

# Class Schedule for the Computational Chemistry Workshop 2000

Monday, June 26 through Friday, July 7

## [Directions](#)

Day	Topics Covered	Assignment
Mon., June 26	<u><a href="#">Introduction</a></u> to <u><a href="#">UNIX</a></u> , <u><a href="#">email</a></u> , the web, and <u><a href="#">C</a></u> .	Exercises in C.
Tue., June 27	More on <u><a href="#">C</a></u> : loops & vectors; Electronic structure lecture.	Implement sorting algorithm in C.
Wed., June 28	<u><a href="#">Introduction to Molecular Dynamics in 1 dimension.</a></u>	<u><a href="#">Write an event driven, 1D MD program in C.</a></u>
Thurs., June 29	Extension of Molecular Dynamics into 2 dimensions.	<u><a href="#">Analyze collisions in 2D.</a></u>
Fri., June 30	<u><a href="#">Introduction to a Molecular Dynamics tool</a></u> ; Set-up projects.	Perform exercises with MD tool.
Mon., July 3	<u><a href="#">Computer generated random number algorithms; The random walk</a></u> ; Set-up projects.	Analysis of random walk distribution.
Tue., July 4	HOLIDAY -- NO CLASS	
Wed., July 5	<u><a href="#">Introduction to Parallel Computing</a></u> ; PowerPoint.	Calculating area by Monte Carlo: serial & parallel.
Thurs., July 6	Finish Projects; <u><a href="#">Special Lecture "SnB"</a></u>	
Fri., July 7	<u><a href="#">Presentations</a></u>	