Characterizing analytical and computational mathematics use during PhD research

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As physics departments increasingly emphasize computational training within the physics curriculum, there is a need for educators to have guiding principles for deciding how and when to use computational approaches over analytical math and vice versa. We investigated the use of analytical and computational mathematics in professional practice by conducting ten semi-structured interviews with PhD students in the physical sciences. The interviews revealed context-rich situations where computational and analytical math were valued and used. Through an emergent and thematic coding process, key contextual features were distilled. Although analytical math was valued as a calculational tool (e.g., manipulating equations), the most prevalent use of analytical math was to develop a preliminary understanding of a problem, which included modeling systems through equations, developing simplified "toy models", understanding background concepts, and understanding how varying parameters affected system behavior. Computational tools had a complementary role of data analysis, complex numerical simulations, and visualization.

I. INTRODUCTION

Analytical math (also referred to as symbolic math) plays a central role in the physics curriculum. Mathematics is regarded as "the language of physics" and provides a means to encapsulate detailed conceptual relationships and quantitative precision at the same time [1]. After the introductory physics sequence, which frequently includes numerical solutions, upper-division physics courses strongly emphasize symbolic expressions and numbers become less common. Several physics educators and PER researchers have developed approaches for going beyond "just math" calculations to foster deeper sense-making through a modeling approach to problem solving. Modeling highlights the links between the real world and abstract models, both when beginning a problem and when reflecting on results at the end of the problem [1, 2].

However, there is a complementary recognition that the physics curriculum should increasingly emphasize computational tools for problem solving and mathematics. The American Association of Physics Teachers (AAPT) has produced specific recommendations for including computation [3]. Additionally, a community-developed collection of computational physics activities is being supported by the Partnership for Integration of Computation into Undergraduate Physics (PICUP) [4].

Given the limited amount of time in any one course there is a need to balance the rich tradition of analytic mathematics with rapidly evolving and increasingly powerful computational tools. The physics community needs to develop curricula that utilize the unique affordances of both symbolic and computational techniques.

One approach to identify affordances and establish balance is to study the practices of professionals and examine how they utilize mathematics, which is the approach of this study. We investigate two research questions: (1) What analytical and computational mathematics activities are utilized in a physics research setting? And (2) How is the use of an-

alytic or computational math impacted by the unique affordances of each approach?

For the purposes of this paper, analytical math (also referred to as symbolic math), includes a variety of tasks that would typically be done with pencil and paper or on a white board, such as solving a system of equations or deriving a formula. Analytical math does not include pencil and paper numerical calculations. Computational math is broader and includes any math-related work involving a computer.

II. METHODS

This study explores math use through the perspectives of ten PhD students engaged in full-time research. The PhD students came from fields such as astronomy, astrophysics, optics, semiconductor fabrication, and photovoltaics. Their research emphasized experimental, computational, and observational approaches. The sample included 5 women and 5 men. Altogether 40 graduate students were contacted via email and offered \$20 for their participation, from which the 10 participants were identified.

The interview was semi-structured, initially exploring the educational background of the student and a short description of their dissertation project. The protocol then focused on eliciting a series of concrete examples of analytical and computational math that occurred in their own research, which began by directly asking "What types of (routine, difficult, or important) tasks do you do for your project that include analytical math?" Follow-up questions elicited additional contextual details, including the methods and tools used. After discussing analytical math, the protocol transitioned to discuss computational math in a nearly identical manner. Then students were asked to "describe the relationship between computational and analytical methods" in their research. Finally, they were given an opportunity to provide additional thoughts or suggestions about teaching analytic and computational math in the undergraduate curriculum. The analysis

presented in Sec. III below focuses on the beginning portion of the interview where students described specific math activities in their own research.

Each interview lasted 30-45 minutes and was transcribed prior to analysis. The coding process involved iterative passes through the transcripts. Initially, two researchers read through the interviews and identified any instances of analytical or computational math. These instances were summarized with short phrases and then grouped together into emergent codes, which were then defined. Both coders applied this 2nd round code dictionary to re-code all instances, during which time the code structure and definitions were refined. All codes were integrated into NVivo qualitative data analysis software to link the audio, transcripts, and codes, and to evaluate the intersection of math activities with either analytical or computational tools.

III. FINDINGS

The emergent coding process identified a number of uses of math within graduate students' research. Both analytical math activities (Sec. III A) and computational activities (Sec. III B) are discussed in turn. Then, Sec. III C reorganizes the uses according to broad categories (i.e., modeling, calculations, and other uses) and highlights unique uses and shared uses shown in Table I. Throughout the discussion below, emergently identified math activities are italicized and their definitions are woven into the discussion.

A. Analytic Math Use

One of the most prevalent uses of analytic math was to gain an early-stage understanding of a problem. Foremost was the use of analytic math to *understand background concepts*, which included gaining background knowledge or articulating underlying principles to solve a problem in their research. One student said, "I think the role that analytical mathematics plays in my research is that it gives me the groundwork and the motivation to do my numerical studies...So, the importance of [analytical math] to my research is a foundation, to show that we're not pulling this out of nowhere." The analytic math is trustworthy because it is directly connected to the fundamental principles governing the system. Another student trained in geometric and physical optics (both classical physics) was discussing changes to lithography processes as integrated circuit features shrink closer to the atomic scale. The student believed that quantum mechanics (a topic he had not studied much before) would be essential for the new simulation tools. "So if we don't use ... less than five nanometers, the quantum optics doesn't come into play. Up to now it doesn't come into play in our research but ...probably within the next one or two years, if anyone wants to do the photolithographic research they need to take account of [quantum mechanics]. Then the analytic work will be more important."

This student anticipated a need to understand the principles of quantum mechanics and quantum optics (fundamentally expressed as equations) because they will be incorporated into the next generation of simulation tools.

Also prevalent was *modeling systems through equations*, which included instances when students used equations to represent a physical system. One student said, "I usually use differential equations for solving the fluid flow to predict trajectories of the particles, or how the electric field gets distributed on the inside of the microchannel. Because this is the only way, or this is the only tools we have for trying to predict what is happening on the inside." Another described a particularly challenging situation. "Probably what was most difficult was to make a model for the evolution of [a galactic phenomena] that I was observing...we had to put this into an analytical form. So I had to write a function which took into account a number of things." Sometimes the *equation was a transitional step to computation*. As another student described, "The amount of work that I do analytically is very dependent on what I'm doing computationally. Basically, I go from having an analytic equation that I need to input to, okay, I need to have that written this way in the code..."

Another emergent practice was *exploring simplified models* (or "toy" models) of systems. Beyond the utilization of mathematics to express a model, many times the analytical models were simplified to allow for an exploratory analysis of the system behavior. This was widely recognized by students. "Usually I have to start off by saying, 'Here is our basic analytical model. This is an example of how this might work analytically in a simple case,' and then we move on." Another example was "a lot of times, we'll design an instrument for a simple aperture, like a circular aperture, and usually these are easy to handle analytically. And then we apply those ideas - the basic ideas - to more complicated systems." "that's the ultimate goal, to have a really simplified expression"

One particular use of simplified models (and mathematical models in general) was to *understand the impact of different parameters* on the behavior of a system. The purpose of analytics math according to one student was "...to get a first order intuitive understanding of the system...it's much easier to dive into the impact of parameters, understanding the impact of parameters when you have an analytical expression. So that's always my first go to when I'm trying to understand a system." Another interviewee, when explaining how various factors in a solar cell affected the quantum efficiency, couldn't refrain from writing an equation to explain how one parameter affected a key experimental quantity, "Can I write out some equations? ... So, if you change temperature here, [the] thermal escape [rate] is so sensitive, ...so at higher temperature, you get higher intensity, due to your higher thermal escape rate."

Calculations and math operations also played a role in research, which included activities like doing an integral, solving an equation, etc.

B. Computational Mathematics Use

One of the most prevalent uses of computational tools was *modeling via computation and simulations*, where students used computational math to gain an understanding of a real-world, physical system. One grad student who used computational models in the design process for a telescope said, “It all comes down to designing realistic situations for my optical system, so designing code that allows you to simulate atmosphere, simulate imperfections in the optics of the telescope. They call them aberrations. Simulating realistic optics...”

A primary reason students’ found computational models to be helpful was the ability to *extend simpler analytic models* and develop models with added realism and complexity. “[it] gets very complicated, at least analytically. There is a point when you cannot use analytical skills and you need to rely on numerical methods.” However, just because computational methods can go beyond analytically-solvable models, it doesn’t mean the work is easy or simple. Again referring to the design of a telescope, a grad student said, “Getting to the level where you’re doing really accurate simulations on the computer is difficult, so that’s where I spend most of my time. I find that to be the most difficult task that I deal with.”

Similar to how analytical models were used, computational modeling also emphasizes *understanding the impact of different parameters* on the behavior of the system. Making predictions in the virtual world is a powerful way to explore a range of parameters and gain insight. In reference to fitting experimental current versus voltage (I-V) data for a solar cell, one student described, “For example, I have an I-V curve– the simulation runs like this, but actually experimental data is like this. So, I need to change parameters to make my theory to fit those experimental [data]. But however, there are a lot of stuff I can change, so I always question myself which parameters I should change, and which others I shouldn’t.” Again, the computer offers new capabilities, but using it appropriately is still a task that requires significant thought.

Computational tools also offer the ability to *visualize data and represent models* in new ways. Visualization and plotting are not only valued for presentations to others, but are key tools for sense-making. A grad student said, “You’d be surprised, I spend almost just as much time visualizing my results than I do actually creating my results.” Another student described their computation use as “...most of it has been using ODE in MATLAB...and then otherwise plotting, lots of plotting.”

Data analysis and interpretation, in addition to visualization, is another frequent activity among grad students. An astronomer described, “what we mostly do is related to analyzing images but also fitting functions to spectra, for example. Types of functions would be Gaussians, Gauss-Hermite polynomials. What I have to do is to write a code which fits these kinds of functions to my signal, and then I have to get some parameters out of the fit.”

The memory and computational power of modern computers makes them very efficient and accurate for both simple

and large *numerical calculations*. Whether it is arithmetic or multiplying enormous matrices, the computational representation used by the researcher (expressed as programming code) can be very brief in both cases. An astronomy graduate student explained, “So you have 1.5 million objects in one database and then 600,000 objects in another database, and what you can do is you can do cross-correlation mapping between the two to see what’s common between the two.”

Another affordance of computational tools was their ability to *interface with data acquisition and databases*. The ability to link complex calculations directly to data sources enables modern science to rapidly answer new questions. Discussing the analysis of publicly available astronomical data a grad student said, “As I said because I’m dealing with a thousand galaxies, I have to have some way of storing them and reading and writing into the database. So, SQL is that language that allows you to access your database using some commands.” Another student discussed interfacing a commercial simulation tool with MATLAB to automate batches of runs and save results. “Usually [the simulation tool] has very simple input and output that can be used in the classroom but when I want to do research I need to go to the programming interface of the product.” Although interfacing with databases and data acquisition may not be considered mathematics, it is tightly integrated with computational mathematics in many real-world problems.

Finally, sometimes computational tools are used to do *symbolic calculations*. “Usually I move on to Mathematica and I [chuckles]– so, a lot of times I will come up with these integrals...a specific example recently I had to take integrals of products of Bessel functions.”

C. Synthesis

Sections III A and III B divide the mathematical activities by whether they involved manipulating symbolic expressions with pencil and paper or involved programming, simulations, or computer-aided visualizations. In order to address our second research question regarding how the math use is linked to affordances of the tools, we have constructed Table I, which regroups the activities into three main categories: *modeling*, *calculations*, and *other*. *Modeling* broadly includes developing and using models. *Calculations* emphasizes activities that lacked the emphasis on sense-making and connection to the real-world. Calculations are typically (but not always) part of some larger activity such as modeling or data analysis. The *other* category encompasses uses that did not fit neatly into modeling or calculations.

While some activities are common to analytical and computational mathematics (e.g., understanding the impact of different parameters), other activities are differentiated. Simplified “toy” models are often best analyzed through symbolic calculations, while more realistic and complex models and visual representations benefit from a computational approach. Table I lists additional shared and differentiated activities.

TABLE I. Mathematical activities are organized by whether they are primarily conducted using analytic math, computational math, or both. Activities are further organized by whether they are part of a larger modeling process, a calculation, or some other use.

	Modeling	Calculations	Other
Analytical and symbolic math	Express models as equations (includes transitional step toward computation), Examine behavior of simplified “toy” models		Understand and communicate background concepts
Shared	Understand the impact of different parameters	Symbolic calculations	Analyze and interpret data
Computational math	Express models using code and simulations, Extend analytical models with realism and complexity, Visually represent models and data	Accurate, complex, and large calculations	Interface with data acquisition and databases

IV. CONCLUSION

The first research question focused on identifying the analytic and computational math activities valued in a physics research setting, which were summarized in Secs. III A and III B. Although the limited sample in this study could not uncover all possible math activities, many were documented and described. The second research question sought to understand why analytical or computational approaches would be preferred in particular mathematical problem-solving situations. Table I highlights the strengths of both analytical and computational tools, which can be used to inspire pedagogical implications for math use in the undergraduate physics curriculum.

The symbolic mathematics developed by our physics community over centuries and taught throughout the physics curriculum is a powerful tool for representing conceptual and quantitative relationships. The PhD students in our sample valued analytic math for its ability to foster early stage sense-making when faced with a new problem. These results suggest analytic problem solving could include more exploratory modeling activities, such as developing models and expressing them as symbolic equations and seeking out trends in the behavior rather than focusing on numerical results in a given special case. Other physics educators and researchers have also proposed a more explicit emphasis on modeling [1].

In the curriculum, computational math could be used to explore more complex and realistic situations by extending idealized “toy” models. These computational models could also be used in an exploratory way by examining qualitative

and quantitative trends, such as the dependency of system behavior on parameters. Computational tools also require expressing math in new representations (e.g., snippets of Python code) and also generate new visual representations for models and data. Computational physics education can go beyond numerical methods to focus on topics such as plotting and visualization, data analysis, large calculations, and rapid access to data. In addition to improving the quality of computational instruction, every interviewee regardless of research specialty mentioned that undergraduate education would be improved by increasing the quantity of computational training.

Although a multi-year PhD research project represents a very different context from a physics classroom, many of the day-to-day activities occurring during research may be suitable for physics courses. Incorporating these research-inspired uses may also provide useful professional preparation for work outside of academia. For example, research projects and engineering projects are typically open-ended, ill-defined, and require a wide range of technical and interpersonal skills [5, 6]. The inclusion of multi-week projects could be a feasible way to incorporate exploratory and complex uses of math in the classroom.

While this study is not an exhaustive investigation, it does show that contexts outside of the classroom, such as workplace settings, can provide useful insights about math use within physics. These insights could guide curriculum decisions that support students’ professional preparation, as well as guide new education research into math use in professional physics settings.

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