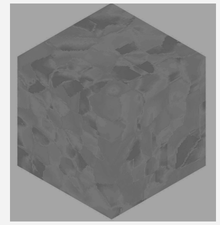
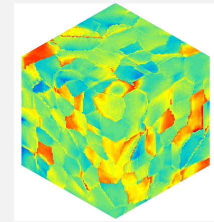
# Contents



# Computations at various scales

| *Black box* | *Realistic aggregate* | *Intermediate level* |
|---|---|---|
|  |  | *Averaging process*<br>(2) phase by phase<br>(2') grain by grain |
| Level (1)<br>*Macroscopic models*<br>*Average stress and strain tensor* | Level (3)<br>*Local information*<br>*Respect local Constitutive Equations*<br>*Equilibrium* | Level (2) or (2')<br>*Local average*<br>*Respect local Constitutive Equations*<br>*no neighbooring effect* |



## FE calculations of crystalline microstructures

*Georges Cailletaud*

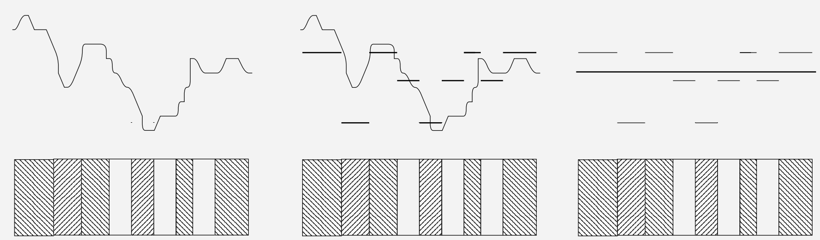
*Centre des Matériaux*
*Ecole des Mines de Paris/CNRS*

# Various scales in heterogeneous material modeling

(a) *Microstructure calculation: take into account local phases and local equilibrium (*This lecture *)*

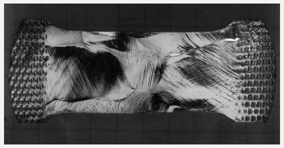
(b) *Uniform field models: take into account local phases only*

(c) *Macroscopic models: do not account for local phases nor local equilibrium*

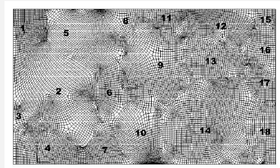


(a) (b) (c)

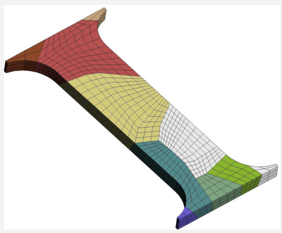
## Multicrystals, real microstructures



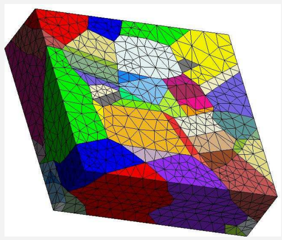
*[Delaire et al., 2000]*



*[Raabe et al., 1981]*



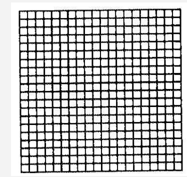
*[Eberl et al., 1998]*

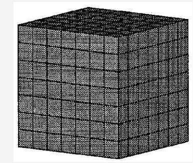


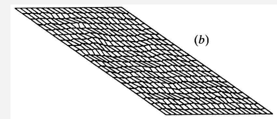
*Next lecture*



## Cubic meshes, cube elements








*2D*
*[Kalidindi et al., 1992]*

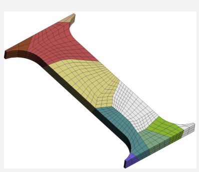
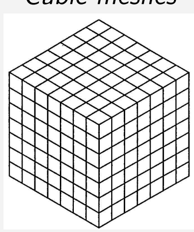
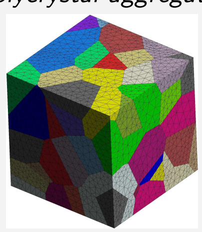
*3D*
*[Miehe et al., 1999]*

Meshes used for homogenization purpose



## Various types of FE computations using crystal plasticity

*Single Crystal models in each Gauss point*

| Multicrystals | Cubic meshes | Polycrystal aggregates |
|---|---|---|
|  |  |  |
| Real specimens | Cubes | Realistic microstructures |
| with a few grains<br>to check local fields<br>With experiments | 1 grain/elt<br>Numerical<br>Homogenization | Many Gauss Pt/grain<br>Homogenization<br>AND Relocalization |

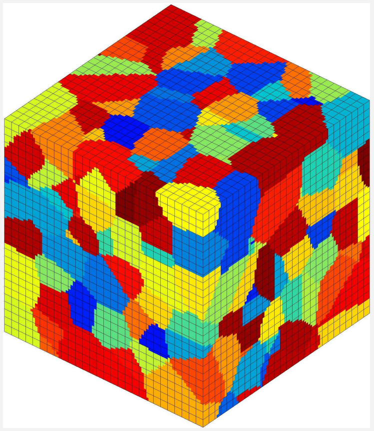


## State-of-the-art on real microstructures

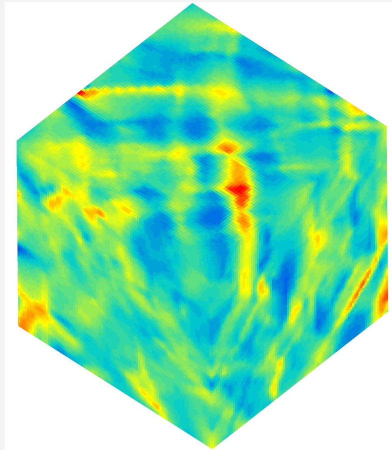
- *Good agreement, specially for large grains*
- *Problems near grain boundaries*
- *Behavior of a grain in its environment $\neq$ single crystal behavior*
- *Primary–secondary slip*
- *Problem surface–volume (2D–3D meshes ?)*
- Example of a OFHC copper specimen, coming soon...

# Polycrystal aggregates

Work by Barbe (2000), Diard (2002), Musienko (2005)



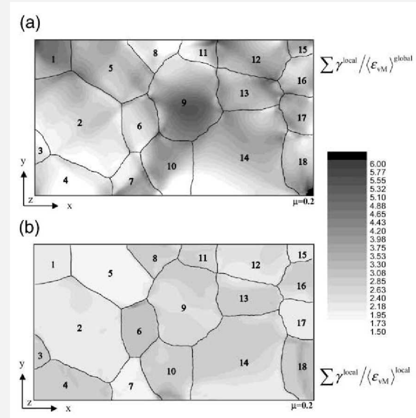
*28×28×28 mesh*



*Local field of total axial strain*



# Influence of GB's




*Global and local Taylor factor*

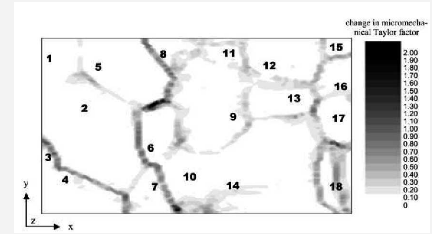
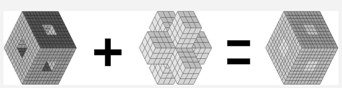


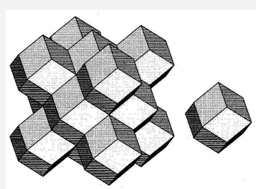

*Illustration of the perturbation due to grain boundary by the variation of the local Taylor factor*

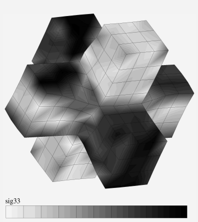
(more in [Raabe et al., 1981])



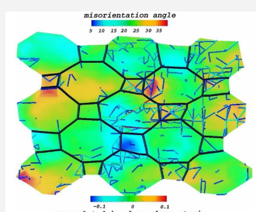
# Polycrystalline aggregates (2)







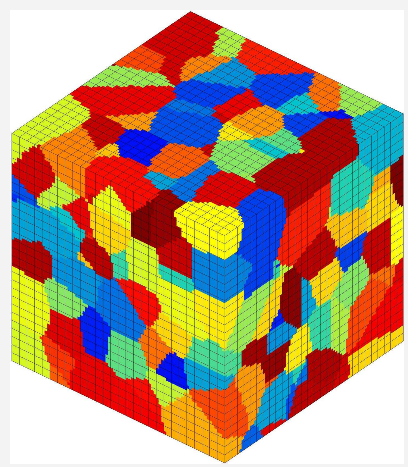

*[Bugat et al., 1999]*
*Looking for level (2) info*



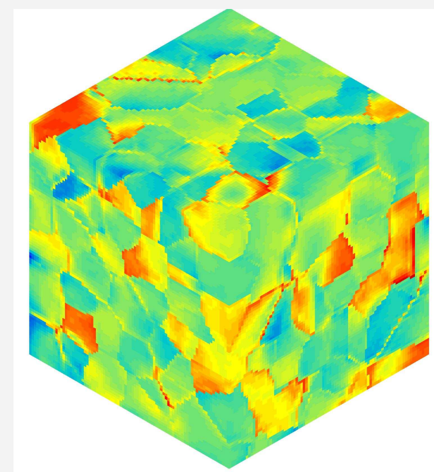

*[Mika and Dawson, 1999]*
*Looking for level (3) info*



# Polycrystal aggregates



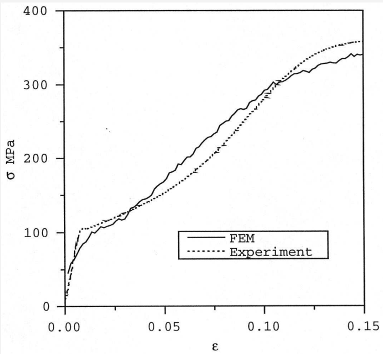
*28×28×28 mesh*



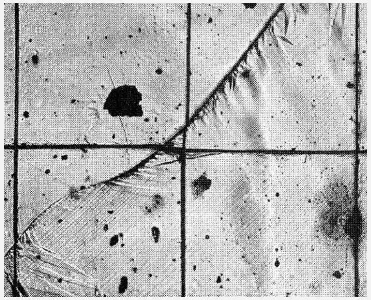
*Local field of von Mises stress*

## Slip and twinning in Magnesium

(more in [Staroselski and Anand, 2003])




*Compression on AZ31 works only with GB model*



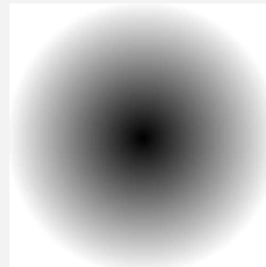
Hauser (1955)

*Slip system contribution + von Mises for GB's*

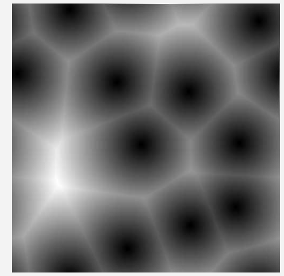
$$\underset{\sim}{\mathbf{L}}^p = (1-\xi)\sum_s \dot{\gamma}^s sign(\tau^s)\underset{\sim}{\mathbf{S}}^s_0 + \xi \underset{\sim}{\mathbf{M}}$$



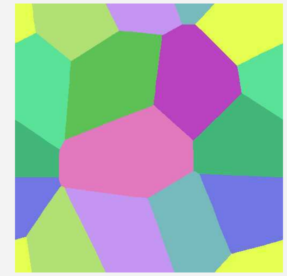
## Construction of Voronoï polyhedra



*Distance function of a single point source*



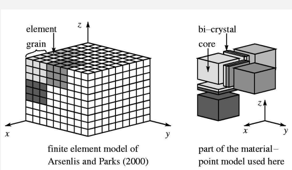
*Distance function of a set of point sources*



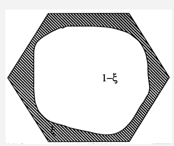
*Final result after construction and labelling*



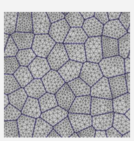
## A need for Grain Boundaries



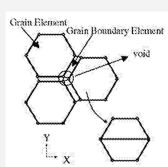

*[Evers et al., 2002]*




*[Staroselski and Anand, 2003]*



*[Cailletaud et al., 2002]*



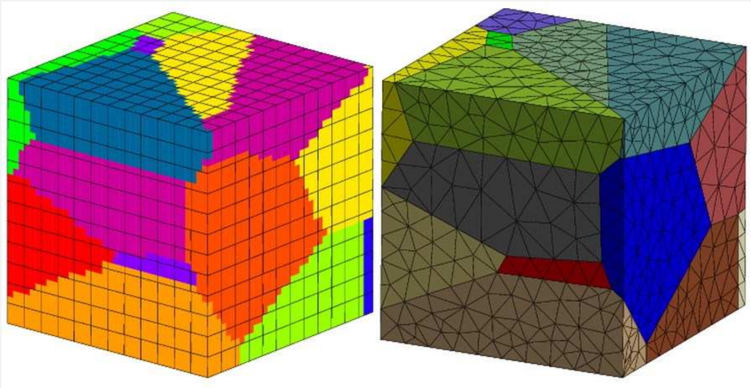

*[Kim et al., 2002]*



## State-of-the-art on cubic meshes and RVEs

- *Periodic cells – Polycrystal RVE*
- *Generally rather good for texture prediction, not so far from Taylor (too stiff)*
- *Representative provided 200–300 grains are used*
- *Validity of the local information on approximative geometries ?*
- Realistic morphologies are necessary to capture local stress and strain fields

## Typical realization and the associated meshes

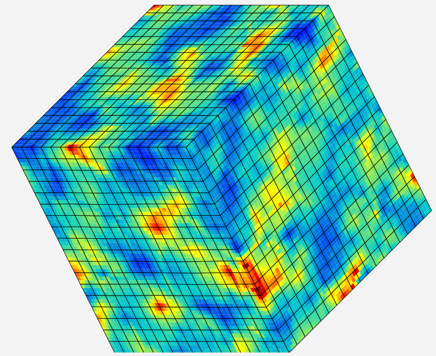


*Multiphase element technique* — *Real 3D mesh respecting grain boundaries*

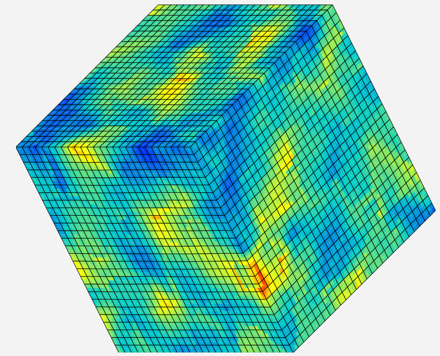


## Effect of the FE interpolation

- *Comparison between two strategies with 157464 integration points*



$18^3$ *= 5832 quadratic elts*

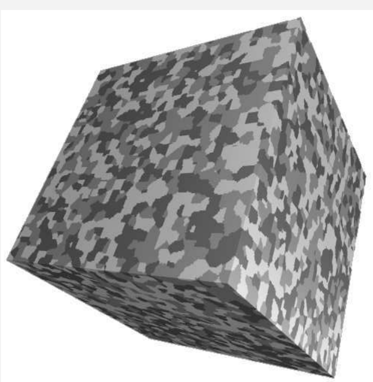


$27^3$ *= 19683 linear elts*

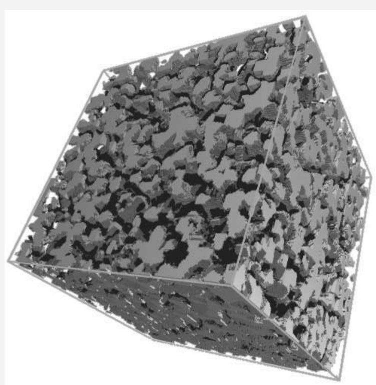
Contour of accumulated slip after 0.015 extension



## Example of a three phase material with 16000 grains



*Cubic domain of* $250^3$ *voxels*



*3D view*
*Extraction of phase 1*



## Tests on various FE configurations

- *Effect of the orientation distribution*
  - *Number of grains*
  - *Number of Euler angle sets*

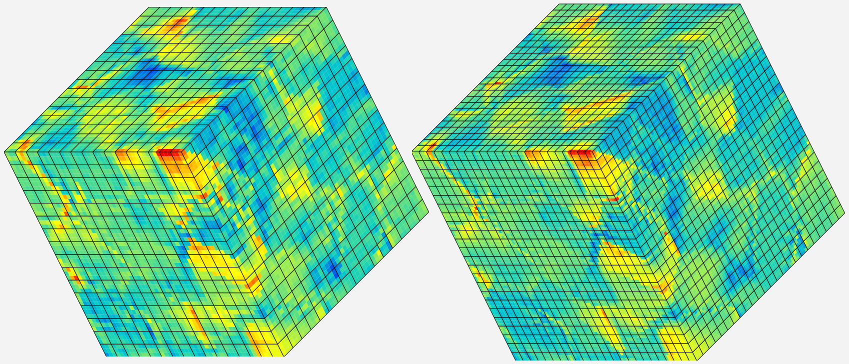
  $\longrightarrow$ 200 grains or more, randomly distributed
- *Effect of the FE interpolation*

  $\longrightarrow$ quadratic interpolation, full integration
- *Effect of mesh size*

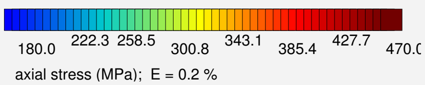
  $\longrightarrow$ 16 for macro, much more for local...

Tests made in tension, with $\underset{\sim}{\varepsilon} = \text{Diag}\,(\varepsilon, -0.5\varepsilon, -0.5\varepsilon)$

## Effect of the mesh size on local stress field



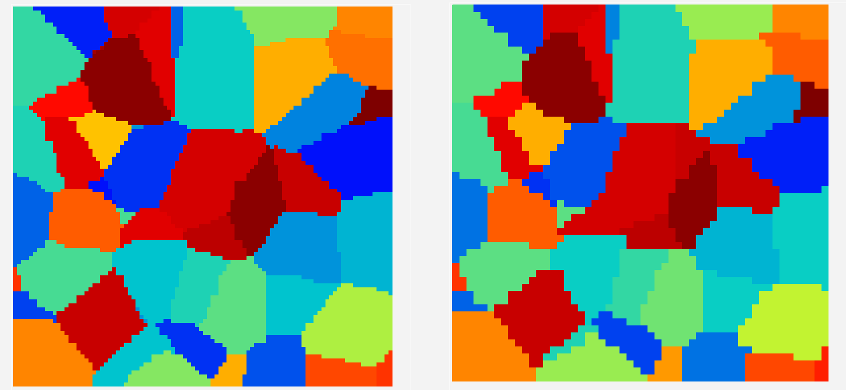
$16 \times 16 \times 16$ *elts* $24 \times 24 \times 24$ *elts*




Quadratic mesh, axial tension 0.2%, 200 grains



## Effect of the mesh size: geometry



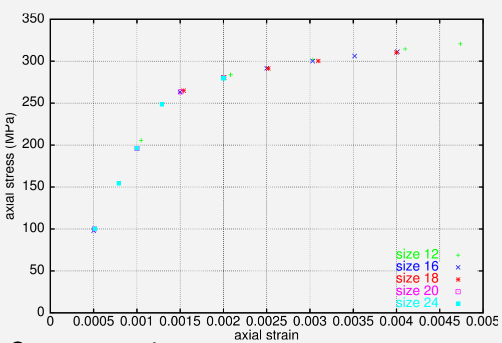
$32 \times 32 \times 32$ *elts* $18 \times 18 \times 18$ *elts*

Quadratic mesh, axial tension, 200 grains



## Effect of the mesh size

*Global response*




*Stress – strain curve*

*Local response*

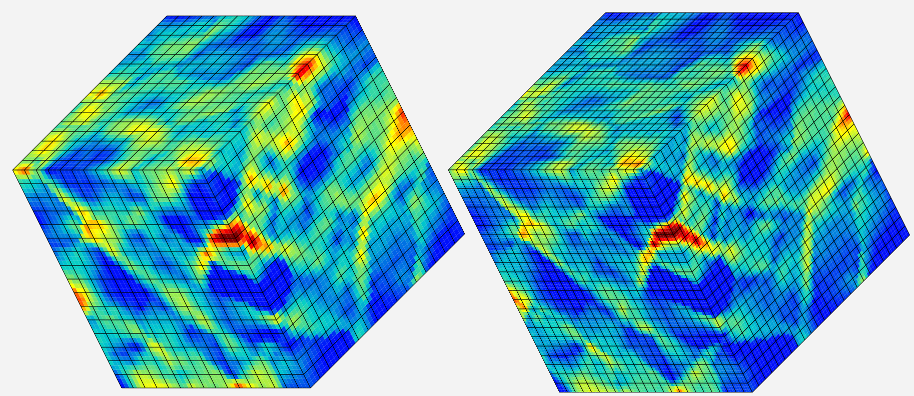
| *elt number* | *min* | *max* |
|---|---|---|
| $12^3$ | *194.80* | *411.02* |
| $16^3$ | *191.42* | *464.42* |
| $18^3$ | *185.68* | *456.90* |
| $20^3$ | *184.19* | *470.94* |
| $24^3$ | *180.37* | *470.91* |

*Min and Max local values of the axial stress*

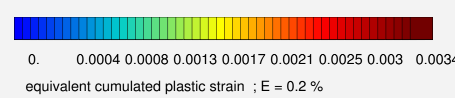
Pure extension to $\varepsilon_{zz} = 0.015$



## Effect of the mesh size on accumulated plastic strain



$16 \times 16 \times 16$ *elts* $24 \times 24 \times 24$ *elts*




Quadratic mesh, axial tension 0.2%, 200 grains

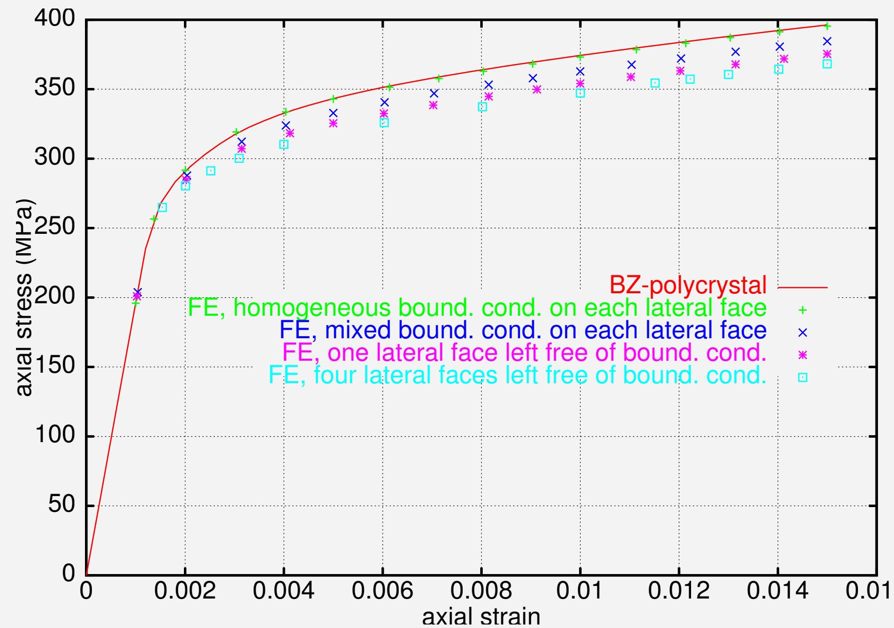
## The problem of the boundary conditions

- *From homogenization theory:*
  - *The macroscopic response of a RVE should be* independent *of boundary conditions*
- *Four boundary conditions have been used*
  - HSB *Homogeneous Strain at the Boundary: full constraint*
  - MB *Mixed Boundary condition: flat lateral faces*
  - 1FF *1 Free Face*
  - 4FF *4 Free Faces*

Tests made in pure tension, trying to keep a zero lateral force



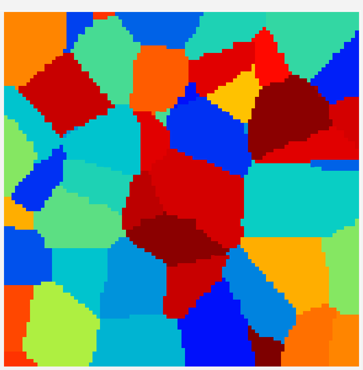
## Macroscopic responses: axial stress–strain curves

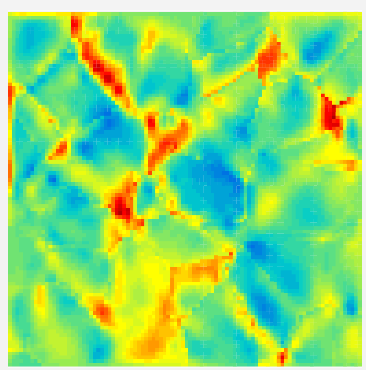



Homogeneous strain BC present the best agreement with BZ model



## Effect of the mesh size on accumulated plastic strain





range: 0.003 – 0.089

*Geometry*

$32 \times 32 \times 32$ *elts*

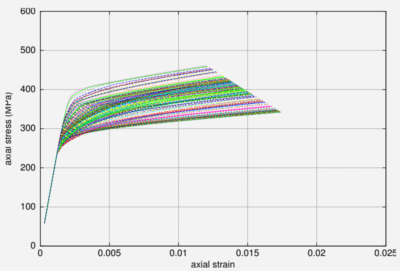
Quadratic mesh, axial tension 0.2%, 200 grains



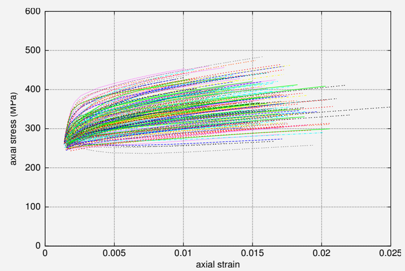
## Effect of the boundary conditions

- *Low on the macroscopic response (level 1)*
  - *Self–consistent model in good agreement with FE*
- *Significant on the mean value in the grain (level 2)*
  - *More scatter in FE than in self–consistent approach*
  - *More scatter in terms of stress for HSB*
  - *More scatter in terms of strain for 4FF*
- *Very high on intragranular fields (level 3)*
  - *Stress and strain gradients inside the grains*

## Grain responses: axial stress–strain curves




*Self–consistent model*



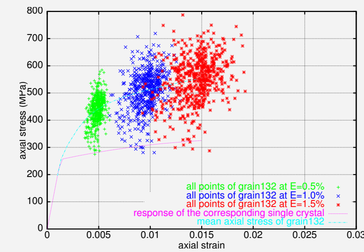

4 free faces

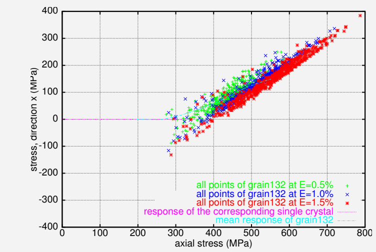
Axial $\sigma$–$\varepsilon$ curves , tension to $\varepsilon_{zz} = 0.015$



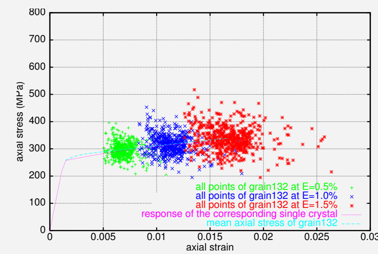
## Local response of the strongest grain

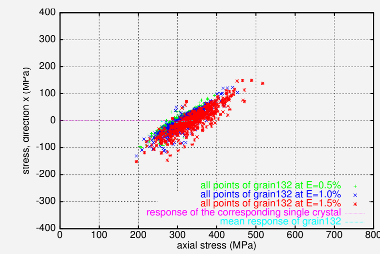
*Homogeneous strain*




*4 Free Faces*

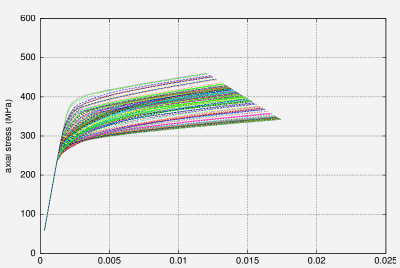


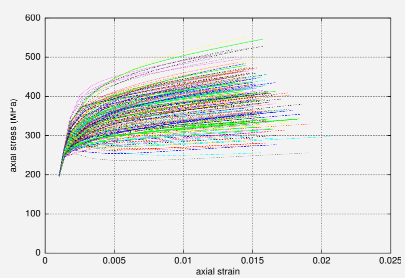

*Axial stress-strain curve* *Lateral* versus *axial stress*



## Grain responses: axial stress–strain curves




*Self–consistent model*



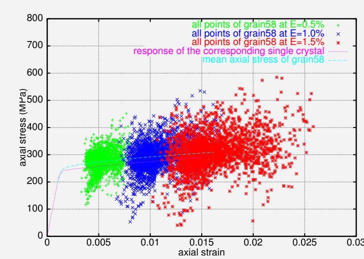

Homogeneous strain BC

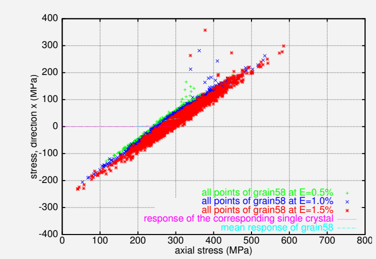
Axial $\sigma$–$\varepsilon$ curves , tension to $\varepsilon_{zz} = 0.015$



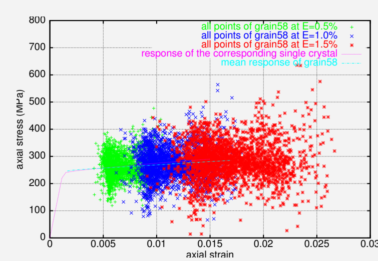
## Local response of the biggest grain

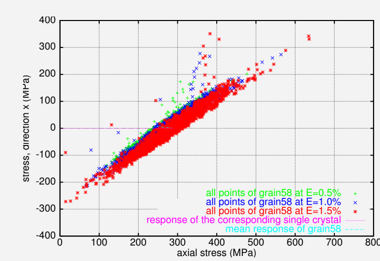
*Homogeneous strain*



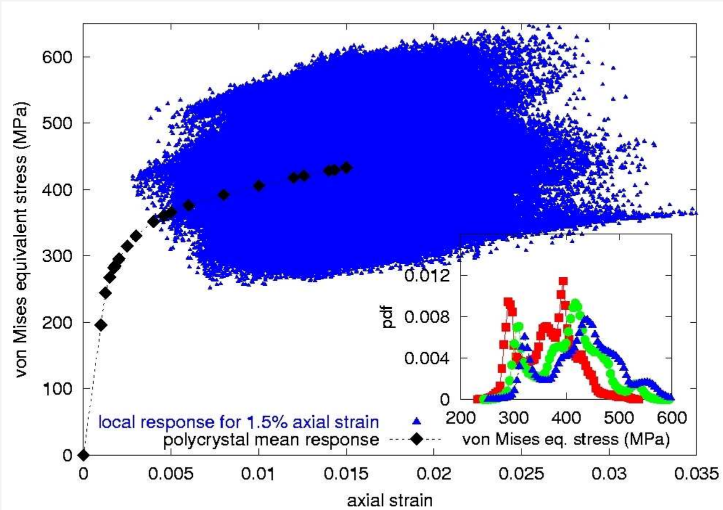

*4 Free Faces*




*Axial stress-strain curve* *Lateral* versus *axial stress*

## A result on all the Gauss points in the cube




Two populations ?

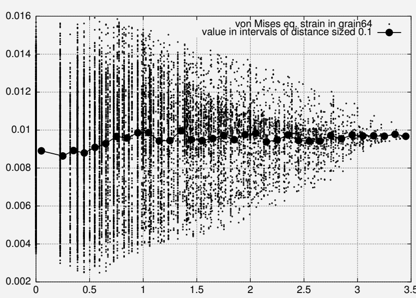


## Parallel computations

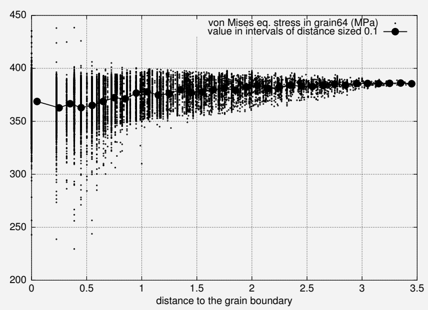
- *ZéBuLoN FE code*
- *Z-mat material library*
- *Computations on a linux PC cluster*
- *FETI method for parallel computation (with Onera/Feyel)*
- *August 2006: 160 64-bit processors*



## Scatter due to grain boundary (GB)




*Equivalent plastic strain*
versus *dist to the GB*




*Equivalent stress (von Mises)*
versus *dist to the GB*



## Perspectives

- *Provide information for the higher level*
- *Take information from lower level*
- *Use finer and finer meshes (parallel computing)*
- *Change the crystalllographic model (*HCP, next lecture *)*
- *Introduce damage (*intergranular damage and cleavage, next lecture *)*
- *Use in stress/strain fields presenting strong gradients, for instance with Cosserat type models, not shown here (*see for instance [Forest et al., 2000] *)*

more in [Barbe et al., 2001a, Barbe et al., 2001b, Barbe et al., 2003] [Cordier et al., 2005]

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