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CMCMM 2015 | HAO LIU (DEN, DEC, SESC)
Supervisors: I. RAMIÈRE (DEN, DEC, SESC) AND
F. LEBON (LMA, AIX-MARSEILLE UNIVERSITY)

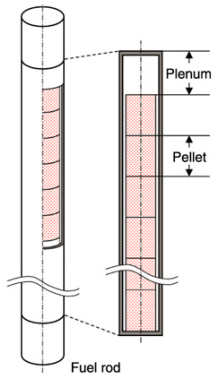
MARCH 22-27, 2015

- **Industrial context**
- **Local Defect Correction Method**
- **A posteriori error estimation in Solid Mechanics**
- **Numerical results of the combination of LDC and ZZ estimator**
- **Conclusions and perspectives**

Industrial context

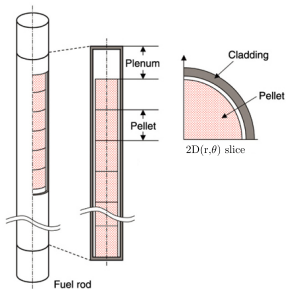
■ Pressurized Water Reactors

■ Fuel and Cladding



■ Pressurized Water Reactors

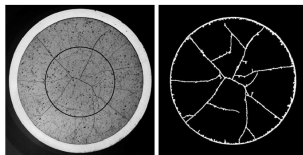
■ Fuel and Cladding



■ During irradiation

■ Pellet cracking

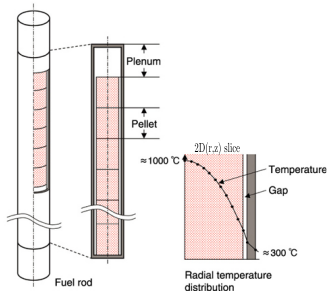
The pellet cracks and swells and the cladding creeps



⇒ **Discontinuous contacts** between pellet and cladding

■ Pressurized Water Reactors

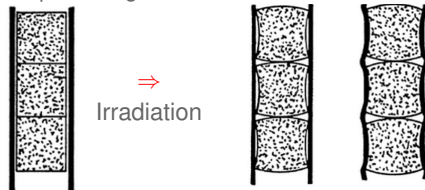
■ Fuel and Cladding



■ During irradiation

■ Hourglass shape deformation

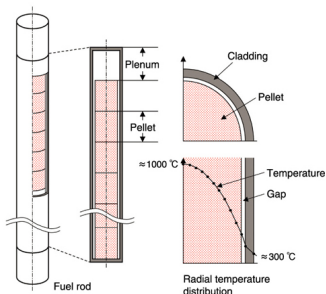
Due to the deforming effects of the high temperature gradient



⇒ **Contacts** occur first in **front of the inter-pellet plane**

■ Pressurized Water Reactors

■ Fuel and Cladding

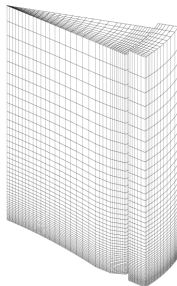


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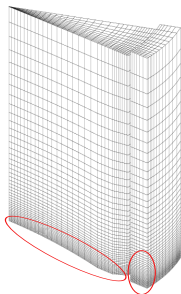
- Pellet cracking
 - Hourglass shape deformation
- ⇒ Localized high stress concentrations on the cladding
- ⇒ Integrity of the cladding (security stake)

- Simulation in PLEIADES fuel performance software environment

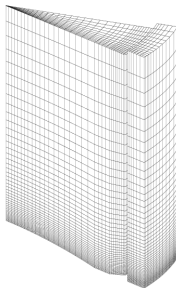
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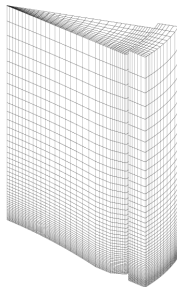
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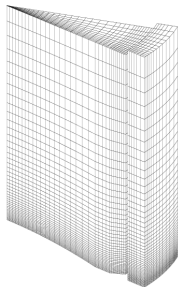
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- Acceptable computational times and memory space



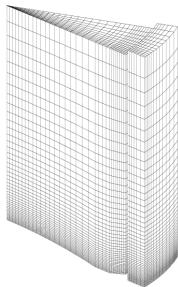
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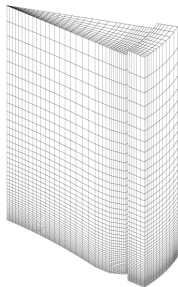
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Local Defect Correction Method

- Adaptive Mesh Refinement methods
 - ≡ Local Multigrid methods

■ Adaptive Mesh Refinement methods

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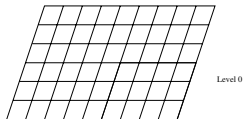
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■ Adaptive Mesh Refinement methods

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■ Inverse multi-grid process :

- Global coarse grid

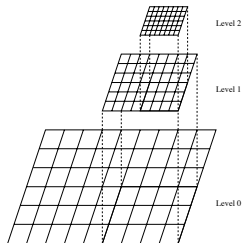


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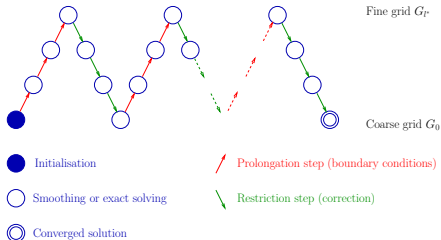
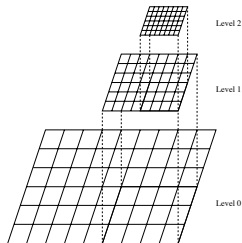
- Global coarse grid
- Local finer grids generated recursively in zones of interest



■ Adaptive Mesh Refinement methods

≡ Local Multigrid methods

- **Inverse multi-grid** process :
 - Global coarse grid
 - Local finer grids generated recursively in zones of interest
- **Prolongation** (BC interpolation) and **Restriction** operators link the grids
- ↪ **Iterative process** (\wedge -cycles)



■ Adaptive Mesh Refinement methods

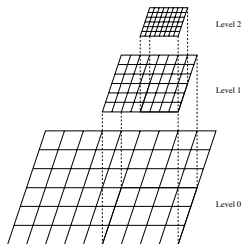
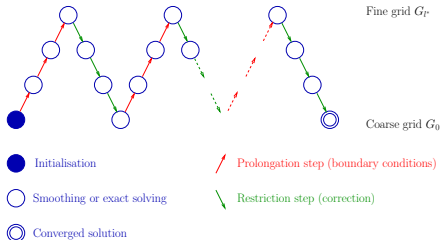
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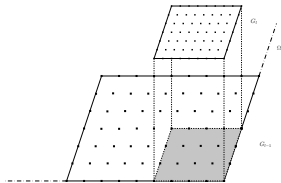
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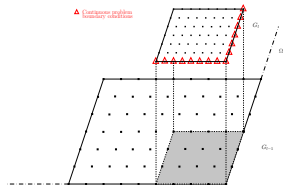
- 😊 Work on local fine meshes, Fast resolution on each sub-grid, Generic method : mesh, solver, model, refinement ratio
- ☹ Several meshes, Iterative process, Accuracy depending on prolongation and restriction operators

- Discrete problem on $G_l : \mathcal{L}_l(u_l^k) = f_l^k \forall l, k$
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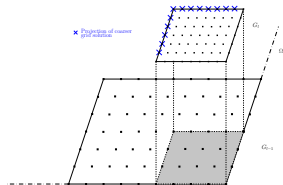


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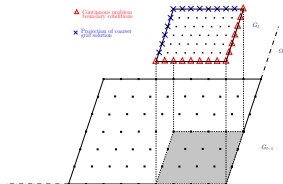
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$$u_{\Gamma_l \setminus (\Gamma_l \cap \Gamma)}^k = P_{l-1}^l(u_{l-1}^k)|_{\Gamma_l \setminus (\Gamma_l \cap \Gamma)}$$



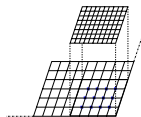
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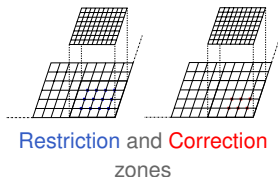
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- Prolongation step : BC definition on the fine grid G_l
- Restriction step : voluminous efforts correction on next coarse grid G_{l-1}
 - Restriction of the next finer solution at interior nodes : $\tilde{u}_{l-1}^k(x) = (R_l^{l-1} u_l^k)(x) \quad \forall x \in \blacksquare$



Restriction and Correction zones

- Discrete problem on $G_l : \mathcal{L}_l(u_l^k) = f_l^k \forall l, k$
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 - Restriction of the next finer solution at interior nodes : $\tilde{u}_{l-1}^k(x) = (R_l^{l-1} u_l^k)(x) \quad \forall x \in \blacksquare$
 - Use the corresponding coarse defect as correction :

$$f_{l-1}^k(x) = f_{l-1}^0(x) + \chi_{\blacksquare} (\mathcal{L}_{l-1}(\tilde{u}_{l-1}^k) - f_{l-1}^0)(x)$$
 ↪ overlaying zone must be large enough



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- Depends on zones of interest : either a priori known, or to be detected automatically

A posteriori error estimation in Solid Mechanics

- Estimation of the discretization error from a preliminary calculation
↳ automatic detection of the zones to be refined

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- Main error estimations in Solid Mechanics
 - Residual type a posteriori error estimators (Babuška and Rheinboldt, 1978)
 - Based on the fact that FE simulation does not verify locally the equilibrium equation
 - Calculation of the interior element residuals and the jumps at the element boundaries
 - Explicit method : post-processing method, easy to implement, dependant on unknown coefficients
 - Implicit method : solve local problems, high computational costs

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- Main error estimations in Solid Mechanics
 - Residual type a posteriori error estimators (Babuška and Rheinboldt, 1978)
 - Constitutive relation error estimators (Ladevèze and Leguillon, 1983)
 - Based on the fact that stress field of FE solution is not statically admissible
 - Define local problems to construct a statically admissible solution
 - High computational costs

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 - Residual type a posteriori error estimators (Babuška and Rheinboldt, 1978)
 - Constitutive relation error estimators (Ladevèze and Leguillon, 1983)
 - Recovery-based error estimators (Zienkiewicz and Zhu, 1987)
 - Based on the fact that the stress field of Lagrange FE method is discontinuous between elements
 - Construction of a smoothed stress field : recover the nodal values of stresses, then construct a continuous stress field using displacement shape functions
 - 2 methods (Projection method, SPR method) based on minimization process
 - Effective, easy to implement, widely used in industrial codes

- Estimation of the discretization error from a preliminary calculation
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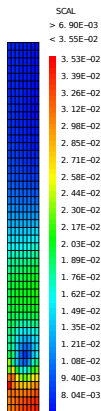
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- ⇒ Use the Zienkiewicz and Zhu error estimator

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↔ **Error = difference** between the FE and the smoothed stress fields

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- One classical method to detect the **zones of interest**
 - **Zone to be refined** : elements K such that

$$e_K > \alpha \% (\max_L e_L)$$
 - 😊 Easy to implement, **works well for every kind of estimators and norms**
 - ☹ **α unknown**, requirement of a **stopping criteria** for LDC Method



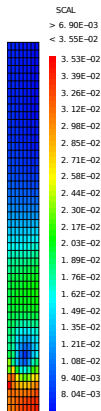
Example of ZZ a posteriori error estimation

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⇒ We want to find a user-independent detection method



Example of ZZ a posteriori error estimation

■ Relative error estimator in energy norm :

$$\|e_K\|_E = \left(\frac{\int_K (\sigma^* - \sigma_h) : (\varepsilon^* - \varepsilon_h) dK}{\int_K \sigma^* : \varepsilon^* dK} \right)^{1/2}$$

with σ^*, ε^* smoothed solutions and $\varepsilon^* = [C]^{-1} \sigma^*$, σ, ε FE solutions

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- Refine the elements for which the stress error is superior to a threshold :

$$\|e_K\|_E > \text{threshold.}$$

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- Global error

$$\begin{aligned} \|e_\Omega\|_E &= \left(\frac{\int_\Omega (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}_h) : (\boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon}_h) d\Omega}{\int_\Omega \boldsymbol{\sigma}^* : \boldsymbol{\varepsilon}^* d\Omega} \right)^{1/2} \\ &= \left(\frac{\sum \int_K (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}_h) : (\boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon}_h) dK}{\sum \int_K \boldsymbol{\sigma}^* : \boldsymbol{\varepsilon}^* dK} \right)^{1/2} < \text{threshold} \end{aligned}$$

■ Error estimator in maximal norm :

$$\|e_K\|_\infty = \max_{\text{Gauss point in } K} |\sigma^* - \sigma_h|$$

with σ^* smoothed solutions and σ FE solutions

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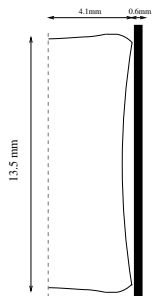
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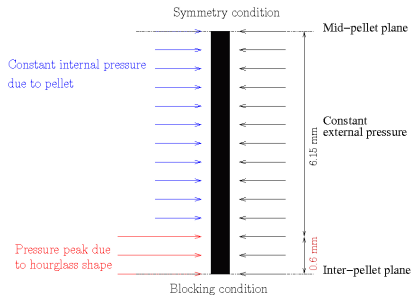
- Not widely used in the literature
- More interesting for mechanical engineer because it gives a local information

**Numerical results of
the combination of LDC
and ZZ estimator**

- Hourglass shape deformation :
 $2D(r, z)$ test case

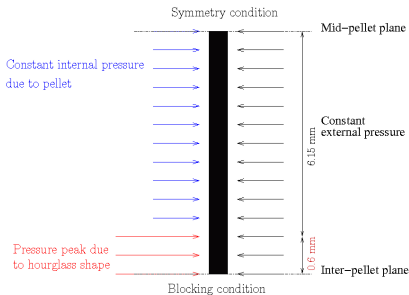


- Hourglass shape deformation :
 $2D(r, z)$ test case
- Focus on the elastic response of the cladding



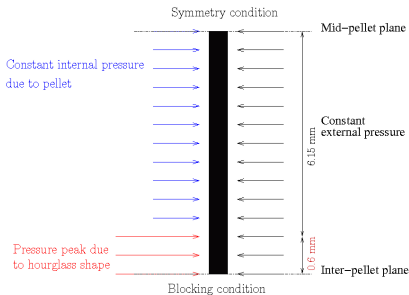
$$E = 100 \text{ GPa}, \nu = 0.3$$

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 $2D(r, z)$ test case
- Focus on the elastic response of the cladding
- Contact with the pellet = discontinuous pressure imposed on the internal radius of the cladding



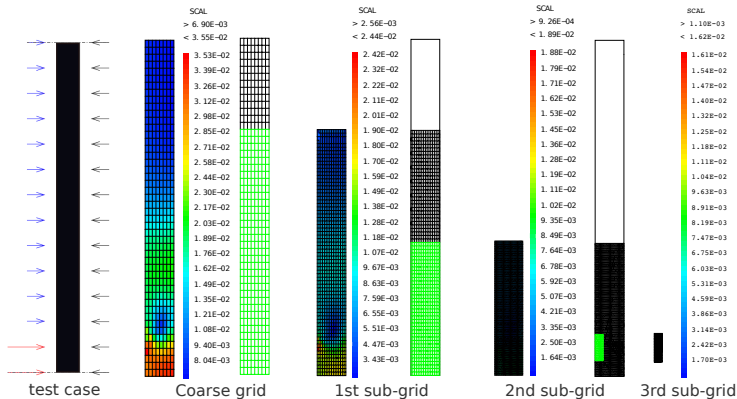
$$E = 100 \text{ GPa}, \nu = 0.3$$

- Hourglass shape deformation :
 $2D(r, z)$ test case
- Focus on the elastic response of the cladding
- Contact with the pellet = discontinuous pressure imposed on the internal radius of the cladding
- LDC coupled with ZZ error estimator
 - Generate sub-grids at the first prolongation step
 - Number of level of sub-grids generated automatically



$$E = 100 \text{ GPa}, \nu = 0.3$$

Relative error in energy norm



Example for threshold 1%

- Number of levels stops automatically
- Sub-grids localized around the pressure discontinuity

■ Relative error in energy norm

mesh	threshold			
	5%	2%	1%	0.50%
hi =328 μm	4.5%	2.04%	0.614%	0.366%
hi/2	4.20%	1.98%	0.614%	0.366%
hi/4	1.92%	1.92%	0.527%	0.366%
hi/8	0.757%	0.757%	0.433%	0.322%

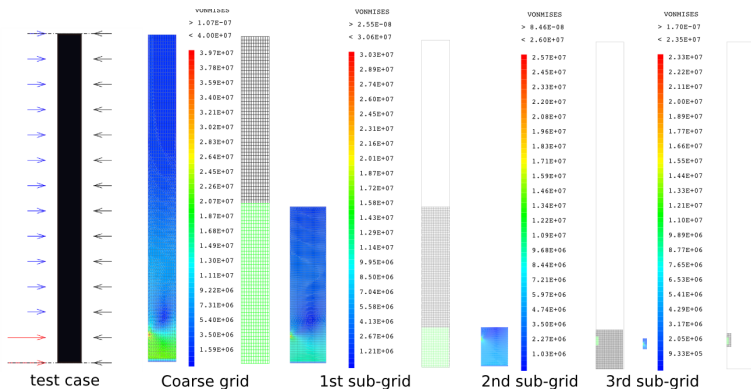
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- Works well, obtained errors inferior to threshold for different thresholds and different initial coarse meshes.
- Error can be sub-estimated by ZZ estimator \rightarrow security coefficient

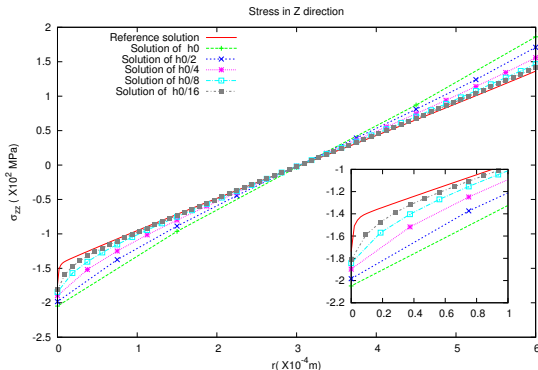
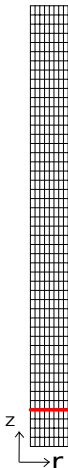
Maximal norm



Example for threshold $5E+6$ Pa

- Generation of sub-levels **doesn't stop**
- Zone detected **more localized**

Maximal norm



Stress for different meshes

Stress singularity near the pressure discontinuity

Never converge with the mesh step

→ Find a method to stop the generation of sub-grids

Conclusions and perspectives

■ Conclusions

- Use the solver as a "black box"
- Coupling of ZZ error estimator and LDC method works well.
- Zones of interest are detected automatically
 - Energy norm : automatically stop
 - Maximal norm : generation of sub-grids doesn't stop (singularity)
- Numerical results of the 2D(r,z) test case are promising as zones of interest are more and more localized and the errors decrease.

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■ Perspectives

- Error in maximal norm
 - Find a user-independent method to stop generating sub-grids
- Nonlinear test case
- Comparison with h-adaptive method (most used space refinement method)

Thank you

This work has been achieved in the framework of the PLEIADES project, financially supported by CEA (Commissariat à l'Énergie Atomique et aux Énergies Alternatives), EDF (Électricité de France) and AREVA.