CSMA Junior 2024
Modèles numériques robustes pour les problématiques d'EDF: le cas de l'incompressibilité plastique

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EDF R&D

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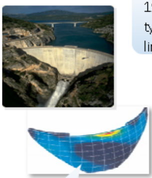
Industrial context : numerical simulation at EDF

- Justifying installations with respect to safety
- Understanding physics or system response
- Qualifying and optimizing processes

Two industrial open-source softwares at EDF

- *code_aster* : finite element code for thermo-hydro-mechanical simulation in structural mechanics
- *code_saturne* : finite volume code for computational fluid dynamics
- Internal development for nuclear applications
- Some advantages but also disadvantages

60 years of computational mechanics

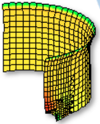


1960-70: First dam linear FE simulation (EDF apps then ASKA)

Pylon Optimization (OPSTAR)

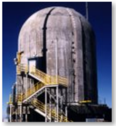
1970-80: design studies, on type of FE, linear, specific limit conditions

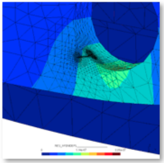
1980: 3D non linear breaking simulation: vessel damage surface detection



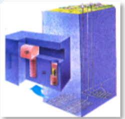
1996: start civil engineering studies

2002: start containment building leakage studies





Now: Civil engineering
Steel thermal fatigue
Damage, lifetime
Earthquake resistance
Coupled Thermal – hydraulic – mechanical



1960 | 1970 | 1980 | 1990 | 2000 | 2010 | 2020

1989: birth of code_aster

2001: code_aster goes open source

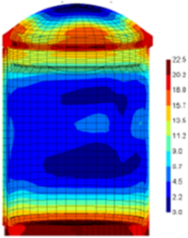
2011: salome_meca becomes the qualified software

code_aster in a nutshell

- A large scope of features
  - Real and complex arithmetics
  - Multiphysics : mechanics, thermal, acoustics, fluid (Darcy)
  - Statics, dynamics, modal, harmonic analysis
  - 400 finite elements : 3D, 2D, shells, beams, pipes ...
  - python API
  - HPC capacities
- Non-linearities and specific features
  - Large deformations
  - Contact and friction
  - Behaviour models ($>$100 laws)
  - Multi-dimensional simulation
  - Kinematics constraints between DoFs (MPC)

Which kind of studies

- A large part of the studies are linear.
  - A good approximation is sufficient
  - Validation with norms and codifications
- A small part are non-linear
  - Need accuracy to have a "best-estimate" model
  - Validation of linear and/or simplified model
  - Going beyond codification and norms. Understanding of fine physical phenomena
- Different applications between R&D and engineering teams (and time-scale)



From reality to simulation

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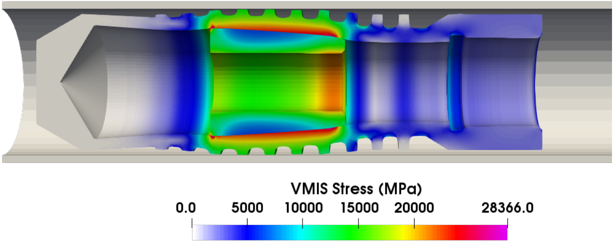
What is nonlinear ?

- Accurate and robust numerical simulations
- Strongly nonlinear mechanical problems to solve
  - nonlinear measure of deformations (geometric nonlinearity)
  - nonlinear stress-strain constitutive relation (material nonlinearity)
  - damage and crack propagation (irreversibility)
  - contact and friction (boundary nonlinearity)
  - coupling between physics and modelizations
- Industrial example : Notch plug



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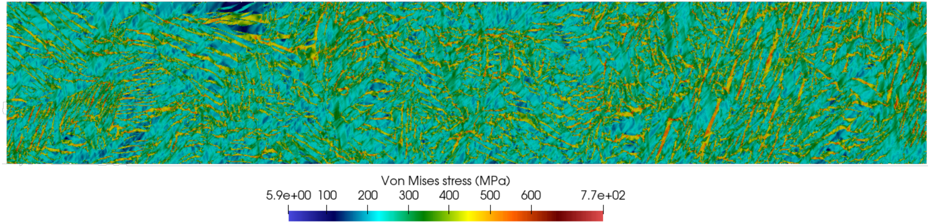
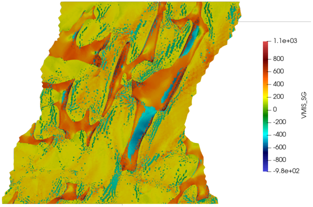
Polycristalline homogenization (Maxime Mollens' PhD)

- 3D-aggregate of 1794 grains of bainitic phase with Méric-Cailletaud's law
- Size of a grain : $100\mu m \times 10\mu m$
- Monotone traction (5% of deformation in x-direction)
- 15 370 535 DoFs and 720 CPUs
- 13 days for the total run and 8.7 days for the Jacobian matrix
- 55 355 time steps (!) (and 352 017 Newton's iterations)
- Performance is killed by the difficult local behavior integration and the incoherent tangent stiffness



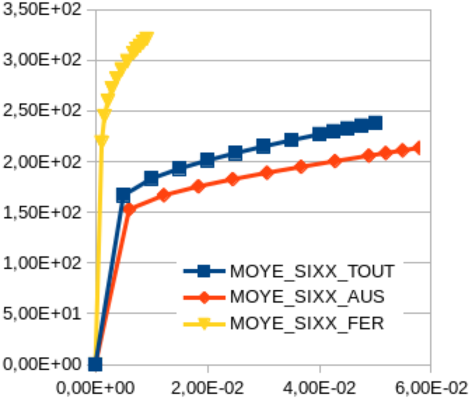
Polycristalline homogenization

(a) micro-structure



(b) von Mises stress (MPa)

Local zoom (on a subdomain)



Homogenized traction curve in x-direction

→ Presence of volumetric locking

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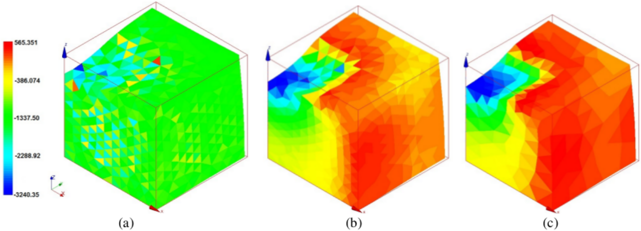
Volumetric locking

- Presence of volumetric locking with primal H^1-conforming formulation due to plastic incompressibility
- An alternative : using mixed methods but more unknowns, more expensive to build, saddle-point problem to solve ...
- Example : pinching of a cube



Trace of the stress tensor for (a) P1 (b) P2 (c) P2/P1/P1

- or using a primal formulation without volumetric locking

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Locking-free primal formulations

- discontinuous Galerkin (dG) (cell-base method)
  - second order elliptic pb. [Arnold, Brezzi, Cockburn, Marini 01]
  - linear elasticity [Hansbo & Larson 03]
- Hybridizable Discontinuous Galerkin (HDG) (face-base method)
  - second order elliptic pb. [Cockburn, Gopalakrishnan, Lozarov 09]
  - linear elasticity [Soon, Cockburn, Stolarski 09]
- Hybrid High-Order (HHO) (face-base method) $\Leftarrow$ this talk
  - diffusion problem [Di Pietro, Ern, Lemaire 14]
  - linear elasticity [Di Pietro & Ern 15]
- Virtual Element Method (VEM) (vertex-base method)
  - linear elasticity [Beirão da Veiga, Brezzi, Marini 13]
  - second order elliptic pb. [Beirão da Veiga, Brezzi, Marini, Russo 16]
- Strong connection between HDG and HHO [Cockburn, Di Pietro, Ern 16]

Main features of HHO for nonlinear solid mechanics

- More advantageous than mixed methods

  $\Rightarrow$ Primal formulation

- More advantageous than FE methods

  $\Rightarrow$ Absence of volumetric locking

- More advantageous than dG methods

  $\Rightarrow$ Integration of the behavior law only at cell-based quadrature nodes

  $\Rightarrow$ Symmetric tangent matrix at each nonlinear solver iteration

- Implementation in the open-source libraries `disk++`
  - Implementation from scratch in `code_aster` (integrated in version 15.0.8)
  - Implementation of the nonlinear mechanical module in `disk++`

- Pave the way to HDG methods

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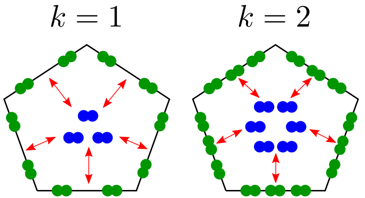
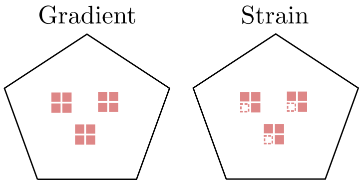
Key ideas of **H**ybrid **H**igh-**O**rder (HHO) methods

- Discontinuous (non-conforming) method
- Primal formulation with cell and face unknowns (poly. of order $k \geq 1$)
  - cell unknowns are eliminated locally by static condensation
- Local gradient/strain reconstruction (poly. of order $k \geq 1$)
  - h^{k+1} convergence in energy-norm (linear elasticity)
- Stabilization connecting cell and face unknowns



cell and face unknowns (2D)



gradient/strain unknowns (2D, k=1)

Other interesting features of HHO methods

- Support of polytopal meshes (with possibly nonconforming interfaces)
- Attractive computational costs
  - Compact stencil (only neighbourhood faces)
  - Reduced size $N_{dofs}^{hho} \approx k^2 \mathrm{card}(\mathcal{F}_h)$ vs. $N_{dofs}^{dG} \approx k^3 \mathrm{card}(\mathcal{T}_h)$
- Local principle of virtual work (equilibrated fluxes)
- Robustness to physical parameters (dominant advection, quasi-incomp.)
- Robustness to distorted meshes (flat cells, small edges)

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Polyhedral meshes

- Convenient framework for multi-domain meshing, local refinement, agglomeration mesh coarsening

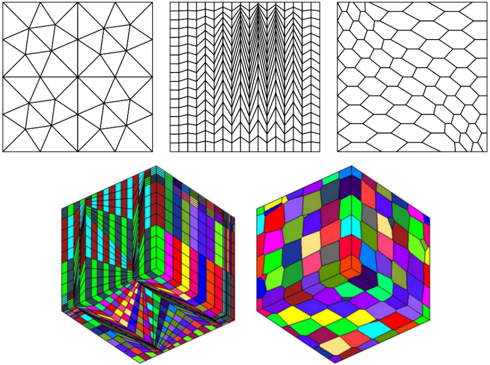

Figure 1 – Polyhedral meshes in 2D and 3D : [Herbin and Hubert, 2008, FVCA5] and [DP and Lemaire, 2015] (above) and [Eymard et al., 2011, FVCA6] (below)

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Bibliography

Seminal papers :

- An arbitrary-order and compact-stencil discretization of diffusion on general meshes based on local reconstruction operators [Di Pietro, Lemaire, Ern, 2014, CMAM]
- A hybrid high-order locking-free method for linear elasticity on general meshes [Di Pietro & Ern, 2015, CMAME]
- A review of hybrid high-order methods : formulations, computational aspects, comparison with other methods [Di Pietro, Lemaire, Ern, 2016]

Book (base of this talk) :

- Hybrid high-order methods. A primer with application to solid mechanics [Cicuttin, Ern, NP, 2021]

Poisson problem

- Let $f \in L^2(D)$ and let $D \subset \mathbb{R}^d$ be a Lipschitz polyhedron
- Homogeneous Dirichlet boundary conditions $u_D = 0 \text{ on } \Gamma := \partial D$
- Find $u \in H_0^1(D)$ s.t.

$$(\boldsymbol{\nabla} u, \boldsymbol{\nabla} v)_{\underline{L}^2(D)} = (f, v)_{L^2(D)}, \qquad \forall v \in H_0^1(D)$$

- Well-posed problem

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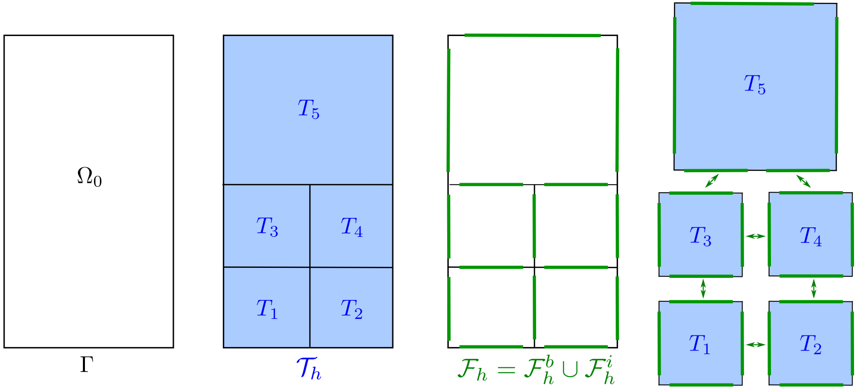
Mesh notation

- $\mathcal{T}_h$: set of cells ; $\mathcal{F}_h$: set of (planar) faces
- Mesh $\mathcal{M}_h := (\mathcal{T}_h, \mathcal{F}_h)$

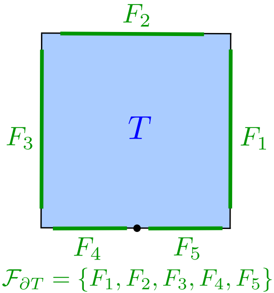


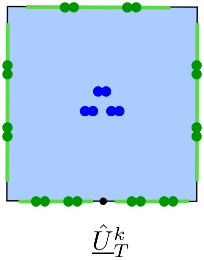
Mesh $\mathcal{M}_h$ composed of 5 cells and 15 faces

Local DOFs space

- $\mathcal{F}_{\partial T}$: set of mesh faces of cell T
- Let a polynomial degree $k \geq 0$; for all $T \in \mathcal{T}_h$, set

$$\hat{v}_T := (v_T, v_{\partial T}) \in \hat{U}_T^k := \underbrace{\mathbb{P}_d^k(T;\mathbb{R})}_{\text{local cell dofs}} \times \underbrace{\mathbb{P}_{d-1}^k(\mathcal{F}_{\partial T};\mathbb{R})}_{\text{local face dofs}}$$





Gradient reconstruction

$$\underline{G}_T : \underbrace{\mathbb{P}_d^k(T;\mathbb{R}) \times \mathbb{P}_{d-1}^k(\mathcal{F}_{\partial T};\mathbb{R})}_{=:\hat{U}_T^k} \to \underbrace{\mathbb{P}_d^k(T;\mathbb{R}^d)}_{\text{local gradient space}}$$

- The reconstructed strain $\underline{G}_T(\hat{v}_T) \in \mathbb{P}_d^k(T;\mathbb{R}^d)$ solves

$$(\underline{G}_T(\hat{v}_T), \underline{\tau})_{\underline{L}^2(T)} = -(v_T, \nabla\cdot\underline{\tau})_{\underline{L}^2(T)} + (v_{\partial T}, \underline{\tau}\cdot\underline{n}_T)_{L^2(\partial T)}$$

for all $\boldsymbol{\tau} \in \mathbb{P}_d^k(T;\mathbb{R}^d)$

  - mimic an integration by parts $(\nabla v, \underline{\tau})_{\underline{L}^2(T)} = -(v, \nabla\cdot\underline{\tau})_{\underline{L}^2(T)} + (v_{|\partial T}, \underline{\tau}\cdot\underline{n}_T)_{L^2(\partial T)}$
  - local scalar mass-matrix of size $\binom{k+d}{k}$ (ex : $k = 2$, $d = 3 \implies$ size $= 10$)

- Local interpolation operator : $\hat{I}_T^k(v) = (\Pi_T^k(v), \Pi_{\partial T}^k(v_{|\partial T})) \in \hat{U}_T^k$

- Commuting property :

$$\underline{G}_T(\hat{I}_T^k(\underline{v})) = \Pi_T^k(\boldsymbol{\nabla} v), \quad \forall v \in H^1(T;\mathbb{R})$$

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Stabilization operator

- "Connect" the face unknowns to the trace of the cell unknowns
- We penalize the quantity $v_{\partial T} - v_{T|\partial T}$ in a least-squares sense
- HHO-stabilization operator $S_{\partial T}(\hat{v}_T) \in \mathbb{P}^k_{d-1}(\mathcal{F}_{\partial T};\mathbb{R})$ s.t.

$$S_{\partial T}(\hat{v}_T) := \Pi^k_{\partial T}\big(\underbrace{v_{\partial T} - v_{T|\partial T}}_{\text{HDG term}} - \underbrace{(\underline{I}_d - \Pi^k_T)R^{k+1}_T(0, v_{\partial T} - v_{T|\partial T})}_{\text{HHO correction}}\big)$$

$\Pi^k_{\partial T}$: L^2-projector on $\mathbb{P}^k_{d-1}(\mathcal{F}_{\partial T};\mathbb{R})$; Π^k_T : L^2-projector on $\mathbb{P}^k_d(T;\mathbb{R})$
R^{k+1}_T : higher-order reconstructed field in $\mathbb{P}^{k+1}_d(T;\mathbb{R})$

- The HHO correction ensures high-order error estimates $\mathcal{O}(h^{k+1})$ on polyhedral meshes (instead of $\mathcal{O}(h^k)$)
- Stability :

$$\|\nabla v_T\|^2_{\underline{L}^2(T)} + h_T^{-1}\|v_{\partial T} - v_{T|\partial T}\|^2_{L^2(\partial T)} \lesssim \|\underline{G}_T(\hat{v}_T)\|^2_{\underline{L}^2(T)} + h_T^{-1}\|S_{\partial T}(\hat{v}_T)\|^2_{L^2(\partial T)}$$

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Local Galerkin contribution

- Local Galerkin contribution

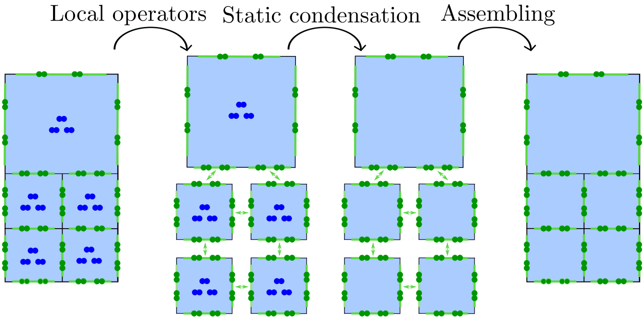
$$\hat{a}_T^G(\hat{v}_T, \hat{w}_T) := \underbrace{(\underline{G}_T(\hat{v}_T), \underline{G}_T(\hat{w}_T))_{\underline{L}^2(T)}}_{\text{FEM-like stiffness term}} + \underbrace{h_T^{-1}(S_{\partial T}(\hat{v}_T), S_{\partial T}(\hat{w}_T))_{L^2(\partial T)}}_{\text{stabilization term}}$$

- Local RHS

$$\hat{\ell}_T(\hat{v}_T) := (f, v_T)_{L^2(T)}$$

Global DOFs space

- Global DOFs : $\hat{u}_h := (u_{\mathcal{T}_h}, u_{\mathcal{F}_h}) \in \hat{U}_h^k := \underbrace{\mathbb{P}_d^k(\mathcal{T}_h;\mathbb{R})}_{\text{global cells dofs}} \times \underbrace{\mathbb{P}_{d-1}^k(\mathcal{F}_h;\mathbb{R})}_{\text{global faces dofs}}$



- Cellwise assembly (fully parallelizable)
- Face unknowns are uniquely defined
- Dirichlet boundary conditions are imposed strongly

$$\hat{U}_{h,0}^k := \left\{ \hat{u}_h \in \hat{U}_h^k \ : u_F = 0 \text{ on } \Gamma_{\mathrm{D}} \right\}$$

Global discrete problem (Poisson problem)

$$
\begin{cases}
\text{Find } \hat{u}_h \in \hat{U}^k_{h,0} \text{ such that} \\
\hat{a}^G_h(\hat{u}_h, \hat{v}_h) = \hat{\ell}_h(\hat{v}_h) \quad \forall\, \hat{v}_h \in \hat{U}^k_{h,0}
\end{cases}
$$

with

$$
\hat{a}^G_h(\hat{u}_h, \hat{v}_h) := \sum_{T \in \mathcal{T}_h} \hat{a}^G_T(\hat{u}_T, \hat{v}_T) \text{ and } \hat{\ell}_h(\hat{v}_h) := \sum_{T \in \mathcal{T}_h} \hat{\ell}_T(\hat{v}_T)
$$

- Well-posed problem
- Optimal convergence
  - h^{k+1}-convergence in energy-norm
  - h^{k+2}-convergence in L^2-norm with elliptic regularity

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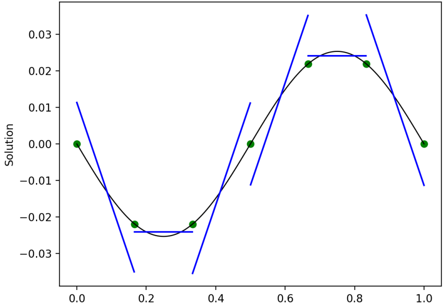
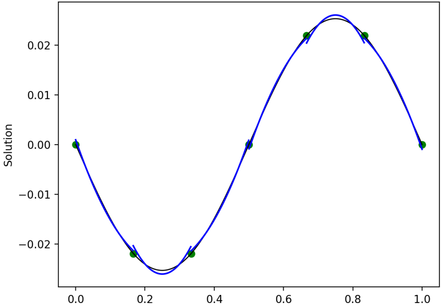
1D-example : local interpolation operator $\hat{I}_T^k$

- HHO methods are really simple in 1D.
- Face unknowns : $\mathbb{P}_{d-1}^k(F;\mathbb{R}) = \mathbb{R} \Rightarrow$ 1 unknown (1D only)
- Analytical solution $u(x) = -\sin(\pi x)$ on $[0,1]$



(a) $k = 1$



(b) $k = 2$

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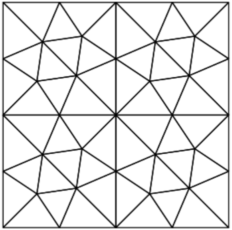
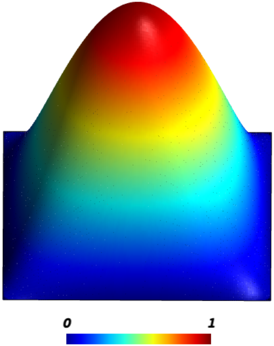
Numerical example :

- Analytical solution $u(x, y) = \sin(\pi x)\sin(\pi y)$ on the unit square
- Solution computed with HHO methods



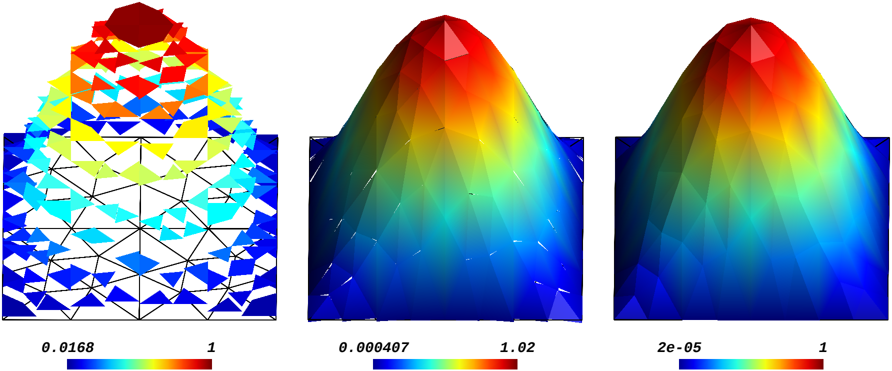
(c) 2D simplicial mesh



(d) Analytical solution

2D-example : p-convergence

For a given mesh (56 cells) and for different order $k = \{0, 1, 2\}$



(e) $k = 0$ (f) $k = 1$ (g) $k = 2$

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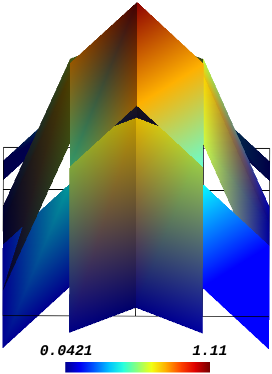
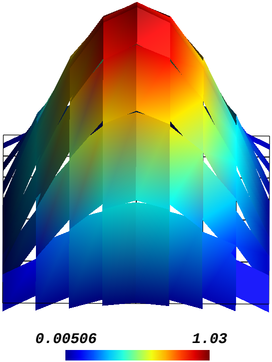
2D-example : h-convergence

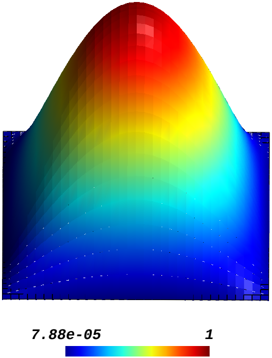
For k=1 and for different cartesian meshes



(h) 4×4



(i) 8×8



(j) 32×32

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Global discrete problem (finite def.)

For all $1 \leq n \leq N$, find $\hat{u}_h^n \in \hat{U}_{h,\mathrm{D}}^k$ such that

$$\sum_{T \in \mathcal{T}_h} (\boldsymbol{P}^n, \underline{G}_T(\hat{v}_T))_{\boldsymbol{L}^2(T)} + \sum_{T \in \mathcal{T}_h} 2\mu\beta_0 h_T^{-1} (S_{\partial T}(\hat{u}_T^n), S_{\partial T}(\hat{v}_T))_{\underline{L}^2(\partial T)}$$
$$= \hat{\ell}_h(\hat{v}_h), \quad \forall\, \hat{v}_h \in \hat{U}_{h,0}^k$$

and for all the cell-quadrature points

$$\boldsymbol{P}^n = \mathrm{FINITE\_PLASTICITY}(\underline{\chi}_T^{n-1}, \boldsymbol{F}_T(\hat{u}_T^{n-1}), \boldsymbol{F}_T(\hat{u}_T^n))$$

with $\boldsymbol{F}_T = \underline{G}_T + \boldsymbol{I}_d$ and $\underline{\chi}_T$ the internal variable states ; and β_0 the stabilization parameter (no general theory, $\beta_0 = 1$ for linear elasticity)

- FINITE_PLASTICITY is a generic function integrate behavior law locally
- Gradient and stabilization are computed by tensorization of scalar operators

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Coercivity (finite def.)

Theorem (Coercivity)

Assume that $k_Q \geq 2k$ and that all the quadrature weights are positive. Moreover, assume that the consistent elastoplastic tangent modulus $\mathbb{A}_{ep}$ is positive-definite, i.e., $\theta_{\mathcal{T}_h,Q} > 0$. Then, the linear system in each Newton's step is coercive for all $\beta_0 > 0$, i.e., there exists $C_{\mathrm{ell}} > 0$, independent of h, such that for all $\hat{v}_h \in \hat{U}^k_{h,0}$,

$$\sum_{T\in\mathcal{T}_h} (\tilde{\mathbb{A}}_{ep} : \underline{G}_T(\hat{v}_T), \underline{G}_T(\hat{v}_T))_{\boldsymbol{L}^2_Q(T)} + \sum_{T\in\mathcal{T}_h} 2\mu\beta_0 h_T^{-1} \|S_{\partial T}(\hat{v}_T)\|^2_{\underline{L}^2(\partial T)}$$

$$\geq C_{\mathrm{ell}} \min\left(\beta_0, \frac{\theta_{\mathcal{T}_h,Q}}{2\mu}\right) 2\mu \sum_{T\in\mathcal{T}_h} |\hat{v}_T|^2_{1,T}.$$

- Give a lower bound $\beta_0 \geq \frac{\theta_{\mathcal{T}_h,Q}}{2\mu} > 0$
- $\theta_{\mathcal{T}_h,Q} = 2\mu \to \beta_0 \geq 1$ for linear elasticity

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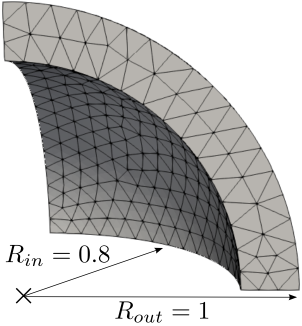
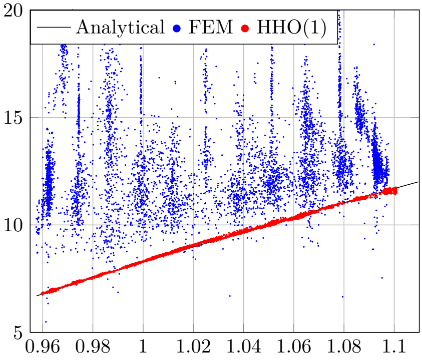
Mech. bench. : Quasi-incomp. sphere under internal forces

- Perfect J_2-plasticity and elastic incompressibility
- Increase the internal radial force until the limit load



(a) Mesh



(b) Trace of the stress tensor at all the quadrature points

- Absence of volumetric locking for HHO methods

Non-local micromorphic approch

- Local damage approach $\rightarrow$ mesh-dependent results
- Non-local damage approach
  - global scalar HHO-unknowns on $\mathcal{T}_h$
  - add regularization term (depends on length scale)
  - strong coupling : displacement/macro-damage/micro-damage formulation
  - mesh-independent results

Micromorphic damage evolution

What is available in code_aster

- Linear and quadratic approximation
- Standard geometric cells (TRIA, QUAD, HEXA, ...) - no polyhedral support
- Linear thermics and non-linear mechanic
- Small and finite deformations
- Static and dynamic analysis
- Projection on Lagrange space for visualization

Conclusion

- Practical sessions :Locking in finite plasticity

CODE aster

Conclusion

- Practical sessions :Locking in finite plasticity

Thanks you for your attention