carried out by submitting bag-of-task (BoT) [14] type jobs to single or distributed systems using the VLab service-oriented cyberinfrastructure [12–14].

On Blue Waters, these calculations were performed using BoTs or MPI directives, "image" parallelization (1st level of parallelization). For a typical system with 20 atoms (e.g., $MgSiO_3$ perovskite or post-perovskite [7,15]), the best performance was achieved with 128 cores per job. Thus, a full thermodynamic calculation could be performed in less than one minute, or a calculation of thermoelastic constants could be performed in a couple of minutes.

WHY BLUE WATERS?

The major reason for using Blue Waters is the number of cores available. We developed wrappers around several modules of the Quantum ESPRESSO software that allow us to use the system for high-throughput calculations. As explained above, phase space sampling for thermodynamics calculations is intrinsically a high-throughput problem.

A future Track-1 system will allow us to expand the dimension of phase space currently sampled. Minerals are solid solutions and a full investigation of phase equilibrium in these solids involves sampling of atomic configurations. We have just started addressing this issue. We are exploring techniques to do maximally efficient sampling of atomic configurations. Nevertheless, multiple configurations (~10^1–10^2) need to be explored in each of up to ~10^4 calculations.

We have essentially investigated all major end-member phases and simple versions of the main mineral solid solutions of the mantle using only a few few atomic configurations. While elastic properties of crystalline aggregates are well described by using few atomic configurations, phase diagrams containing binary (or multi-phase) loops need accurate free energies, which can only be achieved through careful sampling of atomic configurations. An example of this problem can be seen in fig. 1, where OPx and CPx phases "dissolve" into Gt (garnet) within a broad pressure range (i.e. 5 GPa < P < 18 GPa). A detailed description of this phenomenon requires a considerably larger number of (smarter) calculations.

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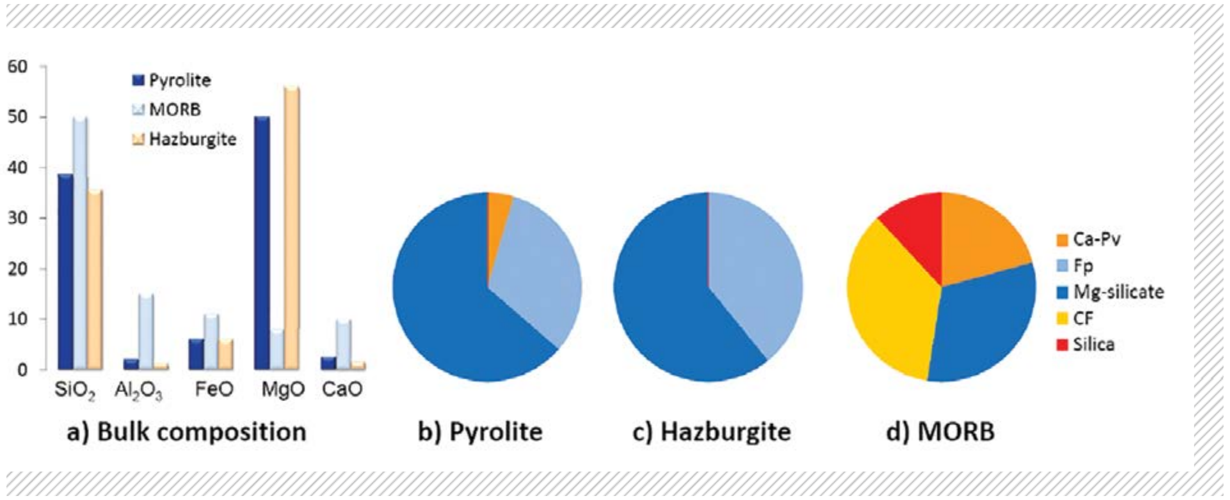

FIGURE 2: (a) Chemical compositions of mantle rocks [85-87]. Mineralogy (in mol%) of (b) pyrolite [88], (c) harzburgite, and (d) basalt [89] in the lowermost mantle. Mg-Silicate: $MgSiO_3$ perovskite and/or post-perovskite, Fp: ferropericlase, Ca-Pv: $CaSiO_3$ perovskite, and CF: calcium-ferrite-type phase.

USING PETASCALE COMPUTING CAPABILITIES TO ADDRESS CLIMATE CHANGE UNCERTAINTIES

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EXECUTIVE SUMMARY:

This collaborative research between the University of Illinois, the National Center for Atmospheric Research (NCAR), and the University of Maryland uses Blue Waters to address key uncertainties in numerically modeling the Earth's climate system and accuracy in analyses of past and projected future changes in climate at a level that would be impossible without petascale computing. Our studies used the latest, most advanced versions of the Community Earth System Model (CESM) and two versions of NCAR's Weather Research and Forecasting Model (WRF and CWRF) for high-resolution regional climate analyses. These model runs put us on the pathway for major international leadership in high-resolution climate modeling studies.

INTRODUCTION

This collaborative research used Blue Waters to address key uncertainties in numerically modeling the Earth's climate system and accuracy in analyses of past and projected future changes in climate. Our studies used the latest versions of the Community Earth System Model (CESM), the Weather Research and Forecasting model (WRF), and the Climate-WRF (CWRF).

We explored the effect of external forcings (e.g., concentrations of greenhouse gases) on globally averaged temperature, focusing on uncertainties associated with the representation of processes and interactions between clouds, aerosols, and radiative transfer in the models and how these uncertainties influence the climate sensitivity.

Our second objective aimed to evaluate CESM with different model dynamical cores and the effects of much higher horizontal (10–30 km) and vertical resolution. There is considerable evidence that increased resolution leads to better simulations of both transient small-scale activity (e.g., eddies and waves) and large-scale features of the mean climate.

We expect that results from our studies will be an integral part of the scientific analysis of climate change for the major international climate assessments (e.g., the follow-on to the Assessment Report 5, AR5, 2014) of the Intergovernmental Panel on Climate Change (IPCC), which will likely influence U.S. and international policies regarding the effects of human activities on the Earth's climate, and provide supplementary data for use in various climate impact assessments at regional to local scales.

METHODS AND RESULTS

CESM

After tuning the physics and testing model settings of (the atmospheric portion of) CESM, we began a series of simulations that will support studies for the next Climate Model Intercomparison Project 6 (CMIP6), which is important to the next IPCC assessment of climate change.

Recent results from simulations that ran 1979 to the present suggested that the global number of tropical storms and hurricanes per year will decrease in a warming climate. However, the maximum intensity seemed to increase, meaning more major hurricanes (category 4 and 5). In the North Atlantic basin the RCP8.5 scenario showed a decrease in the number of tropical cyclones and hurricanes. The selection of a dynamical core can have a significant impact on tropical cyclone intensity and frequency even in the presence of similar climatology and large-scale environments [1]. For example, CAM5 with the spectral element (SE) core produced stronger cyclones, and therefore more hurricanes and major hurricanes per year, than CAM5 with the finite volume (FV) core (figs. 1–2). The exact causes for these differences is an area of continued work.

Compared to the out-of-box model, we improved the performance of CAM5 from 1.3 years/day to 2.5 years/day. Pat Worley (ORNL) and Ryan Mokos (NCSA) helped remove bottlenecks in MPI calls, while John Truesdale

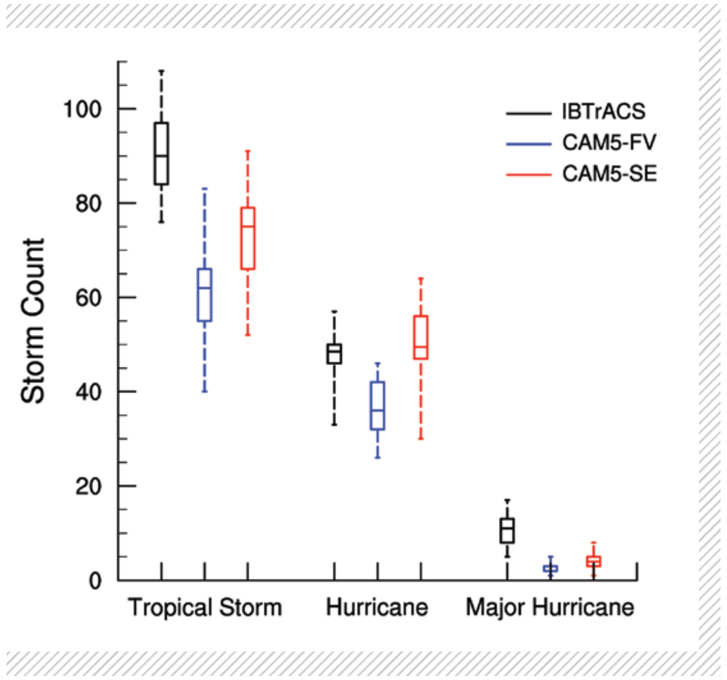

FIGURE 1: Distribution of the global number of tropical cyclones that reach tropical storm, hurricane, and major hurricane (cat. 4-5) strength per year for the CAM5-FV and CAM5-SE simulations 1980-1999. The boxes show the 25th, 50th, and 75th percentiles; values outside the box represent extrema (i.e. years with the most and least number of TCs). IBTrACS observations are included as a reference.

(NCAR) rebalanced the PE layout among the model components. These and future modifications could improve model performance on other machines as well.

WRF at 12 km Resolution

WRF model was used to downscale the GFDL and the Hadley Centre model results, both of which provide ~1° (~100 km) resolution, to 12 km horizontal resolution in one historical simulation and two climate projections using different greenhouse gas scenarios. High-resolution model runs can resolve mesoscale processes and provide better detail of extreme weather, such as heat waves and convective thunderstorms. For instance, at 12 km resolution, long convective storms lead to the majority of flash floods and severe weather. A lower resolution model would have trouble correctly resolving these types of storms. When we compared the GFDL and WRF to the North American Regional Reanalysis (NARR), a gridded dataset derived from observed precipitation, we saw obvious improvements in resolution especially along coasts and in mountainous parts of the country when using WRF (fig. 3).

CWRF Uncertainty Analyses

We also used the regional CWRF [2] to examine uncertainties in the treatment of cloud, aerosol, and radiative transfer processes. We defined a subset of computationally feasible size from the Cloud-Aerosol-Radiation (CAR) [3] ensemble system that can capture the observed climate characteristics, especially those relevant to climate variability and extreme events. We ran an ensemble of 24 CWRF physics configurations, all driven by ERA-Interim reanalysis data. The results showed that mean surface temperatures and summer precipitation over both land and ocean differed dramatically among CWRF configurations despite the same lateral boundary conditions from ERI. Some configurations had overall small biases while others produced much larger errors.

We plan to complete the retrospective integration during 1979–2014 for all 24 configurations to ensure statistically robust results, especially for diagnosing interannual variations and extreme events. Subsequent diagnostic analysis of this initial ensemble output will allow us to form a better strategy to choose a more representative (and likely larger) ensemble to conduct CWRF climate change projections driven by CCSM4.

WHY BLUE WATERS?

The major objectives of the project addressed long-recognized issues associated with model resolution and understanding climate sensitivity. The unique super-ensemble approach used in the climate sensitivity studies and the advanced dynamical model cores used in the high-resolution studies both required petascale capabilities.

CAM5-SE required five wall-clock days to run a decade of model time on Blue Waters using thousands of cores. Several of these decade-long tests were required to determine an optimal set of model parameters, and then we used those settings to simulate a century or longer. To complete all of these model runs at high resolution and in a timely manner required petascale computing resources. Similarly, the high-resolution studies using WRF and CWRF also required a system like Blue Waters.

The next Track-1 system will allow us to run century-long ensembles of high-resolution climate models to quantify and reduce uncertainty. The climate modeling community plans to further increase the ocean/sea ice resolution from 1° to 0.1° and atmospheric resolution from 0.25° to 0.125° and beyond. This would improve representation of ocean eddies, cloud processes, and other important details of the Earth system.

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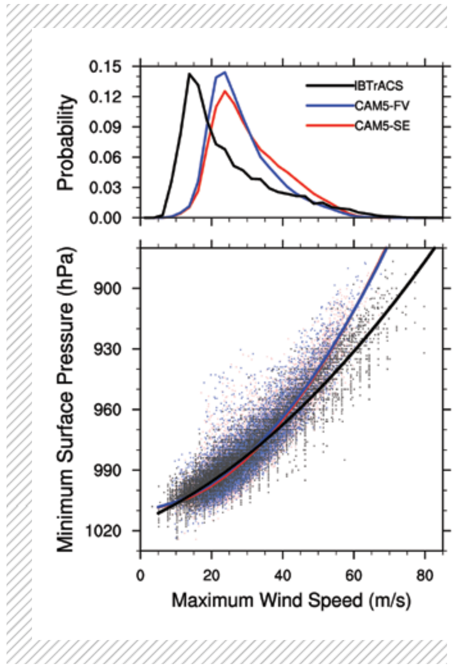

FIGURE 2: Intensity distribution shown as a (top) probability density function of the maximum wind speed and (bottom) minimum surface pressure vs. maximum wind speed relationship with quadratic least squares fit (solid lines) for the CAM5-FV and CAM5-SE simulations 1980-1999. IBTrACS observations are included as a reference.

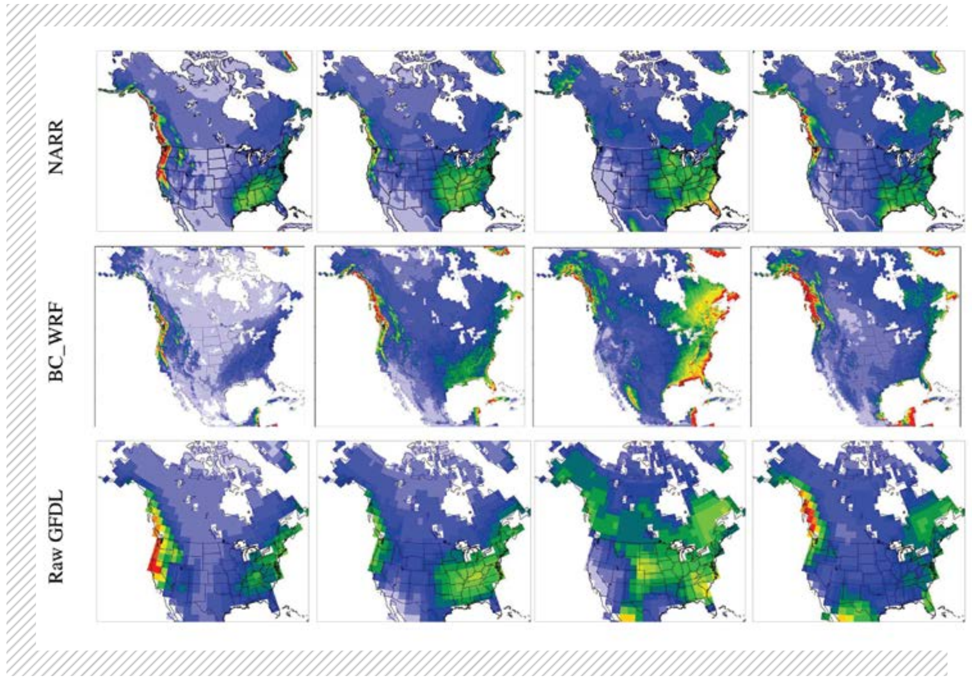

FIGURE 3: WRF simulated, GFDL-ESM2G simulated, and NARR gridded 10-year mean precipitation in winter, spring, summer, and fall (left to right; mm/day).