Modèles hiérarchiques (et réduction de modèles)

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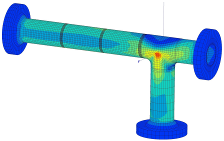
- *Macroscopic models*
- *Uniform fields approaches*
- *Microstructure computations*
- *Examples*

Centre des Matériaux

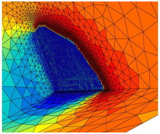
Idea League

http://mat.ensmp.fr

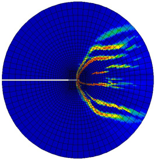
CoCaS: Mechanics of materials and structures



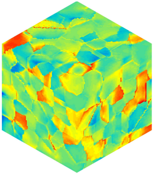
Structural computations



Crack propagation with cohesive zone models



Portevin-Le Chatelier effect



Microstructure calculations

- *Georges Cailletaud*
- *Samuel Forest*
- *David Ryckelynck*

20 PhD students, 3 post-doc

Modèles de calcul

- *Les modèles de conception de structure (modèles, codes)*
  Ces modèles (règles de construction) doivent être simples de manipulation et stocker sous forme éventuellement heuristique les connaissances sur des conceptions analogues. Pour ces modèles, la robustesse prime sur la performance.
- *Les modèles d'analyse de structure (modèles phénoménologiques)*
  Ce sont des modèles, éventuellement raffinés, destinés à l'étude de problèmes de champ sur un objet dont la géométrie, les matériaux, les conditions aux limites et les chargements sont connus. Pour ces modèles, la performance et la robustesse doivent faire l'objet d'un compromis équilibré.
- *Les modèles de compréhension du comportement de la matière (modèles multi-échelles)*
  Leur objectif principal est la compréhension fine du comportement à l'échelle locale. Pour ces modèles, la performance prime complètement sur la robustesse.

Stratégie de développement

- *Développement d'un code de calcul "maison"* Le développement du solveur Eléments finis *Zébulon* a commencé en 1982; le code *Z-set* qui en est issu est maintenant codéveloppé par le CDM, l'ONERA/DMSE, NorthWest Numerics, avec des coopérations à l'UTT et à l'ENS Cachan
- *Une librairie de modèles de matériaux* Une attention toute particulière est mise dans la représentation des comportements non-linéaires des matériaux; la librairie *Z-mat* est interfacée avec les principaux codes commerciaux
- *Les langages "orientés-objet"* Le choix du C++ est fait en 1992, avec réécriture totale du code
- *Le parallélisme* Utilisation d'un solveur parallèle (FETI) valide sur machine à mémoire *distribuée*, en coopération avec l'ONERA

Les buts du calcul de microstructures

- *Comprendre le "fonctionnement" du matériau* Etre capable de reproduire par la simulation un comportement est un gage de compréhension des mécanismes élémentaires
- *Obtenir des champs locaux, entrée des modèles de rupture* Le phénomène de rupture étant local, il est naturel qu'il soit modélisé à l'aide de variables de l'échelle locales, contraintes et déformations à l'échelle des grains dans un alliage, à l'échelle des phases dans un composite, par exemple
- *Créer une véritable "ingéniérie des matériaux"* Etre capable de prévoir des propriétés mécaniques ou physiques sans produire le matériau; optimiser le matériau vis-à-vis d'une sollicitation donnée

Contents

Contents

Ingredients of a mechanical model (small strain)

- *Strain partition*

$$\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^{in} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^p + \underset{\sim}{\varepsilon}^{vp}$$

with

$$\underset{\sim}{\boldsymbol{\sigma}} = \underset{\approx}{\boldsymbol{\Lambda}} : \underset{\sim}{\varepsilon}^e$$

- *Flow rules*
  - *Plasticity*

$$\dot{\underset{\sim}{\varepsilon}}^p = \dot{\lambda}\, \underset{\sim}{\mathbf{n}} \qquad \dot{\lambda} \quad \textit{from } \dot{f} = 0$$

  - *Viscoplasticity*

$$\dot{\underset{\sim}{\varepsilon}}^{vp} = \dot{p}\, \underset{\sim}{\mathbf{n}} \qquad \dot{p} = \left\langle \frac{f}{K} \right\rangle^n$$

- *Hardening rules*

$$\dot{Y}_I = fct(Y_I, \underset{\sim}{\varepsilon}^p, \underset{\sim}{\varepsilon}^{vp})$$

[Besson et al., 2001]

Common formalism for plasticity and viscoplasticity

- Same equations *for the strain partition and hardening rules*
- *Only the flow rule will differ: see for instance a model with von Mises criterion and isotropic hardening,* $f(\underset{\sim}{\sigma}) = J(\underset{\sim}{\sigma}) - R(p) - \sigma_y$
  - Plasticity *(point expected to be on the yield surface at the end of the increment)*

$$f = 0 \qquad J(\underset{\sim}{\sigma}) - R(p) - \sigma_y = 0$$

  - Viscoplasticity *(point expected to be on the relevant equipotential at the end of the increment)*

$$f > 0 \qquad J(\underset{\sim}{\sigma}) - R(p) - \sigma_y + K\dot{p}^{1/n} = 0$$

$$or \quad J(\underset{\sim}{\sigma}) - R(p) - \sigma_y + K\left(\frac{\Delta p}{\Delta t}\right)^{1/n} = 0$$

Common formalism for small and large strain

- Same equations *for the flow and hardening rules*
- *Only the partition rule will differ:*
  - *Small strain*

$$\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^{e} + \underset{\sim}{\varepsilon}^{in}$$

  - *Large strain*

$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{E}}\,\underset{\sim}{\mathbf{P}}$$

Case of multipotential models

- *Strain partition*, unchanged

$$\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^{in} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^p + \underset{\sim}{\varepsilon}^{vp}$$

- *Elasticity*, unchanged

$$\underset{\sim}{\boldsymbol{\sigma}} = \underset{\approx}{\boldsymbol{\Lambda}} : \underset{\sim}{\varepsilon}^e$$

- *Flow rules*
  - *Plasticity (e.g. crystal plasticity)*

$$\dot{\underset{\sim}{\varepsilon}}^p = \sum_s \dot{\lambda}^s \underset{\sim}{\mathbf{m}}^s \qquad \dot{\lambda}^s \text{ from } \dot{f}^s = 0$$

$$\text{for active systems} \qquad f^s = |\tau^s| - \tau_c = 0$$

  - *Viscoplasticity*

$$\dot{\underset{\sim}{\varepsilon}}^{vp} = \sum_s \dot{v}^s \, \underset{\sim}{\mathbf{m}}^s \qquad \dot{v}^s = \left\langle \frac{f^s}{K} \right\rangle^n$$

- *Hardening rules*

$$\dot{Y}_I = fct(Y_I, \underset{\sim}{\varepsilon}^p, \underset{\sim}{\varepsilon}^{vp})$$

Flow under strain rate control

$$\dot{\underset{\sim}{\sigma}} = \underset{\approx}{\mathbf{\Lambda}} : (\dot{\underset{\sim}{\varepsilon}} - \dot{\underset{\sim}{\varepsilon}}^p) \quad \textit{and :} \quad \underset{\sim}{\mathbf{n}} : \dot{\underset{\sim}{\sigma}} = H\dot{p}$$

$$\dot{\lambda} = \dot{p} = \frac{\underset{\sim}{\mathbf{n}} : \underset{\approx}{\mathbf{\Lambda}} : \dot{\underset{\sim}{\varepsilon}}}{H + \underset{\sim}{\mathbf{n}} : \underset{\approx}{\mathbf{\Lambda}} : \underset{\sim}{\mathbf{n}}}$$

$$\dot{\underset{\sim}{\sigma}} = \underset{\approx}{\mathbf{\Lambda}} : (\dot{\underset{\sim}{\varepsilon}} - \dot{\underset{\sim}{\varepsilon}}^p) = \left(\underset{\approx}{\mathbf{\Lambda}} - \frac{(\underset{\approx}{\mathbf{\Lambda}} : \underset{\sim}{\mathbf{n}}) \otimes (\underset{\sim}{\mathbf{n}} : \underset{\approx}{\mathbf{\Lambda}})}{H + \underset{\sim}{\mathbf{n}} : \underset{\approx}{\mathbf{\Lambda}} : \underset{\sim}{\mathbf{n}}} \right) : \dot{\underset{\sim}{\varepsilon}}$$

Continuous tangent operator $\underset{\approx}{\mathbf{L}}_t$

Note: for isotropic elasticity and von Mises material,

$$\dot{\lambda} = \frac{2\mu \, \underset{\sim}{\mathbf{n}} : \dot{\underset{\sim}{\varepsilon}}}{H + 3\mu}$$

Anatomy of constitutive equations

- *Definitions:*
  - External parameters *(*`ep`*) imposed as input*
  - Integrated variables *(*`vint`*)*
  - Auxiliary variables *(*`vaux`*), just for output*
  - Coefficients *(*`coef`*), material parameters*
  - Primal and dual variables, *prescribed variables and associated fluxes*
- *Three sets of equations are to be considered*
  - *Strain partition (1 tensorial variable)*
  - *Plastic/viscoplastic flow (1 scalar variable for each potential)*
  - *Hardening rules (model dependent)*

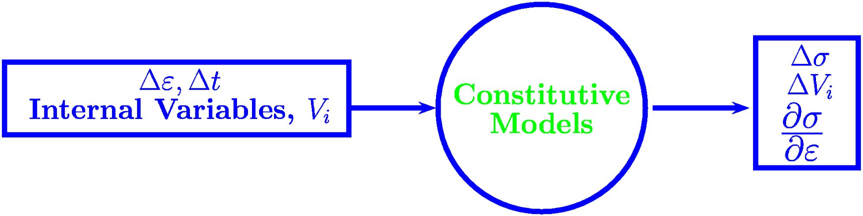
Primal and dual variables in various fields

problem	primal	dual
mechanics, small perturbation	$\underset{\sim}{\varepsilon}$	$\underset{\sim}{\boldsymbol{\sigma}}$
mechanics, large deformation	$\underset{\sim}{\mathbf{F}}$	$\underset{\sim}{\mathbf{\Pi}}$
thermal pb	$(T, \underline{\mathbf{grad}}\, T)$	$(H, \underline{\mathbf{q}})$
diffusion	*concentration*	*flux*
electrostatics	$\underline{\mathbf{grad}}\, V$	$\underline{\mathbf{E}}$
magnetostatics	$\mathrm{rot}\, \underline{\mathbf{A}}$	$\underline{\mathbf{H}}$

$\underset{\sim}{\varepsilon}$ *strain tensor,* $\underset{\sim}{\mathbf{F}}$ *deformation gradient,* T *temperature,* V *electric potential,* $\underline{\mathbf{A}}$ *potential vector,* $\underset{\sim}{\boldsymbol{\sigma}}$ *Cauchy stress tensor,* $\underset{\sim}{\mathbf{S}}$ *second Piola–Kirchhoff stress tensor,* H *enthalpy,* $\underline{\mathbf{q}}$ *thermal flux ,* $\underline{\mathbf{E}}$ *electric field* $\underline{\mathbf{H}}$ *magnetic field.*

Generic interface for any constitutive equation

For each Gauss Point...

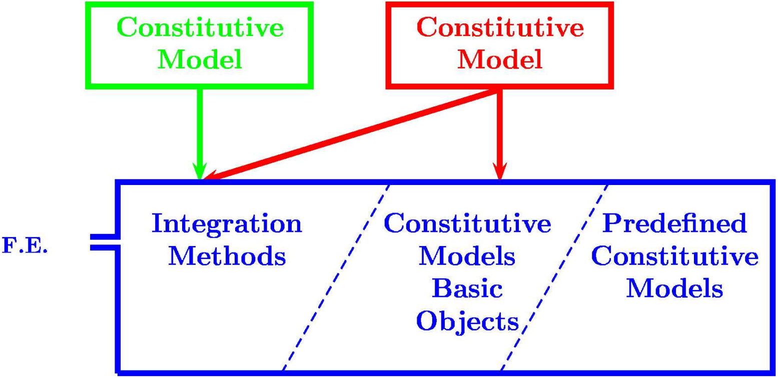


Example of the material library *Z-mat*

- *Numerous material models, plus* user *material*
- *Interface with the classical FE softwares*
- *Provide automatic time stepping and consistent tangent stiffness*
- *Coefficients presenting unlimited dependence on internal variables*
- *ZeBFRoNT, automatic code generation*
- *MuLTiMaT concept, for recursive multiscale modeling*

[zval@mat.ensmp.fr]

What is inside *Z-mat* ?



- **Runge-Kutta**
- **Theta method**

- **Elasticity**
- **Thermal Strain**
- **Isotropic Hardening**
- **Kinematic Hardening**
- **...**

Object oriented modular design in *Z-mat*

Material objects

- Flow
- Behavior
- Isotropic hardening
- Criterion
- Kinematic hardening
- Damage
- Elasticity
- Potential
- Thermal strain
- etc ...

Typical assembly for viscoplasticity

- Behavior
  - Elasticity
  - Thermal strain
  - Potential
    - Criterion
    - Flow
    - Isotropic hardening
    - Kinematic hardening
    - Kinematic hardening

Isotropic and nonlinear kinematic model in *Z-mat*

behavior

elasticity isotropic

thermal_strain isotropic $\underset{\sim}{\epsilon}^{th} = \alpha(T - T_{ref})$

potential ev

criterion mises $f = J\left(\underset{\sim}{\sigma}' - \sum_i \underset{\sim}{\mathbf{X}}_i\right) - R$

flow norton $\dot{p} = \left\langle \frac{f}{K} \right\rangle^n \quad , \quad \dot{\underset{\sim}{\epsilon}}^{ev} = \dot{p}\underset{\sim}{\mathbf{n}}$

isotropic nonlinear $R = R_0 + Q(1 - e^{-bp})$

kinematic nonlinear $\underset{\sim}{\mathbf{X}} = \frac{2}{3}C\underset{\sim}{\alpha} \quad , \quad \dot{\underset{\sim}{\alpha}} = \dot{p}\left[\underset{\sim}{\mathbf{n}} - \frac{3D}{2C}\underset{\sim}{\mathbf{X}}\right]$

Example of data files in *Z-mat*

Plasticity

```
***behavior gen_evp
  **elasticity isotropic
   young    100000.
   poisson  0.3
  **potential gen_evp ep
   *criterion mises
   *flow plasticity
   *isotropic nonlinear
     R0 210. Q 50. b 10.
   *kinematic nonlinear
     C 20000. D 500.
```

Viscoplasticity

```
***behavior gen_evp
  **elasticity isotropic
   young    100000.
   poisson  0.3
  **potential gen_evp ev
   *criterion mises
   *flow norton
     K 1000. n 4.5
   *isotropic nonlinear
     R0 210. Q 50. b 10.
   *kinematic nonlinear
     C 20000. D 500.
```

Crystal viscoplasticity

```
***behavior gen_evp
  **elasticity cubic
   y1111    100000.
   y1122    75000.
   y1212    112000.
  **potential octahedral
   *flow norton
     K 1000. n 4.5
   *isotropic nonlinear
     R0 210. Q 50. b 10.
   *kinematic nonlinear
     C 20000. D 500.
   *interaction slip
  h1 1. h2 1.2 h3 1.4 h5 1.3 h6 1.
```

ZeBFRoNT concept

- *Preprocessor, using building bricks like* `elasticity`, `flow`, *etc...*
- *Use a macrolanguage, with a limited number of keywords like* `Coefs`, `StrainPart`, `derivative`, `implicit`, *etc...*
- *Generate C++ code*

Explicit programming with *ZeBFRoNT*

`@Class NORTON_BEHAVIOR : BASIC_NL_BEHAVIOR`	
`{`	
`@Name norton;`	Nom du comportement
`@SubClass ELASTICITY elasticity;`	Objet matrice d'élasticité
`@Coefs K, n;`	Coefficients de Norton
`@tVarInt eel;`	Variable interne tensorielle : $\underset{\sim}{\varepsilon}_e$
`@sVarInt evcum;`	Variable interne scalaire : p
`};`	
`@StrainPart {`	Calcul de la contrainte après intégration
`sig = *elasticity*eel;`	$\underset{\sim}{\sigma} = \underset{\approx}{\mathbf{E}}\underset{\sim}{\varepsilon}_e$
`m_tg_matrix=*elasticity;`	Matrice tangente approchée (RK !)
`}`	
`@Derivative {`	Calcul du vecteur dérivé $\underline{\dot{Y}}$
`TENSOR2 sprime,norm;`	
`double J;`	
`sig=*elasticity*eel;`	
`sprime=deviator(sig);`	Calcul du déviateur $\underset{\sim}{\sigma}'$
`J=sqrt(1.5*(sprime|sprime));`	Calcul du deuxième invariant
`devcum=pow(J/K,n);`	Fluage de Norton : $\dot{p} = (\frac{J}{K})^n$
`norm=sprime*(1.5/J);`	Direction de l'écoulement
`deel=deto-devcum*norm;`	Déformation élastique
`}`	

Implicit programming with *ZeBFRoNT*

```
@CalcGradF {
  ELASTICITY& E=*elasticity;
  sig = E*eel;
  f_vec_eel -= deto;
  TENSOR2 sigeff = deviator(sig);
  double J = sqrt(1.5*(sigeff|sigeff));
  if (J>(double)0.0) {
    TENSOR2 norm = sigeff*(1.5/J);
    f_vec_eel += norm*devcum;
    f_vec_evcum -= dt*pow(J/K,n);
    SMATRIX dn_ds = unit32;
    dn_ds -= norm ^ norm;
    dn_ds *= theta*devcum/J;
    deel_deel += dn_ds *E;

    deel_devcum += norm;
    double dv_df = tdt*n*pow(J/K,n-1)/K;
    TENSOR2 df_fs = dv_df*norm;
    devcum_deel -= df_fs*E;

  }
}
```

Intégration implicite

$\underset{\sim}{\sigma} = \underset{\approx}{\mathbf{E}}\underset{\sim}{\varepsilon}_e$

$\underset{\sim}{\mathbf{Re}} = \Delta\underset{\sim}{\varepsilon}_{\mathbf{e}} - \Delta\underset{\sim}{\varepsilon}$

Déviateur $\underset{\sim}{\sigma}'$

Deuxième invariant

Si on a plastifié

Direction de l'écoulement $\underset{\sim}{\mathbf{n}}$

$\underset{\sim}{\mathbf{Re}} = \Delta\underset{\sim}{\varepsilon}_{\mathbf{e}} - \Delta\underset{\sim}{\varepsilon} + \Delta p\underset{\sim}{\mathbf{n}}$

$\Delta p = (\frac{J}{K})^n \Delta t$

$\frac{\partial \underset{\sim}{\mathbf{Re}}}{\partial \Delta\underset{\sim}{\varepsilon}_{\mathbf{e}}}$

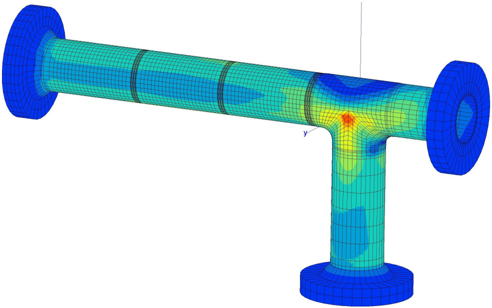
$\frac{\partial \underset{\sim}{\mathbf{Re}}}{\partial \Delta p}$

$\frac{\partial Rp}{\partial \Delta\underset{\sim}{\varepsilon}_{\mathbf{e}}}$

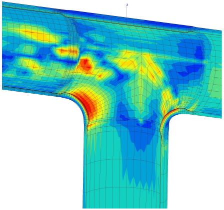
$\frac{\partial Rp}{\partial \Delta p} = 1$

Contents

Tubes in nuclear power plants



Contour of the von Mises stress

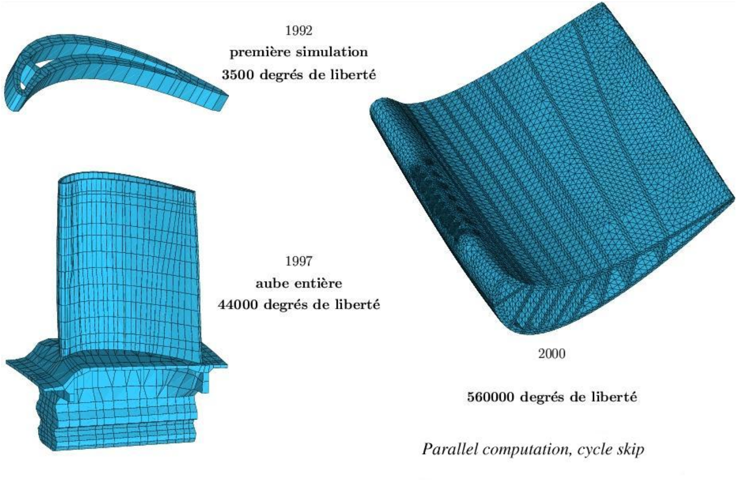


Zoom on the critical area

600 000 dof's, 1000 time steps

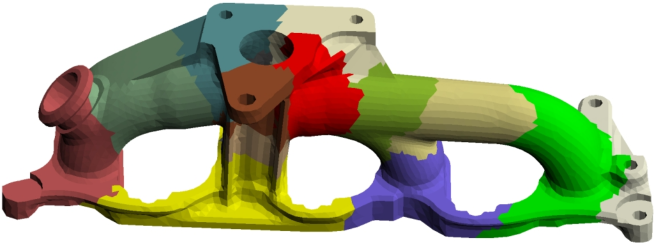
Collaboration with EDF

Turbine blades (SNECMA)



1992: One slice only 1997: Real 3D computation with viscoplastic constitutive equations 2000: Mesh taking into account the detailed geometry

Exhaustion system in car engine (Renault)

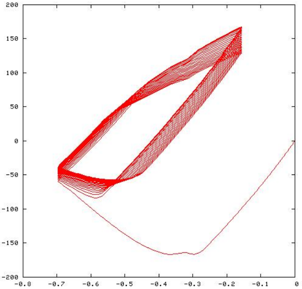


345000 dof's, viscoplastic computation including aging

Subdomains in a mesh for parallel computation

GEN-EVP - Application to Aluminum with aging

If aging is purely time based, direct integration can be used and the effect applied to all material coefficients

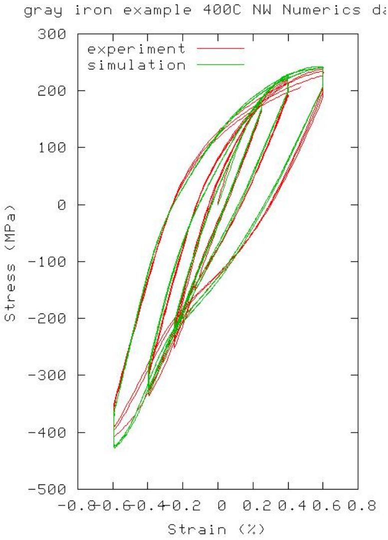



```
%the **auxiliary aging option is part of the base behavior,
%and can therfore be used to implement time based (or
%weakly coupled) coefficient dependencies
%
 **auxiliary aging age_1
     aging_inf   temperature
        0.          0.
        0.5       200.
        0.7       280.
        0.9       324.
     tau         temperature
        1.e+07      0.
        1.e+06    150.
        1.e+05    200.
        12500.    250.
        2500.     280.
        500.      300.
        100.      324.

  *kinematic   nonlinear X1
   C  aging_effects param:age_1 factor:1.0  temperature
         16000.       0.
         15000.      20.
             0.     324.
         D          100.
```

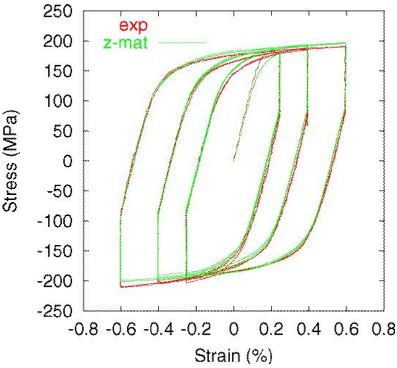
Cast Iron material Model

- **Very general framework including :**
  - *Viscoplasticity and flow rule*
  - *Nonlinear kinematic herdening with no limit on number of terms*
  - *Isotropic hardening / softening*
  - *Adjustable damage evolution strain closure shifts compressive with damage, opening occurs at zero stress*
  - *Fatigue damage terms correlated to peak stress and accumulated plasticity*
- **Successfully used in production FEA (e.g. ABAQUS) for more than 5 years now**



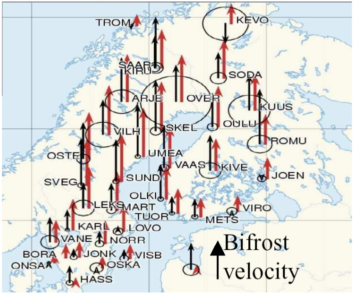
GEN-EVP - SiMo type Materials

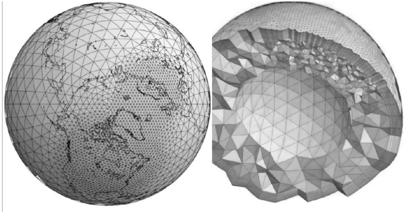
- **Viscoplasticity**
  - *Rate law should take into account wide range of rates ... Norton summation or multiple deformation potentials*
  - *Kinematic hardening is necessary even if yield radius is zero! Kinematic shift of yield locus*
  - *Static recovery required for full relaxation at very high temperatures*
  - *Relatively high number of temperatures required to calibrate e.g. 23, 150, 225, 300, 375, 450, 525, 600, 720, 740, 800...*



For structures like exhaust manifolds, the viscous effects are important to determine transient effects..e.g. frictional movements and structural ratchetting rates

Post-glacial rebound

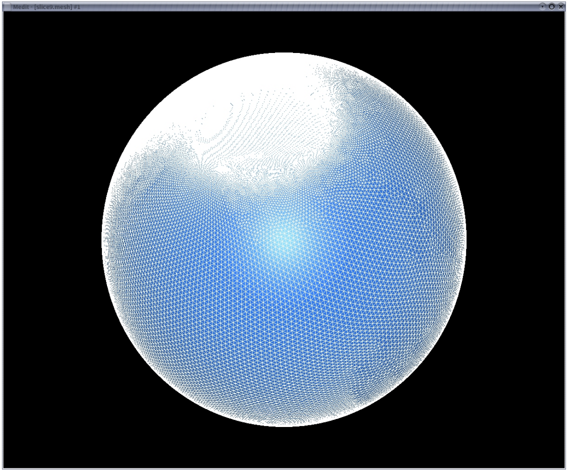




- *20000 years ago, a big amount of ice on Scandinavia and Canada (until 3000 m)*
- *Ice melting, the continents go up*
- *Question 1: Sea level ?*
- *Question 2: Earth mantle viscosity (earthquake prediction)*

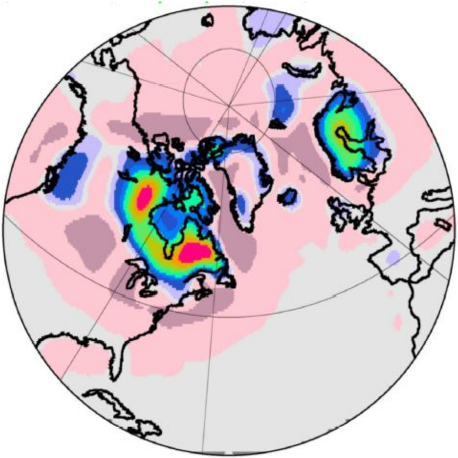
Collaboration with ENS Ulm

Post-glacial rebound: *New meshes*



9600000 dof's, 100 processors

Post-glacial rebound: *First results*

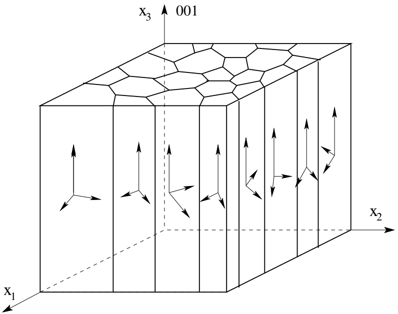


Contents

The limits of the classical yield criteria

- *Initial texture, texture evolution*
  - *Directionnally solidified materials*
  - *Metal forming*
- *Need for a local information in phases*
  - *Phase transformation, several coexisting phases*

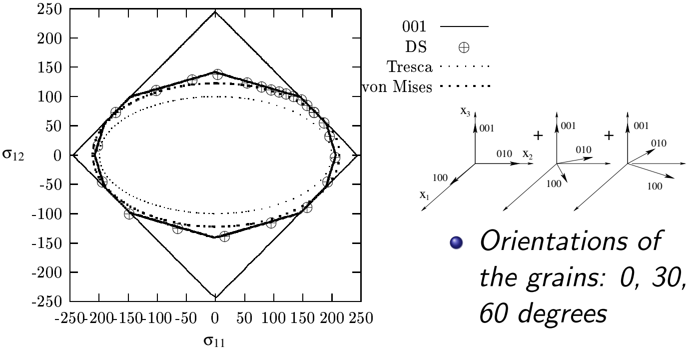
Loading surface of a directionally solidified material (DS)



- *For a DS material, all the grains have a common crystal axis, say (001). The orientation of each grain is then defined by one angle around this axis.*
- *Assuming that elasticity is uniform, the stress is also uniform during the elastic phase.*

[Sai et al., 2006]

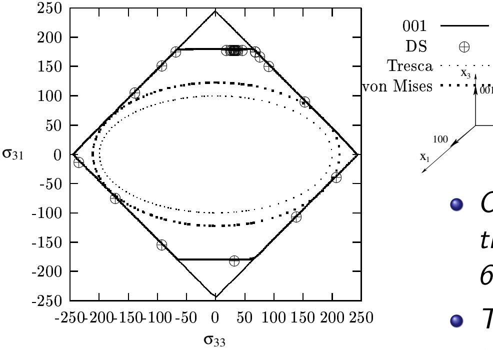
Yield surface for DS material with *3 orientations*

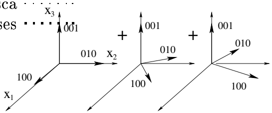


- *Orientations of the grains: 0, 30, 60 degrees*

More slip directions in the plane σ_{11}–σ_{12}: the model turns out to become similar to von Mises/Tresca

Yield surface for DS material with *3 orientations*



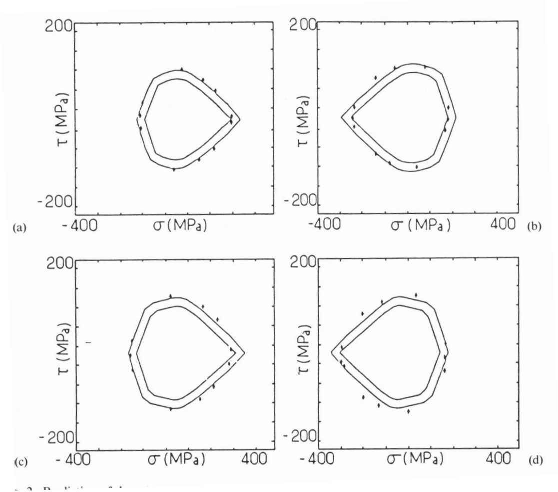


- *Orientations of the grains: 0, 30, 60 degrees*
- *Try an other set* HERE

No additional slip activated by shear in the plane σ_{33}–σ_{13}: the yield stress in shear remains high, and sharp corners are still present

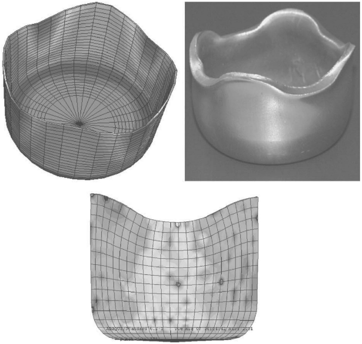
Simulation of the distorsion of a yield surface

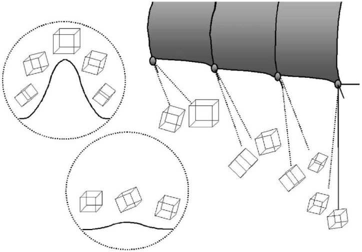
First cycle and second cycles, 2024 luminium alloy



[Cailletaud, 1992]

Deep drawing, one polycristal for each Gauss point





([Raabe and Roters, 2004])

Contents

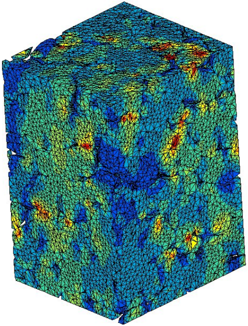
What comes out microstructure computations

- *Homogenization results*
  - *Equivalent properties for a given microstructure*
- *Results in each phase*
  - *Average values in each phase*
- *Intragranular fields, results near grain boundaries*
  - *Local values inside grains*
- *Real fields in critical zones*
  - *when microstructure size is not small wrt stress gradients*

Contents

Two-phase refractory materials

- Aim: predict the thermomechanical behaviour

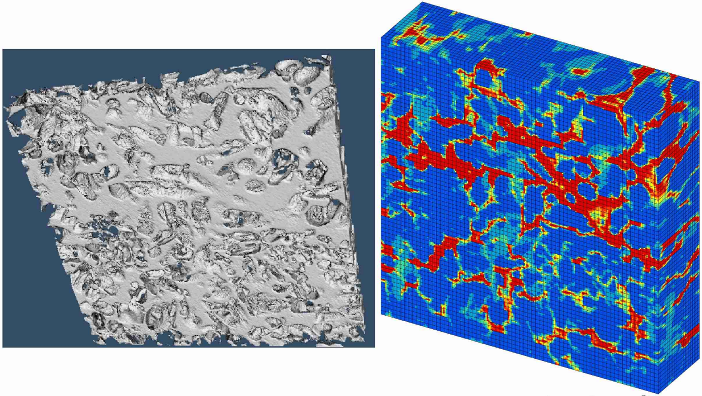


Calculation on a RVE
$350\mu m \times 350\mu m \times 350\mu m$

1300 000 node mesh
$350\mu m \times 350\mu m \times 700\mu m$

[Madi et al., 2007]

Ice cream

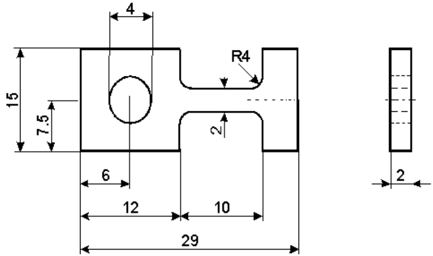


imagerie 3D confocale — calcul parallèle à 10^6 ddl

[Kanit et al., 2003]

Contents

A test on small OFHC copper specimens



Tension tests on a small flat specimen made of OFHC copper

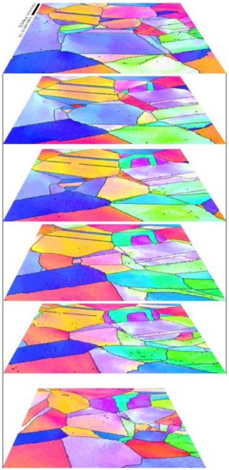
Data available:

- *Macro stress-strain curve*
- *SEM images*
- *OIM scans*
- *Local strain field*

[Tatschl and Kolednik, 2003, Tatschl and Kolednik, 2004]

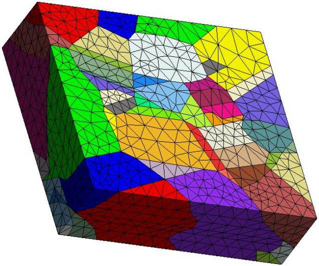
Erich Schmid Institute of Material Science, Leoben, Austria

3D grain morphology information

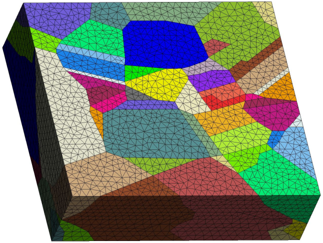


- *After the test, 6 layers of material were successively removed*
- *Final depth – 100 μm*
- *OIM-analysis was made after each removal*
- *3D grain structure can be reconstructed*

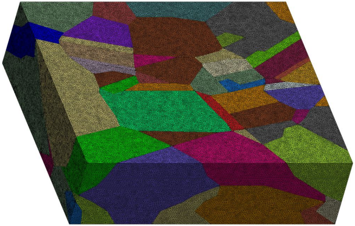
Polycrystal computations



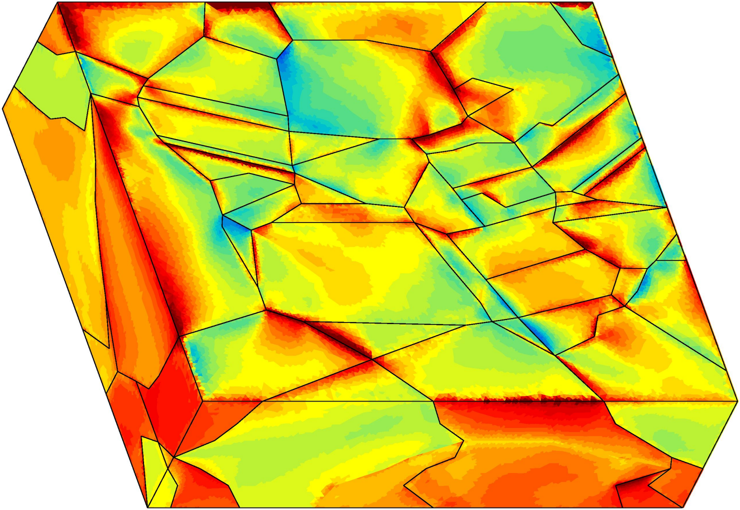
30 000 nodes



130 000 nodes



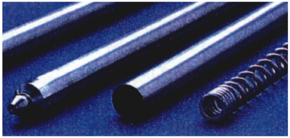
Local strain in a polycrystal



[Musienko et al., 2007]

Contents

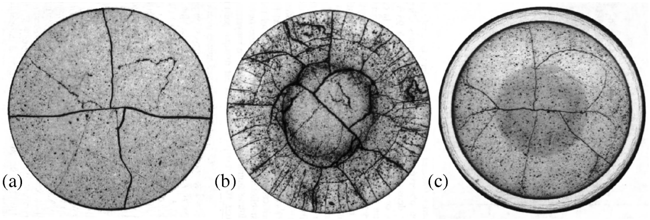
Presentation of the industrial framework



- *Integrity of fuel assemblies of PWR*
- *Fuel rods made of uranium dioxide pellets piled in a Zy4 cladding*
- *Zy4 cladding is the first protection to avoid fission products spreading*
- *Incident called* Pellet – Cladding Interaction

[Diard, 2001, Musienko, 2005]

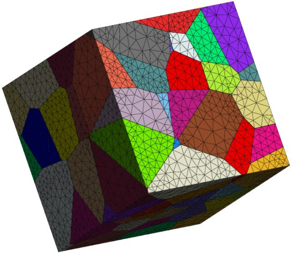
Pellet Crack Patterns

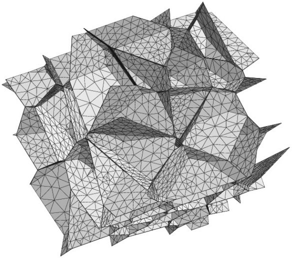


After one irradiation cycle

- *Expansion of the uranium oxide, then indentation of the tube by the fragments*
- *Dimension of the tube : diameter 8 mm, thickness 0.7 mm*

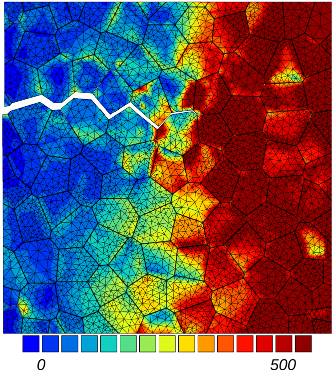
3D - a 100 grain aggregate



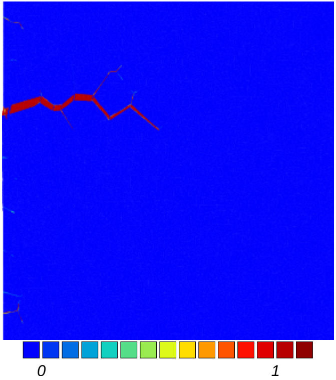


- *2 element boundaries, hexahedra, prisms, tetrahedra, quadratic and quadratic/linear elements*
- *Local orientation to determine normal to the grain boundary*

2D iodine-influenced intergranular fracture (DOS+iodine)

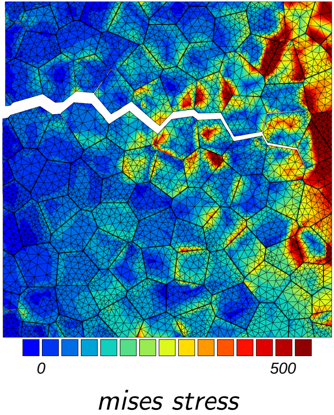


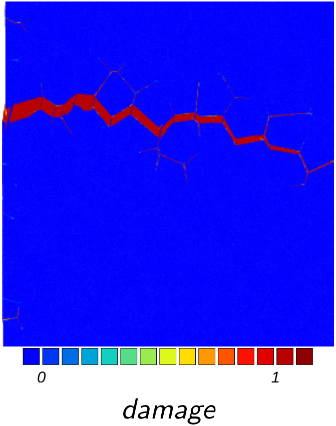
mises stress



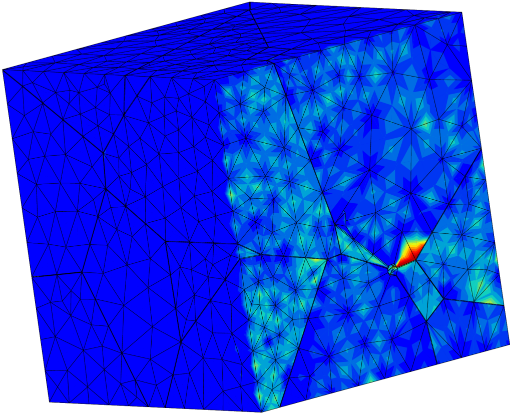
damage

2D iodine-influenced intergranular fracture (DOS+iodine)



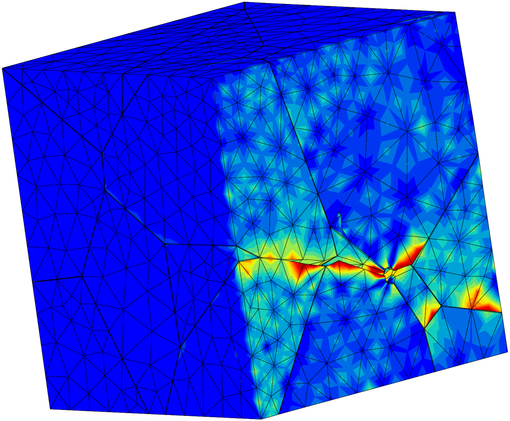


Crack opening



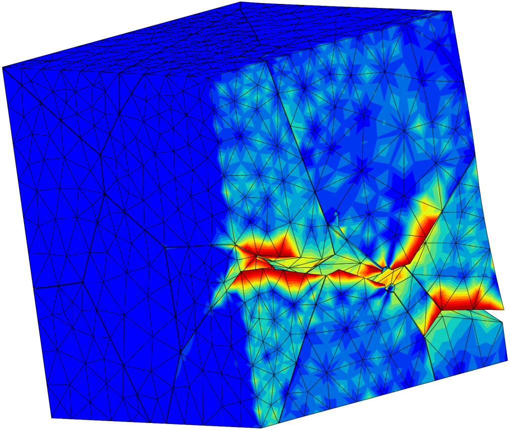
[Cailletaud et al., 2004]

Crack opening



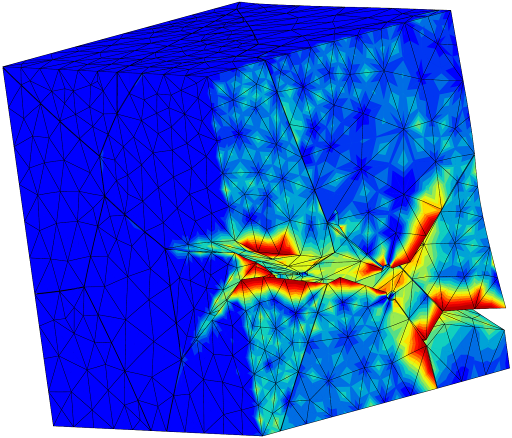
[Cailletaud et al., 2004]

Crack opening



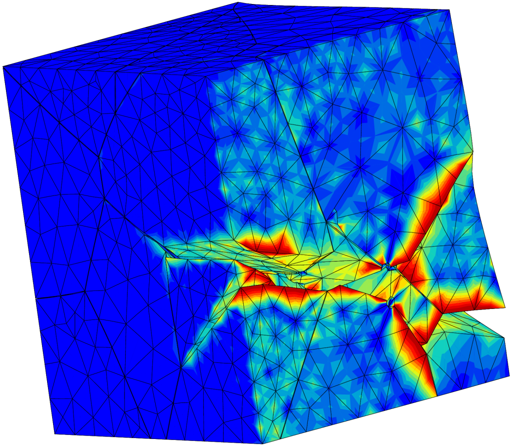
[Cailletaud et al., 2004]

Crack opening



[Cailletaud et al., 2004]

Crack opening



[Cailletaud et al., 2004]

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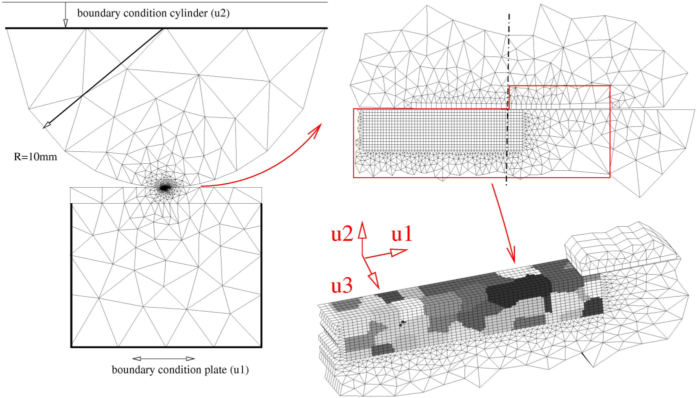
3D FE model of a fretting wear test

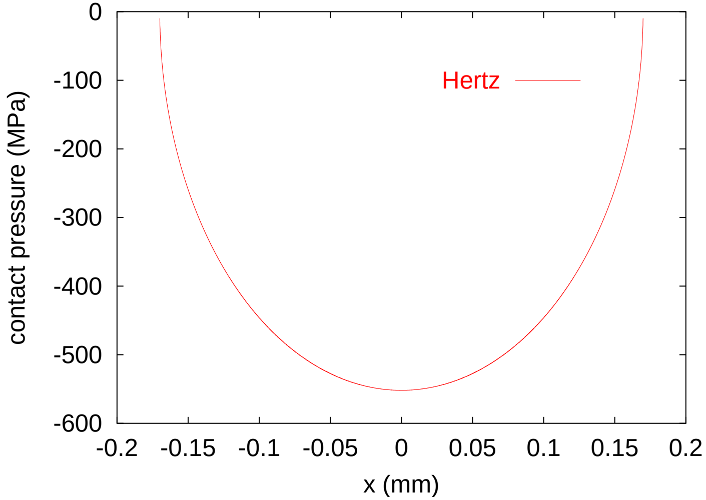


Computation settings	
mesh	*linear plane strain elements*
u3	*zero displacement on front and back planes*
u2	*set to cause vertical force* $\mathrm{P} = 133\ \mathrm{N}$
u1	$\delta_{\max} = 75\ \mu\mathrm{m}$
friction coefficient	*0.8*
cycling frequency	$5\ \mathrm{Hz}$

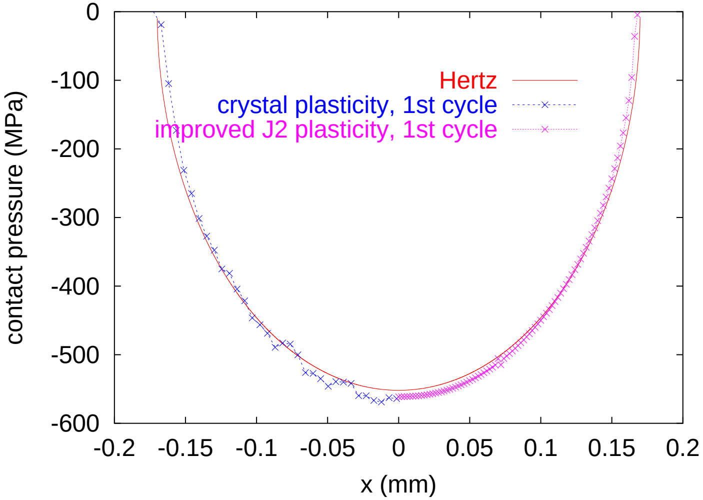
- *element size in contact* $5.4\mu\mathrm{m}$ *x* $5.4\mu\mathrm{m}$ *x* $6.3\mu\mathrm{m}$
- *small deformations formulation*

[Dick et al., 2006]

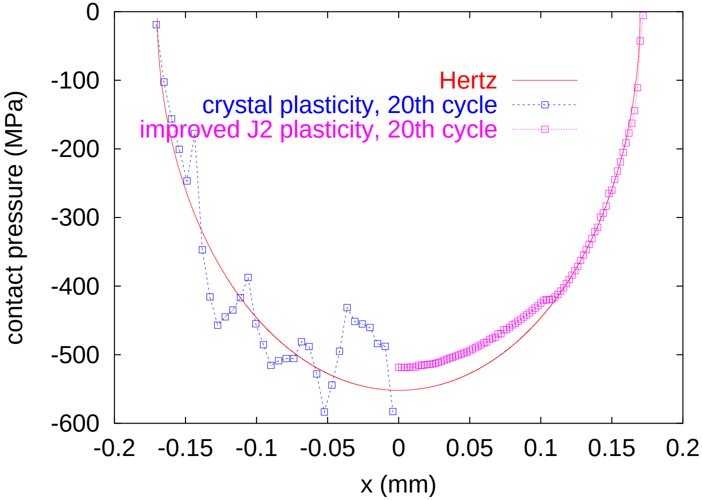
Computation Results: contact pressure



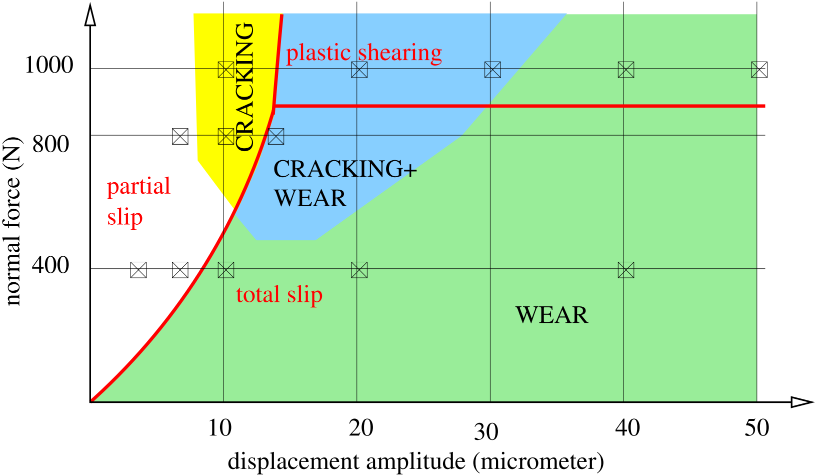
Computation Results: contact pressure



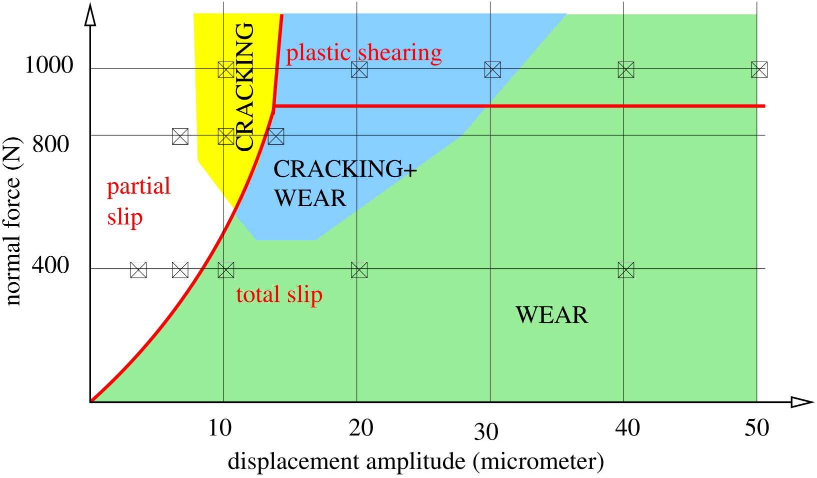
Computation Results: contact pressure



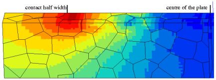
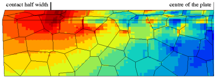
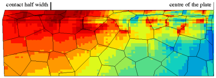
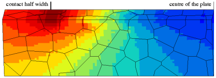
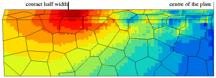
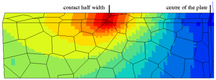
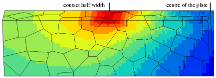
Fretting damage map



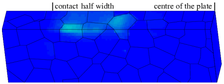
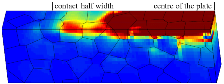
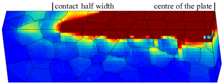
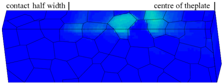
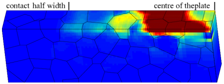
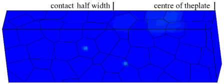
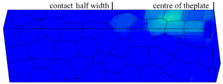
Fretting damage map



Dang Van equivalent stress fields after 20 cycles

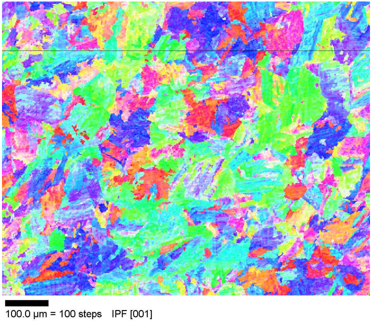
F (N)	δ=6 or 10 μm	δ=20 μm	δ=50 μm
1000	 *Max* = *952 MPa*	 *Max* = *1058 MPa*	 *Max* = *1087 MPa*
800	 *Max* = *911 MPa*	 *Max* = *1002 MPa*	*Crack initiation (end of contact zone) predicted provided the force is larger than 800 MPa*
133	 *Max* = *700 MPa*	 *Max* = *751 MPa*	*Are cracks erased by plasticity in the contact area ?*

Total slip fields after 20 cycles

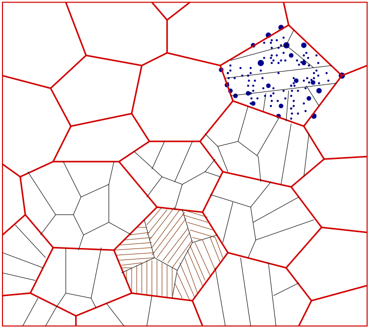
F (N)	δ=6 or 10 μm	δ=20 μm	δ=50 μm
1000	 Max = 0.042	 Max = 0.91	 Max = 2
800	 Max = 0.037	 Max = 0.16	*Wear promoted when total slip is higher than 1% per cycle*
133	 Max = 0.011	 Max = 0.025	*No noticeable effect for total slip lower than 0.1% per cycle*

Contents

Microstructure description, 16MND5 bainitic steel



EBSD image

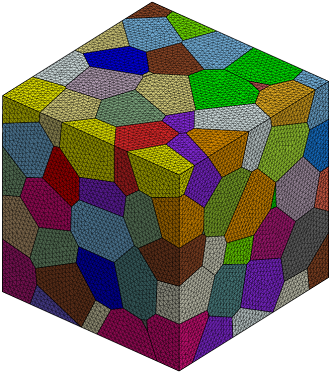


Schematic view

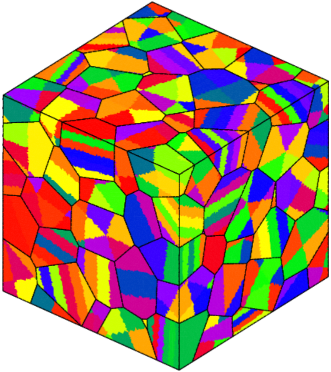
– grain size= 50μm – packet size=15μm – lath size=2μm –
– carbide size = 1μm –

PhD. Nikolay Osipov, dec. 17, 2007

Synthetic microstructure of austenitic and bainitic phases



Austenitic phase represented by 120 Voronoï grains



Bainitic microstructure
$\approx$ 1000 bainitic packets
3 types of cutting

Steps to generate a free–free mesh

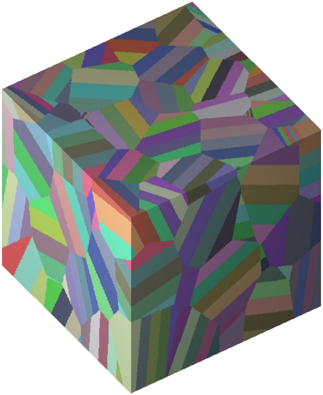


Image generation

Steps to generate a free–free mesh

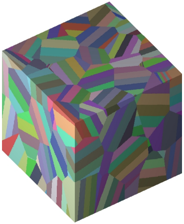
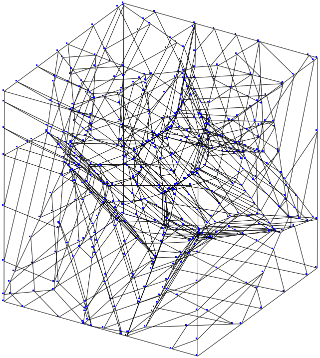


Image generation



Geometry reconstruction

Steps to generate a free–free mesh

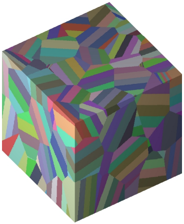
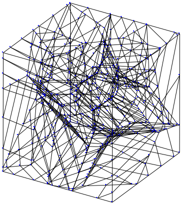
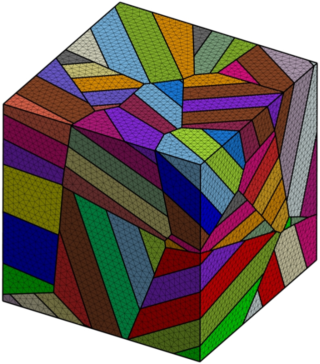


Image generation

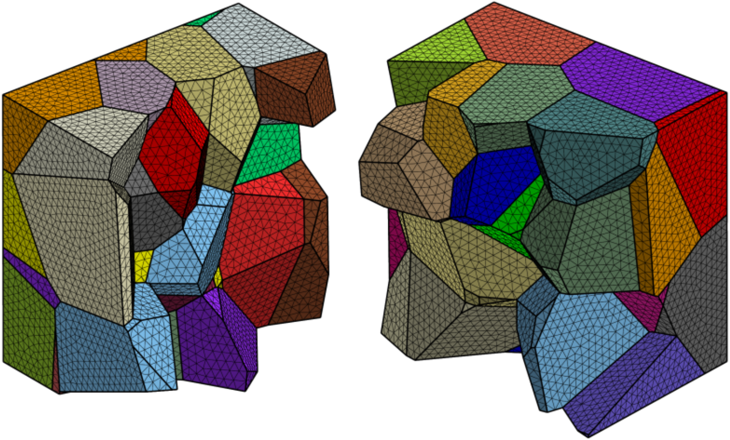


Geometry reconstruction

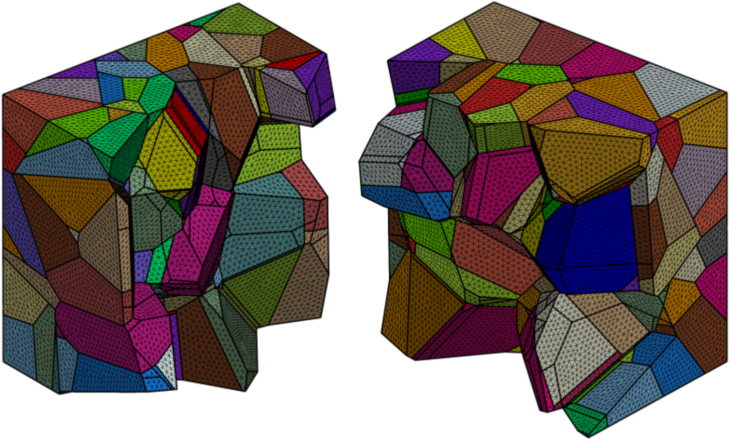


Free mesh generation

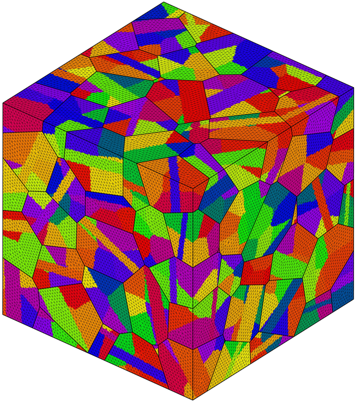
Free mesh of an austenitic microstructure before cutting (50 grains)



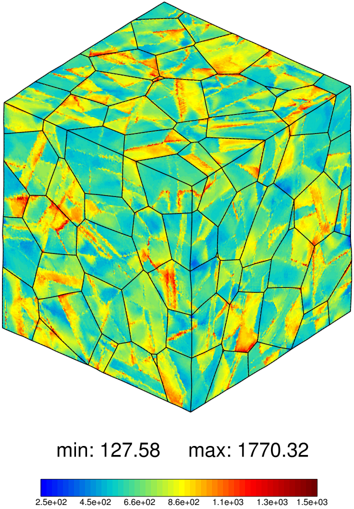
Free mesh of a bainitic microstructure after cutting (50 grains, 245 subgrains)



Von Mises stress in the representative volume element

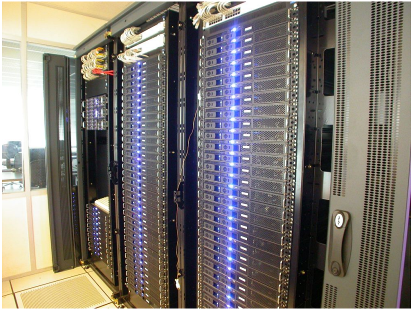


$9 \cdot 10^6$ *dof*



PC clusters

50 processors
32 bits/800 MHz
50 Go memory
2000–2005



224 processors
64bits/2.2GHz
776 Go memory
2005–2009

- *Financial support of Région Ile-de-France and Département de l'Essonne*
- *In connection with Pôle de compétitivité System@tic and Teratec*

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In Ahzi, S., Khaleel, M., Zbib, H., Zikry, M., LaMatina, B., and Cherkaoui, M., editors, Multiscale Modelling and Characterisation of Elastic-Inelastic Behaviour of Engineering Materials (Proc.of the IUTAM Symposium on Multiscale Modelling of Engng. Materials. Marrakech, Oct. 2002), *pages 149–156. Kluwer.*

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Un exemple de couplage comportement–endommagement–environnement dans les polycristaux. Application à l'interaction pastille–gaine.
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Experimental and numerical analysis of local and global plastic behaviour in fretting wear.
Tribology International, *39:1036–1044.*

Kanit, T., Forest, S., Galliet, I., Mounoury, V., and Jeulin, D. (2003).
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