PX425-7.5 High Performance Computing in Physics

21/22

Department
> Physics

Level
> Undergraduate Level 4

Module leader
> Nicholas Hine

Credit value
> 7.5

Module duration
> 5 weeks

Assessment
> 100% coursework

Study location
> University of Warwick main campus, Coventry

Description

Introductory description

The module will address the increased use of computer simulation and data analysis on high performance computers in all fields of computational physics and other sciences. Computing skills are greatly valued across science and beyond and we encourage students to go as far as they can to develop such skills.

[Module web page](#)

Module aims

To continue your training in the use of computers by exploring the use of super-computers. The module should teach how to write scalable, portable programs for parallel computer systems and explore how large-scale physics problems are tackled.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

Programming for efficiency. Modern cache architectures and CPU pipelining. Avoiding expensive and repeated operations. Compiler optimisation flags. Profiling with gprof.

Introduction to parallel computing. Modern HPC hardware and parallelisation strategies. Applications in Physics, super problems need super-computers.

Shared memory programming. The OpenMP standard. Parallelisation using compiler directives. Threading and variable types. Loop and sections constructs. Program correctness and reproducibility. Scheduling and false sharing as factors influencing performance.

Distributed memory programming. The MPI standard for message passing. Point-to-point and collective communication. Synchronous vs asynchronous communication. MPI communicators and topologies.

GPU programming. CUDA vs OpenCL. Kernels and host-device communication. Shared and constant memory, synchronicity and performance. GPU coding restrictions.

Limitations to parallel performance. Strong vs weak scaling. Amdahl's law. Network contention in modern many-core architectures. Mixed mode OpenMP+MPI programming.

Learning outcomes

By the end of the module, students should be able to:

- Use visualisation libraries and desktop visualisation tools; be able to write a scientific application with a graphical user interface, using a toolkit
- Write a parallel program using shared-memory or message passing constructs, for physics applications
- Explain the concepts underlying Grid computing and e-science, and discuss their general areas of applicability.

Indicative reading list

R Chandra et al, Parallel Programming in OpenMP (Morgan Kaufmann, 2000)
P Pacheco, Parallel Programming with MPI (Morgan Kaufmann, 1996)
M Quinn, Parallel Programming in C with MPI and OpenMP (McGraw-Hill, 2003)
D Kirk and W Hwu, Programming Massively Parallel Processors (Elsevier, 2010)

View reading list on Talis Aspire

Subject specific skills

Skills in computer-modelling, reasoning, thinking. Knowledge of mathematics and physics

Transferable skills

Analytical, communication, computing and general IT, problem-solving, self-study

Study

Study time

Type	Required
Lectures	15 sessions of 1 hour (20%)
Demonstrations	5 sessions of 2 hours (13%)
Private study	50 hours (67%)
Total	75 hours

Private study description

Working through lecture notes, formulating problems, writing and testing code, discussing with others taking the module, preparing and submitting coursework

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group A1

	Weighting	Study time
Coding assignments	100%	
Test computing skills		

Feedback on assessment

General feedback addressing common issues arising out of assignments will be given in lectures. Feedback on individual submissions will be given electronically via a web page with customised content for each student.

Availability

Courses

This module is Core optional for:

- Year 1 of TPXA-F344 Postgraduate Taught Modelling of Heterogeneous Systems

This module is Optional for:

- TMAA-G1PE Master of Advanced Study in Mathematical Sciences
    - Year 1 of G1PE Master of Advanced Study in Mathematical Sciences
    - Year 1 of G1PE Master of Advanced Study in Mathematical Sciences
    - Year 1 of G1PE Master of Advanced Study in Mathematical Sciences
- Year 1 of TMAA-G1P9 Postgraduate Taught Interdisciplinary Mathematics
- Year 1 of TMAA-G1PD Postgraduate Taught Interdisciplinary Mathematics (Diploma plus MSc)
- Year 1 of TMAA-G1P0 Postgraduate Taught Mathematics
- Year 1 of TMAA-G1PC Postgraduate Taught Mathematics (Diploma plus MSc)
- Year 4 of UPXA-F304 Undergraduate Physics (BSc MPhys)
- Year 4 of UPXA-F303 Undergraduate Physics (MPhys)

This module is Core option list A for:

- Year 2 of TPXA-F345 Postgraduate Taught Modelling of Heterogeneous Systems (PGDip)

This module is Option list A for:

- Year 1 of TMAA-G1P0 Postgraduate Taught Mathematics
- Year 3 of UMAA-G100 Undergraduate Mathematics (BSc)
- Year 4 of UMAA-G101 Undergraduate Mathematics with Intercalated Year

This module is Option list B for:

- Year 4 of UPXA-FG33 Undergraduate Mathematics and Physics (BSc MMathPhys)
- Year 4 of UPXA-FG31 Undergraduate Mathematics and Physics (MMathPhys)

This module is Option list C for:

- UMAA-G105 Undergraduate Master of Mathematics (with Intercalated Year)
    - Year 3 of G105 Mathematics (MMath) with Intercalated Year
    - Year 5 of G105 Mathematics (MMath) with Intercalated Year
- UMAA-G103 Undergraduate Mathematics (MMath)
    - Year 3 of G103 Mathematics (MMath)
    - Year 4 of G103 Mathematics (MMath)
- UMAA-G106 Undergraduate Mathematics (MMath) with Study in Europe
    - Year 3 of G106 Mathematics (MMath) with Study in Europe
    - Year 4 of G106 Mathematics (MMath) with Study in Europe