南方科技大学 SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

课程详述

COURSE SPECIFICATION

以下课程信息可能根据实际授课需要或在课程检讨之后产生变动。如对课程有任何疑问，请联系授课教师。

The course information as follows may be subject to change, either during the session because of unforeseen circumstances, or following review of the course at the end of the session. Queries about the course should be directed to the course instructor.

1.	**课程名称 Course Title**	计算物理 Introduction to Computational Physics
2.	**授课院系 Originating Department**	物理系 Department of Physics
3.	**课程编号 Course Code**	PHY336
4.	**课程学分 Credit Value**	3
5.	**课程类别 Course Type**	专业选修课　Subject Elective
6.	**授课学期 Semester**	春季 Spring
7.	**授课语言 Teaching Language**	中文 mainly Chinese
8.	**授课教师、所属学系、联系方式（如属团队授课，请列明其他授课教师） Instructor(s), Affiliation& Contact （For team teaching, please list all instructors）**	黄丽，助理教授，物理系 第二科研楼 203 室 huang.l@sustc.edu.cn 0755-88018268 HUANG Li, Assistant Professor, Department of Physics Rm. 203, No.2 Research Bldg. huang.l@sustc.edu.cn 0755-88018268
9.	**实验员/助教、所属学系、联系方式 Tutor/TA(s), Contact**	待公布 To be announced
10.	**选课人数限额(可不填) Maximum Enrolment （Optional）**	40

11.	**授课方式 Delivery Method**	**讲授 Lectures**	**习题/辅导/讨论 Tutorials**	**实验/实习 Lab/Practical**	**其它(请具体注明) Other（Please specify）**	**总学时 Total**
	学时数 Credit Hours	48	16 （另外安排，不占用上课时间，不计入学时）	N/A	复习、考试（2 周，不占用上课时间）	48

12.	**先修课程、其它学习要求 Pre-requisites or Other Academic Requirements**	计算机程序设计基础 B Introduction to Computer Programming B（CS102B） 热力学与统计物理 I Thermodynamics and Statistical Physics I（PHY204） 固体物理 Introduction to Solid State Physics（PHY321-15）
13.	**后续课程、其它学习规划 Courses for which this course is a pre-requisite**	无 N/A
14.	**其它要求修读本课程的学系 Cross-listing Dept.**	无 N/A

教学大纲及教学日历 SYLLABUS

15. **教学目标 Course Objectives**

This course provides an introduction to some of the most widely used methods of computational physics, including numerical solutions of differential equations (initial and boundary value problems), molecular dynamics simulations, and Monte Carlo simulations. In addition to giving the students a basic working knowledge of these particular techniques, the goal is to make them comfortable with scientificc computing in general, so that they will be prepared to tackle also other computational problem that they may encounter in the future. The Fortran 90 and C++ programming languages will be used.

本课程介绍用数值方法求解典型物理问题，使学生掌握常用的普通微分方程和偏微分方程的数值解法和编程技巧（初始值问题、边界值问题、本征值问题），分子动力学模拟、蒙特卡洛模拟等， 并结合计算机技术适当介绍计算科学的进展，为学生进一步从事有关的科学和技术研究打下基础。 课程将主要采用 Fortran 90 和 C++语言来示例各种数值算法

16. **预达学习成果 Learning Outcomes**

It is particularly important in this course that the students should learn by doing. The course is therefore designed such that a significant fraction of the students' time is spent actually programming specific physical problems rather than learning abstract techniques. Students will be expected to be familiar with basic programming. The goal is to make the students comfortable with scientificc computing in general, so that they will be prepared to tackle also other computational problem that they may encounter in the future.

通过计算物理的学习，学生应能够系统地掌握物理模型和数学模型的建立方法和数值计算方法的选取原则，获得分析和处理一些物理问题的基本方法和解决问题的能力，提高逻辑推理和抽象思维的能力，具备独立解决科学研究中的实际问题所必需的数学物理基础，为学生进一步从事有关的科学和技术研究打下基础。

17. **课程内容及教学日历 （如授课语言以英文为主，则课程内容介绍可以用英文；如团队教学或模块教学，教学日历须注明主讲人）**
Course Contents (in Parts/Chapters/Sections/Weeks. Please notify name of instructor for course section(s), if this is a team teaching or module course.)

The tentative schedule for the lectures is the following (the numbers refer to weeks):

课程安排如下（数字 n 表示学期的第 n 周时间）

1) Introduction to basic knowledge of the Unix operating system (including Shells, Vim, Gnuplot…);

介绍 Unix 操作系统的基础知识，包括 shell 编程、Vim 编辑器，意见 Gnuplot 等基本作图软件的使用。

2) Basic knowledge of C++ language;

通过示例介绍基本 C++编程知识。

3) Basic knowledge of Fortran 90 language;

通过示例介绍基本 Fortran 90 编程知识。

4) Data fitting (interpolation and extrapolation);

基本数值方法： 数据拟合

5) Numerical integration；

数值积分

6) numerical differentiation;

数值微分

7) Numerical solutions of ordinary differential equations (ODE) I (Initial value and boundary value problems);

普通微分方程的数值解法 （初始值问题和边界值问题）

8) Numerical solutions of ODE II (quantum eigenfunctions and eigenvalues);

薛定谔方程的本征值和本征矢的数值求解。

9) Panel discussion and student presentation on mid-term projects;

期中 projects 的小组讨论和学生报告。

10) Partial differential equations (Elliptic, parabolic and hyperbolic equations)

椭圆型、双曲线型和抛物线型偏微分方程的数值求解。

11) Linear Algebra (Matrix, BLAS, LAPACK …);

线性代数，科研数学库的使用

12) Fourier transform for PDEs.

傅里叶变换的数值算法。

13) Periodic solids, plane waves, and band structure calculations.

周期性固体和基于平面波为基函数的能带结构方法。

14) Molecular dynamics simulations (basic schemes for classical many-particle dynamics);

经典的分子动力学模拟。

15) Monte Carlo simulations (Random numbers, Metropolis algorithm for equilibrium statistical mechanics);

蒙特卡洛模拟。

16) Kinetic Monte Carlo simulations

动力学蒙特卡洛模拟。

18. 教材及其它参考资料 Textbook and Supplementary Readings

There is no required text book for this course. Lecture notes, along with other material, such as homework assignments and program examples, will be made available during the course. In addition, the following textbooks are recommended reading: 1. Tao Pang, “An Introduction to Computational Physics“, Cambridge University Press, New York, 1997, QC20.7.E4 P36 1997; 2. Computational physics. K. H. Hoffmann and M. Schreiber, QC32 .C65 1996.

课程评估 ASSESSMENT

19.

评估形式 Type of Assessment	评估时间 Time	占考试总成绩百分比 % of final score	违纪处罚 Penalty	备注 Notes
出勤 Attendance				
课堂表现 Class Performance				
小测验 Quiz				
课程项目 Projects				
平时作业 Assignments		60%		
期中考试 Mid-Term Test		20%		
期末考试 Final Exam				
期末报告 Final Presentation		20%		
其它（可根据需要改写以上评估方式） Others (The above may be modified as necessary)				

20. 记分方式 GRADING SYSTEM

☑ A. 十三级等级制 Letter Grading
☐ B. 二级记分制（通过/不通过） Pass/Fail Grading

课程审批 REVIEW AND APPROVAL

21. 本课程设置已经过以下责任人/委员会审议通过
This Course has been approved by the following person or committee of authority

物理系教学指导委员会
Education Instruction Committee of Physics department