2022 SYLLABUS for course PHYD57, Advanced Computational Methods in Physics
Lecturer: prof. Pawel Artymowicz (pawel@utsc.utoronto.ca; please put PHYD57 in the subject line and make sure the address is as shown, otherwise mail may be misplaced and not answered)

Lectures (L1−L12, 2 hrs with 10 min break) on Tuesdays 14:00−16:00
Tutorials (T1−T10) on Tuesdays, 17:00−18:00, on days listed below.
Meetings on zoom, login via Quercus.
Deadlines for 4 sets of assignments/projects are denoted A1−A4 at 2pm.
Expect to see them posted 7−14 days before the deadline.

Jan		Feb		Mar		Apr	
11	L1	1	L4, T3, A1	1	midterm*, L7	5	L12, T10, A4
18	L2, T1	8	L5, T4,	8	L8, T6		
25	L3, T2	15	L6, T5, A2	15	L9, T7, A3		
		22	reading week	22	L10, T8		
				29	L11, T9		

---

*) midterm in class, 1st hour of lecture 7 (14:05−15:00) on 1 March

Syllabus is subject to small changes. Please download the updates every week.

1 Structure iand scope of the course
Syllabus of PHYD57
Numerical Comp. in Physical Sciences: History and Contemporary efforts

2 HPC: need for speed, why and how
History and modernity: microprocessors, Unix, Linux, and Internet
Intro to Linux (CentOS)
Command line interface and shells (bash and tcsh)
Text editors: vi, nano, gedit, micro, ...

3 Connectivity (ssh & sftp, traceroute & ping)
Securing your system against break−ins via /etc/hosts.deny
Basic Linux commands (cd, ls, ps, cd, &, bg, fg, alias, setenv,
output redirection to file via > , rm)
Getting more info: manual pages (man), −h, −−help, or −help modifiers
Recommended compilers: GNU: gcc, gfortran; Intel: icc, ifort;
PGI: pgcc, pgf95
Simple program in C, Fortran95, Python, Matlab and IDL
(Schoerghofer book p.30)
More complex program, example of HPC:
2nd order Laplace operator stencil for diffusion equation
Speed comparison of C/F95 with Python & Numpy: why we learn HPC

4 C and Fortran 95 − compilers, basic usage
Numerical puzzle of 711 − learning C and Fortran
Kruskal counts and their connection to linked lists
Coding Kruskal counts trick in Python and Fortran
C: Language overview, compilers
Integration with Python: calling C from Python
examples of programs

5 More Fortran
Examples of programs: Init. value problems for ODEs
More C
Parallel execution of programs on CPU and MIC
OpenMP in Fortran and C
Parallel implementations: diffusion and wave equation
Modern computing (continued)

6 Multi−dimensional arrays in C vs. Fortran
Bottlenecks: Computation vs. CPU−RAM bandwidth
An example program in C and Fortran.
Parallelization via OpenMP
Automatic vectorization and compiler reports
Segmentation faults due to limited stack

7 Calling C functions from Python

Graphics in Fortran and C: DISLIN library
Efficient computation of tetrahedrons puzzle
Parallel implementations: diffusion and wave equation

8 Computations on GPUs with CUDA
Examples in C and Fortran
N−body and other problems of computational physics
Fourier transforms and FFT

9 Bayesian methods of statistics: Markov chain Monte Carlo
Establishing orbits of extrasolar planets
Numerical Comp. in Physical Sci: Particle disks on MIC cluster
Interaction of protoplanets with disks

10 N−body integration methods and implementations
Introduction to MPI and SPH
Fluids by Eulerian vs. Lagrangian methods

11 Fluid computations on CPU and in CUDA C
Planet in a 3D disk
Optically thick disk calculation (IRI)
Smoothed Particle Hydrodynamics: theory
Discussion of projects

12 SPH Implementation. Linked lists, nearest neighbor search
Can one simulate pandemic?
Machine Learning, Artificial Intelligence, Neural Networks
Optimum Search: Simplex Nader−Mead
Why NNs work despite dimensionality curse
Discussion of projects