A QUANTUM-AI FRAMEWORK FOR EXTREME WEATHER PREDICTION

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FOCAL AREA: PREDICTIVE MODELING

We present a differential equation-AI hybrid approach for high resolution geophysical fluid dynamical simulation to improve extreme weather event prediction. We discuss ways to leverage existing computing technologies and discuss how developments in quantum computing have the potential to significantly enhance existing capabilities.

SCIENCE CHALLENGE

The frequency and intensity of extreme weather events in North America will likely increase with a changing climate[1]. High resolution simulations are necessary to advance process-based understanding of weather events at local scales accompanying future changes in global atmospheric circulation[2].

RATIONALE

Earth system modeling is performed by costly evaluation of many partial differential equations (PDEs) on classical computers. For each Climate Model Intercomparison Project (CMIP) cycle, numerous climate model simulations are organized to include key aspects of the Earth system. To achieve this community comparison effort, the horizontal resolution of the simulation is typically compromised to ~150 km or coarser in the atmosphere and 1° in the ocean[3]. Important climate and weather processes, such as atmospheric convection, are parameterized at this coarse resolution, underestimating the frequency of severe storms that cause fatalities and economic losses. In a recent study utilizing a convection-permitting model, the authors found the summertime storm frequency will more than triple in North America by the end of the century under the Representative Concentration Pathway (RCP) 8.5[4].

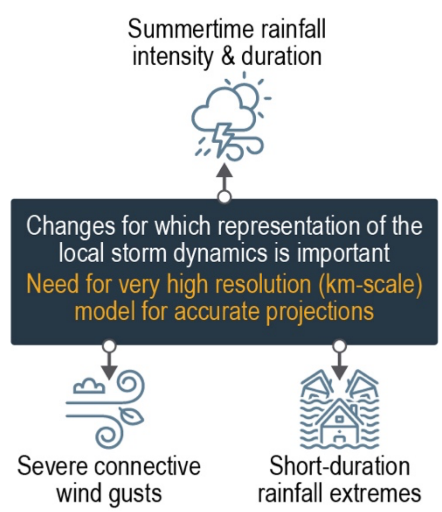

Figure 1: High resolution models are required for accurate projections of extreme weather events. Graphic recreated from [2].

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Modeling of local scale weather impacts requires highly spatially resolved simulations, but the computational resources required to run these simulations are costly. Parameterization of sub-grid scale processes inhibits process-based understanding of local-scale atmospheric dynamics. In the following section, we present a modeling approach which improves computational efficiency while maintaining explicit dynamical modeling to enable interpretability and process-based understanding.

NARRATIVE

SCIENTIFIC AND TECHNICAL DESCRIPTION OF OPPORTUNITIES AND APPROACH

To address an immediate need for more finely resolved simulations, we present a hybrid differential equation-AI approach to maximize computational resource utilization and provide value in the near term and as quantum capabilities mature. There is a rich and active emergent field in the machine learning community applying powerful AI originally developed for medical imaging and computer vision to augment this computation. Incorporating elements of "superresolution" into an iterative PDE solution has been shown to dramatically increase the fine detail of coarsely resolved simulations and reduce error that accumulates through simulated time steps[5]. Many state-of-the-art models performing superresolution utilize the U-Net convolutional neural network (CNN) architecture originally developed for medical image segmentation[6]. The model illustrated in Fig. 2 demonstrates this multi-disciplinary U-Net architecture fitting discretely into a hybrid PDE solver. Strong results have been produced for the system of Rayleigh-Bénard Convection[4,7]. Work remains to extend these methods to 3D where necessary and apply results throughout elements of an Earth system model.

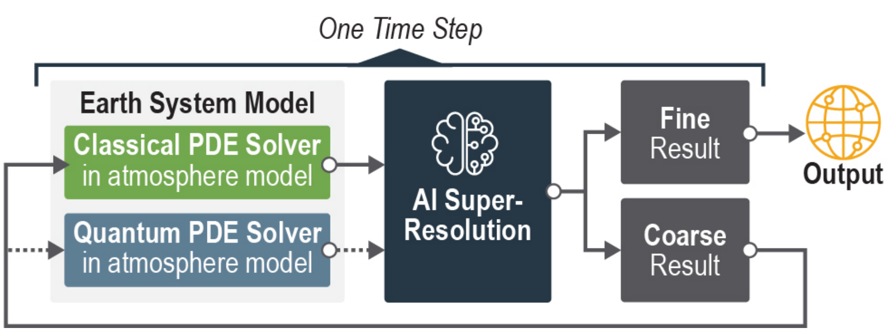

Figure 2: Schematic illustrating a combined machine learning-partial differential equation model in the context of Earth system modeling. Concept adapted from [5]. An iteration begins with low resolution frame that is time stepped with the PDE solver. The new low-resolution frame is upscaled and error corrected with machine learning superresolution. The resulting frame is then saved as output and downscaled to the original resolution to feed into the next iteration. While PDEs are solved by classical computers, the dotted line indicates a possible future where quantum speedups may be realized.

Separately, quantum computation has been proven in theory to speed up Navier-Stokes fluid simulation[8]. The quantum PDE solution offers up to a quadratic speed-up over the best random classical algorithm, and up to an exponential speed-up over the best deterministic classical algorithm. The largest speed-ups are seen on rough, non-differentiable functions, traditionally the most challenging functions to simulate classically. This result indicates the potential for quantum computation to revolutionize the simulation of Earth systems as quantum capabilities grow. This hybrid framework, combining quantum computation for PDE simulation with AI superresolution to resolve fine spatial details provides potential for faster and more accurate simulation of extreme events.

ACTIVITIES THAT WILL ADVANCE THE SCIENCE

A specific example of how this framework would be implemented with the DOE E3SM Atmosphere model would follow the schematic in Fig. 2. The machine learning model to upscale and error correct with machine learning superresolution would be trained on the suite of model runs planned for the E3SM v2 simulation campaign, i.e. the standard low resolution (LR), high resolution (HR), and regional refined model (RRM) for North America. While the training of the machine learning model will be computationally expensive, the inference of the model will be efficient and reusable, allowing the upscaling and error correction operations to be performed at every time step. This approach is an improvement on existing methods of statistically downscaling static climate model output fields. Because the resolution operators are employed at each time step, it enables process-based understanding and interpretability of highly resolved features. Additionally, analyses on the full spatial domain can elucidate the influence of global teleconnections in the atmospheric system on local scale dynamics.

OUTLOOK FOR INCORPORATING QUANTUM COMPUTING

Quantum supremacy, or the real-world demonstration that a quantum computer can perform a specific computational task faster than a classical computer, was first demonstrated in late 2019. Current devices have limited resources, with state-of-the-art chips containing around 50 qubits (quantum bits) prone to errors at modest rates compared to standard desktop computers which use billions of bits with virtually non-existent error-rates. Protocols to perform precise calculations on unreliable quantum computers exist, but they require a large computational resource overhead. Estimates have shown that to run a quantum algorithm of comparable complexity to that for solving differential equations on reasonable inputs requires millions of qubits and many trillions of elementary operations. Given that current device capabilities are roughly doubling each year (akin to Moore’s law), the horizon for realizing full-capability quantum computers can be estimated as roughly 15-20 years out. As with any emerging technology, this forecast is extremely speculative, and unforeseen breakthroughs could place quantum computing protocols useful to climate modeling within reach within 5 years.

The evolving nature of quantum computers and their theoretical demonstration of applicability to climate science motivate continued exploration of these devices as tools for climate study as the technology matures. Despite the speculative nature of forecasting the arrival of scalable, fault tolerant universal quantum computers, the overarching power these systems offer to Earth systems simulation means that, as we develop new approaches, we need to do so in such a way that is consistent with an eventual quantum future. Optimistically, the research effort in both quantum hardware and quantum algorithms is growing exponentially, and DOE is both a leader and driver of new developments through, for example, the Oak Ridge National Laboratory Quantum Computing Institute and various programs administered by the Basic Energy Sciences division. The confluence of DOE leadership in both Earth systems science and quantum computing is therefore exceptionally compelling.

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