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Physics-Informed Recurrent Neural Networks for Predicting Elasto-Plastic Behavior in Hierarchical Finite Element Modeling

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ABSTRACT

Nanoporous gold, with its hierarchical structure comprising interconnected networks on multiple length scales, poses significant computational challenges for traditional modeling methods. To solve this challenge, this study introduces a physics-informed recurrent neural network (RNN) to model the homogenized material response of a diamond beam-based representative volume element representing the lower level of hierarchy (LL), which was integrated as a material subroutine within an upper level (UL) finite element simulation. The RNN predicts the tangent stiffness matrix as a primary output from given strain trajectories. Secondary outputs such as stress, plastic strain, and plastic energy increments are derived through embedded physical relationships, ensuring physical consistency across the outputs. The RNN architecture enforces positive energy dissipation inherently through positive eigenvalues of the tangent stiffness matrix and further through penalization of negative energy increments, promoting thermodynamically consistent predictions. A two-level hierarchical approach is employed, where the 2D UL model is subjected to uniaxial strain, while multiaxial strain conditions naturally arise locally within the structure. The inclusion of the LL significantly modifies the strain trajectories observed at the UL, while stress trajectories, although maintaining their general trend, experience considerable changes in magnitude. This approach demonstrates the capability to efficiently simulate hierarchical materials, capturing the influence of LL porosity on the UL material behavior while maintaining physical consistency. Additionally, the model allows for straightforward integration into finite element frameworks like Abaqus, offering a computationally efficient method for studying complex hierarchical materials.

1 | Introduction

Modern material design spans multiple length scales, from the macroscale of parts to the microstructure and atomic configurations that determine their properties and functionality. Hierarchical materials, characterized by structural organization across multiple length scales, are a prominent example in this context. Hierarchical nanoporous metals, especially hierarchical nanoporous gold (hNPG), serve as an exemplary artificial hierarchical material, with self-assembled interconnected porous

networks on multiple scales [1, 2], see Figure 1. The upper level of hierarchy (UL) consists of a bi-continuous nanoporous network with ligaments on the scale of a few hundred nanometers, while the lower level of hierarchy (LL) describes the network within these ligaments, which exhibit ligaments measuring a few nanometers. While structure–property relationships for these materials at the microscale are increasingly well-understood through experimental methods [1, 2], detailed analysis of stress and strain distribution at the nanoscale or under multiaxial loading conditions is challenging and expensive in experiments [3–5].

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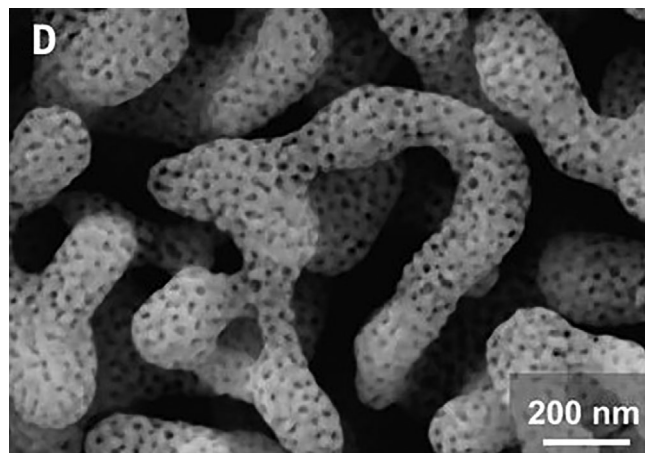


FIGURE 1 | Scanning electron microscopy image of a hierarchical nanoporous gold sample with ligament lengths of 15 and 110 nm for the LL and UL, respectively. Adapted from [1], with permission from American Association for the Advancement of Science.

Finite element (FE) analysis is a tool to effectively simulate the mechanical behavior of complex structures. Huber et al. [6] introduced a randomized diamond FE-beam representative volume element (RVE) to model non-hierarchical nanoporous gold, which shows trends consistent with experiments [7, 8], deepens the understanding of structure–property relationships [7, 9–13] and, thus, material design. However, to model hierarchical nanoporous materials, an efficient method integrating the nanoporous network on both the UL and LL is required. Typically, multiscale approaches manage such computational complexity by separating scales. For instance, macroscale FE models use homogenized RVEs to capture microscale behavior through user-defined material models (UMATs) [14, 15]. The FE^2 method is a common approach that couples simulations on multiple length scales by running RVE simulations at each integration point [16, 17], providing accurate results but at high computational cost.

Machine learning (ML)-based surrogate models can substitute the LL simulations in these approaches by learning material behavior, such as constitutive laws, directly from experimental or simulation data. These models range from purely data-driven techniques to physics-informed approaches that integrate material laws in a weak or strong form [18–21]. Physics informed approaches, such as the physics-informed neural networks introduced in [22], enhance training efficiency by enabling the network to learn relationships with minimal data and ensuring physically meaningful results. Furthermore, hybrid models were suggested, where only specific components of constitutive laws, such as strain energies in elasticity [23–25] or yield surfaces [26–29], plastic potentials [30, 31] and tangent stiffness [32] in plasticity, can be substituted with ML algorithms to enhance efficiency and describe complex material behavior. Although physics-informed and hybrid architectures can mitigate this risk to some extent by embedding physical constraints into the learning process, ML-based constitutive models may still lose accuracy outside the training domain. To address this limitation, a hybrid FE approach was proposed in [33] in which the local nonlinear and iterative elasto-viscoplastic constitutive updates are replaced by a feed-forward neural network to accelerate the

Newton–Raphson procedure, while a residual-based fallback to the classical material update ensures physical consistency whenever the surrogate becomes unreliable. However, this approach requires knowledge of the underlying constitutive laws.

Nanoporous metals exhibit elastic–plastic material behavior, for which path-dependency is essential. In our previous work [27], a comparison between the anisotropic yield surface of the diamond RVE to the Deshpande–Fleck model for isotropic solid foams [34] showed large deviations. While literature provides several descriptions for anisotropic yield surfaces [35–37], they rarely take into account compressible material behavior and require a careful adjustment of parameters. To overcome such limitations, support vector classification and feed forward neural networks (FFNN) were used in [27] to predict the anisotropic yield surfaces of a diamond RVE as a first step toward modeling plasticity in nanoporous materials. For foams, a non-associated flow rule is often necessary, which can be implemented by an additional network [30, 31]. However, scanning yield surfaces requires extensive data, especially for anisotropically evolving surfaces.

Constitutive surrogate models, particularly in the form of physics-informed approaches, can be employed to overcome these limitations. In the literature, approaches for modeling the path-dependent behavior of elasto-plastic materials include, among others, (physics-informed) neural networks and recurrent neural networks (RNN). Although FFNNs do not inherently allow for modeling path-dependency, because each input is processed independently, using input features associated with internal variables that evolve in the material, e.g., plastic strain or variables for hardening, enables FFNNs to capture path-dependent behavior [21, 38]. Extending these approaches with physics-based constraints has been shown to further improve robustness and generalization [20, 21, 39]. For example, a physics-informed elasto-plasticity model was proposed in [21], which incorporates the elastic–plastic strain decomposition, nonlinear incremental elasticity, and the evolution of internal variables directly into the architecture and the loss function. This results in reduced data requirements and improved generalization. A physics-informed neural network for cyclic plasticity was introduced in [39], where internal variables such as plastic strain and the back-stress tensor are predicted by the neural network based on the current internal state and strain increments. The stress response is then obtained through constitutive relationships and included in the loss function. A data-free physics-informed neural network was suggested in [20] to replace the Newton–Raphson return-mapping scheme in FE simulations. By incorporating the known constitutive relationships, such as the formulation of the free-energy function and the yield function, into the loss function, the neural network can find the solution without requiring precomputed stress–strain data.

In contrast to feed-forward neural networks, recurrent neural networks (RNNs) inherently capture path-dependency and are therefore a promising alternative for predicting constitutive relationships. In particular, RNNs with gating mechanisms such as gated recurrent units (GRU) [40] or long short-term memory (LSTM) networks [41] are popular approaches for modeling elasto-plastic material behavior [18, 42–44]. Mozaffar et al. [43] demonstrated that data-driven RNNs can learn constitutive relationships, including stress paths, yield surfaces, and dissipation

energy, directly from stress–strain data. However, similar to physics-informed neural networks, incorporating physical constraints into RNNs can significantly reduce data requirements and improve generalization. For example, Borkowski et al. [44] introduced weak enforcement of physics into a GRU based RNN by penalizing non-zero changes in plastic energy. Danoun et al. [45] proposed a thermodynamically consistent RNN based on LSTM layers that predicts stress increments, internal variables (e.g., plastic strains) and the tangent stiffness as independent outputs. Although, the dissipation energy is constrained in the loss function, the model does not explicitly connect the outputs via physical relationships. In contrast, He et al. [46] developed a strongly physics-informed RNN that predicts the Helmholtz free energy as a function of strain trajectories via internal variables. From this, stresses, entropy, and dissipation rate are derived as partial derivatives of the Helmholtz free energy by automatic differentiation, ensuring thermodynamic consistency. The minimal state cell introduced in [47] and extended in [48] is an alternative to commonly used RNN cells such as GRUs and LSTMs and provides an efficient framework for modeling constitutive relationships for a wide range of materials. This approach significantly reduces the number of parameters by employing a compact set of state variables (memory units in the RNN), offering computational efficiency and better interpretability. A detailed review on data-driven constitutive modeling was published in [19] and a comparative study on different implementations of data-driven and physics-based FFNN and RNN models for the prediction of viscoelasticity and elastoplasticity is provided in [18].

The available studies strongly focus on J2 plasticity with different hardening models. Only a few works [21, 31, 49, 50] consider constitutive modeling of porous or granular materials. However, these either do not take into account hierarchy with complex porous structures and evolving multiaxial trajectories on multiple length scales or do not provide an implementation into the commercial finite element software Abaqus. Therefore, in this work we introduce a physics-informed RNN, which allows a straight forward implementation into Abaqus with stable convergence. The RNN captures the homogenized elastic–plastic material response of a diamond RVE as the LL, considering characteristics of porous material behavior and anisotropic effects.

Similar to [32, 51], the tangent stiffness matrix is predicted by the ML model to describe material behavior. However, in contrast to these works, stresses, plastic strains, and plastic energy are derived as secondary outputs through physical relationships embedded within the architecture, with all output variables trained jointly to ensure physical consistency. Positive energy dissipation is inherently given through predominantly positive eigenvalues of the tangent stiffness matrix and further reinforced by penalization of negative energy increments in the loss function, enabling thermodynamically consistent predictions.

Although motivated by hierarchical nanoporous metals, this work is focused on the introduction of the RNN architecture and employs simplified structures on both hierarchy levels. This choice enables more efficient model development, improves interpretability, and allows for controlled validation before extending it to more realistic structures. At the UL, a simplified 2D model under uniaxial strain is used, leading to bending of the ligaments, which results in a variety of non-linear, multiaxial

trajectories acting on the LL structure. The simplified structure allows for analysis and interpretation of these multiaxial trajectories and how they are affected by the LL material model. The LL, represented by the diamond RVE, captures key characteristics of porosity, including compressibility, anisotropic yield surfaces and a non-associated flow rule. Subsequently, the generalizability is shown by using the RNN trained on an extended data set within a random structure that resembles a slice of a nanoporous gold sample.

The paper is organized as follows: Section 2 describes the implementation of the 2D model representing the UL and the diamond RVE for the LL. Section 3 introduces the RNN architecture and its integration of physical constraints. Section 4 details choice, analysis, and preprocessing of the training data. Section 5 discusses the results, including validation in Abaqus and analysis of the impact of the LL structure on UL trajectories, compared to conventional isotropic hardening models. Finally, the work is concluded in Section 6.

2 | Hierarchical Modeling: Representation of Upper and Lower Level of Hierarchy

With the goal to study hierarchical nanoporous structures, which are complex and computationally demanding, we are aiming for an efficient multiscale modeling approach based on FE simulations and machine learning. Hierarchical relates to a nanoporous structure built of interconnected ligaments measuring a few hundreds of nanometers on the UL, which themselves form a porous network structure on the nanoscale (LL) with ligaments of a few nanometer in diameter, see Figure 1.

For the scope of this article, a simplified 2D FE model is introduced in Section 2.1 as the UL structure. A more random structure is discussed in Section 5.4. To introduce porosity on the LL, a beam model with diamond architecture, as introduced in [6], is employed as an RVE. The modeling approach for replacing the mechanical response on the LL by a RNN as a surrogate model is discussed in Section 2.2.

2.1 | Modeling the Upper Level of Hierarchy

In a first step, on the UL we utilize a 2D FE model as shown in Figure 2. This structure is highly simplified compared to real hNPG samples [1]. This allows for better interpretability of the trajectories and how they're affected by introducing the diamond RVE on the LL than for a realistic 3D structure. It is also more feasible with regard to ML model development and validation. The structure resembles a 4-coordinated node as they commonly occur in nanoporous structures with the central part and the arms representing the node and ligaments of a nanoporous structure, respectively.

The model consists of 2081 2D plane strain elements, including both quadrilateral (CPE4) and trilateral (CPE3) elements. For simplicity, the model has unit length and volume. The simulations are performed using Abaqus. While the simplified upper-level model facilitates interpretability and controlled testing, especially with regard to the Abaqus implementation,

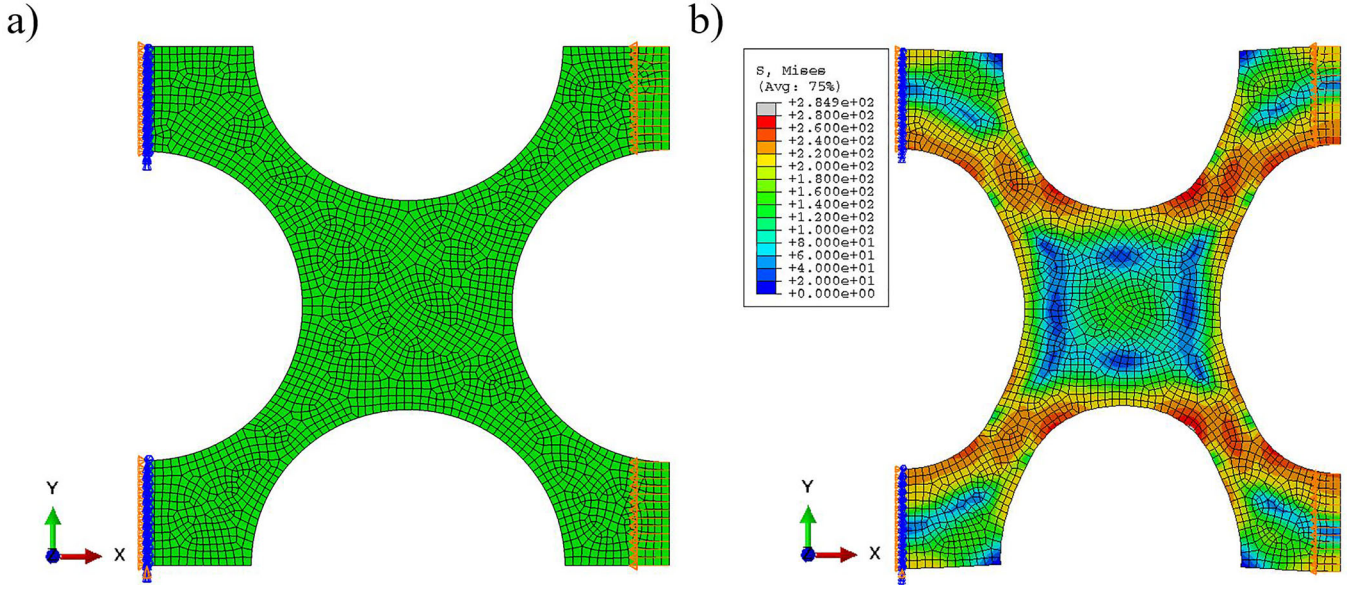


FIGURE 2 | Upper level 2D FE model with CPE4 and CPE3 elements. Shown are a) the undeformed state including applied boundary conditions and b) the local von Mises stresses in the deformed structure after uniaxial compression was applied at the right boundary of the model.

we demonstrate in Section 5.4 that our methodology remains applicable to more complex and realistic structures.

For the initial simulation, the material behavior at the integration points is given by

$$d\vec{\sigma} = \begin{cases} \mathbf{D}^e d\vec{\epsilon} & \text{for } \sigma < \sigma_Y \\ \mathbf{D} d\vec{\epsilon} & \text{else} \end{cases} \quad (1)$$

with the stress increment $d\vec{\sigma}$, total strain increment $d\vec{\epsilon}$, yield stress σ_Y , elastic stiffness matrix $\mathbf{D}^e$ and material tangent stiffness matrix $\mathbf{D}$. Note that stress and strain states as well as the stiffness matrices are given in Voigt notation throughout this work. Thus, stresses are given as

$$\vec{\sigma} = \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \end{pmatrix} \quad (2)$$

for plane strain conditions based on the tensor components σ_{ij} . The same notation is used for the strains with the exception that $\epsilon_4 = 2\epsilon_{12}$.

The isotropic linear elastic behavior is governed by Hooke's Law

$$d\vec{\sigma} = \begin{pmatrix} d\sigma_1 \\ d\sigma_2 \\ d\sigma_3 \\ d\sigma_4 \end{pmatrix} = \mathbf{D}^e d\vec{\epsilon}_{el} = \begin{pmatrix} D_{11}^e & D_{12}^e & D_{12}^e & 0 \\ D_{12}^e & D_{11}^e & D_{12}^e & 0 \\ D_{12}^e & D_{12}^e & D_{11}^e & 0 \\ 0 & 0 & 0 & D_{44}^e \end{pmatrix} \begin{pmatrix} d\epsilon_1^{el} \\ d\epsilon_2^{el} \\ d\epsilon_3^{el} \\ d\epsilon_4^{el} \end{pmatrix} \quad (3)$$

with the elastic stiffness matrix $\mathbf{D}^e$ for plane strain conditions and the elastic strains $\vec{\epsilon}_{el}$. The components of $\mathbf{D}^e$ are determined via

$$D_{11}^e = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \quad D_{12}^e = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad D_{44}^e = G \quad (4)$$

with the elastic properties of gold: Young's modulus $E = 80$ GPa, Poisson ratio $\nu = 0.42$ [27, 52] and isotropic shear modulus $G = \frac{E}{2(1+\nu)} = 28$ GPa.

Plastic deformation begins once the von Mises yield criterion

$$\sigma_m - (\sigma_Y + H\epsilon_m^{pl}) = 0 \quad (5)$$

is fulfilled. Here, the yield stress is assumed with $\sigma_Y = 200$ MPa and the von Mises stress is given by

$$\sigma_m = \sqrt{\frac{1}{2}[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2] + 3\sigma_4^2} \quad (6)$$

for the plane strain state. The equivalent plastic strain ϵ_m^{pl} is calculated in a similar manner. In the plastic region, the material is modeled by von Mises plasticity theory with isotropic linear hardening, with a hardening modulus of $H = 6000$ MPa [27].

In nonlinear FE analysis, the solution for plastic material behavior is obtained incrementally and the relationship between stress and strain increments

$$d\vec{\sigma} = \mathbf{D} d\vec{\epsilon} = (\mathbf{D}^e - \mathbf{D}^{corr}) d\vec{\epsilon}, \quad (7)$$

assumes linearity within sufficiently small increments. The linear transformation matrix $\mathbf{D}$ is the material tangent stiffness matrix, which corrects the elastic stiffness $\mathbf{D}^e$ by $\mathbf{D}^{corr}$ to account for plastic deformations, ensuring that the stress state remains on the yield surface. For von Mises plasticity with linear isotropic hardening, the corrected material tangent stiffness is given by

$$\mathbf{D} = \mathbf{D}^e - \frac{\mathbf{D}^e \vec{m} \vec{m}^T \mathbf{D}^e}{H + \vec{m}^T \mathbf{D}^e \vec{m}}, \quad (8)$$

where $\vec{n} = \partial \sigma_m / \partial \vec{\sigma} = \vec{\sigma}_{dev} / \|\vec{\sigma}_{dev}\| = \vec{m}$ is the normal on the yield surface, which aligns with the deviatoric stress $\vec{\sigma}_{dev}$ and

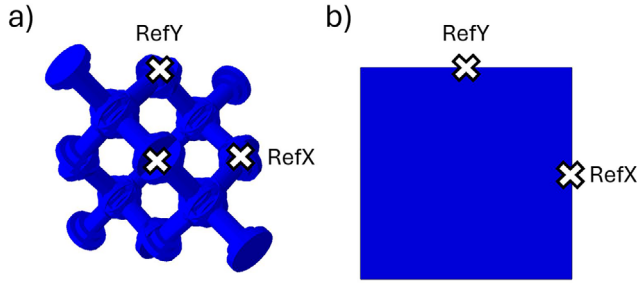


FIGURE 3 | RVEs on the LL: a) 3D diamond beam model representing a porous LL structure and b) CPE4 element for validation of the method. The reference points, used for applying deformations and evaluating the resulting forces, are indicated by crosses.

the direction of plastic strains $\vec{m}$ for von Mises plasticity with an associated flow rule. Note that the used vector notation requires setting $m_4 = 2\sigma_4^{\text{dev}}$. For detailed discussions of von Mises plasticity we refer to standard literature for constitutive model implementation in FE methods [53, 54].

Boundary conditions are applied such that the displacement of the left corner nodes are constrained in x -direction, and the lower-left node is fixed in all directions to prevent rigid body motion, see Figure 2a. For small strain analysis, including the plastic transition, a strain of $\epsilon_1 = -1\%$ is applied as a deformation to the nodes on the right boundary, resulting in uniaxial compression of the UL structure. The resulting stress distribution is shown in Figure 2b. The strain trajectories collected at the integration points serve as input for the ML model and are applied in subsequent RVE simulations to study the LL behavior, as discussed in Section 2.2.

2.2 | Modeling the Lower Level: Representative Volume Elements

In hNPG, the LL represents the nanoscaled ligament network evolving within the UL ligaments. In the context of FE modeling with separated scales, stress and strain trajectories arising from the UL structure act upon the LL. These trajectories are generally multiaxial and non-linear, with contributions from both normal as well as shear stresses and strains, governed by bending of the ligaments [6]. The anisotropy and porosity of the LL, along with its non-associated flow rule and compressibility, makes modeling its material response with established material laws challenging [27, 31]. To address this, strain trajectories obtained from the UL model are applied as deformation inputs to the LL structures, with their response evaluated through displacement-controlled simulations. The resulting data is used to train an RNN, enabling it to predict the material behavior on the LL.

Here, an efficient diamond beam RVE, Figure 3a, is used as a simplified representation of the LL structure. In addition, a single CPE4 element, Figure 3b, is used to validate the approach presented herein. For simplicity, both structures have unit length, area and volume. Periodic boundary conditions are applied to both RVEs according to [13, 55] and displacements are controlled via the indicated reference points.

TABLE 1 | Homogenized elastic material properties, elastic stiffness components (Equation (4)), and plastic material properties for the CPE4 element (gold), as well as the diamond RVE [27]. The beam elements in the diamond RVE and the UL model are modeled using the properties of gold (CPE4).

		CPE4	Diamond
Young's modulus	E [MPa]	80 000.0	3 626.99
Poisson ratio	ν [-]	0.420	0.355
Shear modulus	G [MPa]	28 169.0	2 812.24
Yield stress	σ_Y [MPa]	200	—
Hardening modulus	H [MPa]	6000	—
Elastic stiffness components	$D_{e,11}$ [MPa]	204 225	5 953.45
	$D_{e,12}$ [MPa]	147 887	3 276.71
	$D_{e,44}$ [MPa]	56 338.0	5 624.48

The diamond beam RVE is a 3D structure proposed in [6] as a basis for modeling nanoporous gold and was further developed in [9–11, 13, 52, 56, 57]. For the LL, we utilize cylindrical ligaments by assigning a radius of $r/a \approx 0.1$ to the beam elements, where a is the unit length of the RVE. The beam elements follow the same material model as used for the UL elements, see Table 1 (CPE4). Note that a constant yield stress and hardening modulus are assumed here. For nanoporous metals, experiments suggest that these are a function of the ligament size [58, 59]. For simplification, the size dependency is neglected here, since only a single configuration of the diamond RVE with constant ligament size is considered for validation of the method evaluated herein. For accurate modeling that allows comparison with e.g., experimental data, the size effects should be taken into account. This can be achieved e.g., by assigning size dependent yield stresses locally to the elements using a Hall–Petch type relationship [59]. Further, at these length scales, surface effects influence mechanical properties. To account for such effects in FE modeling, the use of a skin in form of pipe elements, which model the effect of surface energy by imposing a ligament size dependent pre-compressive stress onto the core of the ligament, was introduced in [60].

Compared to a solid model, beam elements do not represent the volume in the nodal areas. This typically leads to a more compliant behavior of the beam models compared to solid models. In addition, beam models can not fully capture the complex plasticity within the nodes and the beams, leading to changes in plastic behavior and yield strength. To circumvent these drawbacks of the more efficient beam model, the node correction introduced in [52] is applied. Therefore, the radii of the elements increase toward the nodes and the yield stress is adjusted within these elements based on the results in [52], ensuring that solid and beam RVEs with otherwise same structure show comparable homogenized mechanical material properties such as Young's modulus and yield stress.

The strain trajectories are applied as displacements at the reference points (RefX, RefY, RefZ), indicated in Figure 3, such that $u_i^{\text{RefX}} = \epsilon_{i1}$, $u_i^{\text{RefY}} = \epsilon_{i2}$ and $u_i^{\text{RefZ}} = \epsilon_{i3}$. Here, ϵ_{ij} denotes the components of the extracted strain tensors. Note that this procedure is

only valid for small deformation and because the RVEs have unit length and volume. For the diamond RVE, displacements of the nodes in the center of the faces are connected to the displacement of the reference points via

$$\vec{u}_{X1} - \vec{u}_{X0} - \vec{u}_{\text{Ref}X} = 0 \quad (9)$$

to satisfy periodic boundary conditions. Here, $\vec{u}$ is the 3-dimensional displacement vector and $X1$ and $X0$ denote the coordinates of the faces that is, faces at $x = 1$ and $x = 0$. The same applies to the points in the Y and Z faces. The corner nodes are constrained such that

$$\vec{u}_{X0Y0Z0} - \vec{u}_{X1Y1Z0} + \vec{u}_{\text{Ref}X} + \vec{u}_{\text{Ref}Y} = 0 \quad (10)$$

$$\vec{u}_{X1Y1Z0} - \vec{u}_{X0Y1Z1} - \vec{u}_{\text{Ref}X} + \vec{u}_{\text{Ref}Z} = 0 \quad (11)$$

$$\vec{u}_{X0Y1Z1} - \vec{u}_{X1Y0Z1} + \vec{u}_{\text{Ref}X} - \vec{u}_{\text{Ref}Y} = 0. \quad (12)$$

This differs from the classic definition of periodic boundary conditions at the corners of cubes, because nodes are only available at every second corner. Furthermore, for plane strain conditions, we set

$$u_1^{\text{Ref}Z} = u_2^{\text{Ref}Z} = u_3^{\text{Ref}Z} = u_3^{\text{Ref}X} = u_3^{\text{Ref}Y} = 0.$$

The homogenized material response is subsequently calculated in a post-processing step using the displacements and reaction forces at the reference points. The deformation gradient is defined by these deformations and is used to calculate the logarithmic strains and, via the reaction forces, the Cauchy stresses.

The homogenized elastic–plastic material behavior of this diamond beam RVE was studied in [27] for linear load paths and multiaxial loading conditions. Orthotropic elasticity followed by a plastic regime with an anisotropic yield surface is required to describe the behavior of this RVE. The homogenized elastic properties from [27] and the stiffness components resulting from Equation (4) are given in Table 1. The plastic behavior of the diamond RVE is complex, due to an anisotropic yield surface in combination with a non-associated flow rule and compressibility [27, 31]. This motivates an alternative formulation of material laws, which allows for higher flexibility.

Here, we propose a RNN to determine the material response by predicting the correction of the material tangent stiffness $\mathbf{D}^{\text{corr}}$ in Equation (7) from given strain trajectories, such that

$$d\vec{\sigma} = \mathbf{D}d\vec{\epsilon} = (\mathbf{D}^e - \mathbf{D}^{\text{RNN}})d\vec{\epsilon} \quad (13)$$

with $\mathbf{D}^{\text{RNN}}$ the prediction of the RNN. Section 3 gives an overview of the architecture and the training procedure of the RNN.

For validation of the method, a 2D CPE4 element with identical material properties to those defined in the elements of the UL model is used. Periodic boundary conditions, connecting displacements of reference and the 4 corner nodes, are applied via

$$\mathbf{u}_{X0Y0} - \mathbf{u}_{X1Y1} + \mathbf{u}_{\text{Ref}X} + \mathbf{u}_{\text{Ref}Y} = 0 \quad (14)$$

$$\mathbf{u}_{X0Y1} - \mathbf{u}_{X1Y0} + \mathbf{u}_{\text{Ref}X} - \mathbf{u}_{\text{Ref}Y} = 0 \quad (15)$$

using the classic definition of periodic boundary conditions [55]. We would like to note that the 2D CPE4 element is used for higher efficiency but gives the same results as a 3D C3D8 element with the same boundary conditions as prescribed on the diamond RVE.

The UL model, governed by von Mises plasticity within the elements, is used as a reference due to its known material response. This allows for a direct comparison between the UL simulation and the results obtained using the proposed method, in which a RNN is trained and implemented into a UMAT. For the RNN trained with data from the CPE4 element, the predicted response is expected to match the UL simulation, Section 2.1, and, thus, allows for validating the RNN's ability to replicate material behavior accurately. Similar to the diamond RVE, data for the CPE4 element is gathered by applying the strain trajectories from the UL model via the reference points. However, for the CPE4 element, the resulting local strains and stresses are extracted at the integration points of the CPE4 element.

3 | Recurrent Neural Network Architecture

The material behavior and properties, such as the yield stress after plastic deformation, are highly dependent on the nanoporous material's load history [27]. To capture such dependencies on the LL, we propose an architecture based on a RNN as the core element, denoted as recurrent layer in Figure 4, due to its efficiency to learn from time-series data, such as stress and strain trajectories by using the same trained weight matrices for each time step and providing information from previous time steps that is forwarded to the next time step. The herein proposed architecture incorporates two key aspects: 1) using inputs and outputs required for the description of plasticity in Abaqus Standard that is, strain increments as input and tangent stiffness components, stress, plastic energy, and plastic strain increments as outputs, and 2) connection of these variables through physical relationships involving multiplication rather than automatic differentiation. Existing architectures often use automatic differentiation of outputs such as energy potentials with respect to the strains given as input to derive stresses, ensuring physical consistency [24, 46]. Similarly, the tangent stiffness components can be determined by automatic differentiation of stresses with respect to strains [61]. Thereby, automatic differentiation is used as a tool to compute the derivatives of a function, such as the outputs of a neural network with respect to its inputs or previous layers. It achieves this by breaking down the operations leading to the output into smaller steps (computational graph) and applying piecewise differentiation using the chain rule, similar to backpropagation during training. While this allows implementing physical relationships within existing python machine learning frameworks, where the algorithm is included and can be easily applied, integrating these differentials for RNNs into Fortran based FE code such as Abaqus is both tedious and error-prone. Therefore, we are focusing on a straight forward implementation using multiplicative relationships and the tangent stiffness as the primary output to allow a straight forward implementation of the trained RNN into Abaqus.

To overcome limitations in learning long-term dependencies in standard RNNs, gated recurrent units (GRUs) [40, 62], as implemented in Keras [63], are used in this work. Each GRU includes

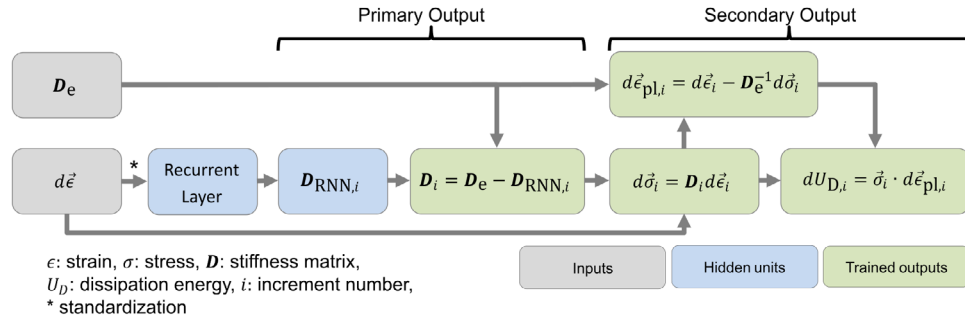


FIGURE 4 | RNN architecture including physical relationships between multiple output variables to predict the material response of the LL RVE. Sequences of strain increments and the elastic stiffness matrix serve as input to predict the material tangent stiffness components as a primary output. Stress, plastic strain, and plastic (dissipation) energy increments are secondary outputs and calculated based on the tangent stiffness. The recurrent layer is a single GRU layer. The strain increments are standardized before passing the recurrent layer as indicated by the asterisk.

two gates, which process the input data x_i (new information) of the current time step i and the hidden states h_{i-1} (history information) of the previous time step $i - 1$. The reset gate in the j -th unit

$$r_i^j = \sigma(\mathbf{W}_r \vec{x}_i + \mathbf{U}_r \vec{h}_{i-1})^j \quad (16)$$

determines how much of the new and old information needs to be considered for the new candidate hidden state

$$\tilde{h}_i^j = \tanh(\mathbf{W}_z \vec{x}_i + \mathbf{U}_z (\vec{r}_i \odot \vec{h}_{i-1}))^j, \quad (17)$$

where $\odot$ is the element-wise multiplication (Hadamard product). The update gate

$$z_i^j = \sigma(\mathbf{W}_z \vec{x}_i + \mathbf{U}_z \vec{h}_{i-1})^j \quad (18)$$

decides how strongly the previous hidden state is overwritten by the candidate hidden state for the new hidden state

$$h_i^j = (z_i \vec{h}_{i-1} + (1 - z_i) \tilde{h}_i^j)^j. \quad (19)$$

The weight matrices $\mathbf{U}$ and $\mathbf{W}$ for each gate and the candidate hidden state are learned during the training process. σ is the sigmoid function used for recurrent activation and $\tanh$ the hyperbolic tangent activation function. The input data x_i relevant for the recurrent layer are standardized using

$$x'_k = \frac{x_k - d\bar{x}_k}{s_k} \quad (20)$$

where x_k denotes each feature of the input, x'_k the standardized feature, $\bar{x}_k$ the mean of the feature in the training set and s is the standard deviation of the feature in the training set. In this work, x represents sequences of strain increments $d\vec{\epsilon}$, which correspond to the applied strain in Equation (13), with each component representing an individual feature.

We use a many-to-many architecture, where the hidden state $\vec{h}_i$ not only serves as input for the next time step but also as the output at each time step. This output is passed to a dense layer with 16 units and linear activation function, resulting in the prediction for the correcting term of the tangent stiffness matrix

$$\mathbf{D}_i^{\text{RNN}} = \mathbf{W}_d \vec{h}_i + \vec{b}, \quad (21)$$

with the weight matrix $\mathbf{W}_d$ and bias vector $\vec{b}$. All other outputs in Figure 4 are derived from this prediction through custom layers without trainable variables within the defined RNN architecture and, therefore, referred to as secondary outputs.

Since the dense layer outputs a vector, it is reshaped into a 4×4 matrix to align with standard conventions and to enable further matrix operations. With the elastic stiffness matrix $\mathbf{D}^e$ and the unstandardized strain increments $d\vec{\epsilon}$ as an input, the material tangent stiffness matrix $\mathbf{D}$ and stress increments $d\vec{\sigma}$ are calculated using the relationships given in Equation (13). Calculating the stress increments from strain increments via the tangent stiffness internally ensures that $d\vec{\sigma} = 0$ if $d\vec{\epsilon} = 0$. The total strain increment can be divided into $d\vec{\epsilon} = d\vec{\epsilon}^{\text{el}} + d\vec{\epsilon}^{\text{pl}}$. The elastic strain increment $d\vec{\epsilon}^{\text{el}}$ is determined through inversion of Equation (3). Thus, the plastic strains are given by

$$d\vec{\epsilon}_i^{\text{pl}} = d\vec{\epsilon}_i - d\vec{\epsilon}_i^{\text{el}} = d\vec{\epsilon}_i - \mathbf{D}_e^{-1} d\vec{\sigma}_i \quad (22)$$

and the plastic energy increments are approximated by

$$dU^D = \vec{\sigma}_i d\vec{\epsilon}_i^{\text{pl}}, \quad (23)$$

given that the RVEs have unit volume.

The tangent stiffness components are the only direct output of the RNN and are included in the architecture to allow a smooth implementation and easy accessibility within an implicit Abaqus subroutine. However, determining the tangent stiffness components is challenging and not fully accurate, especially for the diamond RVE (see Section 4.2). Therefore, when the RNN is only trained on the tangent stiffness, this leads to deviations in the additional outputs (e.g. stresses) that depend on the tangent stiffness. In contrast, stress trajectories are a direct output of the FE simulation and are considered the ground truth for training the RNN together with the plastic strains and the plastic energy. Therefore, adding the stress increments to the training variables allows the RNN to adjust the tangent stiffness to the observed material response. Generally, this architecture also enables unsupervised learning of the tangent stiffness, but we are focusing on supervised learning in this work. The plastic energy is included as an output to further ensure physically and thermodynamically meaningful predictions. The plastic strain is added as an additional output, which provides information about if the structure

is currently deforming elastically or plastically. Thus, training the RNN on all variables marked as output in Figure 4 allows to find more reasonable relationships and accurate prediction of the tangent stiffness components. While no significant improvement in prediction accuracy is observed for the stress response from including plastic strains and plastic energy as output variables for the loading trajectories considered in this study, their inclusion in the model architecture allows a direct prediction of these variables without additional postprocessing and contributes to thermodynamic consistency. Moreover, for complex load paths including unloading and reloading scenarios, which are outside the scope of the present work, these variables are expected to improve the learning process, especially when implemented in a recurrent manner.

Thus, during training, the model is provided with target data for each of these output variables. The loss function

$$\mathcal{L} = \mathcal{L}(\mathbf{D}) + \mathcal{L}(d\vec{\sigma}) + \mathcal{L}(d\vec{\epsilon}^{\text{pl}}) + \mathcal{L}(dU^D) + \mathcal{L}_\lambda + \mathcal{L}_{\text{sym}} \quad (24)$$

takes into account all output variables and is minimized during training using the stochastic gradient descend method implemented in the Adam optimizer [64]. The first three components of the loss are given by the mean absolute error

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |y_i - \hat{y}_i|, \quad (25)$$

where N is the number of samples in the dataset, y is the predicted output and $\hat{y}$ the corresponding target output. For the tangent stiffness components, the RNN is further guided toward meaningful solutions by adding a penalty term to avoid negative eigenvalues λ_i^D

$$\mathcal{L}_\lambda = \omega_\lambda \sum_{i=1}^4 \max(0, -\lambda_i^D) \quad (26)$$

and another penalty term to support symmetry of the tangent stiffness matrix

$$\mathcal{L}_{\text{sym}} = \omega_{\text{sym}} \sum_{i=1}^4 \sum_{j=1}^4 \max(0, |D_{ij} - D_{ji}|) \bar{\delta}_{ij}. \quad (27)$$

Here,

$$\bar{\delta}_{ij} = \begin{cases} i = j & 0 \\ i \neq j & 1 \end{cases} \quad (28)$$

is the complement of the Kronecker Delta and ω_λ and ω_{sym} are loss weights, which are defined as required, see Section 5.1. The additional losses are formulated as unsupervised, layer-level regularization terms that are independent of the target outputs.

While plastic energy increments are inherently positive because of predominantly positive eigenvalues in the tangent stiffness matrix, the loss for the plastic energy increment is defined as

$$\mathcal{L}(dU^D) = \text{MAE}(dU^D) + \omega_U \max(0, -dU^D), \quad (29)$$

which introduces an additional penalty term $\max(0, -dU^D)$ to address negative values in dU^D , preventing unrealistic predictions. The coefficient $\omega_U = 4$ has been determined empirically

to optimize the model's performance. To ensure that all loss contributions have a similar order of magnitude, we divide the tangent stiffness by a factor of 10^4 and the plastic strain by 10^{-4} . This scaling prevents that a single output with a large loss dominates the training. Including all these variables in the training process and giving them a similar importance makes the RNN and the prediction of the tangent stiffness more reliable.

4 | Data Generation and Analysis

Data generation is a crucial step for training machine-learning models. In the literature, randomized loading paths are frequently employed to train constitutive ML models, because they expose the network to a broad range of deformation modes and allow learning generalized constitutive behavior rather than specific trajectories [18, 43, 65, 66]. However, RNN-based approaches typically require on the order of 10^4 such random loading paths [65, 66], which becomes computationally demanding. Although randomized loading paths are beneficial for developing broadly applicable constitutive surrogates, our objective here is an efficient data generation strategy focusing on the mechanical characteristics and relevant loading patterns in nanoporous metals. For example, the upper-scale ligaments of nanoporous metals predominantly experience bending-dominated deformation [1, 6] and reoccurring deformation patterns are expected in the structure under uniaxial loading. Motivated by the beforementioned points, we adopt a data generation strategy based on strain trajectories extracted from an initial bulk 2D upper-level FE simulation under uniaxial loading (Section 2.1), rather than generating fully randomized loading paths. Information on the material response of the LL RVE is then obtained from FE simulations in which these extracted strain trajectories are applied to the RVEs, as described in Section 2.2. The strain trajectories serve as input to the ML model, while the resulting stress trajectories, plastic strain, plastic energy, and tangent stiffness components evaluated on the LL provide the corresponding outputs.

Before training the RNN in Section 5, the following sections outline the generation and analysis of the training data, focusing on strain and resulting stress trajectories as well as the tangent stiffness components. The choice of trajectories for the training procedure and their analysis is discussed in Section 4.1. Section 4.2 describes the process of determining the tangent stiffness components from restart simulations including an analysis of the determined components. The preprocessing of input and output sequences is outlined in Section 4.3.

4.1 | Choice and Analysis of Strain and Stress Trajectories

Strain trajectories are extracted from the UL simulation at a single integration point in 100 of the 2081 elements. The elements were selected randomly, ensuring that at least 50% include plastic deformation. To thoroughly define the training range and prevent values in later simulations from exceeding this range, we included all trajectories where maximum absolute values occurred in any of the observed variables $\{\epsilon_i, \sigma_i, \epsilon_i^{\text{pl}}, U_D\}$ with $i \in \{1, 2, 3, 4\}$. For the validation data, 20 additional elements with plastic deformations were chosen randomly from the remaining

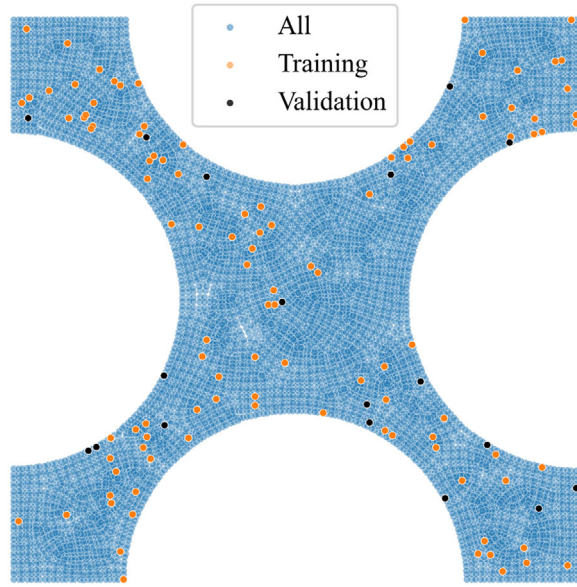


FIGURE 5 | Spatial location of the randomly selected elements, of which the trajectories are used for the training (orange) and the validation (black) of the RNN.

elements. The local distribution of the elements included in the training and validation data are shown in Figure 5. For efficient development of the approach, validation of the Abaqus implementation as well as for good interpretability of changes in trajectories due to inclusion of the diamond RVE, this section and the majority of Section 5 is based on a relatively small data set with trajectories extracted solely from the simple 2D UL simulation under uniaxial compression introduced in Section 2.1. However, we will extend the training to further UL boundary conditions in Section 5.4 to show the applicability to more random structures.

A representative selection of the strain trajectories in the simple training data set are shown in Figure 6a,b, plotted in ϵ_1 - ϵ_2 and ϵ_1 - ϵ_3 -space, respectively. Applying these trajectories to the RVEs produces the stress trajectories shown in Figure 6c,d for the CPE4 element and in Figure 6e,f for the diamond RVE. For most elements, ϵ_1 shows compressive strains according to the applied strain on the UL structure. Elements showing tensile strains in ϵ_1 are located at the bottom and top edges as well as the center of the UL structure. ϵ_2 corresponds to lateral strains occurring normal to the deformation applied to the UL structure. The strong correlation between ϵ_1 and ϵ_2 in the plastic regime, which is observed for most of the trajectories in Figure 6a, is caused by the volume conservation during plastic deformation leading to $d\epsilon_1^{pl} = -d\epsilon_2^{pl}$ for plane strain conditions. In general, the out-of-plane plastic strain increment $d\epsilon_3^{pl}$ can be nonzero under plane strain conditions, due to the associated flow rule and the requirement of plastic incompressibility. Specifically, if $d\epsilon_1^{pl} + d\epsilon_2^{pl} \neq 0$, $d\epsilon_3^{pl}$ must adjust to satisfy plastic incompressibility. In the present setting, $d\epsilon_2^{pl}$ accommodates the incompressibility constraint, resulting in a negligible $d\epsilon_3^{pl}$. In the elastic regime, multiaxial stress states and the absence of a plastic incompressibility constraint allow for more variety in directions of the strain trajectories, which change direction as soon as plastic deformation starts within the element.

Figure 6c,d shows a variety of multiaxial stress trajectories that occur for the CPE4 element. While the stress components increase quickly in the elastic regime, they are only increasing slightly in the plastic regime, as only elastic strains lead to a noticeable increase in stress and the hardening modulus is small compared to the Young's modulus. Therefore, unlike the strain components, stresses are evolving in various directions, also in σ_1 - σ_2 -space. Beside these observations, some trajectories show plateaus or drops in certain stress and strain components. The green curves in Figure 6a-d illustrate this, showing an irregularity in the strain trajectory (see box in Figure 6a), which is reflected within the stress response. The corresponding element is located in a region of early plastic yielding. We propose that the observed stress drops result from 1) stress redistribution due to bending-like deformations within the UL structure and high local shear stresses, and 2) changes in strain direction caused by the onset of plastic yielding in the element itself and its surroundings. Note that while stress drops are observed for certain components, the overall (von Mises) stress response is monotonically increasing, as these drops are compensated by other components. Nonlinearities also occur in purely elastic trajectories (e.g., in brown and violet) and coincide temporally with those observed in the plastic trajectories. This suggests that a local onset of plasticity influences the global mechanical behavior.

For the diamond RVE, the stress trajectories in the σ_1 - σ_2 space are shown in Figure 6e. Initially, these trajectories follow a similar trend to those observed in the CPE4 element. However, as the stresses increase, their direction shifts and begins to resemble the trend observed for the strain trajectories in Figure 6a. In Figure 6a, the onset of plasticity on the UL lead to changes in direction of the strain trajectories and forces trajectories such that $\epsilon_1^{pl} = -\epsilon_2^{pl}$, which likely differ from the natural deformation paths of the diamond RVE. Furthermore, the changes in direction due to plasticity in the UL strain trajectories, do not necessarily intersect with the onset of plasticity in the diamond RVE. Looking at the orange curve in Figure 6, the first change in the stress trajectory refers to the change in the strain trajectories, while subsequent ones are caused by the onset of plastic yielding within the diamond RVE. This highlights the distinct constitutive behavior of the diamond RVE compared to the bulk CPE4 element with isotropic von Mises plasticity, which will be further discussed in Section 5.3.

Figure 6b shows no relationship between shear and normal strains, which is in accordance to the expectations. In the elastic regime, shear and normal strains are uncoupled for structures with cubic anisotropy, which are considered here. In the plastic regime coupling can occur, see Section 4.2, arising from the requirement that the stress state remains on the yield surface, as well as the influence of the yield surface geometry and plastic strains on the tangent stiffness matrix, see Equation (8). Furthermore, plastic incompressibility primarily constrains the volumetric that is, normal strains, but does not directly restrict the evolution of shear strains. As a result, shear strain components can evolve mostly independently from ϵ_1 , leading to scattered directions of the trajectories. The same is observed for the shear stresses in Figure 6d and f. Note that localized non-linearities are observed for the diamond RVE, likely arising from the transition between elastic and plastic behavior, first in the strain trajectories of the UL and subsequently in the diamond RVE, see Figure 6f.

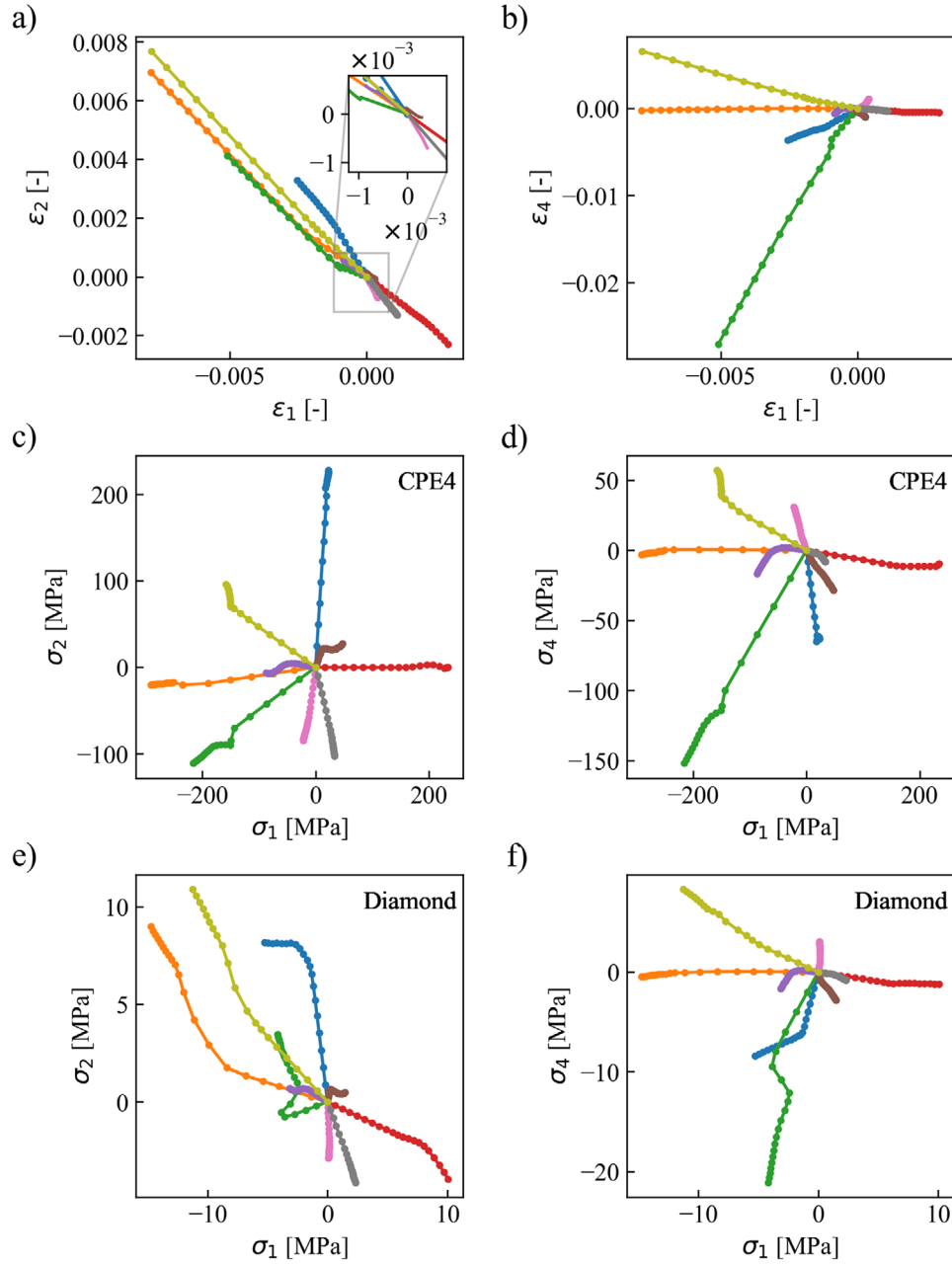


FIGURE 6 | Representative selection of strain and stress trajectories used for training. The strain trajectories shown in a) ϵ_1 - ϵ_2 -space and b) ϵ_1 - ϵ_4 -space are extracted at the UL integration points and subsequently applied to the CPE4 element and the diamond RVE. c) and d) show the resulting stress trajectories for the CPE4 element in σ_1 - σ_2 -space and σ_1 - σ_4 -space, respectively. The ones for the diamond RVE are shown in e) and f).

Furthermore, they are a result of the UL trajectories being forced onto the diamond RVE.

4.2 | Tangent Stiffness Components

The tangent stiffness matrix is not a direct output of the FE simulations, where the UL trajectories are applied on the LL RVEs. Therefore, additional simulations are performed based on these LL simulation. In the following, we will refer to these additional simulations as restart simulations. An Abaqus functionality is used, where a new simulation can be started at any increment of an existing simulation. The initial state of the restart simulation is

the state of a chosen increment in the LL simulation. This allows applying new boundary conditions without affecting the initial LL simulation. The tangent stiffness matrix is defined as $D_{ij} = \partial \sigma_i / \partial \epsilon_j$ with $i, j \in \{1, 2, 3, 4\}$, such that Equation (7) describes the relationship between stress increments and given strain increments. To determine the stress response with respect to the change in a single strain component, three restart simulations are performed per increment in each LL simulation. Thereby, a small strain increment $d\epsilon_i$ is added in form of an equally sized displacement $du_i^j = d\epsilon_{ij}$ to the existing displacements at the given increment of the LL simulation independently for each required strain component ($\epsilon_1 = \epsilon_{11}, \epsilon_2 = \epsilon_{22}, \epsilon_4 = \epsilon_{12}$). This is valid for small strains and the absence of geometrical nonlinearities.

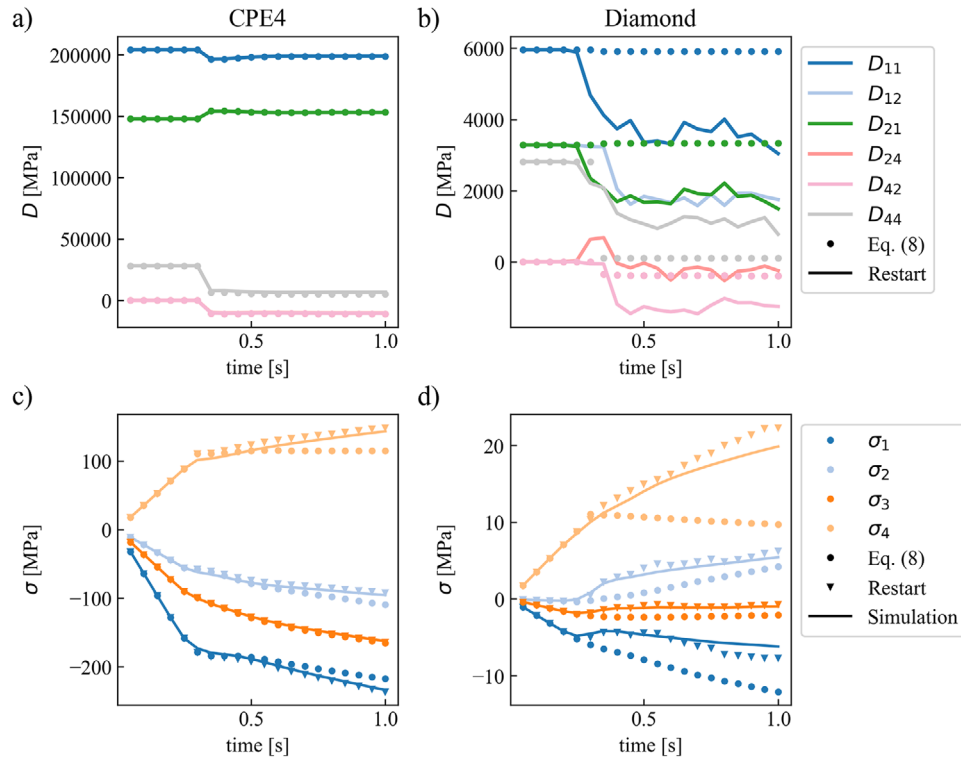


FIGURE 7 | Tangent stiffness components for a) the CPE4 element and b) the diamond RVE, calculated with Equation (8) and determined by restart simulations. c) and d) show the resulting stresses, obtained by applying Equation (7) using the tangent stiffness matrices determined from restart simulations and Equation (8), alongside the target stresses from the LL simulations for the CPE4 element and the diamond RVE, respectively.

The resulting tangent stiffness components are sensitive to the chosen size of strain increments $d\epsilon_i$ and the time increments dt used within the restart simulations, see Appendix B. The choice of these parameters has to be adjusted for different load scenarios and depends on the complexity of the structure and material response. For the CPE4 element $|d\epsilon_i| = 10^{-4}$ and $dt = 0.1$ give good results, see Figure 7a. The diamond RVE is forced onto the trajectories from the UL simulation, which makes the tangent stiffness components more sensitive to the parameters in the restart simulation. Here, $|d\epsilon_i| = 10^{-6}$ and $dt = 0.05$ are used.

For validation of our numerical approach, we compare the determined material tangent stiffness for the CPE4 element with the stiffness components derived analytically from Equation (8). Figure 7a illustrates a selection of determined tangent stiffness components for an example element undergoing plastic deformation and shows a very good agreement between the two methods. The stresses calculated from the tangent stiffness matrix, both determined by Equation (8) and restart simulations, are compared to the CPE4 simulation outputs in Figure 7c. Even though barely visible in Figure 7a, a few of the tangent stiffness components show deviations of up to 5%. This leads to differences in the stress response observed in Figure 7c, where we find better agreement for the stresses calculated using the tangent stiffness components determined from restart simulations. Some elements (not shown here) exhibit discrepancies caused by a later onset of plastic yielding for stresses calculated from the tangent stiffness components. Here, for a strain or stress increment we apply the tangent stiffness from the previous time step. This means, we

do not account for the onset of yielding within the increment, as it is done within FE analysis. Therefore, for some samples, the onset of plastic yielding is shifted by one time increment. These shifts do not pose a problem for training, instead it is a possibility to show the adaptability of the RNN. Due to multiple output variables connected through physical relationships, the RNN is forced to predict the tangent stiffness components such that stresses and further output variables are predicted correctly. Furthermore, artificially increasing the number of increments in the training data, see Section 4.3, reduces deviations introduced by this simplification.

The evolution of the tangent stiffness components of the diamond RVE differ considerably from those of the CPE4 element, see Figure 7b. The components change gradually and less consistently, while a comparably clear transition was observed for the CPE4 element. Furthermore, the relative difference between components in the elastic and plastic regime is more pronounced. The peaks occurring over time within the tangent stiffness components are a result of the small strain increment of $|d\epsilon_i| = 10^{-6}$ within the restart simulation, which is required to get a good agreement with the stresses in Figure 7d.

For some elements, relatively large values are determined for the components coupling shear and normal stresses and strains, see D_{42} in Figure 7b, leading to negative eigenvalues of the tangent stiffness matrix. Within the RNN, this is corrected by including loss terms that guides the components toward solutions without negative eigenvalues and a less pronounced asymmetry, especially with regard to the mentioned components.

Large deviations occur between the tangent stiffness components determined by restart simulations and those calculated by Equation (8). This shows that assuming von Mises plasticity for the diamond RVE with a yield stress of $\sigma_y = 16.2$ determined at $\epsilon_{pl} = 0.2\%$ during uniaxial deformation in x -direction is not sufficient. This was expected and indicates that the plastic behavior of the diamond RVE is more complex than the behavior resulting from von Mises plasticity with linear isotropic hardening and an associated flow rule, as given within the CPE4 element. Therefore, for the diamond RVE, the stiffness components can not be determined by Equation (8). We argue that this is mainly a result of the porosity of the diamond RVE, which, in contrast to the von Mises yield surface, requires an anisotropic yield surface (evolution), allows plastic compressibility [27], and a non-associated flow rule. The influence of porosity on the material response is further discussed in Section 5.3.

In contrast to the CPE4 element, we observe a slightly larger deviation between the stress outputs from the LL simulations and those, where stresses are calculated based on the tangent stiffness components determined by the restart simulations, especially for the shear stress σ_4 , see Figure 7d. However, we will show in Section 5 that the exact tangent stiffness is not required for training, and that such deviations can be corrected by the RNN.

In general, the tangent stiffness components in the plastic regime are influenced by the strain and stress trajectories within the individual elements. Furthermore, note that components corresponding to variations in ϵ_3 were not determined due to the plane strain conditions. While these components are not relevant for the calculated stresses, they might influence the stability in convergence and the eigenvalues of the tangent stiffness matrix and are therefore approximated as follows: $D_{13} = D_{31}$, $D_{23} = D_{32}$, $D_{33} = D_{11}$, such that symmetry is assumed at least within the normal components. D_{43} is set to zero.

4.3 | Preprocessing

The preprocessing of the training and validation datasets functions as a data augmentation step, where sequences with varying length and increment sizes are created. This process ensures that the model's predictions are invariant to increment sizes and sequence lengths within the training range and accounts for variations in increment sizes that might occur in FE simulations.

Each sequence of the raw data, presented in Section 4.1, is used three times in the training set with varying number of increments. The number of increments N for each sequence is drawn from a discrete uniform distribution in the range [20,200]. The distribution of the resulting sequence lengths is shown in Figure 8a.

Next, the size of each increment dt_i is sampled from a uniform distribution in the range [0,1]. These increments are then scaled by

$$dt'_i = \frac{dt_i}{\sum_{j=1}^N dt_j}, \quad (30)$$

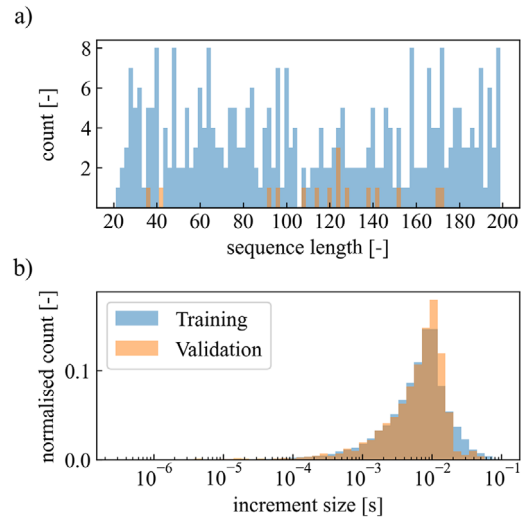


FIGURE 8 | Distribution of a) number of increments per sequence and b) increment sizes of the training and validation datasets. The counts in b) are normalized with the number of total counts for improved visualization.

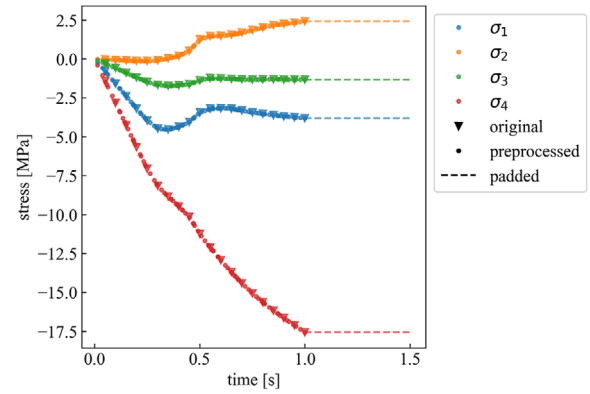


FIGURE 9 | Example of a padded sequence for total stresses. The plot displays original data points as triangles, the new increments as points and the padded part as dashed lines. Note that the padded elements in the sequence are not assigned to specific time frames, so arbitrary times larger than 1.0 are used for visualization.

such that the total time is in agreement with the total time in the raw data. The resulting distribution of increment sizes over the full training and validation set is illustrated in Figure 8b. Subsequently, all sequences are padded to a length of 200 increments for the use in the RNN. During padding, tangent stiffness components remain at their last values, while all incremental input and output variables are set to zero for the padded portions, ensuring that their values remain constant throughout the padded sequence, see Figure 9 for the resulting stress curves.

5 | Results and Discussion

The primary goal of this section is to test the accuracy and applicability of the introduced RNN architecture, see Section 3, and to analyze the mechanical response of the hierarchical structures, after integrating the RNN into Abaqus as a material

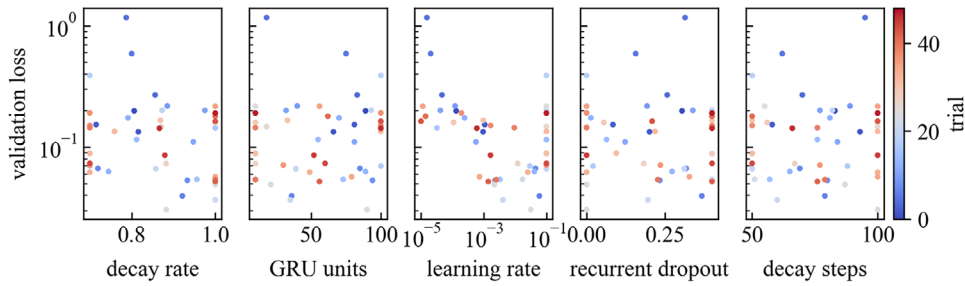


FIGURE 10 | Results for the Bayesian optimization of five hyperparameters (decay rate, GRU units, initial learning rate, recurrent dropout and decay steps) using 50 trials. Colors indicate the trial number. Training is performed across 1000 epochs using a dataset including 50 samples from the diamond RVE. The optimization process is based on minimizing the validation loss.

subroutine. In a first step, Section 5.1, the RNN is optimized and trained such that it captures the stress-strain relationship seen in the RVEs via the tangent stiffness matrix, ensuring stable convergence during the simulation process in Abaqus. In Section 5.2, as a first example, we use the RNN trained on the CPE4 element for validating the implementation of the trained RNN as a material subroutine in Abaqus. The second example is the hierarchical simulation in Section 5.3, where the RNN trained on the diamond RVE is implemented. For both examples, the stress and strain distributions and trajectories obtained from FE simulations with and without the RNN are discussed, giving valuable insights about how the overall material behavior on the UL changes, when introducing a porous RVE on the LL. Finally, to demonstrate the generalizability of the proposed method, the RNN is trained on an extended data set and used within a randomized 2D structure.

5.1 | Training and Optimization of the RNN

Before starting the training process of the RNN architecture, it is essential to carefully choose the hyperparameters in the model architecture. This includes the parameters set in the GRU layer such as the dropout rate and the number of units. The activation functions are kept at default that is, using a sigmoid function for the recurrent activation and a hyperbolic tangent function for the non-recurrent activation, as given in Equation (16) to (18). Additionally, the parameters for the exponential learning rate schedule—initial learning rate, decay steps, and decay rate—are optimized.

As emphasized in Section 4.2, the material behavior, especially the evolution of tangent stiffness components, is more complex in the diamond RVE. Thus, we use a separate, smaller data set of 50 samples for the diamond RVE to analyze which hyperparameters lead to lowest validation losses. The validation loss depending on the choice of hyperparameters is shown in Figure 10 for 50 trials of Bayesian hyperparameter optimization.

Most of the parameters are interdependent and cannot be evaluated separately. The only parameter showing a clear trend is the initial learning rate, which yields lowest losses within the range from 10^{-3} to 10^{-1} , particularly in combination with a high decay rate (greater than 0.88). This sensitivity to the learning rate is expected: if set too low, the learning process risks converging in local minima, while too high learning rates that is, larger than 0.1,

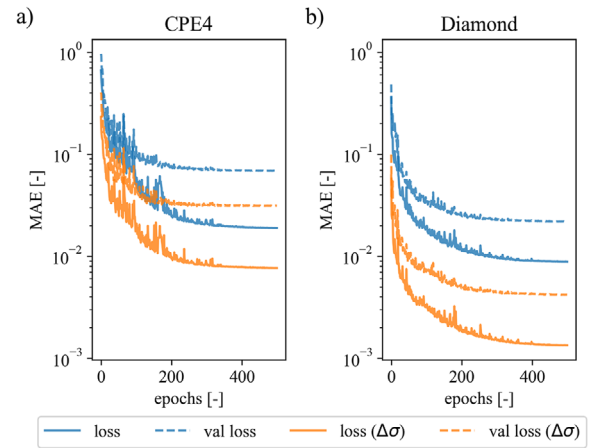


FIGURE 11 | Learning curves illustrating the convergence of the total loss and the loss associated with stress increments $\Delta\sigma$ for the training and validation datasets of a) the CPE4 element and b) the diamond RVE during RNN training over 500 epochs.

can cause gradients to become too large, resulting in overshooting past the optimal minimum. Hyperparameter settings with the lowest validation loss served as a basis and they were fine-tuned empirically. The loss weights ω_Δ and ω_{sym} , introduced in Section 3, are determined empirically and are only required for the diamond RVE. All parameters used for the training procedure are summarized in Table 2 for both RVEs.

Training of the RNNs after 500 epochs and with a batch size of 16 results in the loss curves in Figure 11a,b for the CPE4 element and the diamond RVE, respectively. Even though the material behavior is less complex for the CPE4 element with von Mises plasticity and linear isotropic hardening, because the transition in the tangent stiffness is sharp and the single components stay constant after the transition, the learning curve shows more scattering, especially for the training data set. We link this behavior with the increased tangent stiffness and stress components compared to the diamond RVE, leading to larger gradients and losses.

The validation data gives information about how well the RNN responds to unseen data. A higher validation loss w.r.t. the stress increments is observed for both RVEs in Figure 11. For the diamond RVE, the validation loss for the stress increments of 0.0042 is approximately 3.5 times higher compared to the training

TABLE 2 | Hyperparameters used for training of the RNN for both the CPE4 element and the diamond RVE.

	Recurrent dropout	GRU units	Initial learning rate	Decay steps	Decay rate	ω_λ	ω_{sym}
CPE4	0.0	90	0.01	100	0.94	0.0	0.0
Diamond						10^{-5}	10^{-5}

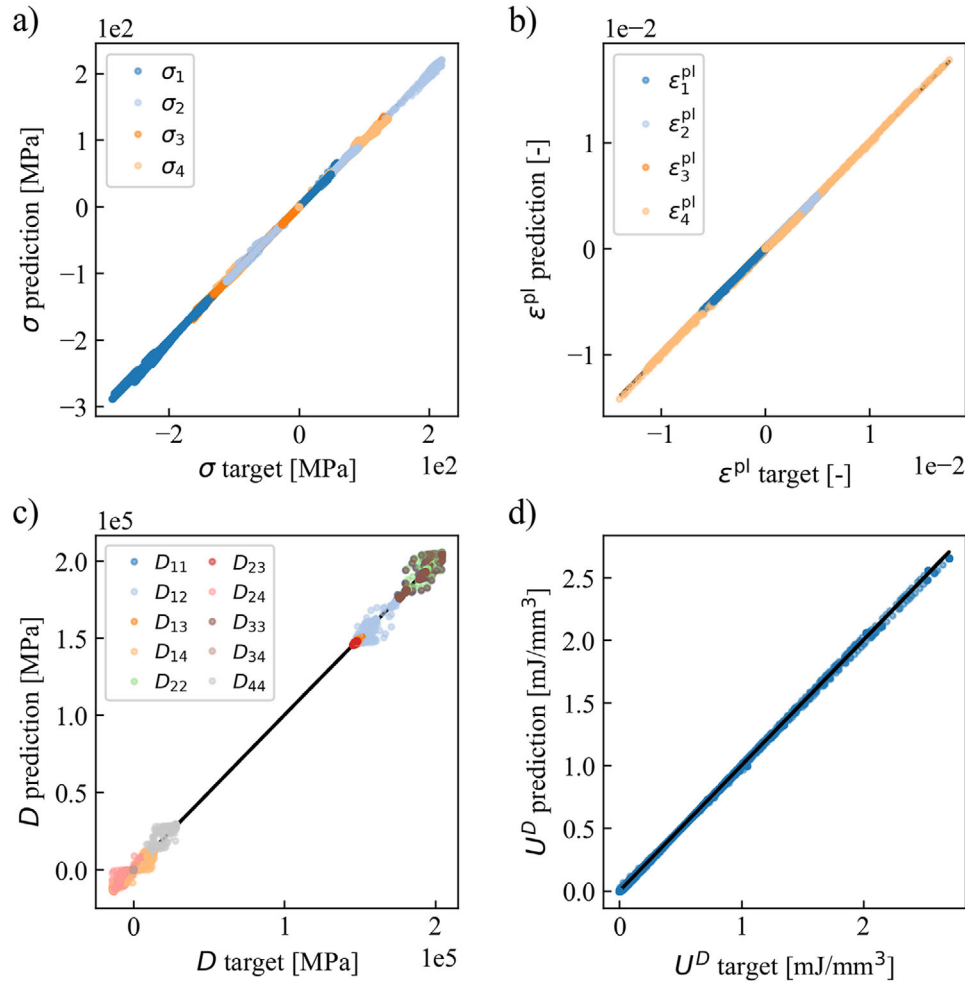


FIGURE 12 | Validation plots after training the RNN with CPE4 data. Shown are the predicted versus target values for each RNN output parameter a) stresses σ , b) plastic strains ϵ^{pl} , c) tangent stiffness components D_{ij} and d) plastic dissipation energy U^D . a), b), and d) are given as total values instead of increments. The scatter in the tangent stiffness components D_{ij} (c) reflects the RNN's adjustments to accurately match the stress outputs, rather than prediction errors.

loss with 0.0012. Similarly, for the CPE4 element, the validation loss for the stress increments is 0.030 compared to 0.0077 for the training set.

Figures 12 and 13 display validation plots for the CPE4 element and diamond RVE, demonstrating strong agreement between predicted and target values for stress (Figures 12a and 13a), plastic strain (Figures 12b and 13b) and plastic energy (Figures 12d and 13d).

This shows that the RNN is generalizing well to unseen data with different increment sizes and sequence lengths, even though the validation loss is considerably higher than the training loss, and

despite the relatively large scattering observed in the learning curves for the CPE4 element.

The tangent stiffness components within the training data set are approximated by restart simulations, see Section 4.2, and do not fully capture the stress response in the LL simulations. As a result, the scattering in the tangent stiffness values, see Figures 12c and 13c, mostly reflect corrections of these components. Together with the correct prediction of the stress trajectories in Figures 12a and 13a this demonstrates the RNN's ability to adjust the tangent stiffness to meet the requirements of accurate stress and plastic strain predictions enforced through physical relationships within the RNNs architecture. For the diamond RVE, the additional loss

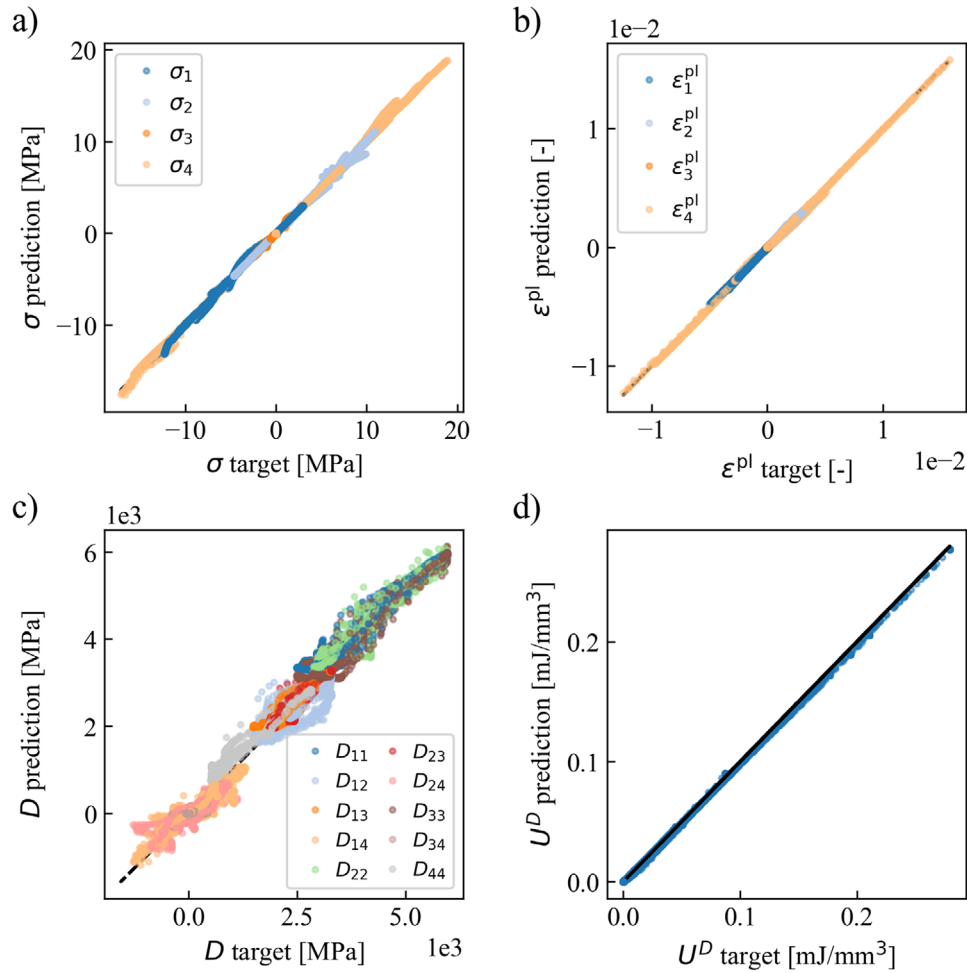


FIGURE 13 | Validation plots after training with diamond RVE data. Shown are the predicted versus target values for each RNN output parameter a) stresses σ , b) plastic strains ϵ^{pl} , c) tangent stiffness components D_{ij} and d) plastic dissipation energy U^D . a), b), and d) are given as total values instead of increments. The scatter in the tangent stiffness components D_{ij} (c) reflects the RNN's adjustments to accurately match the stress outputs, rather than prediction errors.

values successfully avoid negative eigenvalues of the predicted tangent stiffness matrices, see Appendix C.

The tangent stiffness components of the diamond RVE show considerable scattering, both across and along the target line. In comparison, the CPE4 element, displays tightly grouped values for each stiffness component, forming clear clusters, see Figure 12c. These clusters are less distinct for the diamond RVE, particularly in the plastic regime, where the components scatter more widely and overlap, see Figure 13c. This behavior suggests a sensitivity to strain paths and loading history. Furthermore, the overlap can be partially explained by the narrower spread of tangent stiffness components in the diamond RVE's elastic regime, which arises from its cubic anisotropy.

For the analysis of the time invariance of the method, Figure 14 shows the predicted output variables for one example element of the CPE4 validation data set, based on varying input sequence lengths of 20, 100, 150, and 200 increments with randomly chosen increment sizes as described in Section 4.3. The predictions are compared to the target trajectories from the simulations. There is a strong agreement between target and predicted outputs for

all output variables, demonstrating the ability to yield correct predictions. In addition, this example emphasizes the previously mentioned correction of the tangent stiffness components by shifting the onset of plastic yielding, which is in accordance with the observations of the validation plot in Figure 12c.

5.2 | Validation of the Method: Implementation of RNN as Material Subroutine (CPE4)

To validate the RNN-based approach within the FE software Abaqus, we conducted a simulation using the RNN, trained on CPE4 element data, as a user material subroutine (UMAT) in Abaqus Standard. The initial and maximum increment sizes were both set to 0.005, resulting in 200 increments with stable convergence throughout the simulation. Figure 15a,b compare the local von Mises stress distributions from the reference and RNN-based simulation, demonstrating an overall convincing agreement. Figure 15c illustrates the element-wise percentage error field, further highlighting the model's performance. Most errors range between 0% and 7% with only a few localized regions reaching up to 30%, mostly occurring in the elastic regions, which

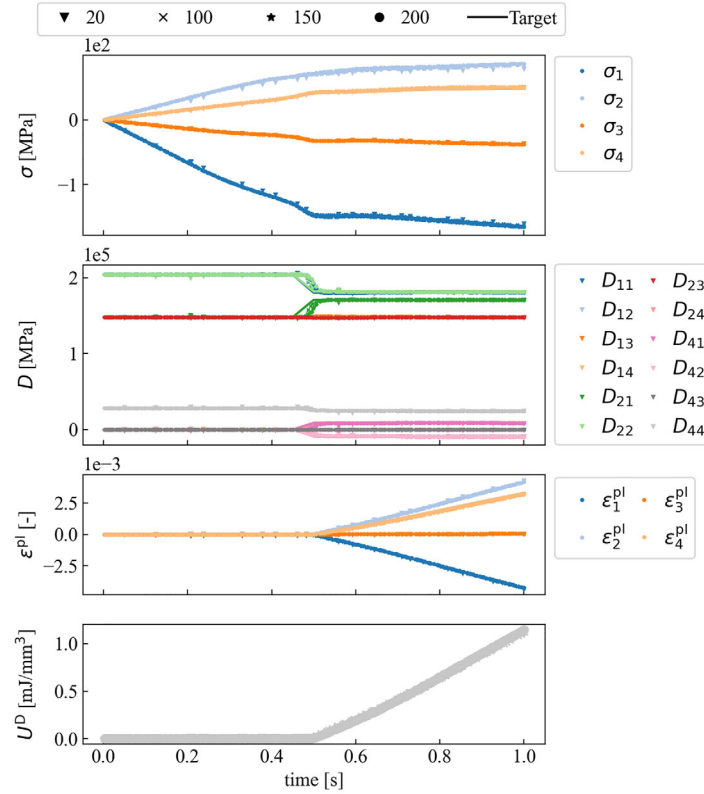


FIGURE 14 | Predictions for one example element from the CPE4 validation data set. The original and the predicted trajectories are shown. The latter were predicted from interpolated strain trajectories with a number of increments between 20 and 200 and randomly chosen increment sizes.

are in proximity to strong plastic deformations. This could be improved by e.g., additional training data in such regions. Despite these outliers, the overall agreement supports the conclusion that the training was successful. A similar level of agreement is observed for the strain distributions, although these results are not included here.

Figure 16 shows the distributions of individual stress and strain components in the RNN-based and reference simulation, confirming their strong alignment. The mean absolute percentage errors

$$\text{MAPE} = \frac{1}{N} \sum_{i=1}^N \frac{|x_i - \hat{x}_i|}{|x_i|} \times 100\% \quad (31)$$

of the stress and strain components within the final increment range between 3% and 6%. For the the calculation of the MAPE values smaller than 1% of the respective maximum values, highlighted as gray area in Figure 16, are excluded to avoid disproportionately large errors caused by division through small values. Based on these results, we consider the training as well as the implementation into Abaqus as successful.

The computational efficiency of the RNN implementation was evaluated, showing that the RNN-based simulation required 280 seconds of CPU time—nearly 10 times longer than the 31 seconds for the original simulation under identical conditions (200 increments). While the RNN-based approach is less efficient than the analytical implementation for isotropic plasticity, it remains at least 50 times faster than the estimated runtime of a full-scale FE^2

simulation without taking into account communication within an FE^2 approach. Furthermore, the benefit increases with more complex structures on the lower level. A reduction in the number of GRU units in the RNN architecture could potentially decrease computation times further, though this was not examined in the current study.

5.3 | Hierarchical Modeling With the Diamond RVE

After successful validation with the CPE4 element, the RNN trained on the diamond RVE data was implemented as a material subroutine. Since a FE^2 method unfortunately is unavailable for validation of the RNN that is trained on the diamond RVE, a simulation based on a material model assuming linear elasticity followed by von Mises plasticity with isotropic hardening was used as a reference. This approach provides further insights into how the material behavior of the diamond RVE differs from that of an isotropic, incompressible model. We use cubic elasticity using the parameters given for the diamond RVE in Table 1. For the plastic regime, the yield stress is determined at different plastic strains by a simulation of the diamond RVE under uniaxial loading in x-direction, see Appendix A.

The local von Mises stress distribution of the reference simulation as well as the RNN-driven simulation are shown in Figure 17a,b. The simulations show a general agreement in stress distributions, however the simulations with the RNN lead to considerably higher stresses especially in the plastic regions. The

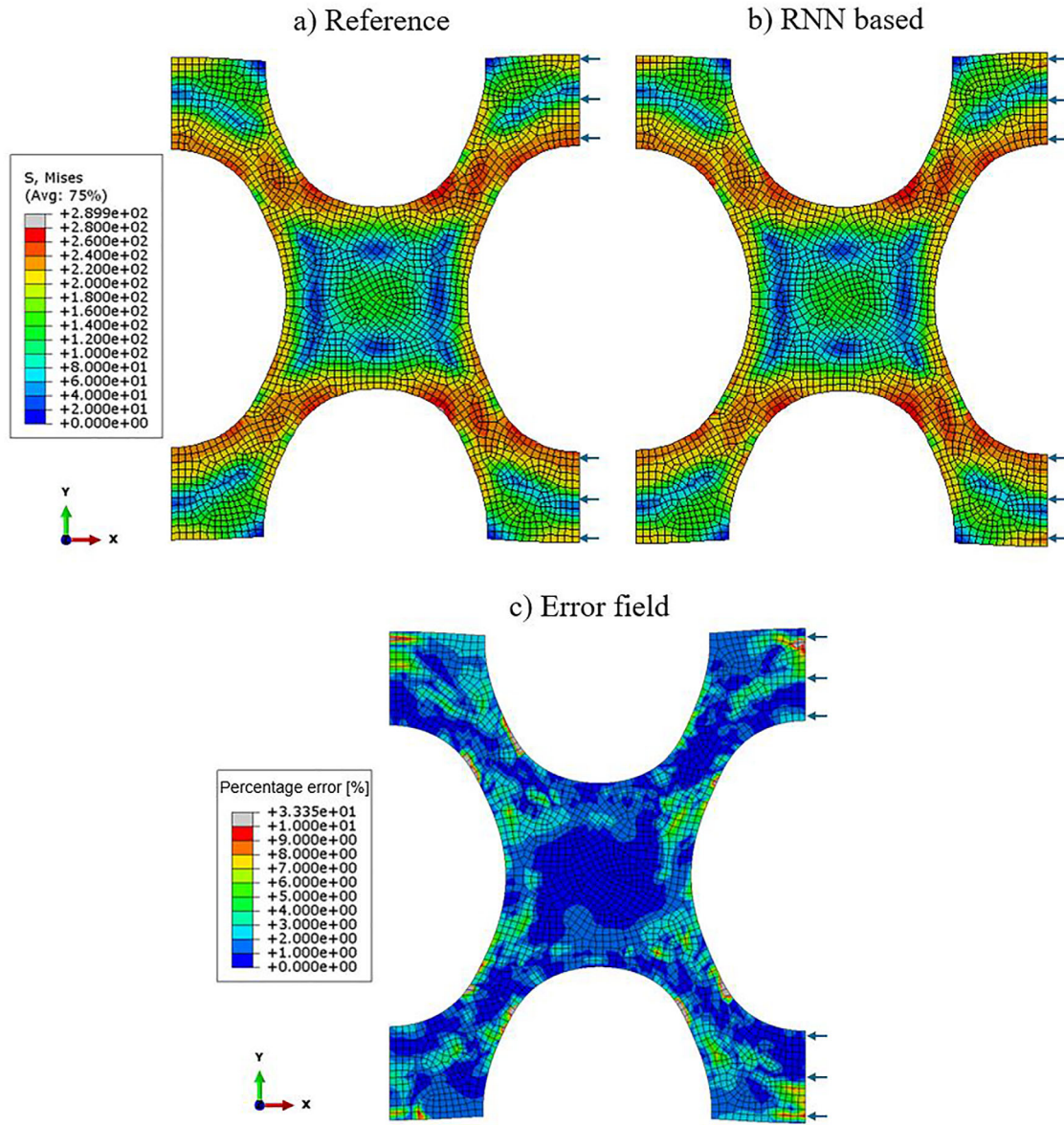


FIGURE 15 | Von Mises stress distribution for the validation of the RNN implementation into a user defined material subroutine (UMAT). Shown are a) the initial UL FE model (reference), introduced in Section 2.1, and b) the simulation using the RNN-based UMAT, with the RNN trained on CPE4 data. The percentage error of the RNN-based simulation with respect to the reference is shown in c) with the error given as $\frac{|x_{\text{ref}} - x_{\text{UMAT}}|}{|x_{\text{ref}}|} \times 100\%$.

strain and stress trajectories in ϵ_1 - ϵ_2 - and σ_1 - σ_2 -space are shown in Figure 18a-d for both the reference and the RNN guided simulation. For the reference simulation with von Mises plasticity and isotropic hardening, a trend of $\epsilon_1^{\text{pl}} = -\epsilon_2^{\text{pl}}$ is observed in the plastic region in Figure 18a, similar to the initial trajectories that were used for training, see Figure 6a. In contrast, Figure 18c shows that the trajectories for the implemented RNN, representing the diamond RVE, are rather non-linear and resemble the trajectories in the elastic regime in Figure 18a, showing no clear relationship between ϵ_1 and ϵ_2 and also no clear transition into the plastic region. The RNN was trained with the trajectories in the UL ligaments, which all include the relationship $\epsilon_1^{\text{pl}} = -\epsilon_2^{\text{pl}}$ in the plastic regime. To account for the new trajectories arising from the inclusion of the diamond RVE as the LL, additional training data was collected. Specifically, the trajectories extracted from the new simulation, partially shown in Figure 18c, were applied to

the diamond RVE to obtain the corresponding material response. Tangent stiffness components were determined through restart simulations, and a new RNN was subsequently trained on the gathered data. The resulting local stress distribution, shown in Figure 17c, yield smaller von Mises stresses in the plastic region compared to the previous RNN-guided simulation. However, the distribution closely matches the simulation with the von Mises plasticity model in Figure 17a. At first sight, this finding is interesting, given the very different strain trajectories found in Figure 18a and e. Furthermore, due to the anisotropy of the yield surface, we expected larger deviations for the stresses and their trajectories. However, considering that stresses resolve due to elastic strains and that we are dealing with comparably small strains of 1% and a simplification to a 2D plane strain problem, this observation can be explained. In addition, the yield surface and flow rule especially affect the plastic region including the plastic

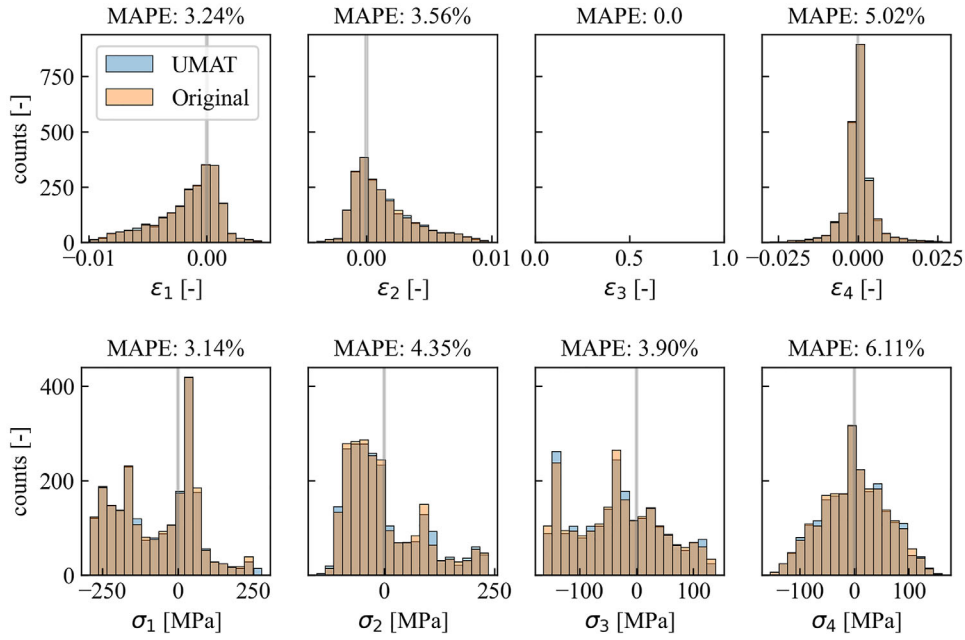


FIGURE 16 | Comparison of the distribution of strain and stress components in the original 2D simulation and the simulation, where the RNN, trained on the data of the CPE4 element, is implemented in a material subroutine (UMAT). The mean absolute percentage error (MAPE) of the RNN guided simulation is given for each component. The gray shaded area corresponds to values smaller than 1% of the respective maximum values, which are excluded from the calculation to avoid large errors due to small target values.

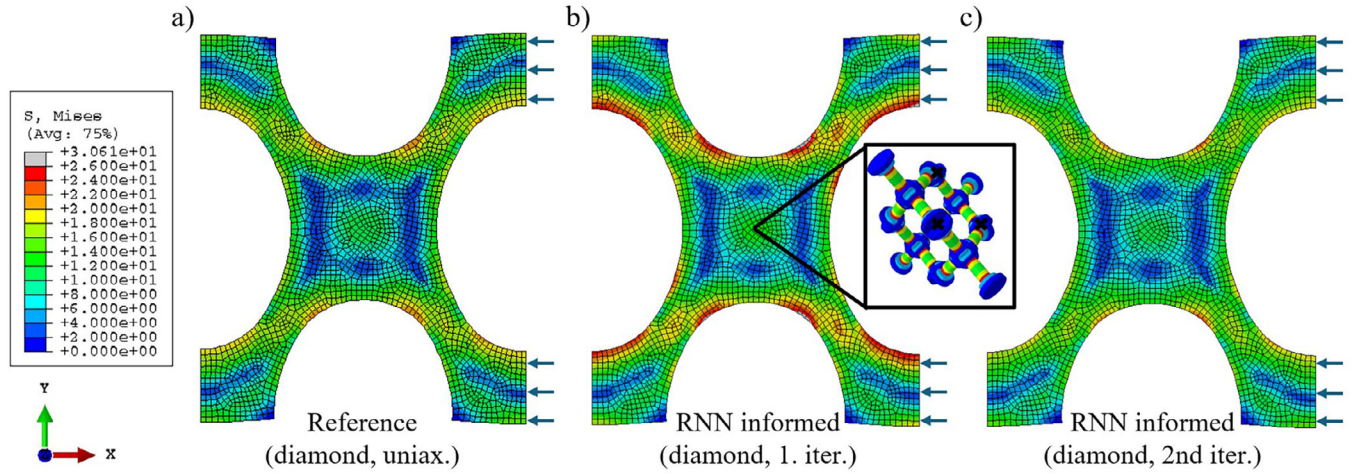


FIGURE 17 | Comparison of von Mises stress distribution between a) the reference simulation, assuming von Mises plasticity with isotropic hardening based on yield stresses of the diamond RVE under uniaxial loading, b) the simulation utilizing an RNN trained on data from the diamond RVE as the material model at the integration points and c) the simulation with the RNN trained on the new trajectories resulting from b) as a material model. The legend is based on b) and the limits are set identical for all simulations.

strains and, therefore, don't have a significant influence on the stress response.

Comparing the strain and stress trajectories in the first and second iteration in Figure 18c–f shows no major changes in the trend of the trajectories. The strain trajectories in Figure 18e show minor changes in magnitude. Additionally, the orange and blue trajectories show a slightly more pronounced transition to the plastic regime compared to the first iteration in Figure 18c, leading to curves that rather diverge from the trend $\epsilon_1^{\text{pl}} = -\epsilon_2^{\text{pl}}$ in

the plastic regime that was observed in Figure 18a for isotropic von Mises plasticity. This behavior can be explained by the compressibility in the plastic regime and might be further affected by the anisotropic yield surface and non-associated flow-rule of the diamond RVE. In Figure 18f, a reduction of stresses is observed compared to Figure 18d, while the main direction of stress trajectories remains similar. Therefore, the first simulation, Figure 18c,d, can be seen as a first approximation, however a second iteration is required. The reason for this is that the network was initially trained on mostly linear trajectories, compare

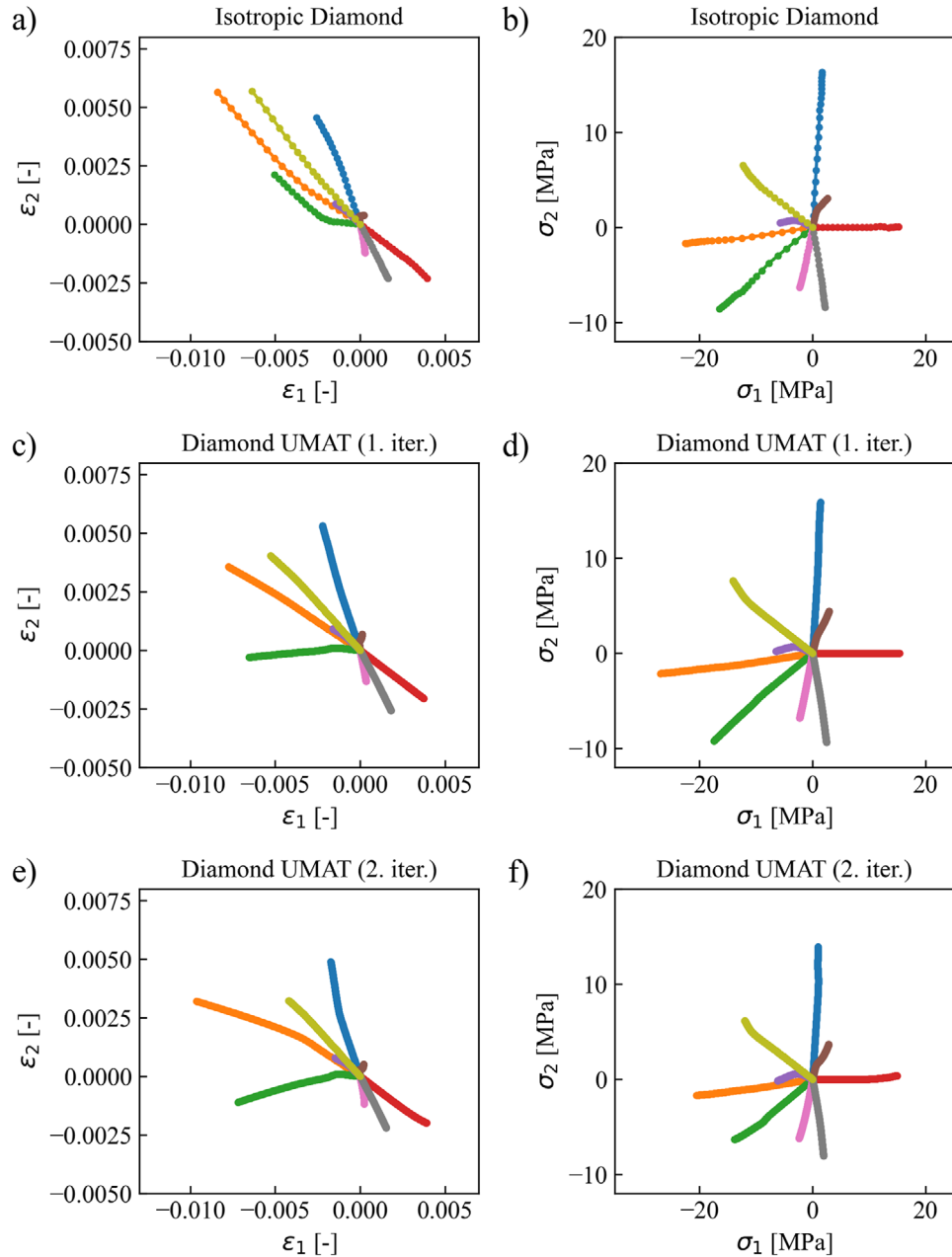


FIGURE 18 | Strain trajectories in ϵ_1 - ϵ_2 -space after the hierarchical simulation with a) the reference material model using von Mises plasticity with isotropic hardening following Figure A1, c) the RNN guided material model after the first training with initial trajectories and e) the RNN guided model trained on the trajectories in c). The corresponding stress responses are given in b), d), and f). The trajectories shown are for the same representative UL elements as those in Figure 6a.

Figure 6a. Keeping this in mind, the first approximation shows the flexibility of the trained RNN, as it was able to handle the non-linear trajectories evolving due to the introduced diamond RVE, even though the stresses were overestimated (due to later prediction of the onset of plastic yielding). This flexibility is caused by the architecture of the RNN and the elastic stiffness matrix, which is provided to the RNN as an input.

The analysis of the tangent stiffness components of the diamond RVE, resulting from applying the initial trajectories (Figure 6a) and updated trajectories (Figure 18c), shows a clear difference (not shown here). The observed limitations in determining the components in Section 4.2 are an effect of the forced trajec-

tories and not a limitation of the method. Forcing the RVE onto trajectories leads to peaks in the tangent stiffness components relating normal and shear components. Furthermore, the high negative values in these tangent stiffness components, which were leading to partially negative eigenvalues, are no longer observed when applying the new trajectories to the diamond RVE.

This study shows that the inclusion of the diamond RVE as the LL structure leads to significant changes in the response in the UL model, introduced in Section 2.1. The porosity results in a reduction of the stresses by a factor of 10, while the general trend of the stress trajectories in Figures 6c and 18f remains

similar. For the strain trajectories, the opposite is observed: while the values remain in the same range of magnitude due to the constant applied strain on the UL structure, the trajectories in Figures 6a and 18e differ considerably. This is a result of smaller lateral strains ϵ_z , which are caused by a smaller Poisson ratio in the elastic regime and by the compressibility in the plastic regime [67]. These observations are not only caused by the introduced porosity but are also a result of the diamond RVEs anisotropy in the elastic as well as the plastic regime. The considerably higher shear modulus compared to the Young's modulus results in smaller shear strains, compared to the initial UL model without including hierarchy. The anisotropic yield surface, non-associated flow rule and compressibility are interdependent causes for the changes in the plastic material behavior and their influence on the material behavior can not be easily separated.

5.4 | Extension to Additional Load Cases and Prediction of a Randomized Structure

In this section, we apply the previously introduced RNN architecture to predict the mechanical response of a randomized upper-level structure resembling a two-dimensional slice of nanoporous gold. As in earlier examples, the material response is evaluated under 1% uniaxial compression in the x -direction, see Figure 19a–c. To ensure direct comparability between the reference simulation and the RNN guided simulation, solely the RNN trained on the CPE4 element with bulk material behavior is considered. The reference simulation shown in Figure 19a uses material properties consistent with those described in Section 2.1, based on von Mises plasticity with linear isotropic hardening, as summarized in Table 1 (CPE4). These same properties are applied in the CPE4 element.

Although the boundary conditions on the upper level remain the same as in previous examples, the resulting strain and stress trajectories differ significantly, particularly in magnitude. Localized strains of up to 10% and stress peaks of up to 800 MPa occur in regions with high plastic deformation, whereas previous structures exhibited strains closer to the applied 1% and von Mises stresses of around 300 MPa. These pronounced differences lead to substantial overestimations in a simulation, which is based on the initially trained RNN considering limited trajectories and small strains. The RNN predicts a set of 1000 stress trajectories from the random structure with a MAPE of around 24% considering stresses exceeding 4 MPa. The early onset of plastic yielding, driven by the high local strains, further contributes to these inaccuracies.

To improve the generalization capability of the RNN, the training dataset was expanded to include a broader range of applied boundary conditions and higher strains. The boundary conditions, including the applied strains that directly translate to deformations in this context, as well as the resulting von Mises stress distributions are provided in Table 3. While the strain levels considered might suggest the need to account for geometric nonlinearity within the simulations, it is demonstrated in [68] that such effects have negligible influence on the overall UL response for complex 3D nanoporous structures and are therefore not considered here.

K-means clustering was applied to identify 200 distinct clusters out of the trajectories from the new UL simulations listed in Table 3. Thereby, clustering was performed on the last increment of these trajectories considering the feature space $[\sigma_i, \epsilon_i^{pl}]$, ensuring diversity within the training data focusing on characteristics of the plastic regime. Taking one trajectory per cluster results in 200 distinct trajectories for the extended training data set. Table 3 provides information about the contribution of each UL simulation to the training data. The strain trajectories are applied to the CPE4 element and the gathered data is preprocessed as described in Section 4.3, except that the trajectories are only augmented two-fold, resulting in a total of 400 training trajectories.

The RNN was retrained using the same parameters as in Table 2 (Section 5.1) for the CPE4 element. Using the extended training data reduced the error from 24% to 15%. While the number of unique trajectories doubled, the overall data volume increased by only 25%, demonstrating that improved data diversity—rather than data volume—can enhance generalization.

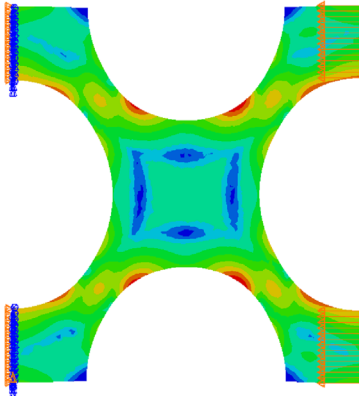
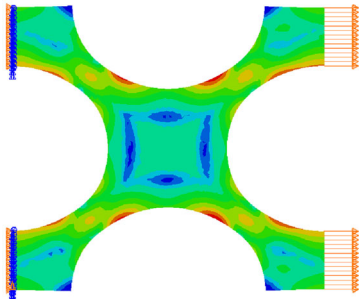
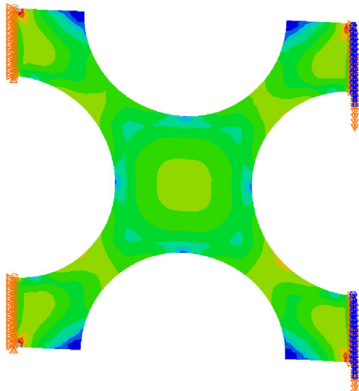
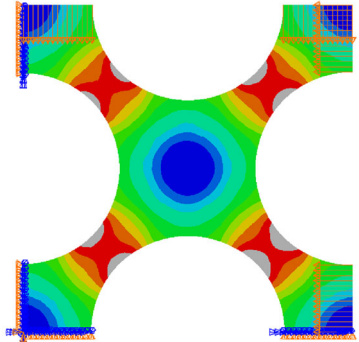
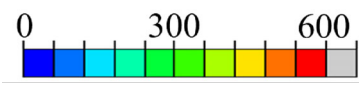
Further improvements are achieved by scaling each loss term by the number of contributing components, reducing the error to MAPE = 10%. Such weighting strategies are commonly applied in multi-output models to balance contributions and avoid bias toward outputs with larger numerical scale or dimensionality [69]. Here, it shifts the focus toward learning the relation between strain and stress increments, instead of learning a pattern in tangent stiffness components, while still leading to consistent values in the tangent stiffness due to the physical relationships in the architecture.

Lastly, including both stress increments and total stress values during training further improves predictions for trajectories from the random structure to MAPE = 7%, likely due to better modeling of the onset of plastic yielding. Additionally, local incorrect estimation of stress increments can lead to a persistent bias in the predicted stress state, even if subsequent increments are accurate. Providing total stress as a reference enables the model to realign its predictions and reduces the risk of error accumulation. The results for the initial RNN and the adjustments described for the RNN trained on the extended data set are summarized in Table 4.

The newly trained RNN is subsequently implemented into the finite element simulation. Figure 19b shows the resulting von Mises stress distribution and Figure 19c the error field, which illustrates the percentage error of von Mises stresses within the RNN-guided simulation compared to the reference. A very good agreement is observed in the plastic regime, with only a few points exceeding errors of 6%. Within the elastic regions, higher errors of more than 10% are observed, in some cases reaching up to 200%. These disproportionately high errors occur in regions with very small stress magnitudes close to zero in the reference simulation, see Figure 19a. Regions with errors of up to 20% also correspond to relatively low stress values in the reference simulation and are therefore negligible in terms of their impact on the overall material response.

The existing deviations could be reduced by adding more complexity to the RNN and the training data. However, the overall good performance of the RNN on a previously unknown structure demonstrates its generalizability. With regard to hierarchical

TABLE 3 | Overview of boundary conditions and corresponding von Mises (v. M.) stress distributions for the new simulations used to extend the training data. The applied strains on the simplified 2D structure are listed alongside the number of trajectories that are included in the training data from each simulation.

Load case	v.M. Stress distribution	Applied UL strain	Trajectories in training set
Compression		$\epsilon_{11} = -5\%$	50
Tension		$\epsilon_{11} = 5\%$	59
Shear		$\epsilon_{12} = -5\%$	34
Biaxial compression	 	$\epsilon_{11} = -2.5\%$ $\epsilon_{22} = -2.5\%$	57

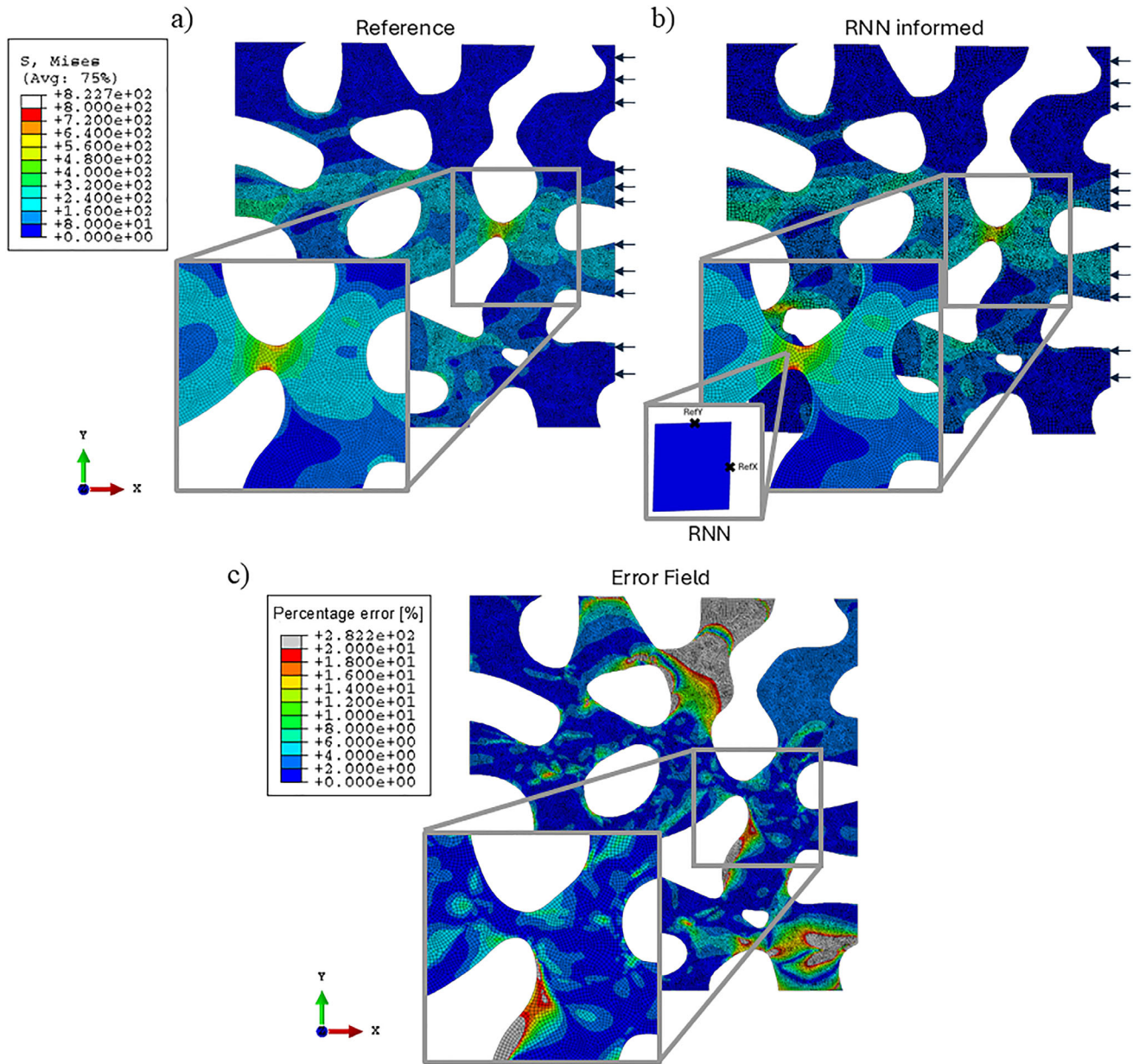


FIGURE 19 | Random 2D structure resembling a 2D nanoporous gold slice with local stress distribution of a) the original simulation with properties of gold given in Table 1 and b) the RNN retrained on the extended data set for a CPE4 element. c) shows the local percentage error of b) w.r.t. a).

nanoporous metals, this paves the way for predictions within structures of different solid fractions and geometries as well as more complex structures. While this work focuses on 2D structures, the method can be extended to 3D structures, however this will be the concern of future work.

6 | Conclusion

In this study, we introduce a physics-informed RNN-based architecture for the description of non-linear deformation behavior of hierarchical materials considering 2D (nano-)porous networks on two length scales. The architecture, which includes GRU cells to capture temporal dependencies in sequential data, was trained on varied increment sizes and sequence lengths to ensure flexibility with regard to varying increment sizes in the FE simu-

lations. Providing physical relationships within the architecture, the RNN predicts the tangent stiffness matrix as a primary output consistent with the relationship between strain and stress increments as well as plastic strain increments, and plastic energy increments. The RNN was successfully implemented in a material subroutine for the FE software Abaqus. Implementing the RNN, trained on CPE4 element data, demonstrated a strong agreement with reference simulations for von Mises stress and strain distributions, with errors mostly below 3%. Despite increased computational time compared to analytic material model definitions, the RNN implementation is significantly faster than full-scale FE² simulations, highlighting its potential for efficient and accurate material modeling.

Incorporating the RNN trained on the diamond RVE as the LL response led to significant changes of the material behavior,

TABLE 4 | Effect of training set complexity and loss weighting on the mean absolute percentage error (MAPE). A selection of 1000 stress trajectories showing plastic deformation from the randomized structure are predicted using the RNN and compared to their target values. The "initial" training set includes only uniaxial compression at 1% strain of the UL structure (Figure 2), while the "extended" set incorporates four loading conditions and larger strains. Loss weights ω_i are partially normalized by the number of components contributing to the error. The final configuration additionally includes total stresses in the training. MAPE is computed for stress values exceeding 4 MPa.

Training set	$\omega_{\Delta U^D}$	ω_D	$\omega_{\Delta\sigma}$	ω_σ	$\omega_{\Delta\epsilon^{pl}}$	MAPE _{σ} [%]
Initial	1	1	1	0	1	23.87
Extended	1	1	1	0	1	14.57
Extended	1	1/16	1/4	0	1/4	10.11
Extended	1	1/16	1/4	0.01	1/4	7.40

e.g., a significant stress reduction within the UL ligaments due to porosity on the LL. Interestingly, while the stress response of the diamond RVE was similar to a model with von Mises plasticity and isotropic hardening, the strain response differed considerably. The anisotropic yield surface, non-associated flow rule, and plastic compressibility of the diamond RVE contributed to observed differences in plastic behavior, which highlights the complex interplay between the structural features of the diamond RVE on the LL and the resulting UL behavior. The RNN's ability to generalize from initial linear trajectories to handle non-linear trajectories introduced by the diamond RVE, as well as the convincing performance for a random structure, demonstrates its robustness and adaptability. Nevertheless, as with most ML-based constitutive models, load cases or deformation magnitudes that deviate substantially from the training domain may lead to increased prediction errors, and the validity of ML-based predictions must therefore always be verified.

Future work could focus on optimizing the RNN architecture to enhance computational efficiency and extending the training data to more complex load cases on the UL structure and a 3D model to represent the UL.

Author Contributions

Lena Dyckhoff: conceptualisation, formal analysis, investigation, methodology, software, visualization, writing – original draft. **Norbert Huber:** conceptualization, funding acquisition, methodology, software, supervision, writing – review & editing.

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Conflicts of Interest

The authors declare no conflicts of interest.

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Appendix A: Hardening of Diamond RVE Under Uniaxial Load

The reference for the hierarchical simulation with the diamond RVE on the LL, introduced in Section 5.3, uses a material model that includes linear elasticity with orthotropic anisotropy followed by a plastic regime described by von Mises plasticity with isotropic hardening. The hardening behavior for the reference was taken from a simulation of the diamond RVE under uniaxial compression. The yield stresses are determined in a range of 0.2% to 2% plastic strain and are given in Figure A1.

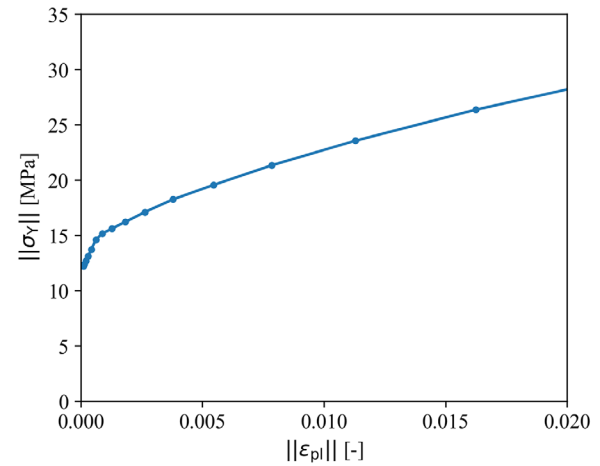


FIGURE A1 | Hardening behavior of the diamond RVE during plastic deformation under uniaxial compression in x-direction. The yield stress is plotted versus the plastic strains.

Appendix B: Analysis of Parameters Influencing the Tangent Stiffness Components From Restart Simulation

The tangent stiffness components are approximated using restart simulations in Abaqus. Stress and strain states from increments within an original simulation are used as initial conditions within the restart simulations and new boundary conditions are applied in form of small deformations $d\vec{u} = d\vec{\epsilon}$. To determine the tangent stiffness, only one strain component is adjusted within one restart simulation. Thereby, the size of the applied strain increment $d\epsilon_i$ as well as the temporal increments dt within one restart simulation affect the approximated tangent stiffness components. As discussed in Section 4.2, especially the diamond RVE shows a higher sensitivity to the choice of parameters. Therefore, we studied how these parameters influence the resulting tangent stiffness for an example case for the diamond RVE.

For a measure of accuracy, the stress trajectories that were calculated using the approximated tangent stiffness components are compared to the stress response from the original simulation that the restart simulations are based on. Figure A2 shows the resulting MAPE for different parameter combinations, while Figure A3 shows a selection of

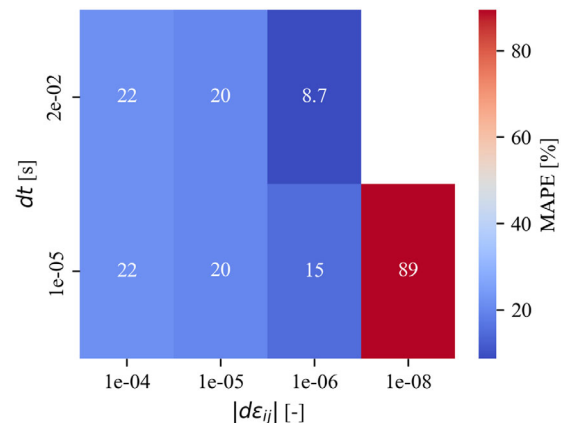


FIGURE A2 | Influence of the size of time increments dt added strain increments $d\epsilon_{ij}$ in the restart simulations on determined tangent stiffness components and subsequently on the stresses. The mean absolute percentage error (MAPE) of the calculated stresses is given. The study was performed on the same sample as it was given for the diamond RVE in Figure 7.

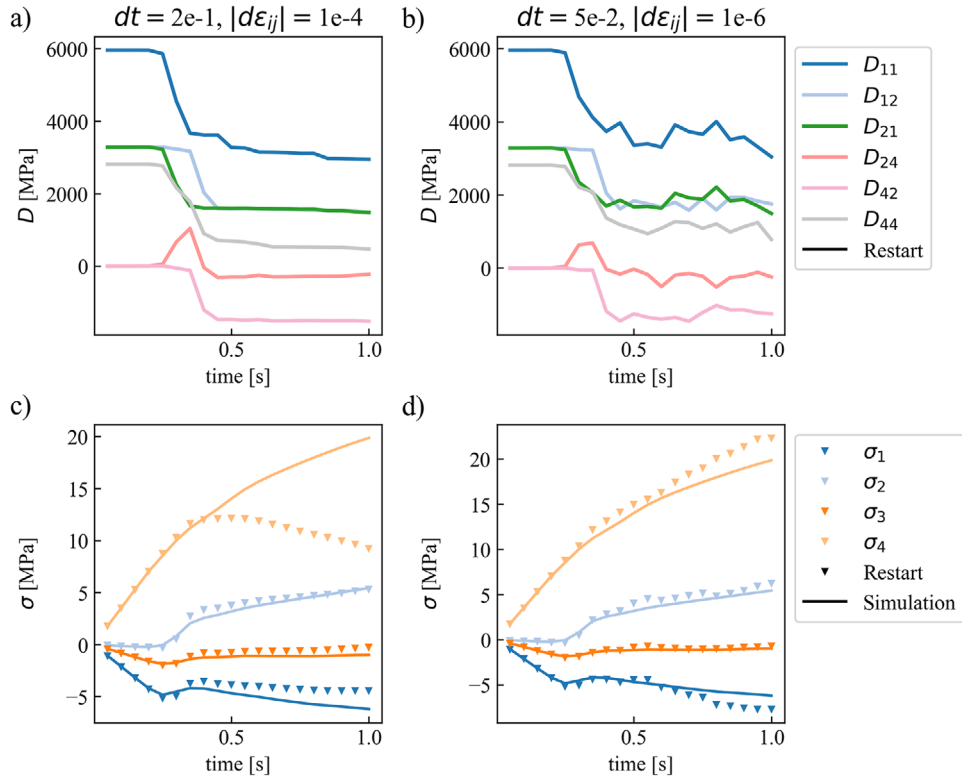


FIGURE A3 | Shown are a), b) the approximated tangent stiffness components and c), d) the resulting stress trajectories for different parameter combinations (dt , $d\epsilon$) in the restart simulation. The calculated stress trajectories are compared to the LL simulation, which is the basis for the restart simulations. The trajectories corresponds to the same diamond RVE sample as used in Figure 7.

tangent stiffness components and corresponding stress trajectories for two distinct parameter combinations. Our findings indicate that smaller strain increments generally lead to more accurate results; however, if the increments become too small, numerical noise might dominate, leading to larger errors, see Figure A2. This behavior likely also explains the error spikes visible in Figure A3b, however in the latter case with a comparably good accuracy for the stress response. Additionally, smaller time increments tend to improve accuracy by allowing the simulation more time to adapt to the new boundary conditions. However, this comes at the cost of increased computational effort.

Appendix C: Eigenvalues

Section 4.2 discusses the occurrence of strongly negative tangent stiffness components for the diamond RVE when applying trajectories from the initial upper level simulation. The distribution of the resulting eigenvalues for the training data is shown in Figure A4. To avoid negative eigenvalues in the predicted tangent stiffness matrices, additional loss terms were introduced in the loss function of the RNN for the diamond RVE (Section 3). Although strictly non-negative eigenvalues cannot be guaranteed, Figure A4 shows that the eigenvalues of the tangent stiffness matrices predicted by the RNN for the same training data are predominantly non-negative, demonstrating the ability of the RNN to correct tangent stiffness matrices toward non-negative eigenvalues. Note that the components D_{13} are assigned based on symmetry assumptions within the stiffness matrix. However, their exact values remain undetermined due to the plane strain conditions, which might further influence the calculation of eigenvalues.

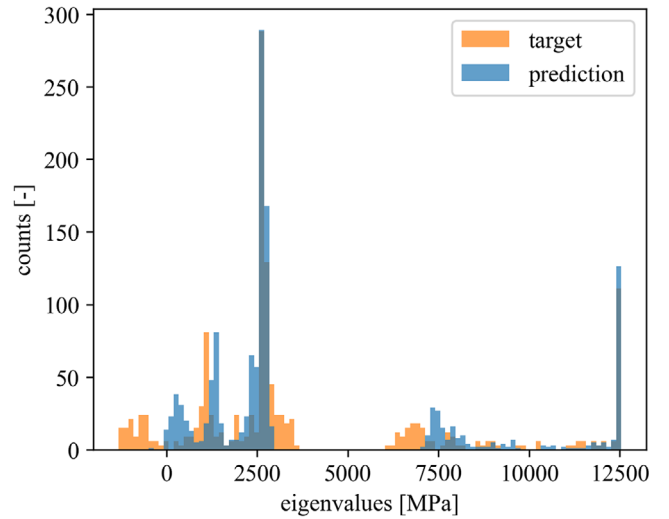


FIGURE A4 | Distribution of eigenvalues for the target data and the RNN predictions of the diamond RVE training data set.