A multigrid method for the design of heterogeneous material in tribology

Hugo Boffy – Kees Venner
Context

- Reduction of the industrial costs and green policy are daily problems
- Higher level of stresses - improvement of performances and fatigue life
- Focus on interfaces between elements
- Advanced numerical methods are required
- Analysis performed by engineers to provide innovative and efficient solutions (materials)!
Objectives

- Modelling of homogeneous and heterogeneous materials
- Be able to deal with low and high property ratios
- Provide accurate solutions in local area/volume
- Fast solution to have low turn around time of computations

Perform 3D simulations involving millions DoF
Be able to get accurate solutions at low numerical costs
Outline

- 3D numerical tool
- Multigrid method
- Advanced numerical tools for heterogeneous material design
- Applications
- Conclusion
3D numerical tool

Lame's equations

- 3 PDE

\[(\lambda u_{j,j})_{,i} + (\mu u_{i,j})_{,j} + (\mu u_{j,i})_{,j} = 0 \quad i,j=1,2,3\]

- \(\lambda, \mu\): Lame's coefficients
depend of material properties: \((E, \nu) = f(x,y,z)\)

- \(u_i\): displacements along \(x, y\) and \(z\) (unknowns)

- Both Neumann and Dirichlet boundary conditions can be imposed
How to solve the equations: finite difference method

Lame's equations can be written as a system of equations: \( L^h<u>_{i,j,k} \)

- The discrete operator \( L^h \) uses a second order scheme

- Residual: \( r^h_{i,j,k} = f^h_{i,j,k} - L^h<u>^h_{i,j,k} \)

- Converged solution: \( r^h_{i,j,k} = 0 \) for all point \( M[i,j,k] \) in the computation domain

- Iterative solver: adjust solution point by point such that the residual is reduced or eliminated.

- Sweep across all points: relaxation (Gauss-Seidel).
Multilevel method

- Highest level should represent solution with the desired accuracy.

- Lower levels are a means to accelerate the convergence speed. The solution and the residuals are transferred between the different level of grids.

- Components with a low frequency relative to a fine grid have a high frequency relative to a coarse grid.
A common multilevel schedule

Full Multigrid cycle

finest grid $k^3$

$k/2^3$

...$

coarsest grid

Final solution

time

● = relax

\ = interpolate

\ = restrict
Local refinement strategy

- Be able to realize very precise local calculations:

- Advantages:
  
  Reduction of memory cost
  
  Reduction of CPU time
  
  Increase of the number of levels
  
  Higher accuracy in the refined volume

- Convergence speed of the algorithm not affected [1]

Polycrystalline media [1]

- Heterogeneous structure:
  
  4000 grains (Voronoi tessellation)
  Gaussian distribution of the properties
  Grain size and shape controlled by the algorithm

- Numerical modeling:
  
  Top surface: Hertzian pressure \((a_0, P_0)\)
  Bulk size \([8a_0, 8a_0, 4a_0]\)
  Meshing: 5 global levels - 3 local levels
  Polycrystalline behavior restrain on \(\Omega_8\)
  Number of points: \(11.10^6\)
  CPU time: 15-20 minutes

Polycrystalline media

Computation of the Von-Mises stresses
Inclusions in an homogeneous media

- Presence of 2 inclusions in an homogeneous media (E, ν):
  
  - Inclusion 1
    size: R1=0.05
    mechanical properties: E1=0.01E , ν₁=ν
  
  - Inclusion 2
    size: R2=0.1
    mechanical properties: E1=5E , ν₁=ν
  
- Numerical modeling :
  Top surface : Hertzian pressure (a₀,P₀)
  Bulk size [8a₀,8a₀,4a₀]
  Meshing : 5 global levels - 3 local levels
  Number of points : 11.10⁶
  CPU time : 15 minutes
Application: spherical hole in an homogeneous material

- Homogeneous material \((E,\nu)\) with a spherical void \((E_v/E=1/1000)\)
- Bulk size: \([0.1;0.1;0.1]\)
- Mesh: \([257;257;257]\)
- BC : Hertzian pressure top surface
  Zero displacements bottom
  Free other boundaries
- CPU time < 10 min
- Principal stress \(\sigma_1\) in the plan \((x,y=0,z)\)
Hard fibers in an infinite matrix

- Two coated copper fibers inside an epoxy matrix.

- Soft and hard interphases are considered

- Bulk size: [0.1;0.1;0.1]

- Mesh: [513;513;513]

- BC: vertical displacement $w_0$ imposed on top and bottom surfaces

<table>
<thead>
<tr>
<th>Phases</th>
<th>$\nu$</th>
<th>$E$ (MPa)</th>
<th>$E/E_{matrix}$</th>
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</thead>
<tbody>
<tr>
<td>Epoxy matrix</td>
<td>0.265</td>
<td>2885</td>
<td>1.0</td>
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<tr>
<td>Copper fiber</td>
<td>0.265</td>
<td>112220</td>
<td>38.9</td>
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<td>Interphase1</td>
<td>0.265</td>
<td>57693</td>
<td>20.0</td>
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<tr>
<td>Interphase2</td>
<td>0.265</td>
<td>193</td>
<td>0.067</td>
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</table>
Hard fibers in an infinite matrix

- Iso-values of the principal stress $\sigma_1$
- Effect of the interlayer on the stress field highlighted:
  Location and intensity of the maxima ($\sigma_{1\text{max}}=1.13$ | 0.68)
  Discontinuity of the stress field
Fiber reinforced material

- Oriented cylinders in a matrix
- Horizontal fiber planes
- Bulk size: [0.1;0.1;0.1]
- Mesh: [513;513;513]
- Boundary conditions:
  Vertical displacement on the top surface: \( w_0 \)
  Zero displacements on the bottom
  Free other boundaries

<table>
<thead>
<tr>
<th>simulation</th>
<th>( \theta_1 )</th>
<th>( \theta_2 )</th>
<th>( E_{f1}/E_h )</th>
<th>( E_{f2}/E_h )</th>
<th>( R_{f12} )</th>
<th>( n_1 )</th>
<th>( n_2 )</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>0</td>
<td>0</td>
<td>10</td>
<td>5</td>
<td>0.005</td>
<td>7</td>
<td>7</td>
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<tr>
<td>B</td>
<td>0</td>
<td>0</td>
<td>10</td>
<td>5</td>
<td>0.005</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>C</td>
<td>0</td>
<td>( \pi/2 )</td>
<td>10</td>
<td>5</td>
<td>0.005</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>D</td>
<td>( \pi/5 )</td>
<td>( -\pi/5 )</td>
<td>10</td>
<td>5</td>
<td>0.005</td>
<td>5</td>
<td>3</td>
</tr>
</tbody>
</table>
Fiber reinforced material

- Aligned fibers ($\Theta_{1,2}=0$)
- Effect of the density of the fibers: stress path (tensile stress)
Fiber reinforced material

- Oriented fibers ($\Theta_2 = \pi/2$) – ($\Theta_{1,2} = \pm \pi/5$)
- Effect of the density and orientation of the fibers: different stress path
Conclusion

- Development of a fast efficient solver to deal with 3D elastic problems involving strongly heterogeneous materials

- Ability to consider hundred millions DoF in order to take into account small scale variations in great detail

- Fast calculations on a PC allowing parametric studies at different scales
Prospects

- Consider other types of heterogeneous materials
- Take into account the material anisotropy
- Design new materials
- Create a path between macro/micro
Acknowledgement

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Thank you for your attention

Questions?

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