Andre Nogueira de Souza

Scientific Machine Learning & AI Physics Engineer | Industrial Simulation, HPC & Surrogate Modeling
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Summary

Scientific Machine Learning / AI Physics engineer with a PhD in applied mathematics and 10+ years of experience across machine learning, high-performance computing, generative modeling, stochastic dynamics, uncertainty quantification, and physical simulation. At Rescale, I build production-oriented AI-for-engineering workflows for industrial simulation data, including surrogate modeling systems, model-selection workflows, training and evaluation pipelines, benchmark methodology, GPU/HPC optimization, and customer-facing technical validation. Research background spans fluid mechanics, climate physics, generative modeling, stochastic dynamics, and high-performance scientific computing.

Core Strengths

- Scientific machine learning for physical systems: surrogate modeling, transformer architectures, neural operators, generative modeling, probabilistic forecasting, and uncertainty-aware evaluation.
- AI Physics and engineering workflows: CFD/FEA-style simulation data, mesh and point-cloud pipelines, model validation, inference workflows, and engineering-relevant metrics.
- HPC/GPU scientific computing: Python/PyTorch, JAX, Julia, Rust, GPU/HPC workflows, mixed precision, async dataloading, and performance-oriented model implementation.
- Cross-functional technical leadership: architecture design, benchmark methodology, customer-facing validation, research-to-product translation, technical roadmap documents, mentoring, and technical hiring.

Professional Experience

Senior HPC Engineer, Data and AI 2025–Present
Rescale, Inc. *San Francisco / Remote*

- Build production-oriented AI Physics and scientific ML workflows for industrial simulation data, spanning data preparation, architecture selection, model training, validation, inference, and product integration.
- Developed transformer-based surrogate modeling methods for large-scale engineering simulation data and integrated them into platform-facing training, evaluation, visualization, and artifact-generation workflows.
- Developing AI Physics AutoML and model-selection workflows for comparing baseline models, advanced architectures, training recipes, accuracy, training cost, inference latency, and deployment constraints.
- Improved difficult engineering prediction workflows for industrial simulation data through architecture design, physics-aware feature construction, sampling strategy, loss-function design, and validation methodology; delivered production-usable surrogate workflows where standard approaches were insufficient.
- Designed benchmark and evaluation methods for engineering AI models, including physical-space metrics, ranking fidelity, uncertainty-aware evaluation, training cost, inference cost, and deployment robustness.
- Optimized large-scale transformer training and inference using PyTorch, GPU/HPC workflows, mixed precision, Torch compile, optimizer tuning, async dataloading, and mesh/point-cloud data pipelines.
- Led technical scoping, validation, and handoff across strategic industrial simulation workflows, translating model behavior, uncertainty, and deployment constraints into engineering decisions.
- Authored architecture, roadmap, and AI-for-engineering strategy documents to align engineering, product, leadership, and go-to-market stakeholders; contributed to hiring and team capability building.

Research Scientist 2019–2025
Massachusetts Institute of Technology *Cambridge, MA*

- Developed scientific ML methods for complex physical systems, including score-based generative models, reduced-order methods, transfer-operator methods, and uncertainty-aware emulators.
- Published research in PNAS, Physical Review Letters, Journal of Fluid Mechanics, Journal of Advances in Modeling Earth Systems, Physica D, and related scientific computing venues.
- Built high-performance research code in Julia, Python, and JAX for scientific machine learning, stochastic dynamics, transfer operators, uncertainty quantification, and physics-based modeling.
- Collaborated across applied mathematics, climate physics, fluid dynamics, and scientific computing groups to turn mathematical methods into working computational tools.
- Supervised undergraduate and graduate research projects and communicated technical results through publications, invited talks, research software, and interdisciplinary collaborations.
- Developed methods connecting generative modeling, statistical physics, turbulence, and reduced-order modeling.

Education

PhD, Applied and Interdisciplinary Mathematics, University of Michigan 2016
Dissertation: *An Optimal Control Approach to Bounding Transport Properties of Thermal Convection*

Selected Publications

- L. T. Giorgini, F. Falasca, and **A. N. Souza**. *Predicting forced responses of probability distributions via the fluctuation-dissipation theorem and generative modeling*. Proceedings of the National Academy of Sciences, 122(41), e2509578122, 2025.
- S. Bouabid, **A. N. Souza**, and R. Ferrari. *Score-Based Generative Emulation of Impact-Relevant Earth System Model Outputs*. Journal of Advances in Modeling Earth Systems, 18(3), e2025MS005558, 2026.
- L. T. Giorgini, K. Deck, T. Bischoff, and **A. Souza**. *Response Theory via Generative Score Modeling*. Physical Review Letters, 133, 267302, 2024.
- **A. N. Souza**, J. He, T. Bischoff, M. Waruszewski, L. Novak, V. Barra, T. Gibson, A. Sridhar, S. Kandala, S. Byrne, L. Wilcox, J. Kozdon, F. Giraldo, O. Knoth, R. Ferrari, J. Marshall, and T. Schneider. *The Flux-Differencing Discontinuous Galerkin Method Applied to an Idealized Fully Compressible Nonhydrostatic Dry Atmosphere*. Journal of Advances in Modeling Earth Systems, 15(4), e2022MS003527, 2023.
- **A. Souza**. *Representing Turbulent Statistics with Partitions of State Space I: Theory and Methodology*. Journal of Fluid Mechanics, 997, A1, 2024.
- **A. Souza**. *Representing Turbulent Statistics with Partitions of State Space II: The Compressible Euler Equations*. Journal of Fluid Mechanics, 997, A2, 2024.
- **A. N. Souza**, T. L. Lutz, and G. R. Flierl. *Statistical Nonlocality of Dynamically Coherent Structures*. Journal of Fluid Mechanics, 966, A44, 2023.
- **A. N. Souza**, I. Tobasco, and C. R. Doering. *Wall-to-wall optimal transport: theory and 2D computations*. Journal of Fluid Mechanics, 889, A34, 2020.
- **A. N. Souza** and C. R. Doering. *Maximal transport in the Lorenz equations*. Physics Letters A, 379(6), 518–523, 2015.
- L. T. Giorgini, **A. N. Souza**, D. Lippolis, P. Cvitanovic, and P. Schmid. *Learning dissipation and instability fields from chaotic dynamics*. Physica D: Nonlinear Phenomena, 2025.
- L. T. Giorgini, **A. N. Souza**, and P. J. Schmid. *Reduced Markovian Models of Dynamical Systems*. Physica D: Nonlinear Phenomena, 462, 134393, 2024.
- O. R. A. Dunbar, M. Bieli, A. Garbuno-Inigo, M. Howland, **A. Souza**, L. A. Mansfield, G. L. Wagner, and N. Efrat-Henrici. *CalibrateEmulateSample.jl: Accelerated Parametric Uncertainty Quantification*. Journal of Open Source Software, 9(97), 6372, 2024.
- M. G. Geogdzhayeva, **A. N. Souza**, and R. Ferrari. *The Evolving Butterfly: Statistics in a Changing Attractor*. Physica D: Nonlinear Phenomena, 462, 134107, 2024.
- **A. N. Souza** and M. Tao. *Metastable transitions in inertial Langevin systems: What can be different from the overdamped case?* European Journal of Applied Mathematics, 30(5), 830–852, 2019.
- **A. N. Souza**, D. J. Perkins, C. E. Starrett, D. Saumon, and S. B. Hansen. *Predictions of x-ray scattering spectra for warm dense matter*. Physical Review E, 89(2), 023108, 2014.

Selected Talks, Honors, and Service

- Invited talks include MIT PAOC Colloquium, MIT Ocean Engineering Seminar, MIT CSE Community Seminar, Nordita WINQ plenary, JuliaEO, LEAP, M2LInES, Brown LCDS, NYU Atmosphere Ocean Science Colloquium, and University of Michigan AIM Seminar.
- Honors and funding include MIT-Google Program for Computing Innovation, NCAR CISL large allocation, Bringing Computation to the Climate Challenge, CliMA Research Scientist, and Woods Hole GFD Fellowship.
- Technical service includes research mentoring, curriculum development, technical interviews, open-source scientific software, and cross-functional architecture documentation.

Tools and Methods

Languages and frameworks: Python/PyTorch, JAX, Julia, Rust, GPU/HPC workflows, AI-assisted software development.
ML and modeling: transformers, neural operators, diffusion/score models, probabilistic forecasting, uncertainty quantification, surrogate modeling, generative modeling.
Scientific computing: HPC/GPU workflows, CFD/FEA-style data, physics simulation, dynamical systems, stochastic processes, PDEs, optimization, large mesh and point-cloud data.