11PHY388 "Advanced Computational Physics"
Part II "Comparison of classical and quantum physics"
September 26 – October 26 2016

Goal	The goal of part II of PHY388 is to strengthen the intuition for quantum mechanical and statistical concepts such as probability distributions and expectation values. We will compare the time evolution of the quantum mechanical wave function to the dynamics of classical ensembles.
Numerics	Monte Carlo simulations of non-interacting classical ensembles, non-uniformly distributed random numbers, Box-Muller algorithm, rejection method, Fast Fourier transformation, split-operator techniques, Mathematica animation.
Class time	MW 12:00-1:15 PM Moulton 307B
Instructor	Prof. R. Grobe, Moulton Hall 216 Phone: 438-5470
Office hours	by appointment, or just walk in.
Texts	Sorry, there are no textbooks for part II of the course.
Lecture notes	Lecture notes will be provided.
References	A recommended references includes: Paul L. DeVries, "A First Course in Computational Physics," John Wiley & Sons, Inc.
Homework	A total of three homework assignments, each worth 50 points, will be distributed. The homework assignments will consist of some theoretical problems and some computer-based problems. The computer-based problems will generally require that you write computer programs in order to solve the problems. Though we will give examples in class using the Fortran programming language, you are welcome to work the problems in c. Please consult one of your instructors to discuss the use of compilers for other languages. Homework assignments will have specific due dates. If the homework is turned in 1 msec after the due date, 50% of the total points will be subtracted. Homework turned in one week after the due date will not be accepted.
Exam	There will be one exam on Wednesday, September 26, 12:00-1:15 in MLT 307B. A make-up exam will not be given unless you can present a legitimate excuse.

Grades		
	3 homework assignments (50 points each)	150 points
	Exam	183 points
		TOTAL 333 points for PART II

Your final letter grade for the entire course is based on the number of points you have gathered in all three parts and it will be determined as follows:

A	90 – 100 %
B	80 – 89 %
C	70 – 79 %
D	60 – 69 %
F	59 % and below

We reserve the right to modify these boundaries downward if appropriate.

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2.9 Temporally resolved scattering off a potential well

III Time-dependent methods to calculate spectra

3.1 Autocorrelation function
3.2 Lineshape fitting techniques
3.3 Integration in imaginary time