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The Uncertainty Budget to Fit Force-Distance Curves from Atomic Force Microscopy

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UAH RCEU 2017 Proposal

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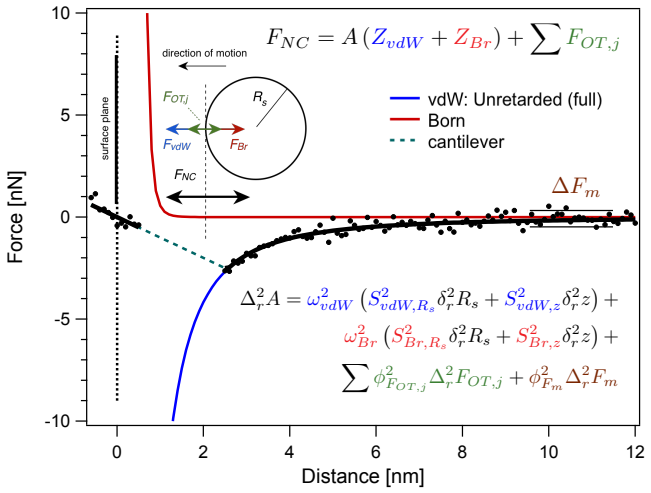
Background and Motivation



In atomic force microscopy (AFM), a finely-pointed tip scans over a surface and measures forces with spatial resolutions on the scale of nanometers. Our group has created a program to plot forces F_{NC} for a sphere scanning over a plate, as seen on the right. In a real system, forces are measured with noise, as shown by the scattered points. Noise causes problems when we try to extract theoretical fitting parameters. Suppose $F_m = Af(z)$. We want to get A by fitting F_m versus z. Noise ΔF_m causes an uncertainty in the fitting parameter $\Delta_r A \equiv \Delta A/A$.

We have started to analyze this problem in an approach called uncertainty budget analysis. Uncertainty budgets are an important topic in the definitions of uncertainty at the National Institute of Standards and Technology. We have theoretical equations for forces in F_{NC}. We also have a program to generate theoretical curves at different values of A with different levels of noise ΔF_M. We have tools to reverse the process. We fit the model noisy "measured" data with different theoretical equations to obtain $\Delta_r A$. We are completing a publication on this effort to submit to a peer-reviewed journal. We now invite you to take part in this insightful, ongoing research study.

Prerequisites

This RCEU project is designed for students who want to expand their skills in advanced statistical analysis of data. You must demonstrate that you can perform rigorous regression curve fitting of data using equations that are not simply $y = mx + b$. This may be in software applications such as MatLab, MathCad, Mathematica, or Maple. You will use Igor Pro for this work. To appreciate the physical background, you should investigate general forms of equations for forces in chemical bonds (e.g. ionic, Lennard-Jones, or even Hook's law). In the case of multiple inquiries, students who demonstrate the clearest interest in and appreciation of the research will be given preference.

Duties

Your first objective is to define where you will go with your research efforts. You will have three weeks to generate a project proposal. You will redo analysis that we have already completed to demonstrate that you can repeat existing results with confidence. In parallel, you will design a protocol for your experiments. What force equations will you use? What variations in noise level will you use? The challenges in this part are to become proficient with the existing software and to document how you will use it productively. Your outcomes are the skills to use Igor Pro and greater confidence to design protocols for an experiment before you actually start to do it.

Your second objective is to perform, document, and report on the analysis that you do. You will have until nearly the end of the program to complete this successfully according to your timeline. You will generate model noisy data and analyze it. Each week, you will present concise written and oral reports on your progress. The challenges in this part are to stay on-task in respect to your proposed time-line while dealing with mistakes, misfortunes, or mis-adventures and to report what you have achieved in a concise, informative, and well-structured manner. Your outcome is an improved ability to analyze data with statistical tools, stay on task, and prepare technical reports.

The final objective is to prepare a final report. You will report your findings in publication-ready style, and you will present them in the RCEU poster session. Your outcome is a public presentation that you can document on your résumé as a primary author. Your contributions will also be fully acknowledged in any further publications that use what you generate.

An advanced level of study is also open. For this, I am looking for clear initiative and independence. Do your experiments have physical significance? How do your results fit in the existing literature? Have you validated a hypothesis or solved a problem in a self-contained way? Your ability to address these questions will go beyond doing just the data analysis on the project. The target outcome is a potential for co-authorship on a journal publication.

Mentor Supervision and Interaction

You will be supervised by me (Dr. J. J. Weimer). I will provide the software and train you in its use. I will give you the add-ons to generate and analyze data. I will guide you on how to design a successful experiment (Objective 1); how to analyze data, stay on task, and prepare technical reports (Objective 2); and how to prepare a publication-ready poster (Objective 3). I will offer suggestions on how to approach the advanced level of study and guidance to tackle it successfully.

We will meet routinely to discuss your progress. I will be openly available to address any questions. We will exchange information directly and via email, Skype, Canvas, and Google Drive.