Centro di Ateneo di Studi e Attività Spaziali
Università di Padova

Request of admission to the third year of the PhD Course

Simulation of damage propagation in materials and structures by using peridynamics

PhD Course: Scienze, Tecnologie e Misure Spaziali (STMS)

Curriculum: STASA
XXXIV Cycle

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Supervisor: Ugo Galvanetto
Co-Supervisor: Mirco Zaccariotto

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RESEARCH BACKGROUND

Need to develop **lighter** and **more efficient components** for **aircraft structures**

↓

Composite and **nanocomposite materials**

Among them, **polymeric composites** reinforced with **nanoscale reinforcements** have recently attracted a tremendous attention

↓

They exhibit **enhanced mechanical**, **thermal**, and **barrier properties**

BENEFITS

↓

Reduction of **airplane mass** and **fuel consumption**

↓

Downturn in the **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 the in-house **CCM-PD coupling software** for possible integration into a reliable **structural integrity assessment** system

III. Study of **wave propagation** features and numerical **modelling techniques**

IV. Development of **PD** based computational **tools** for **nanocomposites mechanical properties prediction**

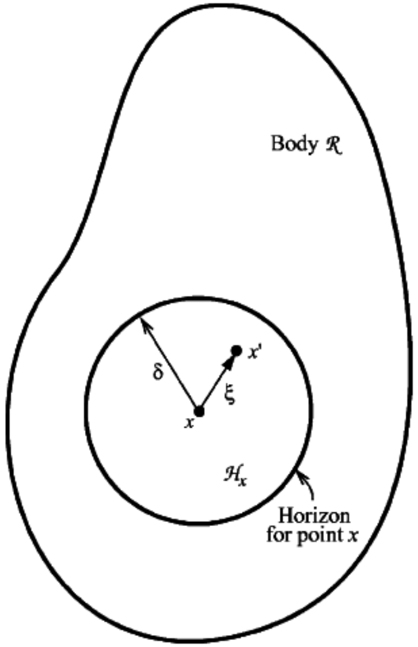
V. **Validation** of numerical simulations through **experimental activities**

CCM = classical continuum mechanics
PD = peridynamics

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 H_x through bonds

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

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

where:

- ρ is the mass density
- **x** is a material point of the domain R
- $\mathbf{H_x}$ 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
- $\underline{\boldsymbol{T}}[\boldsymbol{x},t]\langle\boldsymbol{x}'-\boldsymbol{x}\rangle$ 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:

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

$\xi = \mathbf{x}' - \mathbf{x}$ **is the relative position vector**

$\eta = \mathbf{u}' - \mathbf{u}$ **is the relative displacement vector**

Pairwise force function in BB-PD theory

WORK METHODOLOGIES AND TOOLS (2/3)

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**

↓

Its **application** in **large-scale**, **geometrically complex** simulations is **hindered**

In **nonlocal** theories the **boundaries** are **fuzzy**

↓

Defining **boundary conditions** introduces some **difficulties**

SOLUTION →

Coupling of peridynamics and classical continuum mechanics

It is **common practice** to **couple meshfree discretized PD** models with **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**

  ↓

  All PD nodes have a **fully internal family**

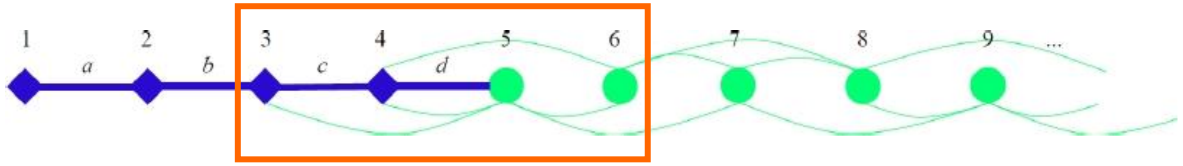
  ↓

  Solution to the "**surface problem**" of PD

WORK METHODOLOGIES AND TOOLS (3/3)

Proposed CCM-PD coupling strategy

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



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:

$$
\begin{bmatrix}
a & -a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \vdots \\
-a & 2a & -a & 0 & 0 & 0 & 0 & 0 & 0 & \vdots \\
0 & -a & 2a & -a & 0 & 0 & 0 & 0 & 0 & \vdots \\
0 & 0 & -a & 2a & -a & 0 & 0 & 0 & 0 & \vdots \\
0 & 0 & -\frac{1}{4}b & -b & \frac{5}{2}b & -b & -\frac{1}{4}b & 0 & 0 & \vdots \\
0 & 0 & 0 & -\frac{1}{4}b & -b & \frac{5}{2}b & -b & -\frac{1}{4}b & 0 & \vdots \\
0 & 0 & 0 & 0 & -\frac{1}{4}b & -b & \frac{5}{2}b & -b & -\frac{1}{4}b & \vdots \\
0 & 0 & 0 & 0 & \cdots & \cdots & \cdots & \ddots & \vdots & \vdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \ddots & \vdots
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ u_N \end{bmatrix}
=
\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ f_N \end{bmatrix}
$$

- $a := EA/\Delta x$, $b := cA^2\Delta x$
- 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
- $\{u_i\}_{i=1,\dots\dots,N}$ = nodal displacements, $\{f_i\}_{i=1,\dots\dots,N}$ = external nodal forces
- c = micromodulus constant

TASKS COMPLETED IN THE SECOND YEAR OF PhD COURSE

- **TASK 1: Bibliographic research on peridynamics and nanocomposites State of Art**
  - **CCM-PD coupling** strategies and coupled Multiphysics problems
  - **Nanocomposites** morphologies, mechanical properties, and main features
  - **Numerical modelling tools** for the prediction of nanocomposites mechanical properties
  - **Experimental techniques** for the characterization of nanocomposites mechanical properties
- **TASK 2: Investigation and improvement of the CCM-PD coupling software developed at the UniPD**
  - **Theoretical** and **numerical** analysis of the **consistency** between linear **BB-PD** and **CCM** models
  - **Theoretical** and **numerical** analysis of the **out-of-balance forces** in coupled **CCM-PD** models
  - Preliminary analysis of the **effect** of the **shape** of the **coupling interface** on the **overall equilibrium**
- **TASK 3: Development of PD based numerical tools for nanocomposites mechanical properties prediction**
  - Preliminary implementation of a **hierarchical multiscale approach** based on a **2D BB-PD** model
- **TASK 4: Development of PD based numerical tools to model crack propagation in nanocomposite materials**
  - Preliminary implementation of a **PD based multiscale approach** to simulate **crack propagation** and **branching**
- **TASK 5: International collaborations**
  - Dr. **Pablo Seleson** (Oak Ridge National Laboratory, US): drafting and publication of a **manuscript**

MODELLING OF HIGH SPECIFIC STIFFNESS MATERIALS PROPERTIES (1/3)

Polymer/clay nanocomposites (PCNs)

Nanocomposites are **multicomponent materials** comprising **different phase domains** in which at least one of the phases has **at least one dimension** on the order of **nanometers**

↓

Polymeric composites reinforced with nanoscale reinforcements have attracted a tremendous attention, since **they exhibit enhanced mechanical properties**

↓

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

↓

By adding **low concentrations** of **clay platelets**, the **polymer matrix** becomes **highly restrained mechanically**

↓

A significant portion of the **applied load** is **carried by** the **fillers**

↓

Significant enhancements of **tensile modulus** and **strength**

MODELLING OF HIGH SPECIFIC STIFFNESS MATERIALS PROPERTIES (2/3)

Numerical modelling of PCNs mechanical properties

Implementation of a **PD hierarchical multiscale approach** for the **prediction** of the **overall mechanical properties** of **PCNs**

↓

The **mechanical analysis** is performed on a mesoscale **Representative Volume Element** (RVE)

↓

The geometrically periodic **RVE** is a sample which is **structurally typical** of the **whole blend on average**

↓

The **random heterogeneity** of the **RVE** domain is modelled by selecting the most **feasible probability distribution function** for **each random characteristic parameter** in the model

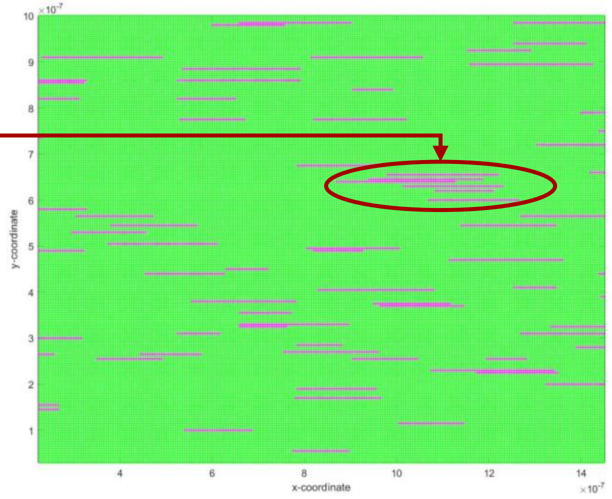
↓

From this **medium-scale analysis**, **the homogenized effective properties** of the nanocomposite are extrapolated

MODELLING OF HIGH SPECIFIC STIFFNESS MATERIALS PROPERTIES (3/3)

Why peridynamics?

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



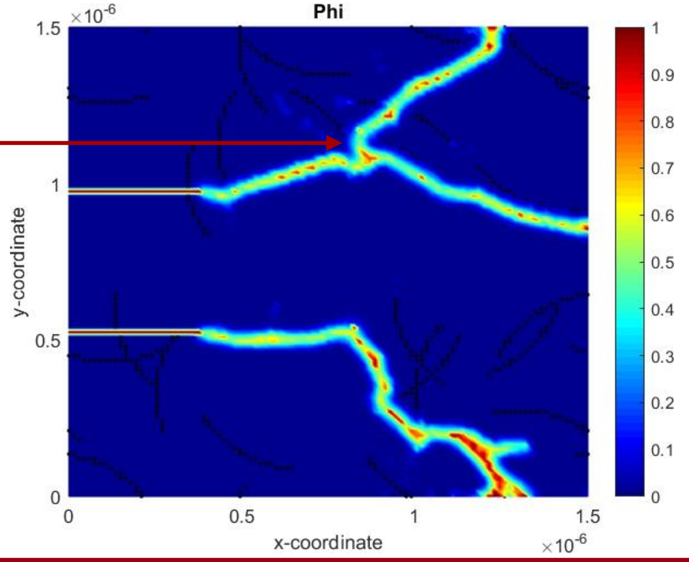
The use of **PD avoids** the **issues** related to the **high aspect ratio** of nanoplatelets, which bring **FEM meshing problems** because of **distorted elements**

↓

Possibility to **simulate high aspect ratio** platelets **values** (i.e., **AR = 1000**)

Possibility to **simulate weak interfacial adhesion** or **interfacial debonding** through **“weakened” PD bonds** or **bonds breakage**

Capability to **model crack propagation** and **branching** phenomena



FUTURE WORK

- **TASK 1: Further development of the PD based numerical method for nanocomposite materials analysis**
  - Extension of the **PD** based **hierarchical multiscale approach** for **mechanical properties prediction**
  - Extension of the **PD** based **multiscale strategy** to model **crack propagation** and **branching**
- **TASK 2: Validation of numerical simulations through experimental activities**
  - **Tensile** and **fracture testing**, use of **Environmental Scanning Electron Microscopy** (**E.S.E.M.**) and of **Transmission Electron Microscopy** (**TEM**)
  - Collaboration with **Prof. R. Bertani**, Department of Industrial Engineering (DII) – University of Padova
- **TASK 3: Study of Multiphysics phenomena and implementation in FEM commercial codes**
  - Simulations on **Multiphysics** problems involving **diffusion phenomena**
- **TASK 4: Implementation of the adaptive refinement/coarsening approach**
  - Implementation of the **adaptive refinement approach** for multi-dimensional analyses
  - Further collaboration with **Dr. P. Seleson**, Oak Ridge National Laboratory, US
- **TASK 5: Writing of PhD thesis**

LIST OF PUBLICATIONS

Journal paper:

G. Ongaro, P. Seleson, U. Galvanetto, T. Ni, M. Zaccariotto, Overall equilibrium in the coupling of peridynamics and classical continuum mechanics, *Accepted for publication* in Computer Methods in Applied Mechanics and Engineering (2021)

Conference contributions:

CFRAC2019 Germany
Overall structural equilibrium in Computational Methods Coupling Peridynamics with Classical Mechanics
M. Zaccariotto, T. Ni, G. Ongaro, P. Seleson, U. Galvanetto

USNCCM15 Austin
Global Equilibrium in Computational Methods Coupling Peridynamics with Classical Mechanics
U. Galvanetto, T. Ni, G. Ongaro, P. Seleson, M. Zaccariotto

ICCM2019 Singapore
The Problem of Static Equilibrium in Computational Methods Coupling Classical Mechanics and Peridynamics
U. Galvanetto, T. Ni, G. Ongaro, P. Seleson, M. Zaccariotto

SIPS2019 Paphos, Cyprus
Is coupling PD with FEM the way forward to solve in an efficient way crack propagation problems?
U. Galvanetto, T. Ni, G. Ongaro, P. Seleson, M. Zaccariotto

IMECE2020 Portland, Oregon
Overall Equilibrium in the Coupling of Peridynamics and Classical Continuum Mechanics
P. Seleson, G. Ongaro, U. Galvanetto, T. Ni, M. Zaccariotto

AIDAA 2019
Computational methods coupling peridynamics with classical mechanics: out-of-balance forces in overall structural equilibrium
M. Zaccariotto, G. Ongaro, T. Ni, P. Seleson, U. Galvanetto

THANK YOU FOR YOUR ATTENTION

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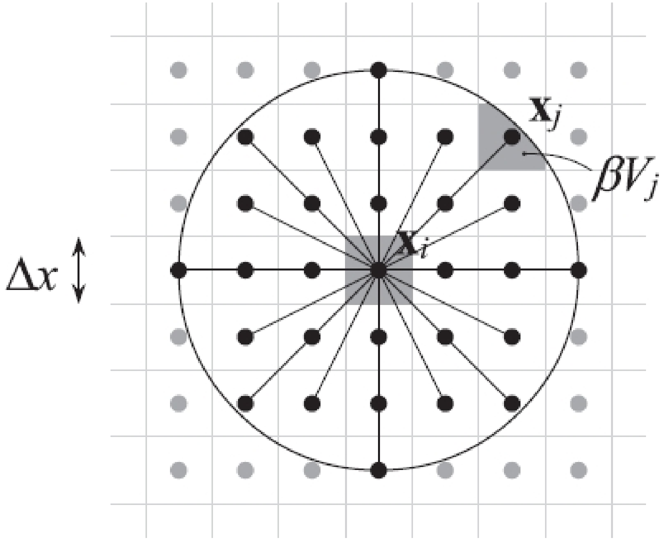
BACKUP SLIDE

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

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

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

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 correction factor used to evaluate the portion of $\boldsymbol{V}_j$ that falls within the neighborhood of the source node $\boldsymbol{x}_i$

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BACKUP SLIDE

Wave propagation in peridynamics

For problems involving **wave propagation**, **peridynamics** can suffer from **anomalous wave dispersion** phenomena

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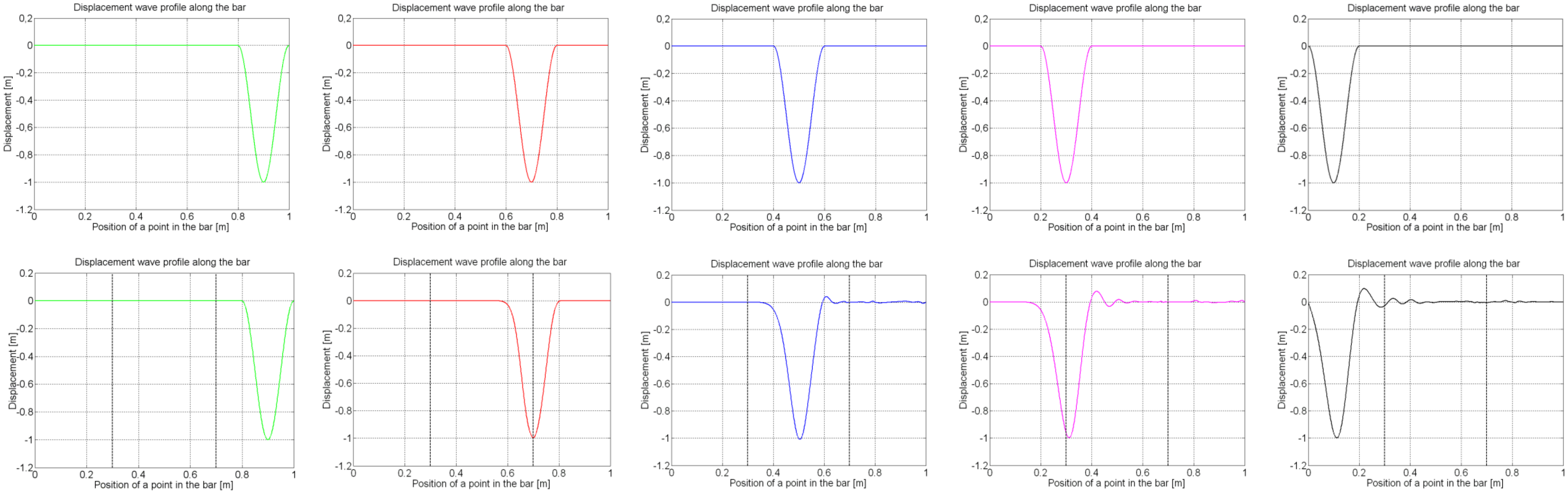
This is the case when the **ratio** between the **horizon** δ and the **wavelength** λ, i.e., δ/λ, is **not small enough**

(a) FEM

(b) PD



t = 0.2 [s] | t = 0.4 [s] | t = 0.6 [s] | t = 0.8 [s] | t = 1.0 [s]

Example of wave propagation and perturbations in a 1D system discretized using (a) FEM and (b) PD. In the example, E=1, ρ=1, A=1, δ=0.031, λ=0.2, and δ/λ = 0.155 in consistent units

Wave propagation in peridynamics

Strategies to **improve** the **dispersion properties** of **PD**

$\delta \ll \lambda$

↓

PD can **accurately** simulate **wave motion** if the ratio δ/λ is **small**

DRAWBACKS

- **Computationally very expensive**
- **Implementation** for large-scale, geometrically complex, **realistic** structures is **difficult**

Modification of the **pairwise force function** (**f**) by introducing **weight coefficients** to **improve** the accuracy of the **dispersion relation**

BENEFITS

No need to satisfy $\delta \ll \lambda$

↓

Possibility to use a **larger** δ

DRAWBACKS

Negative weight coefficients could lead to **numerical instability** when dealing with **crack propagation**

Implementation of **Fourier spectral methods** for peridynamic models

DRAWBACK

Still under development