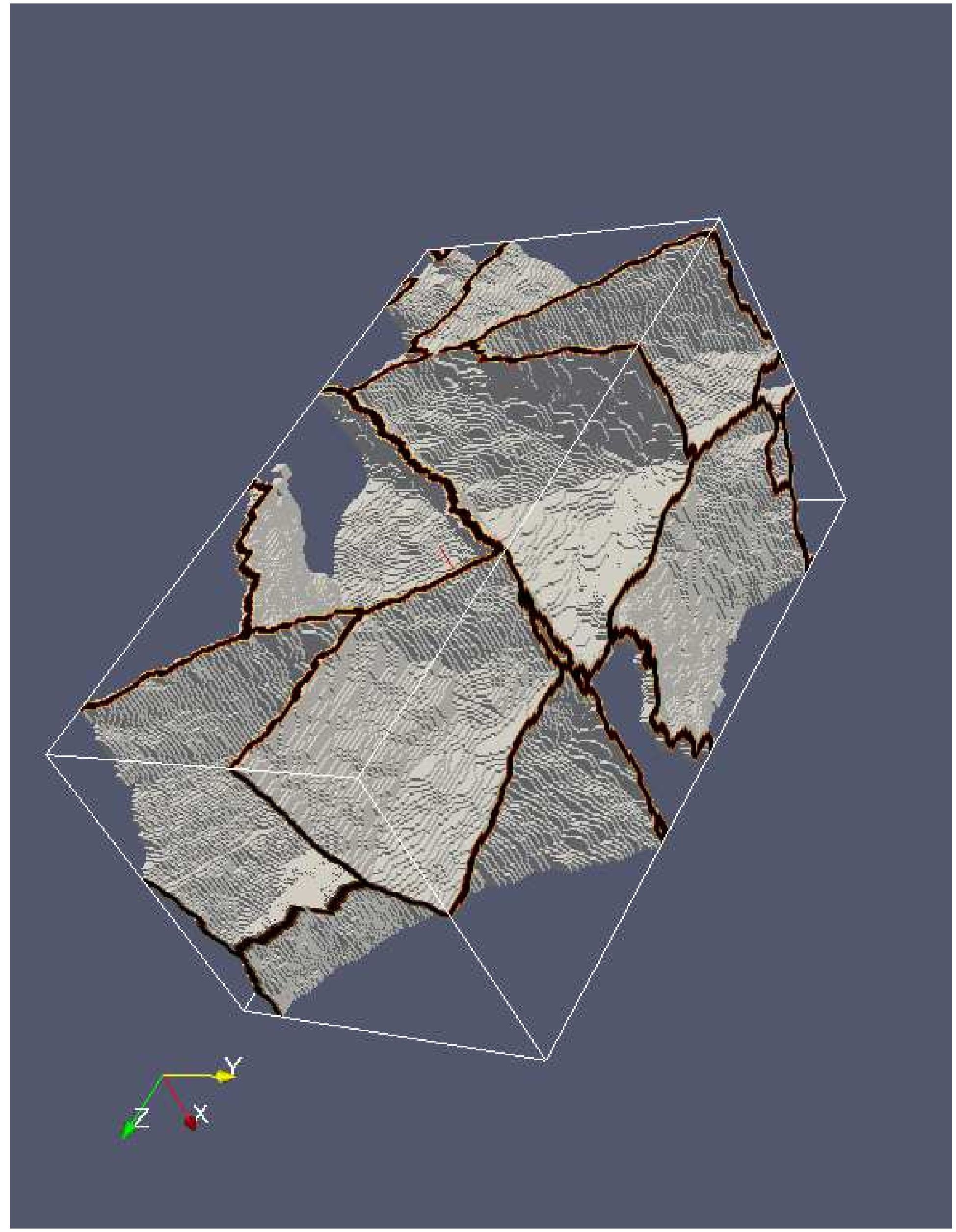




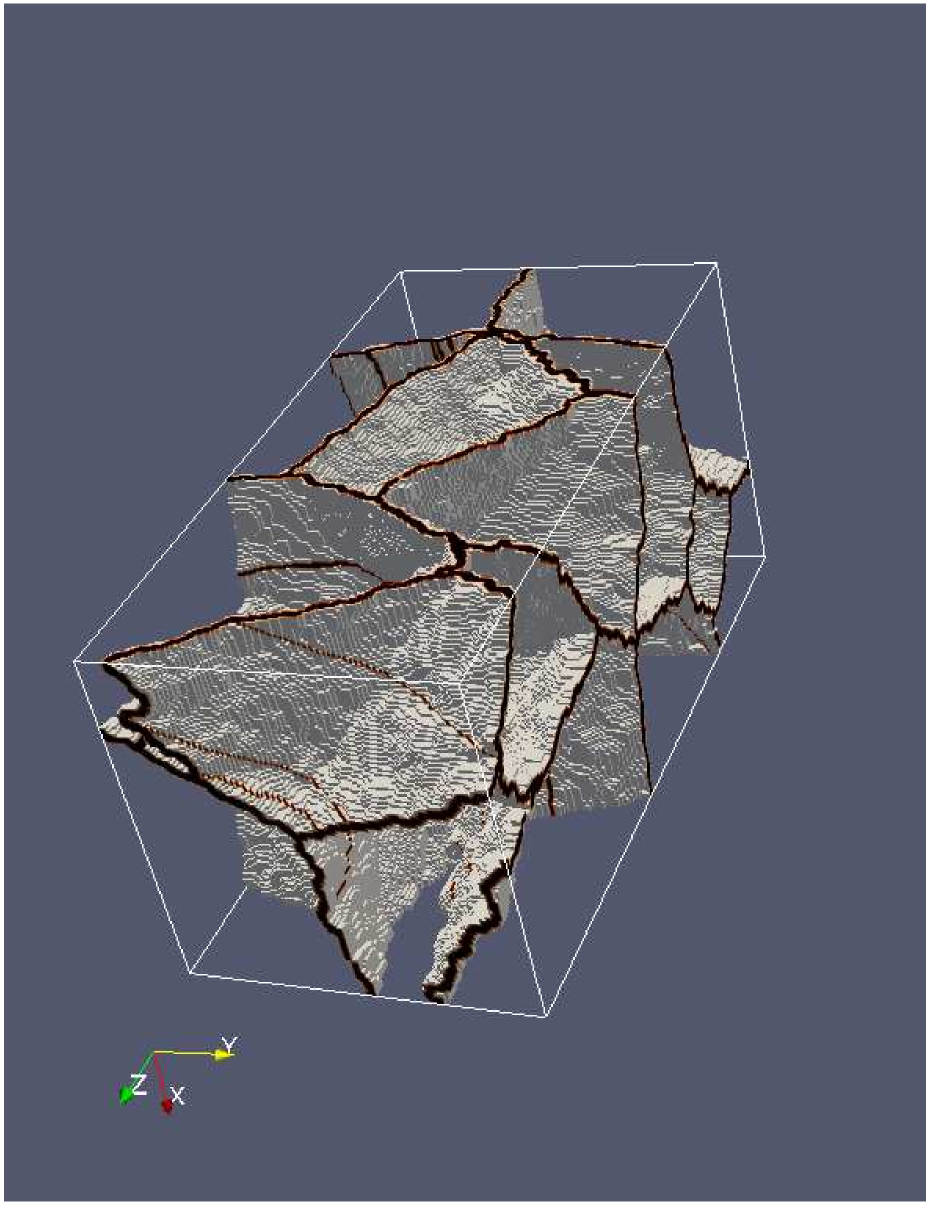


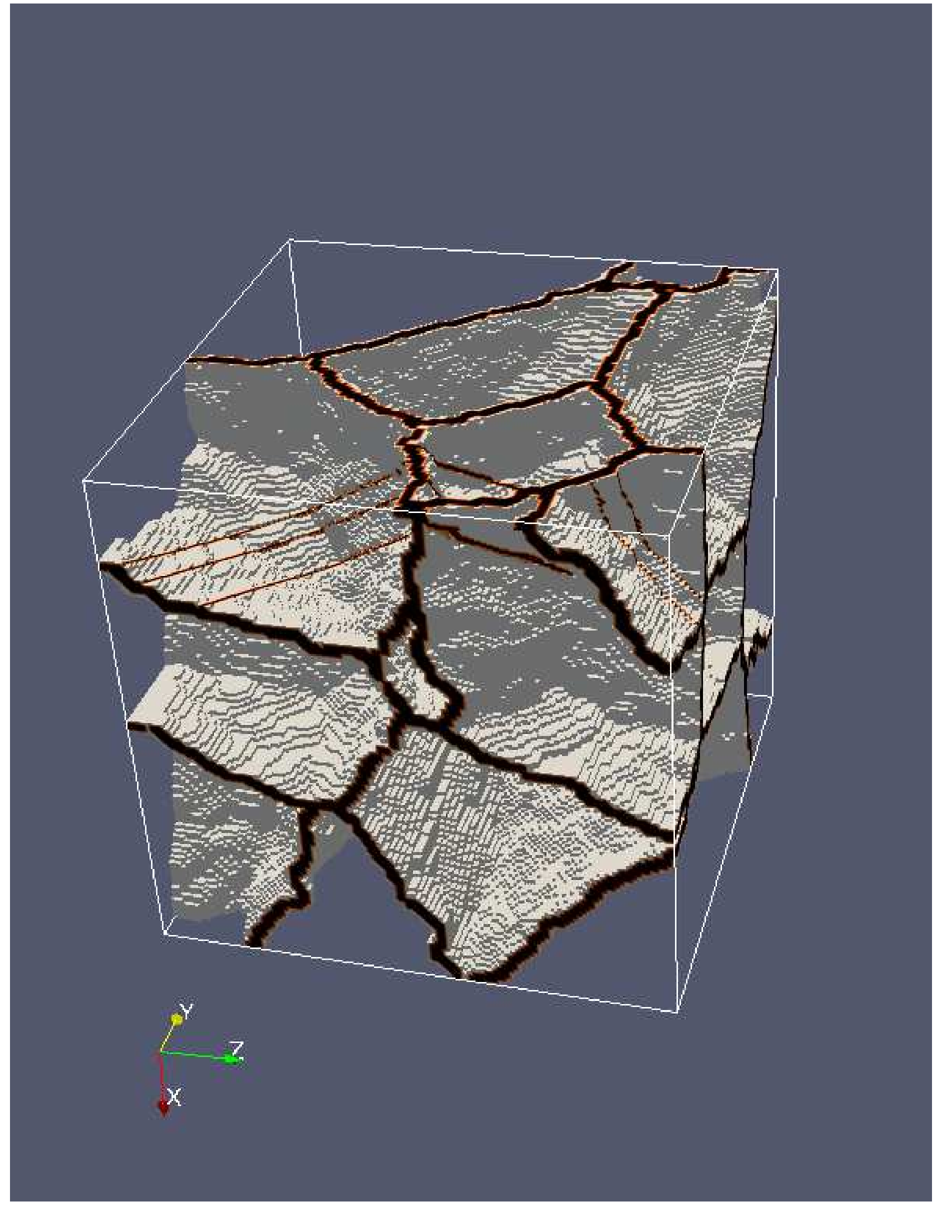
8. Grain boundaries



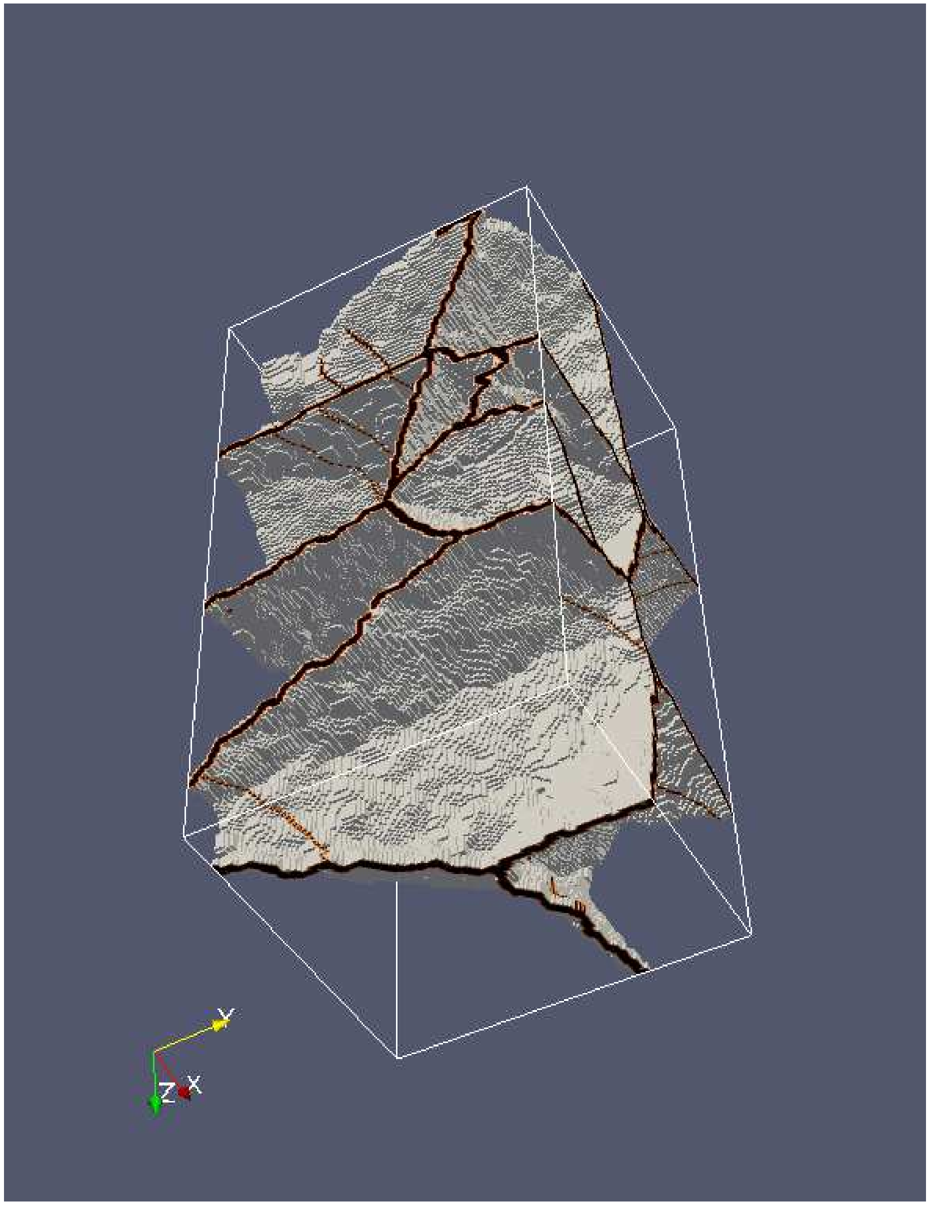


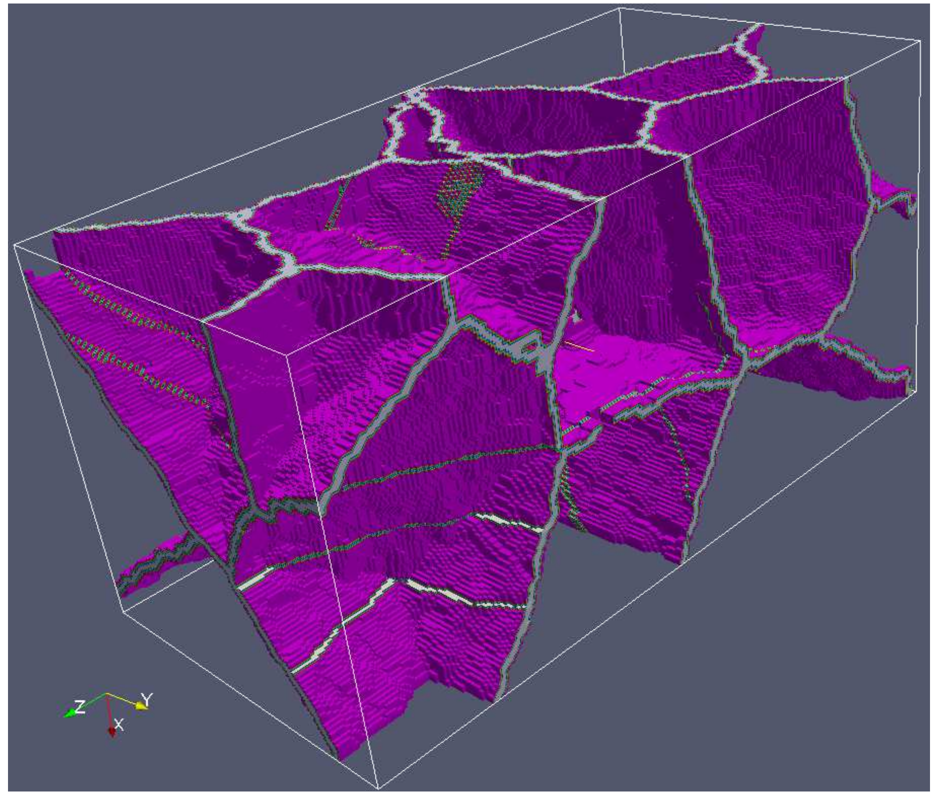
Grain boundaries



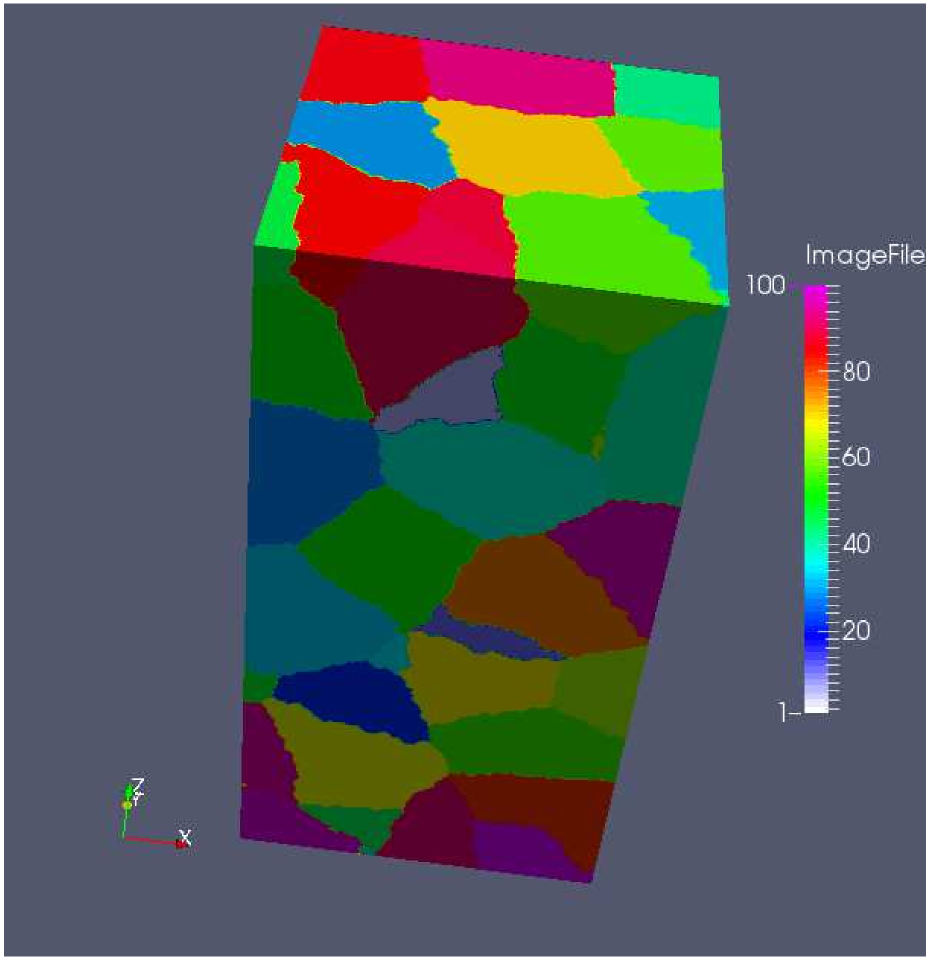


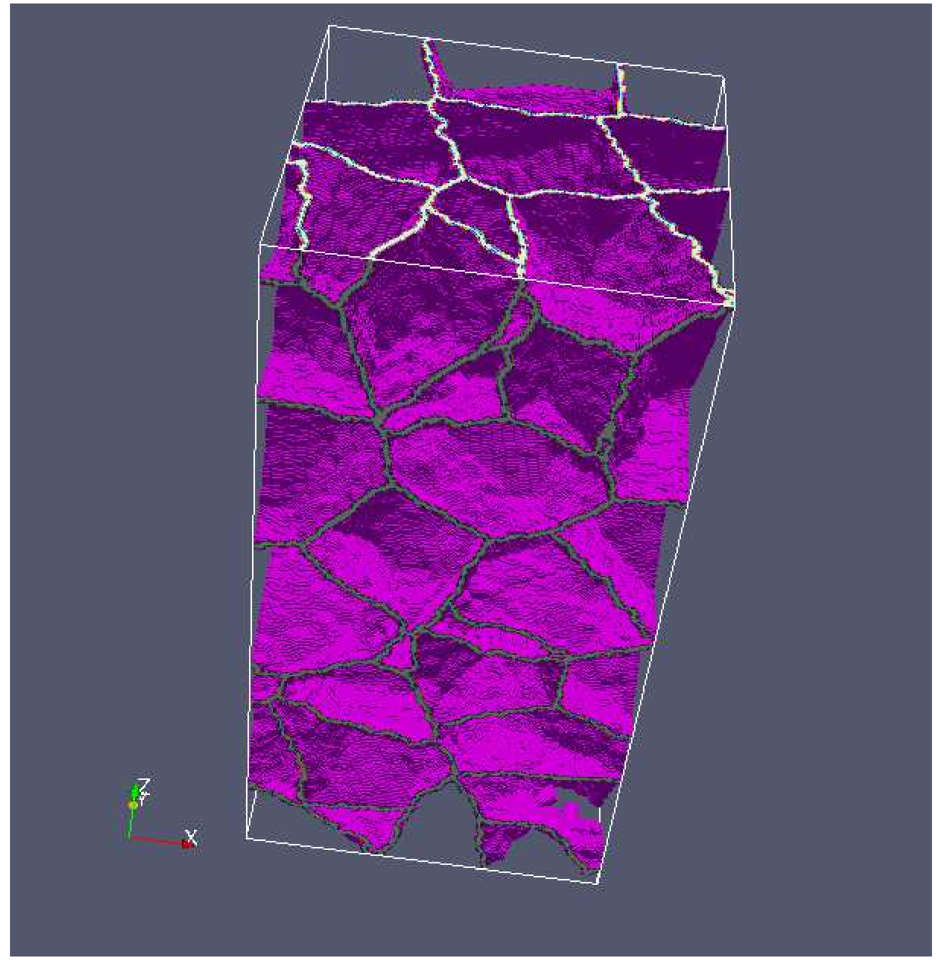
Grain boundaries



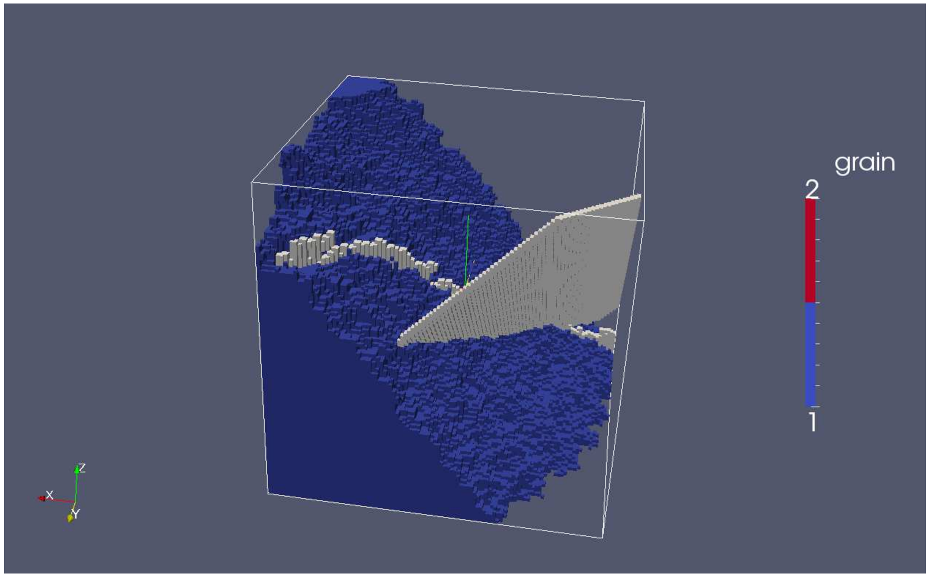


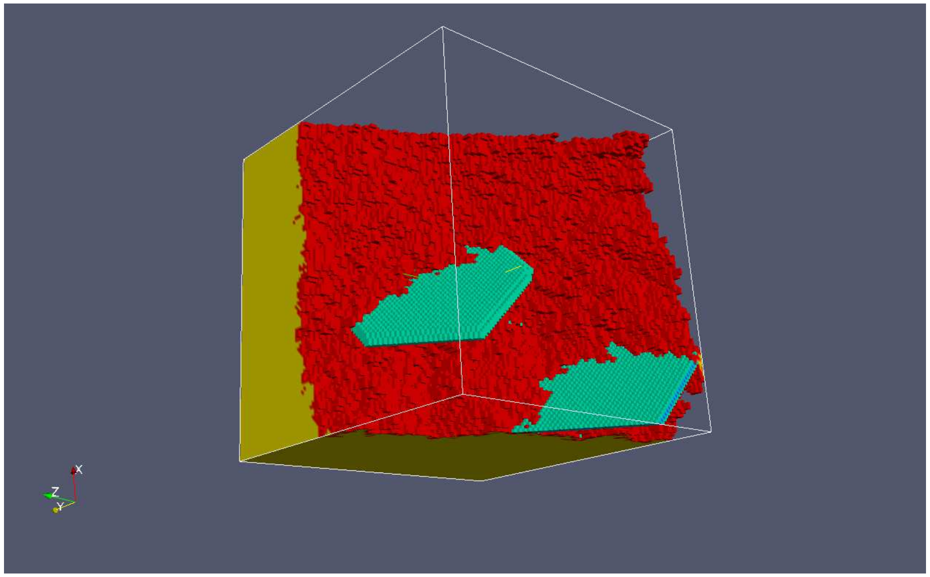
Grain boundaries

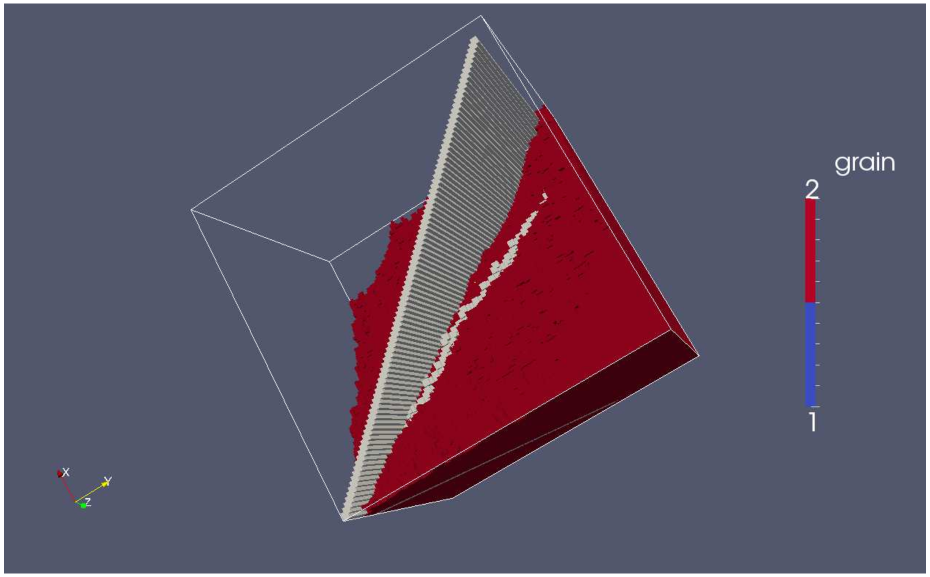


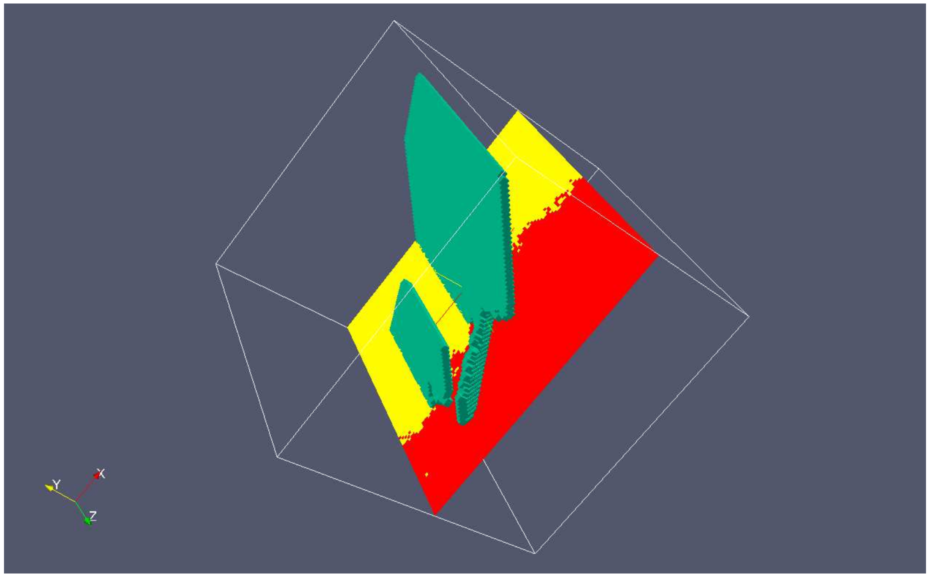


9. Cracks crossing GB

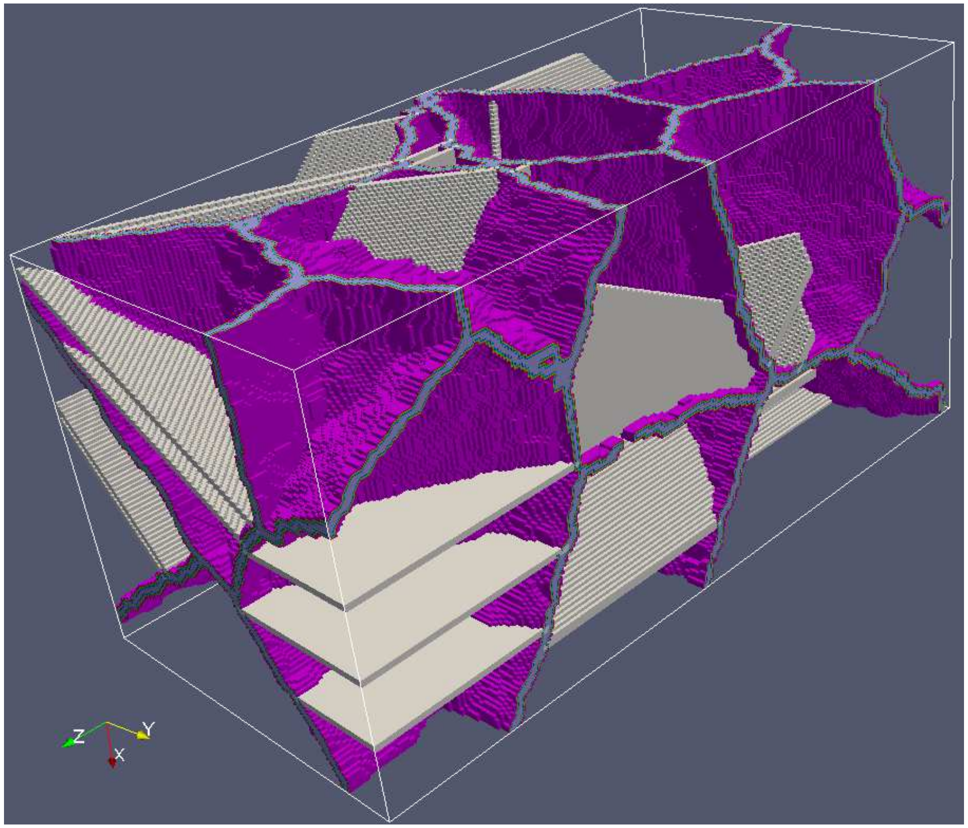


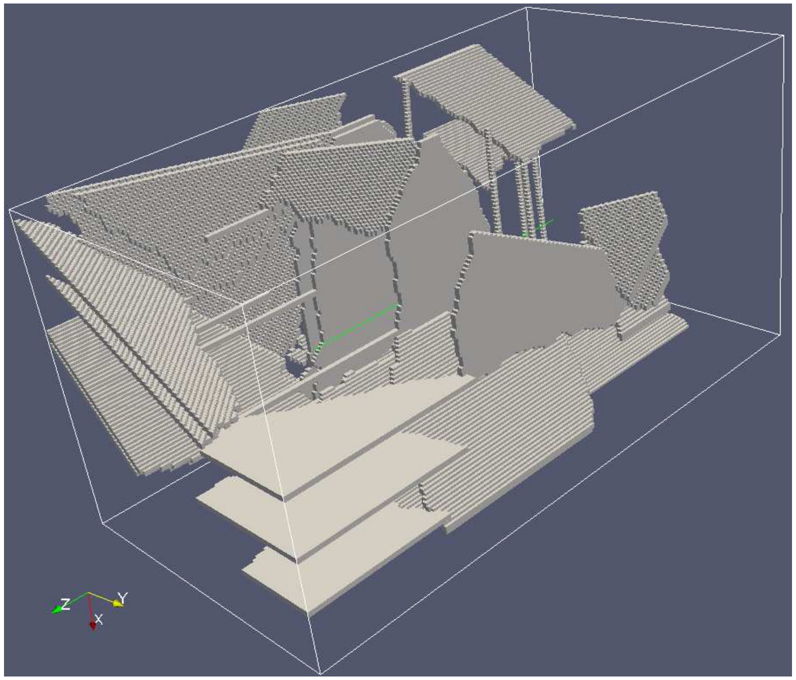


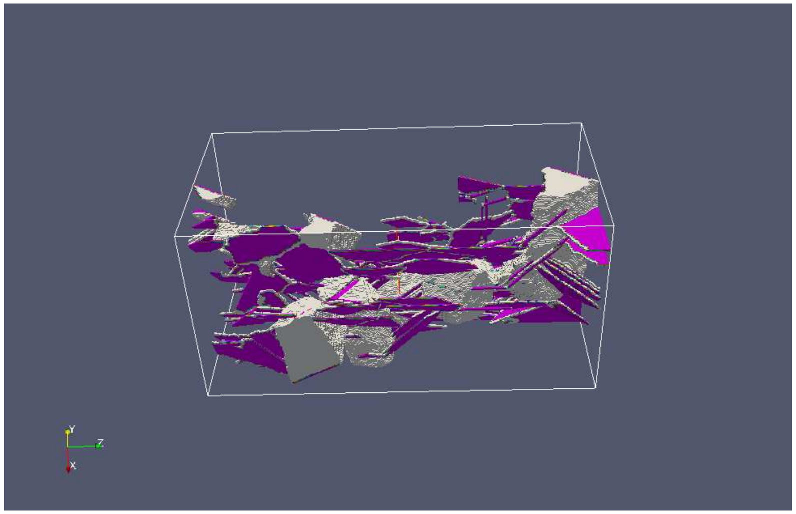




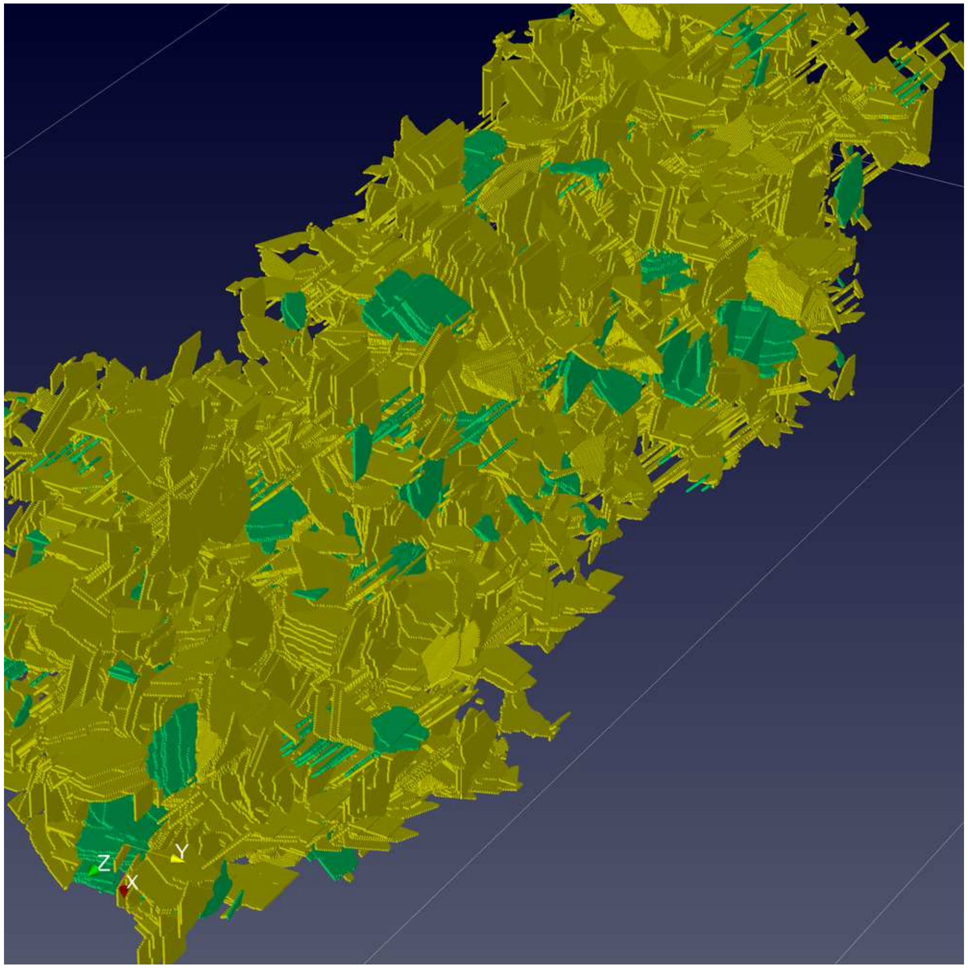
10. Microcracks joining into a macrocrack

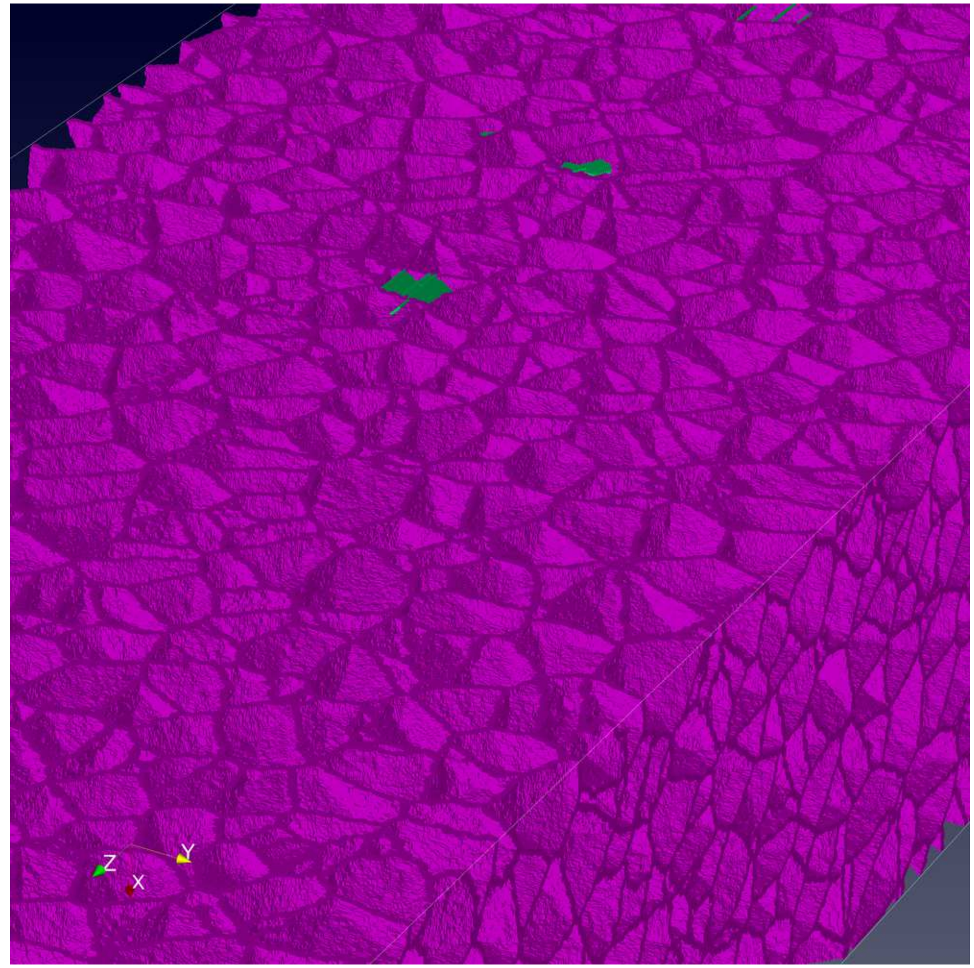




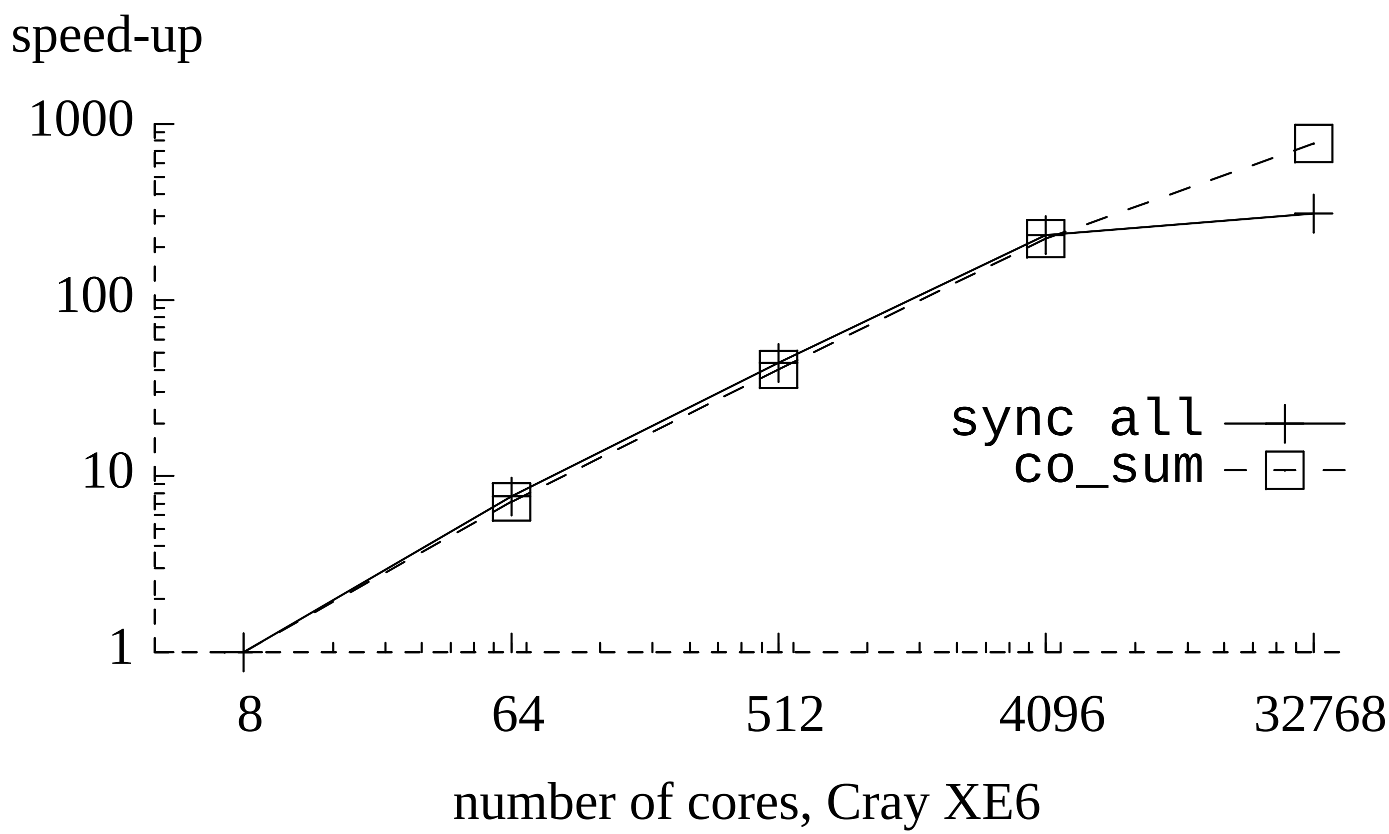


Microcracks joining into a macrocrack, 10^9 cells





11. CA performance, Cray XE6, 10^9 cells[16]

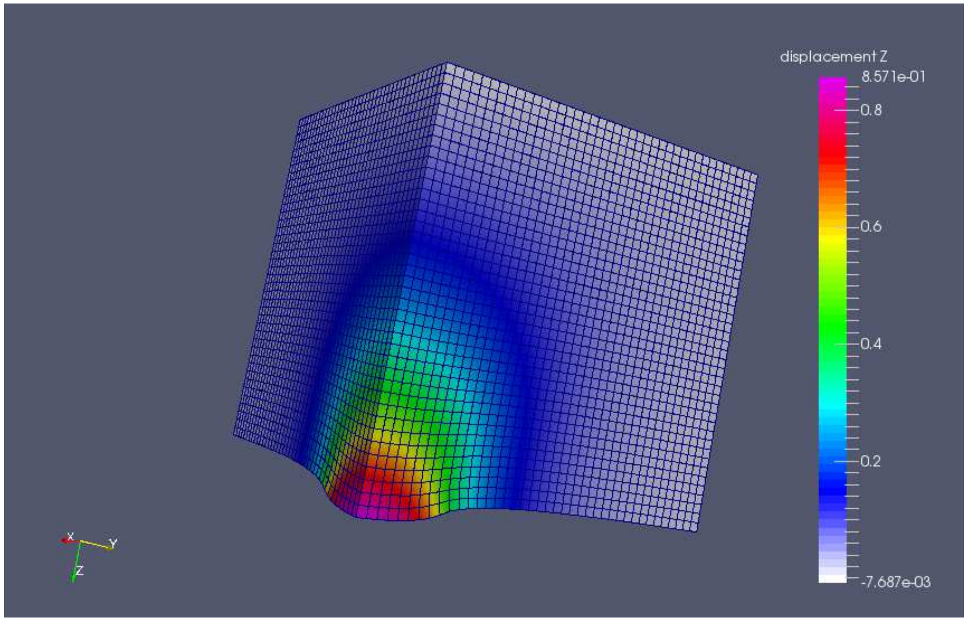


- Scaling due to identical calculations performed for all cells
- No asyncronous execution

12. CAFE sample results[15]

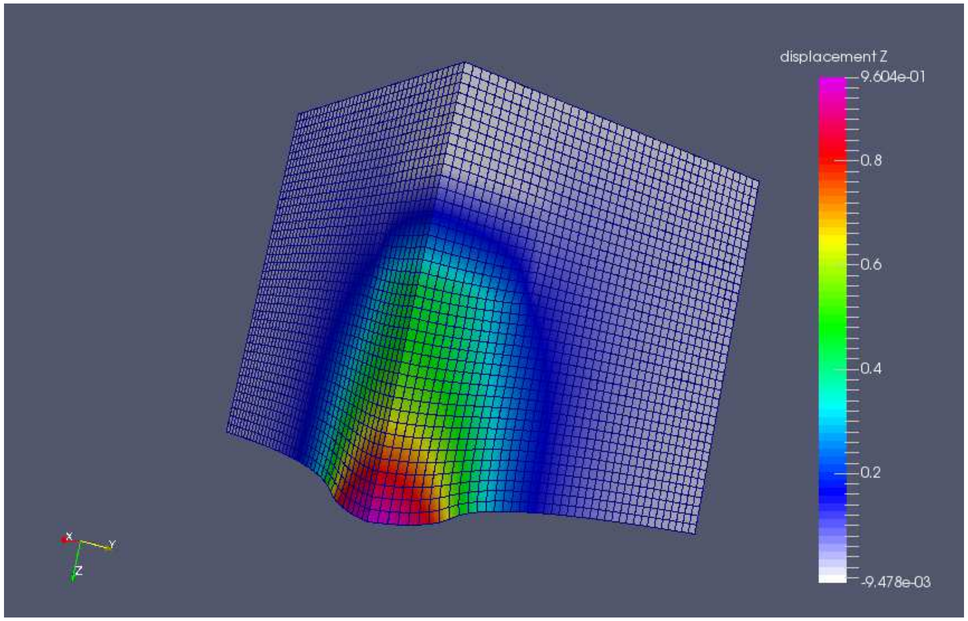
- 3D cube, quasi-static tension
- *D*, the CA damage variable per FE, $D = 1$ - no damage (intact), $D = 0$ - failed
- Update the Young's modulus: $E = E_0 \times D$

No cracking

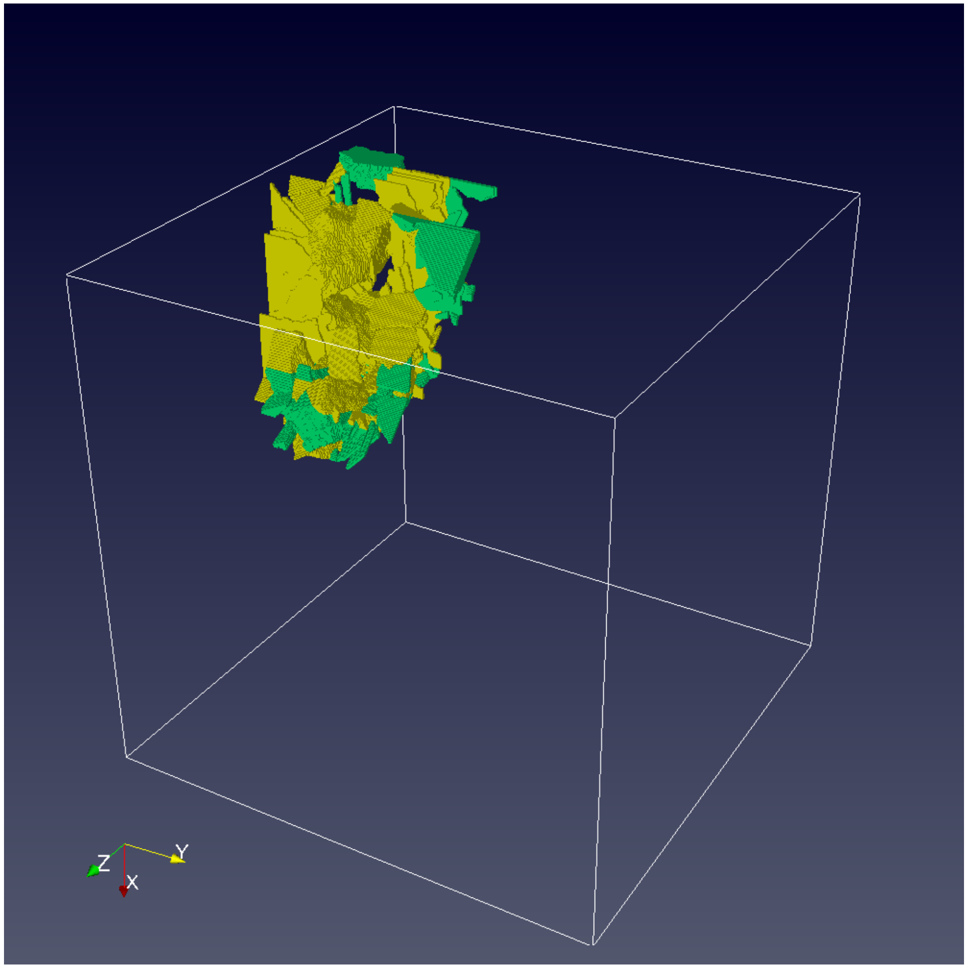


Cracked model

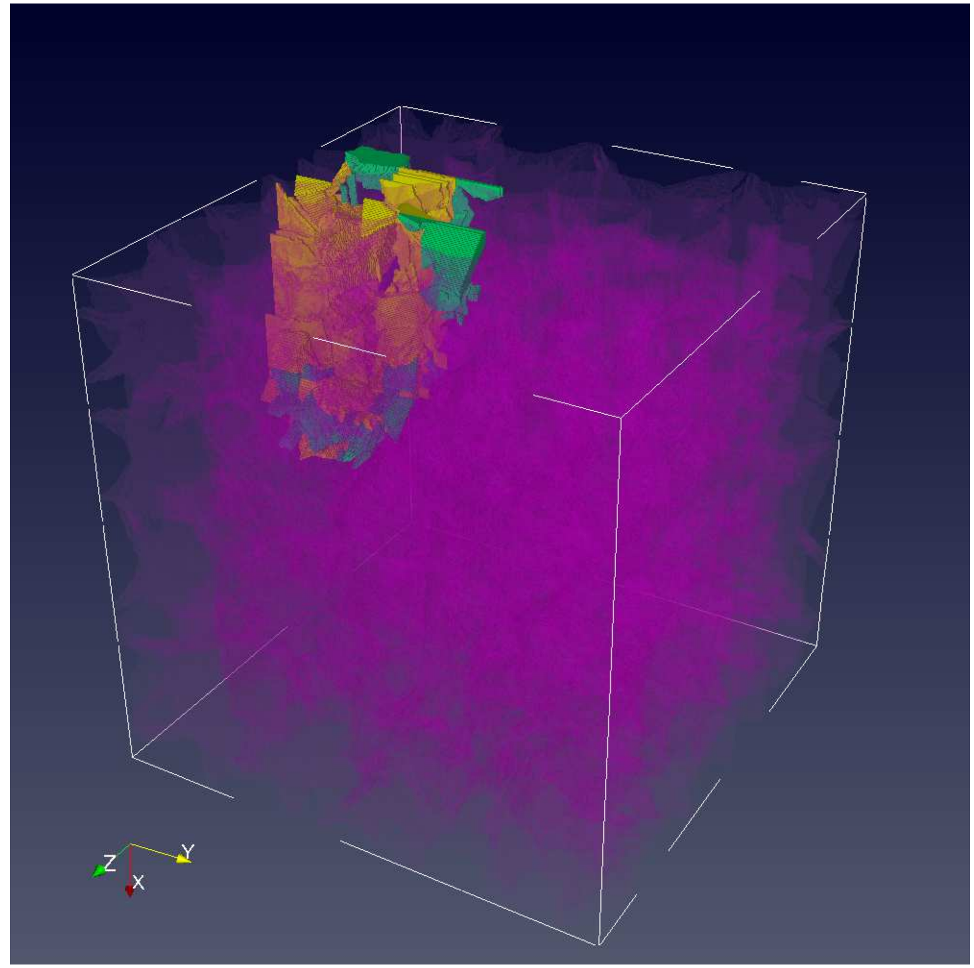
Note discontinuity on the blue band, corresponding to crack front crossing the boundary.



CAFE sample results



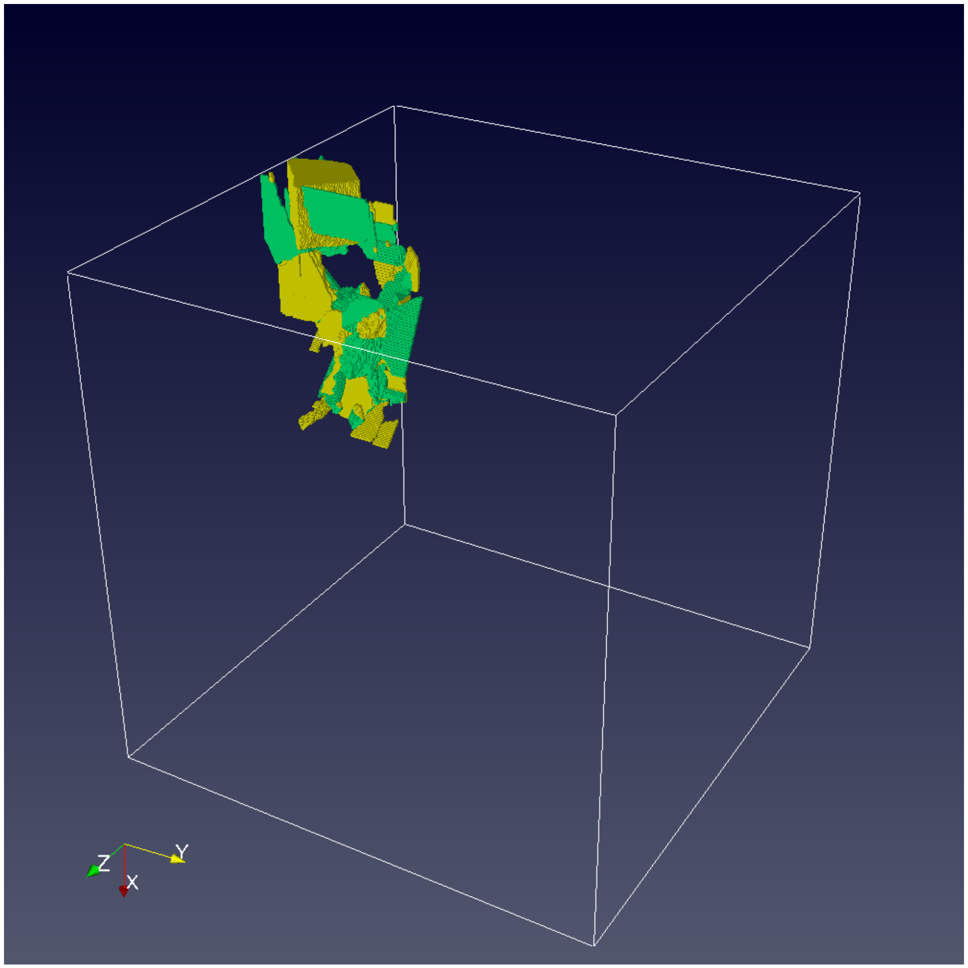
The macro-crack emerges as cleavage cracks in individual grains join up after crossing grain boundaries in poly-crystalline bcc iron. Green cracks - {110} planes, yellow - {100} planes.

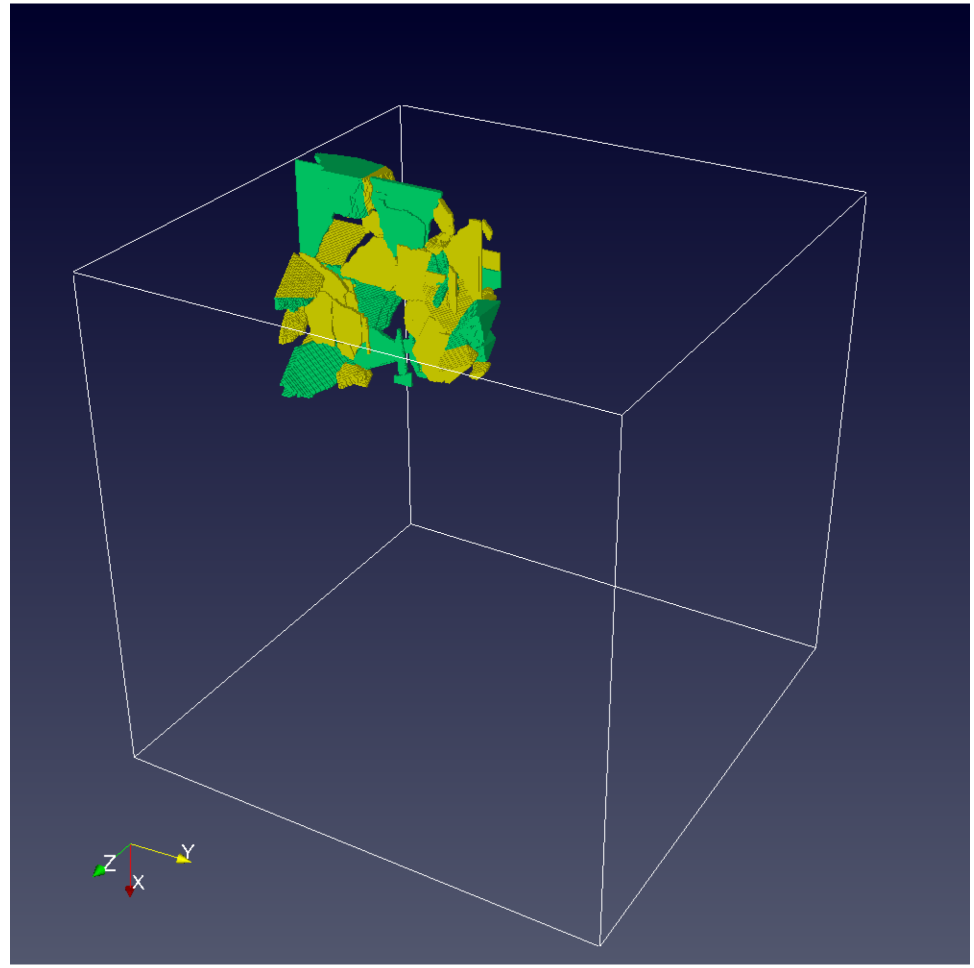


The process is driven by the FE stress fields on the macro-scale.

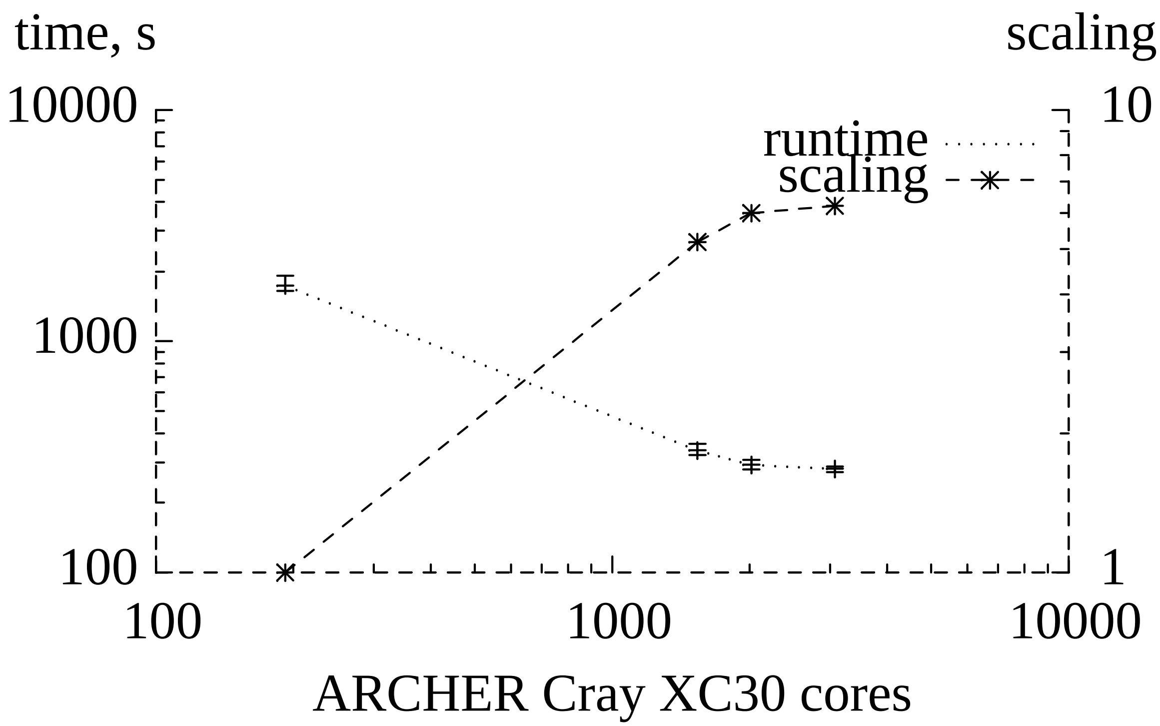
CAFE sample results, exploring uncertainty and scatter

Random samples of microstructure produce different crack paths.





13. ParaFEM/CGPACK CAFE scaling on ARCHER, Cray XC30



- $200 \rightarrow 1,500$ cores = $\times 5$ scaling. Parallel efficiency of > 60%.
- ParaFEM - MPI, CA - CGPACK - Fortran 2008 coarrays
- Hybrid MPI/coarray - novel, risky
- Cray and Intel now, GCC soon

14. Future: generic framework

We need:

- *Framework* for building multi-scale solid mechanics models
- *Flexible*, *expandable*- wide range of problems.
- *API* centred
- Opportunities for *code replacement* and *interoperability*.
- The framework must not not be linked to any particular FE code or any particular microstructure model.
- *Concurrent* simulation at all scales, with a two way information exchange.[18]
- The framework must allow for implementing *homogenisation* and *localisation* (upscaling/downscaling) algorithms, e.g. using the representative volume of material (RVE)[19] or nested homogenisation-localisation.[20]
- Multi-scale models are large. *Petascale* now and *exascale* soon.
- The aim of the framework is to allow researchers to combine their micro- or mesa-scale models with a variety of continuum mechanics FE solvers.
- *Comparison* of different multi-scale models and of different modelling results will be more rigorous and fair.

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