Non-linear mechanical solvers for GMSH

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Introduction

• Different projects going on
  – Fracture of composites
    • ERA-NET
    • CENAERO, e-Xstream, IMDEA, Tudor
  – Mean-field homogenization with damage
    • ERA-NET
    • CENAERO, e-Xstream, IMDEA, Tudor
  – Fracture or MEMS
    • UCL
  – Fracture of thin structures
    • MS3, GDTech
  – Computational multiscale
    • ARC

• Different methods
  – Need of common computational tools
  – Need of maximum flexibility
Flowchart

GMSH (elasticity) Solver

Linear System → Dof Manager (Bi)linear terms Function Space Quadrature Rule Geo tools

Tools for linear finite element analysis
Structure for non-linear finite element analyzes

- Pure virtual classes
- Definition of classical material laws
- Time integration
- Parallel implementation
- ...
Flowchart

GMSH (elasticity) Solver

Linear System

Dof Manager

(Bi)linear terms

Function Space

Quadrature Rule

Geo tools

NonLinear MechSolver

NLSysstem QS & Explicit

NLDofManager QS & Explicit

Part Domain

NLTerms

IPVariable

Material Law

Applications

PartDomain

Terms

Function Space

IPVariable

Material Law

Interface Element

dG3D

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Flowchart

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Solver projects

dgshell

dG3D

2012

Non-linear mechanical solvers for GMSH
Material Law

Structure for non-linear material laws

- Defines constitutive model
- Interface with Abaqus, MFH (e-Xstream)
- Allows defining full coupled problems
- Allows considering fracture

<table>
<thead>
<tr>
<th>MaterialLaw createIPState()=0</th>
</tr>
</thead>
<tbody>
<tr>
<td>mlawJ2Linear constitutive()</td>
</tr>
<tr>
<td>mlawNonLocalDamage constitutive()</td>
</tr>
<tr>
<td>mlawVUMat constitutive()</td>
</tr>
<tr>
<td>mlawTwoLaws bulkLaw * cohesiveLaw *</td>
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</table>
Interface for dG3D

NonLinear MechSolver

MaterialLaw
createIPState() = 0

mlawJ2Linear
constitutive()

mlawNonLocalDamage
constitutive()

mlawVUMat
constitutive()

mlawTwoLaws
bulkLaw *
cohesiveLaw *

Applications

dG3DMaterialLaw
stress(IP0, IP1) = 0

dG3DJ2LinearMaterialLaw
mlawJ2Linear *mlaw

dG3DJ2LinearIPVariable
ipJ2Linear
STensor3 Fp, εp

ipNonLocalDamage
double *

ipVUMat
double *

ipTwoLaws
ipBulk *
ipCohesive *

dG3DIPVariable
dG3DJ2Linear
STensor3 F0, F1, P
SVector3 jump, N

dG3DJ2LinearIPVariable
ipJ2Linear _ipJ2

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Interface for dG3D

- Discontinuous Galerkin formulation
  - Finite-element discretization
  - Same **discontinuous** polynomial approximations for the

  - **Test** functions \( \varphi_h \) and
  - **Trial** functions \( \delta \varphi \)

- Definition of operators on the interface trace:
  - **Jump** operator: \( [\bullet] = \bullet^+ - \bullet^- \)
  - **Mean** operator: \( \langle \bullet \rangle = \frac{\bullet^+ + \bullet^-}{2} \)

- Continuity is weakly enforced, such that the method
  - Is consistent
  - Is stable
  - Has the optimal convergence rate
Interface for dG3D

- Discontinuous Galerkin formulation
  - // & fracture
  - Formulation in terms of the first Piola stress tensor $\mathbf{P}$
    \[ \nabla_0 \cdot \mathbf{P}^T = 0 \text{ in } \Omega \quad \& \quad \begin{cases} 
\mathbf{P} \cdot \mathbf{N} = \mathbf{T} \text{ on } \partial_N \Omega \\
\varphi_h = \varphi_h \text{ on } \partial_D B 
\end{cases} \]
  - Weak formulation obtained by integration by parts on each element $\Omega_e$

\[ \sum_e \int_{\Omega_e} \nabla_0 \cdot \mathbf{P}^T (\varphi_h) \cdot \delta \varphi \, dB = 0 \]

\[ \sum_e \int_{\Omega_e} -\mathbf{P} (\varphi_h) : \nabla_0 \delta \varphi \, dB + \sum_e \int_{\partial \Omega_e} \delta \varphi \cdot \mathbf{P} (\varphi_h) \cdot \mathbf{N} \, d\partial B = 0 \]

New interface terms

\[ \int_{B_0} \mathbf{P} (\varphi_h) : \nabla_0 \delta \varphi \, dB + \int_{\partial B_0} [\delta \varphi \cdot \mathbf{P} (\varphi_h)] \cdot \mathbf{N}^- \, d\partial B = \int_{\partial_N B_0} \mathbf{T} \cdot \delta \varphi \, d\partial B \]
Interface for dG3D

- Interface term rewritten as the sum of 3 terms
  - Introduction of the numerical flux \( h \)

\[
\int_{\partial I B_0} [[\delta \varphi \cdot P(\varphi_h)]] \cdot N^- d\partial B \rightarrow \int_{\partial I B_0} [[\delta \varphi]] \cdot h(P^+, P^-, N^-) d\partial B
\]

- Has to be consistent:
  \[
  h(P^+, P^-, N^-) = -h(P^-, P^+, N^+)
  \]

- One possible choice:
  \[
  h(P_{\text{exact}}, P_{\text{exact}}, N^-) = P_{\text{exact}} \cdot N^-
  \]

- Weak enforcement of the compatibility

\[
\int_{\partial I B_0} \left[ \varphi_h \right] \cdot \left\langle \frac{\partial P}{\partial F} : \nabla_0 \delta \varphi \right\rangle \cdot N^- d\partial B
\]

- Stabilization controlled by parameter \( \beta \), for all mesh sizes \( h^s \)

\[
\int_{\partial I B_0} \left[ \varphi_h \right] \otimes N^- : \left\langle \frac{\beta}{h^s} \frac{\partial P}{\partial F} \right\rangle : \left[ \delta \varphi \right] \otimes N^- d\partial B:
\]

- Those terms can also be explicitly derived from a variational formulation (Hu-Washizu-de Veubeke functional) [Noels & Radovitzky, IJNME 2006 & JAM 2006]
Interface for dG3D

- Taylor impact test
  - Copper bar impacting a rigid wall
Cohesive Zone Method for fracture

- Based on the use of cohesive elements
  - Inserted between bulk elements
- Intrinsic Law
  - Cohesive elements inserted from the beginning
  - Drawbacks:
    - Efficient if a priori knowledge of the crack path
    - Mesh dependency [Xu & Needleman, 1994]
    - Initial slope modifies the effective elastic modulus
    - This slope should tend to infinity [Klein et al. 2001]:
      - Alteration of a wave propagation
      - Critical time step is reduced
- Extrinsic Law
  - Cohesive elements inserted on the fly when failure criterion is verified [Ortiz & Pandolfi 1999]
  - Drawback
    - Complex implementation in 3D (parallelization)
• MATERA project: SIMUCOMP
  – CENAERO, e-Xstream, IMDEA Materials, Tudor, ULg
  – Application to composites
  – Representative nature?
  – First results
Interface for shells

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mlawTwoLaws
bulkLaw *
cohesiveLaw *

DGshellMaterialLaw
stress(IP₀, IP₁)=0

dgshellJ2LinearMaterialLaw
mlawJ2Linear *mlaw

IPVariable
get(int )

ipJ2Linear
STensor3 Fᵣ, εᵣ

ipNonLocalDamage
double *

ipVUMat
double *

ipTwoLaws
ipBulk *
ipCohesive *

dG3DJ2LinearIPVariable
std::vector<STensor3> F
std::vector<STensor3> τ

dG3DJ2LinearIPVariable
std::vector <ipJ2Linear> _i_pJ2
Interface for shells

• Thin bodies
  – FRIA (MS3, GDTech)
  – $C^1$ continuity required
  – Test functions

$C^0$/DG formulation
[Noels & Radovitzky, CMAME 2008]

DG formulation
[Becker & Noels, IJNME 2011, CMAME 2011]

• New DG interface terms
  – Consistency
  – Compatibility
  – Stability
Interface for shells

- **New cohesive law for thin bodies**
  - Should take into account a through the thickness fracture
    - Problem: no element on the thickness
    - Very difficult to separate fractured and not fractured parts
  - Solution:
    - Application of cohesive law on
      - The resultant stress
        \[ n^{11} \rightarrow N(\Delta^*) \]
      - The resultant bending stress
        \[ \tilde{m}^{11} \rightarrow M(\Delta^*) \]
    - In terms of a resultant opening \( \Delta^* \)
      \[ \Delta^* = (1 - \beta)\Delta_x + \beta \frac{h}{6} \Delta_r \]
      \( h_{eq} \) for non-linear materials
• Application
  – Notched elasto-plastic cylinder submitted to a blast
• **Application**
  - Fragmentation of a brittle ceramic ring submitted to centrifugal forces
    • Weibull strength distribution
  - Future application: Rupture of MEMS
    • **UCL**
Interface for Non Local Damage

GMSH (elasticity) Solver

NonLinear MechSolver

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(dG3D) NonLocalDG

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NonLocalDG

PartDomain Interface

Solver – projects

Applications

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Interface for Non Local Damage

NonLinear
MechSolver

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mlawTwoLaws
bulkLaw *
cohesiveLaw *

dG3DMaterialLaw
stress(IP_0, IP_1)=0

NonLocalDG3DMaterialLaw
mlawNonLocalDamage *mlaw

IPVariable
get(int)

ipJ2Linear
STensor3 F_0, ε_0

ipNonLocalDamage
double *

ipVUMat
double *

ipTwoLaws
ipBulk *
ipCohesive *

dG3DIPVariable
STensor3 F_0, F_1, P
SVector3 jump, N

NonLocalDG3DIPVariable
double dε/dp ....
ipNonLocalDamage _ip
Interface for Non Local Damage

- **MATERA project: SIMUCOMP**
  - CENAERO, e-Xstream, IMDEA Materials, Tudor, ULg

- **Mean Field Homogenization**
  - 2-phase composite

\[
\begin{align*}
\langle \sigma \rangle &= \nu_0 \langle \sigma \rangle_{\omega_0} + \nu_1 \langle \sigma \rangle_{\omega_1} \\
\langle \sigma \rangle_{\omega_0} &= \overline{C}_1 : \langle \varepsilon \rangle_{\omega_1} \\
\langle \sigma \rangle_{\omega_1} &= \overline{C}_0 : \langle \varepsilon \rangle_{\omega_0}
\end{align*}
\]

- Mori-Tanaka assumption

\[
\langle \varepsilon \rangle = \nu_0 \langle \varepsilon \rangle_{\omega_0} + \nu_1 \langle \varepsilon \rangle_{\omega_1}
\]

- **Extension to damage?**
Interface for Non Local Damage

- **Damage**
  - Homogenous unique solution
  - Lose of uniqueness
  - Strain localized

  The numerical results change with the size of mesh and direction of mesh

- **Implicit non-local approach**
  - New equation on an internal variable

  \[
  \bar{a} = \frac{1}{V_c} \int_{V_c} awdV \quad \bar{a} - c \nabla^2 \bar{a} = a
  \]

  Green function as weight functions \( w \)

[Peerlings et al., 1996]
• Non-local damage
  
  – Lemaitre-Chaboche
  
  \[
  \dot{D} = \left( \frac{Y}{S_0} \right)^n (\dot{p} + c_1 \nabla^2 \dot{p} + c_2 \nabla^4 \dot{p} + \ldots) = \left( \frac{Y}{S_0} \right)^n \dot{p}
  \]

  • \(S_0\) and \(n\) are the material parameters
  • \(Y\) is the strain energy release rate
  • \(p\) is the accumulated plastic strain

  – New equation in the system
  
  \[
  \overline{p} - c \nabla^2 \overline{p} = p
  \]

  \[
  \begin{bmatrix}
  K_{uu} & K_{u\overline{p}} \\
  K_{\overline{p}u} & K_{\overline{p}\overline{p}}
  \end{bmatrix}
  \begin{bmatrix}
  du \\
  d\overline{p}
  \end{bmatrix}
  =
  \begin{bmatrix}
  F_{\text{ext}} - F_{\text{int}} \\
  F_p - F_{\overline{p}}
  \end{bmatrix}
  \]
Interface for Non Local Damage

- **MFH with Non-local damage**
  - Based on Linear Composite Comparison \[\text{[Wu, Noels, Adam & Dogrhi, CMAME2012]}\]

\[
\begin{align*}
\delta \sigma &= \nu_1 \delta \sigma_1 + \nu_0 \delta \sigma_0 \\
\delta \sigma_0 &= (1 - D) C_0^{\text{alg}} : \varepsilon_0 - \hat{\sigma}_0 \partial D & \& \hat{\sigma}_0 = \sigma_0 / (1 - D) \\
\delta \sigma &= \nu_1 C_1^{\text{alg}} \varepsilon_1 + \nu_0 (1 - D) C_0^{\text{alg}} : \varepsilon_0 - \nu_0 \hat{\sigma}_0 \partial D
\end{align*}
\]

\[
\delta \sigma = \overline{C}^{\text{alg}} D : \varepsilon_0 - \nu_0 \hat{\sigma}_0 \frac{\partial D}{\partial \overline{p}} \delta \overline{p}
\]

- Finite elements with 4 dofs/node

\[
\begin{cases}
\nabla \sigma + f = 0 & \text{for homogenized material} \\
\overline{p} - l^2 \nabla^2 \overline{p} = p & \text{related to matrix only}
\end{cases}
\]

\[
\begin{bmatrix}
K_{uu} & K_{u\overline{p}} \\
K_{\overline{p}u} & K_{\overline{p}\overline{p}}
\end{bmatrix}
\begin{bmatrix}
du \\
d\overline{p}
\end{bmatrix}
= 
\begin{bmatrix}
F_{\text{ext}} - F_{\text{int}} \\
F_p - F_{\overline{p}}
\end{bmatrix}
\]
• **MFH with Non-local damage**
  – Epoxy-CF (30%)
Interface for Non Local Damage

• Application
  – Epoxy - CF (50%)
  – Laminate 45/-45/-45/45 with a hole
  – Finite element mesh in each layer, with appropriate MFH laws
Interface for FE$^2$

- **GMSH (elasticity) Solver**
- **NonLinear MechSolver**
- Applications

### Linear System
- Dof Manager
- (Bi)linear terms
- Function Space
- Quadrature Rule
- Geo tools

### NonLinear System
- NLSys
- QS & Explicit

### NLDofManager
- QS & Explicit

### Part Domain
- NLTerms
- IPVariable
- Material Law

### PartDomain
- Terms
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- Interface Element

### Geo tools

- HODG FE$^2$

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Interface for FE

NonLinear MechSolver

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hoMultiscaleMaterialLaw

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ipJ2Linear
STensor3 Fᵣ, εᵣ

ipNonLocalDamage
double *

ipVUMat
double *

ipTwoLaws
ipBulk *
ipCohesive *

dG3DIPVariable
STensor3 F₁, Fₚ, P

hoMultiscaleIPVariable
std::string _microMesh
nonLinearSolver *solver
std::vector<data *>

2012 Non-linear mechanical solvers for GMSH
• **Computational Multiscale**
  - **Macro-scale**
    - High-order Strain-Gradient formulation
    - C1 weakly enforced by DG
    - Partitioned mesh
Interface for FE²

- Computational Multiscale
  - Macro-scale
    - High-order Strain-Gradient formulation
    - C1 weakly enforced by DG
    - Partitioned mesh
  - Micro-scale
    - Usual 3D finite elements
    - Periodic boundary conditions
    - Non-conforming mesh
    - Use of interpolant functions
    - Stability

[Nguyen, Béchet, Geuzaine & Noels COMMAT2011]
Interface for FE²

- **Computational Multiscale**
  - **Macro-scale**
    - High-order Strain-Gradient formulation
    - C1 weakly enforced by DG
    - Partitioned mesh
  - **Transition**
    - Gauss-Points on different processors
    - Each Gauss point is associated to
      - One mesh
      - One solver
      - Data: IPStates, fields of microproblem
  - **Micro-scale**
    - Usual 3D finite elements
    - Periodic boundary conditions
      - Non-conforming mesh
      - Use of interpolant functions
    - Stability

\[ \begin{align*}
\nabla F_M & \quad \frac{\partial P_M}{\partial F_M} \\
Q_M & \quad \frac{\partial Q_M}{\partial \nabla F_M}
\end{align*} \]

[Nguyen, Béchet, Geuzaine & Noels COMMAT2011]
Interface for FE^2

- Application
Conclusions

• **NonLinearMechSolver**
  – Generic tool to solve mechanical problems
  – // implementation based on DG

• **Applications**
  – Different projects, which include the solver
    • Projects are independent
  – First results
  – More work coming …

• **Efficient tool for collaborations**
  – Can be downloaded
  – Allows defining a new project easily