Modelling with X-FEM
dynamic propagation and arrest
of a cleavage crack in PWR steel

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Outline of the speech

Context and Objectives

I. Numerical tools

II. Experimental support

III. Model of Propagation

step 1: Proposition of a model
step 2: Predictive Simulations

Conclusion and Prospect
Outline of the speech

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Conclusion and Prospect
Context and Objectives

- **PWR life extension**
- **Case of an accidental pressurized thermal shock** of PWR vessel:
  - Lot of work on brittle fracture
  - Ensure the non-initiation of a hypothetical defect
- **What about brittle crack propagation?**
  - After initiation, how will the crack behave?
  - Consequence for the structure integrity?

**Thesis goals:**
- Understand phenomena occurring during propagation of a cleavage crack in a PWR steel up to arrest
- Propose a model of propagation validated by experiments
Context and Objectives

How to deal with dynamic crack propagation?

**Elastic dynamic analysis?**

- **Kalthoff's observations:**
  - Dynamic analysis is relevant

- **Kaninnen's empirical relation:**
  \[
  K_{\text{dyn}}(\dot{a}) = \frac{K_A}{1-(\dot{a}/v_{\text{lim}})^m}
  \]
  - Simple model for a brittle crack
  - Limited when plasticity is not negligible

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Diagram showing crack length over time with symbols for different specimen types: double cantilever beam specimen and three point bend specimen.
How to deal with dynamic crack propagation?

**Elastic-viscoplastic analysis:**

- **Freund's theoretical model:**
  - Crack speed predicted >> observed

- **RKR model used by Hajjaj:**
  - \( \sigma_I(r=100\mu m) = \sigma_{Ic}(T) \)
  - Relatively good predictions, but only 1 configuration studied
Context and Objectives

To investigate crack propagation and arrest, one needs to perform Dynamic analysis taking into account:

→ Inertial effects on mechanical fields
→ Strain rate dependent constitutive law

• Relevant Experimental data should be collected:
  → as crack speed measurements
  → for different configurations (geometries and loadings)

• Efficient Numerical tool should be used to model:
  → any crack propagation
  → with minimal effort,
  → accurately,
  → for any constitutive law or any configuration hypothesis
Outline of the speech

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Conclusion and Prospect
Difficulties encountered with classical numerical methods for modelling arbitrary crack growth in Finite Element:

- Node release method → suppose to know the crack path
- Deletion element → dissipated energy depend on mesh
- Cohesive zone model → mesh-dependency
- Re-meshing → problem with projection of fields
- ...

Efficiency of methods based on Partition of Unity like:

- The **extended Finite Element Method** (*):
  → the implicit representation of a crack by level set
  → ad hoc enrichment of the displacement with additional degrees of freedom

**Implementation of the X-FEM in Cast3M**

* : [Belytschko 99], [Moes 99], [Gravouil 02], ...
Modelling: Numerical tools

The eXtended Finite Element Method:

- **Implicit Crack Description**

→ by a couple of Level Set (or "distance") functions

the crack front: \[ \psi = 0 \]

the crack plane: \[ \phi = 0 \]
Modelling: Numerical tools

The eXtended Finite Element Method:

- **Enrichment of the displacement approximation**

  - **H-enrichment:**
    \[
    H(x) = \begin{cases} 
    +1 & \text{if } \phi > 0 \\
    -1 & \text{if } \phi < 0 
    \end{cases}
    \]

  - **F-enrichment:**
    \[
    F_j(x) = \sqrt{r} \begin{pmatrix} 
    \sin(\theta/2) \\
    \sin(\theta/2) \sin(\theta) \\
    \cos(\theta/2) \\
    \cos(\theta/2) \sin(\theta) 
    \end{pmatrix}
    \]

\[
\mathbf{u}(x) \approx \sum_i N_i(x) \left[ \mathbf{u}_i + H(x_i) \mathbf{a}_i + \left( \sum_{j=1}^{4} F_j(x_i) b_{i,j} \right) \right]
\]
The eXtended Finite Element Method:

- **Enrichment of the displacement approximation**

\[ q^n = \begin{bmatrix} u_i \\ a^n_i \\ b^n_{i,j} \end{bmatrix} \]

\[ q^{n+1} = \begin{bmatrix} q^n \\ a^{n+1}_i \\ b^{n+1}_{i,j} \end{bmatrix} \]

- Crack tip at time \( t^n \):
  - H-enrichment
  - F-enrichment

- Crack tip at time \( t^{n+1} \):
  - New H-enrichment
  - New F-enrichment

**Context and Objectives**

- Numerical tools
- Experimental support
- Proposition of a Model of Propagation
- Predictive Simulations

**Conclusion and Prospect**

Modelling: Numerical tools

The eXtended Finite Element Method:

- Level Set functions defined on a regular auxiliary grid different from the mechanical mesh

→ **mechanical mesh** (not fitted to level set update)

\[ \text{div}(\sigma) = \rho \ddot{u} \Rightarrow M \ddot{q} + \int B^T \sigma = F^{\text{ext}} \]
The eXtended Finite Element Method:

- Level Set functions defined on a regular auxiliary grid* different from the mechanical mesh

→ **auxiliary grid** (easy, fast and accurate level set update)

\[
\frac{\partial \psi}{\partial t} = V_\psi \cdot \nabla \psi \Rightarrow \frac{\psi_{i,j}^{t+\Delta t} - \psi_{i,j}^{t}}{\Delta t} = H(V_{i,j}, \psi_{m,n})
\]

*: [Prabel et al. 07]
Modelling: Numerical tools

The eXtended Finite Element Method:

- Standard Numerical Integration:

  **Usually,** conformed sub-triangle partitioning

  Crack growth → Change in Gauss points location

  → Projection!
Modelling: Numerical tools

The eXtended Finite Element Method:
- Selected Numerical **Integration**:
  Alternative, non-conformed sub-partitioning*

* : [El guedj 06], [Prabel et al. 07]
Modelling: Numerical tools

The eXtended Finite Element Method:
• Selected Numerical **Integration**: Alternative, non-conformed sub-partitioning

→ **Anticipate** the crack arrival, and the plasticity
Modelling: Numerical tools

The eXtended Finite Element Method:

- Selected Numerical **Integration:**

**Alternative**, non-conformed sub-partitioning

→ **Anticipate** the crack arrival, and the plasticity

The eXtended Finite Element Method:

- Numerical Application: → Kalthoff experiment

→ LEFM criteria:

\[ \dot{a} = c_R \left[ 1 - \frac{K_A}{K_{eq}^{dyn}} \right] \quad \theta_c = \{ \theta, \max (\sigma_{\theta\theta}(r_c)) \} = f(K_I, K_{II}) \]
Modelling: Numerical tools

The eXtended Finite Element Method:

- Numerical Application: → Kalthoff experiment
Modelling: Numerical tools

The eXtended Finite Element Method:

- Numerical **Application**: → **Gregoire** experiment*
  Notched PMMA specimen between Hopkinson bars

* : [Grégoire et al. 07]
Modelling: Numerical tools

The eXtended Finite Element Method:

- Numerical **Application**: → *Gregoire* experiment
Modelling: Numerical tools

The eXtended Finite Element Method:
• Numerical Application: → Gregoire experiment
Outline of the speech

Context and Objectives

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Conclusion and Prospect
Experimental support

Available experimental data for 16MND5 steel:
- Very important material characterization* in term of:
  → static constitutive law (from -175°C to 25°C)
  → cleavage initiation (triaxiality, WPS, ...)

Experimental needs for dynamic fracture:
- Dynamic material characterization:
  → strain rate effect (in temperature range)
- Fracture tests:
  → on laboratory specimen (CT)
  → on analytical specimen (Ring loaded in mode I)
  → for various configurations (Ring in mixed mode)
- Fracture surface observations:
  → to determine fracture mechanism
  → for every specimen type,
  → at every stage of the propagation

*: Campaign FISTER (2000-2004); Campaign CRITER (2002-...) ~ sponsored by IRSN
Experimental support

Material:
- French PWR ferritic steel: 16MND5 (A508)
- Temperature characterization:

\[ T = -150 \, ^\circ C \]
\[ T = 25 \, ^\circ C \]
Experimental support

Material:

- **High strain rate characterization** (Split Hopkinson Pressure Bar) \(\rightarrow\) Modified Symonds-Cowper law:

\[
\sigma(T, \varepsilon^{in}, \dot{\varepsilon}^{in}) = \sigma_{stat}(T, \varepsilon^{in}) \cdot \left[1 + H(T, \varepsilon^{in}) \dot{\varepsilon}^{in} 1/p(T)\right]
\]

**Context and Objectives**

Numerical tools

Experimental Support

Proposition of a Model of Propagation

Predictive Simulations

Conclusion and Prospect
Experimental support

- **Geometries** investigated:
  1. Compact Tension specimen
  2. Notched Ring under Compression (mode I)
  3. Notched Ring under Compression (mixed mode)

- **Fatigue pre-cracking**

- **Fracture test:**
  → Isothermal (-125°C)
  → Quasi-static loading
  → Crack speed measurement:
    Crack gages + Fast acquisition board (60MHz)

- Arrest front marked by fatigue
Experimental support

Geometries investigated:
1. Compact Tension specimen:

- clip gage
- crack gage
- thermocouple
- crack arrest
Experimental support

**Geometries investigated:**
2. Ring under Compression (mode I):
Geometries investigated:
3. Ring under Compression (mixed mode):
pre-cracking
mixed mode loading

25°
Fractography:
• What is the fracture mechanism during propagation?

\[ \rightarrow 100\% \text{ Cleavage fracture} \ (\text{no large ductile ligament}) \]
Outline of the speech

Context and Objectives

I. Numerical tools

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III. Model of Propagation

  step 1: Proposition of a model
  step 2: Predictive Simulations

Conclusion and Prospect
Model of Propagation: A part of the mechanical model

Let us consider a body $\Omega(t)$ with a crack of length $a(t)$

- **Dynamic equilibrium:**
  $$\text{div}(\sigma) = \rho \ddot{u}$$

- **Boundary and initial conditions**
  $$\sigma \cdot n = F^{ext} \text{ on } \partial \Omega_F$$

- **Elastic-viscoplastic constitutive equations:**
  $$\varepsilon = \varepsilon^\text{el} + \varepsilon^\text{in}$$
  $$\varepsilon^\text{el} = D^{-1}\sigma$$
  $$\dot{\varepsilon}^\text{in} = \begin{cases} 
  0 & \text{if } \Phi(\sigma^{eq}, \varepsilon^\text{in}, \dot{\varepsilon}^\text{in}) < 0 \\
  p \frac{\partial \Phi}{\partial \sigma} & \text{if } \Phi(\sigma^{eq}, \varepsilon^\text{in}, \dot{\varepsilon}^\text{in}) = 0
\end{cases}$$

- **Crack Propagation Model** to determine:
  $\rightarrow$ does the crack grow?
  $\rightarrow$ if it does, at which speed?
  $\rightarrow$ and in which direction?
Model of Propagation: Methodology

**Goal:** Propose a relevant *model to predict crack propagation and arrest* in PWR reactor steel.

1st Step:
- Modelling the CT experiment
  - **Crack speed imposed** equal to the experimental data
  - **Proposition** of a relevant crack propagation criteria

\[
a(t) = \text{experimental data}
\]
Model of Propagation: Methodology

**Goal:** Propose a relevant model to predict crack propagation and arrest in PWR reactor steel.

**2nd Step:**

Application of the criteria in a Predictive way to:

1. CT
2. Ring under compression in mode I
3. Ring under compression in mixed mode

and... Comparison with experimental measurements
Outline of the speech

Context and Objectives

I. Numerical tools

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III. Model of Propagation

step 1: Proposition of a model
step 2: Predictive Simulations

Conclusion and Prospect
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:
- Crack speed imposed equal to the experimental data
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:

• Proposition of crack propagation criteria

**Global** concepts as $J^{\text{dyn}}$:

→ difficult to dissociate cleavage dissipation ($G^{\text{tip}}$) and plasticity ($G^{\text{plas}}$)

\[
J^{\text{dyn}} = \frac{\partial W^{\text{dissipée}}}{\partial a} = G^{\text{tip}} + G^{\text{plas}}
\]

**Local** models of Cleavage:

→ based on the Maximum Principal Stress $\sigma_1$
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:
• Proposition of crack propagation criteria

**Global** concepts as $J^{\text{dyn}}$:
→ difficult to dissociate cleavage dissipation ($G^{\text{tip}}$) and plasticity ($G^{\text{plas}}$)

$$J^{\text{dyn}} = \frac{\partial W^{\text{dissipée}}}{\partial a} = G^{\text{tip}} + G^{\text{plas}}$$

**Local** models of Cleavage:
→ based on the Maximum Principal Stress $\sigma_I$
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:

- Proposition of crack propagation criteria based on the **Maximum Principal Stress**

→ **RKR** model:

\[ \sigma_I(r=r_c, \theta=\theta_c) = \sigma_c \]

→ **Half Disc** average stress tensor model:

\[
\tilde{\sigma}_I \equiv \left[ \frac{\int w \sigma \, d\Omega}{\int w \, d\Omega} \right]_I = \sigma_c
\]

\[ w = H(\psi) \exp\left(\frac{-r^2}{2l^2}\right) \]
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:

- Proposition of crack propagation criteria based on the **Maximum Principal Stress**

![Graph showing constant crack speed propagation and drop in crack speed with principal stress vs. crack length](image)

- RKR (100μm) and Half Disc (200μm)

Context and Objectives

Numerical tools

Experimental Support

Proposition of a Model of Propagation

Predictive Simulations

Conclusion and Prospect
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:
- Proposition of crack propagation criteria based on the Maximum Principal Stress

Diagram:
- Constant crack speed propagation
- Drop in the crack speed

→ Dependence of the critical stress with rate of phenomena?
Modelling the CT experiment:
- Proposition of crack propagation criteria
  → Dependence of the critical stress with crack speed

\[ \sigma_{Ic}(\dot{a}) = \frac{\sigma_A}{1 - (\dot{a}/v_{lim})^m} \]
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:
- Proposition of crack propagation criteria
  → Dependence of the critical stress with strain rate

\[ \sigma_{Ic} \left( \dot{\varepsilon}^{\text{in eq}} \right) = \sigma_{Ic0} \left[ 1 + \frac{C_1 \left( \dot{\varepsilon}^{\text{in eq}} \right)}{C_2} \right] \]

Half Disc (200μm)
Model of Propagation – Step 1: Proposition of a model

Modelling the CT experiment:

**Review** of crack propagation models identified in step 1

- Quantify the intensity of the **Maximum Principal Stress**:
  - → **RKR** model
    $$\sigma_I(r=r_c, \theta=\theta_c) = \sigma_c$$
  - → **Half Disc** average stress tensor
    $$\tilde{\sigma}_I \equiv \left[ \frac{\int w \sigma \, d\Omega}{\int w \, d\Omega} \right]_I = \sigma_c$$

- Critical stress dependence with:
  - → **crack speed** $\sigma_{Ic}(\dot{a})$
  - → **strain rate** $\sigma_{Ic}(\dot{\varepsilon}^{\text{in eq}})$
Outline of the speech

Context and Objectives

I. Numerical tools

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III. Model of Propagation

step 1: Proposition of a model

step 2: Predictive Simulations

Conclusion and Prospect
Application of the criteria in a **predictive** way to:

1. CT

![Graph showing crack length vs. time for CT context and objectives](image)
Application of the criteria in a **predictive** way to:

1. **CT**

![Graph showing crack length vs. time](image)
Model of Propagation – Step 2: Predictive Simulations

Application of the criteria in a **predictive** way to:

2. **Ring** under compression in **mode I**

![Graph showing crack length vs. time](image)

- **Criteria type**: $\sigma_{lc}(\dot{\varepsilon})$
- **Experimental points**
- **RKR (100\mu m)**

**Context and Objectives**

**Numerical tools**

**Experimental Support**

**Proposition of a Model of Propagation**

**Predictive Simulations**

**Conclusion and Prospect**
Model of Propagation – Step 2: Predictive Simulations

Application of the criteria in a **predictive** way to:

3. **Ring** under compression in **mixed mode**

- Will the crack stop?
- Subsidiary question: **Where will the crack grow?**
Model of Propagation – Step 2: Predictive Simulations

Application of the criteria in a **predictive** way to:
3. **Ring** under compression in **mixed mode**

- Subsidiary question: **Where will the crack grow?**

One can use:
- Direction of the **maximum hoop stress** $\sigma_{\theta\theta}$
- Direction **perpendicular** to the principal stress of the **average stress tensor**

$$\bar{\sigma} = \bar{\sigma}_I (e_I \times e_I) + ...$$
Application of the criteria in a **predictive** way to:

3. **Ring** under compression in **mixed mode**
Application of the criteria in a **predictive** way to:
3. **Ring** under compression in **mixed mode**
Application of the criteria in a predictive way to:
3. **Ring** under compression in **mixed mode**
→ Hydrostatic stress $\sigma_H$
Outline of the speech

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step 1: Proposition of a model

step 2: Predictive Simulations

Conclusion and Prospect
Conclusion and prospect

Conclusion:

**Experimental** work has been realized:
- Material behavior has been identified at high strain rate
- 3 distinct isothermal fracture tests were realized
- **Cleavage** was clearly identified from fracture surface observations

**Numerical** development have lead to:
- The implementation of the X-FEM in Cast3m
- A level set update performed on a auxiliary grid
- A non conforming partitioning technique which enables numerical integration without projection
Conclusion: Crack propagation model have been proposed:

- Based on the evaluation of the intensity of principal stress at crack tip
- Critical stress dependence with rate of phenomena must be taken into account
- Good predictive results were found in term of speed, length at arrest, and orientation of the crack
Conclusion and prospect

Prospect:

- Complete the implantation of X-FEM in Cast3m (in particular 3D element)
- **Confirm** the critical stress dependence with strain rate
- Possible link with the **yield stress dependence**?
Conclusion and prospect

Prospect:

- Perform other isothermal tests at different temperature → Investigate temperature dependence of $\sigma_{lc}$
- Interpretation of the thermal shock problem
The end

Thank you for your attention!

Criteria type for speed : $\sigma_{ic}$ (Å)

- Experimental points
- RKR (100μm) + $\theta_c(\sigma_I)$
- Half Disc (200μm) + $\theta_c(\sigma_I)$
Dynamic analysis is relevant to study crack arrest:

Kalthoff's observations:

Several experiments
- $K_A$ is constant when dynamic is considered
- $K_a$ (static analysis) is variable

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<th>KEY</th>
<th>SPECIMEN NO</th>
<th>$K_{1c}$ MN/m$^{3/2}$</th>
<th>VELOCITY $v_{max}$ m/s</th>
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<td>295</td>
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<td>c</td>
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<tr>
<td>e</td>
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<td>0.74</td>
<td>15</td>
</tr>
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</table>
Fractography:

- Is there any particularity of the arrest front?

→ Cleavage surface with larger shear step due to loss of energy of the crack
Model of Propagation – Step 1: Proposition

Modelling the CT experiment:
- Proposition of a crack propagation criteria based on the **Maximum Principal Stress**

![Graph](image.png)

- **Proposition of a crack propagation criteria based on the Maximum Principal Stress**

**Context and Objectives**
- Numerical tools
- Experimental Support

**Proposition of a Model of Propagation**
- Predictive Simulations

**Conclusion and Prospect**

Model of Propagation – Step 2: Predictive Simulations

Algorithms for crack propagation:

Critical stress dependence with **crack speed**: $\sigma_{Ic}(\dot{a})$

- **Euler**-like scheme
  
  → resolution at time $t_n$:  
  
  $$M \ddot{u}_n + \int B^T \sigma_n = F_n^{\text{ext}}$$

  → criterion calculation: 
  
  $$\dot{a}_n = \sigma_{Ic}^{-1}(\sigma_n)$$

  → crack propagation: 
  
  $$a_{n+1} = a_n + \dot{a}_n \Delta t$$

  $n \leftarrow n + 1$

Critical stress dependence with **strain rate**: $\sigma_{Ic}(\dot{\varepsilon}^{\text{in eq}})$

- **Iterative scheme**

  → crack propagation: 
  
  $$a_{n+1} = a_n + \Delta a$$

  → resolution at: 
  
  $$t^{(i)}_{n+1} = t_n + \Delta t^{(i)}$$  
  
  $$M \ddot{u}_{n+1}^{(i)} + \int B^T \sigma_n^{(i)} = F_n^{\text{ext}}$$

  → criterion calculation: 
  
  $$\sigma_{Ic}^{(i)}(\dot{\varepsilon}_{n}^{\text{in eq}(i)}) = 0 ?$$

  $i \leftarrow i + 1$

  $n \leftarrow n + 1$

<table>
<thead>
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<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
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Application of the criteria in a **predictive** way to:

2. **Ring** under compression in **mode I**
Application of the criteria in a **predictive** way to:

2. **Ring** under compression in **mode I**

![Graph showing crack length vs. time for ring under compression in mode I.](image)

- **Experimental points**
- **RKR (100μm)**
- **Half Disc (200μm)**

**Criteria type**: $\sigma_{lc}(\dot{\varepsilon})$
Application of the criteria in a **predictive** way to:

3. **Ring** under compression in **mixed mode**
Model of Propagation – Step 2: Predictive Simulations

Application of the criteria in a **predictive** way to:
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Application of the criteria in a **predictive** way to:

3. **Ring** under compression in **mixed mode**
Model of Propagation – Step 2: Predictive Simulations

Application of the criteria in a **predictive** way to:
3. **Ring** under compression in **mixed mode**
Prospect:

- Explain differences between crack paths observed for thin specimen:
  - for fracture at low load → straight crack path
  - high fracture load initiation → crack branching