Math 4997-1

Lecture 8: Introduction to bond-based peridynamics

https://www.cct.lsu.edu/~pdiehl/teaching/2020/4997/

Reminder

Lecture 8

What you should know from last lecture

- Lambda functions
- Asynchronous programming

Classical continuum mechanics

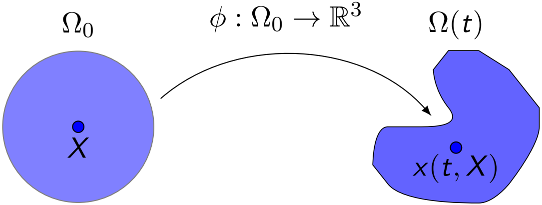


Figure: The continuum in the reference configuration Ω_0 and after the deformation $\phi : \Omega_0 \to \mathbb{R}^3$ with $\det(\text{grad } \phi) > 0$ in the current configuration $\Omega(t)$ at time t.

Prerequisites

- A material point in the continuum is identified with its position $X \in \mathbb{R}^3$ in the so-called reference configuration $\Omega_0 \subset \mathbb{R}^3$.
- The reference configuration Ω_0 is refers to the shape of the continuum at rest with no internal forces.

Prerequisites

- The deformation $\phi : [0, T] \times \mathbb{R}^3 \to \mathbb{R}^3$ of a material point X in the reference configuration Ω_0 to the so-called current configuration $\Omega(t)$ is given by

$$\phi(t, X) := id(X) + u(t, X) = x(t, X)$$

- where $u : [0, T] \times \mathbb{R}^3 \to \mathbb{R}^3$ refers to the displacement

$$u(t, X) := x(t, X) - X \,.$$

- The stretch $s : [0, T] \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ between the material point X and the material point X' after the deformation ϕ in the configuration $\Omega(t)$ is defined by

$$s(t, X, X') := \phi(t, X') - \phi(t, X) \,.$$

Notice

We just covered the prerequisites of classical continuum mechanics which are necessary to introduce the peridyanmic theory. For more details, we refer to

- Liu, I-Shih. Continuum mechanics. Springer Science & Business Media, 2013.
- Gurtin, Morton E. An introduction to continuum mechanics. Vol. 158. Academic press, 1982.

Peridyanmics

What is peridynamics

- A non-local generalization of continuum mechanics
- Has a focus on discontinuous displacement as they arise in fracture mechanics.
- Models crack and fractures on a mesoscopic scale using Newton's second law (force equals mass times acceleration)

$$F = m \cdot a = m \cdot \ddot{X}$$

- Silling, Stewart A. "Reformulation of elasticity theory for discontinuities and long-range forces." Journal of the Mechanics and Physics of Solids 48.1 (2000): 175-209.
- Silling, Stewart A., and Ebrahim Askari. "A meshfree method based on the peridynamic model of solid mechanics." Computers & structures 83.17-18 (2005): 1526-1535.

Principle I

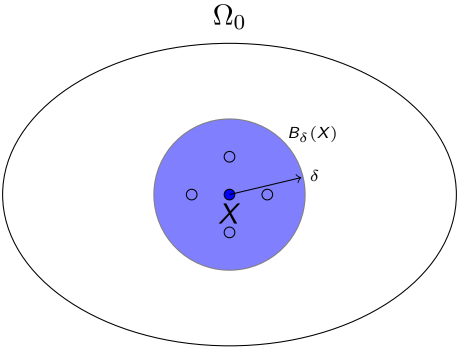


Figure: The continuum in the reference configuration Ω_0 and the interaction zone $B_\delta(X)$ for material point X with the horizon δ.

Principle II

Acceleration $a : [0, T] \times \mathbb{R}^3 \to \mathbb{R}^3$

of a material point at position X at time t is given by

$$\rho(X)a(t, X) := \int\limits_{B_\delta(X)} f\left(t, x(t, X') - x(t, X), X' - X\right) dX' + b(t, X)\,,$$

where $f : [0, T] \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ denotes a pair-wise force function, $\rho(X)$ is the mass density and $b : [0, T] \times \mathbb{R}^3 \to \mathbb{R}^3$ the external force.

Important fundamental assumptions

1. The medium is continuous (equal to a continuous mass density field exists)
2. Internal forces are contact forces (equal to that material points only interact if they are separated by zero distance.
3. Conservation laws of mechanics apply (conservation of mass, linear momentum, and angular momentum).

Conservation of linear momentum

$$f(t, -(x(t, X') - x(t, X)), -(X' - X)) =$$
$$- f(t, x(t, X') - x(t, X), X' - X)$$

Conservation of angular momentum

$$(x(t, X') - x(t, X) + X' - X) \times f\left(t, x(t, X') - x(t, X), X' - X\right) = 0$$

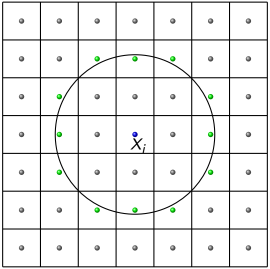
Discretization

EMU nodal discretization (EMU ND)

Assumptions

- All material points X are placed at the nodes $\mathbf{X} := \{X_i \in \mathbb{R}^3 | i = 1, \dots, n\}$ of a regular grid in the reference configuration Ω_0.
- The discrete nodal spacing Δx between X_i and X_j is defined as $\Delta x = \|X_j - X_i\|$.
- The discrete interaction zone $B_\delta(X_i)$ of X_i is given by $B_\delta(X_i) := \{X_j | \, ||X_j - X_i|| \leq \delta\}$.
- For all material points at the nodes $\mathbf{X} := \{X_i \in \mathbb{R}^3 | i = 1, \dots, n\}$ a surrounding volume $\mathbf{V} := \{ \mathbf{V}_i \in \mathbb{R} | i = 1, \dots, n\}$ is assumed.
- These volumes are non overlapping $\mathbf{V}_i \cap \mathbf{V}_j = \emptyset$ and recover the volume of the volume of the reference configuration $\sum_{i=1}^{n} \mathbf{V}_i = \mathbf{V}_{\Omega_0}$.

Discrete equation of motion



$$\rho(X_i)a(t, X_i) = \sum_{X_j \in B_\delta(X_i)} f\left(t, x(t, X_j) - x(t, X_i), X_j - X_i\right) d\mathbf{V}_j + b(t, X_i)$$

Note that we computed the acceleration of a material point $a(t, X)$ and we need to compute the displacement $u(t, X)$ by a

Central difference scheme

$$u(t+1, X) =$$

$$2u(t, X) - u(t-1, X) + \Delta t^2 \left(\sum_{X_j \in B_\delta(X_i)} f(t, X_i, X_j) + b(t, X) \right)$$

to compute the actual displacement $x(t, X) := id(X) + u(t, X)$.

Material models

Prototype Microelastic Brittle (PMB) model

In this model the assumption is made that the pair-wise force f only depends on the relative normalized bond stretch $s : [0, T] \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$

$$s(t, x(t, X') - x(t, X), X' - X) := \frac{||x(t, X') - x(t, X))|| - ||X' - X||}{||X' - X||}.$$

where

- X'-X is the vector between the material points in the reference configuration,
- x(t,X')-x(t,X) is the vector between the material point in the current configuration.

Pair-wise bond force f

$$f(t, x(t, X') - x(t, X), X' - X) := c\, s(t, x(t, X') - x(t, X), X' - X) \frac{x(t, X') - x(t, X)}{\|x(t, X') - x(t, X)\|}$$

with a material dependent stiffness constant c.

More details:

- Silling, Stewart A., and Ebrahim Askari. "A meshfree method based on the peridynamic model of solid mechanics." Computers & structures 83.17-18 (2005): 1526-1535.
- Parks, Michael L., et al. "Implementing peridynamics within a molecular dynamics code." Computer Physics Communications 179.11 (2008): 777-783.

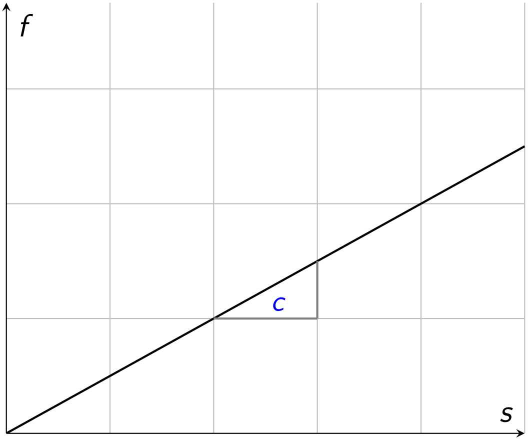


Figure: Sketch of the pair-wise linear valued force function f with the stiffness constant c as slope.

Note that there is no notion of failure/damage in the current material model.

Introducing failure

Introduce a scalar valued history dependent function $\mu : [0, T] \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{N}$ to the computation of the pair-wise force

$$f(t, x(t, X') - x(t, X), X' - X) := \\ cs(t, x(t, X') - x(t, X), X' - X) \\ \mu(t, x(t, X') - x(t, X), X' - X) \frac{x(t, X') - x(t, X)}{\|x(t, X') - x(t, X)\|} .$$

with

$$\mu(t, x(t, X') - x(t, X), X' - X) := \tag{1}$$

$$\begin{cases} 1 & s(t, x(t, X') - x(t, X), X' - X) < s_c \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

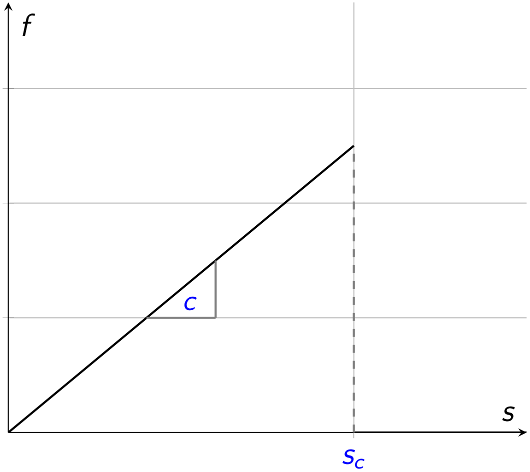


Figure: Sketch of the pair-wise linear valued force function f with the stiffness constant c as slope and the critical bond stretch s_c.

Definition of damage

With the scalar valued history dependent function μ the notion of damage $d(t, X) : [0, T] \times \mathbb{R}^3 \to \mathbb{R}$ can be introduced via

$$d(t,X) := 1 - \frac{\displaystyle\int\limits_{B_\delta(X)} \mu(t, x(t,X') - x(t,X), X' - X) dX'}{\displaystyle\int\limits_{B_\delta(X)} dX'} .$$

To express damage in words, it is the ratio of the active (non-broken) bonds and the amount of bonds in the reference configuration within the neighborhood.

Relation to classical continuum mechanics

Stiffness constant

$$c = \frac{18K}{\pi\delta}$$

Critical bond stretch

$$s_c = \frac{5}{12}\sqrt{\frac{K_{Ic}}{K^2\delta}}$$

With

- K is the bulk modulus
- $K_{I}c$ is the critical stress intensity factor

Notice

We just covered the basics of peridynamics which are necessary to implement peridyanmics for the course project. Fore more details we refer to

- Bobaru, Florin, et al., eds. Handbook of peridynamic modeling. CRC press, 2016.
- Madenci E, Oterkus E. Peridynamic Theory. InPeridynamic Theory and Its Applications 2014 (pp. 19-43). Springer, New York, NY.

Implementation

Algorithm

1. Read the input files
2. Compute the neighborhoods B_δ
3. While $t_n \leq T$
   3.1 Update the boundary conditions
   3.2 Compute the pair-wise forces f
   3.3 Compute the acceleration a
   3.4 Approximate the displacement
   3.5 Compute the new positions
   3.6 Output the simulation data
   3.7 Update the time step $t_n = t_n + 1$
   3.8 Update the time $t = \Delta t * t_n$

Summary

Summary

After this lecture, you should know

- Concept of peridyanmics
- Discretization of peridynamics
- Material models

Note that this lecture is not relevant for the exams, but you should understand the content to implement the course project.

Disclaimer

Some of the material, *e.g.* figures, plots, equations, and sentences, were adapted from P. Diehl, Modeling and Simulation of cracks and fractures with peridynamics in brittle materials, Doktorarbeit, University of Bonn, 2017.