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NONLINEAR INTERACTION IN COMPOSITES USING PHYSICS INFORMED NEURAL NETWORKS

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Abstract. Modelling of composites requires the consideration of various components that work together and interact in a linear and nonlinear way. Linear and nonlinear modelling in view of demanding needs, like representative volume element calculations within numerical homogenization and the advent of new tools, like physics informed neural networks, are reviewed in this article. In particular, a concept is proposed towards the implementation of a unilateral contact mechanics law within physics-informed neural networks. The theoretical framework and related applications are presented. Results indicate that the proposed deep learning approach can further be applied towards solving contact mechanics problems, considering the mechanical interactions between the constituents of composites.

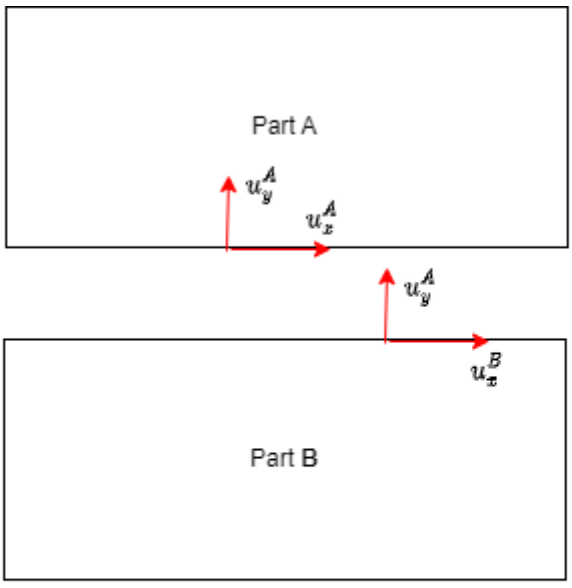
1 INTRODUCTION

Interaction between adjacent constituents within a composite at every scale can be described by nonlinear laws, including unilateral contact and friction that lead to nonsmooth mechanics problems. Numerical evaluation is based on specialized algorithms adopting complementarity formulations, nonsmooth optimization, variational and hemivariational inequalities which have shown their ability to capture highly nonlinear effects [1,2]. Alternatively, if one wants to use classical Newton-type algorithms, appropriate penalty functions can be adopted to enforce inequality and complementarity restrictions [3,4]. Beyond classical numerical approaches, usage of neural networks for calculation of an approximate solution becomes popular, especially within a framework of multi-scale computational homogenization [5-7]. In the latter case the effect of the microstructural response for various loadings, including possible nonlinear

interactions, is transferred to the homogenized medium through the Representative Volume Element (RVE) technique. The solution at the RVE level along the iteration steps may involve some errors, especially if data-driven constitutive laws are adopted [4]. Usage of physics-informed neural networks, combined with complementarity or penalty formulations is proposed here to solve the unilateral contact problem between a two-dimensional structure and a rigid obstacle. This can be considered as a first step towards the numerical solution of the problem of numerical homogenization that includes nonlinear interactions at the RVE level. In this context, PINN training [8,9] can be incorporated at the RVE level in order to provide an approximate solution of the mechanical problem and, subsequently, be integrated within the multi-scale computational homogenization, or FE^2 method. Performance comparisons of various alternatives and discussion for further work in the data-driven framework are included in this article.

2 MODELLING CLASSICAL AND UNILATERAL INTERACTIONS IN COMPOSITES

Different constituent materials must work together within a composite structure. Classical interaction leads to continuity conditions in terms of equalities for displacements and stresses at neighbouring points, see Figure 1. Nonlinear interaction can be modeled with appropriate springs in normal and tangential to the interface directions. Unilateral interaction, including contact and stick-slip friction, can be modelled with a set of inequalities and complementarity conditions, following the techniques of nonsmooth mechanics, see Figure 2.



$$u_x^A = u_x^B \qquad t_x^A = -t_x^B$$

$$u_y^A = u_y^B \qquad t_y^A = -t_y^B$$

Figure 1: Classical interaction between adjacent parts in a composite

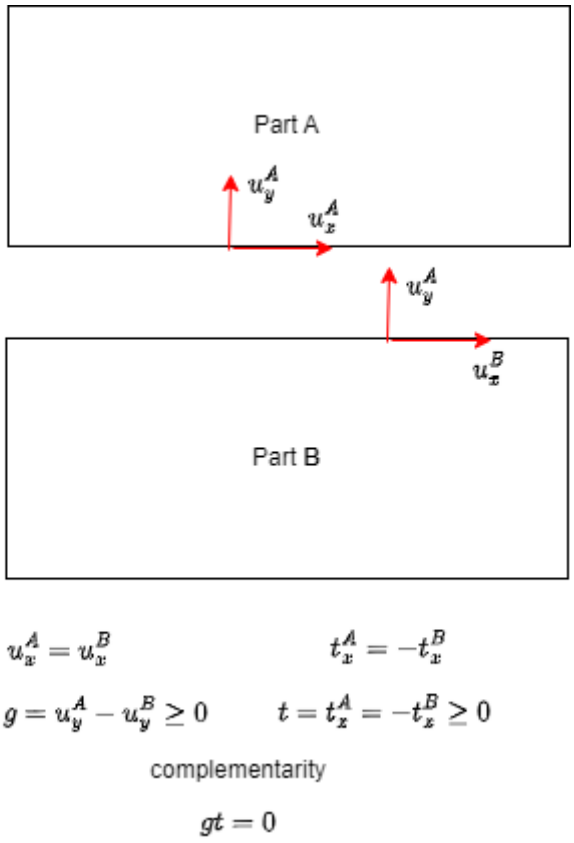


Figure 2: Unilateral interaction between adjacent parts in a composite

Classical solution techniques are described in the literature. Most promising among them are iterative solvers connected with domain decomposition tools that are appropriate for application on parallel computers. In view of data-driven techniques, the Large Time Increment method (LATIN) of macro-iterations should be mentioned.

3 PHYSICS-INFORMED NEURAL NETWORKS

Recently, artificial neural networks have been applied for the solution of partial differential equations. Initial attempts for the solution of elastoplastic and contact problems in mechanics by using the minimization of energy, using Hopfield and Tank neural networks have been proposed by Kortesis and Panagiotopoulos [10] and Avdelas et al. [11]. Feed-forward NNs trained by the backpropagation algorithm, have been used for the approximation of several direct and inverse problems in mechanics based on examples (supervised learning), see among others [12-15].

Based on differentiation of the neural network metamodel, which is available through automatic differentiation within modern packages, an interesting extension of classical data-driven technique rises. Namely, usage of governing differential equations and boundary or interface relations for training of the neural network without the need of having input-output data can be considered. The seminal work, due to Lagaris and his co-workers [16] and recent

developments due to Raisi and Karniadakis led to the method of Physics Informed Neural Networks (PINNs), [17].

The PINNs combine a collocation approach for fitting the governing differential equations and boundary conditions at certain points in the domain and it's boundary and share advantages with more classical collocation and meshless computational mechanics techniques. Previous results of the authors for the solution of beam and rod academic problems [18], and plates in bending including contact [19] demonstrate the usage of this technique.

For complicated problems, including interaction of different domains, PINNs may have convergence difficulties. Ensembles of neural networks or different networks for each domain have been proposed for the effective treatment of such problems. In theory each involved quantity may be approximated by a different neural network and each linear or nonlinear interaction between them can be used for training the resulting PINN. In Figure 3 a schematic Tonti's diagram is presented, showing interaction in a problem of solid mechanics. In Figure 4, a diagram outlining the proposed PINN is provided. In [20] first relevant results in linear plane elastostatics are found and in [21] a recent contribution related to unilateral contact problems is presented.

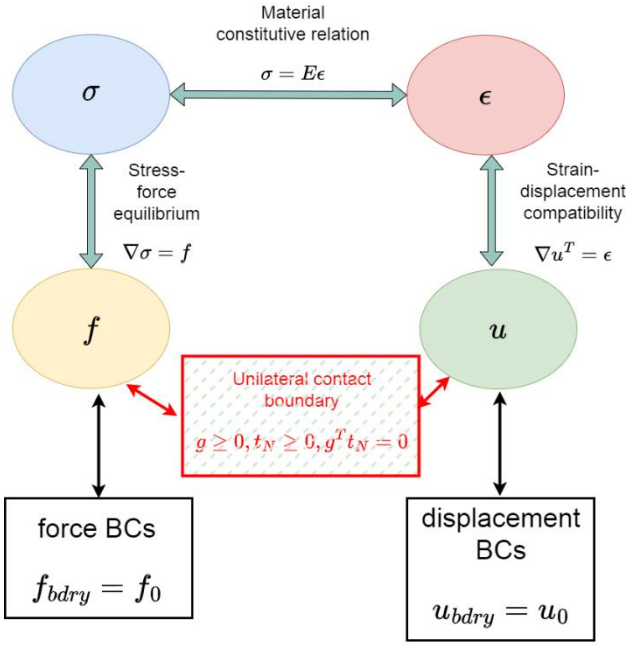


Figure 3: Tonti's diagram indicating all involved quantities and relations. Example of linear elasticity and unilateral contact

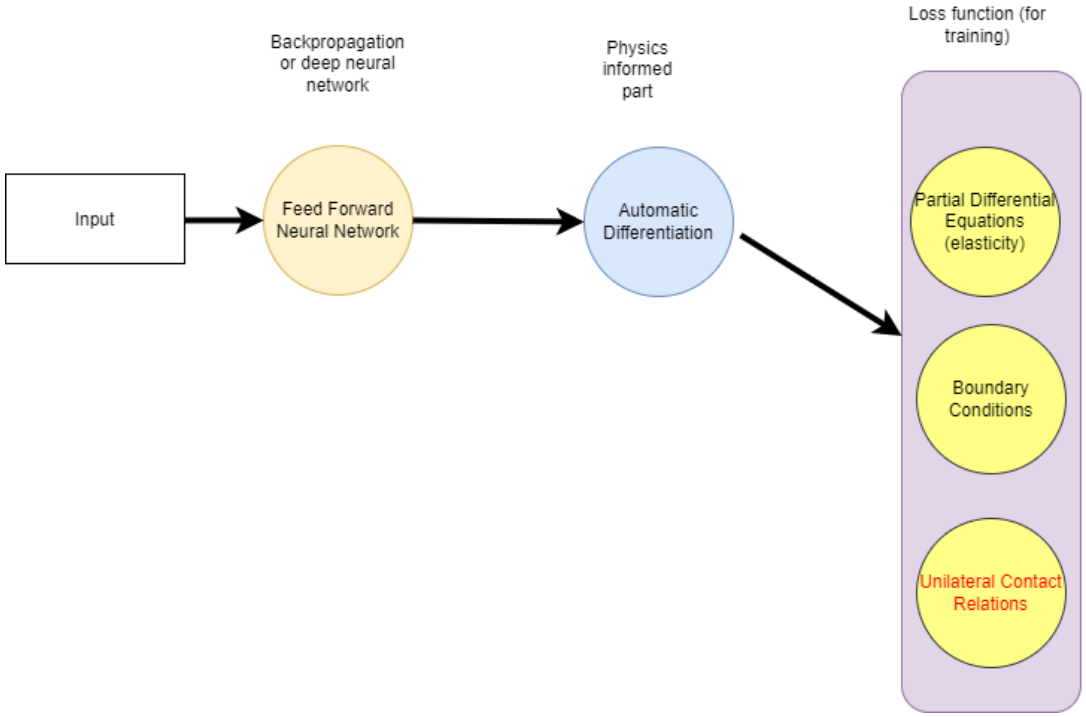


Figure 4: Schematic representation of a PINN approach.

4 PROPOSED APPLICATIONS

The flexibility of PINNs for the solution of complex interaction problems has been outlined. In addition to classical and unilateral contact relations, periodic boundary conditions as required by numerical homogenization schemes are also easily introduced in the loss function of PINNs. On the other hand, complexity of the problem may lead to difficulties in neural network training due to ill-posedness, which manifests itself as a vanishing gradient, appearance of local minima, that lead to premature stop in the iterative process, and similar numerical difficulties.

In this section numerical results of solving the complementarity problem with the Fischer-Burmeister function with the use of PINN for the elasticity equations are presented. The smoothed Fischer–Burmeister function ψ: $R^2 \to R$ proposed in [3], [19], [21] for solving the linear complementarity problems is written as $\psi(a,b) = a + b - \sqrt{a^2 + b^2}$.

It is known that $\psi(a,b) = 0 \iff a \geq 0, b \geq 0, ab = 0$. It is considered a rectangular structure, $0 \leq x \leq l_1, 0 \leq y \leq l_2$, where l_1, l_2 are the lengths of the sides. It is supposed that $l_1 = l_2 = 1$ and the Lamé parameters take the values $\lambda = 1, \mu = 0.5$. For the elasticity equations the following boundary conditions have been taken, $\sigma_{xy}(x, l_2) = 0, \sigma_{yy} = P$, where P is the external loading forces, which is applied on the top of the structure. The forces take the value $P = -0.3$. Furthermore, $u_x(0,y) = u_y(0,y) = 0$, the fixed edge of the considered rectangular domain, $\sigma_{xy}(l_1, y) = 0$, $\sigma_{xx}(l_1, y) = 0$ and $\sigma_{yy}(x,0) = 0$, $\sigma_{xy}(x,0) = 0$.

In our case $a = -u_y - g$, $b = -\sigma_{yy}$ and instead of the condition $\sigma_{yy}(x,0) = 0$ we include the

equation $u_y(x,0) + g + \sigma_{yy}(x,0) + \sqrt{(u_y(x,0)+g)^2 + \sigma_y(x,0)} = 0$ in the loss function. The equation is trained at the corresponding collocation points. The structure under investigated is shown in Figure 5.

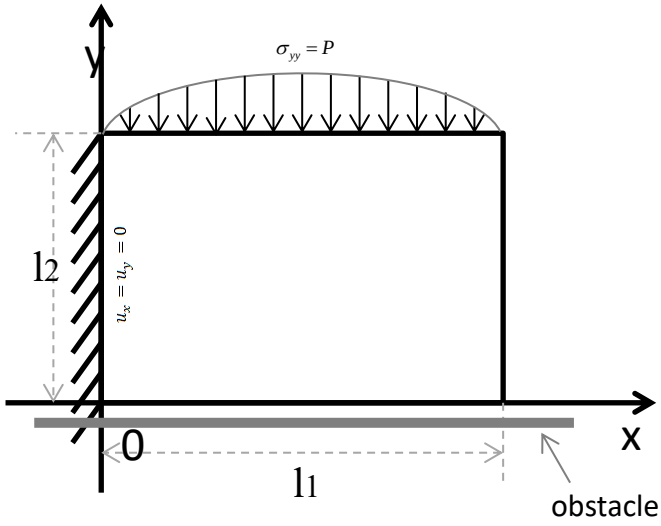


Figure 5: The structure under investigation.

The constructed PINN consists of 4 hidden layers with [15,30,30,15] neurons. For training 40x40 collocation points (samples) and 30x30 test points have been taken. The 26x26 prediction points have been considered. The structure with the rigid obstacle is illustrated on Figure 5. The numerical results are shown on Figures 6-9. The loss error is less than 10^{-4} after 10000 training iterations (epochs) of the multi-PINN.

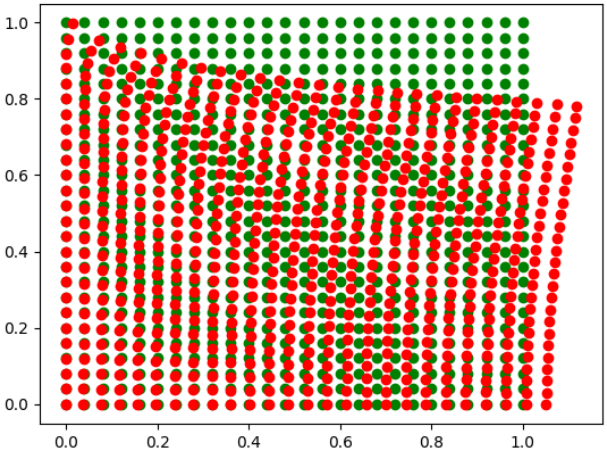


Figure 6: The structure before and after the unilateral contact with g=0.0002 after using the ensemble PINN with epochs=4000.

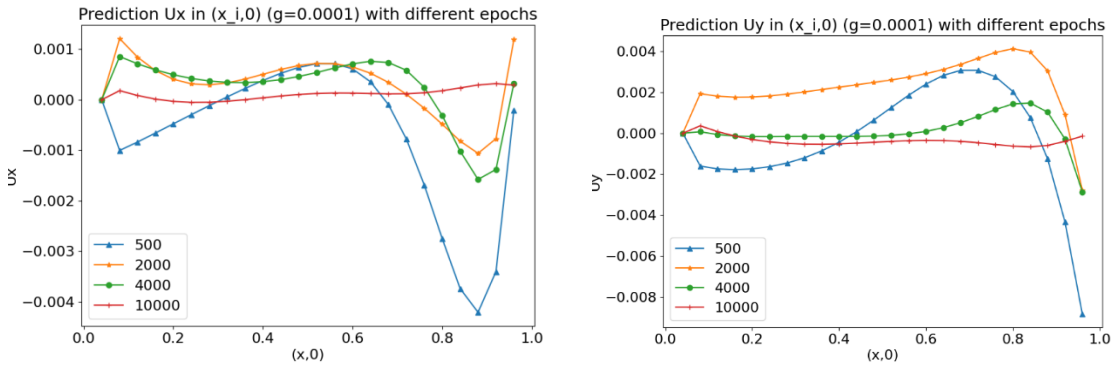


Figure 7: The predictions of u_x, u_y at the points $(x_i, 0)$ with the gap, $g = 0.0001$ between the elastic structure and the obstacle after using the ensemble PINN with different epochs.

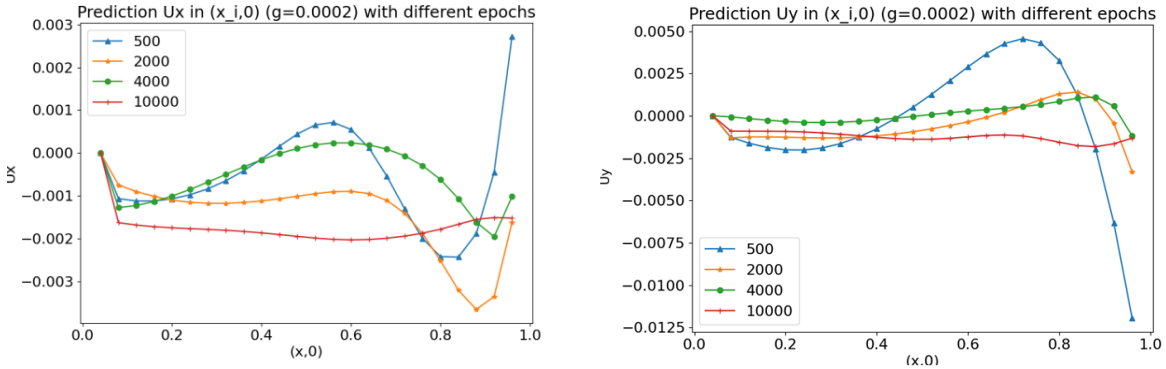


Figure 8: The predictions of u_x, u_y at the points $(x_i, 0)$ with the gap, $g =, 0.0002$ between the elastic structure and the obstacle after using the ensemble PINN with different epochs.

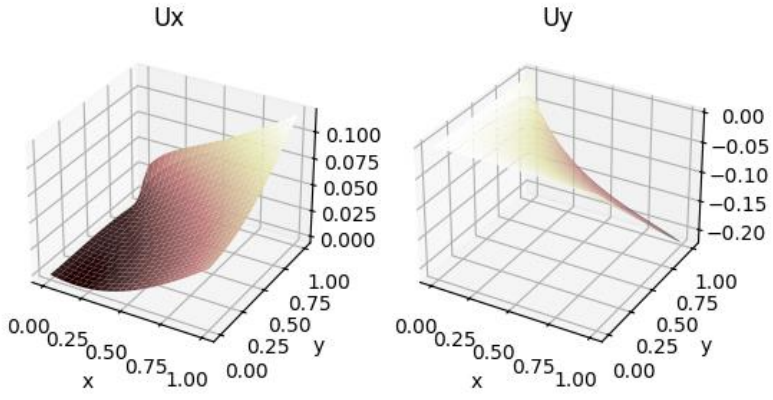


Figure 9. The displacements u_x, u_y of the structure after using the PINN with epochs=4000 and g=0.0002.

4 CONCLUSIONS

A deep learning approach is proposed in this article, aiming to integrate a Physics-informed neural network architecture for an academic plane elasticity problem with unilateral contact conditions. An ensemble approach is adopted to simulate the elastic material properties and the unilateral contact between a two-dimensional structure and a rigid obstacle. Results show a satisfactory performance in terms of the arising error. The work can be extended to simulate the interaction between the constituents of more general heterogeneous materials. This will be the first step towards applications in multi-scale computational homogenization.

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