Research Statement

Dr. Osku Kemppinen

1 Introduction

My research focuses on the interaction of electromagnetic radiation with matter, both how the interaction depends on the properties of the matter in question, i.e. the direct problem, as well as what measurements of the scattered light can tell us about the properties, i.e. the inverse problem. Specifically, I'm interested in particles or other discrete objects, as well as details in larger objects, that fall within the size scale of the wavelength of the radiation in question, where most textbook-level simplifications of electromagnetic scattering can not be utilized. I am experienced in both experimental and computational electromagnetic scattering I can study a wide range of phenomena, and in a wide variety of circumstances, from *in situ* to *in silico*.

Additionally, my practical engineering skillset can be very valuable in experimental research. The combination of three-dimensional design skills, such as various CAD programs, as well as my experience in cutting edge technologies such as rapid prototyping in the form of three-dimensional printing can allow for very fast transfer of technology from benchtop to real world, whether for a field study or collaboration with the private sector. I am also a licensed and experienced unmanned aircraft pilot, and I feel such aircraft are incredibly valuable in many *in situ* measurements of the future, in particular when applied to atmospheric, oceanic, volcanic and other natural phenomena.

At Texas Tech University I would start a research program for experimental electromagnetic and optical studies of condensed matter, focusing on digital holography and its applications in imaging. This builds on my experience with experimental electromagnetic scattering, and the complex data analysis that is required by digital holography greatly benefits from my background as a computational scientist. Importantly, this line of work has applications in multiple other fields of science. For example, at Kansas State University, we are starting to collaborate with agricultural research, as digital holography offers solutions to many of their issues not easily solvable with other imaging methods. Department of Geosciences, especially their Atmospheric Research, can also benefit from aerosol imaging instrument development as well as an improved aerosol scattering database. Thus, I believe there is strong potential for fruitful collaboration within Texas Tech University even outside of the Department of Physics & Astronomy.

2 Dissertation Research

While my dissertation focused on computational electromagnetic scattering, I contributed to another substantial research project in parallel with my dissertation. This arrangement was due to a unique opportunity presented, as well as due to availability of funding. These topics are described separately below for clarity.

2.1 Computational light scattering of irregular atmospheric aerosol particles

Aerosol particles contribute significantly to the radiative balance of Earth, yet the variability of their contribution is almost as large as the mean contribution itself. In practice it means they are very hard to describe with one single model, or to treat as one type of a particle in atmospheric and climate simulations. This is natural if one were to look at images of different types of aerosols. They vary significantly in size, but, importantly, also shape and composition. While much of the early work in light scattering by aerosols focused solely on size, recent advances in modeling have revealed that shape is also a factor. In addition to the gross shape, other morphological details such as sub-wavelength surface roughness and internal structures have been found to be important.

My dissertation work was focused on modeling different previously neglected morphological aspects of atmospheric dust particles. Simulations allow for a systematic control of the particle shape, composition and other details, unlike what is possible in a laboratory. I found that almost all of the commonly-ignored aspects of particle morphology have important consequences, especially for quantities relevant to emerging measurement techniques, such as polarimetry and backscattering, e.g., LIDAR. Finally, I compared simulated scattering by different types of particles, both realistic and simple shapes, with laboratory measurements.

I also found that particle composition inversion via spheroid and ellipsoids is risky, at best. That is, by retrieving the refractive index from the scattering pattern of an irregular particle with a known refractive index using a best-fit ensemble of ellipsoids, I found that the results are consistently inaccurate and that using such retrievals propagates serious inaccuracies in atmospheric radiation simulations.

I proposed a continuation of this research project for my NASA Postdoctoral Fellowship at NASA Langley Research Center, and was happy to learn that they see the importance of the same issue and accepted my proposal. Although I declined the offer in favor of broadening my skills to include experimental work, this fact gives me confidence that there is likely to be fruitful collaboration and funding opportunities in this line of work in the future.

2.2 Mars Science Laboratory relative humidity sensor

Alongside my dissertation work, I served as a sensor expert and a science team member for the relative humidity sensor (REMS-H) on-board NASA's Mars Science Laboratory (MSL). Due to the combination of extreme cold, extremely low pressure, and extreme dryness, humidity measurements on Mars can be challenging, both from instrument design and data analysis point of view. REMS-H is the first instrument on Mars to directly measure relative humidity, by utilizing changes in the capacitance of a porous polymer membrane as a proxy for the humidity. A few months before MSL landed, I worked with the project manager of REMS-H to generate the calibration function to obtain humidity values from the capacitances according to the specific response characteristics of the membrane. We also created an automatic data analysis and plotting pipeline for routine nightly data processing. A week before the landing I traveled to NASA Jet Propulsion Laboratory with a small team to ensure we could respond fast if anything went wrong during the first few weeks of operation.

As it happened, several things did go wrong. We had multiple issues with our electronics and reference capacitors, but eventually found solutions for all of them. We also developed new operational modes to cancel the negative effect of sensor temperature increase, as well as an deconvolution method to mitigate the time lag of the sensor due to the low temperatures. This project was a tremendous learning experience for a second-year Ph.D. student, and I believe many of my latter philosophies for instrument design, data analysis, and measurement procedures can be traced back to that experience. It also allowed me to see how world-class scientists approach high-impact science in real time, balancing priorities and risks, formulating hypotheses in face of uncertainty, and coordinating across large multicultural and multidisciplinary teams.

3 Current Research: Digital Holography

Compared to traditional light scattering analysis of single particles, digital holography offers significant advantages. The main advantage is that because an interference pattern is recorded instead of the conventional intensity pattern, the phase of the scattered light can be retrieved alongside the intensity. This combination of patterns contains significantly more information than the intensity pattern alone, and as a consequence, allows for retrieval of quantities such as the extinction cross-section [Berg et al., 2017]. Importantly, the silhouette-like image of the scatterer can be retrieved from a hologram easily, whereas it is all but impossible to do from just the scattering pattern.

One of the main use cases for holography is lensless single-pulse *in situ* imaging, and that's what my postdoctoral and research assistant professor project has been about. Specifically, this work involves the measurement and analysis of conventional forward-scattered holography, and the results are, essentially, particle silhouette images with limited three-dimensional information of the shape. This work has culminated in me planning, designing and building an *in situ* aerosol particle imaging instrument for large aerosol particles based on digital holography. The instrument is called Holographic Aerosol Particle Imager (HAPI), and it has been designed from scratch to be small and lightweight. Aside from the basic optical components and electronics, HAPI is 3D-printed. I painstakingly custom-designed each mount, holder and support structure to be modular, interchangeable, and to minimize the size and the mass of the instrument. All this was for a good reason: We wanted HAPI to be able to fly on a commercial off-the-shelf drone. I have been able to get scientific flight experience using our group's drone and another instrument, called Portable Optical Particle Counter (POPS) to prepare for HAPI operations. Having a field-portable particle imager capable of measurements in the full three-dimensional space allows for types of measurements that have not been possible so far.

It would be fairly simple to replicate the current experimental setup with forward-scattering holograms from perpendicular directions for more comprehensive particle shape characterization. This would provide simultaneous silhouettes from different directions, yielding more information on the three-dimensional shape. Three mutually perpendicular holograms would be doable as well. It should be stressed that both the two-hologram and the three-hologram versions can be made into field-portable instrument as done with our existing HAPI instrument. While HAPI is a good first step toward atmospheric particle database, a database with simultaneous images of a particle from three different directions, each some depth information in addition to the particle image, would allow for nearly unambiguous characterization of ambient particles.

In addition to the above description of coarse-mode aerosol particle characterization, digital holography can also be used as a simpler particle-counting method with minimal changes in the measurement setup. This is due to its ability to resolve each individual particle in a sensing volume separately, assuming the noise level can be kept small. This is in contrast with traditional optical particle counters that measure total scattering by a sensing volume, and give a best-guess estimate on the number of particles in that volume.

The above work on experiments has been supported by several computational projects. In Kemppinen et al. [2017] we developed a three-dimensional shape reconstruction and automatic focusing procedure for holographic images. In an article currently in preparation we have investigated the ability of Huygens' approximation and Babinet's principle to estimate the forward-scattering pattern of large aerosols when the particle silhouette is known. I have also done preliminary work on alternatives to traditional dense lattice DDA in an effort to speed up calculations in specific situations, such as with soft particles, without compromising the accuracy.

4 Future research

4.1 Atmospheric particle light scattering database

It seems all but inevitable that the field of atmospheric science, from aerosol concentration retrievals to climate simulations, will move toward more realistic aerosol scattering models within the next decade. Currently, there is no scattering database even for a single species of aerosol, or even a statistically significant shape database.

I propose to amend this by producing the first particle database with both the shape information as well as full-angle scattering information, including different polarizations. I propose to start with mineral dust, the most common aerosol type, and one that is critical for e.g. radiative transfer both regionally as well as globally. The approach has three main phases.

The first phase is to gather available information on regional dust particle shapes, preferably with information on the internal structure. I already have an existing collaboration for this, as well as extensive data [Kemppinen et al., 2015a, Jeong et al., 2016]. In addition to microscopy images, the instrument we are developing at Kansas State University, HAPI, will be able to take hundreds of individual particle images every hour, thus providing another source for shape data. In particular, HAPI can image particles directly *in situ* on board a drone platform, allowing for types of sampling not available traditionally in the field.

As part of the effort I would make key improvements to the design to produce a significantly improved version. Importantly, by utilizing two perpendicular laser beams the particle can be imaged from two different sides, thus giving a much better perspective to its three-dimensional structure, which has a major impact on its light-scattering properties. Many design questions have already been solved with HAPI, and thus the improved instrument should be much faster to design and manufacture, even with added complexity.

The second phase is to integrate as much shape information into my pre-existing particle model generation software [Kemppinen et al., 2015a]. This software generates realistic, unique, multi-grained mineral particle simulants. The output format is a list of volume elements in three-dimensional shape, including the refractive index of each element, that together comprise the particle. These particle models can then be fed to a Discrete Dipole Approximation (DDA) simulation software. DDA is an asymptotically accurate electromagnetic scattering simulation software that can work with particles of arbitrary shapes and compositions. I have plenty of experience with DDA, especially on supercomputers, given that was the method of choice for all of the required simulations for my dissertation work.

However, given DDA's extreme computational demand, especially if one wants to provide scattering data at multiple wavelengths, it is not realistic to simulate the single-scattering characteristics of a statistically significant amount of particles in a reasonable time. This is where the third phase comes in. I propose a novel interpolation scheme for scattering patterns: Instead of trying to simulate every combination of particle shape and size, and possible refractive indices, the basic approach is to do simulations at specific combinations of these parameters, and find a scheme that can fill the gaps with minimized inaccuracies. These simulations would be verified against real-world light scattering measurements I would perform in the laboratory with particles captured in the field.

Shortcomings of spheroids and ellipsoids are widely documented [Kemppinen et al., 2015b, Merikallio et al., 2011] in their applicability for direct inversion. However, a geometric shape ensemble should be satisfactory for pure mathematical scattering pattern interpolation. First, a comprehensive, high-resolution simulation database would be created for a small but dense parameter space. Utilizing established machine learning methods that initial database can be used to train and validate the interpolation scheme, and the method can be applied to a larger parameter space to produce a final database. This database can also be extended or refined over time with the main bottleneck being computational resources.

It should be noted that there are several considerations for such an interpolation. Several scattering parameters will have oscillating behavior as a function of the particle size, and as a result, several of the parameters of the interpolation model will have, too. Notably, the ones that will stay constant are likely reflective of the overall particle shape, where small changes in e.g. the size of the particle will have correspondingly small changes in the shape ensemble. However, parameters that correspond to small morphological details such as surface roughness or internal structures will exhibit oscillations whenever their exact characteristic sizes interact strongly with the wavelength of the simulated radiation.

Texas Tech University is an excellent match for this work. Not only will the access to a high-performance computing resource such as the High Performance Computing Center be crucial, but there is also clear potential for collaboration with existing research areas, both in Condensed Matter theory and experiment.

5 Funding

My research has been supported to some extent through external funding since 2013. My final year of Ph.D. was supported by a nationwide Finnish research foundation who distribute awards through a competitive application process. Additionally, during the final months of my Ph.D. I was awarded a NASA Postdoctoral Program Fellowship, though I ended up choosing the position at Kansas State University instead.

During my time in Finnish Meteorological Institute, in addition to personal grants and fellowships, I participated in proposal preparation regularly by writing parts of the narrative, reviewing and producing figures. The key funding agencies involved were the European Research Council and European Space Agency, in addition to Finnish funding organizations. In our large, 100% externally funded group of twenty people at Finnish Meteorological Institute, it was common for students to participate. I also participated in several space-instrumentation proposals as a team member, reviewing pertinent parts of the text and joining preparatory meetings. Even now I am a named collaborator for the environmental sensor package (MEDA) of NASA's upcoming Mars 2020 rover.

Unfortunately, during the first half of my stay at Kansas State University I was not allowed to apply for external grants as a PI due to postdoctoral status. However, I have participated in multiple proposals as a Co-I.

The National Science Foundation has proven supportive of aerosol research, and I plan to pursue funding through them. In addition to the CAREER grant there are several promising individual programs to fund this work, such as Computational and Data-Enabled Science and Engineering. Additionally, due to my previous success and extensive cooperation with NASA, I believe I am well situated to seek funding from them for both terrestrial projects, as well as continuing planetary and other space-related research. Specific calls include New Early Career Fellowship Program, Atmospheric Composition: Radiation Sciences Program and Mars Data Analysis.

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