Writing About Numerical Methods

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Abstract

Numerical techniques are abundant in modern scientific disciplines and are commonly used to solve equations which would be difficult or impossible to solve in closed form or estimate measurements that a research is unable to currently perform. These can include simple methods, such as numerically solving differential and integral equations, to more complex methods such as Monte Carlo for transport theory, or simulations for computational fluid dynamics. When writing about these techniques for a thesis, dissertation, or article, it is prudent to describe several concepts regarding the numerical technique for readers to understand what utility is provided by the technique and why numerical methods were chosen over mathematical calculations or experiments. This report will provide an overview of how to write about numerical techniques and provide an outline for their use.

Introduction

For research projects which are not inherently computational, writing about computational and numerical techniques can pose difficulty for researchers who are more accustomed to writing about theoretical and experimental techniques. As computational methods become more abundant in applied sciences, the ability to explain the code used and the relevance to one's research becomes more and more important. For a paper being published, this may be a subsection of the methodology and methods used, but for a thesis or dissertation, it may require a chapter to explain the computational component of the research. While these may differ in length, the content present will ideally be the same in either case. The following is a short outline for how the author would recommend writing about the techniques used. The audience is primarily experimental and theoretical scientists who do not typically use numerical methods, though it is still applicable to computational scientists who are using their work for an experimental field. The general idea is to write about the physical principles you are trying to measure, the way the code estimates or computes them, and how this data is relevant to other components of your research.

Introducing the Technique Used

When writing about the numerical techniques used, it is important to include a broad overview of the quantities that the code is providing and the utility they will provide for your research. A general summary of the theoretical and experimental techniques may be needed depending on the nature of the research project. For tools that estimate the cross sections of different interactions, this may be a general description of the interaction and why the cross section is required for your research. For optical radiation interactions, this may be a description of how light may be absorbed by the chemical species present. Then describe how knowledge of the cross section can inform the concentration of a particular species within a sample you intend to measure. This section should function as a short introduction in itself for readers who do not care for the detail.

Theoretical Background

Experimental Background

Methods the Tool Uses to Sample Experimental Quantities

Conclusion