End-to-End Differentiability and TPU Computing to Accelerate Materials' Inverse Design

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NEURAL INFORMATION PROCESSING SYSTEMS

New Paradigm to Establish Generative Models for Materials' Inverse Design

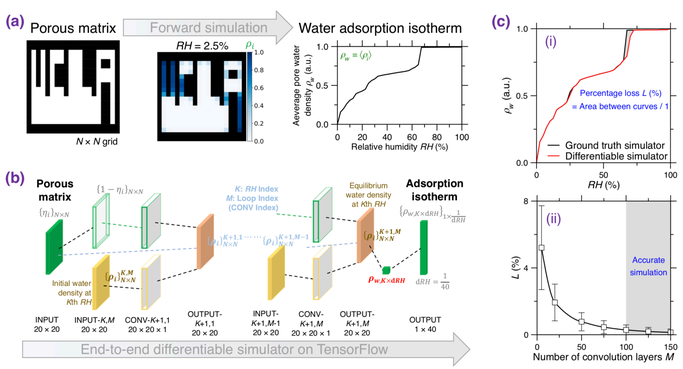
Numerical simulations have revolutionized material design. However, although simulations excel at mapping an input material to its output property, their direct application to inverse design (i.e., mapping an input property to an optimal output material) has traditionally been limited by their high computing cost and lack of differentiability. Here, to address these challenges, we introduce a new paradigm of generative pipeline that Integrates a generator model with an end-to-end differentiable simulator.

- We illustrate the power of this approach by taking the example of the inverse design of a porous matrix featuring targeted sorption isotherm.
- We show that the trained generative model can successfully generate porous structures with arbitrary sorption curves.
- This generator-simulator pipeline leverages for the first time the power of TPU—an emerging dedicated chip, which, although they are specialized in deep learning, are flexible enough for intensive scientific simulations.

I. End-to-End Differentiable Simulator

Water adsorption simulation of porous materials

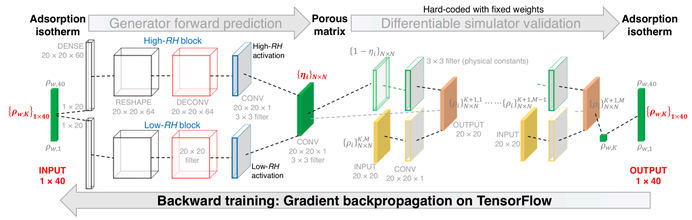
This sorption simulation is enabled by implementing a lattice-based density functional theory (LDFT) code. Such LDFT simulations are traditionally not differentiable. Here, to address this limitation, we decompose the LDFT formula into a series of mathematical operations that can be implemented as differentiable computation layers in TensorFlow, where the CONV layer represents the convolution operation in the formula—i.e., one of the operations that can be efficiently performed by TPUs—and is repeated *M* times until a convergence in the water density is achieved.



End-to-end differentiable simulation of water adsorption in porous materials

II. Generator-Simulator Pipeline Integration

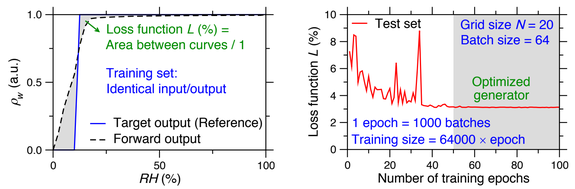
Architecture of the generator-simulator pipeline



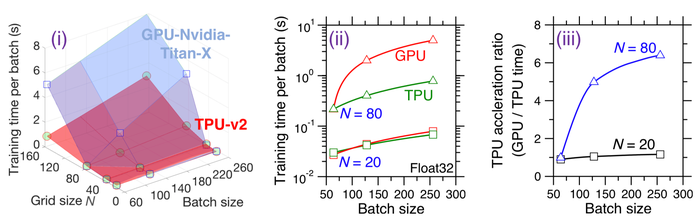
The training pipeline takes as inputs the sorption isotherms curves of the training set, which are transformed into porous matrices by the generator. The generated grids are then fed to the differentiable simulator to compute the "real" sorption curve of the generated porous matrices. The generator can be optimized by gradient backpropagation in TensorFlow to minimize the difference between the input and output sorption curves.

III. Training Acceleration by TPU Computing

Training of the generator-simulator pipeline



The training process comes with a significant computational cost. To mitigate this issue, as a pioneering experiment, the training is conducted on TPUs. We find that, especially for large grid size and batch size, the deliciated TPU hardware results in a training time that is several times faster than that offered by the GPU hardware considered herein (more than 6× faster).

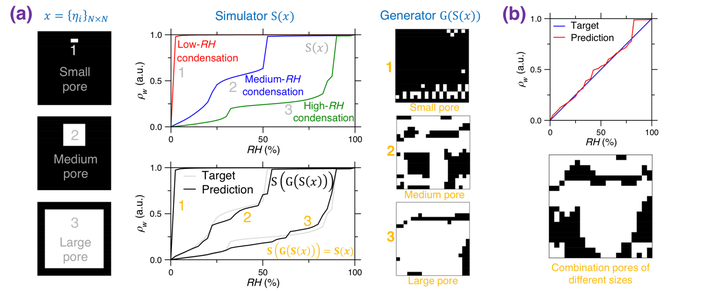


Comparison of the training time per batch as a function of the grid size and batch size offered by Google's TPU-v2 and an NVIDIA TITAN X GPU

IV. Accuracy of the Generative Model

Test of the generator-simulator pipeline

After training, we find that the generator exhibits an average prediction loss of 3% on the test set (which comprises more than 8000 target sorption isotherms), which is here considered very good. Even under challenging tests, we find that the generator model can predict realistic porous matrices, with expected length scales for the pores. Importantly, the simulated sorption curves of the generated porous structures exhibit all the features (in terms of trend, convexity, and value) as the target sorption curves.



(a) Illustration of three porous matrices that are generated to present three archetypical sorption isotherms associated with small, medium, and large pores. (b) Porous matrix generated for a target sorption curve $y = x$.

Conclusion and Broader Impact

Overall, this work establishes a robust pipeline to enable the inverse design of materials by integrating differentiable simulations in machine learning pipelines—which is key to accelerate the discovery of new materials. Importantly, our results establish TPU computing as a promising route to accelerate scientific simulations, which are ubiquitous in various applications. Finally, the ability to design new porous structures with tailored sorption isotherms could leapfrog several important applications, including for CO_2 capture, gas separation, and drug delivery applications.

References

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