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MA50177: Scientific Computing
Information Sheet

This course will be taught jointly by **Dr. Eike Müller** and myself. His contact details are: Office 4W3.35, Email: e.mueller@bath.ac.uk, Tel.: 01225 385633.

Schedule of Classes

There will be three classes per week.

Lecture:	Tuesday	4.15pm	in 1W3.5
Computer Lab:	Wednesday	10.15am	in EB0.9
Tutorial:	Friday	11.15am	in 3E3.1

This structure might vary slightly in some weeks.

In particular, there will be a change to this schedule in Weeks 1 and 2! In Week 2 there will be **no lecture (!)** on Tuesday. However, there will be **two additional** lab sessions

Computer Lab:	Thursday	9.15am	in 3E3.1	**(Weeks 1 & 2 only!)**

Content of lectures

Programming in a high-level language: FORTRAN95**.** Data types, control of flow, arithmetic operations, intrinsic functions, programme units and procedures, array features. Applications.

Typical problems in Scientific Computing. Floating point arithmetic, large scale linear algebra problems, conditioning, complexity, detailed treatment of Gaussian elimination, memory hierarchies, BLAS, scientific software: LAPACK, HSL.
Applications chosen from: Curve fitting, linear regression, analysis of discrete structures, graph partitioning, numerical integration, nonlinear optimisation.

Parallel programming with MPI and applications. The Message Passing Interface (MPI), parallel programming models, performance indicators, introduction to the Mathematical Sciences Beowulf cluster, parallel software packages (e.g. PETSc, HYPRE, ScaLAPACK). Detailed case study of a large scale problem.

IMPORTANT. Each week some **programming exercises** will be set in the labs and on **problem sheets**. Doing the exercises is an **essential** part of the course. Even though they are not part of the assessed coursework, in the later tests and assessed assignments it will be **assumed** that you have done these exercises. Moreover the content of the classes in subsequent weeks will be designed on the assumption that you have done them.

Assessment scheme

Class Test	on programming in FORTRAN95, Friday 24th February 2012	[30%]
Assignment 1	set in Week 6 and due in Week 8	[35%]
Assignment 2	set in Week 10 and due in the Revision Week	[35%]

(Note that the exact dates for the assignments will be announced later.)

Resources

The Moodle page for the course is

http://moodle.bath.ac.uk/course/view.php?id=1134

referred to throughout the course as the homepage. It will contain lecture notes, handouts, pages with useful links, etc. You should automatically be enrolled. If not, please contact us.

Programs for the examples/exercises will be available at ~masrs/ma50177. More about copying them to your home directory and other useful Linux commands in the lab on Thursday. All directories mentioned during the course will be subdirectories of this directory. If there are problems I can also make them available from the homepage.

Main References

Throughout the course the following books will be referenced using the initials noted below. [MeRe] and [Sm] are the most important for the first part of the course.

[De] JW. Demmel, *Applied Numerical Linear Algebra*, SIAM, 1997 (511.84 DEM: 1 copy on 28 day loan, 2 on 7 day loan and 1 on 3 day loan).

[GrLu] W. Gropp, E. Lusk & A. Skjellum, *Using MPI*, 2nd Ed., MIT Press, 1999 (518.721 GRO: 1 copy in the library (1st ed.), 6 in the MSc room).

[He] MT. Heath, *Scientific Computing: An Introductory Survey*, 2nd Ed., McGraw Hill Paperback, 2002 (512.97 HEA: 1 copy on 28 day loan, 3 on 7 day loan).

[MeRe] M. Metcalf & J. Reid, *FORTRAN 90/95 Explained*, 2nd Ed., Oxford University Press, 1999 (518.542 FOR: 2 on 28 day loan, 2 on 7 day loan, 6 in the MSc room)

[Pa] PS. Pacheco, *Parallel Programming with MPI*, Morgan Kaufmann Publishers, 1997 (3 copies in theMSc room)

[Sm] IM. Smith, *Programming in FORTRAN90*, John Wiley, 1995 (518.542FOR: 2 copies on 28 day loan, 6 copies in the MSc room).

We sincerely hope you will enjoy the course. If you have any problems please do not hesitate to see us at the end of a lecture or email us.

Robert Scheichl & Eike Müller 7th February 2012.