



New Graduate Course Announcement: Computational Structural Biology. CS6104, Spring 04.

When: Every Tuesday 3:30 - 6:00; **Where:** WILLIAMS 334

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Molecular interactions are the basis of life. Understanding their intricate details is critical to progress in many areas of life sciences, from the most fundamental level of "how it works?" to the pharmaceutical applications such as design of revolutionary new drugs. Since even the most powerful of available experimental methods do not provide us with a complete picture of what is going on at this microscopic level, computer modeling becomes an indispensable research tool. The complexity of biological molecules and interactions involved makes modeling of these macromolecular systems a highly non-trivial exercise. The key questions are:

1. How to assess what is possible and what is not?
2. How to construct reasonable models based on relevant physical principles?
3. How to interpret the results in a meaningful way?

The topics covered in this course will include an introduction into the theory of biopolymers, molecular dynamics simulations, biomolecular electrostatics, molecular databases, and, if time permits, rational drug design.

Through lectures, student presentations, and work on "real-world" projects you will acquire skills needed to enter the new, rapidly growing field of molecular modeling and simulations – an area of science which has recently been enjoying expanding job market in both academia and industry.

The course is inherently interdisciplinary, and so students of all backgrounds are welcome. Projects require a combination of skills, team work is key, and you can always choose to work on a part where your skills will be put to good use, whether you come from computer science, physics, chemistry or biology. Feel free to e-mail me if you have any questions. More info on my current work is available on my web site (above).