Graph neural network preprocessing for purpose of digital twin of mechanical system

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***Abstract*—Graph neural networks might be brilliant tool how to effectively build digital twin of mechanical system and more.**

The suggested pre-step technique of of novel hybrid modelling is introduced as subset of the main hypothesis, where is assumed synergy between positives of hybrid modelling. Those are especially descriptiveness of model, which is characteristic for physical based modelling. Fast execution and results delivering is than underlying approach of data driven modelling.

Therefore is explored possibility into building empirical model based on extraction of FE model structure with aim to reinforcing whole model by new by information, f.g. measurement data.

***Index Terms*—digital twin, graph neural networks, finite element method, Fibonacci's spring**

I. Introduction

Digital twin (DT) is currently well known words (one can say - nearly cliche) whose cannot be such easily overlooked. This term is carrying a simple idea in imitation of a real system in a virtual environment. DT has been usually connected in context with artificial intelligence and that is fact for most scientific fields. Since it is not absolutely clear what DT should have covered, it is obvious that there exist various approaches on how to build a DT of a certain system. This tool might have a big potential from a whole perspective to solving specific tasks, where different types of information are available. Those information might be measured data, but also models with certain accuracy describing particular phenomena.

Following lines are devoted to the topic of designing DT by usage of graph neural networks (GNN) with combination of finite element method (FEM) in order to store knowledge of some kind of mechanical or multi-physical system. For this purpose, it has to be initially defined the whole mechanical system in FEM software and then, this representation can be transferred to the graph network, which will be further used for the purpose of GNN in order to closely imitate behaviour of a real system.

First three subsections are aiming to briefly describe basic topics DT, GNN and FEM. Those are necessary ingredients for final compilation to a hybrid model of mechanical system. Next section is then describing how to pre-process and create GNS based on the geometry extracted from FEM model representation.

A. Digital twin

The concept of DT might be defined as an adaptive model of a physical system combining various approaches of mathematical modelling with connection of current technologies [1]. Those technologies can be multi-physical solvers, cybernetic of big data, artificial intelligence, augmented and virtual reality. DT can be also defined as the next milestone of simulations connected to the real world. This milestone was aptly depicted in [1] as a successor of product life cycle management approach (PLM), which is in exaggeration simple tool managing database of models and measured data concerned to a specific product.

B. Hybrid modelling

Term Hybrid modelling can be described as approach, which is combining two different types of model building - data driven modelling (DDM) and physical based modelling(PBM). DDM si not more, than building empirical model based on experimental data with usage of statistical methods, or with help of AI and machine learning (ML) methods. On other hand PBM is more transparent approach, with contrary to DDM. Usually, geometrical description of system with combination of FEM is helping to analyse system very deeply and inaccuracy can be easily found, since the partials equation of specific tasks are known. Main cons of PBM are traditionally very high computational cost, which should be reduced when the DDM is used.

C. Graph neural networks

GNN is used for model creation by nodes and edges [2]. Interaction between neighbours are defined by edges, which can (not) have specified direction concerning information exchange. A graph can describe various systems, from social networks in order to investigate voting preferences, or for purpose weather forecasts based on data from weather stations. Most Likely, GNN can be used for compiling information from FEM, where the model already has defined nodes and between them are specified behaviours by element information.

Architecture of probably the latest neural network is by author understood as a more corresponding architecture of the biological brain. The view is coming from naive idea, that the brain has no really defined input and output layer of neurons as

it is usual in standard feed forward neural networks (FFNN), but has specific areas, which are activated in time based on different actions. In other words, specific groups of neurons are excitated by certain subjects. Another comparison GNN to FFNN is the fact that the biological brain is not built by a neat structure of layers of neurons, yet the chaotic graph is more representative, when close neurons are connected.

II. Illustrative mechanical system - Fibonacci's spring

For demonstration of main idea were designed simple geometry of Fibonacci's spring (FBS). FBS is not really following the standard golden spiral and geometry has a slightly different growing ratio of logarithmic spiral. The purpose of designed part is to have mechanical system with visually helpful geometry in order to briefly describe main topic of article.

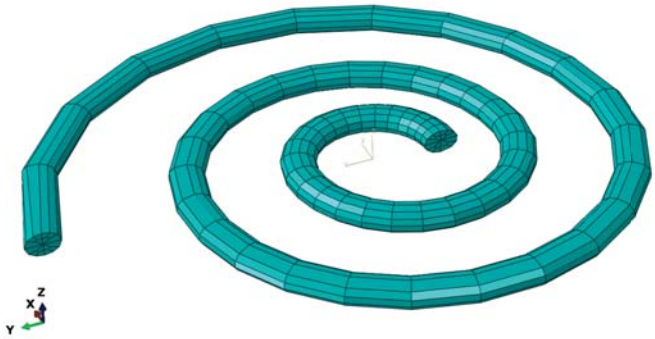

Fig. 1. Representative example of mechanical system - Fibonacci spring

A. Mesh of FBS

Continuously growing mesh seed applied on the part is established only by hexahedral elements. The path defining sweeped pattern on the cross section is located on the inner edge of FBS. This pattern is chosen due to expectations of not sharp bricks in mesh structure, which brings at least usually good convergence behaviour of the FEM model important for potential further investigation.

Linear Hexahedral elements of the FBS part were chosen for the aspect of following simple numbering convention and therefore can be the shape of the part imitated back, once a GNN is built. Mentioned element is in Abaqus software well known abbreviation C3D8, which is not really recommended for tasks, where accurate model is needed, but for our purpose to initiate GNN is more than sufficient.

B. Input information for GNN

Input file (INP) generated in computer aided engineering (CAE) software is containing information regarding the whole FEM model needed for solver performing than calculation of task. INP is not more than a text file representing by its keywords the most important behaviour of a model, such as the

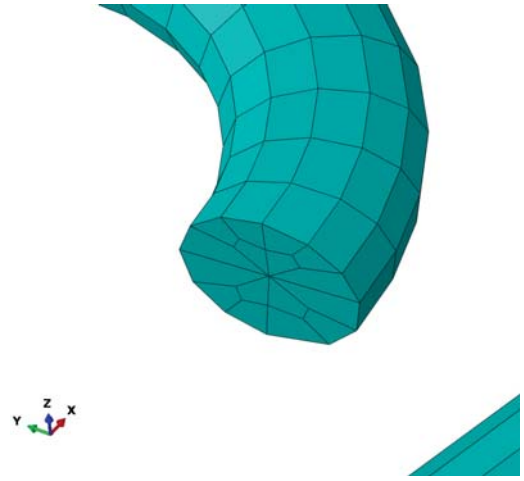

Fig. 2. Detail of sweeped pattern along the inner edge of FBS

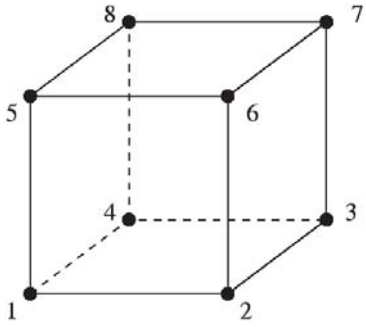

Fig. 3. Element C3D8 and convention of nodes numbering

geometry of the model, materials used, boundary conditions, load, etc. In this INP we will for the next step need information concerning mesh representation. Our essential keywords are:

- *Node ... specification of node label and its space position
- *Element ... with type definition (f.e.: type=C3D8) with element label and nodes shaping certain element

C. Building GNN

Once the information regarding FEM model mesh is available the GNN architecture can be initiated. For this purpose it is selected to use programming language Python and especially Deep Graph Library (DGL) which is mainly developed for deep learning applied on a graph structure. By DGL tool can then be defined graph G based on previously extracted nodes information N and edges E.

$$G = (N, E) \tag{1}$$

One interesting aspect about graphs is that not usually euclidean dependency is required and for their function, position of nodes in space are not really important. Therefore, following possible visualisation of FBS in GNN is not a big

surprise. On 4 can be seen detail of small area focusing on connection made between neighbouring nodes.

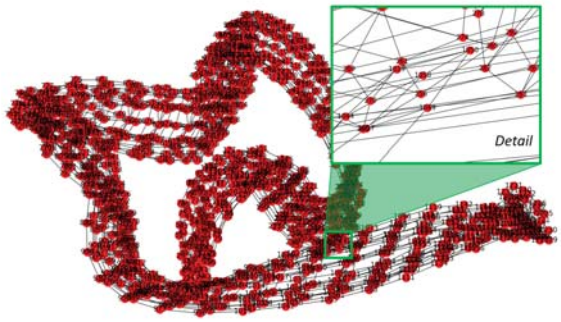

Fig. 4. Possible visualisation of PBS by GNN

Human eye needs to see the initial model and this need can be fulfilled, of course. Since, the INP is still available we can to G put information of N position and then visualise back the full part accordingly to specifications needed.

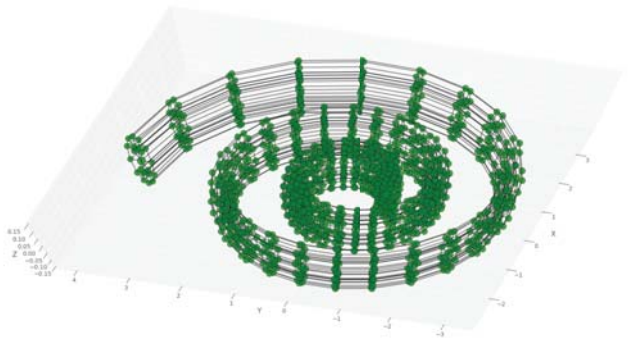

Fig. 5. Visualisation of PBS GNN with positions of nodes in order to validate correctness of built GNN

III. Further works in GNN and FEM hybrid modelling

Previous lines has briefly introduced the main idea of author hypothesis, that graph neural networks as representative of data driven modelling, might be an elegant tool for building a digital twin with help of physical based modelling such as finite element method and was shown as initial step into exploration of topic.

Since, there are many hidden steps, the next one is to distinguish between hierarchical graph structures focusing on idea of loads definition present in system.

Another obvious milestone will be into extracting results data from FEM model and pre-process them (deflections, stresses, etc.) in order to have correctly prepared data-set for learning developed architecture of GNN.

IV. Conclusions

In the article were introduced 3 essential topics which are necessary for compilation of presented pre-processing of GNN.

Next section was devoted to a brief description of workflow dealing with conversion of the FEM model - FBS into the final requested graph.

Last but not least point of article was dealing with few lines introducing next author's intentions in the area focusing to develop theory concerning of building DT by a hybrid modelling with mentioned combination of mathematical approaches.

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