DTU Technical University of Denmark

DANISH CENTER FOR APPLIED MATHEMATICS AND MECHANICS DCAMM

High Performance Computing

FORTRAN, OpenMP and MPI

41391

Content of Course

- Week 1: FORTRAN

Prof. J. H. Walther
DTU MEK
jhw@mek.dtu.dk

Week 2: OpenMP

- With 02614

Asso. Prof. B. Dammann
DTU Compute
beda@dtu.dk

- Week 3: MPI

Prof. J. H. Walther
DTU MEK
jhw@mek.dtu.dk

Learning Objectives

- read programs written in FORTRAN.
- write programs in FORTRAN.
- read programs with OpenMP directives.
- write programs with OpenMP directives.
- read programs using MPI.
- write programs using MPI.
- understand the difference between shared and distributed memory parallelism.
- perform serial benchmarking of code.
- perform code debugging.
- measure parallel efficiency
- use Amdah's law.

FORTRAN

High level procedural language developed by IBM in the 1950ies:

- Mathematical **FOR**mula **TRAN**slating System.
- Suited for scientific and engineering computing.
- ANSI standards: ‘66, ‘77, ‘90, ‘95, ‘03, ’08, ‘18.
- Key features:
  - ‘77: arrays, characters, **modular** programming.
  - ‘9x: allocatable arrays, **object-based** programming.
  - ‘0x: **object-oriented**, generic programming.

OpenMP

- **Open M**ulti-**P**rocessing (**OpenMP**) is a standard **A**pplication **P**rogramming **I**nterface (API) that supports multi-platform **shared memory** multiprocessing programming in C/C++ and FORTRAN.
- OpenMP consists of compiler directives, library routines, and environment variables that enable shared memory parallelism and execution.
- Relatively easy parallelization:
  - Line-by-line strategy for distribution of work load.
  - No need for distributing the data/memory!
- Limited scalability (beyond 4-8 cores):
  - Congestion of the shared memory network.
  - Expensive hardware – limited memory.

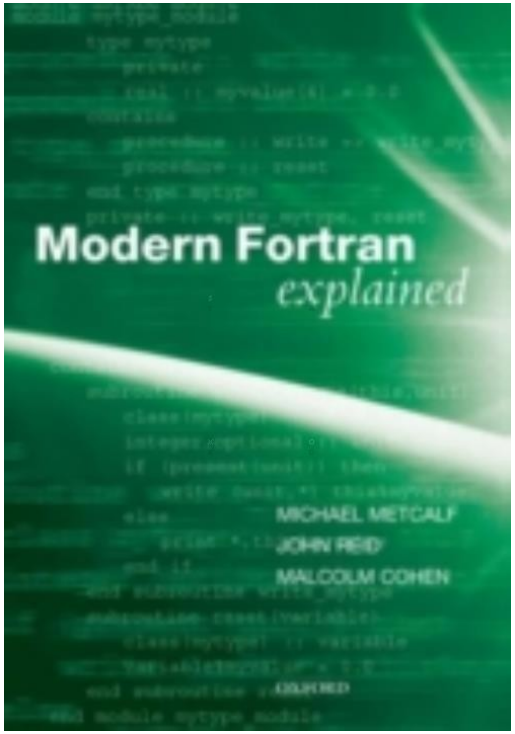
MPI

- **M**essage **P**assing **I**nterface (**MPI**) is the de-facto standard for programming portable message-passing parallel applications on **networked** computers (clusters).
- Has bindings to C/C++ and FORTRAN and is available from single core laptops to massively parallel supercomputers.
- Relatively difficult to implement:
  - Explicit spatial distribution of the problem: data/memory.
  - Complete revision of the algorithms and implementation may be required.
- Good scalability (to thousands/million of cores):
  - The memory is local – so access to local memory is efficient.
  - Inexpensive hardware – unlimited memory/processors.

Content FORTRAN 95

- Day 1:
  - Introduction.
  - Language elements.
  - Expression and assignments.
  - Control constructs.
- Day 2:
  - Program units and procedures.
- Day 3:
  - Array Features.
  - Makefiles.
- Day 4:
  - Specification statements.
  - Intrinsic procedures.
- Day 5:
  - Data transfer.
  - Operations on external files.
  - Advice for the road.
  - Fortran 2003/2008 extensions.

Class Homepage:
learn.inside.dtu.dk



Modern Fortran Explained
John Reid, Malcolm Cohen & Michael Metcalf

Computer accounts

- Computer system: login.gbar.dtu.dk:
  - UNIX/linux (SunOS/linux):
    - www.gbar.dtu.dk
    - www.gbar.dtu.dk/faq/43-thinlinc (remote access - Windows).
  - Access:
    - Use DTU username/passwd (guest account for non-DTU students).
    - Remote access using Thinlinc or ssh:
      - `ssh –Y s111111@login.gbar.dtu.dk`
      - continue to linux nodes by typing the command: `linuxsh –X`
  - UNIX/linux documentation available in **man** pages. Accessed in a shell window/terminal through the command ‘`man <command>`’ e.g., `man ls`

Compiler

- Sun FORTRAN 90/95 compiler:
  - To setup the ENV variables to point to the Sun compiler on the gbar, type, in the terminal:
    - `module add studio`
    - `module add mpi/3.1.3-oracle-12u6`

      You may also download the compiler at:

      www.oracle.com/technetwork/server-storage/solarisstudio/downloads/index.html
  - Documentation: type ‘`man f90`’ or ‘`f90 -help`’ `in the terminal.`
- To compile a simple serial program:

```
     f90 –free example.f
```

- To compile a simple parallel program:

```
     mpif90 –free example.f
```

Lectures and Exercises

- Lectures: 9:00 – 11:30 (2022 recordings available on Learn).
- Exercises: 13:00 – 16:00.
  - Work in groups of 1-2.
  - Hand in report (minimum 4 out of 5) at the end of each week; report = source code (+ plots/figures)