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Thermodynamics-informed neural networks for physically realistic mixed reality[☆]

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Abstract

The imminent impact of immersive technologies in society urges for active research in real-time and interactive physics simulation for virtual worlds to be realistic. In this context, realistic means to be compliant to the laws of physics. In this paper we present a method for computing the dynamic response of (possibly non-linear and dissipative) deformable objects induced by real-time user interactions in mixed reality using deep learning. The graph-based architecture of the method ensures the thermodynamic consistency of the predictions, whereas the visualization pipeline allows a natural and realistic user experience.

Two examples of virtual solids interacting with virtual or physical solids in mixed reality scenarios are provided to prove the performance of the method.

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Keywords: Deep learning; Augmented reality; Thermodynamics; Structure preserving; Real-time simulation

1. Introduction

Computer science advances in the last decades led us to experience in a relatively short lapse of time three major technological innovations: the personal computer, the Internet, and mobile devices. Currently, we are at the beginning of a fourth paradigm of computing innovations involving immersive technologies such as Virtual Reality (VR), Augmented Reality (AR) or Mixed Reality (MR). All this is possible due to huge advances in machine learning techniques and hardware improvements applied to computer graphics and computer vision.

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It is clear that this new paradigm seeks to revolutionize technology in the next years and will have a great impact in society such as smart cities [1,2], new teaching methods [3] or economic paradigms [4]. Technology companies have already created numerous digital platforms, such as the Metaverse [5,6] or the Omniverse [7,8], in order to develop their own immersive technologies.

In most of the cases, virtual worlds are required to resemble our real world as much as possible, so many disciplines come into play (traditionally, computer graphics and computer vision). However, virtual worlds need to be dynamic rather than static so the user can responsively interact with a changing virtual world. From that perspective, physics simulation plays a major role and it is required to be real-time. On the one hand, current real-time physics engines rely on severe simplifications of the governing dynamical equations and are limited to very simple material models and constitutive phenomena. On the other hand, classical engineering methods for solid and fluid simulations, such as the finite element or finite differences methods, have the consistency of decades of theoretical research in terms of the convergence to a consistent physical solution but are too expensive to achieve real-time framerates. However, these last methods can be used to generate a rich and consistent database to train a fast AI accelerated by the recent advances in machine learning procedures.

In this work, we aim to merge the physical consistency of classical simulation methods with the speed of real-time physics engines using a deep learning approach. Although the formulation is general for a wide variety of dynamical systems, in this work we focus on nonlinear solid mechanics. The results are consistent with the laws of thermodynamics by construction and are able to achieve real-time performance in general load cases which were not previously seen by the network. In Section 2, we explore some of the related work involving real-time reality simulators and physics-informed deep learning. In Section 3 we introduce the thermodynamically-informed graph neural networks together with the vision and visualization system used to record the demo videos. Section 4 shows the application of the proposed algorithm in two different solids together with error plots, and future work, limitations and conclusions are provided in Section 5.

2. Related work

Real-time physics engines such as PhysX [9,10] or Havok [11] have mostly been developed in the videogame industry. Even if those engines allow to program custom dynamical models, they usually rely on simplified mass-spring models or rigid body dynamics to achieve high framerates in modern videogames. Multiple research lines remain open trying to leverage the physical consistency of the results with low computational requirements.

2.1. Model order reduction-based simulators

Several authors solved the mentioned problems by creating a reduced order model of the system. These methods consist of a two-stage procedure: an offline phase where the solution space is precomputed in a compressed representation, lying on a reduced-order manifold, and an online phase where the solution can be evaluated in real-time. The difference between each method lies on the specific projection technique used to compute the reduced manifold.

Classical linear methods such as Principal Component Analysis [12,13] or reduced basis [14,15] are fast and simple to implement but fail to capture more complex nonlinear phenomena. This inconvenience can be solved using nonlinear methods such as kernel-Principal Component Analysis [16], Locally Linear Embedding [17,18] or Proper Generalized Decomposition [19,20]. Those techniques have similar disadvantages: as the solution is already precomputed, they are unable to handle different mesh discretizations and fail to generalize to unseen configurations.

2.2. Deep learning based simulators

The use of deep learning in real-time simulations has been widely explored in recent manuscripts, using neural networks as powerful function approximators with fast evaluation performance. The spirit is similar to the reduced order modeling: in the offline phase a neural network is trained with a set of examples and in the online phase the network can be fast evaluated in unseen scenarios.

For instance, several works avoid the real-time restrictions by decreasing the dimensionality of the problem by using autoencoders [21,22] in a similar fashion to the reduced order modeling methods. Other approaches are based on standard multilayer perceptrons, used as a collocation method for residue minimization [23,24]

or specific formulations for contact mechanics [25,26]. Those approaches require the prior knowledge of the governing equations. In the field of physics-informed machine learning, many methods have recently proposed to use neural networks such as solvers of partial differential equations (PDE) residues in the context of general physics [27,28] or fluid mechanics [29–31], identification and simulation of the dynamics of complex systems [32] or structure-preserving algorithms [33–35] with promising results. However, none of the mentioned methods have been implemented nor tested in an augmented or virtual reality setup, to the best of our knowledge.

This work presents a method to simulate real-time dynamics of one or more virtual systems interacting with physical objects in a mixed reality application. We require no governing equation, as it is learned from data using a thermodynamics-based formulation for non-equilibrium dynamical systems together with geometric deep learning. Furthermore, the trained graph neural network achieves real-time performance which enables a smooth user experience in the interaction of several virtual objects.

3. Methodology

3.1. Problem statement

The present work focuses on the deformation of virtual solid objects. Thus, we use the dynamical equilibrium equation of non-linear solid mechanics which balances the external and internal body forces with the acceleration of the solid. This is,

$$\nabla \mathbf{P} + \mathbf{B} = \rho \ddot{\mathbf{u}} \text{ in } \Omega_0, \quad (1)$$

where \mathbf{B} represents the volumetric force applied to the body and \mathbf{P} the first Piola–Kirchhoff stress tensor. $\Omega_0 = \Omega(t = 0)$ represents the undeformed configuration of the virtual solid. The solution is subjected to appropriate boundary conditions

$$\begin{aligned} \mathbf{u}(\mathbf{X}) &= \bar{\mathbf{u}} \text{ on } \Gamma_u, \\ \mathbf{P}\mathbf{N} &= \bar{\mathbf{t}} \text{ on } \Gamma_t, \end{aligned}$$

with Γ_u and Γ_t representing the essential (Dirichlet) and natural (Neumann) portions of the boundary $\Gamma = \partial\Omega$ of the solid. \mathbf{X} is the undeformed position, \mathbf{N} is the unit vector normal to $\Gamma = \partial\Omega_0$ and $\bar{\mathbf{u}}$, $\bar{\mathbf{t}}$ are the applied displacement and traction respectively. To complete the problem, some relationship between kinematic variables (displacements, strain) and dynamic variables (stresses) must be assumed. The constitutive equation is here chosen to be hyperelastic, with a strain energy function per unit volume Ψ defined such that

$$\mathbf{S} = \frac{\partial \Psi}{\partial \mathbf{E}} \quad (2)$$

where \mathbf{S} is the second Piola–Kirchhoff and \mathbf{E} is the Green–Lagrange strain tensor. Viscoelastic effects are also considered using variable shear relaxation modulus via Prony series. The objective of the method is to solve Eq. (1) in a real-time interactive interface with a physics-based neural network trained with high fidelity solutions.

3.2. Thermodynamics-informed graph neural networks

We use a novel deep learning method [36] which aims to learn the dynamical evolution of a physical system using a graph-based approach. Its objective is to learn not the outcome of a given simulation under different conditions such as forces or boundary conditions, but to be able to learn the *physics* taking place, such that the learned simulator is not sensitive to changes in the mesh, for instance.

The graph neural network architecture is thus constructed on top of a graph structure $\mathcal{G} = (V, \mathcal{E}, \mathbf{g})$, where $V = \{1, \dots, n\}$ is a set of $|V| = n$ vertices, $\mathcal{E} \subseteq V \times V$ is a set of $|\mathcal{E}| = e$ edges and $\mathbf{g} \in \mathbf{R}^{F_g}$ is the global feature vector. Each vertex and edge in the graph is associated with a node in the finite element model from which data are obtained. The global feature vector defines the properties shared by all the nodes in the graph, such as constitutive properties.

To ensure translational invariance of the learned model, the position variables of the system \mathbf{q}_i , are assigned to the edge feature vector $\mathbf{e}_{ij} \in \mathbb{R}^{F_e}$ so the edge features represent relative distances ($\mathbf{q}_{ij} = \mathbf{q}_i - \mathbf{q}_j$) between nodes. The rest of the state variables are assigned to the node feature vector $\mathbf{v}_i \in \mathbb{R}^{F_v}$, while the external forces are included in

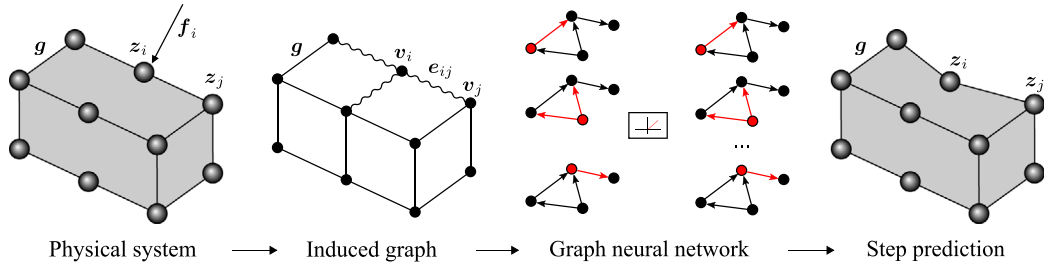


Fig. 1. Thermodynamics-informed graph neural network architecture. The system is described as a set of state variables z_i , global simulations parameters g and external boundary conditions f_i . A graph \mathcal{G} is constructed from the information of the physical system, defining vertex features v_i , edge features e_{ij} and global features g . The graph features are processed with a message-passing graph neural network. The step prediction is performed using the GENERIC integration scheme in Eq. (3), which is repeated iteratively to get the complete rollout of the simulation.

a vector $f_i \in \mathbb{R}^{F_f}$. We employ an encode-process-decode scheme [37], built upon multilayer perceptrons (MLPs) shared between all the nodes and edges of the graph.

We use this architecture to learn the GENERIC structure of the evolution in time of the variables governing the virtual system [38,39]. It consists on splitting the system into a conservative and dissipative contribution. The conservative dynamics are defined using an energy potential E and a symplectic Poisson matrix L , which recover the Hamiltonian formalism, whereas the dissipative dynamics are described by the entropy potential S and the dissipative or friction matrix M , which accounts for the non-reversible dynamics. The time evolution of the state variables of the system z is described by the following equation

$$\frac{dz}{dt} = L\nabla E + M\nabla S. \tag{3}$$

By enforcing the so called degeneracy conditions $L\nabla S = M\nabla E = \mathbf{0}$ together with the algebraic properties of the L (skew-symmetric) and M (symmetric and positive semidefinite) matrices we ensure the energy conservation and the entropy inequality. Thus, we guarantee the thermodynamical consistency of the predictions. The neural network learns the parametrization of the Poisson and friction operators in lower triangular matrices, l and m respectively, and the energy and entropy potentials, E and S . The GENERIC operators are then assembled as $L = l - l^\top$ and $M = mm^\top$, which enforces the skew-symmetry and positive semi-definiteness of the operators. A scheme of the algorithm is presented in Fig. 1.

We assume our virtual solids to be viscous-hyperelastic, so that the state variables for the proper description of their evolution in terms of the GENERIC formalism are the position q , velocity v and the stress tensor σ ,

$$S = \{z = (q, v, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^6\}. \tag{4}$$

The edge feature vector contains the relative deformed position between nodes, to give a distance-based attentional flavor to the graph processing blocks and translational invariance. The velocity and stress tensor components are part of the node feature vector, concatenated to a two-dimensional one-hot vector n which represent the encastre and solid nodes respectively. The external load vector f_i is included in the node processor MLP as an external interaction. No global feature vector is needed in this case, resulting in the following feature vectors:

$$e_{ij} = (q_i - q_j, \|q_{ij}\|_2), \quad v_i = (v, \sigma, n). \tag{5}$$

Thus, the dimensions of the feature vectors are $F_e = 4$, $F_v = 11$, $F_f = 3$ and $F_g = 0$.

3.3. Vision system

For an augmented or mixed reality application, we need to include virtual objects in a real scene. For that, it is necessary to have a sensor able to get information about the physical environment and a screen device to plot the resulting image. In the present work, we use a ZED Mini stereo vision system from Stereolabs, which is able to retrieve both a depth and RGB image of the captured snapshot. We plot the resulting real-time video stream in a computer screen, but could be extended to a VR headset or AR glasses.

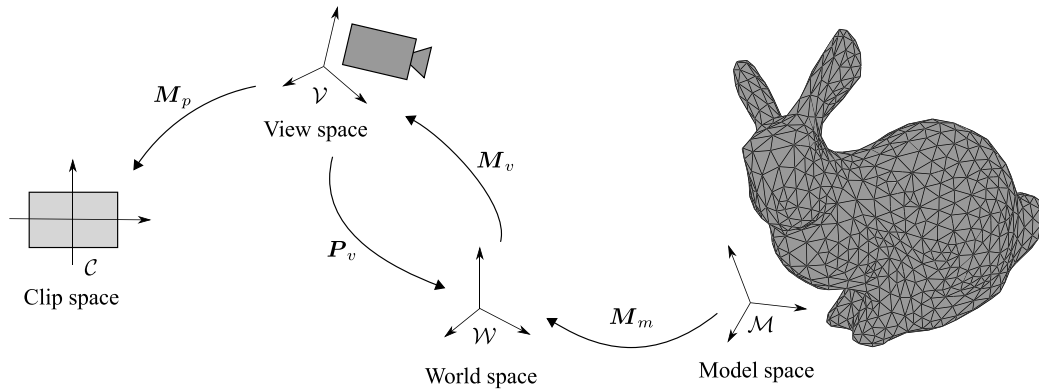


Fig. 2. Model-view-projection transformation between the model and the clip coordinates. The dynamics and interactions are computed in the model space as 3D coordinates, whereas the visualization pipeline requires a 2D clipping coordinates in a fixed range between -1 and 1 .

As the laws of motion are independent with respect to any frame of reference (objectivity), we use the model space to compute the dynamical state variables of the system. However, the visualization pipeline requires the coordinates to be in a normalized range of $\mathcal{C} = [-1, 1] \times [-1, 1]$ called the clip space. The transformation between the 3D model space and the 2D clip space is achieved by the definition of the Model-View-Projection matrix (see Fig. 2). From now, the point coordinates are supposed to be in homogeneous coordinates.

- **Model:** The dynamics are computed in a local frame of reference called the model space \mathcal{M} . The position, orientation and scale of the model can be defined as a set of transformation matrices T_m , R_m and s_m respectively with respect to the world space \mathcal{W} , considered to be the usual Euclidean space \mathbb{R}^3 .

$$\mathbf{x}_{\text{world}} = M_m \mathbf{x}_{\text{model}} = T_m R_m s_m \mathbf{x}_{\text{model}}. \quad (6)$$

- **View:** In a similar fashion, the viewing camera also has a model matrix defining its position in the world space, which is commonly designed as the extrinsic parameters P_v of the camera pose. This information can be obtained using a monocular pose estimator or triangulating with a stereo vision system. Thus, the camera or view space \mathcal{V} can be determined by a set of transformations from the world space using the camera extrinsic parameters given by a rotation R_v and translation T_v matrices.

$$\mathbf{x}_{\text{view}} = M_v \mathbf{x}_{\text{world}} = P_v^{-1} \mathbf{x}_{\text{world}} = (T_v R_v)^{-1} \mathbf{x}_{\text{world}}. \quad (7)$$

- **Projection:** The last transformation is in charge of projecting the 3D coordinates into the 2D clip space \mathcal{C} . First, in order to get a realistic visualization, we use a perspective projection M_p based on the camera viewing frustum

$$M_p = \begin{pmatrix} \cot \frac{\alpha}{2} & 0 & 0 & 0 \\ 0 & \cot \frac{\alpha}{2} & 0 & 0 \\ 0 & 0 & -\frac{z_{\text{far}} + z_{\text{near}}}{z_{\text{far}} - z_{\text{near}}} & -\frac{2z_{\text{far}}z_{\text{near}}}{z_{\text{far}} - z_{\text{near}}} \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad (8)$$

where α is the field of view of the camera and z_{near} and z_{far} are the minimum and maximum distance of the clipping plane. This creates a normalized 3D viewing box of the camera, which is then projected in the 2D clip space by the vertex shader. Thus, the final coordinates can be computed using the following equation:

$$\mathbf{x}_{\text{clip}} = M_p \mathbf{x}_{\text{view}} = M_p M_v M_m \mathbf{x}_{\text{model}}. \quad (9)$$

By defining the Model-View-Projection matrix as $M_p M_v M_m$ we can compute the clip coordinates directly from the model coordinates computed by the thermodynamics-informed neural network.

3.4. Visualization system

The visualization of the resulting image is performed using OpenGL and the GLU library. This pipeline requires the definition of two spatial functions, run sequentially on the GPU, called the vertex and fragment shaders. The vertex shader defines the vertex position of the entities to display whereas the fragment (or texture) shader define the RGBA colors for each rasterized pixel.

Each vertex position is computed using Eq. (9) from the deformed configuration coordinates and the polygons are drawn based on the connectivity matrix of each solid. The color of each vertex is computed directly from the neural network prediction using a fixed colormap. Additionally, a basic lighting model was added to the fragment shader to increase the realism of the virtual objects using the Phong shading. This model computes each RGB pixel intensity as

$$\mathbf{I} = k_a \mathbf{i}_a + k_d (\mathbf{l} \cdot \mathbf{n}) \mathbf{i}_d + k_s (\mathbf{r} \cdot \mathbf{v})^\beta \mathbf{i}_s, \quad (10)$$

where k_a , k_d and k_s are the ambient, diffuse and specular reflection constants, β is the shininess constant of the material and \mathbf{i}_a , \mathbf{i}_d and \mathbf{i}_s are the RGB color intensities of the ambient, diffuse and specular components. The illumination varies depending on the geometry of the scene and camera position, where \mathbf{n} is the surface normal vector, \mathbf{l} and \mathbf{r} are the directions of the light source and its perfect reflection, \mathbf{v} is the viewing direction and “ \cdot ” is the dot product.

We have also implemented a depth or z -buffer in the fragment shader which compares on each pixel the depth of virtual and real objects on the scene and renders only the closest to the camera. This accounts for every occlusion that the vision system may encounter. The depth of the scene seen by the camera is computed directly using the stereo vision system.

3.5. Collision and contact

We use a high-fidelity hand tracker from MediaPipe [40] which provides an accurate localization of the finger tips. By using the inverse transformation of Eq. (9), we can compute the 3D coordinates of the finger tips in the model space and compute the distance to each node of the virtual object. When this distance is less than a small threshold, collision is detected and a prescribed force is applied to the model. A similar procedure is applied to the collision of several virtual objects.

The code is implemented in Python using the PyOpenGL wrapper for the visualization and Pytorch Geometric [41] for the deep learning training and evaluation. The videos are generated using a standard desktop computer with a single Nvidia RTX2070 GPU and provided as supplementary material. The code for the implementation of the thermodynamics-informed neural networks and the video sequences are publicly available at <https://github.com/quercushernandez>.

4. Results

4.1. Bending beams

The first system is composed of two interacting viscoelastic beams. Both identical beams are assembled with a small gap between each other, allowing for a contact interaction, as depicted in Fig. 3.

The dimensions of the beams are $H = 10$, $W = 10$ and $L = 40$. The finite element mesh from which data are obtained consists of $N_e = 500$ hexahedral linear brick elements and $N = 756$ nodes. The constitutive parameters of the hyperelastic strain energy potential are $C_{10} = 1.5 \cdot 10^5$, $C_{01} = 5 \cdot 10^3$, $D_1 = 10^{-7}$ and $\bar{g}_1 = 0.3$, $\bar{g}_2 = 0.49$, $\tau_1 = 0.2$, $\tau_2 = 0.5$ respectively for the two-term Prony series. A distributed load of $F = 10^5$ is applied in 52 different positions with a perpendicular direction to the solid surface. Each simulation is composed of $N_T = 20$ time increments of $\Delta t = 5 \cdot 10^{-2}$ s. Both beams are assembled in 90° with a gap of $g = 10$.

The graph neural network vertex and edge MLPs have two layers of $F_h = 100$ neurons each, with 10 message passing sequential blocks. The training was performed for $N_{\text{epoch}} = 1800$ epochs and learning rate $l_r = 10^{-4}$.

Fig. 4 shows a real-time video sequence generated using the presented algorithm. The interaction of both the real objects (finger tips) and the virtual objects are simulated smoothly at more than 30 frames per second. It is important to highlight that during a video sequence the trained neural network is able to generalize to previously

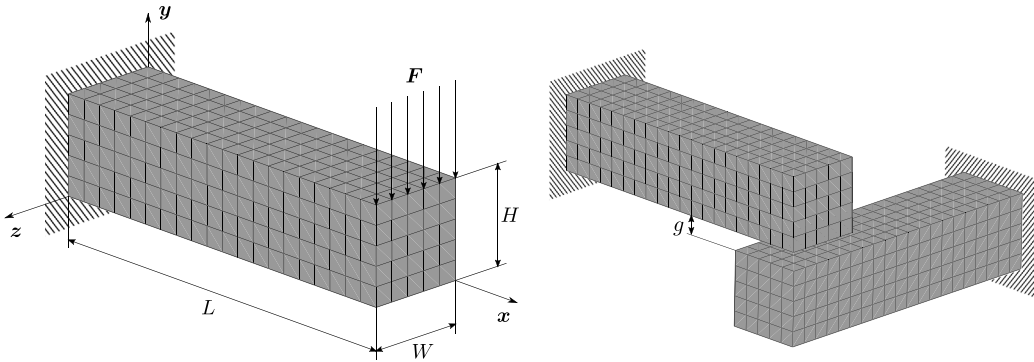


Fig. 3. Interacting beams geometry scheme. Both beams are angled with a gap between both, enabling their interaction.

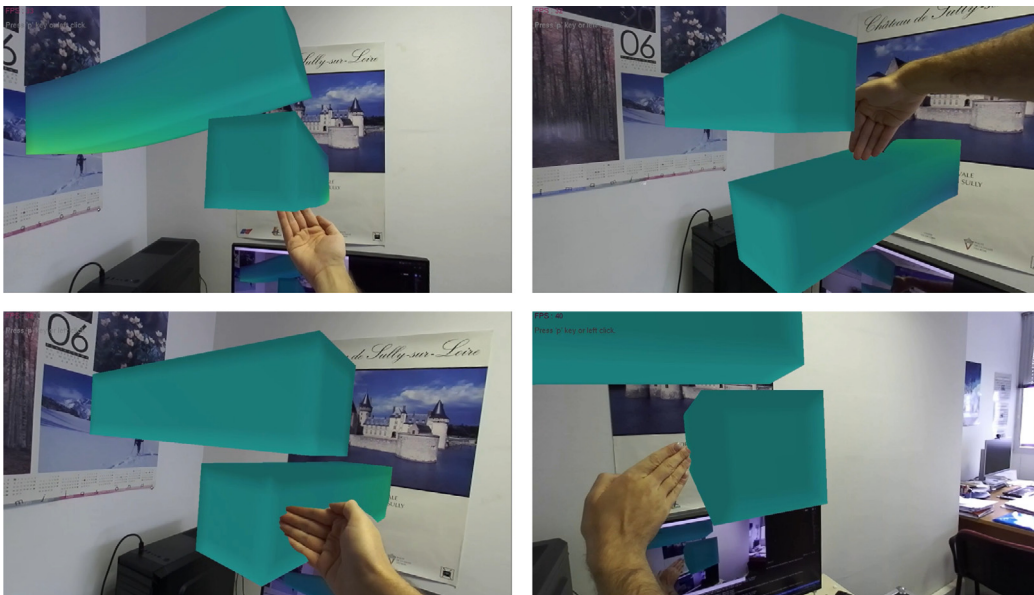


Fig. 4. Frames extracted from the interacting beams sequence. Color encodes the x-x stress field component associated with the displacement imposed by contact with a real object.

unseen configurations. The quantitative errors by the neural network in the real-time rollout predictions are shown in Fig. 7a, which remain below 1% in position and velocity and 10% in the stress tensor field.

The computational cost of the high fidelity FEM simulations used for the training of the neural network is 15 s per simulation, up to 795 s for the whole dataset, and 243 Mb in memory storage. Conversely, the training time of the neural network is 4.5 h and the mean evaluation time is 9 ms with a memory storage of 12.3 Mb. Thus, the use of a deep learning approach allows a drastic reduction of the online computation time with the inconvenient of larger offline training time. It is also worth noting that the network parameters are more than 10 times lighter in terms of memory storage.

4.2. Stanford bunny

The second example is a bunny mesh from the Stanford 3D scanning repository, which is a more complex geometry as the one shown in the previous example. It is a standard reference model in computer graphics research. The model is represented in Fig. 5.

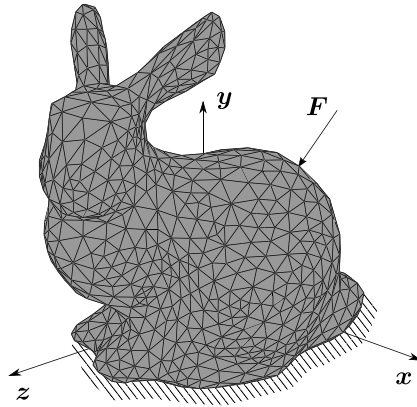


Fig. 5. Bunny mesh geometry with a concentrated application force and bottom encastre.

The finite element mesh from which data are obtained consisted of $N_e = 4941$ tetrahedral linear elements and $N = 1352$ nodes. The constitutive parameters of the hyperelastic strain energy potential are $C_{10} = 2.6 \cdot 10^{-1}$ and $D_1 = 4.9 \cdot 10^{-2}$. Similarly as the previous case, a concentrated load of $F = 1$ is applied in 100 different positions with a perpendicular direction to the solid surface. The body was fixed to the ground plane by disabling displacements and rotations at the lower model nodes. Each simulation is composed of $N_T = 20$ time increments of $\Delta t = 5 \cdot 10^{-2}$ s.

The graph neural network vertex and edge MLPs have two layers of $F_h = 100$ neurons each, with 10 message passing sequential blocks. The training was performed for $N_{\text{epoch}} = 1800$ epochs and learning rate $l_r = 10^{-4}$.

Fig. 6 shows a real-time video sequence generated using the bunny model, also with a minimum framerate of 30 frames per second. In this case the stress field errors reported in Fig. 7b are higher due to the stress peaks at the single-node force application, which causes that the elasticity phenomena remain very local in space.

In this case, the computational cost of the high fidelity FEM simulations is 27 s per simulation, up to 2700 s for the whole dataset and 833 Mb in memory storage. The dataset and edge count is much larger in this example, which increases the training time of the neural network to 20 h and the evaluation time to 11 ms with the same memory storage as the previous example. Thus, the data compression is even bigger in this case. To address the high training time and errors due to stress peaks, several future improvements are discussed in the next section.

5. Conclusions

We presented a real-time augmented reality simulator, which enables a user to interact with virtual deformable solids. The predictions are computed using the GENERIC structure of the system learnt with a message passing graph neural network. The enforcement of such physics constraints guarantees the fulfillment of the first and second laws of thermodynamics. The resulting algorithm has a wide variety of applications not only in the entertainment industry, but also in engineering design or manufacturing, where the visualization of augmented data superimposed in a real or virtual object might redefine the next generation of industry 4.0 and digital twins.

Our method has several limitations which might be addressed as future work. The scalability to bigger meshes is a challenging task, as graph neural networks can suffer from over-squashing or bottlenecks [42,43]. The use of graph reduction techniques via graph autoencoders [44] or U-nets [45] configurations can significantly reduce the computational requirements in larger meshes. This would also reduce the stress peaks discontinuities due to concentrated forces. The message passing algorithm itself is not able to handle domains where the boundary conditions are very far away from the prescribed forces. This can be mitigated by implementing a global attention vector so that certain dynamical information is reached to all the nodes of the domain instantly.

The visualization and data acquisition are possible due to the graphics acceleration. Even if the current work was implemented in a desktop computer as a proof of concept, only a small fraction of all the computational resources were used, so it can be extended to AR/VR headsets or to modern mobile devices. For the same reason, higher

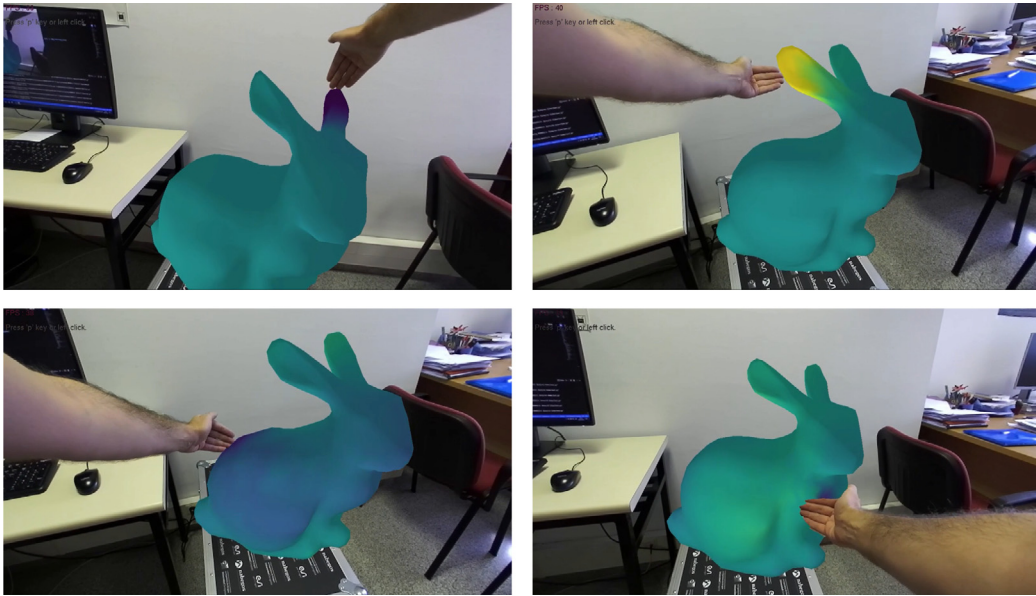


Fig. 6. Frames extracted from the bunny sequence. Color encode the x displacement field component imposed by contact with a real object.

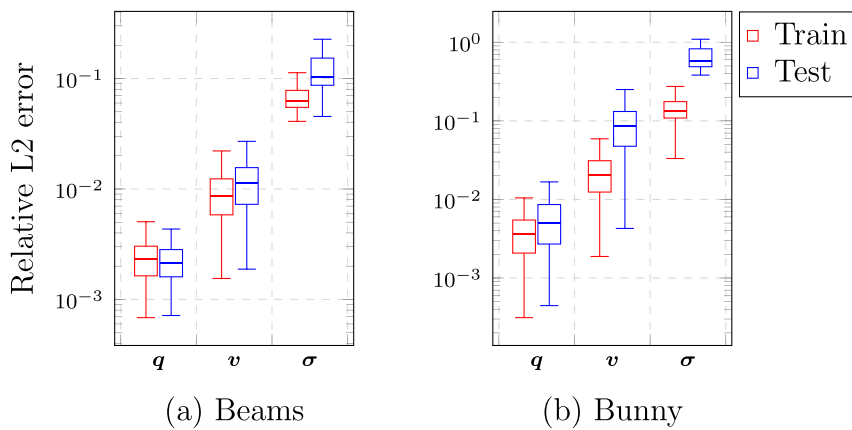


Fig. 7. Box plots for the relative L2 error for all the rollout snapshots of the bunny dataset in both train and test cases. The state variables represented are position (q), velocity (v), and stress tensor (σ).

framerates might be achieved by fine-tuning and optimizing the proposed network structure or porting the code to a higher-performance language such as C++. Occlusions in real-time augmented reality software still remain as an open problem in the computer vision community [46,47]. The stereo depth estimation is an approximation which might cause image artifacts in singular camera poses. For instance, some works handle the problem by using deep learning [48] but it is out of the scope of this manuscript.

This work is just a small step forward towards the new immersive technologies which can potentially deeply change our society. It is a multidisciplinary problem where computer vision, computer graphics, machine learning and computational mechanics must meet to define new algorithms for a new digital revolution.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Elias Cueto reports financial support was provided by Spanish Ministry of Science. Elias Cueto

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Data availability

Data will be made available on request.

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