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AUTOMATIC ADAPTIVE MESH REFINEMENT WITH CONTROLLED ACCURACY IN A MULTISCALE CONTEXT FOR NONLINEAR SOLID MECHANICS

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ABSTRACT
During irradiation in reactors, a variety of phenomena of different natures are occurring at different scales. It is crucial to understand such phenomena and to be able to simulate their evolution in time with a controlled accuracy. In this context, we propose to develop an efficient numerical tool enabling us to perform accurate nonlinear quasi-static mechanical simulations with evolving local phenomena. This tool is based on adaptive mesh refinement (AMR) techniques. We adopt a fully automatic algorithm governed by user-prescribed tolerances on errors. We show that the multilevel Local Defect Correction (LDC) method is the most efficient AMR approach in terms of computation time to achieve desired precisions. Its key advantage lies in the separate resolution of problems of limited sizes on a hierarchy of meshes evolving in time.

1 INTRODUCTION
In the nuclear field, the understanding of phenomena occurring during irradiation, in particular through their numerical simulation, is extremely important with regards to the safety and design procedures. This work is encompassed in the framework of study of a wide range of multiscale and multiphysical phenomena occurring in Pressurized Water Reactor (PWR) during irradiation. We are interested more precisely in the numerical simulation of the localized contact between the fuel pellet and its surrounding cladding. This phenomenon is called Mechanical Pellet-Cladding Interaction (PCI) [1], cf. Figure 1. In order to guarantee integrity of the cladding, first barrier of confinement of fission products, this phenomenon must be studied and simulated with the best precision. The approach currently applied in PLEIADES[1] [2] consists in using a conforming mesh *a priori* refined in the region of interest – pellet-cladding contact zone. Such approach is not sufficiently predictive, elements in the critical region are not sufficiently fine, and computations are costly. Thus, the main motivation of this work consists in proposing a numerical tool allowing us to simulate multiscale problems with phenomena localized at the structural scale in a precise (respecting user-prescribed accuracies) and efficient (in terms of

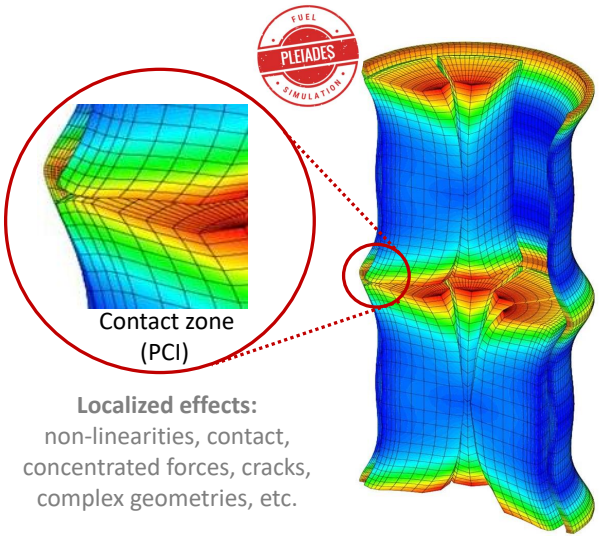

Figure 1: Simulation of multiscale phenomena

[1]Multi-concept fuel software environment for irradiated fuel elements in sub-assemblies for demonstration, experimentation or service, co-developed by CEA (French Alternative Energies and Atomic Energy Commission, www.cea.fr), EDF (Électricité de France, www.edf.fr) and FRAMATOME (ex-AREVA, www.framatome.com)

memory space and computational time) ways. One of the major challenges is the possibility to follow the evolution of a studied phenomenon in time in the case of nonlinear mechanical behaviours (e.g. evolution of the PCI phenomenon).

2 ADAPTIVE MESH REFINEMENT ALGORITHM

To meet the aforementioned challenges, we adopt in this work an adaptive mesh refinement (AMR) algorithm aiming to capture local phenomena at structural scale [7] by automatically enriching the mesh in critical regions – regions with high discretization error[2]. The proposed algorithm is fully automatic and governed by user-prescribed tolerances on errors. It is dedicated to the hierarchical refinement of quadrilateral/hexahedral meshes appealing for their great advantages in industrial applications. Such algorithm follows an iterative refinement loop, whose each iteration is based on a sequence of modules: **SOLVE** $\rightarrow$ **ESTIMATE** $\rightarrow$ **MARK** $\rightarrow$ **STOP** $\rightarrow$ **REFINE**. These modules are briefly introduced hereafter. The interested reader is referred to [3] for more detailed presentation of the refinement algorithm.

Among a wide range of AMR approaches available in the literature [4, 5, 6], we focus on the methods targeting the mesh step h which have gained widespread success within solids mechanics community due to their simplicity and efficiency in particular in presence of singularities [8]. Two main classes of h-based refinement methods have been integrated in the proposed generic AMR algorithm, cf. Figure 2.

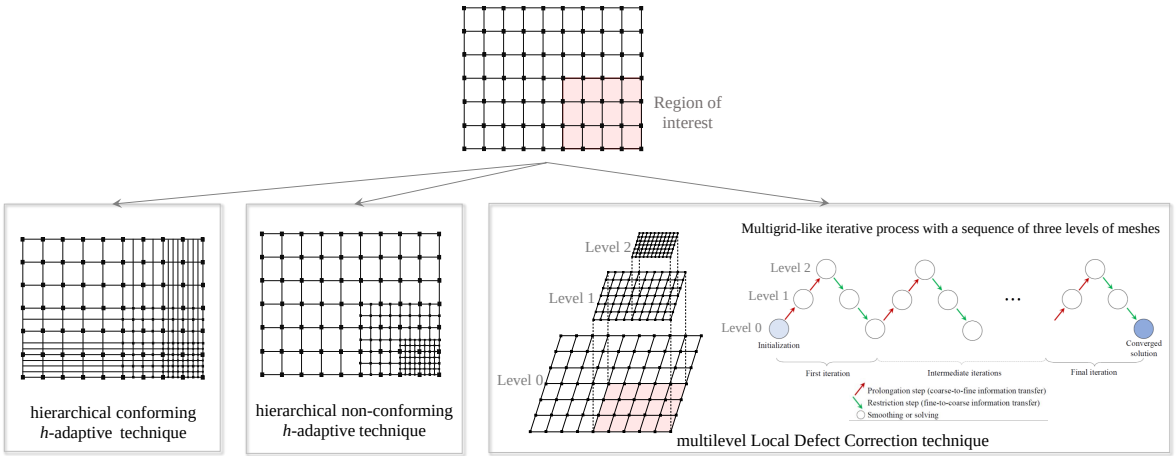

Figure 2: AMR methods based on the mesh step h refinement

The first class involves the well-known h-adaptive strategies [9], conforming and non-conforming techniques, which aim to generate locally refined meshes covering the whole computational domain, cf. Figure 2 left and middle. The conforming h-adaptive strategy aims to generate a conforming locally refined mesh by propagating the refinement outside regions of interest. The non-conforming technique consists in refining only elements in the region of interest and thus generally leads to the appearance of hanging nodes (requiring a dedicated solver).

The second class of h-based AMR methods involves locally adaptive multigrid or multilevel methods. These methods exploit the mesh refinement on several levels of meshes (nested levels of meshes with finer and finer mesh sizes added locally), cf. Figure 2 right. The solution process consists in solving problems associated to different levels of meshes in a sequential manner and coupling solutions through an iterative multigrid-like process based on prolongation and restriction operators [10]. We adopt in this study the multilevel Local Defect Correction (LDC) method [11, 12, 13] as it seems to be the most pertinent choice for solid mechanics problems with localized effects. The LDC prolongation operator is used to define Dirichlet boundary conditions on the internal boundary of the next finer mesh levels by projecting the next coarser solution. The restriction operator aims to obtain a restriction of the next finer solution on the

[2]behaving as $\mathcal{O}(h^p)$ with h being the mesh step and p being the degree of interpolation function

coarse mesh, which serves to derive a residual (also called defect) acting as an additional source term in the current level problem.

The aforementioned methods rely on the mesh step h refinement (**REFINE**) but exploit conceptually different solution processes (**SOLVE**). In the generic algorithm, the module **REFINE** takes into account the specificities of each considered here AMR method to construct refined meshes (e.g. conservation of the mesh conformity, restriction of the non-conformity level, or refinement on several levels). Furthermore, we integrate in the module **SOLVE** the solving specificity of each AMR method (managing hanging nodes, carry out an iterative process for multigrid methods...). These modules are formulated in such a way to be easily implementable in industrial solvers, while being generic and suitable for different geometries, dimensions, etc.

Beyond the AMR strategies, the refinement algorithm involves the following modules. The module **ESTIMATE** stands for the application of an error estimator [5] aiming to automatically drive the mesh adaptation process. This module outputs an elementwise estimated error distribution allowing us to detect the critical regions. In this study, the widely used recovery-based Zienkiewicz and Zhu *a posteriori* error estimator [14] is adopted thanks to its robustness, simplicity of implementation and performance (limited computational cost).

Based on the elementwise estimated error distribution, elements to be refined are detected with the module **MARK**. Various detection criteria has been studied in [3]. In this paper, we rely on the marked strategy based on the mesh optimality criterion introduced in [15] aiming to control both, global and local errors.

The module **STOP** aims to turn off the AMR process when the solution computed at a given refinement iteration respects the user-defined global and local accuracies. The global error control, classical in the literature, consists in verifying if the estimated global discretization error satisfies the prescribed tolerance ϵ_Ω. One of the novelties of this work is to control in addition the local elementwise error which is important for industrial applications, but very little studied in the literature. This local error is quantitatively evaluated by a local error parameter η representing the measure of a discrete approximation of the critical region (set of elements whose estimated local error exceeds the prescribed tolerance ϵ_Ω). This parameter is weighted by the domain's measure (thus, is expressed in percent for convenience), and is compared to the user-prescribed one δ.

3 AMR METHODS COMPARISON

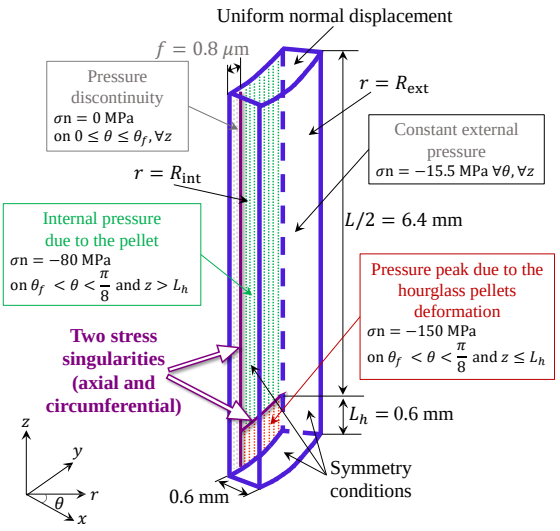

Figure 3: 3D test case of the PCI

The previously presented algorithmic framework allows us to numerically compare the chosen AMR techniques in the most rigorous and objective way. For this comparative study we place ourselves in a linear elastostatic framework. Denoting Ω a bounded domain in $\mathbb{R}^D$ (with D – the dimension) with $\partial\Omega$ its boundary, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ the stress and elastic strain tensors, $\boldsymbol{u}$ the displacement field and $\mathbf{C}$ the fourth order elasticity tensor, the problem reads:

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma}(\boldsymbol{u}) = 0 & \text{in } \Omega \\ \boldsymbol{\sigma}(\boldsymbol{u}) = \mathbf{C} : \boldsymbol{\varepsilon}(\boldsymbol{u}) & \text{in } \Omega \\ \boldsymbol{\varepsilon}(\boldsymbol{u}) = \dfrac{1}{2}(\operatorname{grad} \boldsymbol{u} + \operatorname{grad}^{\mathrm{T}} \boldsymbol{u}) & \text{in } \Omega \\ \text{Boundary conditions} & \text{on } \partial\Omega \end{cases} \tag{1}$$

We present in this contribution the results of the test case representing the Mechanical Pellet-Cladding interaction (PCI) phenomenon. We simulate the cladding's response to the pellet

modifications (the hourglass deformation and the pellet fragmentation) on a 3D test case depicted in Figure 3. Due to the discontinuous contact with the pellet, two crossed singularities (axial and circumferential) of different characteristic length-scales are revealed in the cladding. For symmetry reasons, the cladding in front of $1/32$ of a pellet is represented. Computational domain and boundary conditions are presented in Figure 3. The material of the cladding is supposed to be linear elastic with Young's modulus $E = 10^{11}$ Pa and Poisson's ratio $\nu = 0.3$. From the numerical point of view, finding an accurate solution to such problem is a challenging task since it involves two stress singularities of different characteristic length scales in opposite directions. Thereby, this problem justifies the necessity to apply an AMR strategy. We verify here different global error tolerances ϵ_Ω, while the local error control parameter δ is set to 3%. The reference solution is inaccessible for this problem, thus the estimated final errors are shown.

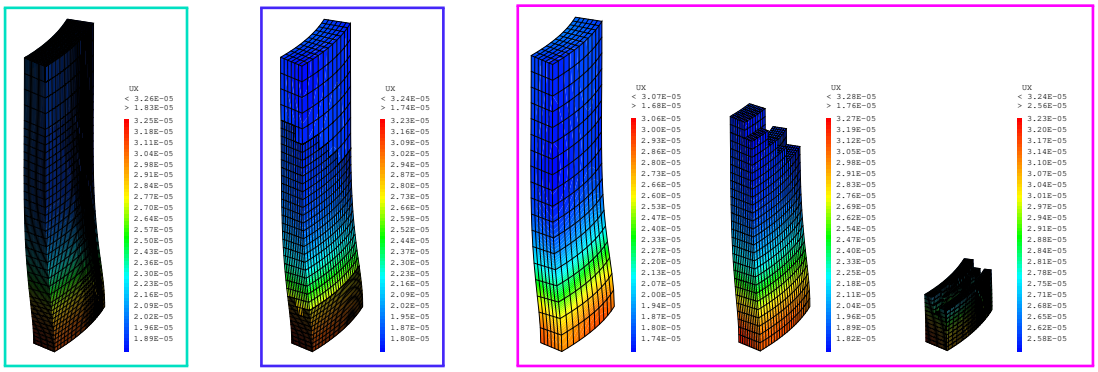

Figure 4: Computed displacement field $\boldsymbol{u}_x$ for $\epsilon_\Omega = 4\%$ on the final refined mesh for *(left)* the conforming h-adaptive method ($\mathbf{e}_{\text{glo}}^{\text{est}} = 1.44\%$), *(center)* non-conforming h-adaptive method ($\mathbf{e}_{\text{glo}}^{\text{est}} = 1.93\%$) and *(right)* on the hierarchy of meshes for the LDC method ($\mathbf{e}_{\text{glo}}^{\text{est}} = 1.95\%$)

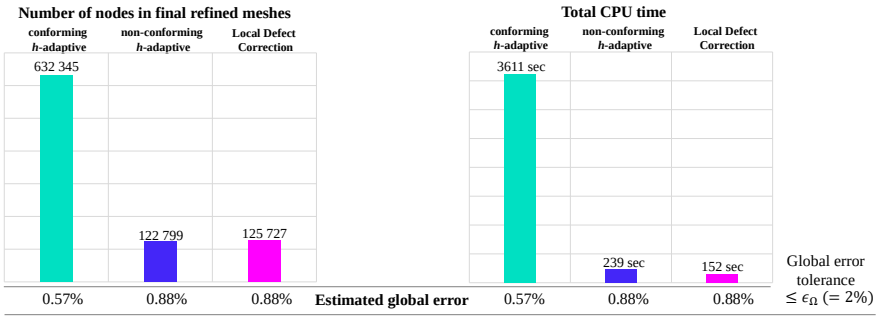

Figure 5: AMR methods comparison for $\epsilon_\Omega = 2\%$: total number of nodes (*left*) and CPU time (*right*)

Figures 4 and 5 present the main qualitative and quantitative results, respectively. In Figure 4 we show the displacement fields in the x direction (plotted on the deformed configuration) obtained with each studied AMR method for the global error tolerance $\epsilon_\Omega = 4\%$. In Figure 5 the main results in terms of the number of nodes and computational time for $\epsilon_\Omega = 2\%$ are depicted. First, it has to be noted that all AMR techniques permit to reach the prescribed local precision (local error control parameter respects fixed $\delta = 3\%$). It implies that the global accuracy is generally over-respected. We observe that the conforming h-refinement generates over-refined final meshes requiring expensive computations. The final mesh of the non-conforming h-adaptive approach is similar to the composite one of the LDC method. However, the non-conforming h-refinement is more demanding in CPU time and requires a dedicated solver to handle hanging nodes. The LDC approach leads to considerable computational savings thanks to its capability to solve problems on a hierarchy of meshes of limited sizes.

Conclusions of the comparative study. Thanks to this comparative numerical study we show that the multilevel LDC method is the most efficient AMR technique which permits to reach

desired accuracies in an attractive computational cost (CPU time and memory space). This opens the way to apply this approach on nonlinear solids mechanics problems.

Remark. In [3, 16] the same conclusions have been derived for other industrial and more academic numerical examples. In addition to the AMR methods comparison, we have revealed the most efficient refinement strategy for quad/hexa meshes. It consists in combining the marking criterion aiming to control global and local errors [15] and the refinement ratio fixed to 2.

4 AMR STRATEGY FOR NONLINEAR QUASI-STATIC PROBLEMS

4.1 Nonlinear quasi-static mechanical problem

In this study we place ourselves in a general nonlinear framework. The constitutive law of the problem 1 thus reads:

$$\boldsymbol{\sigma}(\boldsymbol{u}) = \mathcal{F}(\boldsymbol{\varepsilon}(\boldsymbol{u}), \dot{\boldsymbol{\varepsilon}}(\boldsymbol{u}), ...) \tag{2}$$

The solution of such problem is done by dividing the history into time steps. Generally, a Newton-like algorithm is used at each time step to linearize the variational formulation of the problem. With $\mathbf{H}$ a linearization operator, n the Newton's iteration, and for all field $\boldsymbol{v}$ kinematically admissible to zero, after linearization we obtain the following variational form:

$$\int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{v}) : \mathbf{H}^{n-1} : \boldsymbol{\varepsilon}(\boldsymbol{u}^n - \boldsymbol{u}^{n-1}) \, \mathrm{d}\Omega = \int_{\Gamma_\mathbf{N}} \mathbf{F_N} \, \boldsymbol{v} \, \mathrm{d}\Gamma_\mathbf{N} - \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{\sigma}^{n-1} \, \mathrm{d}\Omega = R^{n-1} \tag{3}$$

The iterative process tends to minimize the residual of the nonlinear problem written as:

$$R^{n-1} = \boldsymbol{F}^{ext} - \boldsymbol{F}^{int}(\boldsymbol{\sigma}^{n-1}) \tag{4}$$

where $\boldsymbol{\sigma}^{n-1}$ is updated at each iteration n using the nonlinear constitutive law 2.

4.2 Extension of the LDC method

We proposed in [7] a theoretical extension of the LDC method to quasi-static mechanical problems with nonlinear material behaviours and variable loadings.

The underlying idea of the LDC method is to make the global displacement tend towards the restricted fine one in the region of interest. It is done in a weak sense via the LDC residual. In the case of nonlinear problems, the LDC algorithm aims to update the nonlinear residual (cf. Eq. 4) of problems associated to coarse mesh levels. Thus, in the region of interest this updated residual can be seen as a minimization of the difference between internal forces computed with the stress coming from restricted fine computations and internal forces computed in the classical way. The key features related to the practical implementation of the LDC method within a black-box nonlinear industrial solver are presented in [16, 17] The efficiency of the LDC method as proposed in this work has been demonstrated on several numerical examples.

Remark. It is important to note that in the analytical study [7], we have developed a unified algorithmic setting in which a large number of multiscale methods based on iterative coupling can be integrated. The conceptual and algorithmic similarities between multilevel AMR methods and numerical homogenization approaches have been highlighted. Moreover, we have shown that the LDC technique can be seen as a meso-homogenisation approach suitable for problems with small scale separation parameter where homogenization-based methods are limited.

4.3 Evolving mesh

The main challenge of this work is to propose a strategy based on moving refined mesh regions which would allow us to capture the phenomenon evolution with a controlled precision. It has to be highlighted that even though many studies have been conducted to propose efficient AMR-based algorithms for time-dependent problems, several important issues, mainly associated with field transfer and error control, still remain open. These questions have been addressed in this thesis, cf. [16, 17].

In the nonlinear framework, as refined mesh is supposed to evolve between time steps, an additional module **TRANSFER** has been introduced in the AMR algorithm detailed in section 2. This module aims to define initial conditions on the mesh at the current time t based on

the converged solution (in terms of the Newton iterations) obtained at the previous time $t-1$. It involves two key features: the fields transfer step and the equilibration step.

There exist two main types of fields to be transferred. For nodal quantities (e.g. displacement), the basis functions of the previous mesh are generally used. The transfer of variables known at integration points (e.g. stress, strain fields and internal variables) is generally more complex and requires the use of a dedicated operator (precision/cost balance, minimization of the numerical diffusion, ...). In our study we have proposed a precise and robust strategy aiming to minimize the numerical diffusion. It lies on an elementwise extrapolation to discretisation nodes, cf. [16] for more details.

Moreover, an important step consists in recovering the equilibrium of transferred fields. We propose here an approach lying on the introduction of the initial non-equilibrated residual, denoted R_{ne}^{t-1}, as a source term of the problem. This residual aims to minimize the initial non-equilibrium (arising from the field transfer) and reads $R_{\text{ne}}^{t-1} = \boldsymbol{F}^{ext,t-1} - \boldsymbol{F}^{int}(\hat{\boldsymbol{\sigma}}^{t-1})$. It involves internal forces $\boldsymbol{F}^{int}(\hat{\boldsymbol{\sigma}}^{t-1})$ computed with $\hat{\boldsymbol{\sigma}}^{t-1}$ – the stress field resulting from the projection of $\boldsymbol{\sigma}^{t-1}$ on the current refined mesh. The residual R_{ne}^{t-1} is added to the initial (standard) one $\tilde{R}^{0,t} = \boldsymbol{F}^{ext,t} - \boldsymbol{F}^{ext,t-1}$, as follows:

$$R^{0,t} = \tilde{R}^{0,t} + R_{\text{ne}}^{t-1} \tag{5}$$

That returns in practice to consider the initial residual of the following form

$$R^{0,t} = \boldsymbol{F}^{ext,t} - \boldsymbol{F}^{int}(\hat{\boldsymbol{\sigma}}^{t-1}) \tag{6}$$

The proposed strategy enables us to not accumulate the non-equilibrium residual and thus to efficiently control the error over time and to adapt the mesh when needed. The importance of this equilibration step has been clearly shown in [16]. Moreover, no evaluation of the constitutive law 2 is required in this equilibration step.

4.4 Numerical results on the PCI industrial benchmark

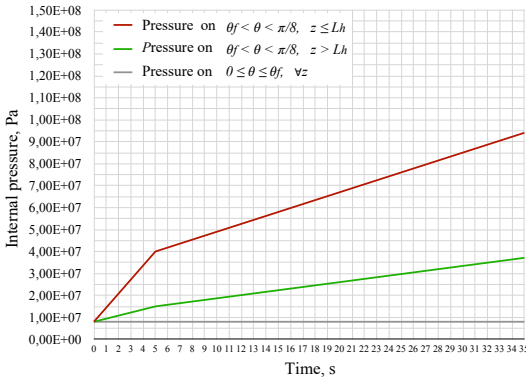

Figure 6: Loading history

We consider here a numerical benchmark of the PCI representing the transient stage with nonlinear visco-plastic behaviour of the cladding and stress singularities generated by variable pressures exerted by the pellet [1]. The main problem setting is detailed in Figure 3. Pressures prescribed on the internal part of the modeled cladding are assumed to vary linearly with time with two different slopes, cf. Figure 6. The first slope corresponds to a conditioning of the pellet (5 seconds), while the second one to a transient of power (30 seconds). The time step is considered to be equal to 1 second.

The cladding's nonlinear behavior is characterized by a Norton creep constitutive law without hardening. Here, the nonlinear strain is related to the stress through its velocity as $\dot{\boldsymbol{\varepsilon}}^{nl} = (\frac{J}{K})^{n-1}\boldsymbol{\sigma}_d$ with $n = 5$ and $K = 2.6 \cdot 10^{11}$ Pa$^{\frac{5}{4}}$ s$^{\frac{1}{4}}$ two given material coefficients, $\boldsymbol{\sigma}_d$ the deviatoric stress tensor and J the second invariant of $\boldsymbol{\sigma}_d$. In this numerical example we set the global error tolerance $\epsilon_\Omega = 10\%$ and the local error control parameter $\delta = 10\%$. The estimated final errors are reported due to inaccessibility of the reference solution.

We present in Figure 7 the Von Mises stress fields obtained for various time steps on composite LDC meshes (superposition of all mesh levels). At the beginning of the modeled time history, the internal pressure is assumed to be constant, thus the refinement is not required to meet the prescribed accuracy. While increasing pressure values applied to the different zones and thus generating the gradual appearance of stress singularities, we observe the automatic evolution of the refined mesh levels. We demonstrate the possibility to automatically add local mesh levels with finer elements to follow the evolution of pressure singularities, cf. Figure 7.

It has also to be emphasized that the proposed LDC-based refinement algorithm allows us to generate meshes with much finer elements in the regions of interest than currently attainable in PLEIADES, cf. [1]. It thus permits to reach better precision than ever.

Remark. It has also to be highlighted what we rely here on a proposed optimized refinement algorithm enabling us to limit the number of remeshing over time (thanks to a proposed remeshing indicator) while guaranteeing the verification of prescribed error tolerances, cf. [16, 17]. Thus, only 5 remeshing have been automatically carried out for 35 time steps.

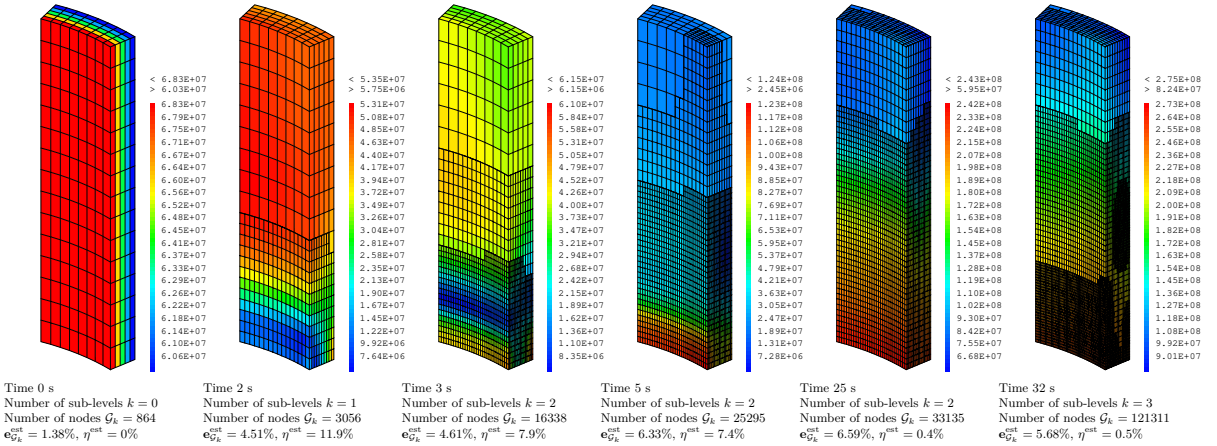

Figure 7: Following in time of the PCI phenomenon with a visco-plastic model – evolving mesh levels (composite meshes) of the LDC multilevel method

Figure 8 presents the evolution of the estimated global errors and local error measures in time. We can see that very satisfying results in terms of reached accuracies have been obtained: the prescribed global and local tolerances are generally well respected. We observe significant decrease of errors which are related to remeshing. Especially, remeshes are carried out at time steps following steps where the local error measure exceeds the prescribed tolerance. It would be possible to avoid exceeding the prescribed thresholds by redoing the computations at the same time step, cf. [16].

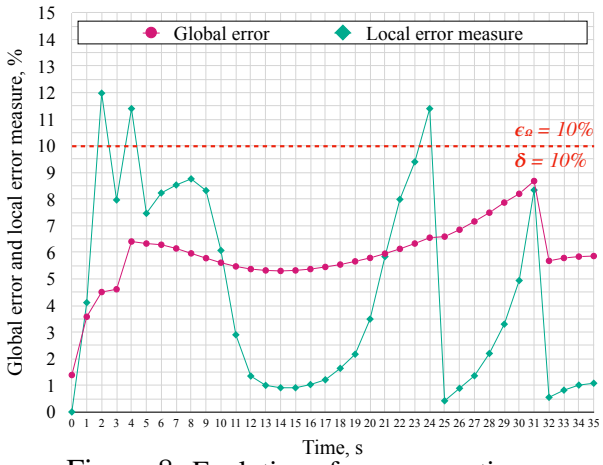

Figure 8: Evolution of errors over time

CONCLUSIONS AND PERSPECTIVES

In this thesis we have proposed a powerful AMR algorithm allowing us to meet one of the industrial challenges related to the Mechanical Pellet-Cladding Interaction simulation. Based on the multilevel Local Defect Correction method, it permits us to reach currently inaccessible accuracies in an attractive computational cost (CPU time and memory space). Moreover, the natural ability of LDC to generate a hierarchy of meshes evolving in time permits to dynamically follow the temporal evolution of the studied phenomenon. We have illustrated the efficiency of the proposed algorithms on a range of mechanical (academic and complex industrial) problems with localized effects of different complexities. Motivated by a specific nuclear problem, a great deal of effort has been consecrated to propose generic and transversal algorithms, which opens ways to apply them to engineering fields other than those of nuclear fuel.

As perspective, it would be interesting to explore the capacity of the LDC approach to address different type of problems (other material behaviors, dynamic problems, large deformations,

crack propagation, etc.). Another perspective of this work is to add the pellet-cladding contact for a more efficient simulation of the PCI phenomenon. It would also be interesting to treat the multiphysics coupling.

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