# High Performance Scientific Computing (HPSC)

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## Contents

- Survey on parallel computing, parallel algorithms
- Programming tools in message passing systems - MPI
- Ordinary differential equations, initial value problem,
- Boundary value problem,
- Case Study: Molecular Dynamics,
- Iterative methods for the solution of linear systems
- Partial differential equations, some examples of applications (electric field, fluid flow).
- Case Study: Diffusion Equation and Heat Transfer



## Lessons

- Before this course you should be able to understand basic ideas of: linear system, matrix algebra, eigenvalues, linear least square, non-linear equations, polynomial approximation, numerical differentiation and integration - topics from CMDIE.
- During this course you should obtain a knowledge on designing parallel algorithms and implementing them by using MPI communication library.
- Foundations of Partial Differential Equations will be explained and several practical problems solved in more details in order to obtain an impression how a real problem could be solved and calculation results represented.



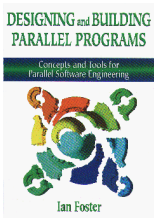
## Labs

- We will have Labs in the small computer room in combination with lessons. Usually the material from lessons will be tested on computers.
- MatLab will be used for testing and solving some basic and well defined problems.
- MPI parallel programs will be designed and implemented on MPICH implementation of the MPI, which is already installed on all computers in the small computer room.
- Practical examples from lessons on partial differential equations will be solved by both of the mentioned programming tools.



## Reference Book 1

- I.Foster: *Designing and Building Parallel Programs,* Addison-Wesley, 1996, (acronym PP is used in this course); Network version accessible on*:* http://swt.cs.tu-berlin.de/pa/dbpp
- Lecture notes available on Class Web.
- A sample of this book is available by me.






## Reference Book 2

- M.T.Heath: *Scientific Computing: An Introductory Survey*, *Second Edition,* McGraw Hill, New York 2001, (SC);
- *First Edition* from 1997;
- Lecture notes accessible on*:* http://www.cse.uiuc.edu/heath/scicomp/notes
- and also on Class-Web

## Supplementary Books

- V. Kumar, A. Grama, A. Gupta, and G. Karypis: *Introduction To Parallel Computing: Design And Analysis Of Algorithms*, Benjamin/Cummings, 1994, (PC)
- Hennessy, J. L, and Patterson, D. A., *Computer Architecture: A Quantitative Approach, 2nd Edition*. Morgan Kaufmann, 1996, (CA)



## Some Scientific Journals

- Siam Journal on Scientific Computing (journal),
- Computing in Science & Engineering (magazine),
- International Journal of High Performance Computing Applications
- Applicable Algebra in Engineering Communication and Computing (mathematics) ,
- Parallel Computing (computer science with applications),
- … and many others



## Some Internet Links

- http://www.scientific-computing.com/
- http://wotug.ukc.ac.uk/parallel/
- . . .



## Course Organisation

- Teaching
  - Lessons with slides (all slides on Class Web Page)
  - Practice with student presentations of solution to problems, theory, homework (announced after lessons)
  - Homework and project published on Class Web-page
- Examination and Grading
  - Homework: 20%
  - Project: 30%
  - Final written exam: 50%
    (see further details on Class Web Page)
- Personal communication
  - Labs, E-mail



## Homework

- Students will solve either exercises from the textbooks or problems defined by themselves.
- It is expected that seven homework assignments will be finished individually.
- The problem and results should be send by e-mail, when accepted they will be posted on the Class Web page, for other students.
- Some of the solved homework will be used in the final exam.



## Project

- Up to three students can work together on a research project,
- It has to involve an practical component– i.e. it is not a paper and pencil exercise, some working program is expected,
- Prepare the project proposal, either your own topic or a suggested one,
- Two months to work on the project and to finish a written report including: overview, methods, results, and possible extensions.
- Projects should be send to my e-mail.
- Start thinking about potential project ideas soon!

## In-class discussions

- A part of some lessons can be set aside for student-led in-class discussions.
- Recent news and areas of research and innovation in parallel and scientific computing can be selected as starting point for the discussion.
- Student candidates can lead one discussion instead of doing the project, however, written report is expected in the same way as for the project.



## Exam

- There will be a final written exam with books and notes, covering the complete course material.
- Questions will be selected from the review questions given for all chapters.
- Some questions will be selected from solved homework.
- Provisional exam terms:
- June/04??; Oct./04; Jan./05
- Homework and projects should be finished before written exam.
- Registration for the exam by e-mail at least one week before the exam term!



## Lecture and Labs Grading

- The final success measured in percentage =
  percentage of accepted homework * lecturer's grade * 0.3 +
  percentage of accepted project * lecturer's grade * 0.2 +
  percentage of solved questions on the exam * 0.5
- Note: The accepted homework and project are graded on the basis of lecturer's judgement in the range from 0.6 to 1.
- Lecture grade according to the final success:
  5 < 60%; 60 <= 4 < 70%; 70 <= 3 < 80%; 80 <= 2 < 90%; 1 >= 90%
- Labs grade depends on grades of labs exercises (labswork) and homework:
  (=Lecture grade) if more than 80% of labswork and homework accepted;
  (=Lecture grade + 1) if all labswork, homework and project accepted.
  (=Lecture grade - 1) if less than 80% of labswork and homework accepted.



## Provisional Scheduling

Once per month on two consecutive days:

Tuesday
- 10 - 11:30 a.m, Lessons, Room T05
- 11:45 - 12:30 p.m, Labs, Small computer room
- 14 - 15:30 p.m, Lessons, Room T05
- 15:45 - 16:30 p.m, Labs, Small computer room

and Wednesday (one hour earlier !)
- 9 - 10:30 a.m, Lessons, Room T06
- 10:45 - 11:30 p.m, Labs, Small computer room
- 13 - 14:30 p.m, Lessons, Room T06
- 14:45 -15:30 p.m, Labs, Small computer room

- Details and final schedule will be arranged with students (see syllabus on Class Web for details).