Characterizing and Predicting Atypical Behavior in Thermal-Mechanical Systems

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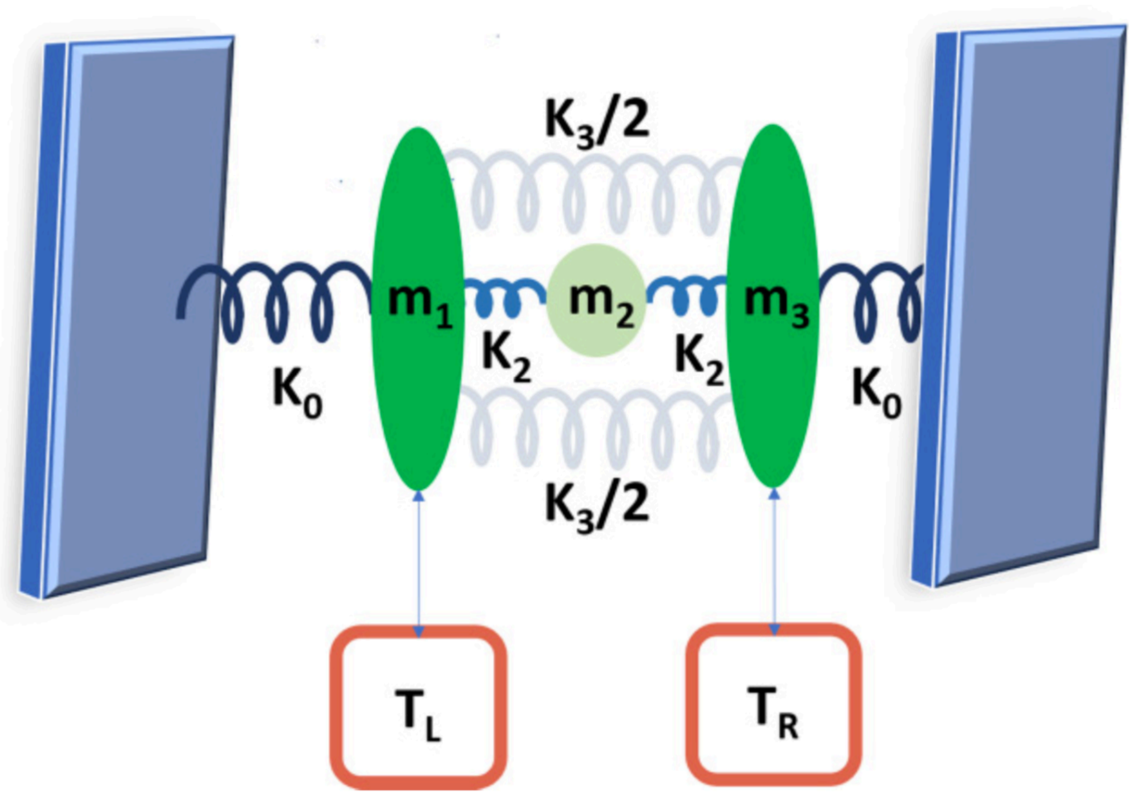
Many simulations are needed to discover interesting behavior



The above system has 3 masses, two of which are connected to thermal reservoirs at different temperatures. Each mass starts at rest, but is driven by the reservoirs (modeled mathematically as Langevin Reservoirs) according to a Stochastic Differential Equation (SDE).

Underlying dynamics:

$$\frac{dX}{dt} = f(X) + \eta$$

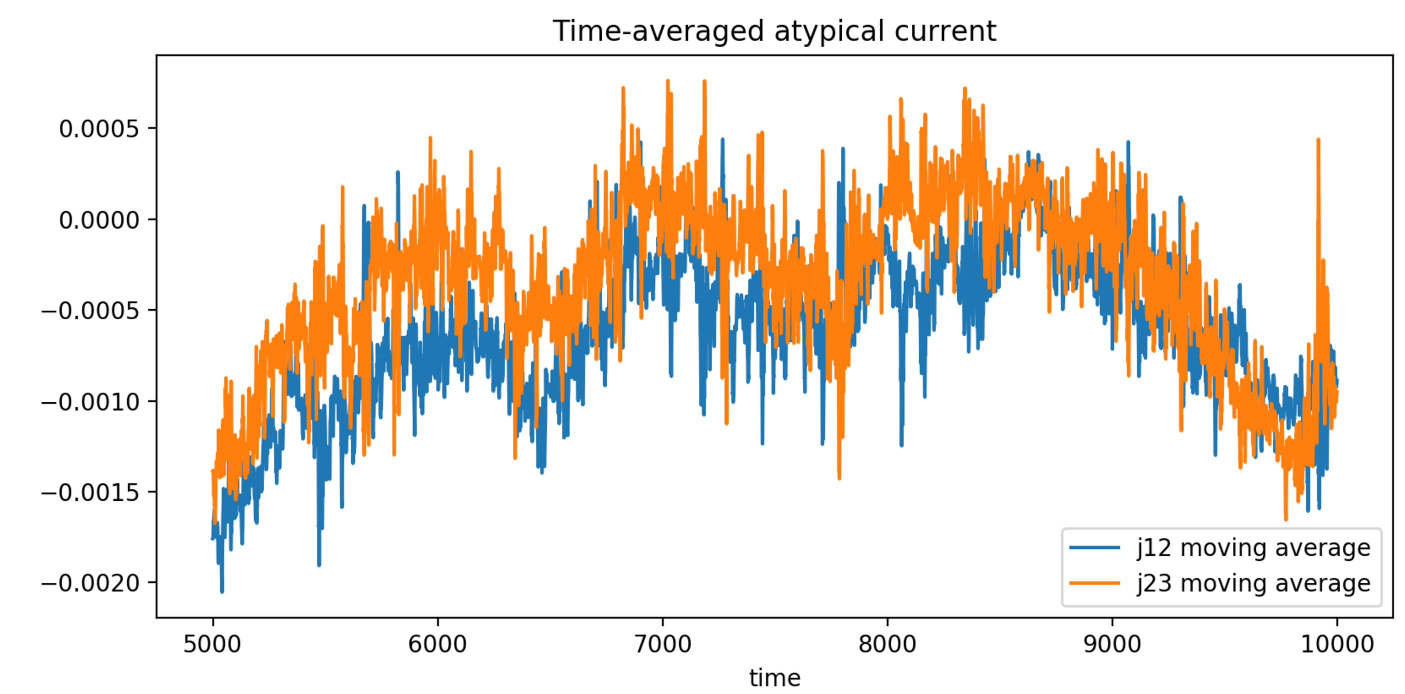
We can compute thermal currents with the following equations:

$$\langle J_{12} \rangle = \langle \dot{x}_2 (K_2 x_1) \rangle$$

$$\langle J_{13} \rangle = \langle \dot{x}_3 (K_2 x_2 + K_3 x_1) \rangle$$

Under certain configurations of the system, J_{12} can be negative, representing a local thermal current moving from cold to hot. This is interesting because it locally contradicts the 2nd law of thermodynamics, even though globally the 2nd law still holds, since the total current still moves from the hot reservoir to the cold reservoir.

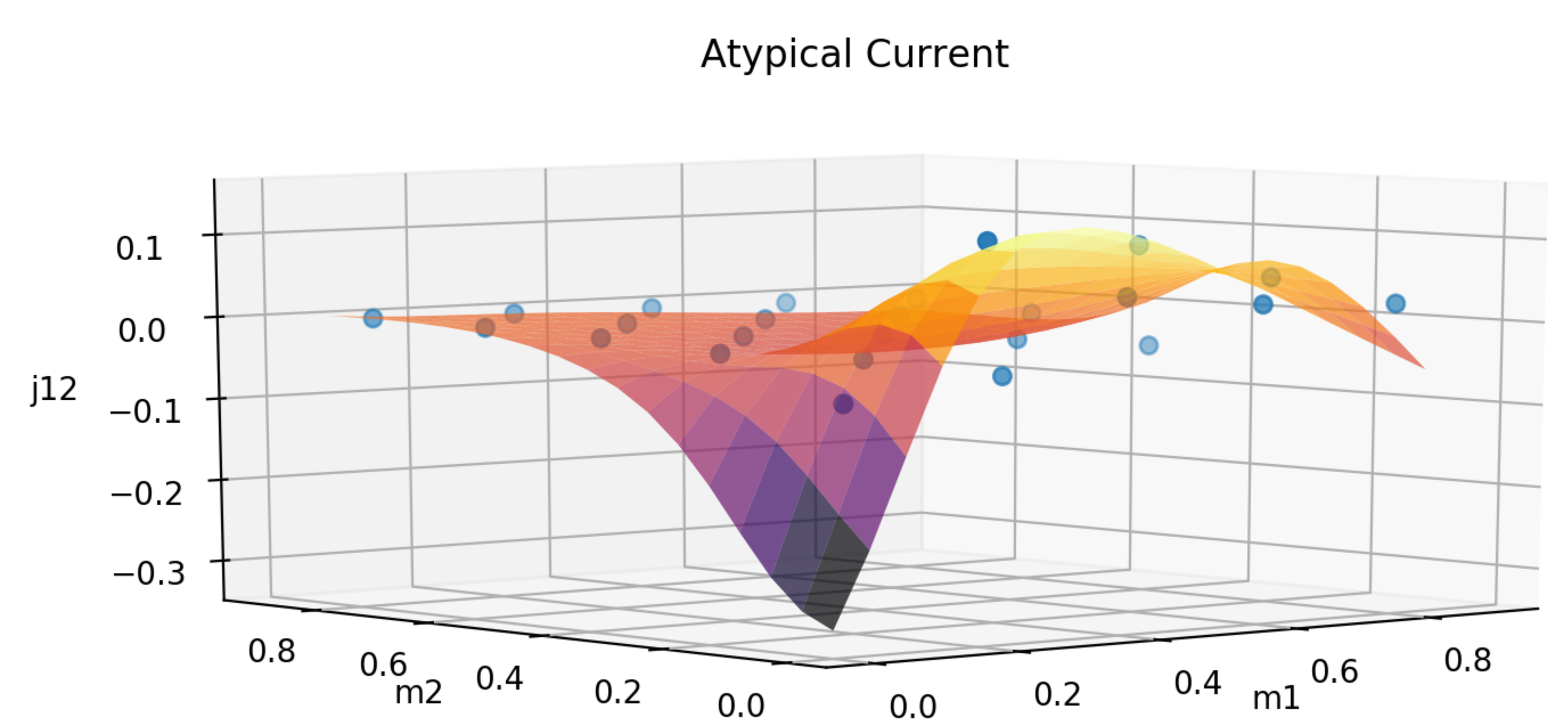
Only certain configurations produce interesting results



Leveraging LC to explore parameter space of system

Expensive simulations are needed to accurately compute steady-state current values. I optimized the original code provided by our UC Merced collaborators, and parallelized it to be run on LC. Simulations ran ~3000x faster when executed on nodes of Surface.

Surrogate model predicts behavior without simulations



Grid search simulation results are in blue, and the model-predicted current values are depicted by the surface

Surrogate model guides parameter search

Once a surrogate model is trained, it can be used to guide more targeted parameter searches. Standard optimizers can be used to maximize or minimize atypical current in parameter space.

Applications

The techniques presented here are important for the future of applied science. This problem exhibits many of the properties that we see in ICF simulations. Many design problems, in fields such as materials science and manufacturing, require computationally expensive simulations. These simulations slow down the process of optimizing the properties of a material or process. Building a surrogate model can accelerate this design process.

The specific system studied could be used as the basis of a “thermal computer”. Positive vs. negative thermal current could represent 1 and 0, and this value could be flipped by adjusting system parameters

Next Steps

To reduce complexity, a subset of 4 of the 10 total system parameters were varied. To train a model on the larger parameter space, a more sophisticated sampling technique could be used, such as an evolutionary algorithm or Merlin, LLNL’s workflow framework for active learning with scientific simulations. The ongoing goal of this work is to develop the field of Scientific Machine Learning (SciML), to help bridge the gap between scientific simulation and machine learning.

We are now interested in characterizing transport not only in Thermal-Mechanical systems, but also quantum transport in both photonic and spin systems.

Affiliations and Acknowledgements

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We found parameters which yield atypical thermal current and built a surrogate model to predict it

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