DEPENDENCE OF THE DIRECTIONAL INTENSITY AND POLARIZATION OF LIGHT SCATTERED BY SMALL ICE CRYSTALS ON THEIR SHAPE AND SIZE: APPLICATIONS FOR AIRBORNE CLOUD PROBES

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EXECUTIVE SUMMARY

Current probes installed on aircraft for measuring the sizes of ice crystals smaller than 50 micrometers assume the intensity of light scattered by particles passing through the sample volume is a function of particle size. The relationship between particle size and scattered light used in current probes is based on Mie theory, which assumes the refractive index of a particle is known, and that all particles are spherical. Not only are small crystals not spherical, but they also can have a wide variety of shapes. To improve airborne measurements of small crystals, precise relationships between the light scattered by nonspherical particles and their size and shape are required and are based on accurate calculations of crystal scattering properties. However, such calculations use numerically exact methods and hence require a large amount of computing time and memory, which increase with crystal size. Thus, we use Blue Waters for these calculations.

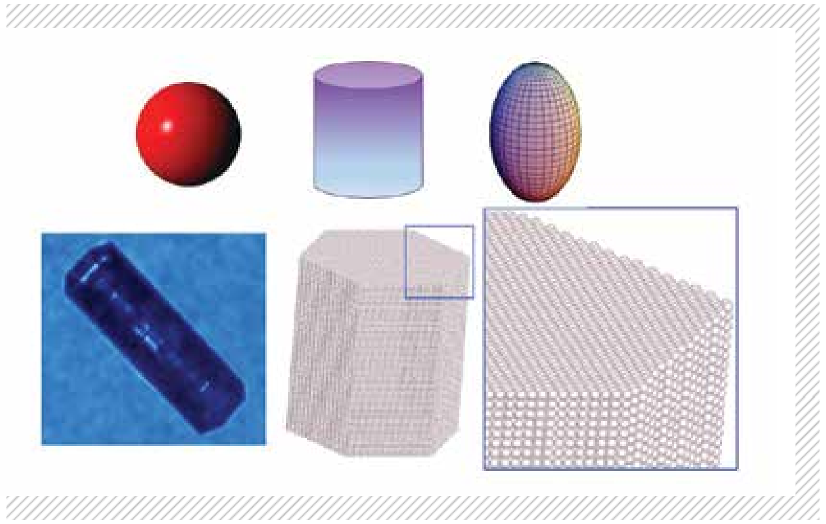

FIGURE 1: Top: A sphere, cylinder, and spheroid represent shapes of ice crystals in previous studies. Bottom: Real image (left) of ice crystals and its representation in DDA calculations.

INTRODUCTION

Cloud particle size distributions measured by cloud probes installed on aircraft are used to both develop parameterizations for and evaluate the results of satellite retrieval algorithms, and numerical models. Some current cloud probes (e.g., forward scattering spectrometer probes) measure the sizes of ice crystals smaller than 50 micrometers assuming that the intensity of light scattered by particles in the forward, and sometimes backward direction is a function of particle size. The retrieval of ice crystal sizes from satellites and application of parameterization schemes for numerical models also rely on relationships between light scattering and particle size.

The relationship between particle size and scattered light used in current forward scattering probes is based on Mie theory, which assumes that the refractive index of a particle is known and that all particles are spherical. Small crystals are not spherical, and a wide variety of shapes have been used to represent them. Although it is known that the scattering properties of non-spherical ice crystals differ from those of spheres, the impacts of non-sphericity on retrieved sizes for airborne probes, satellite retrievals, and model parameterizations are unknown. Further, more advanced forward scattering probes and satellite sensors that use the polarization and intensity of light also require knowledge of the scattering properties of non-spherical ice crystals.

Although a few studies have calculated the scattering properties of nonspherical particles assuming cylindrical and spheroidal shapes (Fig. 1), the shapes used are far different from realistic shapes of small ice crystals. Thus, to improve airborne measurements of small crystals, satellite retrieval algorithms, and numerical models, precise relationships between the intensity and polarization of light scattered in multiple directions with the size and shape of nonspherical crystals are required. However, accurate calculations of the scattering properties of crystals using numerically exact methods (i.e., solving Maxwell's equations) require large amounts of computing time and memory, which increase with crystal size. Thus, Blue Waters is an important resource for these calculations.

METHODS & RESULTS

The scattering properties (i.e., angular dependence of scattering, intensity of scattering, and polarization) of ice crystals with a maximum dimension (D_{max}) smaller than 50 micrometers are calculated at a non-absorbing wavelength (λ=0.55 μm) using a numerically exact method (i.e., the discrete dipole approximation, DDA) [1]. For these calculations, hexagonal ice crystals with varying aspect ratios (*AR*=length/width, AR=0.1, 0.25, 0.5, 1.0, 2.0, and 4.0) are used to represent the shapes of natural small ice crystals (Fig. 1). In DDA calculations, a hexagonal ice crystal is divided into elementary polarization units called dipoles (Fig. 1) with each or a group of dipoles assigned to a single core of Blue Waters for the calculations.

To quantify errors in the sizing of ice crystals used in current forward scattering probes, Figure 2 shows differences in the calculated D_{max} assuming spherical (i.e., Mie calculations) and hexagonal (i.e., DDA calculations) shapes of ice crystals. For a given amount of scattered light measured by a forward scattering probe, multiple selections of particle size are possible because of variations in crystal shapes. In Figure 2, blue dots represent the average differences in calculated diameters, whereas red dots are the maximum and minimum differences in diameters. These differences represent the errors in sizing nonspherical ice crystals using current forward scattering probes. The errors depend on the sizes and ARs of ice crystals (i.e., each panel of Fig. 2). It is shown that differences in sizing particles are smallest for D_{max}=~10 μm, while larger for D_{max}<10 μm (due to light interference structures) and for D_{max}>10 μm (due to nonsphericity) regardless of the *AR*. The differences are larger when the shapes are more nonspherical (i.e., *AR*=0.1 and 4.0). The average differences are up to 41% with a prolate shape (i.e., *AR*=4.0). These differences, representing errors in the retrieval of particle sizes from current forward scattering probes, determined using realistic shapes (i.e., hexagonal shapes) of ice crystals are larger than those determined assuming either cylinder or spheroid shapes in previous studies. Thus, to improve the retrieval of particle sizes from current forward scattering probes, accurate calculations of the scattering properties of realistic shapes of ice crystals are required.

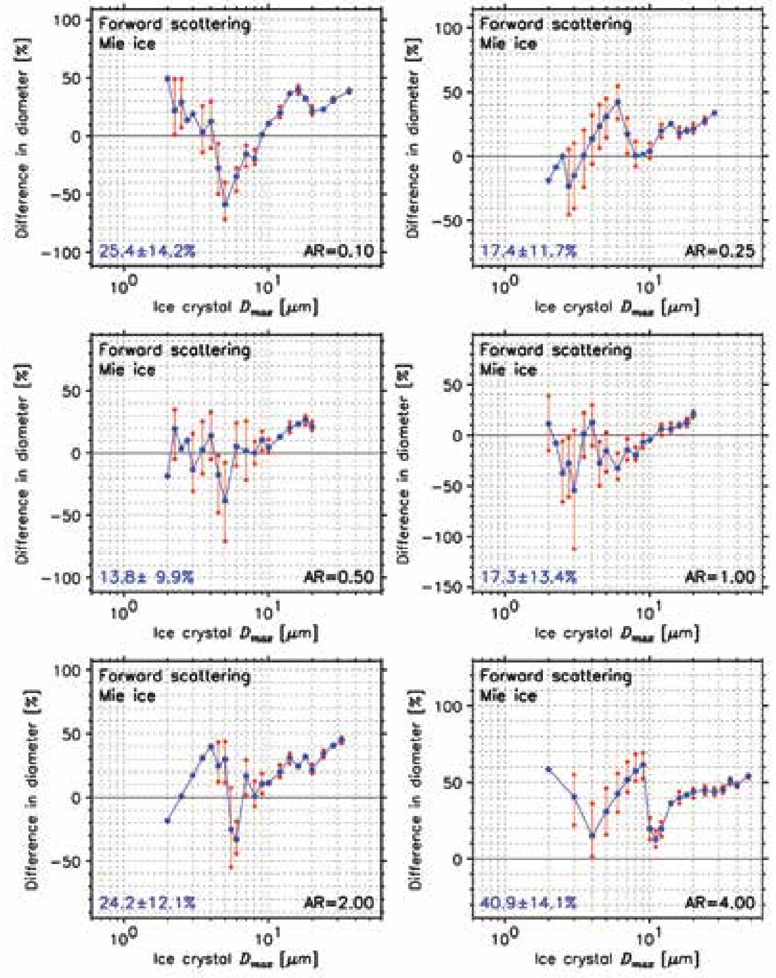

FIGURE 2: Differences (100% × (D_{max} − Mie D_{max})/D_{max}) between actual sizes of ice crystals and those determined based on Mie calculations in forward directions as a function of *AR* of hexagonal ice crystals (each panel). Mean and standard deviation of absolute values of blue circles are embedded in each panel.

WHY BLUE WATERS

Much larger computing resources are required to compute accurate scattering properties of realistic shapes (e.g., hexagonal columns and plates) of ice crystals compared to previous studies that used approximate shapes (e.g., spheres, cylinders and spheroids). The exact discrete dipole method was needed for particles with the small sizes used here. Although the exact methods provide more accurate results, they require more computing time and memory that rapidly increases with particle size. The accuracy of measurements of particle sizes with airborne probes, radiative transfer models, and satellite retrieval algorithms depends heavily on accurate calculations of single-scattering properties of ice crystals. The petascale Blue Waters is an important resource for completing these calculations.

NEXT GENERATION WORK

Natural ice crystals larger than 50 micrometers have various shapes with much more complex internal (e.g., inclusions) and external features (e.g., surface roughness) compared to small ice crystals. Thus, calculations of scattering properties of larger ice crystals will require much larger computing resources than available on Blue Waters. We want to perform such calculations using a next-generation Track-1 system.

PUBLICATIONS AND DATA SETS

Um, J., and G. M. McFarquhar, Formation of atmospheric halos and applicability of geometric optics for calculating single-scattering properties of hexagonal ice crystals: Impacts of aspect ratio and ice crystal size. *J. Quant. Spectrosc. Radiat. Transfer*, 165 (2015), pp. 134-152, doi:10.1016/j.jqsrt.2015.07.001

Um, J., and G. M. McFarquhar, Light scattering by atmospheric ice crystals: Application to forward scattering probes. *International Symposium on Radiation*, Auckland, New Zealand, April 16-22, 2016.

McFarquhar, G. M., and J. Um, Light scattering by atmospheric hexagonal ice crystals for determination of applicability of geometric optics and formation of atmospheric circumscribed halos, *International Symposium on Radiation*, Auckland, New Zealand, April 16-22, 2016.

BUILDING A DATA ASSIMILATION FRAMEWORK FOR FORECASTING VOLCANIC ACTIVITY DURING PERIODS OF UNREST

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EXECUTIVE SUMMARY

A primary goal of the University of Illinois Urbana-Champaign Volcano Lab is to develop innovative strategies for combining volcano-monitoring datasets with thermomechanical models to better understand the dynamics of triggering a volcanic eruption. We use Blue Waters to develop and test a framework for **multi-data stream data assimilation** by conducting a series of eruption "hind casts" for recent eruptions at Sinabung Volcano in Indonesia.

Blue Waters is uniquely capable of handling the computational expense for our ensemble-based modeling approach, which has compute times and storage requirements considerably outside the capabilities of traditional high-performance computing (HPC) resources. Ultimately, this work will provide a critical foundation for future interdisciplinary efforts to model volcano evolution and mitigate volcano disasters for vulnerable populations worldwide.

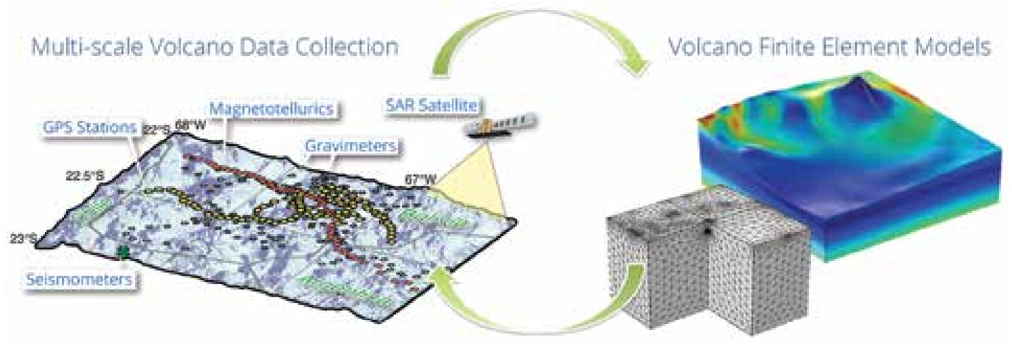

FIGURE 1: Statistical data assimilation techniques combine disparate observations with models to produce forecasts of an evolving system. The data inform the trajectory of the models and the models in turn inform future data targets and collection strategies. Left: A map depicting the NSF PLUTONS Project at Uturuncu Volcano, Bolivia [7]. Right: FEM mesh and modeled stress for Sinabung Volcano, Indonesia.

INTRODUCTION

A primary motivation for investigating volcanic systems is to develop the ability to predict eruptions and mitigate disaster for vulnerable populations. In recent decades, the evaluation of volcanic activity has been greatly enhanced by coupling remote (e.g., satellite and global seismic arrays) and local observations (e.g., GPS, gas emissions, and seismometers) to provide early warning of an imminent eruption or information on the evolution of a magma system during a volcano crisis. Concurrently, thermomechanical models of magma reservoirs have significantly advanced our understanding of eruption-triggering mechanisms beyond the temporal and spatial limitations of our observations [1,2].

Volcano monitoring datasets are commonly analyzed using analytical inversions techniques or by optimizing finite element models [3,4]. While these approaches work well for combining models with one or two data streams, they are static assessments of the system state that do not provide updates or forecasts and are limited in their scope. Alternatively, statistical data assimilation methods were developed to systematically link data with models to provide model updates. Significant advancements in data assimilation have been made in many fields, including engineering, hydrology, physical oceanography, and climate modeling, to incorporate disparate datasets into dynamic, nonlinear models and provide model forecasts [5]. Sequential model-data fusion methods provide a framework for integrating large, disparate data sets into time forward, forecast models (Fig. 1). Data are used to nudge the model trajectory and provide updates of the system's evolution, and models inform future data targets.

Our current efforts on Blue Waters are focused on developing strategies for rapid assimilation of monitoring datasets into evolving geodynamic models to provide near-real-time forecasts and assessment of volcanic unrest. To that end, we are adapting data assimilation methods developed in other fields to combine observations from volcanoes experiencing unrest with thermomechanical finite element models (FEMs) to calculate volcano evolution [6].

METHODS & RESULTS

We have adapted the Ensemble Kalman Filter (EnKF, [5]) sequential data assimilation method to assimilate volcano-monitoring data from satellite and ground-based observations into geodynamic models. The EnKF utilizes a Markov Chain Monte Carlo (MCMC) approach to create suites, or ensembles, of models that are updated sequentially as new observations become available.

Preliminary results indicate that the EnKF is a powerful tool well suited for the problem of forecasting volcanoes experiencing unrest. Our Blue Waters Exploratory Allocation is allowing us to test the feasibility of a large-scale data assimilation approach for volcano monitoring. This is the **first** effort of its kind and has great potential for significantly advancing the field of volcano hazards.

WHY BLUE WATERS

The EnKF is an ensemble based sequential data assimilation method that requires calculating hundreds to thousands of finite element models at each time step. While the EnKF analysis step has been optimized to run very swiftly, the computational expense of running and storing hundred to thousands of finite element models for each time step in the EnKF analysis is cost prohibitive for traditional HPC resources. Blue Waters is uniquely positioned to handle our computational needs and has allowed us to make rapid progress and develop **ambitious** approaches without being hampered by computational limitations.