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RESEARCH ARTICLE

Why develop twice? Integration of continuum mechanical material models in Peridynamics

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Abstract

To harvest the full potential of the peridynamic approach, the state-of-the-art material models should be usable without redeveloping or reimplementing them from classical continuum mechanics theory. User materials (UMAT) in finite element codes allow the researchers or engineers to apply their own material routines. Simple interfaces are specified to allow the utilization of material behaviors in software. In order to use these already existing and often validated models with Peridynamics, a UMAT interface is presented. It allows the simplified use of already existing material routines in the peridynamic framework Peridigm. The interface is based on the finite element (FE) software Abaqus UMAT definition and allows the integration of Fortran routines directly into Peridigm. In addition, the same material model implementations are applicable in finite element applications as well as peridynamic simulations. In the presentation, the interface is presented and various material models are utilized and compared between Peridynamics and FE methods. The effect of the horizon and nonlocal boundaries are analyzed and discussed.

1 | INTRODUCTION

Peridynamics is a theory that addresses the limitations of classical continuum mechanics when dealing with discontinuities, such as cracks, where spatial derivatives of the underlying partial differential equations are not well-defined. To overcome this issue, Peridynamics employs an integral formulation instead of a differential one [1]. This necessitates the rewriting of existing material models. In 2007, Silling et al. developed the correspondence formulation, which introduced a nonlocal integral deformation gradient [2]. This formulation enables the utilization of classical continuum mechanical models within the Peridynamics framework. By employing the nonlocal deformation gradient, it becomes possible to calculate classical strain and stress measures for the entire nonlocal domain. More recently, this approach has been extended even to the bond level [3].

Given Peridynamics' focus on analyzing crack propagation processes, mesh-free methods are commonly employed for numerical solving. One of the advanced frameworks in this domain is Peridigm, developed by Sandia National Labs [4, 5]. This framework facilitates parallelization of large-scale models and includes a post-processing interface to the open-source software ParaView[1]. Over the years, Peridigm has seen various extensions, such as the incorporation

[1] https://www.paraview.org/, access date: 07/03/2022

of energy-based ordinary state-based damage models, anisotropy, and correspondence energy damage models [6, 7]. Additionally, an interface to existing Abaqus user materials (UMAT) has been developed to integrate already-established material routines. UMATs are typically implemented in Fortran and serve as the quasi-standard in this research domain, although alternative formats exist. Therefore, the objective of this publication is to present a direct interface between Peridigm and Abaqus UMAT. This interface aims to reduce the challenges associated with material modeling in Peridynamics and significantly enhance the advantages of the Peridigm framework. The paper provides an overview of the theoretical background, details the interface implementation, and presents two verification examples. It is important to note that despite using the same material models, the results may differ due to the nonlocal nature of Peridynamics. However, as the nonlocality decreases, the results will eventually converge.

2 | APPROACH

In Peridynamics, the conservation of momentum is an integral formulation as is shown in Equation (1) [2].

$$\int_{\mathcal{H}} \left[\underline{\mathbf{T}}(\mathbf{x},t)\langle \mathbf{x}-\mathbf{x}'\rangle - \underline{\mathbf{T}}(\mathbf{x}',t)\langle \mathbf{x}'-\mathbf{x}\rangle dV\right] + \mathbf{b} = \rho\ddot{\mathbf{u}} \tag{1}$$

This equation describes the interactions of one point $\mathbf{x}$ with points $\mathbf{x}'$, called a bond, in a neighborhood $\mathcal{H}$ of volume V. With

$$\boldsymbol{\xi} = \mathbf{x} - \mathbf{x}' \tag{2}$$

the force density $\mathbf{T}(\mathbf{x},t)\langle\boldsymbol{\xi}\rangle$ state can be determined as

$$\mathbf{T}(\mathbf{x},t)\langle\boldsymbol{\xi}\rangle = \underline{\omega}\langle\boldsymbol{\xi}\rangle \mathbf{P}\mathbf{K}^{-1}\boldsymbol{\xi} \tag{3}$$

with the influence function $\underline{\omega}\langle\boldsymbol{\xi}\rangle$. This function is able to scale the behavior of the bond, for example, $\underline{\omega}\langle\boldsymbol{\xi}\rangle = 0$ if the bond is zero. Thereby,

$$\mathbf{P} = \det\mathbf{F}\boldsymbol{\sigma}\mathbf{F} \tag{4}$$

is the the nonlocal first Piola–Kirchhoff stress tensor known from continuum mechanics. It is easy to notice that if utilizing the nonlocal deformation gradient

$$\mathbf{F} = \left[\int_{\mathcal{H}} \underline{\omega}\langle\boldsymbol{\xi}\rangle \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \otimes \underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle dV\right]\mathbf{K}^{-1} \tag{5}$$

with the shape tensor

$$\mathbf{K} = \int_{\mathcal{H}} \underline{\omega}\langle\boldsymbol{\xi}\rangle \underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle \otimes \underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle dV \tag{6}$$

an arbitrary strain measure comparable to the continuum mechanics theory can be defined. The states $\underline{\mathbf{X}}$ and $\underline{\mathbf{Y}}$ are the undeformed reference state and deformed state of one bond. $\underline{\mathbf{X}}$ can be the original configuration and is than equal to Equation (2) or the deformation state of an arbitrary time with $\underline{\mathbf{Y}} = \underline{\mathbf{X}} + \underline{\mathbf{u}}$ and $\underline{\mathbf{u}}$ the displacement state. As an example, the Green–Lagrange strain tensor shown in Equation (7) is utilized.

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left[\mathbf{F}^T\mathbf{F} - \mathbf{I}\right] \tag{7}$$

These strains be used to model continuum mechanical material models and finally to obtain the Cauchy stresses $\boldsymbol{\sigma}$. As example, for the simple linear elastic case and small deformations, Hook's law can be applied utilizing the fourth-order

elasticity tensor $\mathbf{C}$

$$\boldsymbol{\sigma} = \mathbf{C} \cdot \cdot \boldsymbol{\varepsilon}. \tag{8}$$

For a general anisotropic material, the Cauchy stresses depend on several other parameter, for example, the time t, the strain history $\boldsymbol{\varepsilon}$, and so forth.

$$\boldsymbol{\sigma} = f(\boldsymbol{\varepsilon}, d\boldsymbol{\varepsilon}, t, ...) \tag{9}$$

The interface definition is given by Abaqus and shown in Listing 1.

From a software perspective, Peridigm is written in C++, while UMATs are generated in Fortran. However, both languages are generally compatible through the passing of memory addresses. However, the material names cannot be cleanly passed in this form. Therefore, the interface to the external UMAT is structured to work in a Fortran-to-Fortran manner. The C++-to-Fortran interface remains within Peridigm, where the necessary transformations from C++ to Fortran are performed [7]. This approach allows for the full functionality to be provided, and the interface becomes more robust. To use the UMAT, the Fortran file has to be precompiled. This library is then copied in a folder and replaces a placeholder. If multiple materials are used in the Fortran routine they can be selected for example via the material name. In the current implementation, the tangent matrix DDSDDE is not needed, because of the solver architecture of Peridigm.

3 | RESULTS

As a first example, we consider a simple dogbone model made of elastic material and subjected to tension. The model, user material, and all definitions can be found in the provided dataset [8]. The material routine is compiled and utilized in both Peridigm and Abaqus. The resulting displacement distributions for the Peridigm and Abaqus solutions are shown in Figures 1A and 1B, respectively. It should be noted that the u_1 displacement was applied as a boundary condition, which explains the observed displacement patterns.

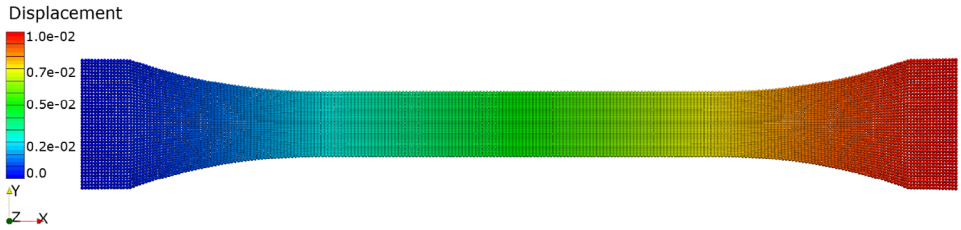
The stress distribution, specifically σ_{11}, is illustrated in Figures 1C and 1D. Some differences can be observed between the two sets of results. These differences arise due to the inherent dissimilarities in the numerical representation between Peridigm and Abaqus. In the peridynamic model, each point represents a volume, making it challenging to apply surface boundary conditions without introducing errors. Furthermore, classical continuum mechanics theory and Peridynamics are distinct formulations, and even when fully converged, they can yield minor differences in results.

To test the interface with a more complex material and to prove the idea of integrating an arbitrary material model in Peridigm, an arbitrary plasticity routine available on GitHub is used. This example serves to highlight the advantages of reduced development effort. The routine includes the Chaboche plasticity model for small strains and incorporates various multiaxial extensions of the Armstrong–Frederick kinematic hardening rule. Specifically, it incorporates the Ohno–Wang model and the multiaxial modification based on Ref. [9]. Both rate-independent and rate-dependent forms of the models are provided, with the latter offering three different overstress functions. The complete material routines were used in Ref. [10].

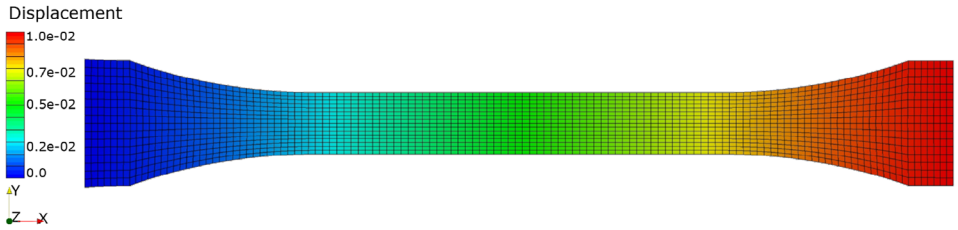
To perform the analysis, nine parameters are required, which are listed in Table 1 and given as an example at Github to test the UMAT function. Additionally, 12 state variables are employed to describe the material behavior and its history.

The dogbone model from the previous example has been utilized and simulated in both Abaqus and Peridigm. The force–displacement outcomes are presented in Figure 2. The displacements in the x direction and the reaction forces in the x direction are normalized to the maximum value of the Abaqus reference solution. The Abaqus model employs a quasi-static iterative Newton–Raphson approach, while the Peridigm model utilizes a Verlet solver. This can be observed in small oscillations within the linear elastic range. It is noticeable that the transition from linear elastic behavior to plastic behavior occurs at the same position for both the normalized displacement and the normalized forces. The slope in the linear elastic and plastic regions is consistent in both results, indicating that the integral behavior of the models is equivalent.

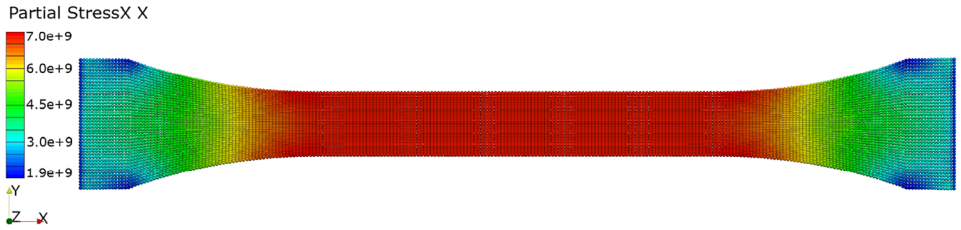
To comparethe local behavior, the Cauchy stresses for the final time step are displayed in Figure 3. The scale for the Peridigm solution in Figure 3A and the Abaqus solution in Figure 3B has been chosen to be equal. The overall stress distribution is similar; however, variations can be observed at different positions along the dogbone. First, the boundary conditions differ because the peridynamic model employs a nonlocal boundary condition. Consequently, a small volume



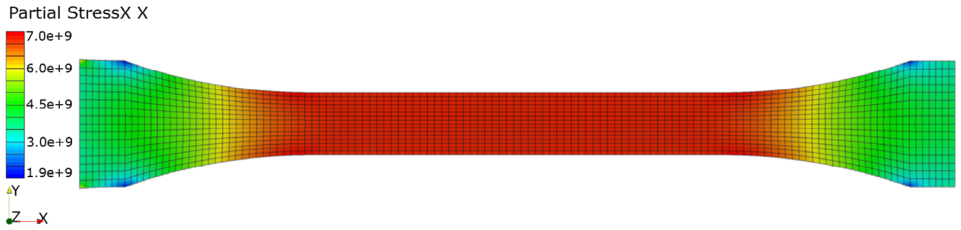
(a) Resulting displacements u_{res} using Peridigm



(b) Resulting displacements u_{res} using Abaqus



(c) Resulting σ_{11} stresses using Peridigm



(d) Resulting σ_{11} stresses using Abaqus

FIGURE 1 Aluminum ($E = 7.24 \times 10^{10}\mathrm{N\,m^{-2}}$, $\nu = 0.33$ and $\rho = 2.7 \times 10^{3}\mathrm{kg\,m^{-3}}$) dogbone loaded under tension ($u_1(x_1 = l) = 0.01$ m).

TABLE 1 Property definition within the material model.

Prop	Parameter	Value	Description
Prop(1)	E [N m^{-2}]	1.6×10^{11}	Young's modulus
Prop(2)	ν [-]	0.3	Poisson's ratio
Prop(3)	Y_0 [N m^{-2}]	4.54×10^{8}	Initial yield limit
Prop(4)	H [N m^{-2}]	3.7×10^{8}	Isotropic hardening modulus
Prop(5)	$1/\kappa_\infty$ [m^2 N^{-1}]	2.720 27×10^{-9}	Inverse of isotropic saturation stress
Prop(6)	$H_{k,1}$ N m^{-2}]	8.921×10^{9}	Kinematic hardening modulus nr. 1
Prop(7)	$1/Y_{k,1}$ [m^2 N^{-1}]	3.311 26×10^{-9}	Inverse of kinematic saturation stress nr. 1
Prop(8)	$H_{k,2}$ N m^{-2}]	1.046×10^{9}	Kinematic hardening modulus nr. 2
Prop(9)	$1/Y_{k,2}$ [m^2 N^{-1}]	3.690 04×$^{-9}$	Inverse of kinematic saturation stress nr. 2

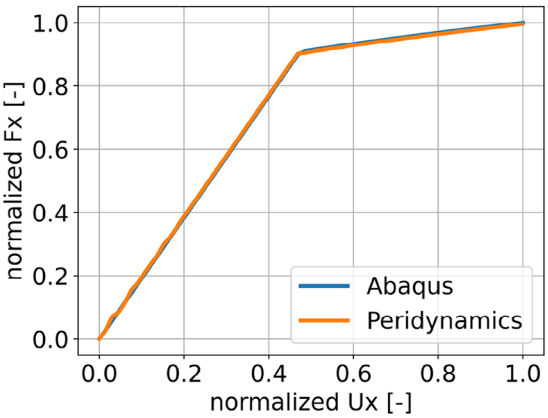
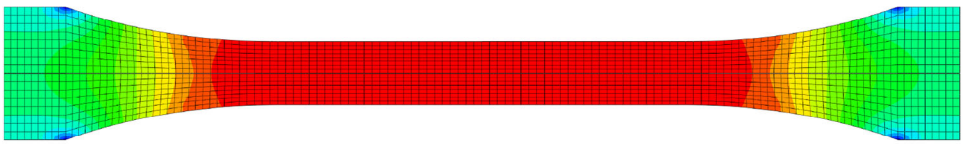


FIGURE 2 Force–displacement plot for the peridynamic and the Abaqus dogbone model.

(a) Cauchy stresses σ_{11} using Peridigm



(b) Cauchy stresses σ_{11} using Abaqus

FIGURE 3 Comparison of the σ_{11} at the end of the simulation utilizing the same scale.

at the left- and right-hand sides exhibits zero stresses since the displacements are equal for the entire block, resulting in no strain inside the block. Second, in regions with localized stress gradients, the nonlocal stress peridynamic formulation requires a higher resolution to accurately describe this behavior. In summary, the User Material (UMAT) integration is well-executed and functions as intended.

4 | CONCLUSION

The paper presents a method to integrate existing User-Defined Material Models (UMATs) into the Peridigm simulation framework. The authors demonstrated this approach through two verification examples, involving linear elastic and elastic plastic materials. Both verification examples address all of the software interface elements and they work as expected. That does mean that the UMAT integration works fine, but says nothing about the interaction of the UMAT with the Peridigm solver, for example, time step determination, and so forth. The physical results obtained from both examples were found to be comparable. However, there were some discrepancies observed in terms of applying boundary conditions and stress distributions.

Since Peridynamics is a nonlocal approach, achieving accurate local stress distributions requires a higher resolution with smaller horizons (δ). Nevertheless, these differences can be addressed by implementing discretization or boundary condition layers to improve the application of boundary conditions.

The primary advantage of this integration method is evident. It eliminates the need to redevelop material models, as validated models can be directly utilized within the Peridynamics framework.

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