Burn wounds immune response 3D surrogates

1 Project Description

We have assessed long short-term memory (LSTM) and physics-informed neural networks (PINNs) for surrogate modelling of an agent-based model of burn wound immune response in a 2D space [1]. We aim to utilize the methods from our paper [1] and improve them. Inspiration could be drawn from recent work utilizing Deep Operator Networks (DeepONets) [2] combined with PINNs [3] entitled OL-PINNs [1], which have been shown to be effective in diffusion systems.

The student must take into account the fact that the model will be extended to a 3D domain in the future, as such Gate Recurrent Units (GRUs) should be considered as they are less computationally expensive. More specifically, the student should also consider ConvGRUs [4].

Multiple neural network architectures can be constructed and assessed, where we also aim to study functions to ensemble predictions of different neural network architectures to deal with uncertainty in our predictions.

Modifications can also be introduced to the model to increase model robustness so ML techniques (e.g: transfer learning) could be applied and the model could be extended to different domains.

2 Requirements

DeepONets approximate mathematical operators in ODE/PDEs, so the student must be able to understand what they have to approximate in order to construct and assess the NNs effectively. The implementation of DeepONets/PINNs through the DeepXDE library is not that hard as long as you understand what the neural network must learn, however, DeepXDE allows you to experiment with a number of things (for example you can set ’hard’ or ’soft’ boundary conditions, which again requires an understanding of the agent-based model).

Prior experience with deep learning and HPC is helpful but not necessary. The ability to understand the PDEs and the ABM is much more important for this project.

Expectations: Biological knowledge is also not a prerequisite, but you will learn the meaning behind the numbers you see and what this translates to a real human simulation, so you know you are not getting “out of the world” results. All our students usually end with at least one publication of their work in a peer-reviewed journal or conference. You are expected to be able to explain your results/methods in Layman speech (able to explain to a kid in normal everyday words).

3 References

[1] Bin Lin, Zhiping Mao, Zhicheng Wang, and George Em Karniadakis. Operator learning enhanced physics-informed neural networks for solving partial differential equations characterized by sharp solutions, 2023.

[2] Lu Lu, Pengzhan Jin, and George Em Karniadakis. Deeponet: Learning nonlinear operators for identifying differential equations based on the universal approximation theorem of operators. *CoRR*, abs/1910.03193, 2019.

[3] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378:686–707, 2019.

[4] Jiyong Zhang, Tao Deng, Fei Yan, and Wenbo Liu. Lane detection model based on spatio-temporal network with double convolutional gated recurrent units. *IEEE Transactions on Intelligent Transportation Systems*, 23(7):6666–6678, July 2022.