

Computational Physics I

PHYS 499

Lect. Thursday 9:30–12:30, ST 061

Lab. Friday 9:00–12:00, ST 026

September – December 2005

Note: 10–13 November is Reading Week,

Calendar:

2005

September							October						
Su	Mo	Tu	We	Th	Fr	Sa	Su	Mo	Tu	We	Th	Fr	Sa
				1	2	3							1
4	5	6	7	8	9	10	2	3	4	5	6	7	8
11	12	13	14	15	16	17	9	10	11	12	13	14	15
18	19	20	21	22	23	24	16	17	18	19	20	21	22
25	26	27	28	29	30		23	24	25	26	27	28	29
							30	31					
November							December						
Su	Mo	Tu	We	Th	Fr	Sa	Su	Mo	Tu	We	Th	Fr	Sa
		1	2	3	4	5					1	2	3
6	7	8	9	10	11	12	4	5	6	7	8	9	10
13	14	15	16	17	18	19	11	12	13	14	15	16	17
20	21	22	23	24	25	26	18	19	20	21	22	23	24
27	28	29	30				25	26	27	28	29	30	31

MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
<u>Sep 12</u>	13 IDL	14	15 IDL (lab)	16
19	20 Runge–Kutta revisited	21	22 Runge–Kutta (lab)	23
26	27 Boundary value prob- lems	28	29 Boundary value prob- lems (lab)	30
<u>Oct 3</u>	4 Monte Carlo	5	6 Monte Carlo (lab)	7
10	11 Monte Carlo	12	13 Monte Carlo (lab)	14
17	18 MC, Optimiza- tion	19	20 MC, Optimiza- tion	21
24	25 CVS, PDEs	26	27 CVS, PDEs (lab)	28
31	<u>Nov 1</u> PDEs	2	3 Midterm Exam	4
7	8 Midterm Exam (contd)	9	10 <i>[Reading Day]</i>	11

MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
<i>14</i>	<i>15</i> 16 PDEs	<i>16</i>	<i>17</i> 17 PDEs (lab)	<i>18</i>
<i>21</i>	<i>22</i> 18 PDEs	<i>23</i>	<i>24</i> 19 PDEs (lab)	<i>25</i>
<i>28</i>	<i>29</i> 20 PDEs	<i>30</i>	<i>Dec 1</i> 21 PDEs (lab)	<i>2</i>
<i>5</i>	<i>6</i> 22 Pencil Code, visualization	<i>7</i>	<i>8</i> 23 Pencil Code, visualization (lab)	<i>9</i>
<i>12</i>	<i>13</i> Final Exam	<i>14</i>	<i>15</i> Final Exam	<i>16</i>

Software:

- g95
- IDL
- Mathematica (?)
- CVS
- Data explorer

Handouts:

- IDL reference card
- IDL presentation
- Data explorer overview (to write)
- CVS handout

Table 2: Plan for Computational Physics II (not all of this will be covered):

<i>Topic</i>	<i>Details</i>	<i>Reference</i>	<i>Example</i>
<i>A. IDL</i>	language, plotting, etc.	[IDL]	
1. Runge–Kutta revisited	step-size control, stability, systems of ODEs	[CK, §10.3,11], [NR77, §16.2], [I96]	3-body problem, charged particle
2. Boundary value problems	shooting method, relaxation, Riccati(?)	[CK, §14], [NR77, §17], [I96]	oscillations of string and plate
<i>B. CVS</i>	setting up and using a repo, collaborative projects	[CVS]	
3. Random Numbers + Monte Carlo	random distributions, central limit theorem, generators (uniform, quasi-uniform), Monte Carlo, Metropolis	[CK, §13], [NR77, §7]	Monty Hall, momentum of inertia, Ising model, QM integrals
4. Optimization (minimization/maximization)	conjugate gradient, simulated annealing, genetic algorithms	[CK, §16], [NR77, §10]	travelling salesman, partitioning of compute nodes
5. Partial Differential Equations	hyperbolic + parabolic equations, shocks	[CK, §15], [NR77, §19], [I96]	Schrödinger: potential well; hydro: sound waves, Parker wind; MHD: Alfvén waves
6. Eigensystems	Givens + Householder transform, matrix exponential (?), SVD (?), EISPACK	[CK, §8.3], [NR77, §11]	Helmholtz, QM, α^2 -dynamo
7. Fourier Methods	FFT, convolution	[NR77, §12,13]	power spectra, gravity in periodic universe
8. Visualization of 2-d and 3d data	advanced visualization	[IDL]	convection (Rayleigh), forced-boundary, Meissner effect, Solar corona
<i>C. Pencil Code; Gridengine</i>	running and adapting samples	[Penc]	

References

- [CK] W. Cheney and D. Kincaid (2003) *Numerical Mathematics and Computing*, 5th edition, Brooks/Cole, Monterey.
- [NR77] W.H. Press, S.A. Teukolsky, W.T. Vetterling and B.P. Flannery (1996) *Numerical Recipes in Fortran 77: The Art of Scientific Computing*, 2nd edition, Cambridge University Press, Cambridge. [Online available at <http://www.library.cornell.edu/nr>]
- [NR90] W.H. Press, S.A. Teukolsky, W.T. Vetterling and B.P. Flannery (1996) *Numerical Recipes in Fortran 90: The Art of Scientific Computing*, 2nd edition, Cambridge University Press, Cambridge. [Online available at <http://www.library.cornell.edu/nr>]
- [I96] A. Iserles (1996) *A first course in the numerical analysis of differential equations*, Cambridge University Press, Cambridge.
- [Penc] W. Dobler & A. Brandenburg (2001–2005) *The Pencil Code: A High-Order MPI code for MHD Turbulence — User's and Reference Manual*, [Online available at <http://www.nordita.dk/software/pencil-code/>]
- [CVS] P. Cederqvist et al. (1993–2005) *CVS — Concurrent Versions System*, [Online available at http://ximbiot.com/cvs/wiki/index.php?title=CVS-Concurrent_Versions_System_v1.12.12.1]
- [IDL] Research Systems Inc. (1993–2005) *Getting Started with IDL*, [Available on Obelix at </opt/rsi/idl/help/getstart.pdf>, along with a number of other PDF manuals, in particular </opt/rsi/idl/help/quickref.pdf>]