
Adaptive Online Emulation for Accelerating Complex Physical Simulations

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Abstract

Complex physical simulations often require trade-offs between model fidelity and computational feasibility. We introduce Adaptive Online Emulation (AOE), which dynamically learns neural network surrogates during simulation execution to accelerate expensive components. Unlike existing methods requiring extensive offline training, AOE uses Online Sequential Extreme Learning Machines (OS-ELMs) to continuously adapt emulators along the actual simulation trajectory. We employ a numerically stable variant of the OS-ELM using cumulative sufficient statistics to avoid matrix inversion instabilities. AOE integrates with time-stepping frameworks through a three-phase strategy balancing data collection, updates, and surrogate usage, while requiring orders of magnitude less training data than conventional surrogate approaches. Demonstrated on a 1D atmospheric model of exoplanet GJ1214b, AOE achieves 11.1× speedup (91% time reduction) across 200,000 timesteps while maintaining accuracy, potentially making previously intractable high-fidelity time-stepping simulations computationally feasible.

1 Introduction

Complex physical simulations are fundamental to scientific discovery, but computational costs often force researchers to choose between model complexity and feasibility. Time-stepping simulations in domains like climate modeling [Schneider et al., 2017], molecular dynamics [Allen and Tildesley, 2017], and fluid dynamics [Pope, 2000] are particularly challenging due to their sequential nature and stability requirements [Durran, 2010].

While surrogate modeling approaches replace expensive components with neural network approximations [Brunton and Kutz, 2019], existing methods require extensive offline training and struggle when simulations explore previously unseen parameter regions—common in scientific discovery where interesting phenomena occur at boundaries or in rare regimes.

We introduce Adaptive Online Emulation (AOE), which dynamically learns surrogate models during simulation execution using Online Sequential Extreme Learning Machines. AOE addresses two critical limitations: (1) the need for extensive offline training and data generation, and (2) poor generalization across parameter space. By leveraging fast, sample-efficient online learning, AOE continuously refines emulator accuracy along the actual simulation trajectory where needed most.

2 Methodology: Adaptive Online Emulation

2.1 Extreme Learning Machines

Extreme Learning Machines (ELMs) [Schmidt et al., 1992, Pao et al., 1994, Huang et al., 2004] are single-hidden-layer networks where, given an input matrix $\mathbf{X} \in \mathbb{R}^{N \times d}$ where N is number of samples and d is input dimensionality, a target matrix $\mathbf{Y} \in \mathbb{R}^{N \times m}$ where m is target dimensionality, and a number of hidden layer neurons H , input weights $\mathbf{W} \in \mathbb{R}^{d \times H}$ and biases $\mathbf{b} \in \mathbb{R}^H$ are randomly fixed, while output weights $\beta \in \mathbb{R}^{H \times m}$ are learned via regularized least squares:

$$\beta = (\mathbf{H}^T \mathbf{H} + \alpha \mathbf{I})^{-1} \mathbf{H}^T \mathbf{Y}$$

where $\mathbf{H} \in \mathbb{R}^{N \times H}$ is the hidden layer output matrix computed as $\mathbf{H} = g(\mathbf{X}\mathbf{W} + \mathbf{1}\mathbf{b}^T)$, $g(\cdot)$ the nonlinear activation function, $\mathbf{1} \in \mathbb{R}^N$ a vector of ones for bias broadcasting, $\alpha > 0$ the regularization parameter, and $\mathbf{I} \in \mathbb{R}^{H \times H}$ the identity matrix. This closed-form solution enables rapid training with computational complexity $\mathcal{O}(NH^2 + NHm + H^3)$.

2.2 Numerically Stable Variant of OS-ELM

To support our adaptive emulation methodology, we employ a numerically stable variant of OS-ELM [Liang et al., 2006] that maintains cumulative sufficient statistics rather than iteratively updating matrix inverses [Foster et al., 2018, Haykin, 2002].

The key insight is that the regularized least squares solution can be expressed using sufficient statistics matrices that decompose additively across data batches:

$$\beta_t = (\mathbf{S}_t^{HH} + \lambda \mathbf{I}_H)^{-1} \mathbf{S}_t^{Hy}$$

where $\mathbf{S}_t^{HH} = \sum_{j=0}^t \mathbf{H}_j^T \mathbf{H}_j$ and $\mathbf{S}_t^{Hy} = \sum_{j=0}^t \mathbf{H}_j^T \mathbf{Y}_j$.

Upon receiving batch $(\mathbf{X}_t, \mathbf{Y}_t)$, we: (1) compute $\mathbf{H}_t = \sigma(\mathbf{X}_t \mathbf{W})$, (2) accumulate $\mathbf{S}_t^{HH} = \mathbf{S}_{t-1}^{HH} + \mathbf{H}_t^T \mathbf{H}_t$ and $\mathbf{S}_t^{Hy} = \mathbf{S}_{t-1}^{Hy} + \mathbf{H}_t^T \mathbf{Y}_t$, and (3) periodically resolve β_t every T updates.

This approach avoids the numerical instability of traditional OS-ELM's iterative matrix inversions [Huang et al., 2015] while providing exact solutions for all accumulated data. The computational complexity is $\mathcal{O}(ldH + lH^2 + lHm + H^3/T + H^2m/T)$ per update.

2.3 Integration with Time-Stepping Frameworks

Our framework implements a state machine governing when to use numerical computation, collect data, train, update, or evaluate the surrogate. The simulation operates through three phases:

Phase 1: Initialization ($1 \leq t \leq N_{\text{init}}$) uses numerical computation to handle initial transients.

Phase 2: Training ($N_{\text{init}} < t \leq N_{\text{init}} + N_{\text{train}}$) collects input-output pairs and performs initial ELM training (at $t = N_{\text{init}} + N_{\text{train}}$).

Phase 3: Adaptive Execution ($t > N_{\text{init}} + N_{\text{train}}$) alternates in fixed cycles of length $N_{\text{cycle}} = N_{\text{update}} + I_{\text{update}}$, between (1) data collection for N_{update} timesteps, (2) an OS-ELM β update, and (3) surrogate usage for I_{update} timesteps, where $I_{\text{update}} \gg N_{\text{update}}$.

The computational complexity per adaptive cycle is $\mathcal{O}(N_{\text{update}}H^2 + H^3 + I_{\text{update}}dH)$, where the first term represents statistics accumulation during data collection, the second term represents weight updates, and the third term represents cheap surrogate evaluations.

3 Results

We evaluate AOE on a 1D atmospheric model (the OASIS model; Mendonça and Buchhave [2020]) of exoplanet GJ1214b over 200,000 timesteps. The simulation models pressure-temperature (p-T) evolution through computationally intensive radiative transfer calculations. The ELM predicts radiative flux profiles that then undergo spatial differentiation to compute atmospheric heating rates, and thus compute the atmospheric p-T profile per timestep. The ELM uses $H = 1000$

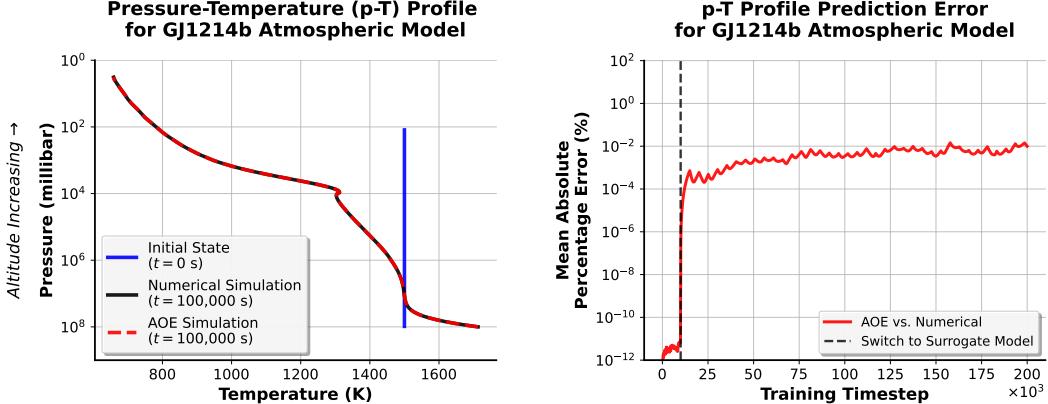


Figure 1: AOE performance on GJ1214b atmospheric simulation. (Left) Pressure-temperature profiles showing strong agreement between numerical (black) and AOE (red dashed) solutions after 200,000 timesteps ($\Delta t = 0.5\text{s}$). (Right) Prediction error remains below $\sim 0.01\%$ throughout the simulation.

hidden neurons with $d = 200$ atmospheric layers \times 3 physical variables = **600** input features and $m = 201$ atmospheric levels \times 2 targets \times 8 directions = **3216** outputs, using a warm-up period of $N_{\text{init}} = \mathbf{5000}$ and collecting $N_{\text{train}} = \mathbf{5000}$ initial samples followed by periodic β updates every $I_{\text{update}} = \mathbf{5100}$ timesteps using $N_{\text{update}} = \mathbf{100}$ update samples. Table 1 includes the timings of components of our AOE framework applied to our test simulation, benchmarked on one NVIDIA V100-16GB GPU.

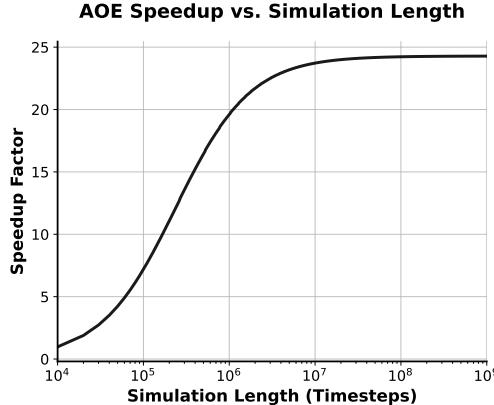


Figure 2: Fixed initialization costs (warmup + training) are amortized over longer simulations enabling a larger speedup. While this speedup factor is unique to this particular simulation and the chosen AOE hyperparameters (N_{update} , N_{cycle} , H), the overall trend is simulation-agnostic.

4 Discussion

The AOE framework demonstrates high accuracy in predicting atmospheric pressure-temperature profiles, as shown in Figure 1. The emulated simulation closely tracks the numerical reference throughout the 200,000 timestep simulation, with the final atmospheric state (red dashed line) nearly indistinguishable from the pure numerical result (black line). Mean absolute percentage errors remain consistently around 0.01% for the majority of the simulation. Notably, this high accuracy is achieved despite the challenging nature of the prediction task: the ELM predicts radiative flux profiles that then undergo spatial differentiation to compute heating rates, meaning small prediction errors could potentially be amplified in the temperature evolution. This level of accuracy, maintained over an extended simulation period, validates the viability of online emulation for scientific computing applications that require large numbers of time steps.

Table 1: Computation time breakdown of Adaptive Online Emulator over 200,000 timesteps benchmarked on one NVIDIA V100-16GB GPU. System overhead includes copying data between arrays and preprocessing and postprocessing input and output data.

Simulation Phase	Duration	Time/Step	Total Time	Speedup
<i>Initialization Phase</i>				
Warmup (numerical only)	5,000 steps	14.14 ms	70.7 s	1.0×
Data collection (numerical + overhead)	5,000 steps	14.21 ms	71.0 s	1.0×
Initial training	1 event	3.09 s	3.1 s	—
<i>Emulation Phase</i>				
ML prediction	186,300 steps	0.19 ms	35.4 s	74.4×
System overhead	186,300 steps	0.12 ms	21.6 s	—
<i>Adaptive Learning</i>				
Retraining data collection	3,700 steps	14.21 ms	52.6 s	1.0×
Model updates	36 events	17.8 ms	0.6 s	—
Effective emulation	186,300 steps	0.31 ms	57.0 s	46.4×
Total simulation	200,000 steps	1.28 ms avg	255.0 s	11.1×
Time if all numerical	200,000 steps	14.14 ms	2,828.0 s	1.0×
Net time savings	—	—	2,573.0 s	91% faster

The AOE framework achieves substantial computational acceleration, reducing simulation time from 2,828 seconds (pure numerical) to 255 seconds (AOE-enabled), representing a 11.1× speedup. This performance improvement scales favorably with simulation length as shown in Figure 2: while initial phases require numerical computation for data collection and training, the majority of timesteps benefit from fast surrogate evaluation. The speedup increases asymptotically with longer simulations as the fixed initialization costs are amortized over more emulated timesteps.

To contextualize this acceleration, the original numerical computation involves a complex CUDA kernel that executes across multiple dimensions: spectral channels, spatial layers, and 8 directional sampling points. For each combination, the kernel performs multi-dimensional interpolations across 4D lookup tables (pressure × temperature × species × wavelength), computes scattering coefficients, applies transport calculations through 200 atmospheric layers, and solves coupled differential equations for upward/downward propagation. This multi-dimensional computation with nested loops, table interpolations, and iterative solvers requires 14.14ms per timestep. In contrast, surrogate evaluation involves a single forward pass through the ELM network requiring only 0.31 ms per timestep (including system overhead of copying and scaling data)—a 46× acceleration per timestep where emulation is used.

The overall simulation acceleration of 11.1× represents a conservative baseline using fixed hyperparameters rather than optimized control policies. The update frequency N_{cycle} and update batch size N_{update} directly control the accuracy-efficiency trade-off, and intelligent optimization of these parameters could yield additional speedup while maintaining high accuracy.

5 Future Work

The current AOE framework has several key areas for improvement that motivate future research:

1. **Adaptive control policies:** Replace fixed hyperparameters N_{update} and N_{cycle} with data-driven policies that adjust update frequency based on observable metrics such as recent prediction variance, rate of state change, or time since last update.
2. **Active Learning:** Implement methods to intelligently sample input space for training and updates to boost emulator performance.
3. **Operational quality control:** Implement real-time surrogate validation through uncertainty quantification (using prediction confidence bounds or ensemble variance estimates).

These developments could significantly enhance the robustness of the AOE framework while enabling greater computational acceleration through intelligent adaptation. The demonstrated effectiveness of AOE on atmospheric modeling suggests potentially broad applicability to computationally intensive scientific domains where expensive physics calculations dominate runtime. By making previously prohibitive simulations tractable while maintaining the accuracy essential for reliable scientific insights, Adaptive Online Emulation has substantial potential to accelerate scientific discovery across physics-based modeling applications.

References

- Michael P. Allen and Dominic J. Tildesley. Molecular dynamics. In Michael P. Allen and Dominic J. Tildesley, editors, *Computer Simulation of Liquids*, page 0. Oxford University Press, June 2017. ISBN 9780198803195. doi: 10.1093/oso/9780198803195.003.0003. URL <https://doi.org/10.1093/oso/9780198803195.003.0003>.
- Steven L. Brunton and J. Nathan Kutz. *Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control*. Cambridge University Press, Cambridge, 2019. doi: 10.1017/9781108380690. URL <https://www.cambridge.org/core/books/datadriven-science-and-engineering/77D52B171B60A496EAFE4DB662ADC36E>.
- Dale Durran. Numerical Methods for Fluid Dynamics. *Numerical Methods for Fluid Dynamics by Dale R. Durran*. New York: Springer, 2010. ISBN: 978-1-4419-6411-3, 32, January 2010. ISSN 9781441964113. doi: 10.1007/978-1-4419-6412-0_1.
- Dylan J. Foster, A. Rakhlin, and Karthik Sridharan. Online Learning: Sufficient Statistics and the Burkholder Method. *ArXiv*, March 2018. URL <https://www.semanticscholar.org/paper/Online-Learning%3A-Sufficient-Statistics-and-the-Foster-Rakhlin/46ea9b781c38ca723aa11e00c55ad00321133be9>.
- S. Haykin. Adaptive Filter Theory 4th Edition. 2002. URL <https://www.semanticscholar.org/paper/Adaptive-Filter-Theory-4th-Edition-Haykin/58af19190dfa172df90d7ef6b8bad0535662950>.
- Gao Huang, Guang-Bin Huang, Shiji Song, and Keyou You. Trends in extreme learning machines: A review. *Neural Networks*, 61:32–48, January 2015. ISSN 08936080. doi: 10.1016/j.neunet.2014.10.001. URL <https://linkinghub.elsevier.com/retrieve/pii/S0893608014002214>.
- Guang-Bin Huang, Qin-Yu Zhu, and Chee Siew. Extreme learning machine: A new learning scheme of feedforward neural networks. volume 2, pages 985–990 vol.2, August 2004. ISBN 9780780383593. doi: 10.1109/IJCNN.2004.1380068.
- Nanying Liang, Guang-Bin Huang, P Saratchandran, and Narasimhan Sundararajan. A Fast and Accurate Online Sequential Learning Algorithm for Feedforward Networks. *IEEE transactions on neural networks / a publication of the IEEE Neural Networks Council*, 17:1411–23, December 2006. doi: 10.1109/TNN.2006.880583.
- João M. Mendonça and Lars A. Buchhave. Modelling the 3D Climate of Venus with OASIS, July 2020. URL <http://arxiv.org/abs/2002.09506>. arXiv:2002.09506.
- Yoh-Han Pao, Gwang-Hoon Park, and Dejan J. Sobajic. Learning and generalization characteristics of the random vector functional-link net. *Neurocomputing*, 6(2):163–180, April 1994. ISSN 0925-2312. doi: 10.1016/0925-2312(94)90053-1. URL <https://www.sciencedirect.com/science/article/pii/0925231294900531>.
- Stephen B. Pope. *Turbulent Flows*. Cambridge University Press, Cambridge, 2000. ISBN 9780521598866. doi: 10.1017/CBO9781316179475. URL <https://www.cambridge.org/core/books/turbulent-flows/69322053C06F73F7EB7124915F9256BD>.
- W.F. Schmidt, M.A. Kraaijveld, and R.P.W. Duin. Feedforward neural networks with random weights. In *Proceedings., 11th IAPR International Conference on Pattern Recognition. Vol.II. Conference B: Pattern Recognition Methodology and Systems*, pages 1–4, August 1992. doi: 10.1109/ICPR.1992.201708. URL <https://ieeexplore.ieee.org/document/201708>.

Tapio Schneider, Shiwei Lan, Andrew Stuart, and João Teixeira. Earth System Modeling 2.0: A Blueprint for Models That Learn From Observations and Targeted High-Resolution Simulations. *Geophysical Research Letters*, 44(24):12,396–12,417, 2017. ISSN 1944-8007. doi: 10.1002/2017GL076101. URL <https://onlinelibrary.wiley.com/doi/abs/10.1002/2017GL076101>.