3D X-FEM modeling of crack coalescence phenomena in the Smart-Cut^{TM} process

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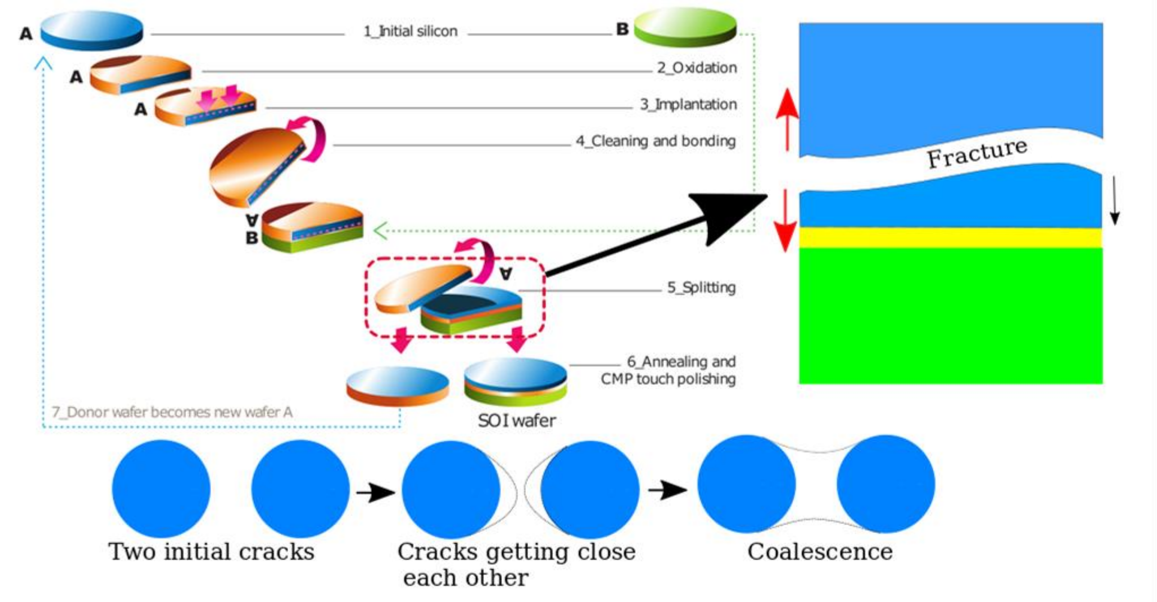
Outlines

- Context and motivations
- 3D X-FEM formulation and discretization
- Prediction of the pressure in the cracks
- Application to the modeling of 3D crack coalescence
- Conclusion and other expected applications

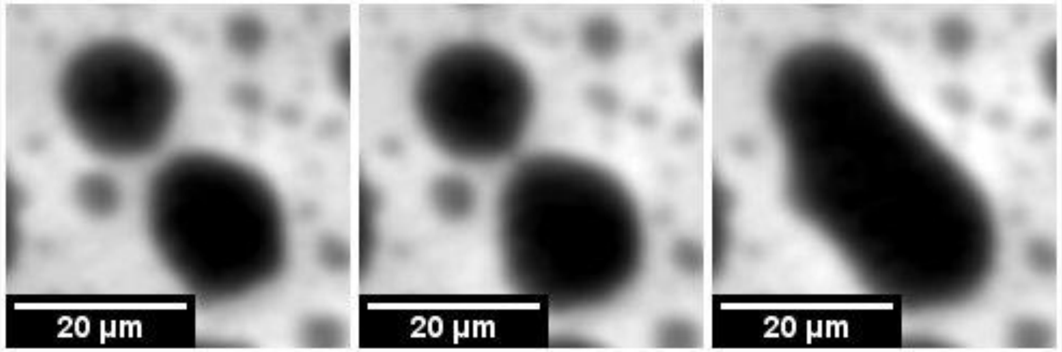
Context and motivations

Smart-Cut^{TM}, SOI, Coalescence phenomenon



Fabrication of SOI using Smart Cut^{TM} [SUT10]

- Smart Cut^{TM}: technological process of transfering a thin layer from one substrate on to another;
- SOI (Silicon-On-Insulator): transfer of a thin layer of silicon on to a substrate (=> SOITEC);
- Applications: starting material for electronic devices;



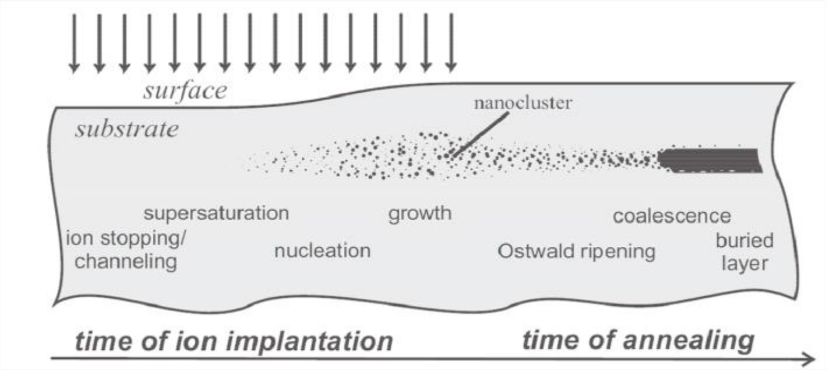
Observation of crack coalescence phenomenon using IR microscopy [COL 21]

[SUT 16] D. Sutula. Energy minimising multi-crack growth in linear-elastic materials using the extended nite element method with application to Smart-CutTM silicon wafer splitting (2016).
[COL 21] L. Colonel, F. Mazen, D. Landru, O. Kononchuk, N. Ben Mohamed, and F Rieutord, In situ observation of pressurized microcrack growth in silicon , Physics Status Solidi A 221 (2021).

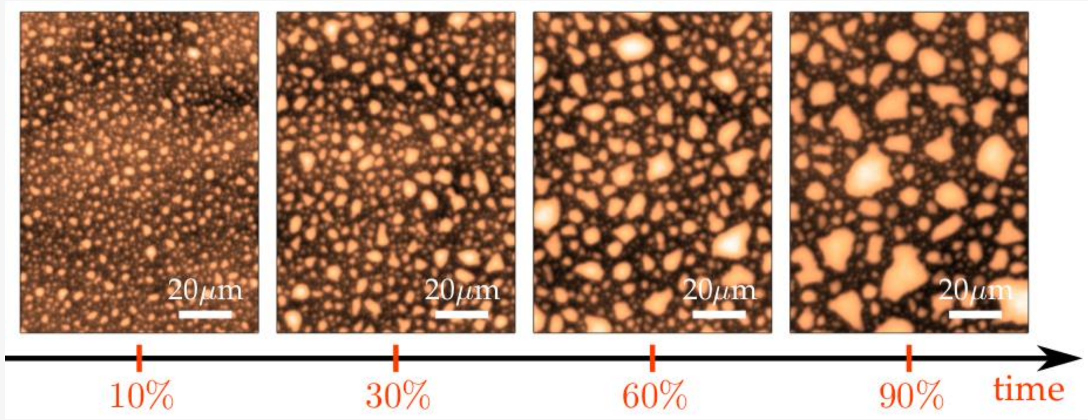
Context and motivations

Implantation and crack growth during annealing

- Implantation : introduction of H-ions or He-ions creating a damaged zone and then platelets [PEN 10, SUT 16];



Implantation of H-ions inside the donor wafer [PEN 10]



Crack growth observation by optical microscopy [PEN 10]

- Annealing: growth of platelets under internal H_2 gaz pressure;

- Separation of the donor wafer during annealing due to the growth and coalescence of microcracks under H_2 internal gaz pressure.

[SUT 16] D. Sutula. Energy minimising multi-crack growth in linear-elastic materials using the extended finite element method with application to Smart-Cut™ silicon wafer splitting (2016).
[PEN 2010] Fragilisation et dynamique de la rupture du silicium implanté, PhD thesis, Université de Grenoble, 2010.

Context and motivations

Problematics and objectives

- Availability of experimental data on the Smart CutTM [PEN 10, MAS 15, DAG 18, COL 21];
- The physics of crack evolution mechanisms difficult to be deduced from analytical approaches ;
- Need of numerical approaches.

Actual limitations :

- Interactions effects on the coalescence of cracks;
- Internal pressure of a growing crack;
- Some 2D numerical approaches have been carried out [GER 10, SUT 16] but 3D models have been very less discussed.

Main objectives:

- Modeling 3D coalescence of cracks under pressure;
- Predict internal pressure of a growing crack using a constitutive law in pressure;
- Criteria of the coalescence of cracks;
- Post-split and post-coalescence roughness.

[MAS 15] D. Massy, F. Mazen, S. Tardif, J. D. Penot, J. Ragani, F. Madeira, D. Landru, O. Kononchuk, and F. Rieutord, Fracture dynamics in implanted silicon , Applied Physics Letters 107 (2015), no. 9, 092102, Publisher: American Institute of Physics.
[DAG 18] N. Daghbouj, N. Cherkashin, and A. Claverie, A method to determine the pressure and densities of gas stored in blisters: Application to H and He sequentialion implantation in silicon , Microelectronic Engineering 190 (2018), 54-56.
[SUT 16] D. Sutula. Energy minimising multi-crack growth in linear-elastic materials using the extended nite element method with application to Smart-Cut^{TM} silicon wafer splitting, PhD. Thesis (2016).

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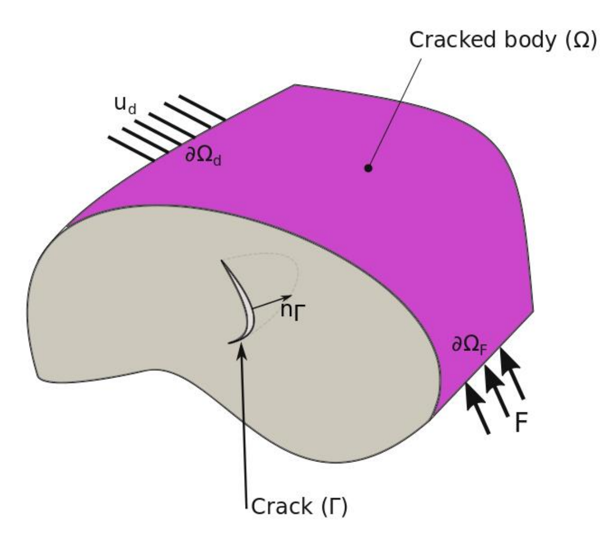
3D X-FEM formulation and discretization

Implantation and crack growth during annealing



3D cracked body [PAL 23]

- Strong formulation:

$$\begin{cases} div\ (\boldsymbol{\sigma}) = 0 \ \text{ dans } \ \Omega \\ \boldsymbol{\sigma}.\mathbf{n} = \mathbf{F} \text{ sur } \partial\Omega_F \\ \mathbf{u} = \mathbf{u}_d \ \text{ sur } \ \partial\Omega_d \\ \boldsymbol{\sigma} = \mathbf{C} : \epsilon \ \text{ dans } \ \Omega \\ \boldsymbol{\sigma}.\mathbf{n} = p(t)\mathbf{n}_\Gamma \ \text{ sur } \ \Gamma \\ p(t) : \text{governing law in pressure} \end{cases}$$

Where **C** is the Hooke's tensor and σ the Cauchy stress tensor.

- weak formulation:

$$\begin{cases} \int_\Omega \boldsymbol{\sigma} : \epsilon(\mathbf{u}^*) dV = \int_\Gamma p(t)\mathbf{n}_\Gamma.\mathbf{u}^* dS, \\ \forall \ \mathbf{u}^* \in \mathfrak{U}_0 \end{cases}$$

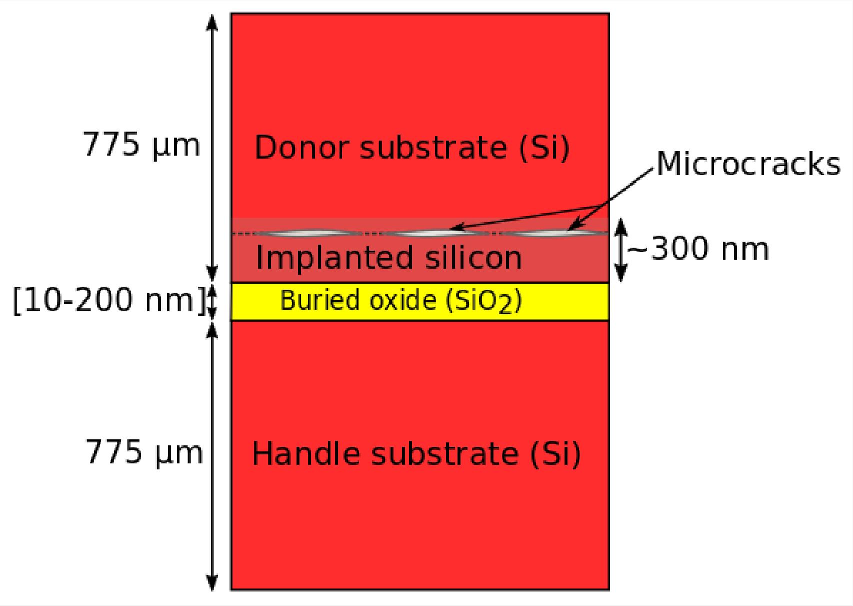
With :

$$\begin{cases} \mathbf{u} \in \mathfrak{U}, \ \mathfrak{U} = \{\mathbf{u} \in H^1(\Omega\backslash\Gamma) \ / \ \mathbf{u} = \mathbf{u}_d \text{ on } \partial\Omega_d\} \\ \mathbf{u}^* \in \mathfrak{U}_0, \ \mathfrak{U}_0 = \{\mathbf{u}^* \in H^1(\Omega\backslash\Gamma) \ / \ \mathbf{u}^* = 0 \text{ on } \partial\Omega_d\} \end{cases}$$

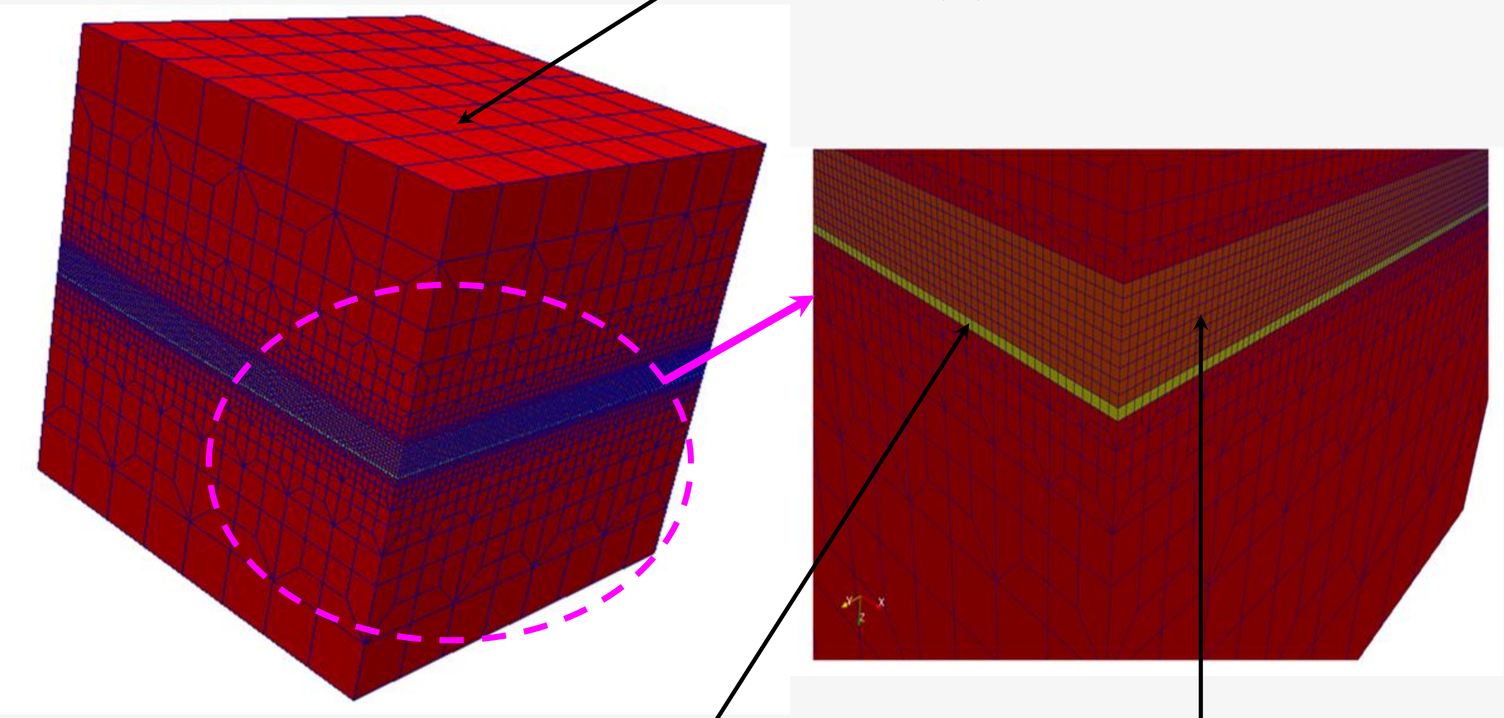
[PAL 23] E. PALI, A. Gravouil, Anne Tanguy , O. Kononchuk and D. Landru, Three-dimensional X-FEM modeling of crack coalescence phenomena in the Smart Cut™ technology, 2023.

3D X-FEM formulation and discretization

Geometry and discretization aspects



Cross-section 2D representative geometry of SOI [PAL 23]

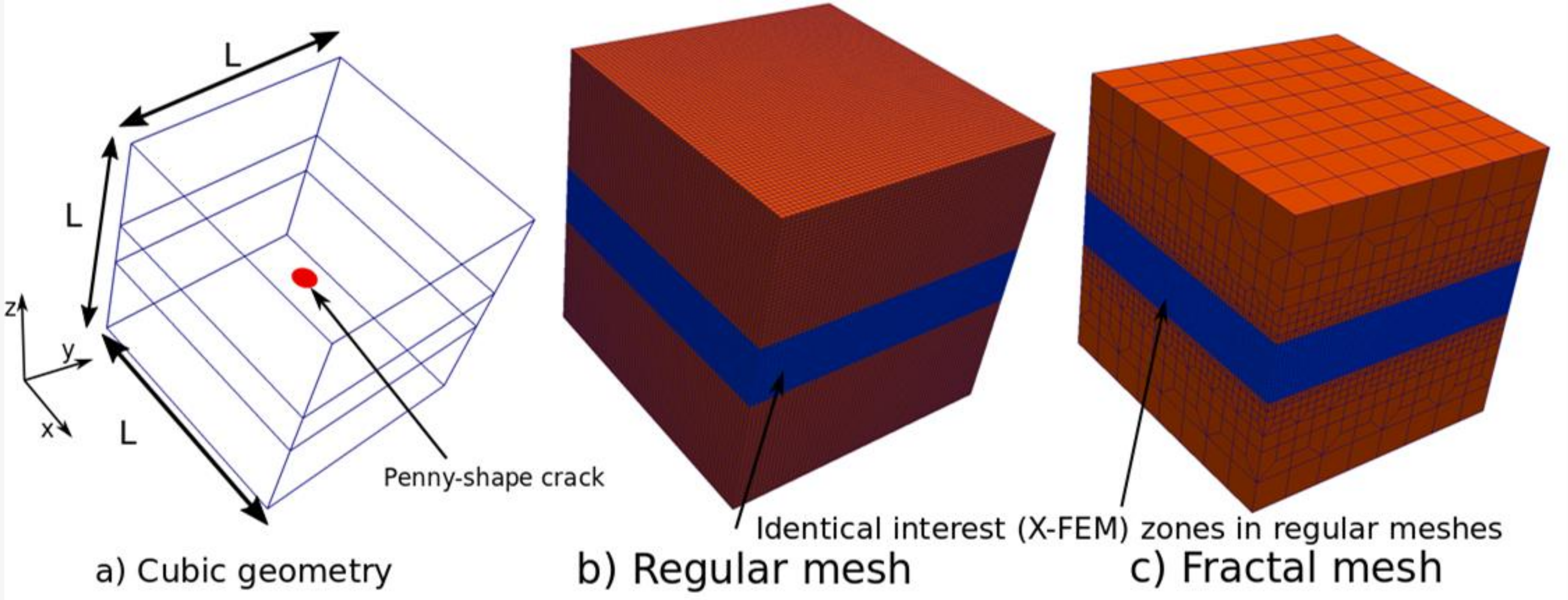


3D Fractal mesh using cast3M [PAL 23]

[PAL 23] E. PALI, A. Gravouil, Anne Tanguy , O. Kononchuk and D. Landru, Three-dimensional X-FEM modeling of crack coalescence phenomena in the Smart Cut™ technology, 20223.

3D X-FEM formulation and discretization

Robustness and efficiency (gain in computation time)



Comparison of gain in CPU time: b) Structured regular mesh and c) Fractal mesh with interest zone discretized with regular mesh

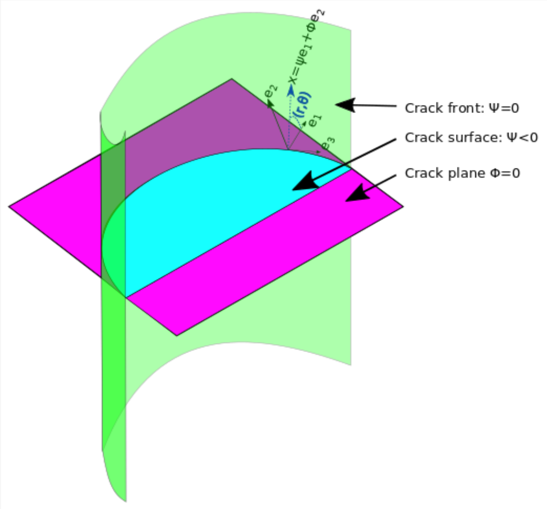
⇒ Number of finite elements reduced on the entire mesh using fractal mesh with respect to structured regular mesh for the same discretisation of the interest zone[PAL 23];

⇒ About 90% gain in CPU time using fractal mesh with respect to structured regular mesh [PAL 23].

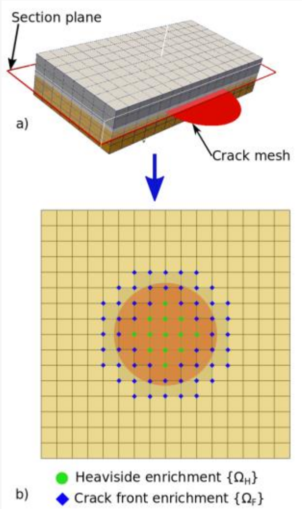
3D X-FEM formulation and discretization

Methods: X-FEM approach

- X-FEM: eXtended Finite Elements Method [MOE 99] based on the partition of the unity approach [MEL 96];
- Implicit representation of the crack (level sets [GRA 02]);



Implicit representation of the crack (level sets).



Explicit definition of the crac and 3D enrichment technique.

$$\begin{cases} \phi(\mathbf{x}) = 0 \text{ and } \psi(\mathbf{x}) < 0 \rightarrow & \text{crack surface} \\ \phi(\mathbf{x}) = 0 \text{ and } \psi(\mathbf{x}) = 0 \rightarrow & \text{crack front} \end{cases}$$

- Explicit representation of the crack and enrichments :
  - ❖ Heaviside enrichment (H):

$$H(\mathbf{x}) = \begin{cases} +1 \text{ if } \phi(\mathbf{x}) > 0 \\ -1 \text{ if } \phi(\mathbf{x}) < 0 \end{cases}$$

  - ❖ Crack front enrichment:

$$\{\mathcal{F}_k\}_{k=1-4} = \sqrt{r}\{\sin\frac{\theta}{2}, \cos\frac{\theta}{2}, \sin\frac{\theta}{2}\sin\theta, \cos\frac{\theta}{2}\sin\theta\}$$

- Displacement field approximation using X-FEM :

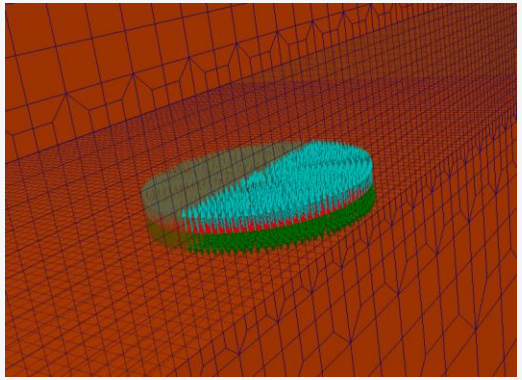
$$\mathbb{U}(\mathbf{x}) = \underbrace{\sum_{i\in\Omega} N_i(\mathbf{x})\boldsymbol{u}_i}_{\text{standard}} + \underbrace{\sum_{j\in\Omega_H} N_j(\mathbf{x})H(\mathbf{x})\boldsymbol{a}_j}_{\text{H-enrichment}} + \underbrace{\sum_{l\in\Omega_F}\left[N_l(\mathbf{x})\sum_{k=1}^{4}\mathcal{F}_k(\mathbf{x})\boldsymbol{b}_{lk}\right]}_{\text{crack front enrichment}}$$

[MOE 99] N. Moës, J. Dolbow, and T. Belytschko, A finite element method for crack growth without remeshing , International Journal for Numerical Methods in Engineering 46 (1999), no. 1, 131-150.
[GRA 02] A. Gravouil, N. Moës, and T. Belytschko, Non-planar 3D crack growth by the extended finite element and level sets-Part II: Level set update , Int. J. Numer. Methods in Eng. 53 (2002), no. 11, 2569-2586.

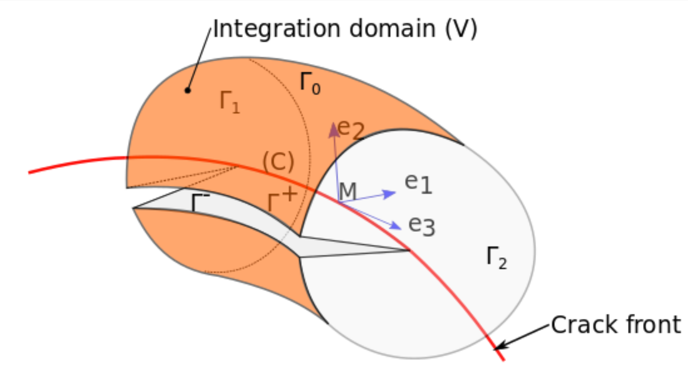
3D X-FEM formulation and discretization

Computation of stress intensity factors (SIFs)

- Domain along the crack front:



Crack under internal pressure



Domain along the crack front to integrate fields

- Domain integral from Eshelby tensor Pij taking into account pressure on crack faces:

$$\boldsymbol{P}_{ij} = \frac{1}{2}\boldsymbol{\sigma}_{kl}\epsilon_{kl}\delta_{ij} - \boldsymbol{\sigma}_{kj}\mathbf{u}_{k,i}$$

$$J = -\int_V (\boldsymbol{P}_{ij}\boldsymbol{q}_i)_{,j}\, dV + \int_{\Gamma^+\cup\Gamma^-} \boldsymbol{P}_{ij}\boldsymbol{q}_i\boldsymbol{n}_j\, dS$$

- Interaction integral to extract SIFs at both modes I, II and III (K_I, K_{II} and K_{III} respectively):

$$J^{R,aux} = J^R + J^{aux} + I$$

- Interaction integral obtained taking into account internal pressure normal to crack faces expressed in the local basis [PAL 23, TRO 2013]:

$$I = \int_V \left[\boldsymbol{\sigma}^R_{ij}\boldsymbol{u}^{aux}_{i,1} + \boldsymbol{\sigma}^{aux}_{ij}\boldsymbol{u}^R_{i,1} - W_I^{R,aux}\delta_{1j}\right] - \int_{\Gamma^+\cup\Gamma^-} \left[\boldsymbol{\sigma}^R_{22}\boldsymbol{u}^{aux}_{2,1} + \boldsymbol{\sigma}^{aux}_{22}\boldsymbol{u}^R_{2,1}\right]\mathbf{q}\, dS$$

[TRO 2013] B. Trolé, Simulation multi-échelles de la propagation des fissures de fatigue dans les rails, PhD. Thesis, 2013.
[PAL 23] E. PALI, A. Gravouil, Anne Tanguy , O. Kononchuk and D. Landru, Three-dimensional X-FEM modeling of crack coalescence phenomena in the Smart CutTM technology, 20223.

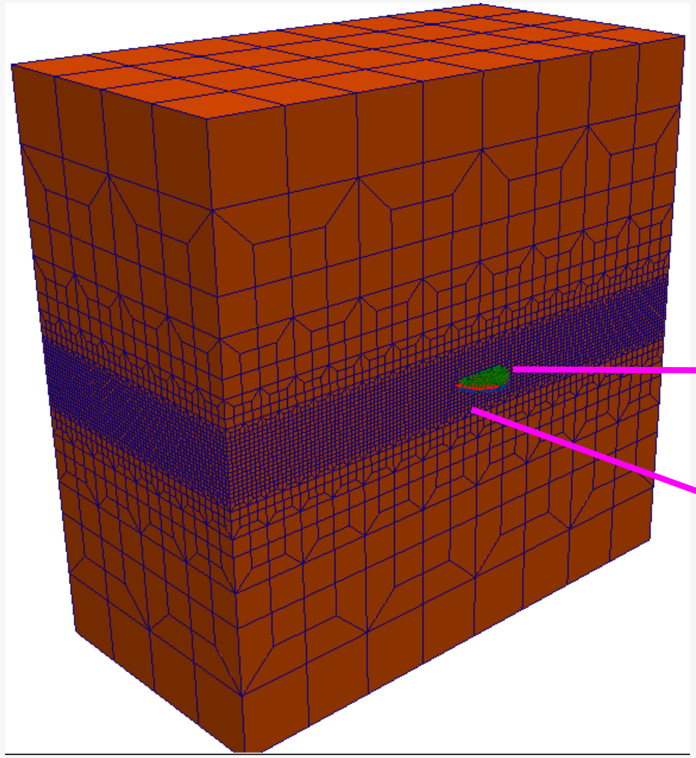
3D X-FEM formulation and discretization

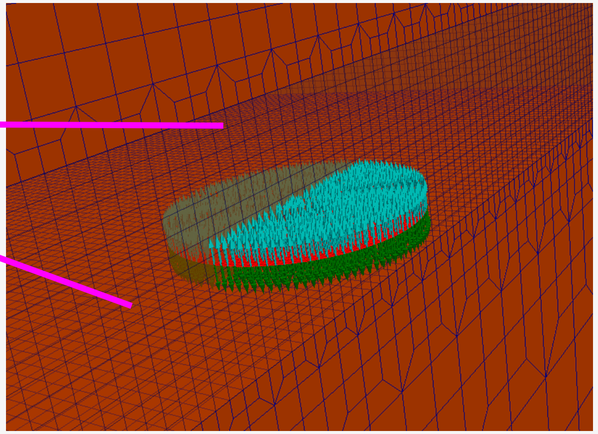
Verification of X-FEM SIF computation with respect to analytical solution: model

- Specifications for the model:
  - ❑ A penny-shape crack under internal pressure normal to its faces ;
  - ❑ Crack radius: R = 2µm (Diameter D = 4µm);
  - ❑ Cube of side 10D;
  - ❑ Applied pressure: P = 10 MPa;
  - ❑ Young's modulus: E = 138.6 GPa;
  - ❑ Poisson ratio: v = 0.28;

- Analytical solution of KI: and averaged error:

$$\begin{cases} K_{I\ (analytical-infin.syst.)} = 2p\sqrt{\frac{R}{\pi}} \\ errorK1 = \frac{|K_{I(analytical-infin.syst.)} - K_{I(X-FEM)}|}{K_{I(analytical-infin.syst.)}} \end{cases}$$



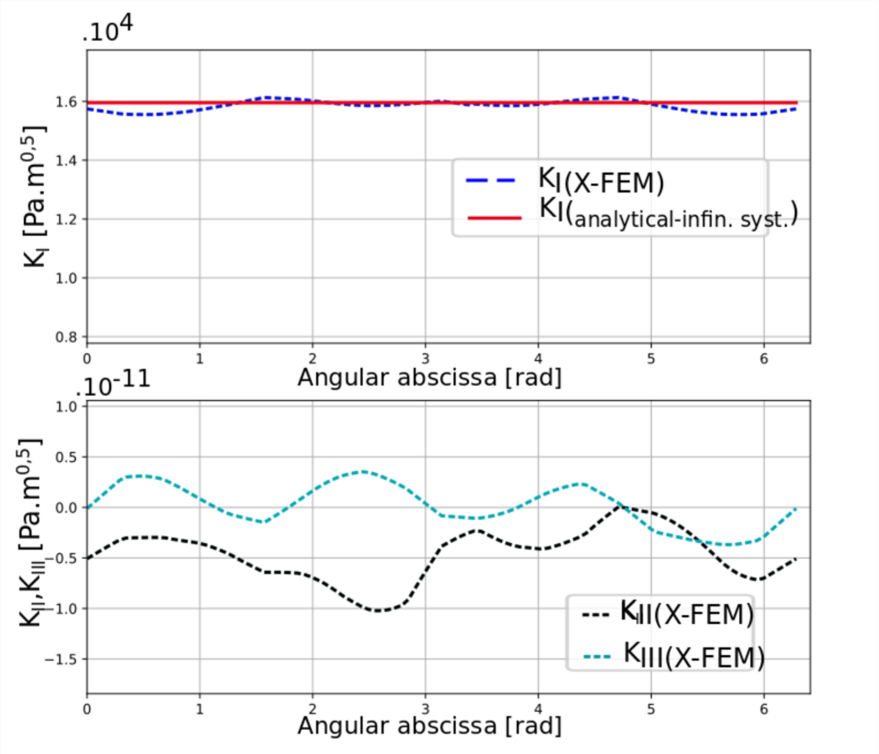


Penny-shape under internal pressure

3D X-FEM formulation and discretization

Verification of X-FEM SIF computation with respect to analytical solution: results

- Averaged relative error of K_I(X-FEM) with respect to its analytical value:
  Averaged relative error on K_I = 0.7%
- Good approximation of K_I with respect to its analytical value (relative error < 1%);
- $K_{II} << K_I$ and $K_{III} << K_I$: agreement to the loading in mode I;



SIFs along a penny-shape crack under pressure in mode I

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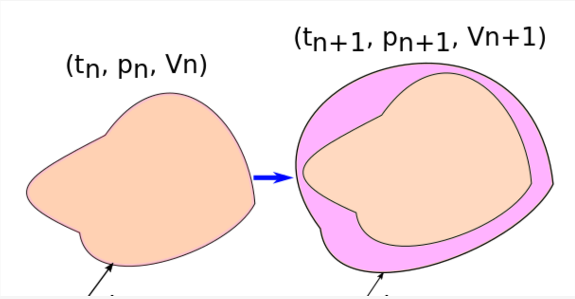
Prediction of the internal pressure in the cracks

Problem statement and X-FEM proposed algorithm

- Idea: predict the pressure in a growing crack from an evolution law in pressure;



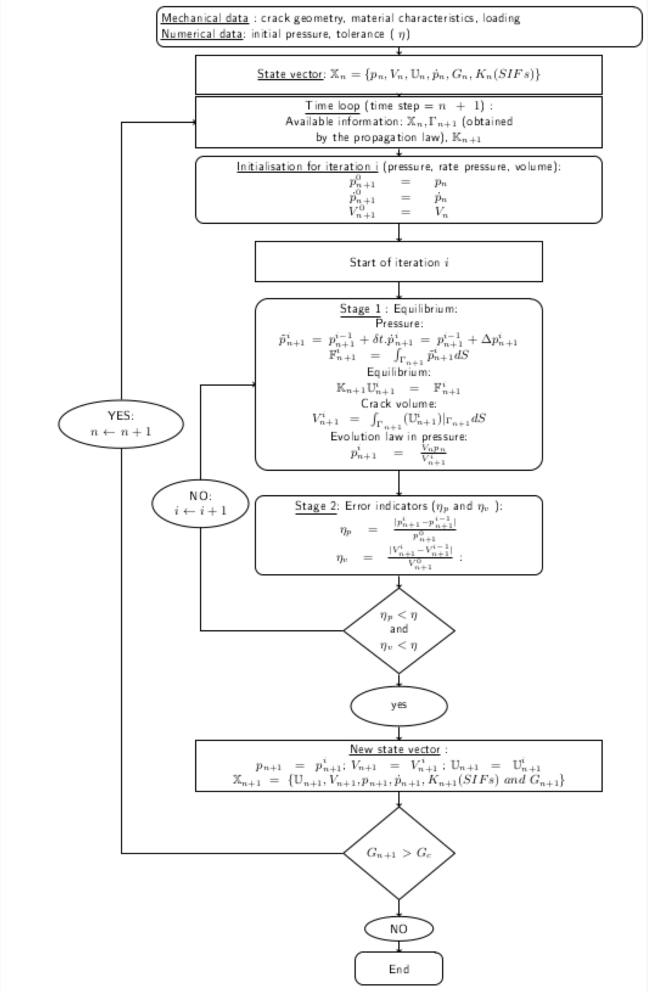
Crack at time step t_n. Crack at time step t_{n+1}.

- Proposed evolution law in pressure: the quantity of H_2 gaz in the crack remains constant:

$$\begin{cases} p(t)V(t) = \text{const} \\ p_{n+1} = \dfrac{V_n}{V_{n+1}} . p_n \end{cases}$$

Non-linear problem

- An algorithm implemented in cast3M based on the Euler implicit method to predict pressure (p_{n+1}) at each time step (t_{n+1}) [PAL 23];



Flowchart

[PAL 23] E. PALI, A. Gravouil, Anne Tanguy , O. Kononchuk and D. Landru, Three-dimensional X-FEM modeling of crack coalescence phenomena in the Smart Cut^{TM} technology, 2023.

Prediction of the internal pressure in the cracks

Validation of the prediction of pressure

- The incremental pressure (pn) in the crack at each time step (tn) is expressed analytically for a penny-shape crack in an infinite medium as follows [PAL 23]:

$$P_{n\ (analytical)} = \sqrt{\frac{3EP_0V_0}{16(1-\nu^2)R_n^3}}$$

Where P_0 is the imposed initial pressure, V_0 the initial volume of the crack and Rn the crack radius at time step tn.

- Crack extension assumed to be proportional to (G-Gc), based on Griffith's energy criterion:

$$\begin{cases} \delta a_j = \beta_j \left(G_j - G_c\right) \ \text{with} \\ \beta_j = \left(\frac{\delta a_j^{max}}{G_j^{max} - G_c}\right) \end{cases}$$

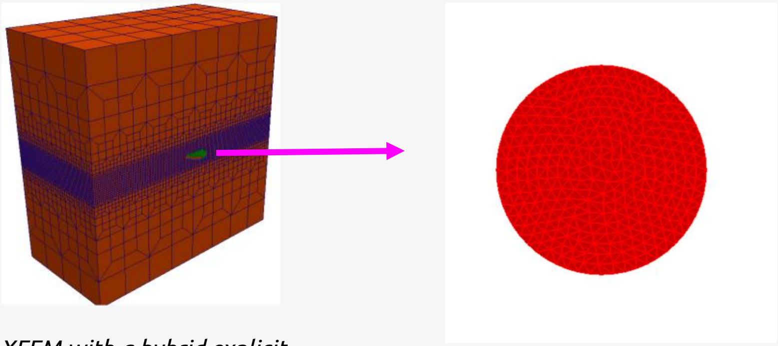
- X-FEM crack propagation using level sets as in [FRI 12];

- Example of an initial penny-shaped crack of radius R_0 = 2µm embedded in a cube;

- Two test cases varying the initial pressure P_0 = {$1.2P_c$; $1.5P_c$} with Pc the critical pressure of a penny-shape [PEN 10]:

$$P_c = \sqrt{\frac{\pi E \gamma}{2R(1-\nu^2)}}$$

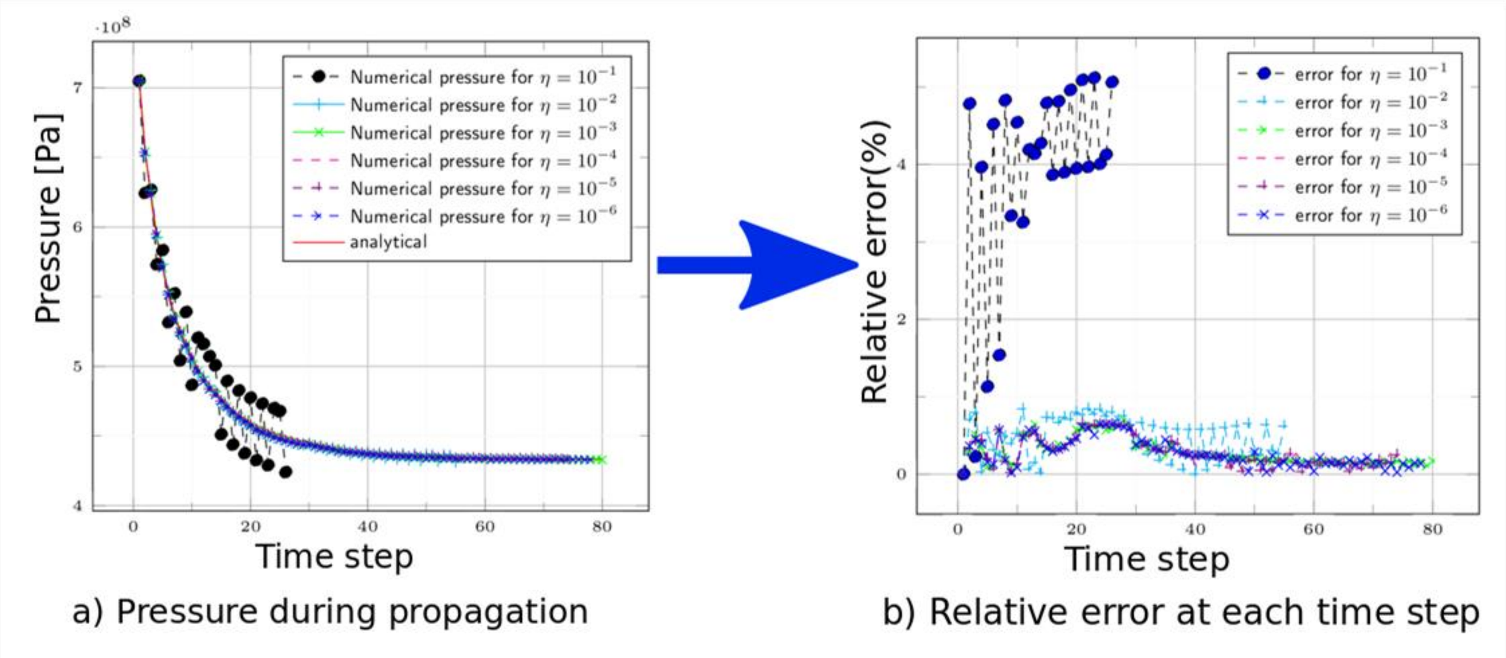
- Six (6) values of the convergence tolerance tested: η = {10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}}



[FRI 12] T.-P. Fries and M. Baydoun, Crack propagation with the extended finite element method and a hybrid explicit-implicit crack description: XFEM with a hybrid explicit-implicit crack description , Int. J. Numer. Meth. Engng 89 (2012), no. 12, 1527-1558.

Prediction of the internal pressure in the cracks

Results: comparison to analytical solution [PAL 23]



- Decrease of the pressure when the crack propagates;
- Relative error between X-FEM approximation with respect to analytical solution less than 1% for small convergence tolerance ($\eta < 10^{-2}$);
- The crack reaches a stability because of the decrease in pressure.

[PAL 23] E. PALI, A. Gravouil, Anne Tanguy , O. Kononchuk and D. Landru, *Three-dimensional X-FEM modeling of crack coalescence phenomena in the Smart Cut™ technology*, 2023.

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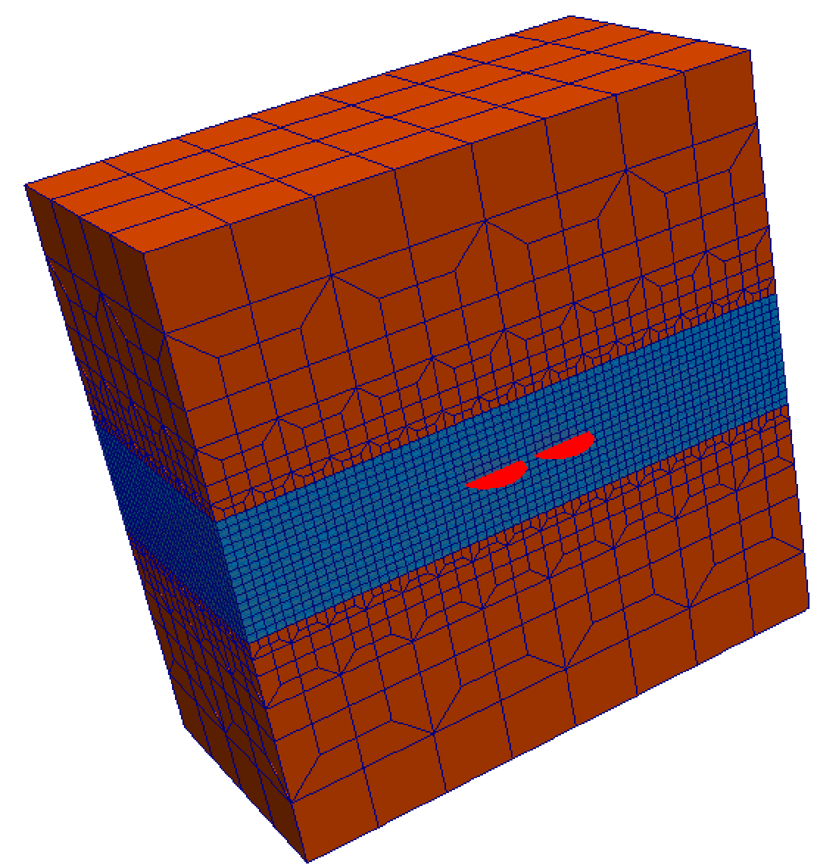
Application to the modeling of 3D crack coalescence

X-FEM discretization aspects

- Explicit representation of the crack: no need to remesh the hole bulk when cracks get closer to each other;
- The use of level sets and enrichments makes it possible to reach coalescence ;
- Let us consider 2 penny-shape cracks of the same dimensions initially spaced by a certain distance embedded in a homogenous cube;
- Cracks are initially submitted to pressure sufficient to allow the coalescence ($P_0 = 2P_c$);
- Application of the implicit algorithm to compute a new pressure at each time step.



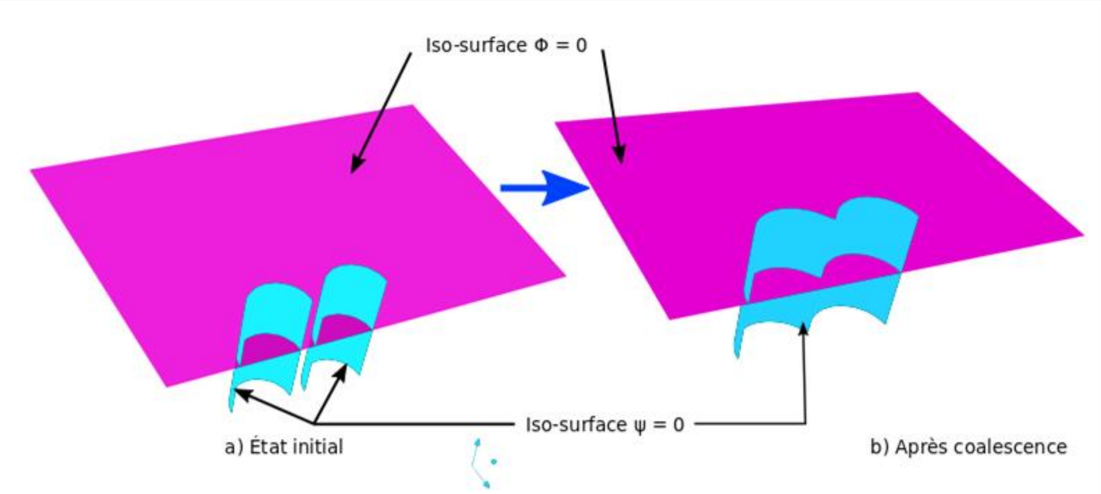
Two (2) penny-shaped cracks in 3D

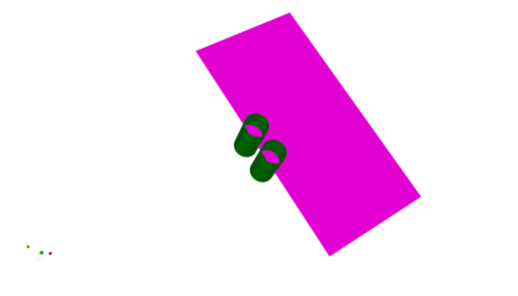
[PAL 23] E. PALI, A. Gravouil, Anne Tanguy , O. Kononchuk and D. Landru, Three-dimensional X-FEM modeling of crack coalescence phenomena in the Smart Cut™ technology, 2023.

Application to the modeling of 3D crack coalescence

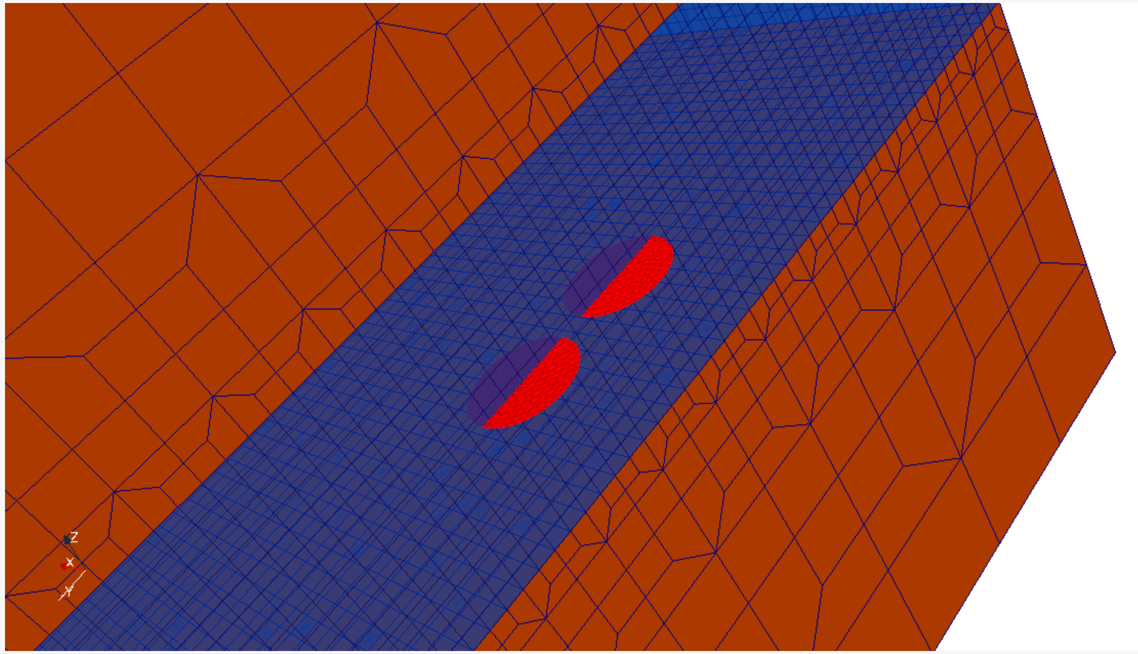
X-FEM discretization aspects

- Illustration by level sets evolution [PALI 23]:





- Illustration by the evolution crack mesh:



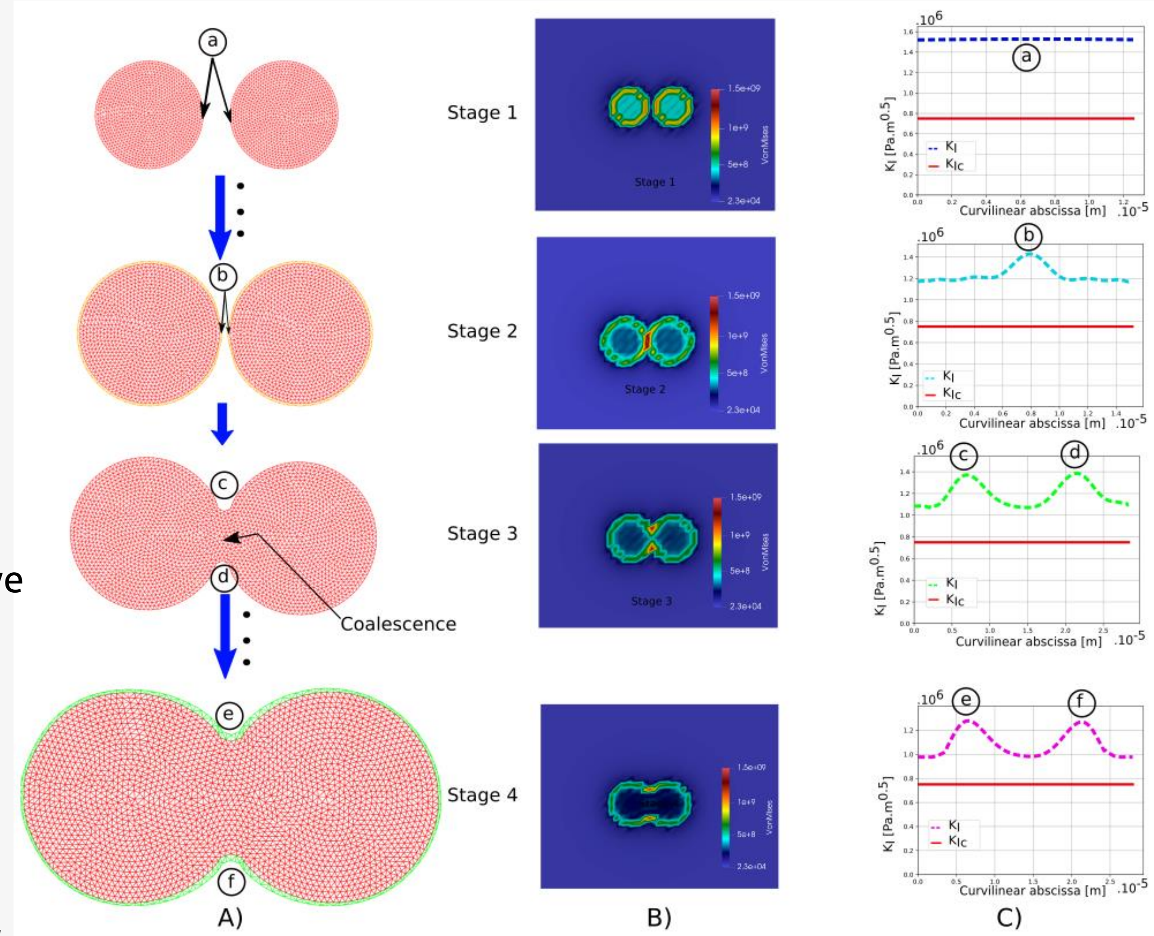
3D coalescence of two cracks

[PAL 23] E. PALI, A. Gravouil, Anne Tanguy , O. Kononchuk and D. Landru, Three-dimensional X-FEM modeling of crack coalescence phenomena in the Smart Cut™ technology, 2023.

Application to the modeling of 3D crack coalescence

Qualitative analysis of stresses [PAL 23]

- **Stage 1**: local stresses and KI almost uniform along crack fronts => neighboring effects negligible;
- **Stage 2**: cracks get closer, maximum stresses are concentrated in regions where the crack fronts are closest inducing a local maximum of K_I: crack interaction effects;
- **Stage 3** and **stage 4**: after coalescence, maximum stresses and KI are now localize in regions of the resulting crack with negative curvatures (concavities); crack will advance preferentially in concave regions as experimentally observed in [COL 21].



Stress evolution along the cracks [PAL 23]

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[COL 21] L. Colonel, F. Mazen, D. Landru, O. Kononchuk, N. Ben Mohamed, and F Rieutord, In situ observation of pressurized microcrack growth in silicon , Physics Status Solidi A 221 (2021).

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Conclusion and other expected applications

- **Key points:**
  - Development of 3D fractal mesh to model cracks under pressure in the Smart Cut^{TM}: accuracy, robustness and efficiency;
  - Modified 3D interaction integral adapted to take into account internal pressure on crack faces in cast3M with X-FEM;
  - Implementation of an implicit algorithm to predict pressure in a propagating crack of any shape;
  - Modeling of 3D coalescence of two cracks using X-FEM.
- **Other expected applications:**
  - Coalescence criteria of two cracks with identical or different sizes and relative orientations;
  - Roughness: post-fracture and post-coalescence;
  - Coalescence of multiple cracks with experimentally measured profiles;
  - Taking into account heterogeneities in material properties.

Thank you for your attention

Any question ?

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Special thanks for their contributions to:

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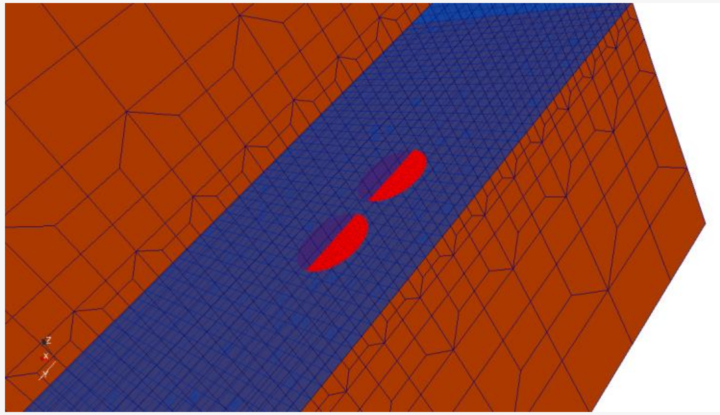

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