Research Statement

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Deep learning techniques have led to major scientific breakthroughs in the past few years, from solving the protein folding problem [Jumper et al., 2021] to better predicting extreme weather events [Price et al., 2025] and discovering millions of new materials [Merchant et al., 2023]. Many scientific challenges remain to be overcome, but these successes show the potential of carefully crafted deep learning approaches to solve scientific problems. Hence, my research lies at the intersection of deep learning and physics simulation, with the goal of combining data-driven approaches and physical science to solve complex scientific problems. Applications in which I am interested include numerical simulations, meteorological forecasts, material discovery, and astrophysics.

Contributing to future success implies developing deep learning methods that have high capacity - for meaningfully processing very large amounts of unstructured data - and provide coherent predictions that follow governing physical laws and ensure interpretability. My research aims to leap towards these objectives by focusing on:

1. **Encoding physical priors in deep learning models:** When modeling phenomena from environments subject to known physical governing laws, we can provide these physical priors to the models in numerous ways. For instance, physics-informed neural networks (PINNs) [Raissi et al., 2019] solve partial differential equations (PDEs) by evaluating the residuals of these PDEs in their loss functions. I will use this method to achieve physical coherence and higher performance for forecasting and inverse problems [Hammoud et al., 2022] (e.g., numerical weather prediction and climate downscaling).

2. **Exploring generative models for physics:** Generative models offer a powerful framework for capturing the inherent variability of complex physical systems while enabling quantification of uncertainty in predictions. However, a persistent challenge lies in assessing the meaningfulness of the variability learned by these models across various scientific applications. My research aims to address this issue by leveraging advanced generative deep learning techniques, such as diffusion models and flow matching, to tackle complex scientific problems. Furthermore, I seek to integrate the Physics-Informed Neural

Networks (PINN) framework — originally developed for deterministic modeling — into generative modeling approaches [Bastek et al., 2024]. This hybrid methodology aims to combine the strengths of PINNs with generative models, fostering more robust and interpretable solutions for challenging scientific domains.

Current research. In an ongoing research project aligned with **(1)**, I improve downscaling of extreme precipitation events by regularizing the loss function with Clausius-Clapeyron scaling, a known physical relationship between relative humidity and temperature [Moustakis et al., 2020]. Regarding **(2)**, in a manuscript currently under review, I implement a probabilistic U-net and outperform deterministic approaches on a climate downscaling task, better capture precipitation spatial patterns, and improve performance on extreme precipitation events.

References

[Bastek et al., 2024] Bastek, J.-H., Sun, W., and Kochmann, D. M. (2024). Physics-informed diffusion models.

[Hammoud et al., 2022] Hammoud, M. A. E. R., Titi, E. S., Hoteit, I., and Knio, O. (2022). Cdanet: A physics-informed deep neural network for downscaling fluid flows. *Journal of Advances in Modeling Earth Systems*, 14(12):e2022MS003051. e2022MS003051 2022MS003051.

[Jumper et al., 2021] Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Žídek, A., Potapenko, A., Bridgland, A., Meyer, C., Kohl, S. A. A., Ballard, A. J., Cowie, A., Romera-Paredes, B., Nikolov, S., Jain, R., Adler, J., Back, T., Petersen, S., Reiman, D., Clancy, E., Zielinski, M., Steinegger, M., Pacholska, M., Berghammer, T., Bodenstein, S., Silver, D., Vinyals, O., Senior, A. W., Kavukcuoglu, K., Kohli, P., and Hassabis, D. (2021). Highly accurate protein structure prediction with AlphaFold. *Nature*, 596(7873):583–589.

[Merchant et al., 2023] Merchant, A., Batzner, S., Schoenholz, S. S., Aykol, M., Cheon, G., and Cubuk, E. D. (2023). Scaling deep learning for materials discovery. *Nature*, 624(7990):80–85.

[Moustakis et al., 2020] Moustakis, Y., Onof, C. J., and Paschalis, A. (2020). Atmospheric convection, dynamics and topography shape the scaling pattern of hourly rainfall extremes with temperature globally. *Communications Earth & Environment*, 1(1):11.

[Price et al., 2025] Price, I., Sanchez-Gonzalez, A., Alet, F., Andersson, T. R., El-Kadi, A., Masters, D., Ewalds, T., Stott, J., Mohamed, S., Battaglia, P., Lam, R., and Willson, M. (2025). Probabilistic weather forecasting with machine learning. *Nature*, 637(8044):84–90.

[Raissi et al., 2019] Raissi, M., Perdikaris, P., and Karniadakis, G. (2019). 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.