INTRODUCTION TO PERIDIGM - INTEGRATION OF PERIDYNAMIC METHODS INTO AN HPC CAPABLE FRAMEWORK

Dr.-Ing. Christian Willberg

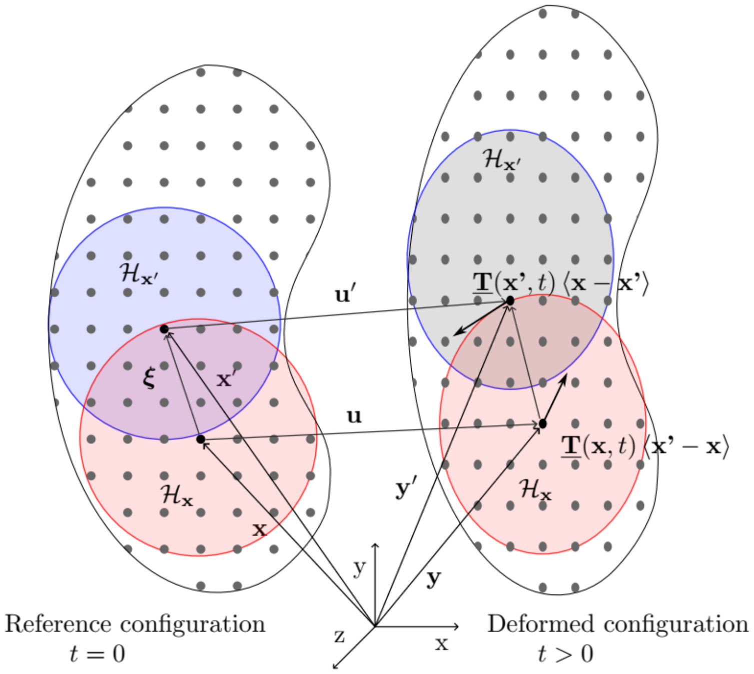
Numerical PD modelling

$$\int_H \left[\underline{\mathbf{T}}(\mathbf{x},t)\langle\mathbf{x}'-\boldsymbol{x}\rangle - \underline{\mathbf{T}}(\mathbf{x}',t)\langle\mathbf{x}-\mathbf{x}'\rangle\right]dV + \mathbf{b} = \rho\ddot{\mathbf{u}}$$

Time integration

Spatial modeling

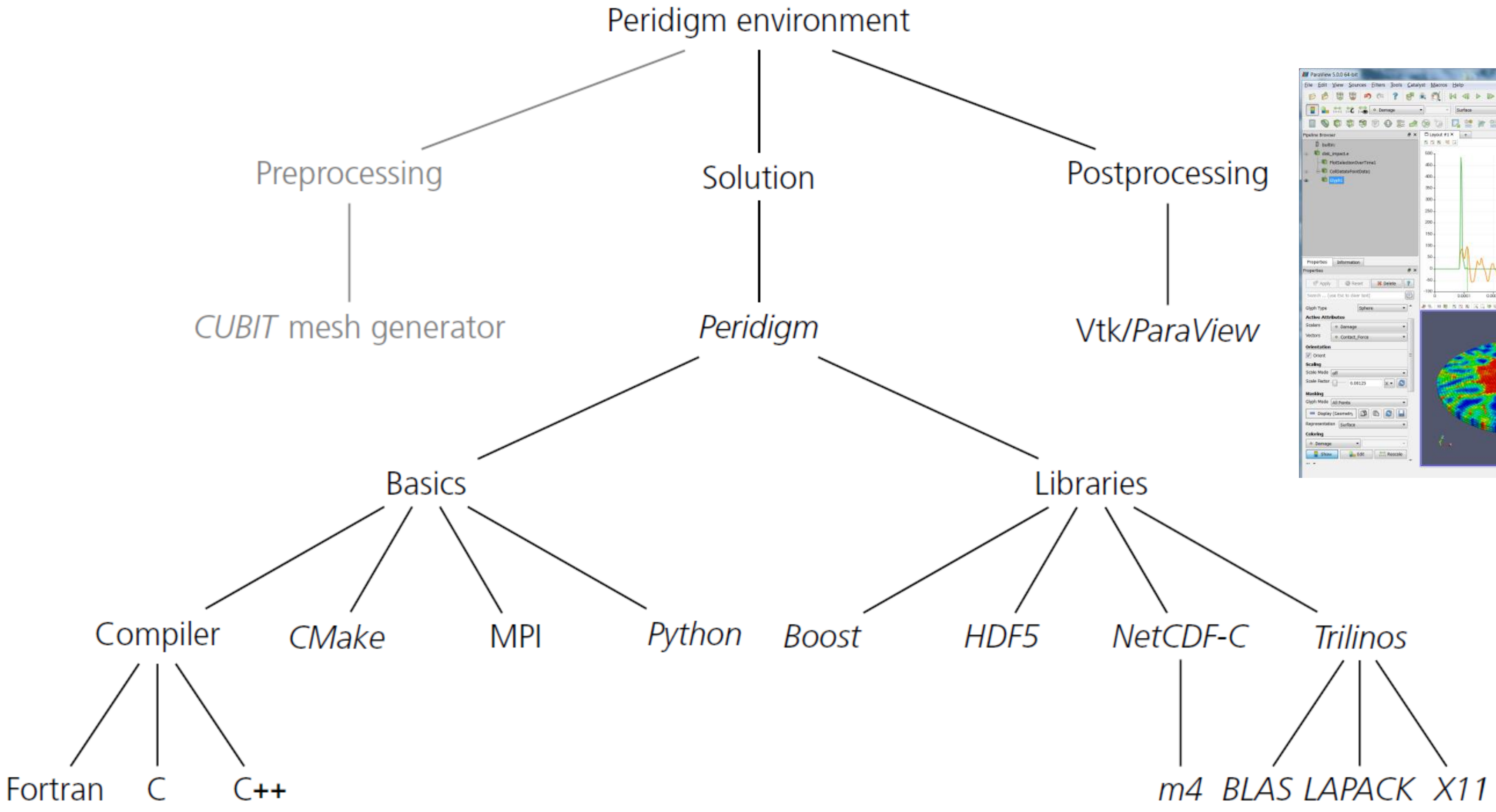
- Non-local mesh free approach
- Fracture is realized by disconnecting interactions
- Simpler discretization, but loss of information (surfaces, edge, etc.)



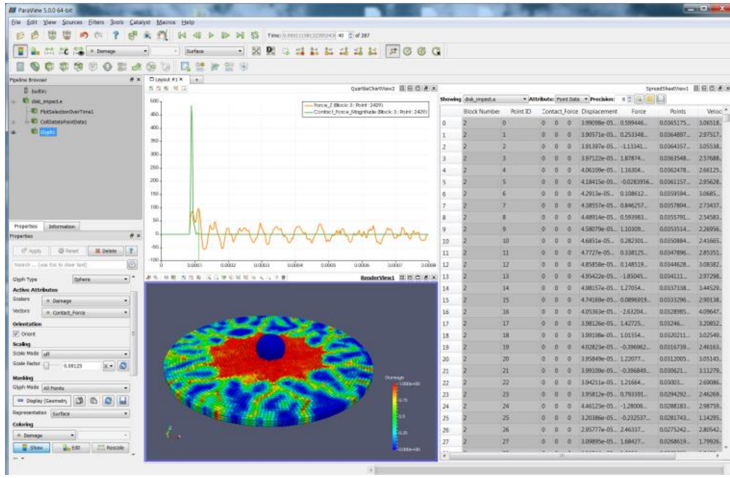
Software

Name	Focus	Language	Maturity level	License
PeriPy	bond-based	Python	medium	MIT
PeriDem	Digital image correlation	C++, Python	low	
PeriPyDIC	2D	Python	low	BSL
PeriPyVFM	Virtual field	Python	low	GPLv3.0
BB_PD	2D, bond-based,	Matlab, C	low-medium	no defined
LAMMPS	Molecular dynamics, bond-based	Python	low	GPLv2
PeriFlakes	2D, coupling FEM	Python, C	low	GPLv3.0
NLMech	2D	C++	medium	
Relation-Based Software	ordinary state-based, bond-based	C++	medium	MIT
EMU	3D, multiphysics, large scale problems	Fortran	high	closed source
Peridigm	3D, multiphysics, large scale problems	C, C++	high	BSD
PeriHub	2D & 3D, Extension of Peridigm	C, C++	high	BSD

Peridigm

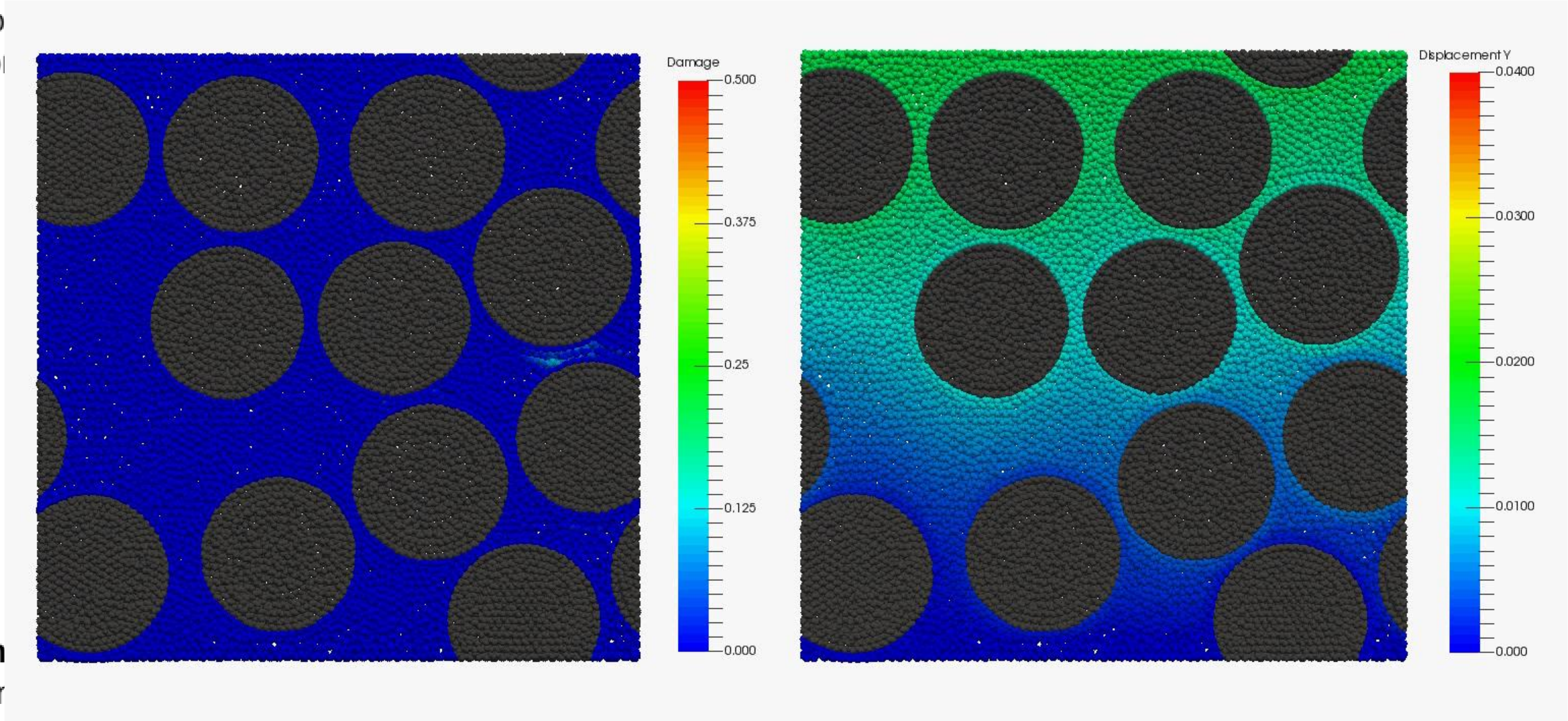


Peridigm environment
Preprocessing
Solution
Postprocessing
CUBIT mesh generator
Peridigm
Vtk/ParaView
Basics
Libraries
Compiler
CMake
MPI
Python
Boost
HDF5
NetCDF-C
Trilinos
Fortran
C
C++
m4
BLAS
LAPACK
X11



How to

initialization;
up
fo



en
syr
timeIntegrationInGlobalVector;

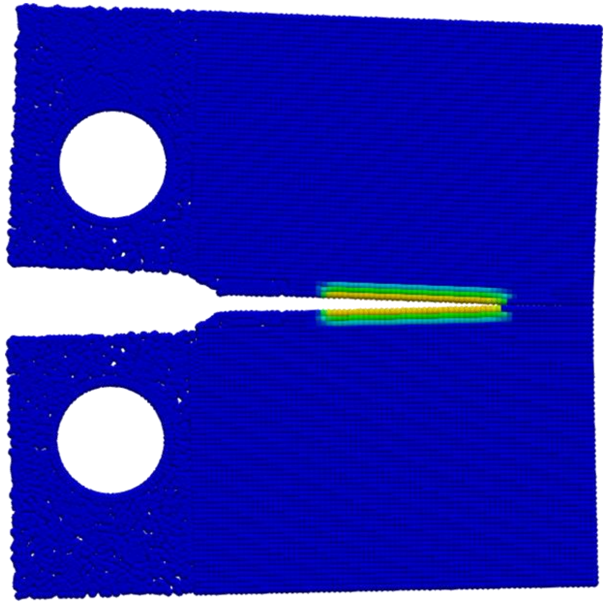
Input

- Exodus FEM standard (binary or ascii) or text based
    - Mesh type influences some options

- Text file input
    - # x y z block_id volume
    - Extensions
        - # x y z block_id volume angle_x angle_y angle_z time
- Yaml or xml
    - Defines blocks, material, solver, etc.

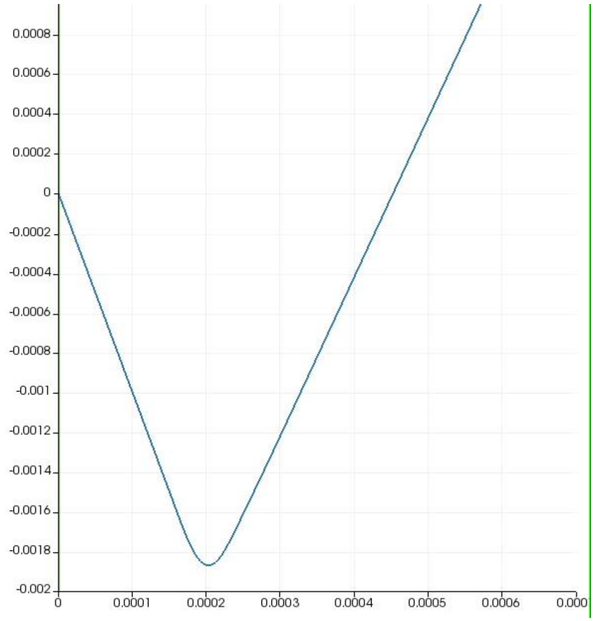
Besides the material

- Bond filter for pre cracks



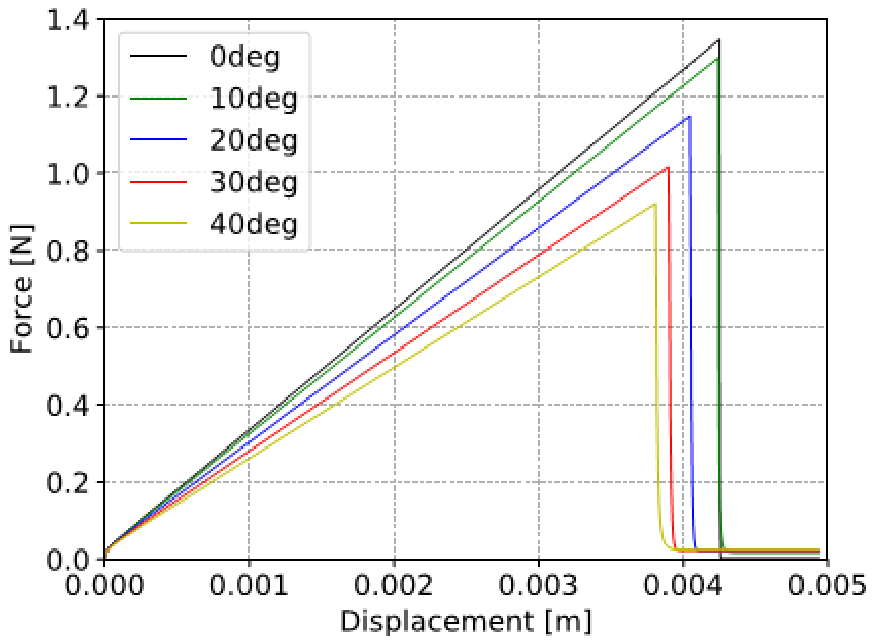
Besides the material

- Bond filter for pre cracks
- Simple contact formulation



Besides the material

- Bond filter for pre cracks
- Simple contact formulation
- Computation class, e.g. create global variables



Besides the material

- Bond filter for pre cracks
- Simple contact formulation
- Computation class, e.g. create global variables
- Equation interpreter, e.g. boundary conditions, variable horizons

Communication

- MPI based

$$\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{pmatrix} = \begin{pmatrix} f_1^{core_1} \\ f_2^{core_1} \\ f_3^{core_1} \\ f_4^{core_1} \\ f_5^{core_1} \\ f_6^{core_1} \end{pmatrix} + \begin{pmatrix} f_1^{core_2} \\ f_2^{core_2} \\ f_3^{core_2} \\ f_4^{core_2} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} f_1^{core_3} \\ f_2^{core_3} \\ 0 \\ 0 \\ f_5^{core_3} \\ f_6^{core_3} \end{pmatrix}$$

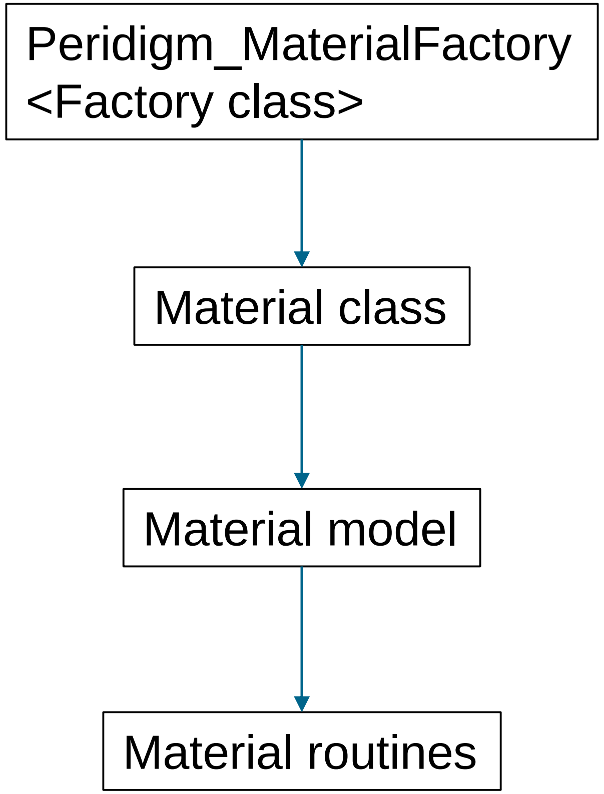
- Not all information is synchronizable
- Field sizes are pre-defined as 1, 3 and 9

Material classes

Class	Numerical effort	Robustness	Convergence	Limitations
Bond-based	1	4	1	Fix Poisson‘s ratio Bad geometrical approximation
Peridynamic solid	2	4	2	Bad geometrical approximation
Correspondence	3	1	3	Zero energy modes
Bond associated correspondence	4	3	4	Numerically demanding

1 - low to 4 - high

How to implement



Correspondence

- Calculated deformation gradient and shape tensor
- Calculate forces and distribute

User correspondence

- Get specific material data

Calculated stresses

- Material law

Peridynamics

Modelling classical continuum mechanics models in Peridynamics

$$\int_H \left[\underline{\mathbf{T}}(\mathbf{x},t)\langle\mathbf{x}'-\boldsymbol{x}\rangle - \underline{\mathbf{T}}(\mathbf{x}',t)\langle\mathbf{x}-\mathbf{x}'\rangle\right]dV + \mathbf{b} = \rho\ddot{\mathbf{u}}$$

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \underline{\omega}\langle\boldsymbol{\xi}\rangle\mathbf{P}\mathbf{K}^{-1}\boldsymbol{\xi}$$

$$\mathbf{P} = \det\mathbf{F}\boldsymbol{\sigma}\mathbf{F}^{-1}$$

$$\mathbf{F} = \left[\int_H \underline{\omega}\langle\boldsymbol{\xi}\rangle\,\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \otimes \underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle dV\right]\mathbf{K}^{-1}$$

$$\mathbf{K} = \int_H \underline{\omega}\langle\boldsymbol{\xi}\rangle\,\underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle \otimes \underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle dV$$

$$\boldsymbol{\sigma} = \mathbf{C}\cdot\cdot\,\boldsymbol{\varepsilon}$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I})$$

$$\boldsymbol{\sigma} = \mathbf{R}\frac{\partial\sigma_{local}}{\partial\varepsilon_{local}}\mathbf{R}^{\boldsymbol{T}}\boldsymbol{\varepsilon}\mathbf{R}\mathbf{R}^{\boldsymbol{T}}$$

Peridynamics

UMAT Fortran Routine

$$\mathrm{d}\boldsymbol{\sigma} = f(\boldsymbol{\varepsilon}_i, d\boldsymbol{\varepsilon}, \boldsymbol{F}_i, \boldsymbol{F}_{i+1}, \boldsymbol{status}, \boldsymbol{prop}, \ldots)$$

$$\boldsymbol{\sigma}_{i+1} = \boldsymbol{\sigma}_i + \mathrm{d}\boldsymbol{\sigma}$$

```
      SUBROUTINE UMAT(STRESS,STATEV,DDSDDE,SSE,SPD,SCD,
     1 RPL,DDSDDT,DRPLDE,DRPLDT,
     2 STRAN,DSTRAN,TIME,DTIME,TEMP,DTEMP,PREDEF,DPRED,CMNAME,
     3 NDI,NSHR,NTENS,NSTATV,PROPS,NPROPS,COORDS,DROT,PNEWDT,
     4 CELENT,DFGRD0,DFGRD1,NOEL,NPT,LAYER,KSPT,JSTEP,KINC)
C
      INCLUDE 'ABA_PARAM.INC'
C
      CHARACTER*80 CMNAME
      DOUBLE PRECISION, DIMENSION(NTENS) :: STRANNP1
      DIMENSION STRESS(NTENS),STATEV(NSTATV),
     1 DDSDDE(NTENS,NTENS),DDSDDT(NTENS),DRPLDE(NTENS),
     2 STRAN(NTENS),DSTRAN(NTENS),TIME(2),PREDEF(1),DPRED(1),
     3 PROPS(NPROPS),COORDS(3),DROT(3,3),DFGRD0(3,3),DFGRD1(3,3),
     4 JSTEP(4)

      ...

      RETURN
      END
```

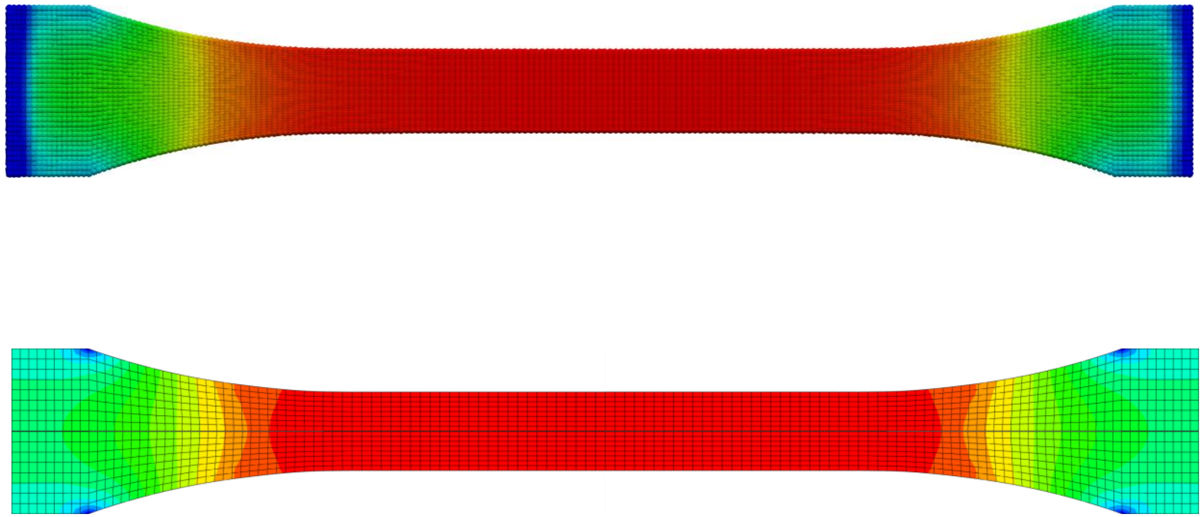
Plasticity

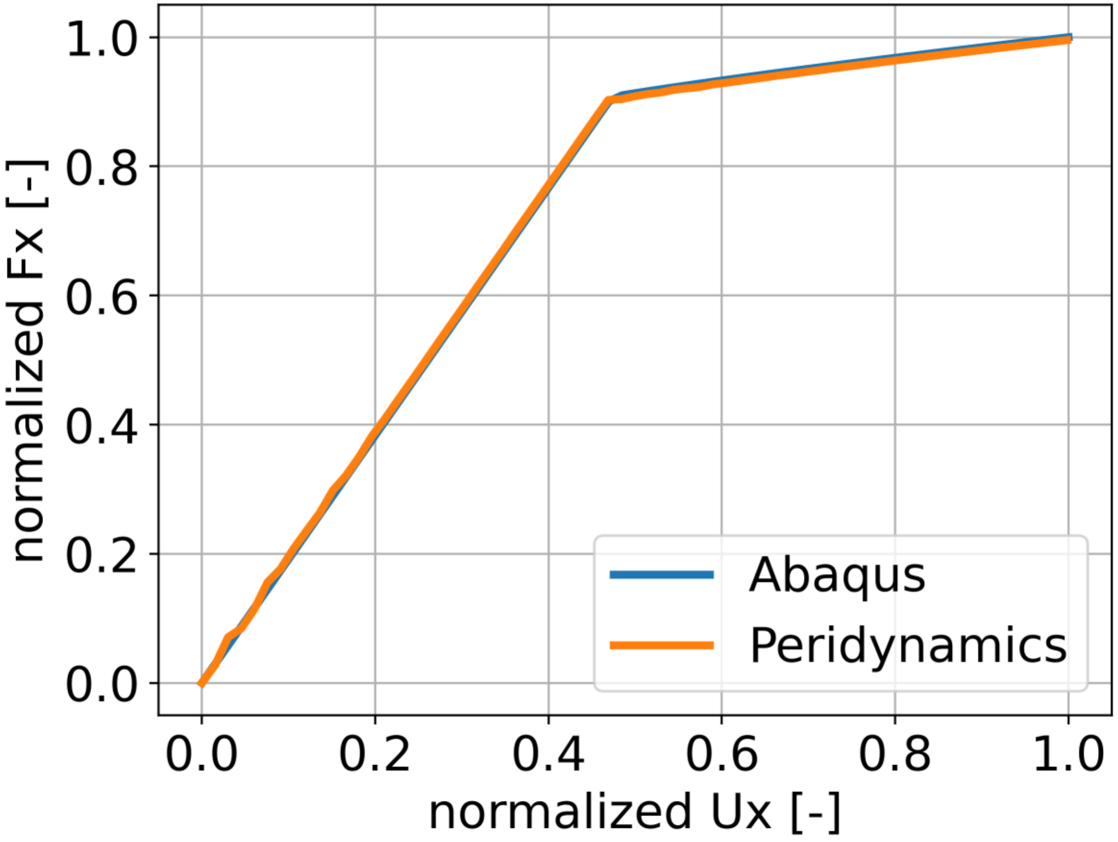
- E (Elastic modulus)
- nu (Poissons ratio)
- Y0 (Initial yield limit)
- Hiso (Isotropic hardening modulus)
- invYiso (Inverse of isotropic saturation stress)
- Hk1 (Kinematic hardening modulus nr. 1)
- invYk1 (Inverse of kinematic saturation stress nr 1)
- Hk2 (Kinematic hardening modulus nr. 2)
- invYk2 (Inverse of kinematic saturation stress nr 2)

https://github.com/KnutAM/MaterialModels

K. A. Meyer, M. Ekh, and J. Ahlström (2018) "Modeling of kinematic hardening at large biaxial deformations in pearlitic rail steel," Int. J. Solids Struct., vol. 130–131, pp. 122–132. https://doi.org/10.1016/j.ijsolstr.2017.10.007

Plasticity - example





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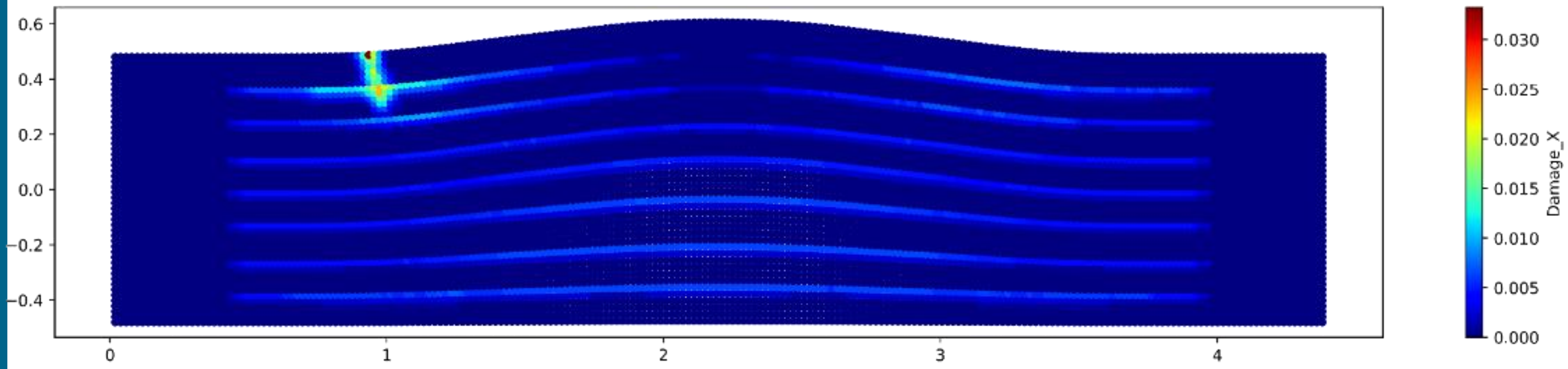
Advantages

- Large scale problems are solveable
- Interface to post processing exists
- Many models are already included
- Moderate test coverage

Disadvantages

- Code repetitions
- New information from mesh file is very hard to distribute
- Dof = 3 hard coded
- Synchronization is not optimal

Thank you


0.6
0.4
0.2
0.0
−0.2
−0.4
0
1
2
3
4
0.030
0.025
0.020
0.015
0.010
0.005
0.000
Damage_X