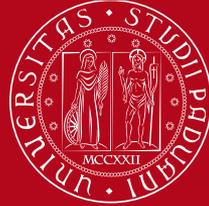


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An improved peridynamic framework for the accurate solution of multi-physics problems

Francesco Scabbia - 36th Cycle

Admission to the thesis evaluation procedure - 14/09/2023

Supervisor: Prof. **Ugo Galvanetto**

Co-supervisor: Prof. **Mirco Zaccariotto**

PhD course in **Sciences, Technologies and Measurements for Space (STMS)**

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 - Mitigation of boundary problems
 - New algorithm for quadrature
 - Coupling with local models
 - Modeling of ZrC oxidation
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Problem

Multi-physics phenomena causing damage in aerospace structures



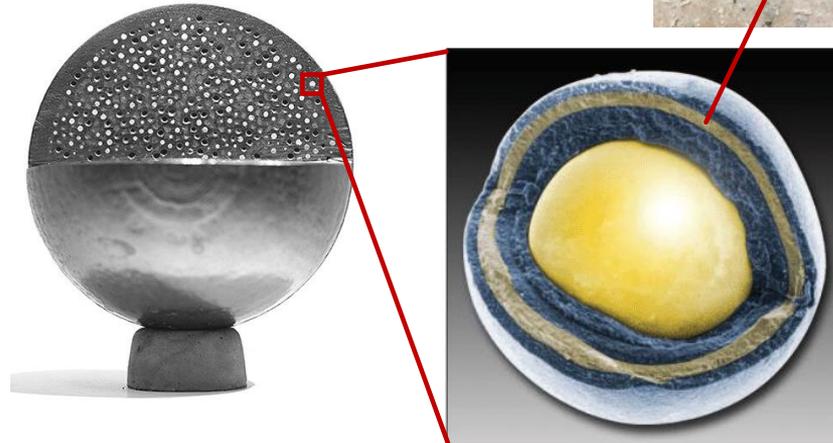
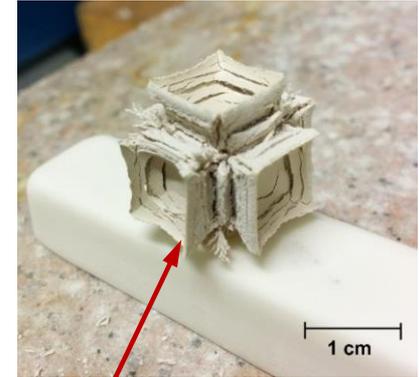
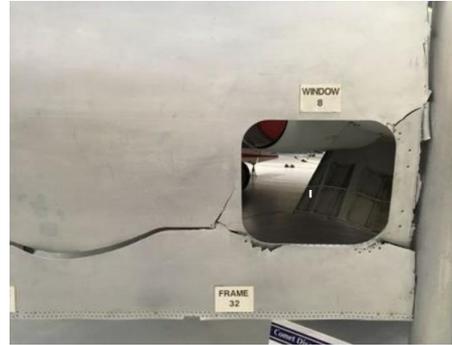
Current solution

Design with high safety margins, with consequent increase of costs



Proposed solution

Development of a reliable numerical tool to improve safety and limit financial losses



2. Research background

Peridynamics is a nonlocal continuum theory with an integral formulation capable of modeling discontinuities in the displacement field, such as crack initiation and evolution of any type.



Equation of motion of point \mathbf{x}

$$\rho(\mathbf{x}) \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{x}, \mathbf{x}', t) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

ρ : density

\mathbf{u} : displacement vector field

δ : horizon

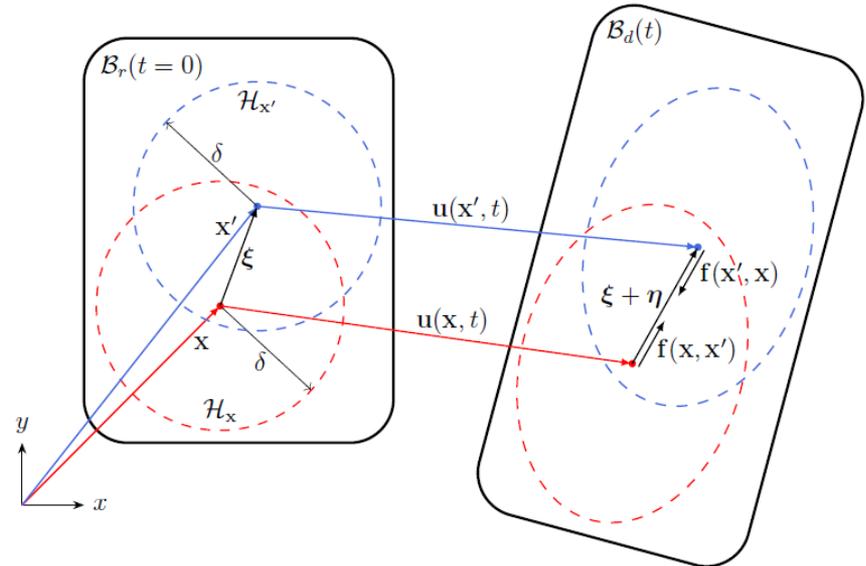
\mathbf{b} : body force vector

$\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$: relative position vector (bond)

$\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t)$: relative displacement vector

$\mathbf{f}(\mathbf{x}, \mathbf{x}', t)$: pairwise force density

$\mathcal{H}_{\mathbf{x}}$: neighborhood



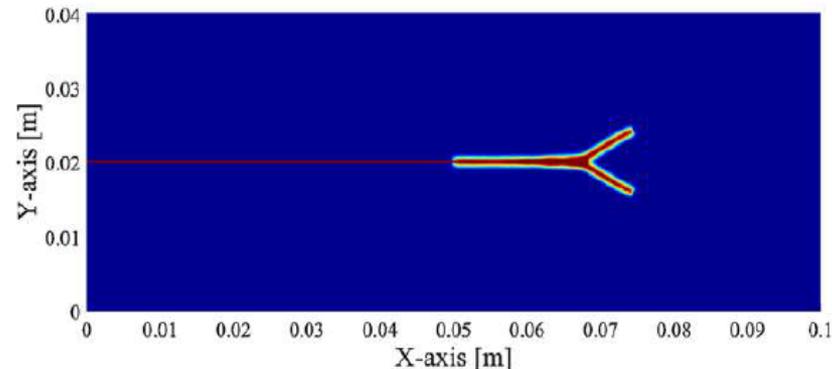
Reference and deformed configuration of a peridynamic body B : each point \mathbf{x} interacts with the points \mathbf{x}' in its neighborhood $\mathcal{H}_{\mathbf{x}}$ through the bonds.

Main advantages

1. Introduction of the concept of structural damage for a material point
2. No ad-hoc criteria to model crack initiation and propagation

Disadvantages

1. Issues on mechanical properties near the boundary (surface effect) and on the imposition of boundary conditions
2. Accurate quadrature is required
3. Higher computational cost than classical continuum models

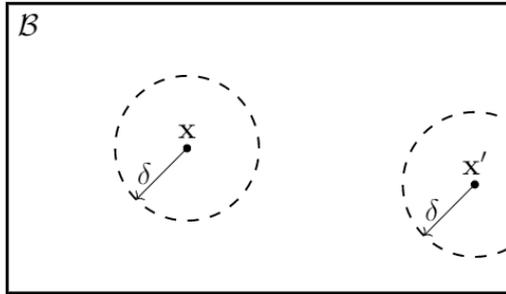


Simulation of a crack propagation in a pre-notched specimen modeled with Peridynamics.

3. Project objectives

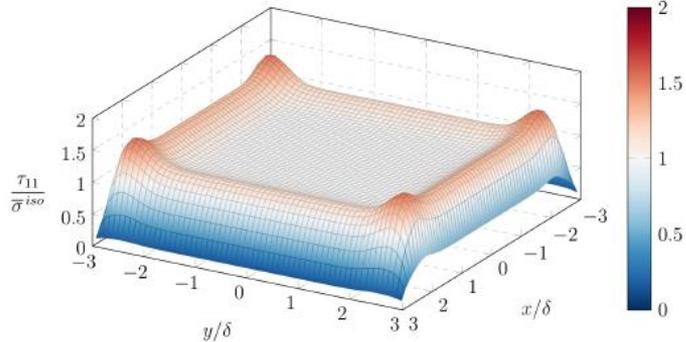
1. Development of an innovative method to mitigate boundary problems due to peridynamic nonlocality.
2. Improvement of currently used algorithms to compute quadrature weights.
3. Coupling of Peridynamics with local models to reduce the overall computational cost.
4. Solution to complex multi-physics problems with the improved peridynamic framework.

4.1 Mitigation of boundary problems

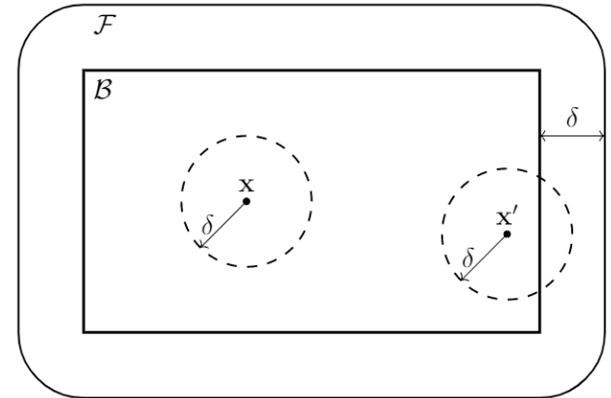


Peridynamic body without boundary corrections.

The Surface Node Method (SNM) is proposed in order to mitigate the surface effect and impose local boundary conditions in Peridynamics.



Stiffness fluctuation (surface effect) near the boundary due to the incomplete neighborhoods.

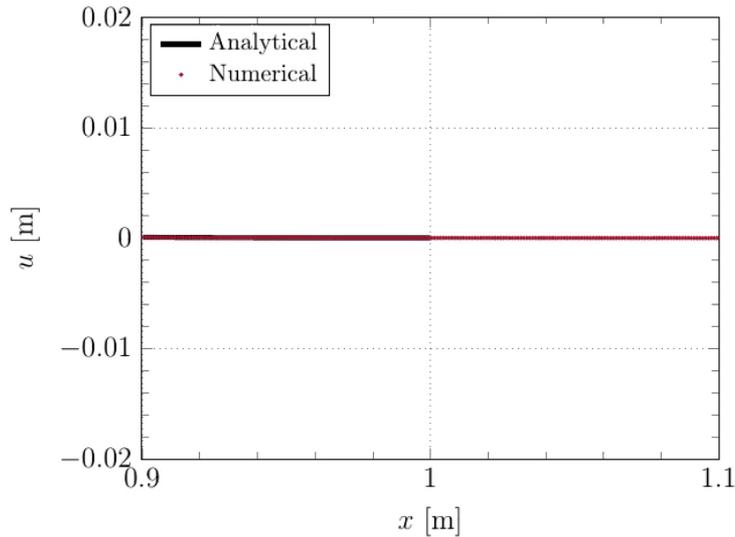


4.1 Mitigation of boundary problems

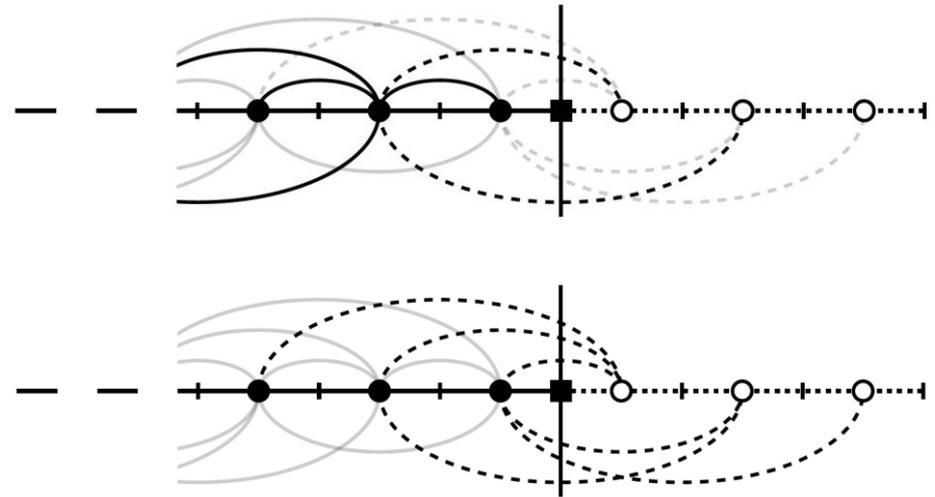
Discretized 1D model with the addition of the surface nodes:



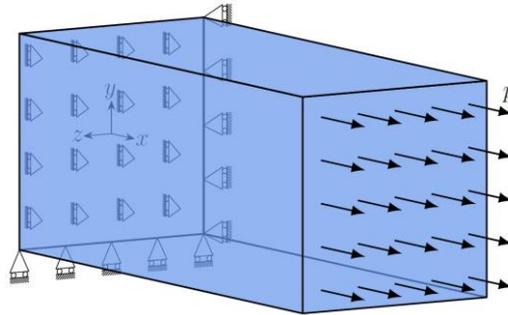
Linear Taylor-based extrapolation to impose local constraints.



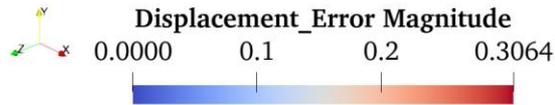
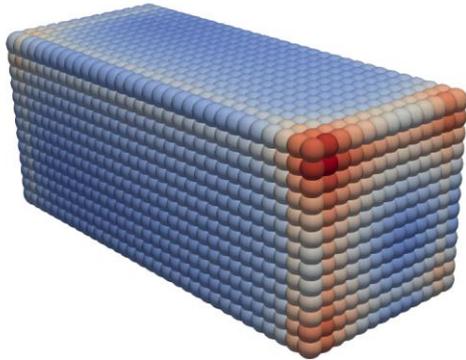
Force flux (peridynamic stress) equation at the surface nodes to impose local loads.



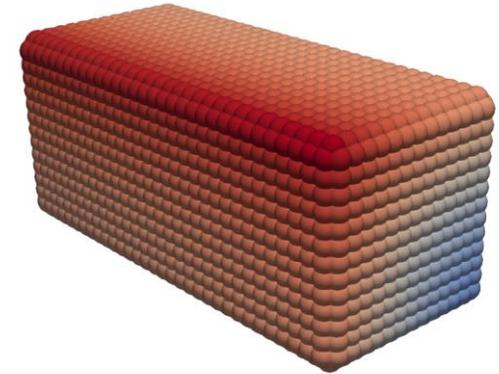
4.1 Mitigation of boundary problems



3D static example.

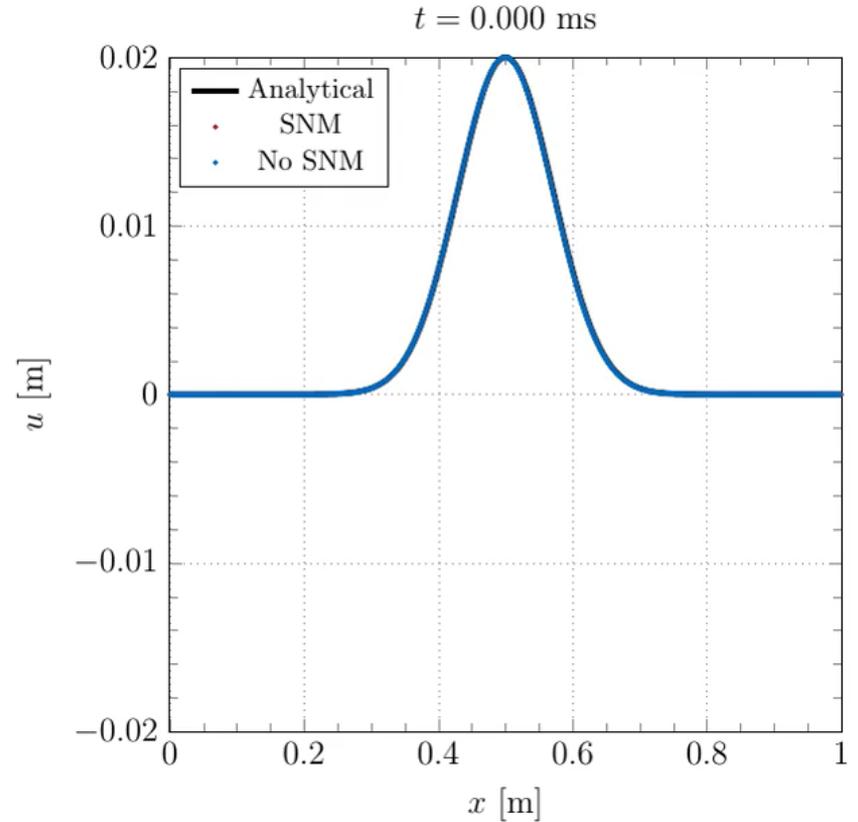
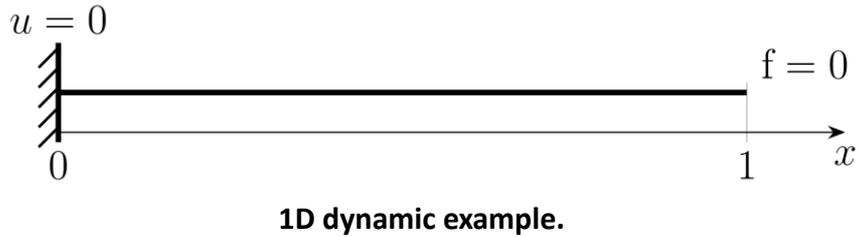


Errors of the solution without correction.



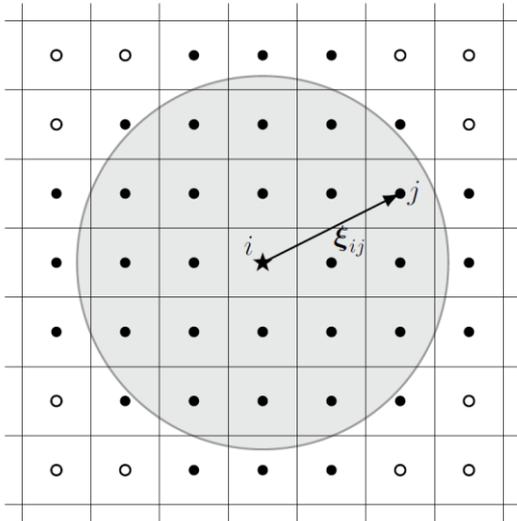
Errors of the solution with the proposed method.

4.1 Mitigation of boundary problems

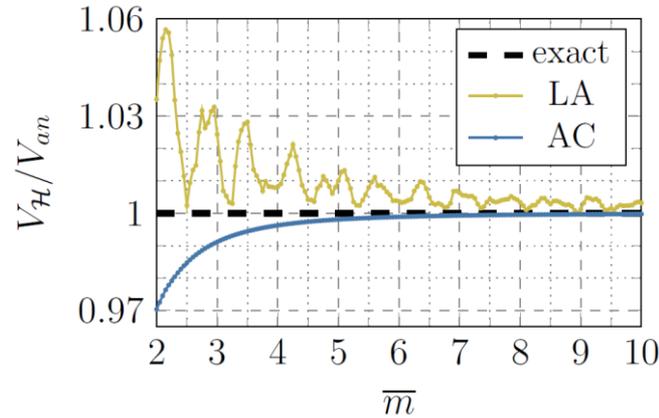


4.2 New algorithm for quadrature

An algorithm to accurately compute quadrature weights in 3D peridynamic models is developed.

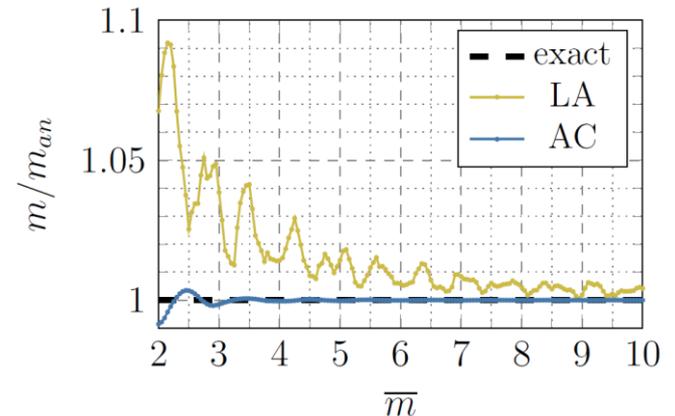


Discretization of the neighborhood (2D model for image clarity).



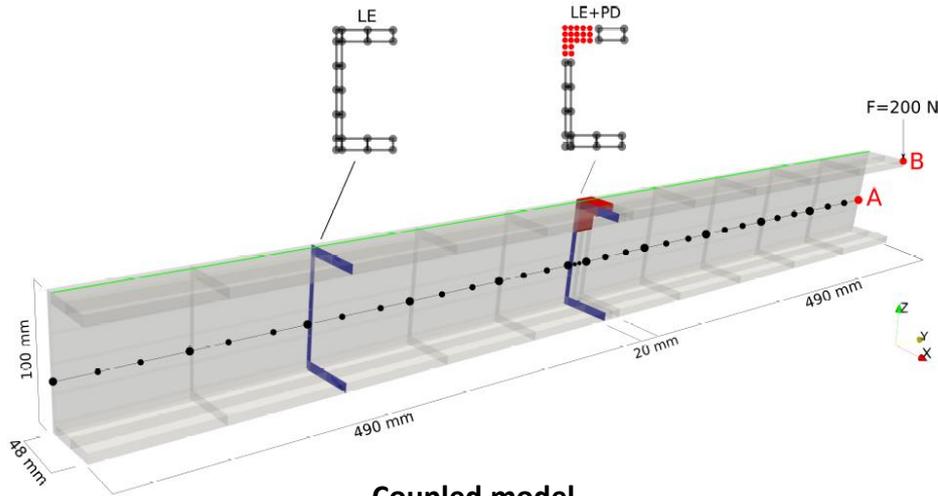
Normalized volume of the neighborhood.

Normalized weighted volume.

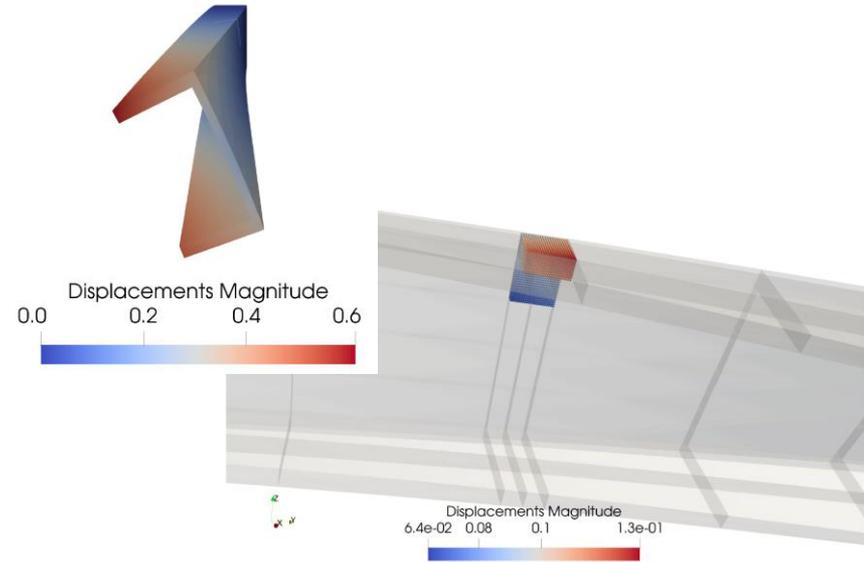


4.3 Coupling with local models

Peridynamics is coupled with Carrera Unified Formulation (CUF), a local theory based on the Finite Element Method (FEM) able to reproduce arbitrary kinematic models, to reduce the overall computational cost.



Coupled model.

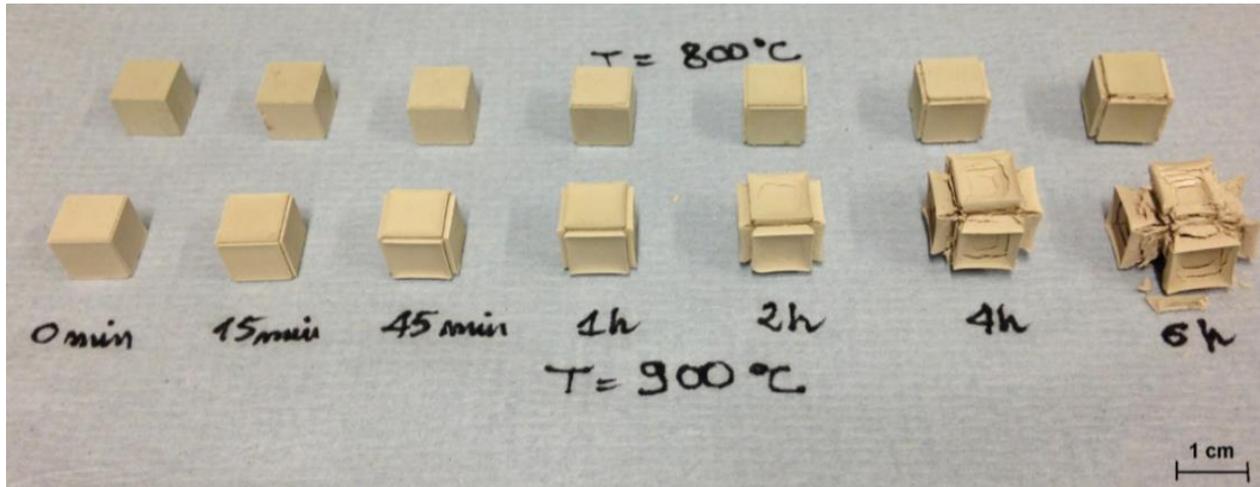
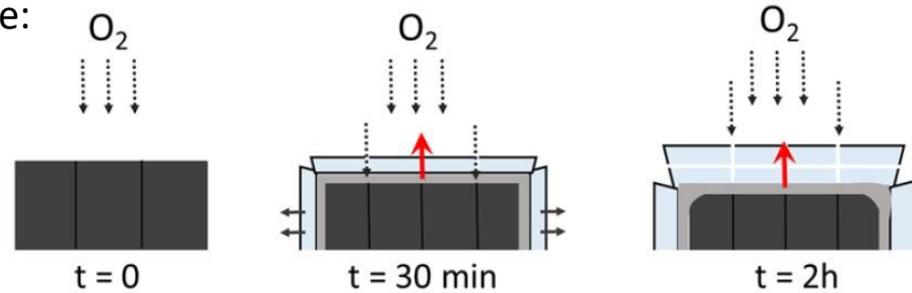


Numerical results, in good agreement with the results of a refined 3D FEM model.

4.4 Modeling of ZrC oxidation

Zirconium carbide (ZrC) oxidation at high temperature:

- Oxygen diffusion within ZrC and oxidation
- Volumetric expansion due to oxidation
- Crack initiation and propagation
- Flow of oxygen within the cracks



Oxidation of a cube made of zirconium carbide.

4.4 Modeling of ZrC oxidation

Stability condition for classical diffusion equation:

$$\Delta t \leq \mathcal{O}(\Delta x^2) \quad \text{as } \Delta x \rightarrow 0$$

Stability condition for peridynamic diffusion equation without considering the influence of boundary conditions:

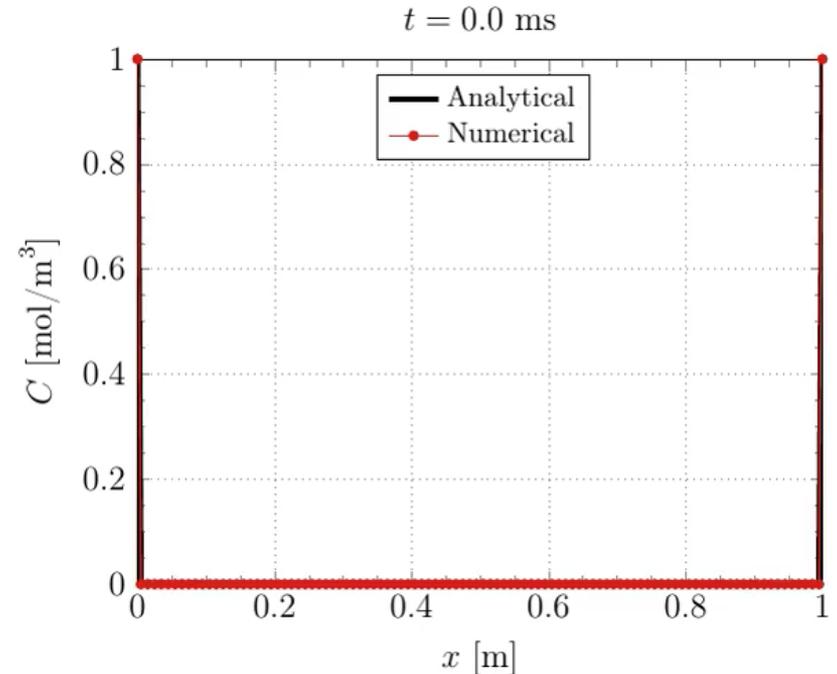
$$\Delta t \leq \frac{1}{d \sum_{m=1}^{\bar{m}} \mu(m\Delta x) \Delta x} = \mathcal{O}(\delta^2) \quad \text{as } \delta \rightarrow 0$$

New stability condition for peridynamic diffusion equation:

$$\Delta t \leq \frac{1}{d \sum_{m=1}^{\bar{m}} \mu(m\Delta x) (m+1) \Delta x} = \mathcal{O}(\delta^2) \quad \text{as } \delta \rightarrow 0$$

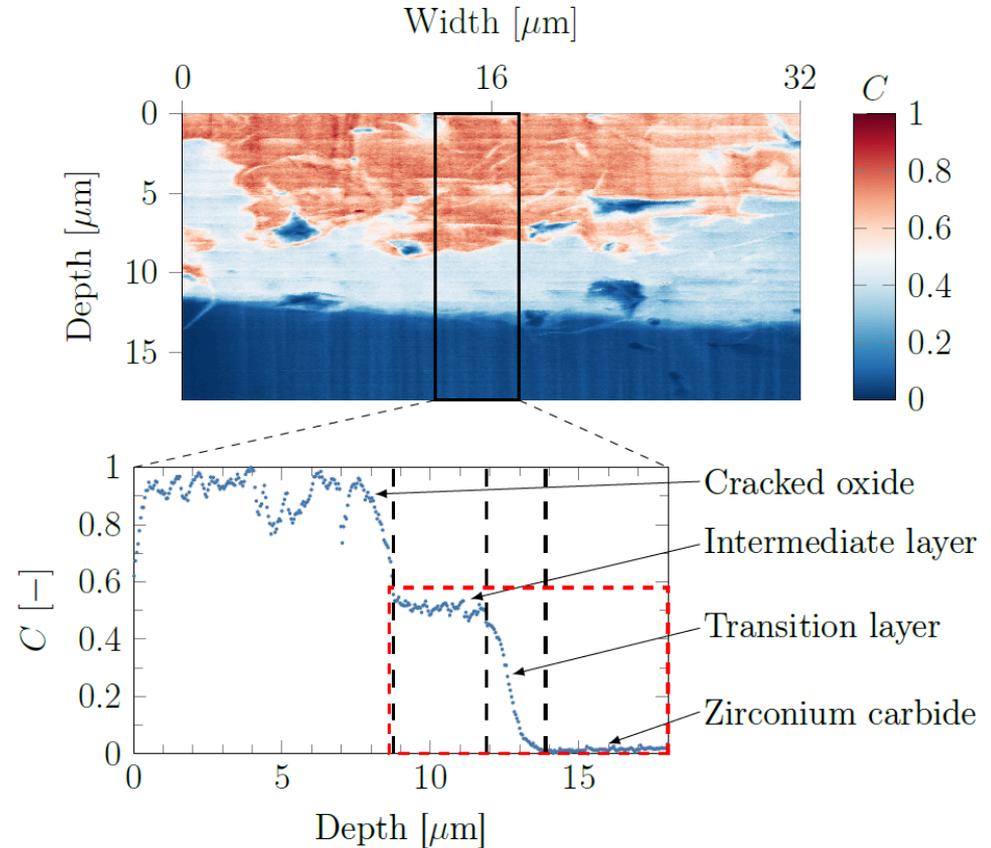
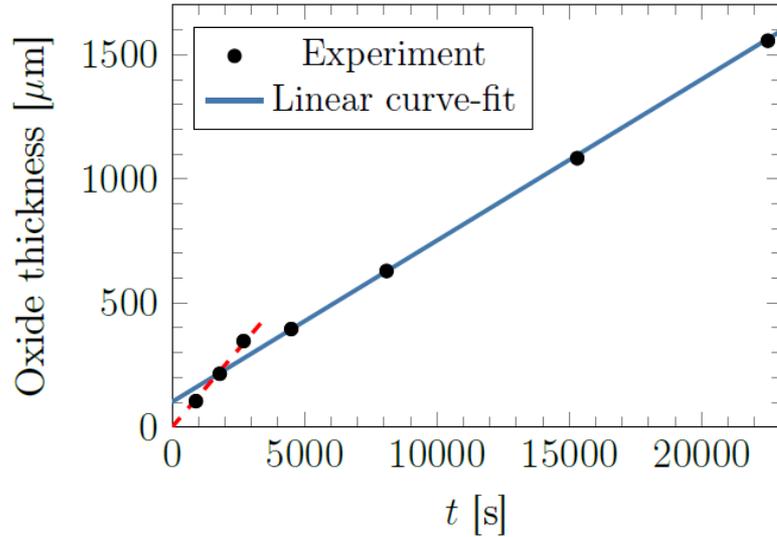
$\bar{m} = \delta/\Delta x$: m-ratio $\mu(\cdot)$: kernel function d : micro-diffusivity

Sudden exposure to oxygen is modeled as a discontinuity in the initial conditions:



4.4 Modeling of ZrC oxidation

Experimental observations of ZrC oxidation



6. Final remarks and future work

1. An innovative method to mitigate boundary issues in peridynamic models has been implemented for static and dynamic problems.
2. A new algorithm to compute 3D quadrature weights in peridynamic models has been developed, resulting in a considerable gain in accuracy and convergence rate.
3. Peridynamics has been coupled with CUF to reduce the overall computational cost. The spurious forces arising at the interfaces have been decreased by improving the coupling technique.
4. The multi-physics problem of the ZrC oxidation has been modeled within the improved peridynamic framework. In future work we will investigate the oxidation-induced damage by coupling the diffusion-based model with a mechanical solver simulating fracture.

Papers:

- F. Scabbia**, M. Zaccariotto, U. Galvanetto. “A novel and effective way to impose boundary conditions and to mitigate the surface effect in state-based Peridynamics”. *International Journal for Numerical Methods in Engineering*, 2021.
- F. Scabbia**, M. Zaccariotto, U. Galvanetto. “A new method based on Taylor expansion and nearest-node strategy to impose Dirichlet and Neumann boundary conditions in ordinary state-based Peridynamics”. *Computational Mechanics*, 2022.
- F. Scabbia**, M. Zaccariotto, U. Galvanetto. “A new surface node method to accurately model the mechanical behavior of the boundary in 3D state-based peridynamics”. *Journal of Peridynamics and Nonlocal Modeling*, 2023.
- F. Scabbia**, M. Zaccariotto, U. Galvanetto. “Accurate computation of partial volumes in 3D peridynamics”. *Engineering with Computers*, 2023.
- F. Scabbia**, M. Enea. “An improved coupling of 3D state-based peridynamics with high-order 1D finite elements to reduce spurious effects at interfaces”. *International Journal for Numerical Methods in Engineering*, 2023.
- F. Scabbia**, C. Gasparri, M. Zaccariotto, U. Galvanetto, A. Larios, F. Bobaru. “Moving interfaces in peridynamic diffusion models and the influence of discontinuous initial conditions: Numerical stability and convergence”. *Computers and Mathematics with Applications*, 2023.
- F. Scabbia**, C. Gasparri, M. Zaccariotto, U. Galvanetto, F. Bobaru. “A peridynamic model for oxidation and damage in zirconium carbide ceramics”. Submitted to *International Journal of Heat and Mass Transfer*, 2023.

Conference proceedings:

F. Scabbia, M. Zaccariotto, U. Galvanetto. “An effective method for imposing peridynamic boundary conditions and mitigating the surface effect”. AIDAA XXVI International Congress, August 31 and September 1-3, 2021, Pisa, Italy.

M. Enea, **F. Scabbia**, A. Pagani, M. Zaccariotto, E. Carrera, U. Galvanetto. “One-dimensional high order finite elements embedding 3D state-based peridynamic subdomains”. AIDAA XXVI International Congress, August 31 and September 1-3, 2021, Pisa, Italy.

U. Galvanetto, **F. Scabbia**, M. Zaccariotto. “Accurate numerical integration in 3D meshless peridynamic models”. 8th International Conference on Structural Engineering, Mechanics and Computation (SEMC), September 5-7, 2022, Cape Town, South Africa.

F. Scabbia, M. Zaccariotto, U. Galvanetto. “Exact computation of the cube-sphere intersection volume to improve peridynamic numerical integration”. 10th International Conference on Design, Modelling and Experiments of Advanced Structures and Systems (DeMEASS2020), May 1-4, 2022, Scopello, Italy.

M. Enea, **F. Scabbia**, A. Pagani, M. Zaccariotto, E. Carrera, U. Galvanetto. “Analysis of beam structures by combined 3D peridynamics and refined 1D finite elements”. 10th International Conference on Design, Modelling and Experiments of Advanced Structures and Systems (DeMEASS2020), May 1-4, 2022, Scopello, Italy.

F. Scabbia, M. Zaccariotto, U. Galvanetto, F. Bobaru. “Peridynamic simulation of elastic wave propagation by applying the boundary conditions with the surface node method”. III Aerospace PhD-Days, April 16-19, 2023, Bertinoro, Italy.

F. Scabbia, M. Zaccariotto, U. Galvanetto. “Surface node method for the peridynamic simulation of elastodynamic problems with Neumann boundary conditions”. AIDAA XXVII International Congress, September 4-7, 2023, Padova, Italy.

Abstracts:

- U. Galvanetto, T. Ni, F. Pesavento, M. Zaccariotto, **F. Scabbia**, B.A. Schrefler. “Hybrid FEM and peridynamic simulation of hydraulic fracture propagation in saturated porous media”. Workshop on Experimental and Computational Fracture Mechanics (WFM), February 26-28, 2020, Baton Rouge, Louisiana, USA.
- **F. Scabbia**, M. Zaccariotto, U. Galvanetto. “A note on the surface effect in OSB-PD models”. 3rd annual meeting of the SIAM Texas-Louisiana Section, October 16-18, 2020, College Station, Texas, USA.
- U. Galvanetto, **F. Scabbia**, M. Zaccariotto. “How to reduce the surface effect and to apply the boundary conditions in 1D peridynamic models”. 16th U.S. National Congress on Computational Mechanics, July 25-29, 2021, virtual event.
- **F. Scabbia**, M. Zaccariotto, U. Galvanetto. “An innovative method to manage non-local boundaries in ordinary state-based Peridynamics”. XVI International Conference on Computational Plasticity, Fundamentals and Applications (COMPLAS2021), September 7-9, 2021, Barcelona, Spain.
- **F. Scabbia**, M. Zaccariotto, U. Galvanetto. “An innovative method to correct the boundary issues in Peridynamics”. 11th European Solid Mechanics Conference (ESMC2022), July 4-8, 2022, Galway, Ireland.
- **F. Scabbia**, M. Zaccariotto, U. Galvanetto. “On the imposition of non-local boundary conditions in Peridynamics to avoid undesired stiffness fluctuations”. 9th GACM Colloquium on Computational Mechanics for Young Scientists from Academia and Industry (GACM2022), September 21-23, 2022, Essen, Germany.
- **F. Scabbia**, M. Zaccariotto, U. Galvanetto. “How to improve the numerical integration in peridynamic models”. 10th International Congress of Croatian Society of Mechanics (ICCSM2022), September 28-30, 2022, Pula, Croatia.
- U. Galvanetto, **F. Scabbia**, M. Zaccariotto. “A method to reduce the surface effect and to impose in a local way the BC in Peridynamics models”. Society of Engineering Science Annual Technical Meeting (SES2022), October 16-19, 2022, College Station, Texas, USA.
- U. Galvanetto, **F. Scabbia**, M. Zaccariotto. “On the surface effect and the imposition of the BC in Peridynamics”. Conference on Computational Science and Engineering (CSE2023), February 27-28 and March 1-3, 2023, Amsterdam, Holland.
- M. Zaccariotto, **F. Scabbia**, U. Galvanetto. “A unified strategy to mitigate the surface effect and to impose in a local way the boundary conditions in Peridynamics models”. 7th International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC2023), June 21-23, 2023, Prague, Czech Republic.
- U. Galvanetto, T. Ni, **F. Scabbia**, A. Pirzadeh, M. Zaccariotto. “New trends in applied computational peridynamics”. NanoInnovation Conference and Exhibition 2023, September 18-22, 2023, Rome, Italy.

Thanks for the attention!
Any questions?

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