# Mathematics of Physical Chemistry Boot Camp

## Fall 2015

The Physical Chemistry Division is offering the *Mathematics of Physical Chemistry Boot Camp* prior to the first week of classes, in order to prepare students for key mathematical and numerical approaches they will encounter in class and research. The boot camp is completely voluntary and is open to new and current graduate students or ambitious undergraduates interested in reviewing mathematical methods and their physical chemistry applications. The classes will meet on two Saturday mornings around the first week of classes. Each meeting will be be motivated by an application in physical chemistry and will review the mathematical modeling and solutions necessary to explore the problems. The format for each session will entail two lectures and hands-on tutorials. The lectures will outline the mathematics and theory behind a given problem, while the tutorials will focus on the practical tools to approach the challenge. Outcomes include working knowledge of common mathematical concepts in physical chemistry and the numerical tools used to solve such problems.

**Instructors**:

- Peter Kekenes-Huskey, Ph.D.
- Chad Risko, Ph.D.
- Caitlin Scott, Ph.D. (co-instructor)

## Schedule and Format

Weekends before/after first day of class (August 26 – Wednesday - First day of classes) in the Chemistry-Physics Building (room TBD). The schedule is as follows:

- Session 1: Saturday, Aug 22, 8a to early afternoon
- Session 2: Saturday, Aug 29, 8a to early afternoon

Each session will consist of

- Two 1-hour lectures centered about an application and the underlying theory
- Two 1-2 hour tutorials to explore analytical tools and numerical approaches to solve the problems

## Topics

**Session 1:** Methods for Quantum Chemistry (Risko)

1. Electronic structure methods in chemistry & materials science
2. Change of basis and the eigenvalue problem (linear algebra)
3. The variation principle and the Schrödinger equation

**Session 2:** Reactions and Transport (Kekenes-Huskey)

1. Unifying lecture on reactions and transport in chemical systems
2. Reaction kinetics for enzyme catalysis (ordinary differential equations)
3. Chemical transport in cells (partial differential equations)

## Materials

- Scratch paper and pen
- Laptop (optional, but highly recommended)
- Recommended text: Mathematical Tools for Physics
  http://www.physics.miami.edu/~nearing/mathmethods/
- We may later suggest installing free software for the tutorials

## Registration

Email instructors (pkekeneshuskey@uky.edu) by August 17 and

- provide linkblue id
- specify if you will be bringing a laptop (and if so, operating system)