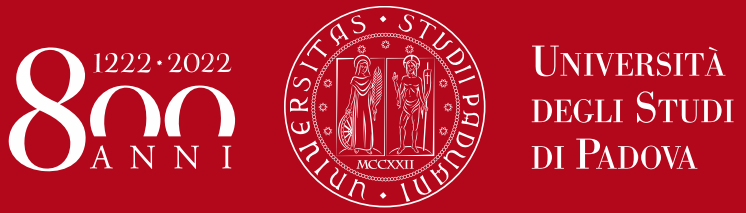


Simulation of damage propagation in materials and structures by using peridynamics

Greta Ongaro - 34th Cycle

Supervisor: Prof. Ugo Galvanetto
Co-Supervisor: Prof. Mirco Zaccariotto

Request of admission to the thesis evaluation procedure - December 15th, 2021

Outline

- **Research background**
- **Project objectives**
- **Work methodologies and tools**
  - Peridynamic theory
  - Classical continuum mechanics-peridynamics coupling strategy
- **Tasks completed throughout the three years of the PhD Course**
- **Study of the in-house CCM-PD coupling software**
- **Modelling of high specific stiffness materials properties**
- **Final remarks and possible future developments**
- **List of publications**

Research background

Need to develop lighter and more efficient components for aircraft structures

↓

Composite and nanocomposite materials

↓

They exhibit enhanced mechanical, thermal, and barrier properties

BENEFITS: Reduction of airplane mass and fuel consumption, downturn in costs and in carbon emissions

MAIN PROBLEM: Unavoidable presence of cracks in aeronautical and aerospace structures

MAJOR CHALLENGES:

Understanding of fracture phenomenon and damage initiation and evolution mechanism

↓

Development of innovative computational methods for material properties characterization and damage prediction

↓

Achievement of an accurate description of large and complex structures

Example of a crack in an aircraft fuselage

Project objectives

I. Study of **CCM-PD coupling methods**: equipping of CCM-based models with the capability to simulate crack formation and propagation

II. Improvement of in-house **CCM-PD coupling software**: study of tools for FEM analysis, analysis of **structural equilibrium** and **convergence** issues to reduce **coupling errors**

III. Development of a **PD-based method** for the numerical modelling of the **mechanical properties** of polymer-based **nanocomposites**

IV. Validation of numerical simulations through **experimental activities**

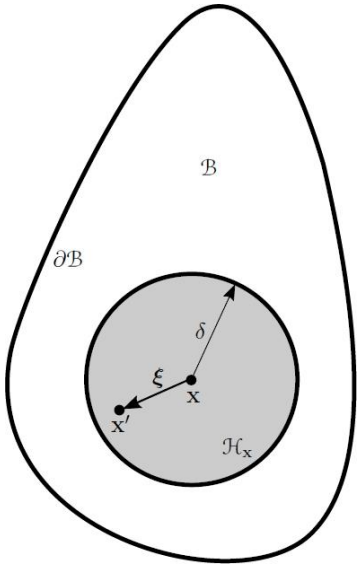
CCM = Classical continuum mechanics
PD = Peridynamics

Work methodologies and tools

Peridynamic theory

Nonlocal reformulation of classical continuum mechanics (CCM) based on integro-differential equations

Two versions of the theory → bond-based (BB) version and state-based (SB) version



Each point **x** in the body interacts with all the points located within its neighbourhood $\mathbf{H_x}$ through bonds

The state-based PD equation of motion for any material point x ∈ *B* is given by:

$$\rho(x)\ddot{u}(x,t) = \int_{H_x} \{\underline{T}[x,t]\langle x' - x\rangle - \underline{T}[x',t]\langle x - x'\rangle\} dV_{x'} + b(x,t), \qquad x' \in H_x$$

where:

- ρ is the mass density
- **x** is a material point of the domain *B*
- $\mathbf{H_x}$ is the finite neighbourhood centred at point **x**
- δ is the horizon radius
- **u** is the displacement vector field
- **b** is a prescribed body force density field
- $\underline{T}[x,t]\langle x' - x\rangle$ is the force density vector that point **x′** exerts on point **x**

The relation between SB-PD models and BB-PD models is given by:

$$\underline{\mathbf{T}}[\mathbf{x},t]\langle\boldsymbol{\xi}\rangle = \frac{1}{2}\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})$$

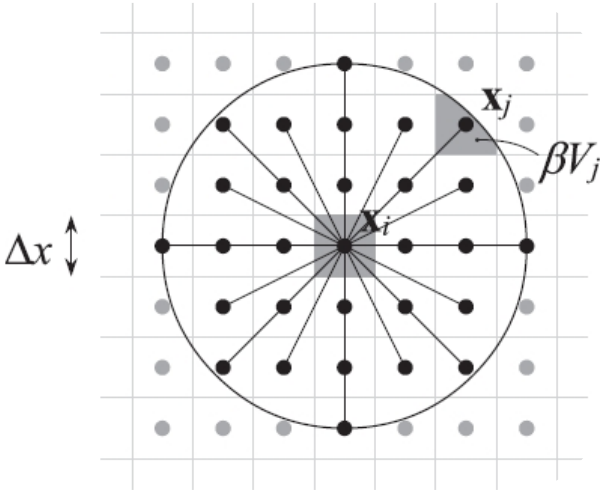
f is the pairwise force function in BB-PD theory
$\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ is the relative position vector
$\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}$ is the relative displacement vector

Work methodologies and tools

PD numerical discretization

The domain is discretized into a grid of points called nodes, each with a known volume (V) in the reference configuration

The method is meshfree → no geometrical connections between the nodes



Representation of a generic horizon in a discretized form. Δx is the grid spacing of the discretized model. $m = \delta/\Delta x = 3$ in the figure **[1]**

The discretized form of the SB-PD and BB-PD equation of motion can be written as:

$$\rho \ddot{\boldsymbol{u}}_i^n = \begin{cases} \sum_j \left\{ \underline{\boldsymbol{T}}[\boldsymbol{x}_i^n]\langle \boldsymbol{x}_j^n - \boldsymbol{x}_i^n \rangle - \underline{\boldsymbol{T}}[\boldsymbol{x}_j^n]\langle \boldsymbol{x}_i^n - \boldsymbol{x}_j^n \rangle \right\} \beta(\boldsymbol{\xi}) \boldsymbol{V}_j + \boldsymbol{b}_i^n, \quad for\ OSB - PD \\ \sum_j \boldsymbol{f}(\boldsymbol{u}_j^n - \boldsymbol{u}_i^n, \boldsymbol{x}_j - \boldsymbol{x}_i)\, \beta(\boldsymbol{\xi}) \boldsymbol{V}_j + \boldsymbol{b}_i^n, \quad for\ BB - PD \end{cases} , \forall \boldsymbol{x}_j \in H(\boldsymbol{x}_i)$$

where:

- n is the time step
- subscripts i, j denote the node number (e.g., $\boldsymbol{u}_j^n = \boldsymbol{u}(\boldsymbol{x}_j, t_n)$)
- $\beta(\boldsymbol{\xi})$ is a partial volume correction factor used to evaluate the portion of $\boldsymbol{V}_j$ that falls within the neighborhood of the source node $\boldsymbol{x}_i$

[1] Shojaei, A., Mossaiby, F., Zaccariotto, M., & Galvanetto, U. (2018). An adaptive multi-grid peridynamic method for dynamic fracture analysis. International Journal of Mechanical Sciences, 144, 600-617.

Work methodologies and tools

CCM-PD coupling

Weak points of peridynamic numerical methods

PD is a nonlocal theory
↓
Bandwidth of the stiffness matrix in PD is bigger than that in CCM
↓
PD is computationally very expensive

In nonlocal theories the boundaries are fuzzy
↓
Defining boundary conditions introduces some difficulties

Coupling of peridynamics and classical continuum mechanics

Coupling of meshfree discretized PD models and CCM models discretized using the FEM

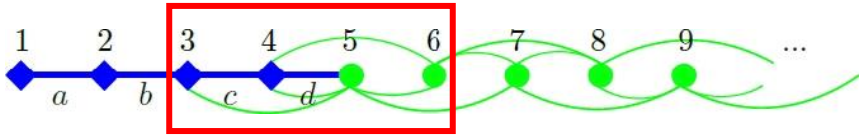
PD grids applied only to portions of the domain where cracks are likely to develop
↓
The remaining part is modelled with the more efficient FEM

FEM can be used at the boundaries
↓
Solution to the “surface effect” of PD

Work methodologies and tools

In-house CCM-PD coupling strategy

The coupling method can be introduced with the help of a 1D model



[2]

A **coupling zone** is defined where **forces** are **exchanged** between the **FEM** and **PD parts** of the domain

Internal forces acting on a **node** are of the **same nature** as the **node itself**

Equilibrium equations of **FEM** (**PD**) **nodes** contain only **terms** coming from the FEM (PD) **formulation**

This 1D coupled model produces the following system of equations:

$$\begin{bmatrix} l & -l & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \vdots \\ -l & 2l & -l & 0 & 0 & 0 & 0 & 0 & 0 & \vdots \\ 0 & -l & 2l & -l & 0 & 0 & 0 & 0 & 0 & \vdots \\ 0 & 0 & -l & 2l & -l & 0 & 0 & 0 & 0 & \vdots \\ 0 & 0 & -\frac{1}{4}p & -p & \frac{5}{2}p & -p & -\frac{1}{4}p & 0 & 0 & \vdots \\ 0 & 0 & 0 & -\frac{1}{4}p & -p & \frac{5}{2}p & -p & -\frac{1}{4}p & 0 & \vdots \\ 0 & 0 & 0 & 0 & -\frac{1}{4}p & -p & \frac{5}{2}p & -p & -\frac{1}{4}p & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cdots & \cdots & \ddots & \vdots & \vdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \ddots & \vdots \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ \vdots \\ \vdots \\ \vdots \\ u_N \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ \vdots \\ \vdots \\ \vdots \\ F_N \end{bmatrix}$$

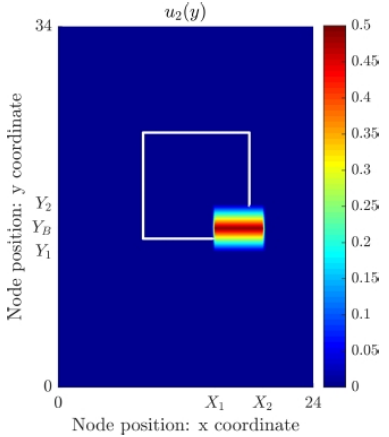
- $l := EA/\Delta x, p := cA^2\Delta x$
- EA = product between Young's modulus E and cross-sectional area A
- Δx = grid spacing of the discretized numerical model
- N = total number of nodes
- $\{\boldsymbol{u}_i\}_{i=1,\dots,N}$ = nodal displacements, $\{\boldsymbol{F}_i\}_{i=1,\dots,N}$ = external nodal forces
- c = micromodulus constant

[2] Ongaro, G., Seleson, P., Galvanetto, U., Ni, T., & Zaccariotto, M. (2021). Overall equilibrium in the coupling of peridynamics and classical continuum mechanics. Computer Methods in Applied Mechanics and Engineering, 381, 113515.

Tasks completed throughout the three years of the PhD Course

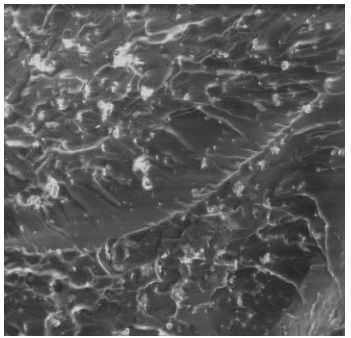
- **TASK 1: Bibliographic research on peridynamics and polymer/clay nanocomposites State of Art**
- **TASK 2: In-depth study and extension of the in-house CCM-PD coupling software**
- **TASK 3: Further development of the coupling method: theoretical and numerical analyses of overall static equilibrium issues**
- **TASK 4: Development of peridynamics-based computational tools for nanocomposite mechanical properties prediction**
- **TASK 5: Writing of PhD thesis and reports throughout the PhD course**
- **TASK 6: National and international collaborations**

Dr. **P. Seleson** (Oak Ridge National Laboratory, US), Prof. **R. Bertani**, Prof. **F. Faleschini**, Prof. **M. Quaresimin**, and Prof. **M. Zappalorto** (University of Padova)



[2]

Numerical study of overall static equilibrium issues



Experimental characterization of nanocomposite properties

[2] Ongaro, G., Seleson, P., Galvanetto, U., Ni, T., & Zaccariotto, M. (2021). Overall equilibrium in the coupling of peridynamics and classical continuum mechanics. Computer Methods in Applied Mechanics and Engineering, 381, 113515.

Study of the in-house CCM-PD coupling software

Consistency between linear BB-PD and CCM models

Often-overlooked issue in the use of **coupled computational methods** → **lack of overall static equilibrium**

↓

Traditionally, the **consistency** between **CCM** and **PD models** is studied through the **analysis** of the **corresponding governing equations**

↓

Theoretical formulations and **supporting numerical simulations** show that for **smooth displacement fields**

↓

If **fourth-order** (and higher) **derivatives** in both **1D and 2D PD equations** can be neglected

PD and **CCM** models possess the **same static solution** for problems with **constant**, **linear**, **quadratic**, or **cubic solutions**

Leading term in the **discrepancy** between **PD** and **CCM models** is of **order** $O(\delta^2)$

However, this analysis does **not reveal** the **culprit responsible** for the existence of **out-of-balance forces** in **CCM-PD** coupled systems

Study of the in-house CCM-PD coupling software

Out-of-balance analysis in CCM-PD coupling

Theoretical formulations and **supporting numerical simulations** show that

↓

The **main reason** for the existence of **out-of-balance forces** is a **lack of balance** between the **local** and **nonlocal tractions** at the **coupling interface**

1D

If the **deformation** around the **interface** is **smooth** and **third-order** (and higher) **derivatives** of displacements are **negligible**

↓

The **nonlocal traction converges** to the **local traction** and **overall equilibrium** is **attained**

↓

The **traction discrepancy** depends upon **third-order** (and higher) **derivatives** of displacements and the **leading term** is of order $\boldsymbol{O(\delta^2)}$

Analytical net out-of-balance force

$$\mathcal{F} = \frac{1}{12}\frac{3-\alpha}{5-\alpha}E\delta^2\left(\frac{d^3u}{dx^3}(x_{IL}) - \frac{d^3u}{dx^3}(x_{IR})\right) + \dots$$

$\neq$

2D

For a **straight interface** and a **smooth deformation**, if **second-order** (and higher) **derivatives** of displacements are **negligible**

↓

The **nonlocal traction converges** to the **local traction** and **overall equilibrium** is **attained**

↓

The **traction discrepancy** depends upon **second-order** (and higher) **derivatives** of displacements and the **leading term** is of order $\boldsymbol{O(\delta)}$

Components of the analytical net out-of-balance force

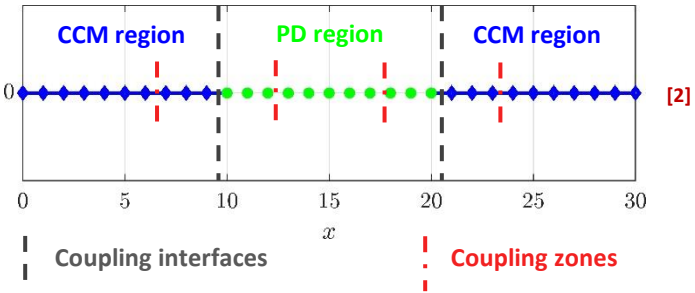
$$\mathcal{F}_1 \approx -\int_\Gamma \frac{2E}{5\pi}\frac{6-\alpha}{7-\alpha}\delta\left(\frac{3}{2}\frac{\partial^2 u_1}{\partial x^2}(x,y_0) + \frac{\partial^2 u_2}{\partial x \partial y}(x,y_0)\right)dx + \dots$$

$$\mathcal{F}_2 \approx -\int_\Gamma \frac{2E}{5\pi}\frac{6-\alpha}{7-\alpha}\delta\left(\frac{\partial^2 u_1}{\partial x \partial y}(x,y_0) + \frac{\partial^2 u_2}{\partial x^2}(x,y_0)\right)dx + \dots$$

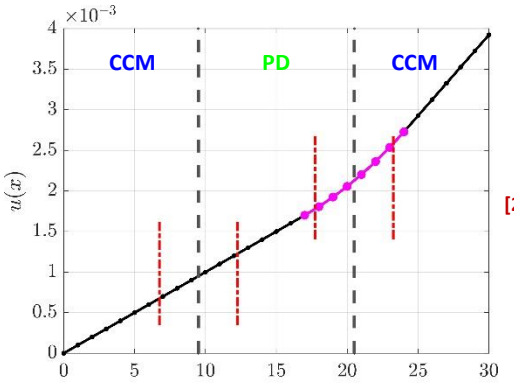
Study of the in-house CCM-PD coupling software

Out-of-balance forces in CCM-PD coupling

1D Case



[2]



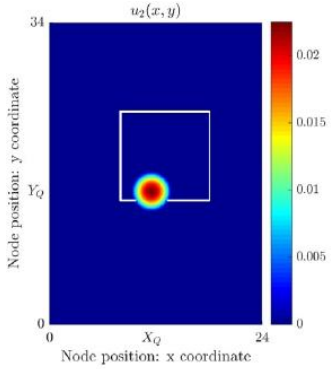
[2]

If **displacements across the coupling interface** are characterized by **cubic or higher-order** polynomial distributions, lack of overall equilibrium is experienced

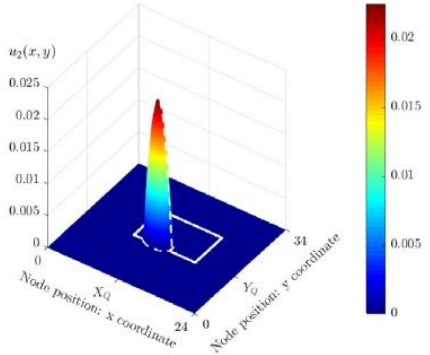
Relative out-of-balance error

$$e_r := \frac{\left|\sum_{i=1}^{N} F_i\right|}{\sum_{i=1}^{N} |F_i|} \rightarrow 5.78 \times 10^{-04}$$

2D Case



[2]



If **displacements across a straight (horizontal or vertical) coupling interface** are characterized by **quadratic or higher-order** polynomial distributions, lack of overall equilibrium is experienced

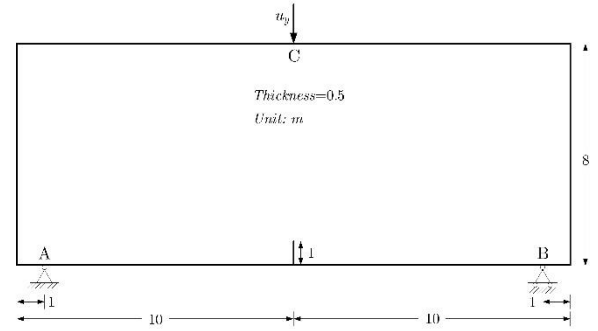
Relative out-of-balance error

$$e_{r_y} := \frac{\left|\sum_{i=1}^{N} F_{2\,i}\right|}{\sum_{i=1}^{N} |F_{2\,i}|} \rightarrow 5.00 \times 10^{-04}$$

[2] Ongaro, G., Seleson, P., Galvanetto, U., Ni, T., & Zaccariotto, M. (2021). Overall equilibrium in the coupling of peridynamics and classical continuum mechanics. Computer Methods in Applied Mechanics and Engineering, 381, 113515.

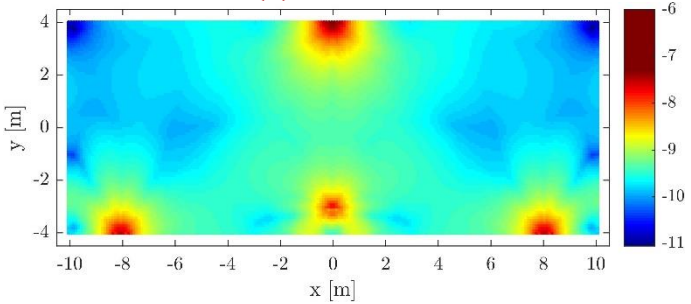
Study of the in-house CCM-PD coupling software

Simulation of crack propagation using the CCM-PD coupled model: three-point bending test



[2]

Distribution of $D^2(u)$ for the three-point bending test

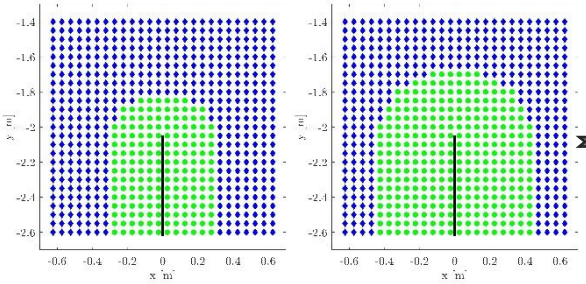


[2]

Distribution of the overall second-order derivatives of the displacement field

$$D^2(u) := \left|\frac{\partial^2 u_1}{\partial x^2}\right| + \left|\frac{\partial^2 u_1}{\partial y^2}\right| + \left|\frac{\partial^2 u_1}{\partial x \partial y}\right| + \left|\frac{\partial^2 u_2}{\partial x^2}\right| + \left|\frac{\partial^2 u_2}{\partial y^2}\right| + \left|\frac{\partial^2 u_2}{\partial x \partial y}\right|$$

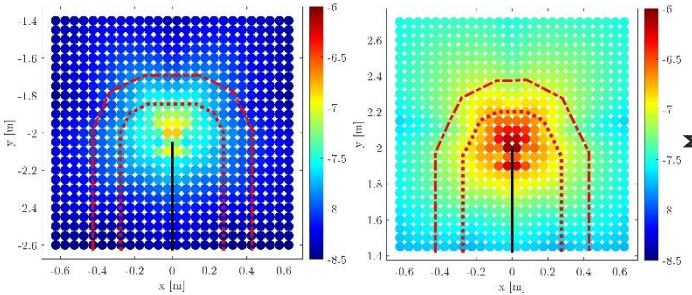
Switching schemes to convert FEM nodes to PD nodes around the crack tip



Switching scheme 1 | Switching scheme 2

[2]

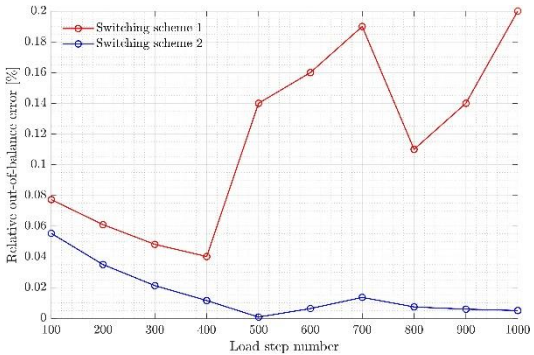
Distribution of $D^2(u)$ around the crack tip for (a) load step= 200 and (b) load step= 1000



(a) (b)

[2]

Out-of-balance error reduction: coupling interface moved away from regions of high gradients of displacements



[2] Ongaro, G., Seleson, P., Galvanetto, U., Ni, T., & Zaccariotto, M. (2021). Overall equilibrium in the coupling of peridynamics and classical continuum mechanics. Computer Methods in Applied Mechanics and Engineering, 381, 113515.

Modelling of high specific stiffness materials properties

Polymer/clay nanocomposites (PCNs)

Polymeric composites reinforced with nanoscale reinforcements exhibit **enhanced mechanical properties**

Clay nanoparticles are the best candidates to **strengthen polymers**, due to their **mechanical** properties, high aspect ratio (AR), high availability and low-cost of production

Three clay morphologies can be distinguished: **aggregated**, **intercalated** and **exfoliated**

Interphase region properties have a **strong influence** on the **overall characteristics** of the nanocomposites

Why peridynamics?

Possibility to incorporate **different materials** and to model **material junctions** without the need of any special treatments

Capability to simulate the **interphase region** between matrix and nanoplatelets, and the nanoclay **agglomeration** by tuning the properties of the PD bonds

The use of PD avoids problems related to the **high aspect ratio** of **nanoplatelets**, which brings FEM meshing issues due to distorted elements

Capability to model **crack nucleation** and **propagation**

Modelling of high specific stiffness materials properties

PD-based Representative Volume Element approach: Different phases of the modelling procedure

1. Characterization of the properties of the constituents

Mechanical and geometrical properties of the constituents are obtained from experimental data reported in literature

Nanofiller aspect ratio, orientation and location are modelled by selecting the most suitable probability distribution functions

2. Selection and numerical modelling of a suitable RVE

The RVE contains enough inclusions for the overall moduli to be independent of the traction and displacement surface values

The statistical properties of the material are computed by constructing many RVEs and by aggregating their results

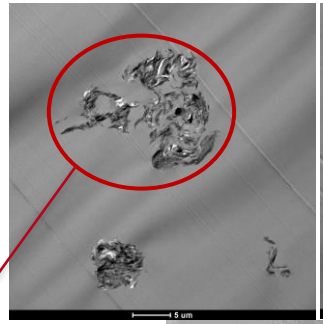
3. Static analysis implementation

4. Computation of the elastic constants to obtain the effective material properties

Modelling of high specific stiffness materials properties

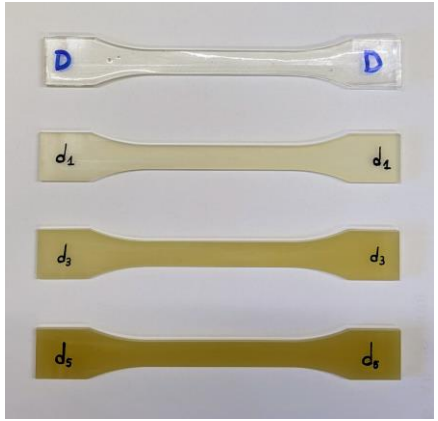
Experimental analysis of epoxy/clay nanocomposites

Transmission Electron Microscopy



Tensile tests on dog-bone specimens (ISO 527-2)

The nanomodification resulted in a slight decrease in the elastic modulus of the resin. The lowest elastic moduli were related to the presence of large agglomerated clay stacks and to the inhomogeneous distribution of nanoclays



Examples of dog-bone specimens with different clay contents

Extension of the study to nanocomposite fracture properties prediction

Mode I fracture tests on compact tension specimens (ASTM D5045-14)

Mode I fracture toughness

$$K_{Ic} = \frac{P_{cr}}{BW^{0.5}} f(x) \longrightarrow \text{measured in } [MPa \cdot m^{0.5}]$$

where:

- P_{cr} is the peak or fracture load measured in [kN]
- B is the specimen thickness measured in [cm]
- W is the specimen ligament measured in [cm]
- $x = a/W$, where a is the crack length measured in [cm]

and:

$$f(x) = \frac{(2+x)(0.886 + 4.64\,x - 13.32\,x^2 + 14.72\,x^3 - 5.6\,x^4)}{(1-x)^{1.5}}$$

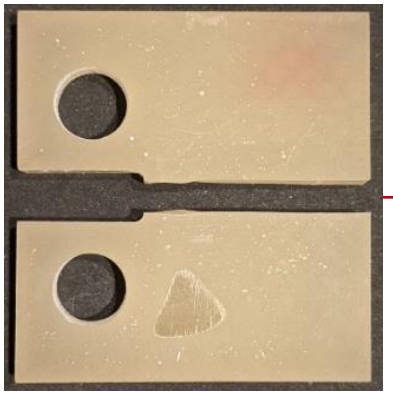
valid for $0.2 < x < 0.8$

Critical energy release rate

$$G_0 = \frac{K_{Ic}^{\ 2}}{E}(1-\nu^2) \longrightarrow \text{measured in } [kJ/m^2]$$

where:

- E is the Young's modulus from tensile tests measured in [GPa]
- v is the Poisson's ratio
- the equation is valid under plane strain conditions



The specimen fractured along the initial crack plane

Crack path of a CT specimen with 5% wt of clay content

Final remarks and possible future developments

Final remarks

- The **out-of-balance forces** are related to the **order** of the **derivatives of displacements** in the **coupling zone**
- The relative **out-of-balance error** is a fraction of a percent and **reduces** as **$\delta \rightarrow 0$**
- It is possible to **reduce** the out-of-balance error by **moving** the coupling **interface away** from regions of **high gradients of displacements**
- The **proper location** and **shape** of the coupling **interface** in a computational problem can be defined by using an **adaptive approach** to convert FEM nodes into PD nodes
- The study confirms that the quality of **nanofiller dispersion** and **distribution** has a **strong influence** on the **interphase properties** and, therefore, on the **tensile performance** of nanocomposites
- The **PD-based method** can model **randomly distributed nanofillers** with different sizes, shapes, and orientations, and can simulate **interphase regions** with different properties and nanofiller **agglomeration phenomena**
- The **properties** of nanocomposites with **various characteristics** can be **accurately reproduced** by the proposed approach

Possible future developments

- **Further extension** of the **out-of-balance analysis** in CCM–PD coupled models to **control** the **relative out-of-balance error** by **optimizing** the **shape** of the **interface** between the PD and CCM portions of the domain
- **Further development** of the **PD-based strategy** to **predict** nanocomposite **fracture toughness** and to **model crack** nucleation and propagation

List of publications

Journal Papers:

Greta Ongaro, Pablo Seleson, Ugo Galvanetto, Tao Ni, and Mirco Zaccariotto. Overall equilibrium in the coupling of peridynamics and classical continuum mechanics. Computer Methods in Applied Mechanics and Engineering, 381:113515, 2021.

Conference Proceedings:

Greta Ongaro, Roberta Bertani, Ugo Galvanetto, and Mirco Zaccariotto. Peridynamic modelling and experimental verification of nanocomposite properties. In: Proceedings of the XXVI AIDAA International Congress of Aeronautics and Astronautics, *In Press*, Persiani Editore, 2021.

Mirco Zaccariotto, **Greta Ongaro**, Tao Ni, Pablo Seleson, and Ugo Galvanetto. Computational methods coupling peridynamics with classical mechanics: out-of-balance forces in overall structural equilibrium. In: Proceedings of the XXV AIDAA International Congress of Aeronautics and Astronautics, Persiani Editore, 2021.

Selected Conference Abstracts:

Greta Ongaro, Roberta Bertani, Ugo Galvanetto, and Mirco Zaccariotto. Peridynamic modelling and experimental characterization of polymer/clay nanocomposites. XVI International Conference on Computational Plasticity. Fundamentals and Applications (COMPLAS 2021), Barcelona, Spain, September 7 - 10, 2021.

Greta Ongaro, Roberta Bertani, Ugo Galvanetto, and Mirco Zaccariotto. Peridynamic modelling and experimental verification of nanocomposites properties. Italian Association of Aeronautics and Astronautics (AIDAA) XXVI International Congress, On-line event hosted by the Tuscany AIDAA Section in Pisa, August 31 - September 3, 2021.

Greta Ongaro, Pablo Seleson, Ugo Galvanetto, Tao Ni, and Mirco Zaccariotto. Overall Equilibrium in the Coupling of Peridynamics and Classical Continuum Mechanics. 16th U.S. National Congress on Computational Mechanics (USNCCM16), Chicago, Illinois, USA, July 25 - 29, 2021.

Mirco Zaccariotto, **Greta Ongaro**, Tao Ni, Pablo Seleson, and Ugo Galvanetto. Out-of-balance forces in computational methods coupling peridynamics with classical mechanics. 14th World Congress on Computational Mechanics (WCCM XIV and ECCOMAS 2020), Virtual Congress, January 11 - 15, 2021.

Greta Ongaro, Ugo Galvanetto, Tao Ni, Pablo Seleson, and Mirco Zaccariotto. Overall Equilibrium in Coupled FEM-PD Models. International Mechanical Engineering Congress & Exposition (IMECE 2019), Salt Lake City, Utah, USA, November 10 - 14, 2019.

Tao Ni, **Greta Ongaro**, Pablo Seleson, Mirco Zaccariotto, and Ugo Galvanetto. Is coupling PD with FEM the way forward to solve in an efficient way crack propagation problems?. In: 2019-Sustainable Industrial Processing Summit, Vol. 7, pp. 83-84, Flogen Star Outreach, Sustainable Industrial Processing Summit & Exhibition, Paphos, Cyprus, October 23 - 27, 2019.

Ugo Galvanetto, Tao Ni, **Greta Ongaro**, Pablo Seleson, and Mirco Zaccariotto. Global Equilibrium in Computational Methods Coupling Peridynamics with Classical Mechanics. 15th U.S. National Congress on Computational Mechanics (USNCCM15), Austin, Texas, USA, July 28 - August 1, 2019.

Ugo Galvanetto, Tao Ni, **Greta Ongaro**, Pablo Seleson, and Mirco Zaccariotto. The Problem of Static Equilibrium in Computational Methods Coupling Classical Mechanics and Peridynamics. The 10th International Conference on Computational Methods (ICCM2019), Singapore, July 9 - 13, 2019.

Mirco Zaccariotto, Tao Ni, **Greta Ongaro**, Pablo Seleson, and Ugo Galvanetto. Overall structural equilibrium in Computational Methods Coupling Peridynamics with Classical Mechanics. VI International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC 2019), Braunschweig, Germany, June 12 - 14, 2019.

Thank you for your attention

Any questions?

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Backup slide: Work methodologies and tools

Peridynamic theory

The **pairwise force function** expresses the vector force of the **interaction** (called **bond**) between the material points $\mathbf{x}$ and $\mathbf{x}'$

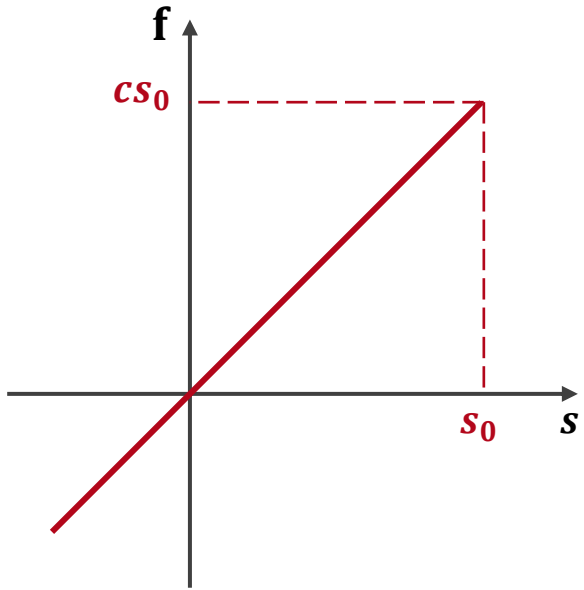
The **Prototype Microelastic Brittle (PMB)** model for a **linear elastic** material is introduced, so that $\mathbf{f}$, for the case of **small deformations**, is determined by:

$$\mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}, t) = \mu(\xi, t)\frac{c\omega(\xi)}{\|\xi\|}\|\mathbf{u}(\mathrm{x}') - \mathbf{u}(\mathrm{x})\|\mathbf{e} = \mu(\xi, t)c(\|\xi\|)s\mathbf{e},$$

where:

- μ is a history dependent damage function that, based on the bond status, takes either the value of 0 (broken bond) or 1 (active bond)
- $c(\|\xi\|)$ is the micromodulus function
- c is the micromodulus constant expressed in terms of material classical constants E (Young's modulus) and ν (Poisson's ratio)
- ω is the influence function that specifies the degree of nonlocal interactions between material points
- s is the relative elongation of a bond defined as $s = (\|\xi + \eta\| - \|\xi\|)/\|\xi\|$
- $\mathbf{e}$ is the unit vector along the direction of the relative position vector in the current configuration

In the **PMB** model, the **failure** of a bond happens when s **exceeds** a predefined value s_0 which is **related to** the material's fracture energy G_0

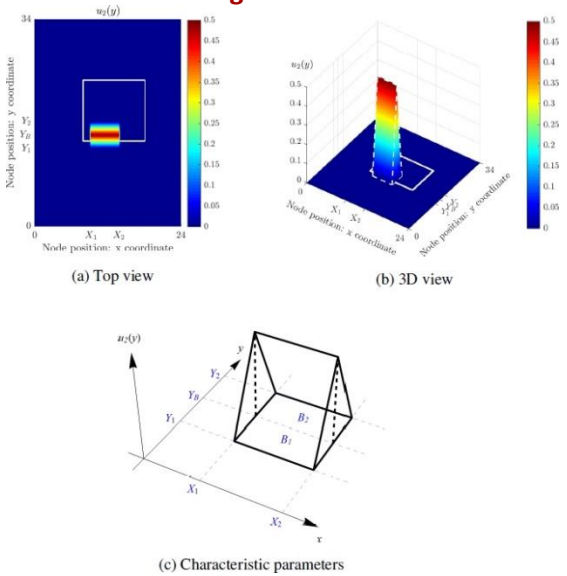


PD bond force versus strain for the PMB model

Backup slide: Study of the in-house CCM-PD coupling software

Out-of-balance forces in CCM-PD coupling

Case I: Bilinear displacement over a straight interface

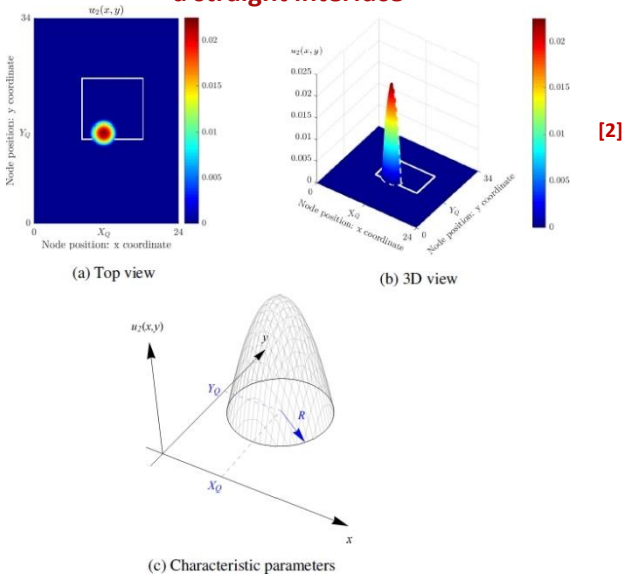


[2]

Coupled model	e_{r_x}	e_{r_y}
Case I	3.28×10^{-16}	5.64×10^{-17}

NO out-of-balance error

Case II: Quadratic displacement over a straight interface

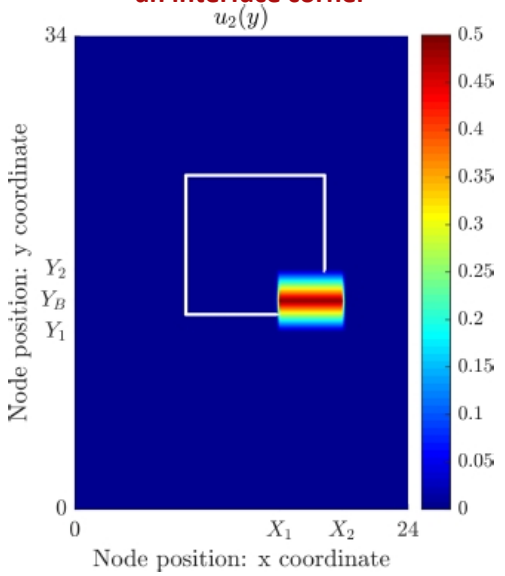


[2]

Coupled model	e_{r_x}	e_{r_y}
Case II	1.40×10^{-16}	5.00×10^{-04}

Out-of-balance error

Case III: Bilinear displacement over an interface corner



[2]

Coupled model	e_{r_x}	e_{r_y}
Case III	4.31×10^{-03}	3.09×10^{-16}

[2] Ongaro, G., Seleson, P., Galvanetto, U., Ni, T., & Zaccariotto, M. (2021). Overall equilibrium in the coupling of peridynamics and classical continuum mechanics. Computer Methods in Applied Mechanics and Engineering, 381, 113515.