Blue Waters Professor Allocation Annual Report: February 1, 2015 – January 31, 2016

Title: 3D radiative transfer modeling for improved weather and climate predictions and satellite remote sensing of the cloudy atmosphere

PI: Larry Di Girolamo, Department of Atmospheric Sciences, University of Illinois at Urbana-Champaign

Collaborator(s): Guangyu Zhao, Alexandra Jones, Brian Jewett, Dongwei Fu, Ming Su, University of Illinois at Urbana-Champaign; Lusheng Liang, SSAI and NASA Langley Research Center

Corresponding Author: Larry Di Girolamo, gdi@illinois.edu

Executive Summary:

Our multi-pronged approach for tackling key problems in weather and climate research that are rooted in 3D radiative transfer has had an incredible year of success: (1) development and benchmarking of the first spectrally integrating, atmospheric 3D Monte Carlo radiative transfer model, (2) improvements to NASA's infrastructure for the transfer of a PB of Terra data to Illinois, (3) a published discovery of the Earth getting bluer and smoother over the 15-year Terra record, (4) a published paper that uncovered, quantified, and corrected large biases in the drop size distribution of water clouds in the MODIS satellite record through data fusion of Terra instruments, (5) development of new initiatives involving Blue Waters and ROGER, and (6) Blue Water Graduate Fellow Alexandra Jones' successful completion of her Ph.D. degree (now a postdoc at Princeton University). Blue Waters allocation was underutilized owing to Jones' fellowship allocation, bench testing and use of ROGER, and time spent bringing results to publication and developing new initiatives.

Description of Research Activities and Results:

Research in weather and climate has massive societal benefits, and indeed has been one of the leading drivers for advancing supercomputing infrastructures. One of least understood and most important aspect of the weather and climate system are Earth's clouds. Clouds cover about 68% of our planet. They are one of the most interconnected components of the Earth System, playing a key role in the Earth's hydrological cycle, regulating the incident solar radiation field more than any other atmospheric variable, and acting as the most important greenhouse constituent in our atmosphere. As such, they modulate a wide range of processes on Earth. The Intergovernmental Panel on Climate Change (IPCC) affirms that the role of clouds remains the leading source of uncertainty in anthropogenic climate change predictions. In addition, the role of cloud microphysics and cloud-radiation interactions in the timing and intensity of weather events remains an active area of research.

Currently, radiative transfer (RT) in models used in weather and climate research is represented in a primitive manner (mostly in a single dimension-up/down) because of the exceptional computational expense. Computational resources have always been a constraint on how radiation can be explicitly represented in dynamic models of the atmosphere such as the Weather Research and Forecasting Model (WRF), especially at LES (large eddy simulation) scales with grid spacing ranging from 10m-100m. As the numerical representation of other physical processes have advanced (e.g. cloud microphysical processes), the representation of radiative processes have remained markedly unsophisticated. This is true even at the finest LES resolutions where the approximations that allow for computationally inexpensive treatments break down even further. These crude representations of radiative transfer can result in localized orders-of-magnitude error in radiative heating in the presence of clouds with complex morphology. The resulting errors, when allowed to feedback on cloud dynamics, feedback as errors in cloud size, lifetime, and physical properties. These changes in turn may impact weather and climate by, for example, affecting rainfall, surface atmospheric heating, and photolysis rates. While 3D radiative transfer is a solved problem (e.g., by way of a Monte Carlo solution), albeit a computationally expensive one, *a full 3D RT model has never before been coupled to a cloud dynamics model*. Here our research aims to do just that. This coupled model, for the first time, will allow us to study and understand how errors from the crude RT approximations used in the past feedback on cloud properties and their evolution. We anticipate that the contributions from radiative cooling at cloud edge and other radiative effects could close the current gap between numerical results and observations, not only of dynamical properties but of micro- and macro-physical cloud properties. In carrying out this project, we will address longstanding significant computational challenges inherent in solving 3D radiative transfer in cloudy atmospheres.

Simulating 3D RT coupled to WRF is a Blue Waters-class computational problem that far exceeds traditional XSEDE resources, as demonstrated in our original Blue Waters proposals. Developing a full 3D radiative physics package for an LES model will provide a solid foundation for testing hypotheses involving the two-way interaction of cloud systems and radiation. This model will also become a test-bed for the development of practical RT parameterizations that capture the most important 3D RT effects at lower resolution and lower computational cost, which will benefit the broader modeling community striving to improve weather and climate predictions. Our new model will also address other unresolved issues related to the role of 3D RT in the interpretation of aircraft and satellite observations of clouds and aerosols, which is a key component of Prof. Di Girolamo's NASA-sponsored research program (more on this below).

In the second year of the Blue Waters Professorship, our RT model has evolved in its development to be capable of simulating broadband radiative transfer through complex 3D cloud scenes. The end result is the first spectrally integrating, Monte Carlo 3D radiative transfer model that includes both internal and external sources, and accounts for absorption, emission, and scattering by the atmosphere, clouds, and the surface. This required the development of large databases of atmospheric optical properties. For example, the optical properties for a particular gamma distribution of liquid water droplets at approximately 250 Hz spectral resolution was created. This database requires about 5TB of storage and is the most comprehensive database of its kind. An unanticipated benefit of developing this database is that it can be mined to provide updated parameterizations of optical properties at lower spectral resolution; the most popular of the sort haven't been updated in almost 30 years. The accuracy of our RT model has been verified with extensive comparison to analytical solutions and results from the world's most advanced 1D Line-by-Line RT model. Our model is now ready to act as the first 3D broadband standard of accuracy for comparison by other RT models that make simplifying assumptions. It will be released for public use and development as a community model upon publication (see Plan for Next Year).

The completion of our 3D RT model and its databases also marked the completion of Alexandra Jones' Ph.D. dissertation (see Publications), which was successfully and impressively defended on January 7, 2016, and deposited on January 20, 2016. She begins her postdoc at Princeton University in mid-February. Alexandra received a Blue Waters Graduate Fellowship this past year, which provided allocation on Blue Waters on top of the Blue Waters Professorship allocation that she was using.

The advancement of science is also rooted in observations. Therefore, to make headway in reducing uncertainty in weather and climate predictions, the World Meteorological Organization and the IPCC defined a list of Essential Climate Variables (ECVs) requiring global satellite observations (http://www.gosic.org/gcos). It has been established that ~2/3 of the ECVs derived from satellite do not meet accuracy requirements, therefore calling for improvements in the algorithms and technologies used by satellites. One of the key recommendations from the NRC 2007 Decadal Survey on Earth Science and Applications from Space (NRC 2007) is clear: *"… experts should… focus on providing comprehensive data* *sets that combine measurements from multiple sensors."* This, in part, targets NASA's flagship of the Earth Observing System where, for the past 15 years, the Terra satellite mission has provided very few ECVs that are based on a multi-sensor, data-fusion approach with its five instruments. The challenge is now particularly acute for Terra, given its growing volume of data (> 1 PB), the storage of different instrument data at different archive centers, the different file formats and projection systems employed for different instrument data, and the inadequate cyberinfrastructure for scientists to access and process whole-mission fusion data (including Level 1 data). This has led to the *Terra Data Fusion Project*, which is supported through Di Girolamo's NCSA Faculty Fellowship that has led to a much larger proposal (PI Di Girolamo) that is currently under review by the NASA ACCESS (Advancing Collaborative Connections for Earth System Science) program. In these proposal, we demonstrate that efficient generation and delivery of Terra data fusion ECVs, followed by analysis, are possible with Blue Waters.

To make headway, we have been working with the Blue Waters staff and NASA on data transfer issues. This has led to improvements to NASA's infrastructure for data deliver, including a five-fold improvement in data transfer from NASA Langley's Atmospheric Science Data Center. When the time came to move the Terra data, ROGER came online. Since we were a Senior Collaborator for ROGER, we decided to move two of the Terra instrument datasets, MISR and MODIS (~0.6 PB), to streamline and test ROGER's capabilities for this project, which also helped provide results provided below. This unplanned effort for ROGER also contributed to our under utilization of our Blue Waters allocation.

Use cases for the Terra Data Fusion Project are already supported by several of the PI's NASA-sponsored projects that specifically call for development and processing of new ECV algorithms for Terra on Blue Waters. One focuses on the fusion of MISR and MODIS data to advance the effective radius of the cloud drop size distribution (an ECV) that is currently derived from MODIS alone. Here, through MODIS and MISR fusion, we have uncovered large biases in the original MODIS effective radius product. The space-time varying biases were determined to range from 3 – 11 μm for marine liquid water clouds, which, when removed, provides a very different understanding of the distribution of liquid cloud drop sizes in our atmosphere compared to what was previously determined from the original MODIS data. This greatly advances the utility of the Terra data for weather and climate research. Our results were reported in the *2015 Blue Waters Annual Report* and published in the *Journal of Geophysical Research – Atmospheres (Liang, et al., 2015)*.

The biases in the MODIS effective radius product arise from the use of a 1D radiative transfer framework for the solution to the inverse problem. In fact, most of the ECVs derived from satellites are also based on a 1D RT framework. [Note, this provides further motivation for the development of our Monte Carlo 3D radiative transfer model discussed above.] This 1D RT assumption, like all assumptions used in remote sensing algorithms, may induce systematic errors in the long-term trends in ECVs, the magnitudes of which depend on the validity of the assumptions for the scenes observed by a satellite. Since systematic and sampling errors co-vary with the underlying conditions in which the retrievals are made (including sun-view geometry), they are often difficult to impossible to quantify and remove from the ECVs. This makes it difficult to decouple true space-time variability found in nature from algorithm-related space-time variability within ECV datasets (*e.g., Di Girolamo, et al., 2010*). Consequently, our most robust evidence for satellite-derived decadal variability in the Earth system would be based not on ECVs, but on the direct underlying radiance measurements.

This led us to directly examine the spectral, textural (spatial), and angular properties of the upwelling radiance field from scattered sunlight sampled by MISR over its 15-year record. Here we identify statistically significant trends in the color and spatial texture of Earth as viewed from multiple directions from MISR. Globally, our results show that the Earth has been appearing relatively bluer (up to 1.6% per decade from both nadir and oblique views) and smoother (up to 1.5% per decade only from oblique views) over the past 15 years. The magnitude of the global bluing trends is comparable to that of uncertainties in radiometric calibration stability. Regional shifts in color and texture, which are significantly larger than global means, are observed, particularly over polar-regions, along the boundaries of the subtropical highs, the tropical western Pacific, Southwestern Asia, and Australia. We demonstrate that the large regional trends cannot be explained either by uncertainties in radiometric calibration or variability in total or spectral solar irradiance; hence they reflect changes internal to Earth's climate system. The 15-year-mean true color composites and texture images of the earth at both nadir and oblique views are also presented for the first time, and shown below as Figure 1. Our results are published in the *IEEE Transactions on Geoscience and Remote Sensing* (*Zhao, et al., 2016; accepted pending minor revisions*).

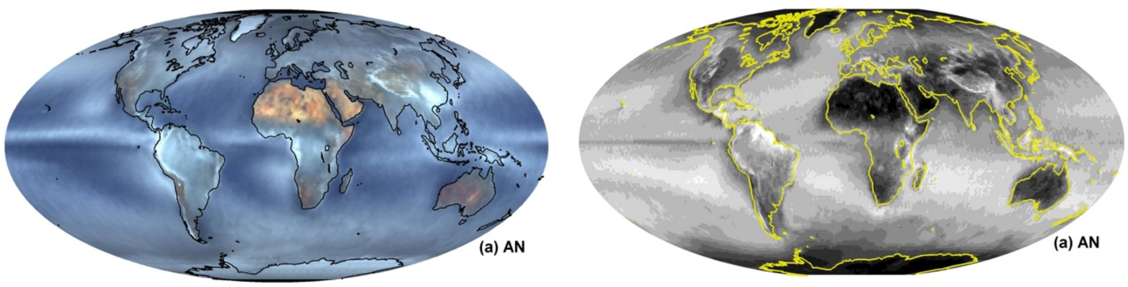

Figure 1. Average true color (right) and texture (left) of the Earth from the nadir-pointing MISR camera. The MISR data is from the descending branch only of Terra's sun-synchronous orbit, which has an equator crossing time of 10:30 am.

Publications and Presentations Associated this this Work

Liang, L., L. Di Girolamo, and W. Sun (2015), Bias in MODIS cloud drop effective radius for oceanic water clouds as deduced from optical thickness variability across scattering angles, *J. Geophys. Res. Atmos.,* 120, doi:10.1002/2015JD023256.

Zhao, G., L. Di Girolamo, D. J. Diner, C.J. Bruegge, K. Muller, and D.L. Wu (2016), Rional changes in Earth's color and texture as observed from space over a 15-year period. *IEEE Trans. Geosci. Remote Sens. (accepted pending minor revisions).*

Jones, A. L. (2016), *Development of an Accurate 3D Monte Carlo Broadband Atmospheric Radiative Transfer Model*, Ph.D. Dissertation, University of Illinois, Urbana, IL.

Di Girolamo, L., A. L. Jones, L. Liang, and G. Zhao, (2015), Global observations of cloud microphysics through Terra data fusion, *2015 Blue Waters Annual Report*, University of Illinois Press, Urbana, IL.

Jones, A.L., Development of a Highly Accurate 3D Radiative Transfer Model, *University of Illinois Atmospheric Sciences Colloquia Series*, Urbana, IL, April 1, 2015.

Di Girolamo, L., L. Liang, and W. Sun, 2015: Bias in MODIS cloud drop effective radius for oceanic water clouds as deduced from measured cloud optical thickness variability across scattering angles. *Joint Assembly of the AGU-GAC-MAC-CGU*, May 2015, Montreal, PQ, ***(Invited)***

Di Girolamo, L., L. Liang, and W. Sun, 2015: Bias in MODIS cloud drop effective radius for oceanic water clouds as deduced from measured cloud optical thickness variability across scattering angles. *MODIS Science Team Meeting*, May, Silver Spring, MD.

Jones, A, and L.Di Girolamo, 2015: High accuracy 3D radiative transfer in cloudy atmospheres. *Blue Waters Symposium*, May 10 - 13, Sunriver, OR.

Plan for Next Year:

Our work for the upcoming year extends much of the work we need this past year. The spectrally integrating, atmospheric Monte Carlo 3D radiative transfer model, and its sister monochromatic version, will be made available to the public. These models have been developed in an object-oriented style, meant to allow for further community development. Before public release later this year, we will work on developing the needed peer-reviewed publications and finalize user and developer documentation for these models. Some work to improve the memory utilization and fine tune the performance of the model at scale on Blue Waters will be carried out. Optimization of these codes on Blue Waters is essential since the intent is to make them available to the broader community, some of whom may wish to carry out their research with these codes on Blue Waters. The models will then be utilized to provide highly accurate standards of comparison for other radiative transfer models. This contribution will allow for inclusion of parameterizations of 3D effects in the simpler, less expensive, more commonly used radiative transfer models that are either coupled to climate and weather models, or used to invert satellite observations, for example. Additional experiments, highlighting the bias in satellite products due to 3D effects will also be conducted. Based on our experience with these models over the past year and our planned experiments, we anticipate approximately 180,000 node hours to bring this work to completion.

Terra data fusion product development is currently supported under two NASA-sponsored projects: NNX14AJ27G for the cloud drop effective radius of liquid water clouds and NNX15AQ25G for ice crystal roughness for cirrus clouds. In both cases, allocation on Blue Waters within Di Girolamo's current Blue Waters Professorship allocation was defined. In addition, our proposal that is currently under review by NASA's ACCESS program also provides allocation under Di Girolamo's current Blue Waters Professorship allocation, as well as a separate storage allocation as stipulated in a separate commitment by the OVCR. We are also launching an education initiative that processes the MISR and MODIS data in a manner that is both informative and appealing to a broader public (like Figure 1) who are interested in Earth sciences. For the upcoming year, we anticipate only 60,000 node hours on Blue Waters for the processing and analysis of the Terra data over all these projects. This is based on our experience in our current processing of the Terra data and our continued off-loading of some of the Terra processing and analysis on ROGER.

We therefore request 240,000 node hours for next year. We expect the usage break down by quarter to be the following:

Q1: 20% Q2: 20% Q3: 30% Q4: 30%

The storage requirement for the 3D radiative transfer modeling work is not anticipated to be large relative to Blue Waters capacity. Tables of scattering properties will need to be retained for each unique atmospheric domain, however total storage for those tables and the corresponding output should not exceed 50 TB. The model requires only two input files and produces one output file, so there is no anticipated taxing of the file system expected due to large numbers of files. The radiative transfer model is comprised mainly of logical operations to determine the fate of the bundle of light, i.e. comparisons of random numbers to cumulative distribution functions and simple arithmetic calculations to tally the contribution of each bundle as it travels through the domain. Memory usage will depend on domain size.

The storage requirement for the Terra work can be large. At the moment, we have stored ~0.6 PB of Terra data (all MISR and MODIS L1B2 data) on ROGER for testing the system and result-oriented processing. We have always envisioned this as a temporary situation, and that the data should eventually move to Blue Waters as we shift our focus back to the Terra Data Fusion Project and the NASA-sponsored research. We still need to transfer from NASA data centers another ~0.6 PB of satellite data (from the ASTER, CERES, and MOPITT instruments on Terra). Since we will be producing large mission scale ECVs from these datasets, we will be creating an additional ~0.8 PB of data for analysis and distribution. **Therefore, we request 2 PB of storage on Nearline Projects.** We note that this storage request is the same as that requested for our proposal to the NASA ACCESS program for the Terra Data Fusion work and serves the same purpose (i.e., we still only need 2 PB and not 4 PB of storage).