A physics-guided recurrent machine learning model for long-time prediction of nonlinear partial differential equation

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I. Introduction

The apparition of hot spots is one of many challenges that slow the adoption of second-generation high temperature superconductor coated conductor (2G HTS CC). Hot spots appear due to the variation of the critical current along the length of the tape. When the injected current reaches a low local critical current, it results in the generation of heat and a rapid rise of the local temperature (hot spot). This generation of heat can lead to the formation of a normal zone (quench) and its propagation under certain conditions.

It is possible to simulate the quench dynamics of 2G HTS CC by solving the coupled electro-thermal equations using a finite element method. Indeed, the heat equation and the current continuity equation are coupled by the heat source, which is defined by the Joule losses generated by the hot spots. One of the challenges of this problem is the nonlinear nature of superconductor conductivity which can make the computation expensive and unstable. Moreover, for particular architecture of HTS tape, the simulation has to be done in 3D, which leads to simulations that last many hours.

Instead of using deterministic methods like the finite element method to simulate the quench dynamics, we propose in this work to use a "physics-guided" data-driven method in order to speed up the computation. The model we propose is inspired by recent work on machine learning (ML) models that have been developed to solve nonlinear dynamical systems [1], [2]. It is also inspired by some studies who tried to incorporate some structure of classical numerical methods (like finite difference and finite volume methods) in their model architecture [3].

II. Machine learning model

The model we propose is a physics-guided recurrent ML model used to make long-time predictions of the temperature evolution over time in the presence of hotspots of a 2G HTS CC. Our model speeds up substantially the resolution of the full 3D electro-thermal coupled problem. The ML model is trained with multiple simulations of quench propagation generated by a standard finite element solver (COMSOL). The different simulations are run with randomly generated parameters like the tape architecture, the initial conditions and the heat source. The model is expected to predict the quench dynamics for any architecture and initial condition without the need for retraining. The model is then used in a recursive way to predict the temperature along the tape at every time step. To test the ML model progressively, we decided to decouple the thermal and electrical problem. To do so, two ML models are defined: a model to predict the electric field (f_E) and a model to predict the temperature (f_T). The architecture of f_E is a simple neural network. This model is trained using values of temperature (T) and electric field (E) along the tape, extracted directly from the 3D COMSOL simulation. This model is relatively easy to fit since the relationship between T and E is related to the power law (imposed in the COMSOL simulation) and the current sharing between the layers of the HTS tape.

The model f_T is the real innovation of this work. It is characterized by an architecture that uses hard physical constraints under a Dufort-Frankel discretization scheme of the nonlinear heat equation in order to guide the solution to respect the conservation of energy and heat fluxes. The model is implemented using the deep learning library PyTorch. The material properties (defined as a function of temperature) are implemented as two neural networks, which give some degree of freedom to the model. The spatial derivatives of the material properties are obtained using the "automatic differentiation" described by Raissi [4]. Also, the finite differences, defined by the Dufort-Frankel discretization scheme are implemented using convolution layers implemented with PyTorch. The weights of the different filters of these layers add additional degrees of freedom to the model.

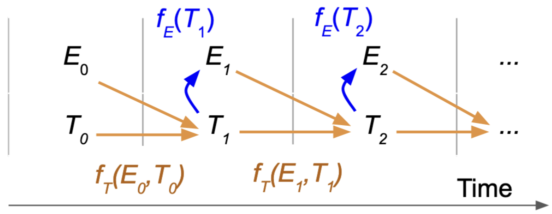

Fig. 1. Decoupling of the thermal and electric problem with two ML models (f_E and f_T)

The two models (f_E and f_T) are used in a recursive, way as describe in figure 1. The model f_T is first used to predict the temperature at the next time step. Then, f_E predicts the electric field at this new time step. The same process is repeated every time step in a recursive manner. In order to reduce the accumulation of errors due to the recursive nature of the model, an adaptive training strategy is used [1]. One could say that, to avoid the accumulation of error, a non-recursive technique could be employed in order to avoid the problem of error accumulation. However, because the heat source changes every time step and depends on the previous predictions, the model has to be recurrent and the problem has to be solved step-by-step.

Many COMSOL simulations were generated for different heat source profiles in order to generate a dataset that can feed f_T. Ten simulations were run using a randomly generated time-varying heat source that emulates the dynamics of hot spots. The nonlinear heat equation was solved in 3D using the heat transfer module of COMSOL on a geometry consisting in a stack of silver, YBCO and hastelloy thin films. The problem could have been solved in 1D, but we created a 3D COMSOL model in order to consider 3D effects on the quench dynamics in a near future.

III. Results

Figure 2 shows the root mean squared error (RMSE) of the ML model on the test set compared to the finite element true solution (COMSOL) along time. The error is the average of the temperature distribution along the tape at each time step. The predictions are compared with a solution computed using a standard finite difference method (FDM) in 1D. One can see that the ML model (trained with the 3D COMSOL simulations) outperform the standard FDM and seems less affected by the accumulation of error.

Figure 3 shows an example of prediction of the material properties learned during the training. The neural networks learned properly the temperature-dependent material properties in the range of temperature seen during the training (vertical dotted lines).

IV. Conclusion

We showed that our machine learning model can minimize the accumulation of error compared to a standard

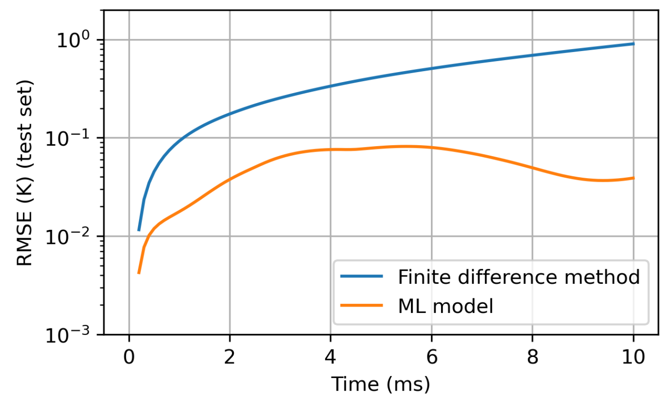

Fig. 2. Error of the ML model and the finite difference method vs. time

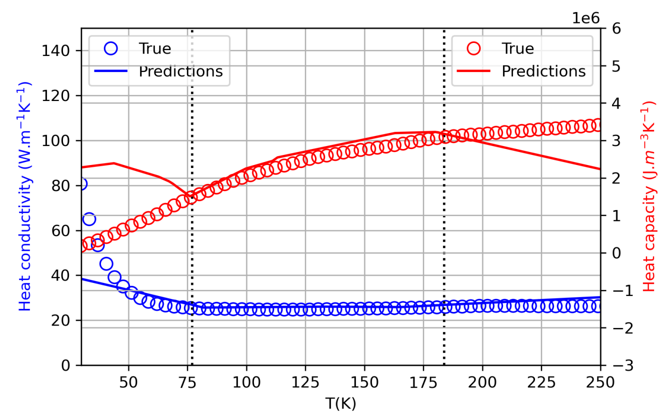

Fig. 3. The true values of material properties were used to generate the dataset. The prediction are made using the two neural network (after training) used to describe the temperature dependence of these variables. Only values lying between the vertical dotted lines were learned by the ML model.

numerical method (here the finite difference method). We also showed that the temperature-dependent material properties can be learned from finite element simulation results. Finally, we showed that for simple cases, the model converges to a classical finite difference method, but it has the potential to generalize to more complex cases and include effects that a simple classical numerical methods cannot take into account.

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References

[1] S. Li and Y. Yang, Journal of Sound and Vibration, vol. 506, p. 116167, 2021.

[2] Q. Teng and L. Zhang, AIP Advances, vol. 9, no. 8, p. 085311, 2019.

[3] B. Stevens and T. Colonius, arXiv preprint arXiv:2002.03014, 2020.

[4] M. Raissi, P. Perdikaris, and G. E. Karniadakis, Journal of Computational Physics, vol. 378, pp. 686–707, 2019.