A numerical study of brittle fracture in monocrystalline silicon

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Dynamic Brittle fracture

Accelerating cracks

Dynamic loading (impact, shock …)

Crack velocity approaching *Cr*

Under constant or quasi-static loading

Main objectives :

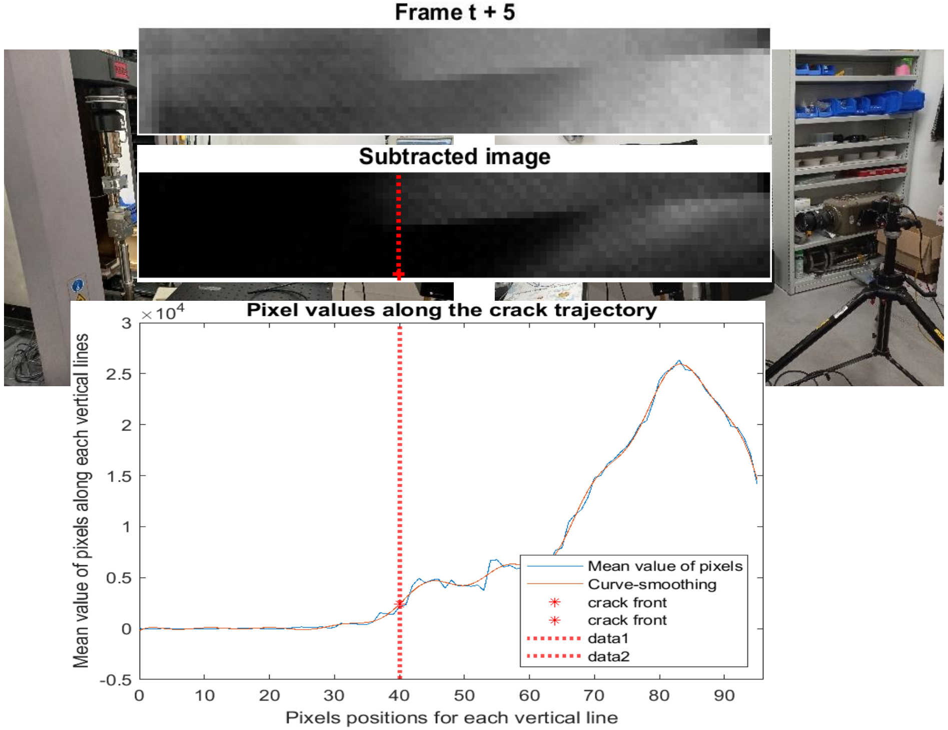
- *Model this rapidly moving cracks numerically*
- *Compute their velocities*
- *Compare it to experimental data*

Background : Crack velocity measurement

- Crack speeds nearing waves' velocities ~ *Cr*
- Small experimental specimen → Very short phenomena

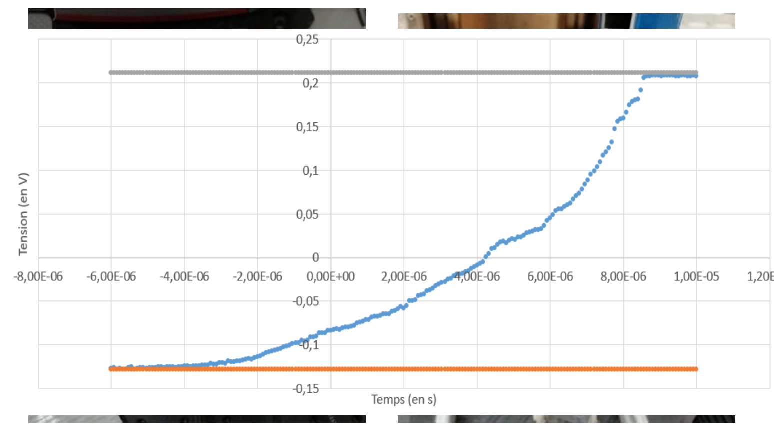
Measurement methods

High-speed camera



Potential drop technique

High data frequency acquisition (up to 50MHz)



Background : Crack velocity measurement on monocrystalline silicone

- Brittle material
- Used in photovoltaic cells (wafers)
- Interesting fracture properties (cleavage fracture)

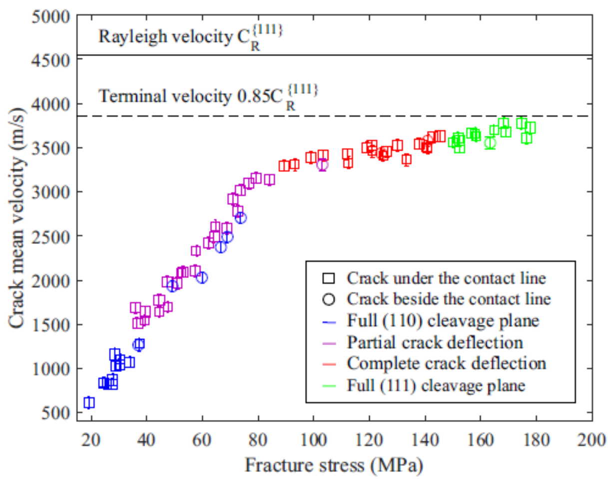


Figure 1 : Measurement of crack speed using high-speed camera (Wang, 2018) [1]

Terminal velocity

- ➢ *Depends on* :
  - Notch length
  - Fracture stress
- ➢ *Max value* ~ 85% of *Cr*

[1] M. Wang, L. Zhao, M. Fourmeau, D. Nelias, Journal of the Mechanics and Physics of Solids 122 (2019) 472–488

Background : Crack velocity predictions vs Crack velocity measurement

- Freund's analytical solution for elastodynamics problems of brittle fracture :

$$V_{crack\_max} = C_r$$

- Experimental data :

Polymethylmetacrylate (PMMA)	*Monocrystalline Silicone (Si)*
$V_{crack\_max} \sim 60\% \; C_r$	$V_{crack\_max} \sim 85\% \; \mathrm{C_r}$

What are the dynamic processes behind this limiting/terminal velocity ?

- Energy dissipation ?
- Waves' interaction with the crack front ?
- Micro-structure effects ?

Dynamic brittle fracture model : Numerical settings

For cracks propagating through the material thickness
→ Bending test [1] : Elliptical crack front → **3D model**

A representation of the crack (discontinuity) within the finite element framework → **XFEM approach**

Short-time varying quantities → **Explicit Time integration scheme**

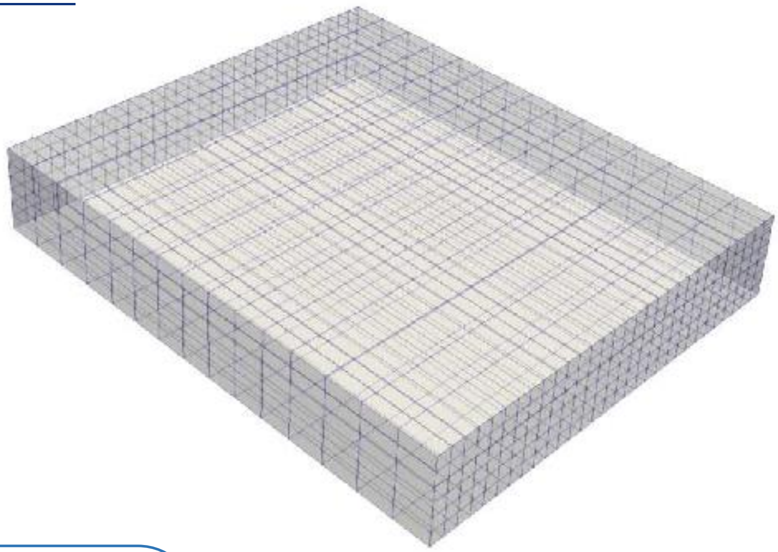
Crack initiation criteria → **Energetic approach** *J-integral*

↓

Software : Cast3M (CEA)

[1] *M. Wang, L. Zhao, M. Fourmeau, D. Nelias, Journal of the Mechanics and Physics of Solids 122 (2019) 472–488*

Numerical model : Specimen dimensions and mesh properties



Specimen mesh :

- Spatial discretization → Coarse mesh: 15 x 30 x 6 éléments
- A simplified model → Dimensions: 7 x 6 x 1 mm
- Element type → Structural linear Hexahedron – CUB8

Material properties:

- Monocrystalline silicone

Poisson's ratio = 0.28

Young's modulus= 130 GPa

Density = 2.33 $* 10^{-9}\ tons/mm^3$

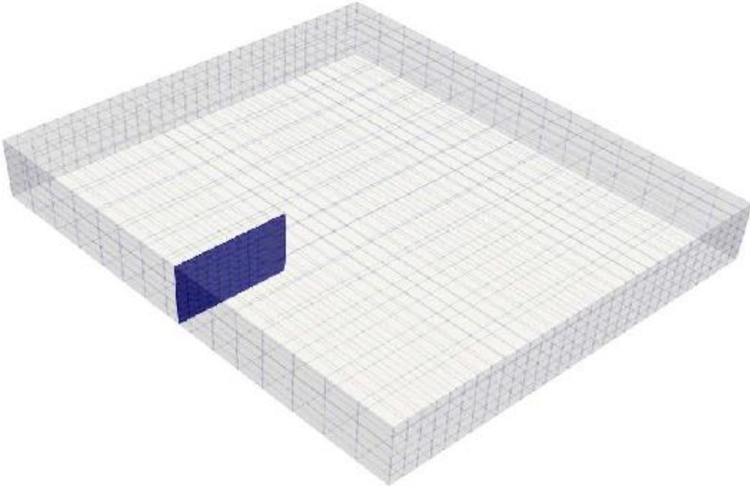
Fracture energy [3] = 1.73 $* 10^{-3}$ mJ$/mm^2$

[3] *Masolin et al., « Thermo-Mechanical and Fracture Properties in Single-Crystal Silicon ».*

Numerical model : Specimen dimensions and mesh properties

Crack representation:

- Type → Straight-through notch
- Length → 1.2 mm – breaking 6 elements
- XFEM → Discontinuity enrichment only – Heaviside function

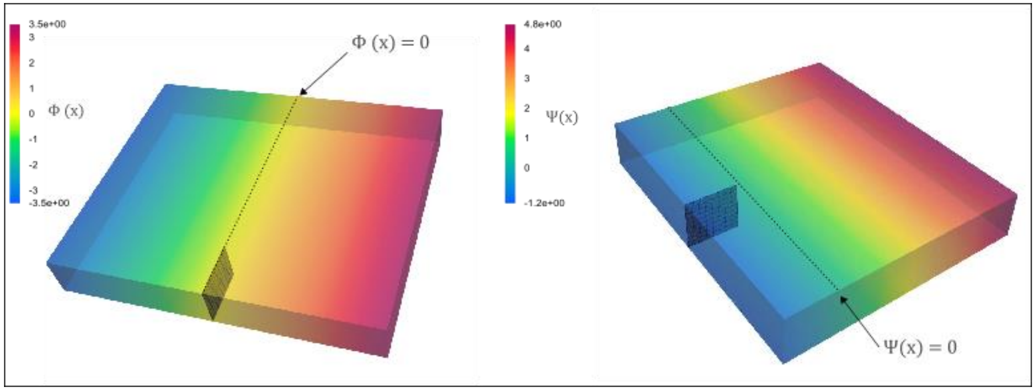


$$H(x) = \begin{cases} +1 & \text{if } x > 0 \\ -1 & \text{if } x < 0 \end{cases}$$

Crack tracking :

- Using both level sets : ϕ(x) and ψ(x)

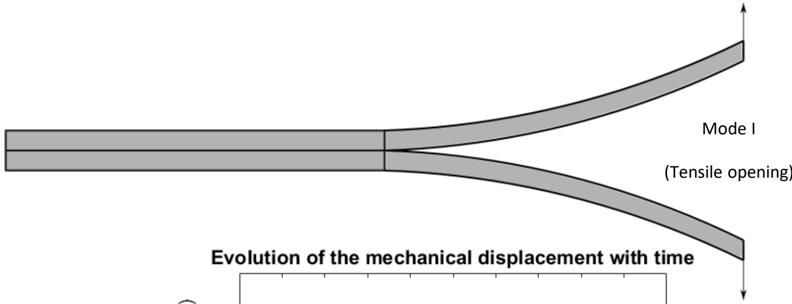
$$\begin{aligned} \text{crack surface} &= \{\phi(\mathbf{x}) = 0 \quad \& \quad \psi(\mathbf{x}) < 0\} \\ \text{crack front} &= \{\phi(\mathbf{x}) = 0 \quad \& \quad \psi(\mathbf{x}) = 0\} \end{aligned}$$

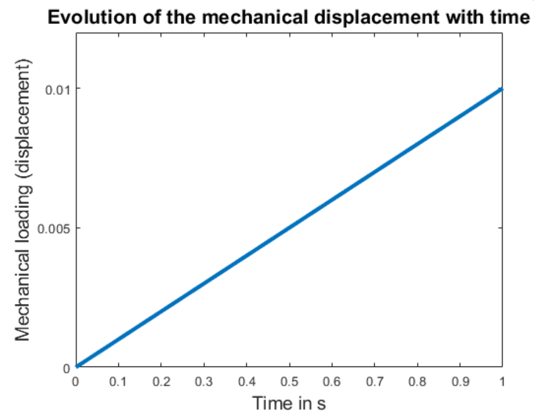


Numerical model : Mechanical loading

- Tensile loading → Imposed displacement

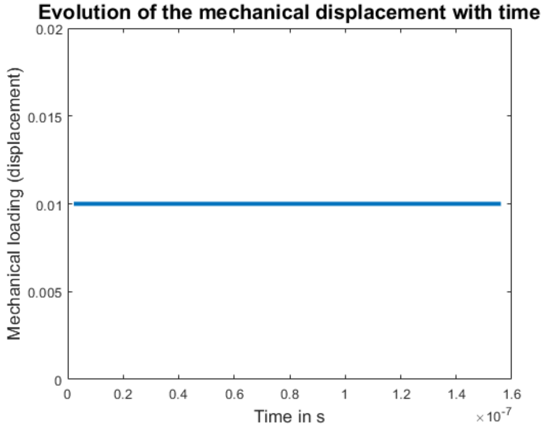
- Two mechanical loadings are applied successively





1. Quasi-static loading

- **Static** computations
- Retrieve the first value of the displacement loading above which the crack onset is initiated *(checked by computing the J-integral)*



2. Constant loading

- **Dynamic** computations
- The value of the applied loading is constant. The applied displacement is the one retrieved after undergoing a quasi-static loading

Numerical model : Temporal integration

1. Implicit integration scheme

- Large time step → Fast calculations
- No dynamic phenomena is considered
- Store enough energy within the specimen to trigger crack propagation afterwards

Using the available method PASAPAS – Cast3m

2. Explicit integration scheme

- Small time step → $2.23 * 10^{-9}$ s
- Follow the dynamic behaviour of crack propagation
- Follow the rapid crack propagation without providing any external work

Implementing Finite Difference Scheme in Cast3M

Numerical model : Temporal integration – Mass lumping

- XFEM : discontinuous enrichment
  → New DoF : 'AX' , 'AY' and 'AZ'
- A mass lumping technique including the new Dofs [4]

↓

Implementing the mass lumping strategy within Cast3M

↓ MASS3D procedure ⟷ MESHXF procedure ↓

- MASS3D procedure: Addition of elementary mass matrices for cracked elements
- MESHXF procedure: Updates the mass matrix to take into account the new cracked elements

[4] Menouillard, T.; Réthoré, J.; Moes, N.; Combescure, A.; Bung, H. Mass lumping strategies for x-fem explicit dynamics: application to crack propagation. International Journal for Numerical Methods in Engineering 2008, 74, 447–474

Numerical model : Crack propagation

Computing the *J-integral* at each time step
Method GTHETA – Cast3m

Compare J to $G_c = 2\gamma$

If $J > G_c$ → Crack initiation criteria is met → The excess of energy is converted to newly created crack surfaces →

$$2 * A_{created} = \frac{J - G_c}{G_c}\ mm^2$$

→

$$l_{crack} = \frac{A_{created}}{e}\ mm$$

If $J < G_c$ → No Crack initiation

Numerical model : Results

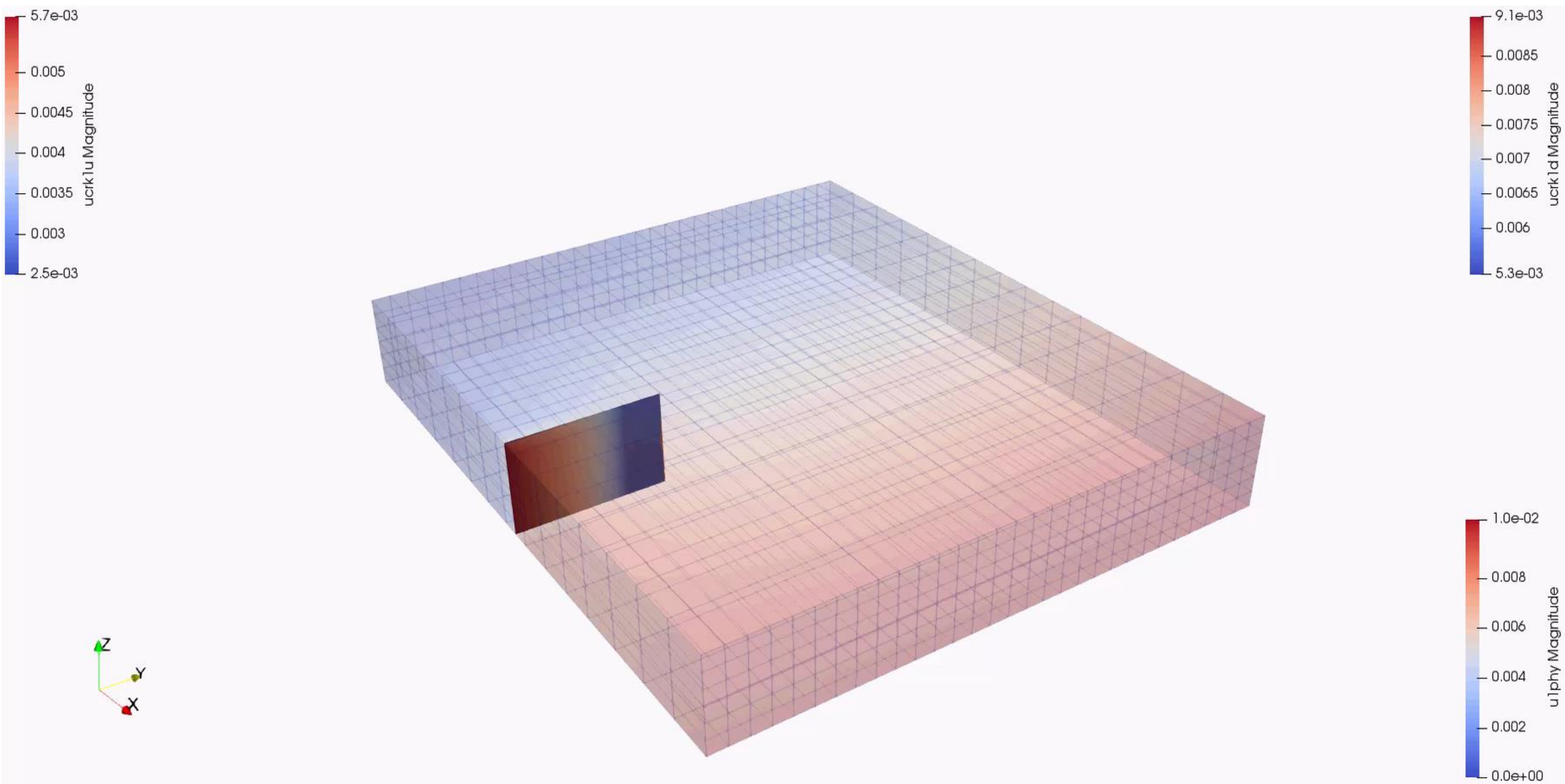


Figure 2 : Crack propagation – Amplification = 1

Numerical model : Results

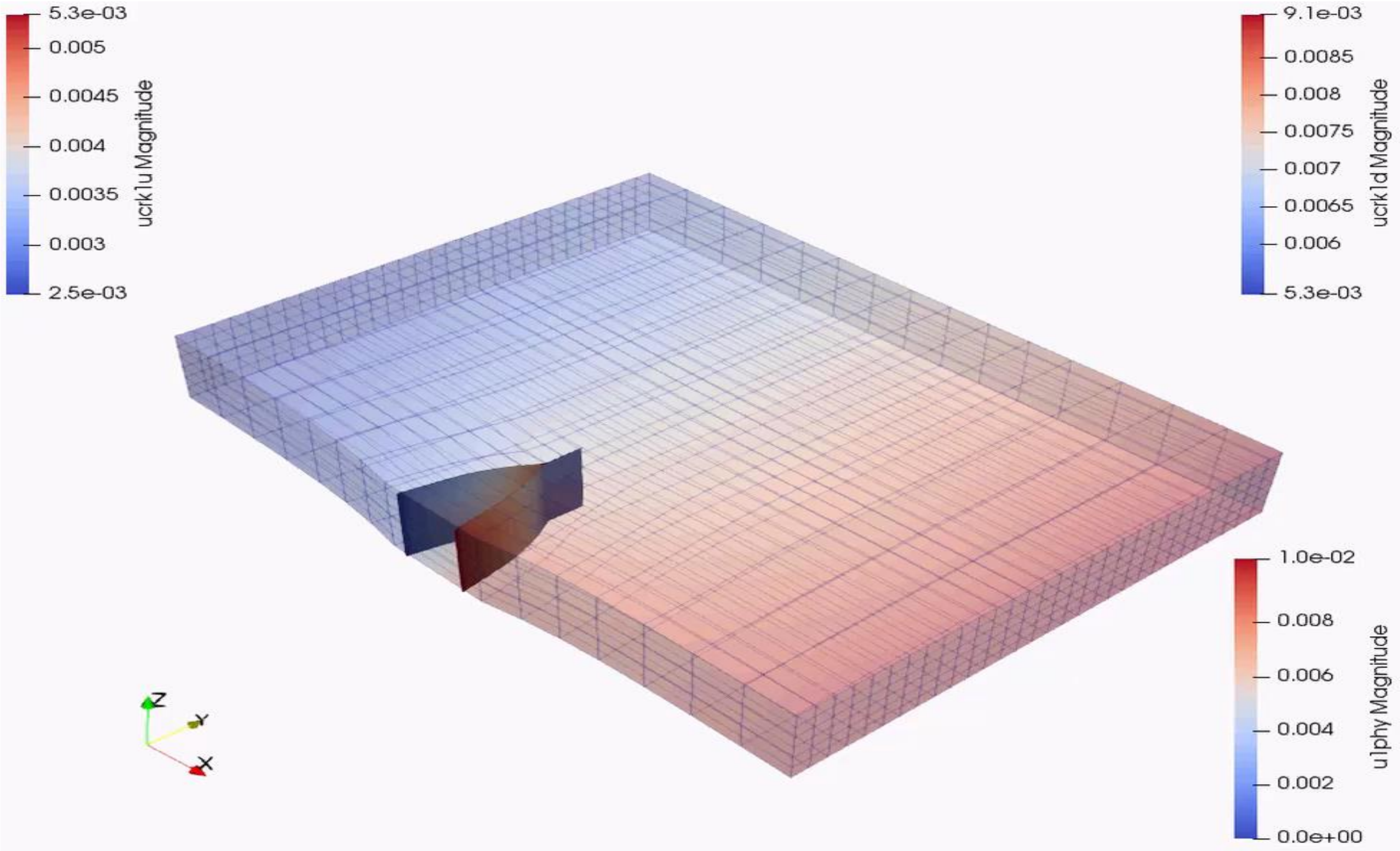
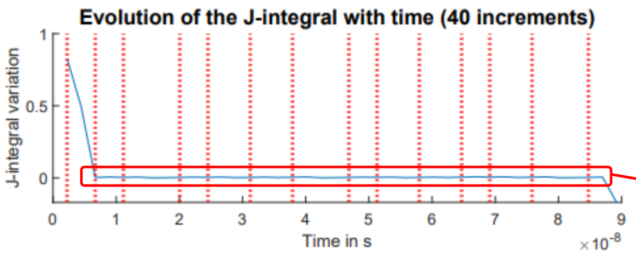
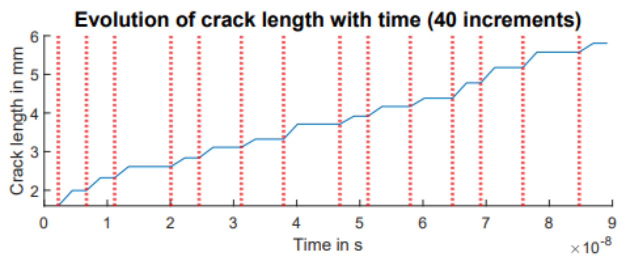


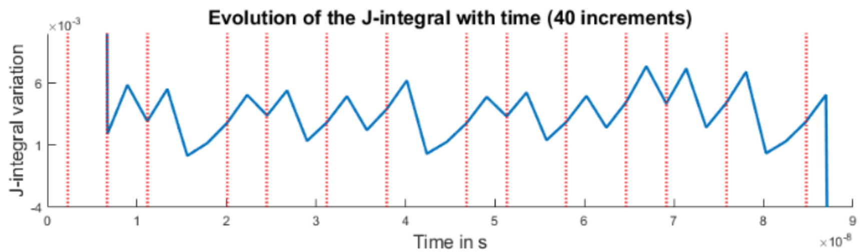
Figure 3 : Crack propagation – Amplification = 100

Numerical model : Results

- J-integral and crack length calculations







- Oscillation of J values : *reaching negative values !*
- Crack propagation is very constrained

unless J values allow 1,2,… elements' fracture → discontinuous enrichment only

Numerical model : Future perspectives

Future perspectives

- Evaluate the dynamic J integral (Depending on the crack speed)
- Use of the singular enrichment
- Mass lumping technique using both the discontinuous and the singular enrichment

Thank you for your attention

Background : On simulating high crack velocities

1- Crack inititation criteria :

- Energetic approach:

$$dW_{fiss} = 2\gamma dA$$

$$G = \int_{\partial\Omega_2} \mathbf{F}_d . \frac{\partial \mathbf{u}}{\partial A} dS + \int_{\Omega} \mathbf{f}_d . \frac{\partial \mathbf{u}}{\partial A} d\Omega - \frac{\partial W_{elas}}{\partial A}$$

If $G < 2\gamma$: No propagation
If $G = 2\gamma$: Crack initiation and stable crack growth
If $G > 2\gamma$: Unstable crack growth

- Local approach : stress intensity factors

$$K_1 = K_1^{cin} = \lim_{r\to 0} \sqrt{2\pi r}\sigma_{22}(\theta = \pi) = \lim_{r\to 0} \frac{\mu}{1+k}\sqrt{\frac{2\pi}{r}}\,[u_2(\theta=\pi)]$$

$$K_2 = K_2^{cin} = \lim_{r\to 0} \sqrt{2\pi r}\sigma_{12}(\theta = \pi) = \lim_{r\to 0} \frac{\mu}{1+k}\sqrt{\frac{2\pi}{r}}\,[u_1(\theta=\pi)]$$

$$K_3 = K_3^{cin} = \lim_{r\to 0} \sqrt{2\pi r}\sigma_{23}(\theta = \pi) = \lim_{r\to 0} \frac{\mu}{4}\sqrt{\frac{2\pi}{r}}\,[u_3(\theta=\pi)]$$

- Maximum circumferential stress Criterion
- Maximum Radial Shear Stress Criterion
- Minimum Strain Energy Density Criterion
- Modified Twin Shear Stress Factor Criterion [2]

2- Crack propagation criteria :

In general, crack velocity/crack extension is governed by empirical laws, such as :

- **Kanninen Law** (*Crack velocity*)

$$\dot{a} = \left(1 - \frac{K_{1c}}{K_{\theta\theta}^{dyn}}\right)^{1/m} c_r$$

- **Paris' Law** (*Rate of growth of a fatigue crack*)

$$\frac{da}{dN} = C(\Delta K)^m$$

[2] Huang, R. Q.; Wu, L. Z.; Li, B. Crack Initiation Criteria and Fracture Simulation for Precracked Sandstones. Advances in Materials Science and Engineering 2019, 2019, e9359410, Publisher: Hindawi.