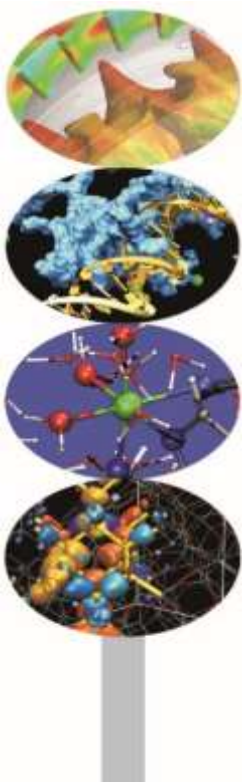
Parallel I/O and management of scientific data



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The Agenda

Monday, 5th

- ✓ 09:30-10:00 Registration
- ✓ 10:00-11:30 I/O: state of the art
- ✓ 11:30-12:30 HDF5: theory & practice
- ✓ 12:30-13:30 Lunch
- ✓ 13:30-17:00 HDF5: theory & practice

Tuesday, 6th

- ✓ 10:00-11:00 Brief MPI introduction/reprise
- ✓ 11:00-12:30 MPI2-IO: theory & Practice
- ✓ 12:30-13:30 Lunch
- ✓ 13:30-17:00 MPI2-IO: theory & Practice

Wednesdey, 7th

- ✓ 10:00-12:30 MPI2-IO: theory & Practice
- ✓ 12:30-13:30 Lunch
- ✓ 13:30-15:00 Management of large scientific data
- ✓ 15:00-17:00 Question & Answer

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Hands-out

- Hands-out and examples can be downloaded at:

1. https://hpc-forge.cineca.it/files/CoursesDev/public/
2. go to 2017
3. go to Parallel_I_O_and_management_of_large_scientific_data/
4. go to Roma

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Using desktop

- Choose linux at boot…
- Use module
  - ✓ `module purge`
  - ✓ `module available (av)`
  - ✓ `module list (li)`
  - ✓ `Module load`
  - ✓ `Module load autoload`

```
[caspurc-05-usere@caspurc-05] $ module av
-------------------- /usr/local/Modules/3.2.10/modulefiles ----------
autoload                          hdf5/intel-serial/1.8.16
gcc/5.2                           intel/compilers/pe-xe-2016
grace/5.1                         intel/mkl/11.3
gromacs/5.0.4                     intel/vtune/16.1
hdf5/gnu-api16-serial/1.8.16 openmpi/1.10.1/gcc-5.2
hdf5/gnu-parallel/1.8.16     openmpi/1.8.5/gcc-4.8
hdf5/gnu-serial/1.8.16            paraview/4.4.0
hdf5/intel-parallel/1.8.16   vmd/1.9.2
```

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Using desktop

- Loading compiler
  - ✓ `module load gcc/5.2`
  - ✓ `module load intel/compilers/pe-xe-2016`
- Using mpi
  - ✓ `module load autoload openmpi/1.10.1/gcc-5.2`
- Using serial hdf5
  - ✓ `module load autoload hdf5/gnu-serial/1.8.16`
  - ✓ `module load autoload hdf5/intel-serial/1.8.16`
  - ✓ `module load autoload hdf5/gnu-api16-serial/1.8.16`
- Using parallel hdf5
  - ✓ `module load autoload hdf5/gnu-parallel/1.8.16`
  - ✓ `module load autoload hdf5/intel-parallel/1.8.16`

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Using cluster GALILEO

- Connect to GALILEO front-end
  - ✓ **`ssh -X a08traXX@login.galileo.cineca.it`**
    - ✓ **where XX can be 01,02,-,20**
    - ✓ **password will be provided during classroom**
- Using MPI
  - ✓ **`module load autoload openmpi`**
- Compiling
  - ✓ **`mpicc -O3 -std=c99 source.c -o executable.exe`**
  - ✓ **`mpifort -O3 source.F90 -o executable.exe`**
- Running
  - ✓ **`mpirun -np N ./executable.exe`**

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exampleHDF5.tar

To expand **exampleHDF5.tar** file, syntax:

…

```
tar -xvf exampleHDF5.tar
```

…

Now a directory HDF5 is created, with this structure:

```
HDF5
├── u_00001000.h5
├── sample.h5
├── PARALLEL
│       └── RUN
└── SERIAL
        └── RUN
```

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exampleMPIIO.tar

To expand **exampleMPIIO.tar** file, syntax:

…

```
tar -xvf exampleMPIIO.tar
```

…

Now a directory MPI_IO is created, with this structure:

```
MPI_IO
├── F90
│     └── sources.F90
└── C
      └── sources.c
```

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