Working with supercomputer HPCFS

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Agenda

- **Model of HPCFS usage** (prof. dr. Janko Slavič, 5 min)
- **Introduction to supercomputing** (as. *dr. Pavel Tomšič, 10 min)*
- **Accessing HPCFS** (*Grega Tomažin, 20 min)*
- **Overview of software on HPCFS** (izr. prof. dr. Janez Povh, 10 min)
- **Start up and first steps: *Ansys, Matlab, Mathematica*** (izr. prof. *dr. Janez Povh, as. dr. Borut Černe, 20 min)*
- **Current projects on HPCFS** (users of HPCFS, 15 min)
- **Discussion** (10 min)

HPCFS – nodes, cores and costs

HPCFS:

- 20 nodes installed in 2016 (N2016): 24 cores, 64GB RAM (20x24x30=14.4knh: **price 0,144€/nh**)
- 20 nodes installed in 2021 (N2021): 2x24 cores, 128GB RAM (20x24x30=14.4knh: **price 0,288€/nh**)

Free nh [N2021] per lab in 2022

Lab	N2021 [nh]
Center za eksperimentalno mehaniko	697
Laboratorij za aeronavtiko	9
Laboratorij za alternativne tehnologije	2993
Laboratorij za digitalne in mikroprocesorske sisteme in elektrotehniko	632
Laboratorij za dinamiko strojev in konstrukcij	6700
Laboratorij za energetske delovne stroje in tehnično akustiko	287
Laboratorij za fotoniko in laserske sisteme	1087
Laboratorij za hladilno tehniko	3720
Laboratorij za lasersko tehniko	3552
Laboratorij za meritve v procesnem strojništvu	387
Laboratorij za modeliranje elementov in konstrukcij	2662
Laboratorij za motorje z notranjim zgorevanjem in elektromobilnost	3904
Laboratorij za nelinearno mehaniko	2479
Laboratorij za numerično modeliranje in simulacijo v mehaniki	2795
Laboratorij za odrezavanje	1481
Laboratorij za ogrevalno, sanitarno in solarno tehniko ter klimatizacijo	589

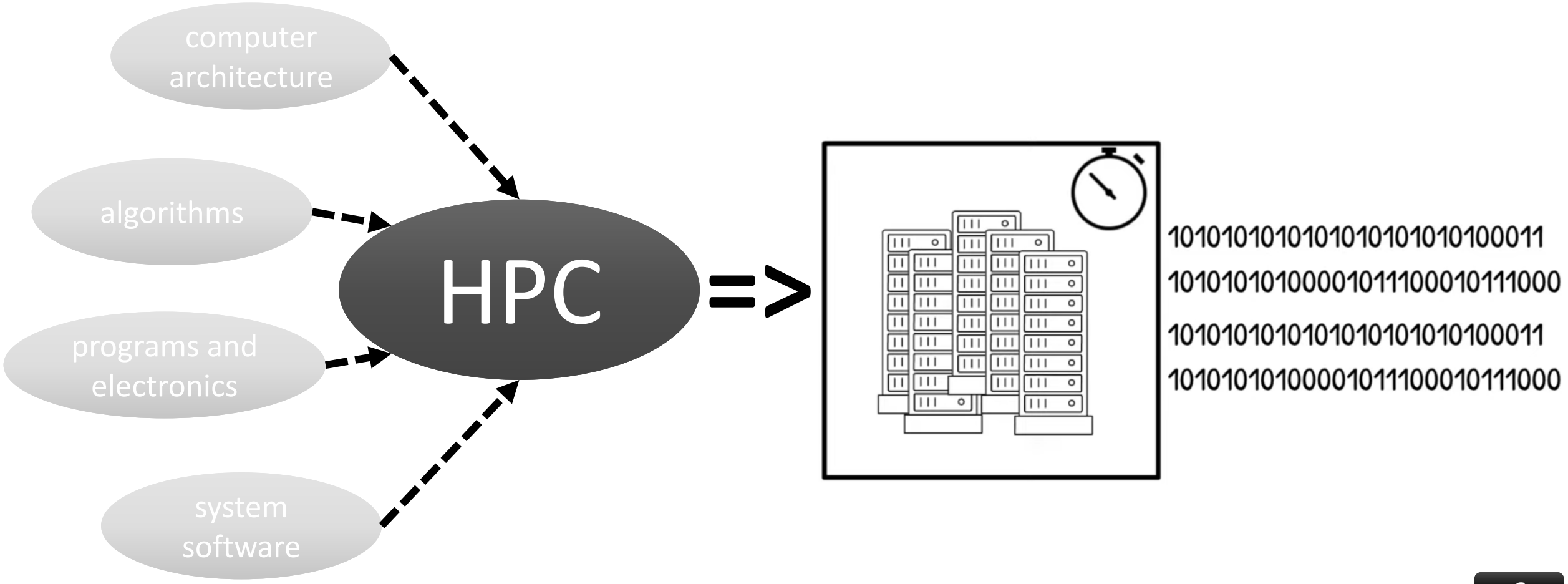
Presenter: Dr. Janko Slavič

Free nh [N2021] per lab in 2022

Laboratorij za okoljske tehnologije v zgradbah	727
Laboratorij za preoblikovanje	204
Laboratorij za procesno avtomatiko	228
Laboratorij za proizvodne sisteme in laboratorij za pripravo in vodenje proizvodnje	208
Laboratorij za sinergetiko	887
Laboratorij za snovanje in optimiranje konstrukcij	2224
Laboratorij za strego, montažo in pnevmatiko	857
Laboratorij za strojne elemente in mehanizme	2576
Laboratorij za tehnično kibernetiko, obdelovalne sisteme in računalniško tehnologijo	338
Laboratorij za termoenergetiko	1033
Laboratorij za toplotno obdelavo in laboratorij za preizkušanje kovin	451
Laboratorij za toplotno tehniko	2941
Laboratorij za tribologijo in površinsko nanotehnologijo	3957
Laboratorij za varjenje	530
Laboratorij za vrednotenje konstrukcij	657
Raziskovalna skupina za matematiko	285

Introduction to supercomputing

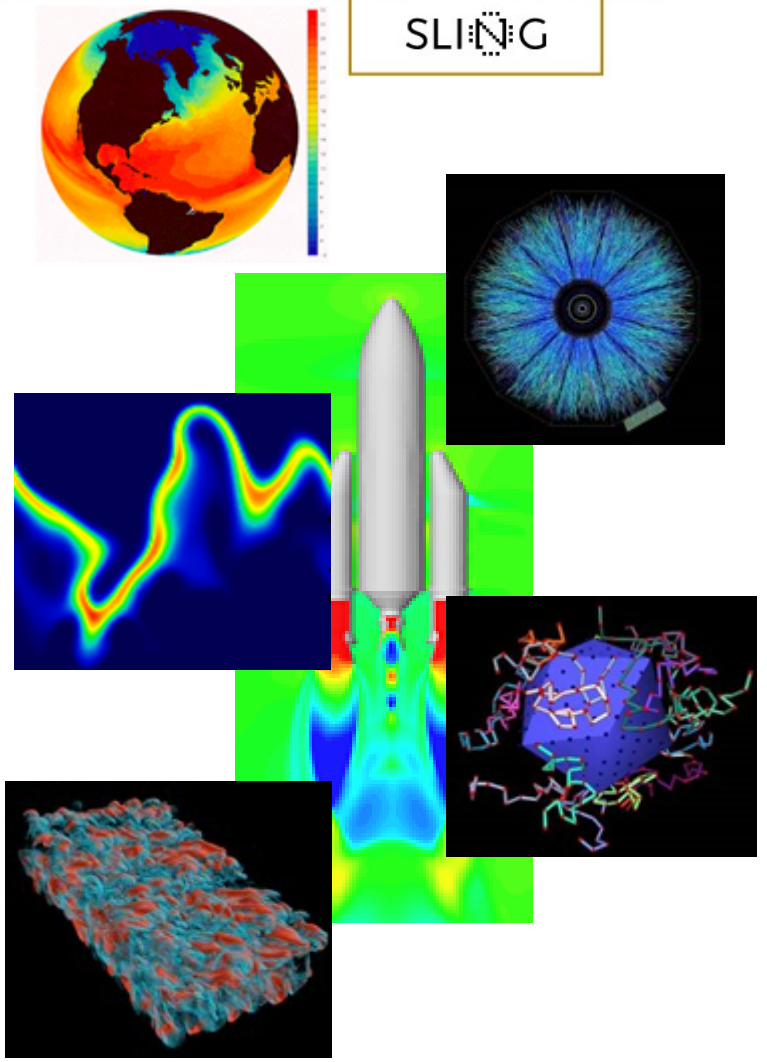
What is High Performance Computing (HPC)



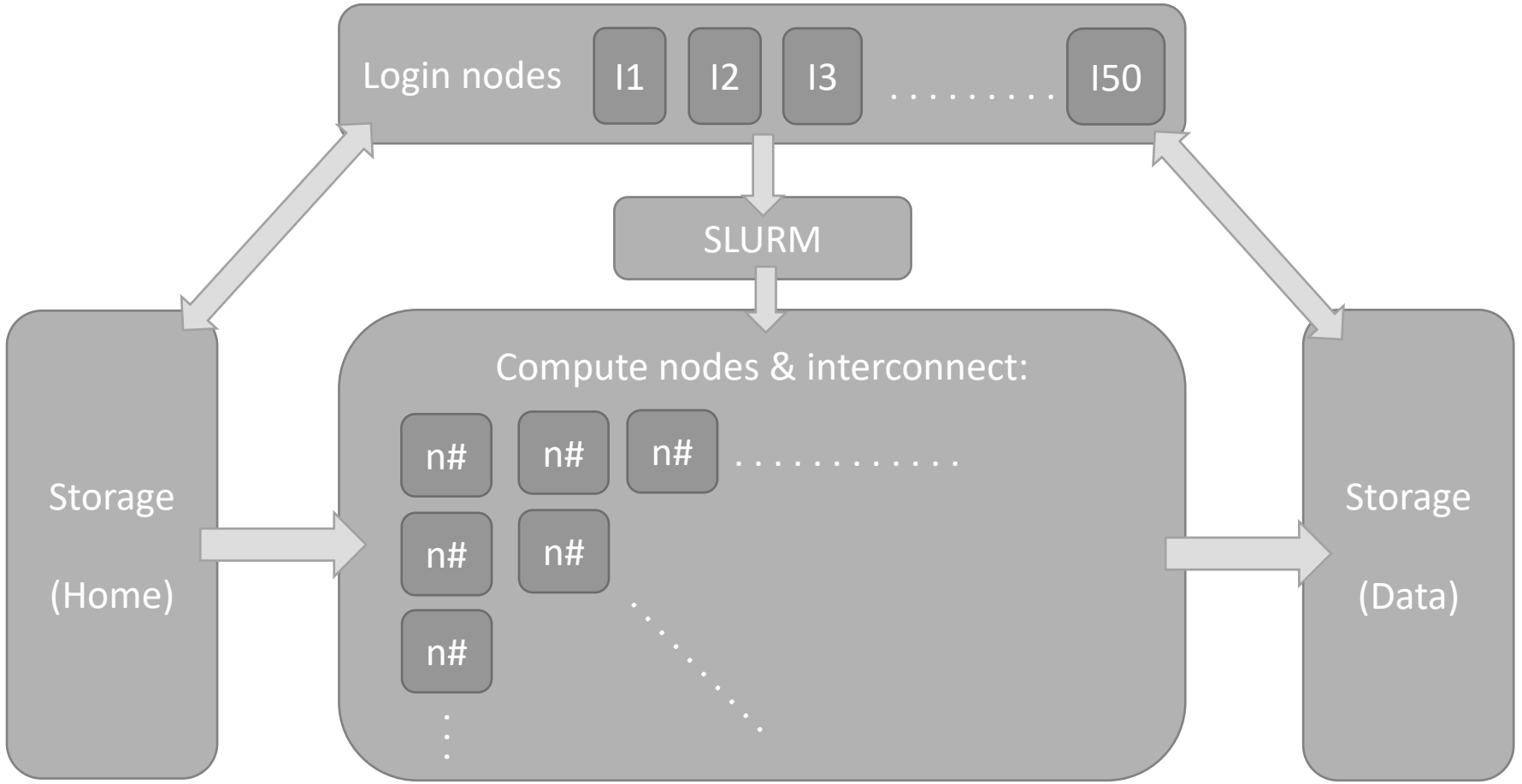
Introduction to supercomputing

Usage

- **Weather, Climatology, Earth Science**
  - degree of warming, scenarios for our future climate.
  - understand and predict ocean properties and variations
  - weather and flood events
- **Astrophysics, Elementary particle physics, Plasma physics**
  - systems, structures which span a large range of different length and time scales
  - quantum field theories like QCD, ITER
- **Material Science, Chemistry, Nanoscience**
  - understanding complex materials, complex chemistry, nanoscience
  - the determination of electronic and transport properties
- **Life Science**
  - system biology, chromatin dynamics, large scale protein dynamics, protein association and aggregation, supramolecular systems, medicine
- ***Engineering***
  - complex helicopter simulation, biomedical flows, gas turbines and internal combustion engines, forest fires, green aircraft,
  - virtual power plant



Components of HPC cluster



Login nodes

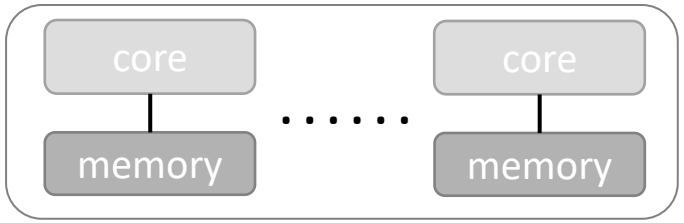
Compute nodes

Shared (login, storage)

Exclusive (compute nodes)

Parallel hardware

Serial computing



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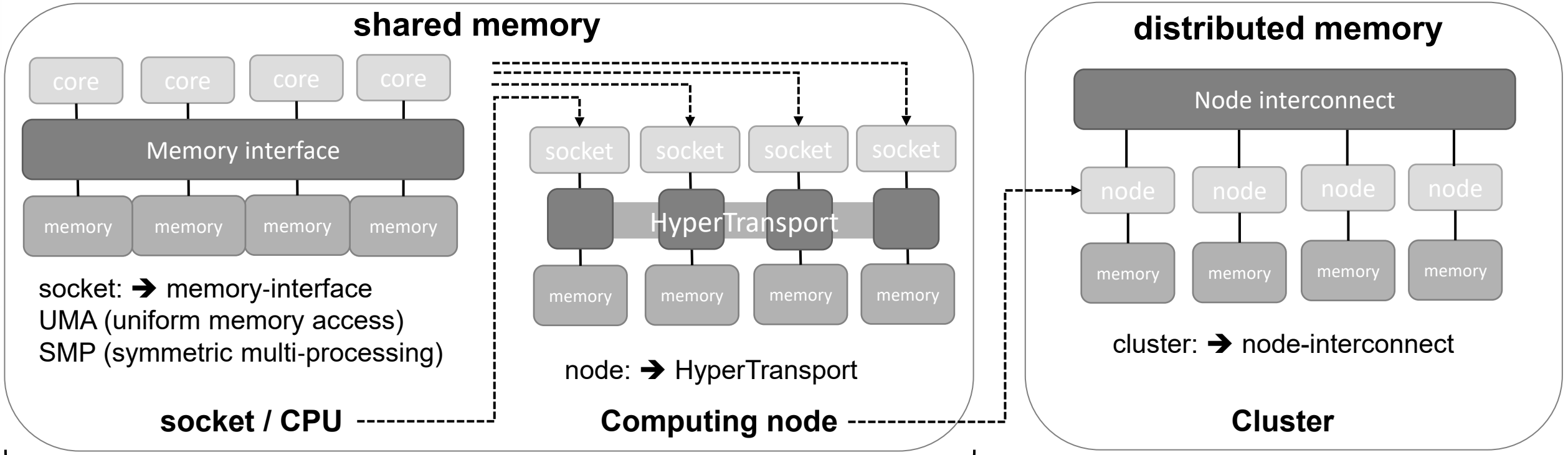
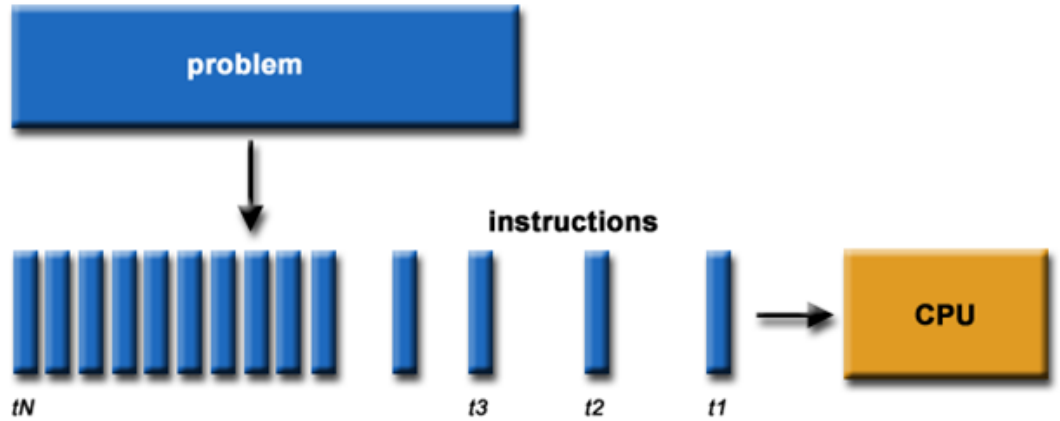
Parallel hardware



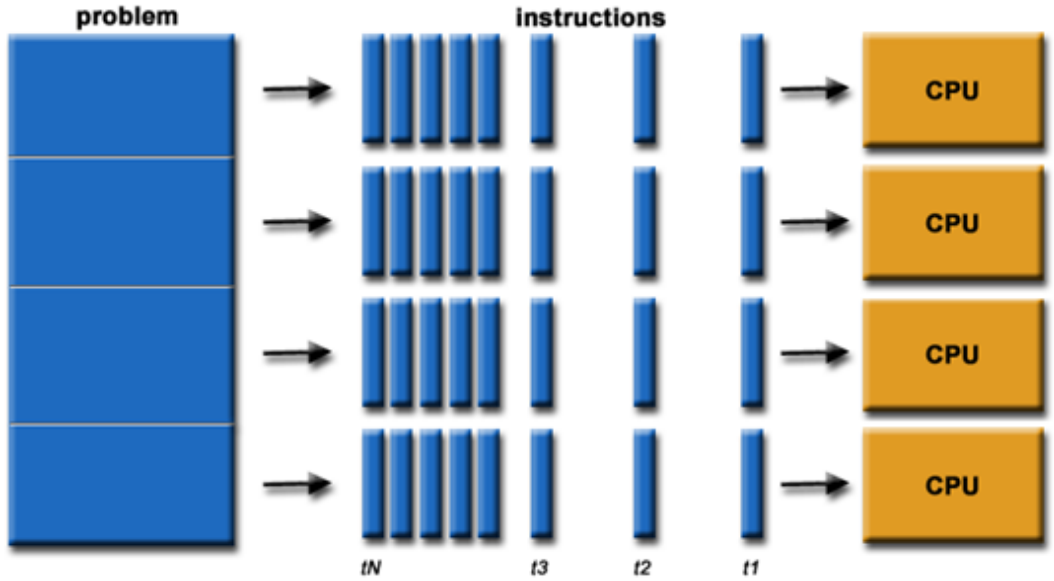
A simple parallel process

Problem discretisation

Serial computing



Problem paralelisation



Program scalability

- Parallel portion of the code determines code scalability
- Amdahl's law:

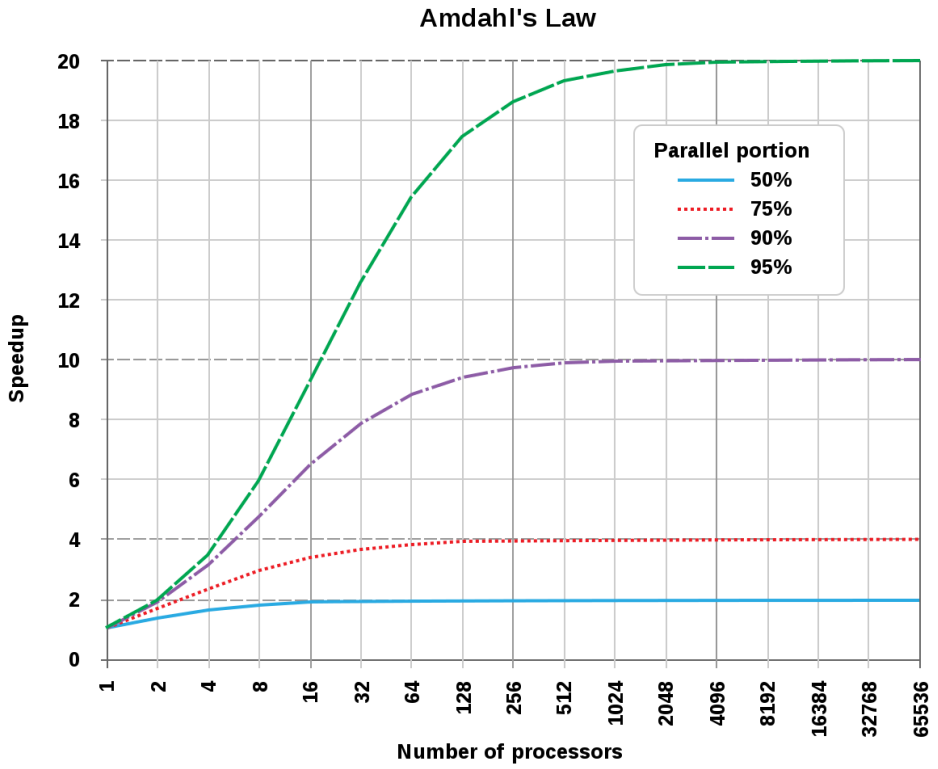
f ... sequential part of code
p … #processors

neglecting time for communication
neglecting load imbalance

$$S_p = T_{serial} / T_{parallel,p} = 1 / (f + (1-f) / p)$$

Speedup is limited: $S_p < 1 / f$

- Development of parallel codes
  - Good understanding of the problem being solved
  - How much of the problem can be run in parallel
  - Bottleneck analysis and profiling
  - We optimize and parallelize parts that consume most of the computing time
  - Problem needs to be dissected into parts functionally and logically



Source: Wikipedia

Accessing HPCFS

- You can access the supercomputer HPCFS by **username and password** OR by **ssh key**.
  In both cases, you first need **approval** by computing center of UL FME. To get it, you need to send to hpc@fs.uni-lj.si **two things:**

1. a completed form (fill it out, sign it, provide a signature from the head of research unit (laboratory) whose computing resources you will spend);
2. encrypted password **OR** SSH key:
   - **password:** click on the password to obtain the encrypted password. Send this password to hpc@fs.uni-lj.si;
   - **SSH key:** you can create and distribute SSH key

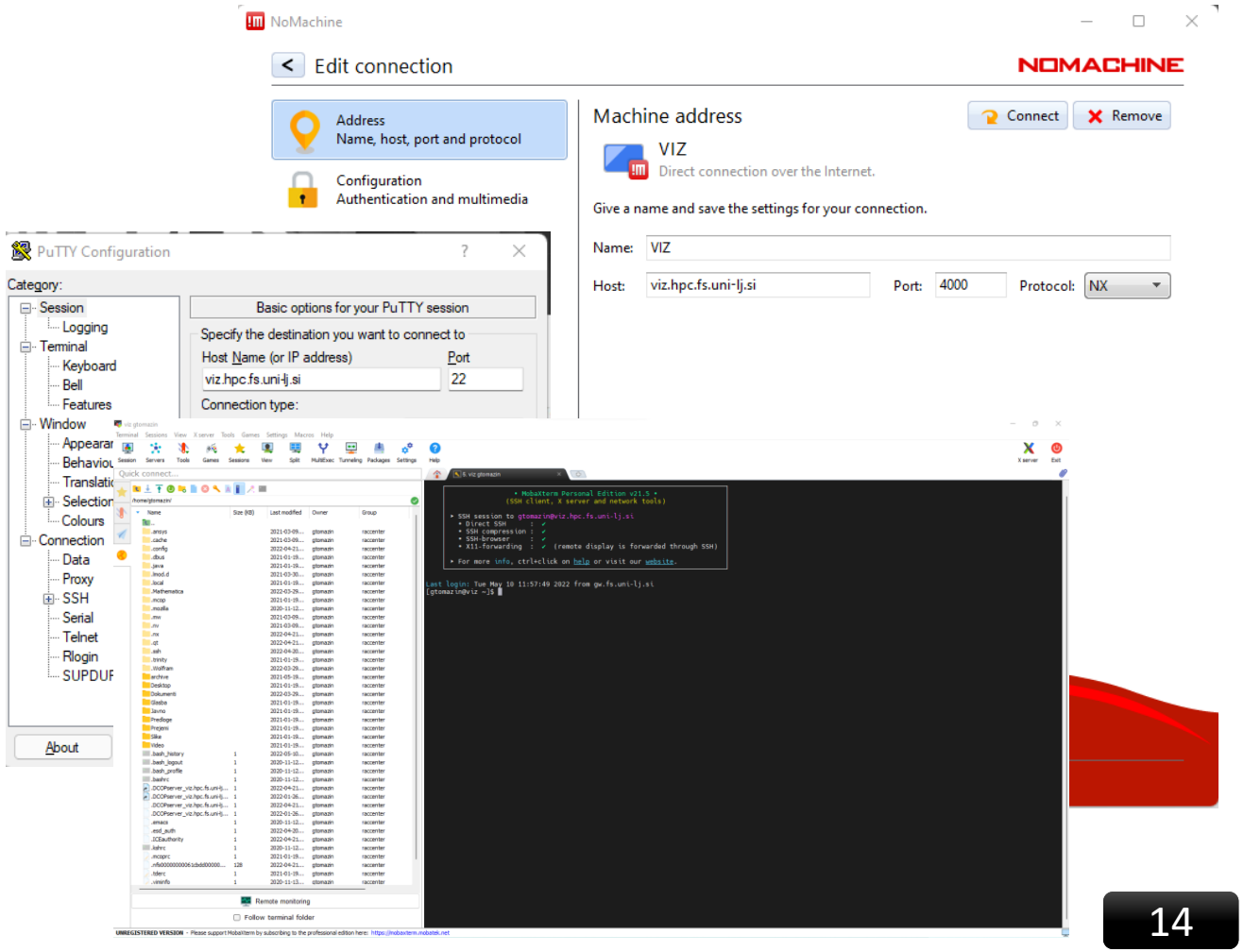
Accessing HPCFS

- **Accessing HPC software**

1. NoMachine NX or SSH
2. Putty
3. MobaXterm (console and files)
4. …

- **viz.hpc.fs.uni-lj.si**

SSH:22, NX:4000



Accessing HPCFS

- **Basic Slurm commands**
- Srun, sbatch, sinfo, squeue, scancel <jobid>
  - LD_PRELOAD= srun --pty bash –I
  - env --unset=LD_PRELOAD TMOUT=600 srun --mem=100G --time=4:0:0 -p rome --x11 --pty bash -I

- **More about Slurm usage you can read here:**
  https://wiki.hpc.fs.uni-lj.si
  https://slurm.schedmd.com/documentation.html

WIKI
HPC FS

SLURM
DOC

Overview of software on HPCFS

- Ansys Multiphysics
- Ansys CFX, Fluent, Maxwell, HFSS
- OpenFOAM CFD + extend
- VisIt in ParaView postprocesor
- Intel F90, CC
- TotalView, Allinea DDT
- Siemens NX in ProEngineer
- Octave, R, Mathematica, Matlab
- OpenMP, OpenMPI, HPMPI, IntelMPI
- ATLAS, BLAS, BLACS, FFTW, GOTO, MUMPS, NetCDF, HDF5, Sparsekit, Scalapack

Overview of software on HPCFS

Module environment

- Module concept is available on most supercomputers
- It simplifies the use of different software (versions) in a controlled way.
- Settings for each SW (version) are encapsulated into "environment modules" maintained by the module system.
- *Do not mix with "perl" or "python" modules*

Basic module commands

- To get list currently loaded modules on the node

[jpovh@cn62 ~]$ **module list**

No modules loaded

- To list all available modules on HPC

[jpovh@cn62 ~]$ **module avail**

```
[jpovh@cn62 ~]$ module avail

------------------------------------------------------------------------------ /opt/pkg/modules/all ------------------------------
   ANSYS/20.1                                                  Tcl/8.6.9-GCCcore-8.2.0
   ANSYS/21.R1                                        (D)      Tcl/8.6.9-GCCcore-8.3.0
   ANSYS/21.1                                                  Tcl/8.6.10-GCCcore-9.3.0
   ANSYS/2021R2                                                Tcl/8.6.10-GCCcore-10.2.0                                  (D)
   ATK/2.22.0-foss-2016b                                       TensorFlow/1.10.1-foss-2018b-Python-3.6.6
   ATK/2.28.1-fosscuda-2018b                                   TensorFlow/1.10.1-fosscuda-2018b-Python-2.7.15
   ATK/2.32.0-GCCcore-8.2.0                           (D)      TensorFlow/1.13.1-foss-2019a-Python-3.7.2
   ATLAS/3.10.2-GCC-5.4.0-2.26-LAPACK-3.6.1                    TensorFlow/1.13.1-fosscuda-2019a-Python-3.7.2
   Arrow/0.17.1-foss-2020a-Python-3.8.2                        TensorFlow/2.0.0-foss-2019a-Python-3.7.2
   Autoconf/2.69-foss-2016b                                    TensorFlow/2.0.0-fosscuda-2019b-Python-3.7.4               (D)
```

More module commands - keyword

- To search for a module starting with some **keyword**

[jpovh@cn62 ~]$ **module keyword Ansy**

-

The following modules match your search criteria: "Ansys"

-

ANSYS: ANSYS/20.1, ANSYS/21.R1, ANSYS/21.1, ANSYS/2021R2

ANSYS simulation software enables organizations to confidently predict how their products will operate in the real world. We believe that every product is a promise of something greater.

More module commands - whatis

- To see details about some module

jpovh@cn62 ~]$ **module whatis** MATLAB

MATLAB/2019a : Description: MATLAB is a high-level language and interactive environment

that enables you to perform computationally intensive tasks faster than with

traditional programming languages such as C, C++, and Fortran.

MATLAB/2019a : Homepage: http://www.mathworks.com/products/matlab

More module commands - spider

- For slightly more details about given module

[jpovh@cn62 ~]$ **module spider MATLAB**

MATLAB: MATLAB/2019a

Description:

MATLAB is a high-level language and interactive environment that enables you to perform computationally intensive tasks faster than with traditional programming languages such as C, C++, and Fortran.

More module commands - show

- For even more details about given module

[jpovh@cn62 ~]$ **module show MATLAB**

Most important commands

[jpovh@cn62 ~]$ **module load MATLAB/2019a**

[jpovh@cn62 ~]$ **module list**

Currently Loaded Modules:

1) Java/1.8.0_202 2) MATLAB/2019a

[jpovh@cn62 ~]$ **module unload MATLAB/2019a**

If you want to remove all the currently laoded modules:

[jpovh@cn62 ~]$ **module purge**

Some other modules

- Intel compiler

[jpovh@cn62 ~]$ module load intel/2020a

- GCC compiler

[jpovh@cn62 ~]$ module load intel/2020a

If NO module

- If the software package you need isn’t available under the modules system then try to build it yourself first in your home directory.
- Contact the support team for assistance with doing this, or to request that the software is included in the modules system in the future.

Start up and usage: *Ansys Workbench*

- 2 methods of access and use: **interactive** and **batch mode**

1. Interactive mode access commands:

a) Alocate ANSYS/2021R2 license dir:

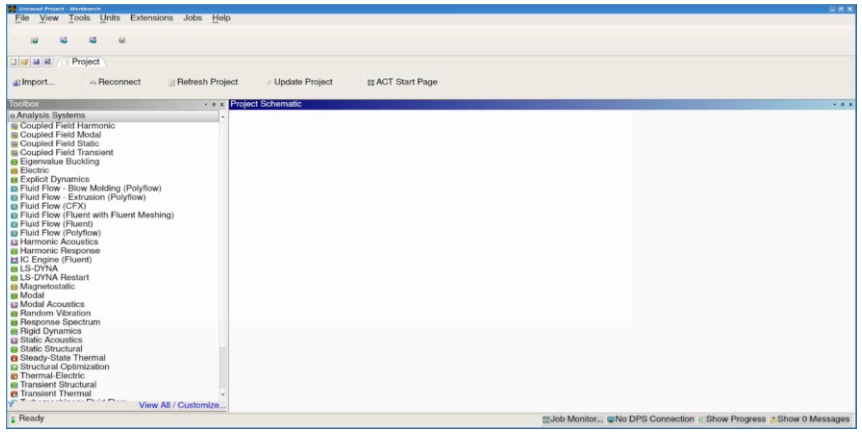
```
[user@viz~]$ LD_PRELOAD=/opt/pkg/software/ANSYS/2021R2/v212/commonfiles/MPI/Intel/2018.3.222/linx64/lib/libstrtok.so
```

b) Alocate new node:

```
[user@viz ~]$ srun -n 48 --time=60:00 --export=ALL --x11 -p rome --mem=120G --pty bash -I
```

c) Run ANSYS/2021R2 module and GUI:

```
[user@cnXX ~]$ module load ANSYS/2021R2
[user@cnXX ~]$ runwb2
```



Start up and usage: *Ansys Workbench*

2. Batch mode:

1. Create ANSYS Workbench project and model on local machine
2. Export case input file (e.g. Analysis.dat)
3. In HPC Linux terminal run batch script ANSYS_CRun.txt:

[user@viz **dir**] sbatch ANSYS_CRun.txt:

Directory where input file and batch script are stored

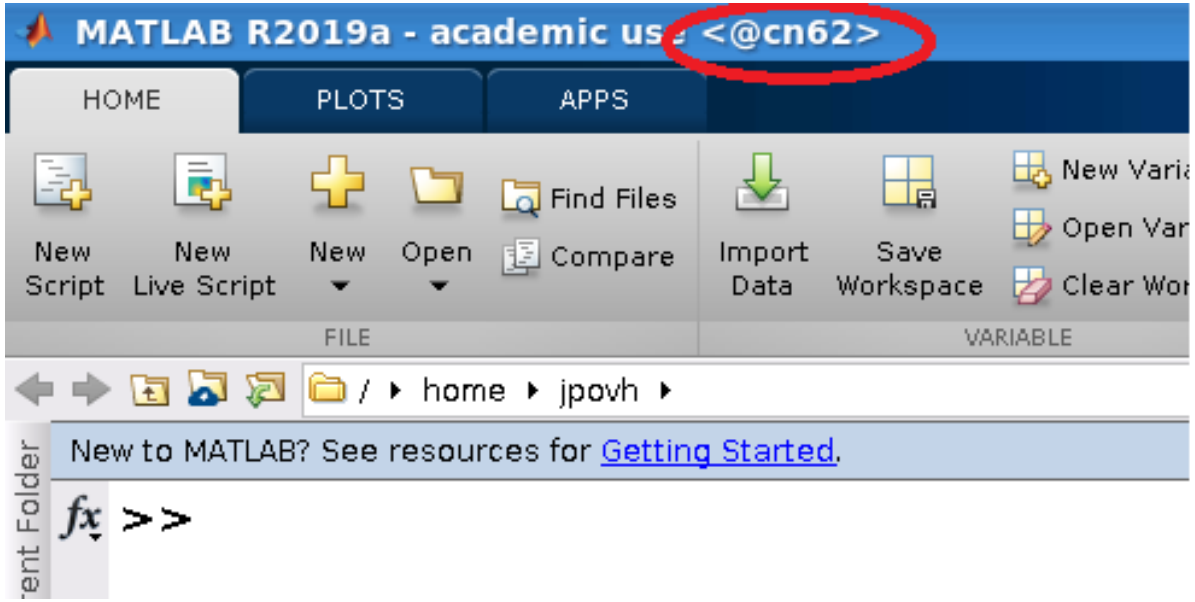
ANSYS_CRun.txt batch script:

```
#!/bin/bash
#SBATCH --export=ALL,LD_PRELOAD=/opt/pkg/software/ANSYS/2021R2/v212/commonfiles/MPI/Intel/2018.3.222/linx64/lib/libstrtok.so
#SBATCH --partition=rome
#SBATCH --mem=120G
#SBATCH --time=1-00:00:00
#SBATCH -n 48
module purge
module load ANSYS/2021R2
srun hostname -s &> $(pwd)/slurmhosts.$SLURM_JOB_ID.txt
ansys212 -dis -np 48 -b -machines=$(pwd)/slurmhosts.$SLURM_JOB_ID.txt -i Analysis.dat -o Output.dat
```

Start up: *Matlab*

[jpovh@cn62 ~]$ module load MATLAB/2019a

[jpovh@cn62 ~]$ matlab



First parallelization with *Matlab*

Define the function that generates a random *n* x *n* matrix and computes it arithmetic mean

```
function m=inner_fun(n)
    m=sum(sum(rand(n)))/n^2;
```

First parallelization with *Matlab*

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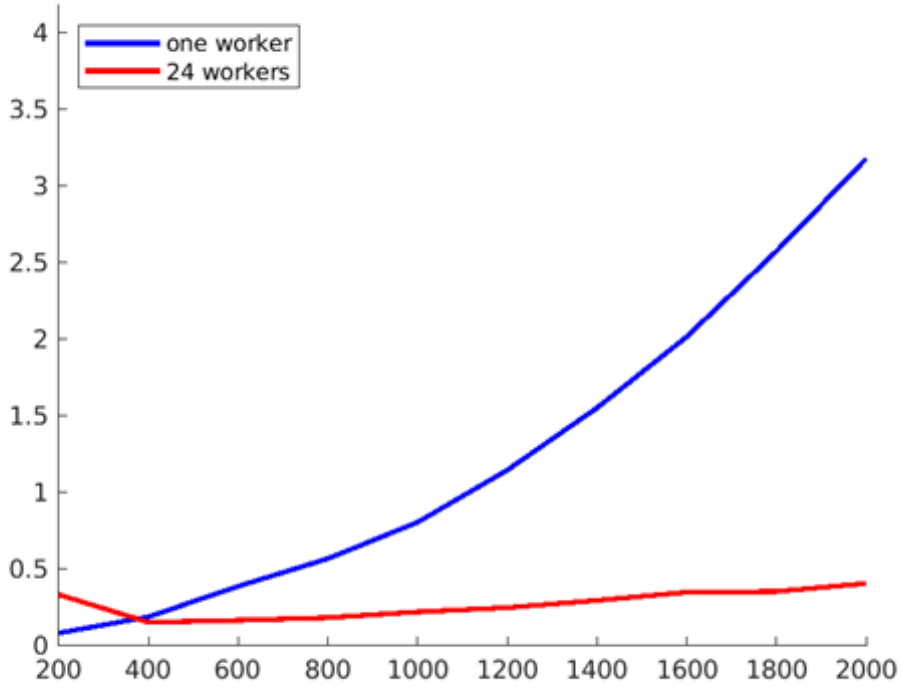
Call inner function using one worker and 24 workers

```
1 -    output_file='/home/jpovh/jpcode/jobs/seminar_matlab/results/plot_2.png'
2
3 -    N=10
4 -    T=zeros(N,2);
5 -    my_pool = parpool('local',24);
6 -    for i=1:N
7 -        n=200*i;
8 -        tic;
9 -        parfor ind=1:100
0 -            a(ind)=inner_fun1(n);
1 -        end
2 -        T(i,2)=toc;
3 -    end
4 -    delete(my_pool)
5 -    for i=1:N
6 -        n=200*i;
7 -        tic;
8 -        for ind=1:100
9 -            b(ind)=inner_fun1(n);
0 -        end
1 -        T(i,1)=toc;
2 -    end
```

First parallelization with *Matlab*

Scaling diagram



Starting *Mathematica*

- [jpovh@viz ~]$ **module keyword Mathema**

The following modules match your search criteria: "Mathema"

Gurobi: Gurobi/9.0.0, Gurobi/9.0.1

- The Gurobi Optimizer is a state-of-the-art solver for mathematical programming. The solvers in the Gurobi Optimizer were designed from the ground up to exploit modern architectures and multi-core processors, using the most advanced implementations of the latest algorithms.
- Mathematica: Mathematica/12.0.0, Mathematica/12.1.1, Mathematica/13.0.0

Mathematica is a computational software program used in many scientific, engineering, mathematical and computing fields.

Starting *Mathematica*

```
[jpovh@viz ~]$ module load Mathematica/12.1.1
[jpovh@viz ~]$ mathematica
```

Starting *Mathematica*

EigV[n_] := Eigenvalues[RandomReal[{-1, 1}, {n, n}]]

Timing_serial = Table[{n, EigV[n]}, {n, 1000, 2000, 50}]; // AbsoluteTiming

Timing_parallel = ParallelTable[{n, EigV[n]}, {n, 1000, 2000, 50}]; // AbsoluteTiming

Current projects on HPCFS - LeCAD

- Area of usage: integrated modelling and engineering design (ELMER, Ansys), heat flux simulations (ELMER), big data analysis, mathematical optimization
- Usage of HPCFS: up to 20 nodes
- Advantages of usage – faster computations, invitations to new projects

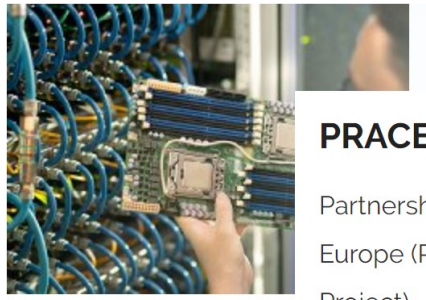
Current research work in LeCAD

ITER IMAS

Integrated Modelling Analysis Suite

EUMaster4HPC

HPC European Consortium Leading Education Activities



PRACE-6IP

Partnership for Advanced Computing in Europe (PRACE 6th Implementation Phase Project)

SCtrain

Supercomputing knowledge partnership

Current research work in LeCAD

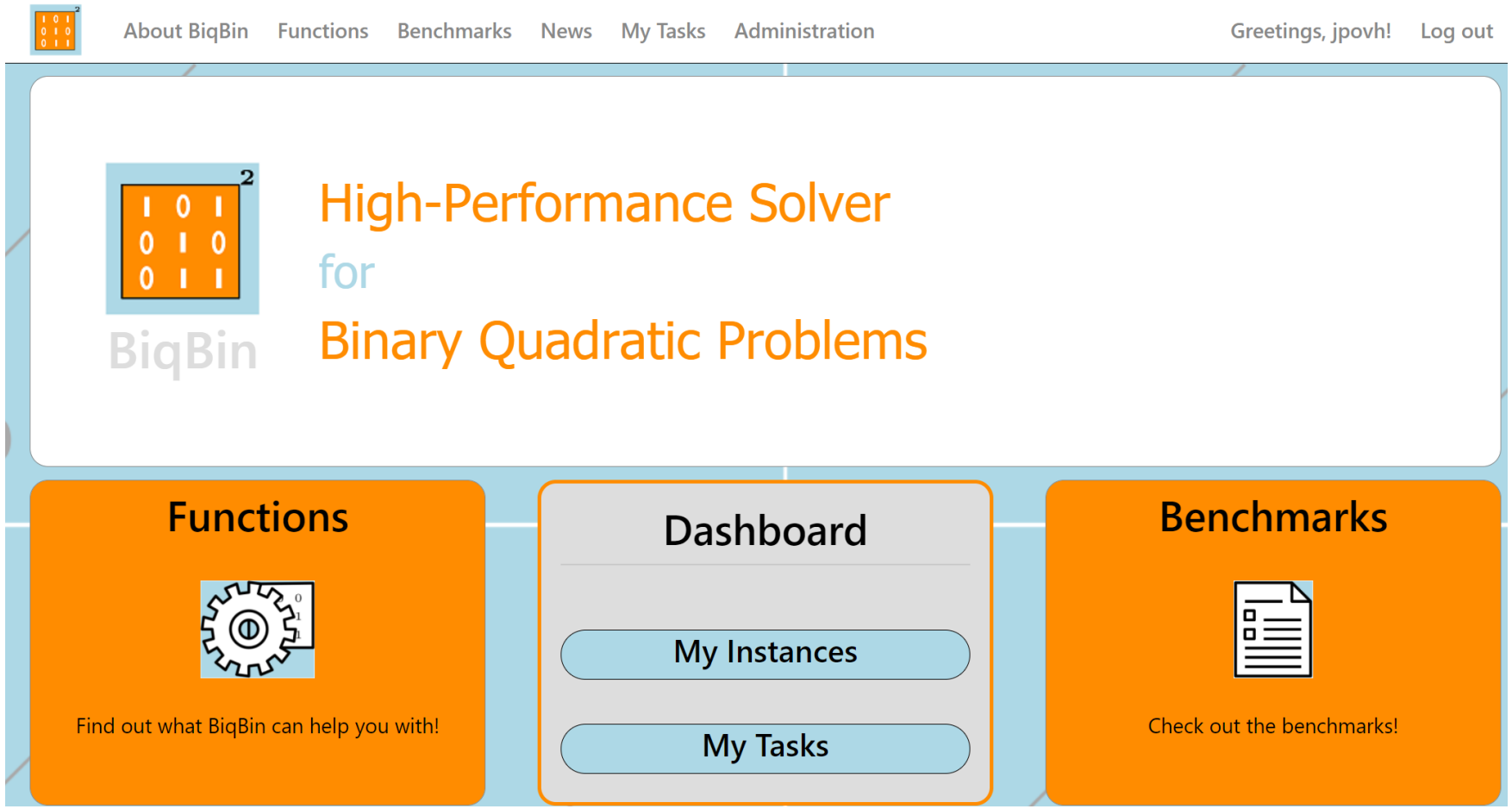
EUROCC

National Competence Centres in the framework of EuroHPC

J5-2552

Predicting collaboration between researchers by discovering patterns from the literature

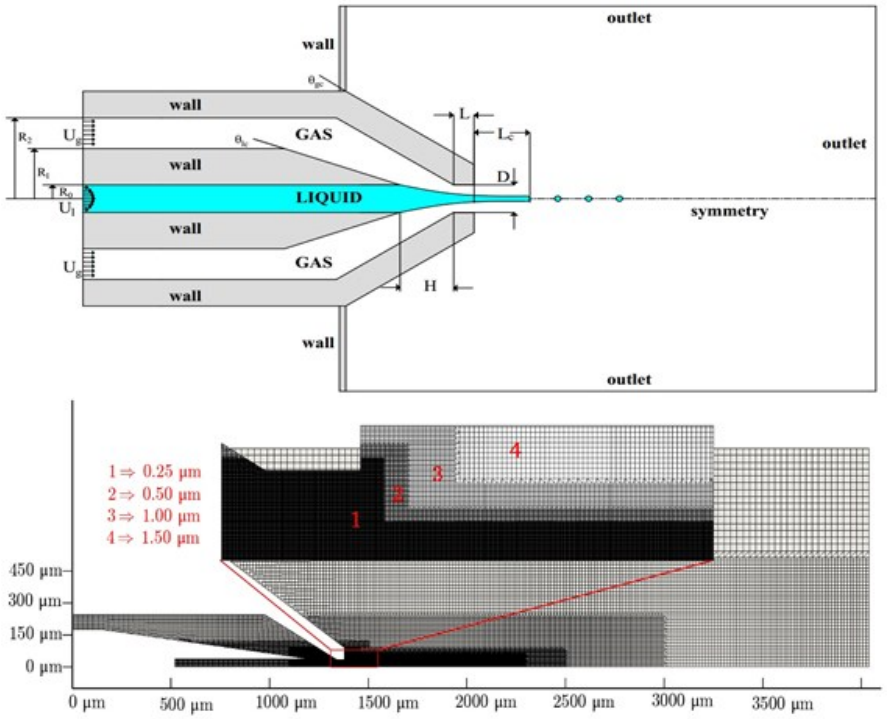
Current research work in LeCAD



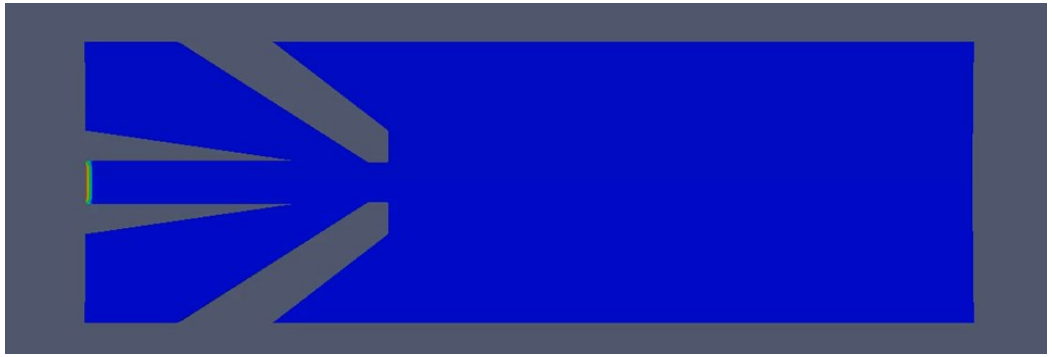
Current projects on HPCFS - LFDT

- Jet delivery system – flow focusing nozzles

Concept of FF nozzle and mesh



Single flow focusing



Double flow focusing

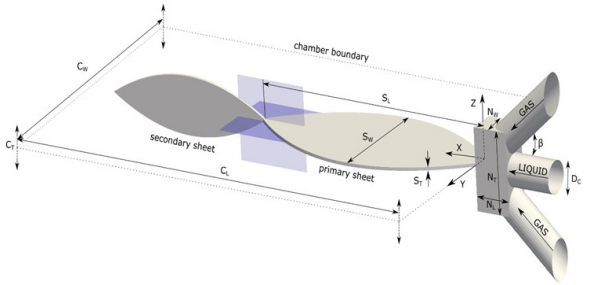
Apporx. 300000 cells on 6 nodes for 2 weeks

Presenter: dr. Jurij Gregorc

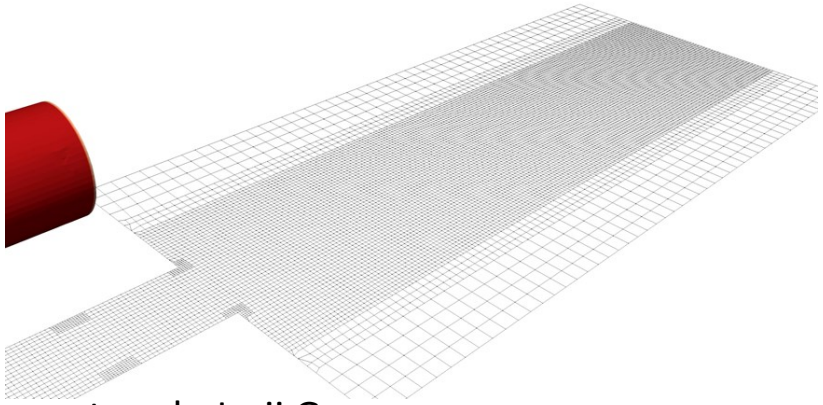
Current projects on HPCFS - LFDT

- Other delivery system

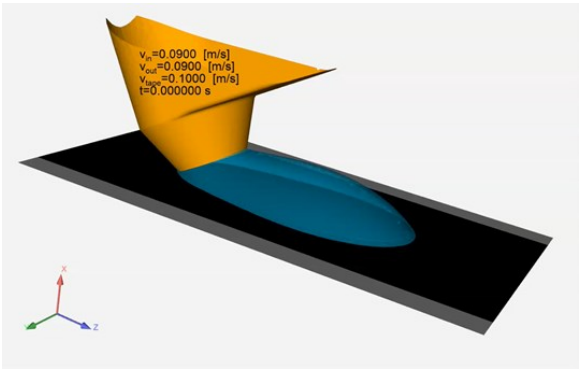
Liquid sheets



Liquid sheet & adaptive meshing



TapeDrive



Apporx. 300000 cells on 6 nodes for 2 weeks

Current projects on HPCFS - LVTS

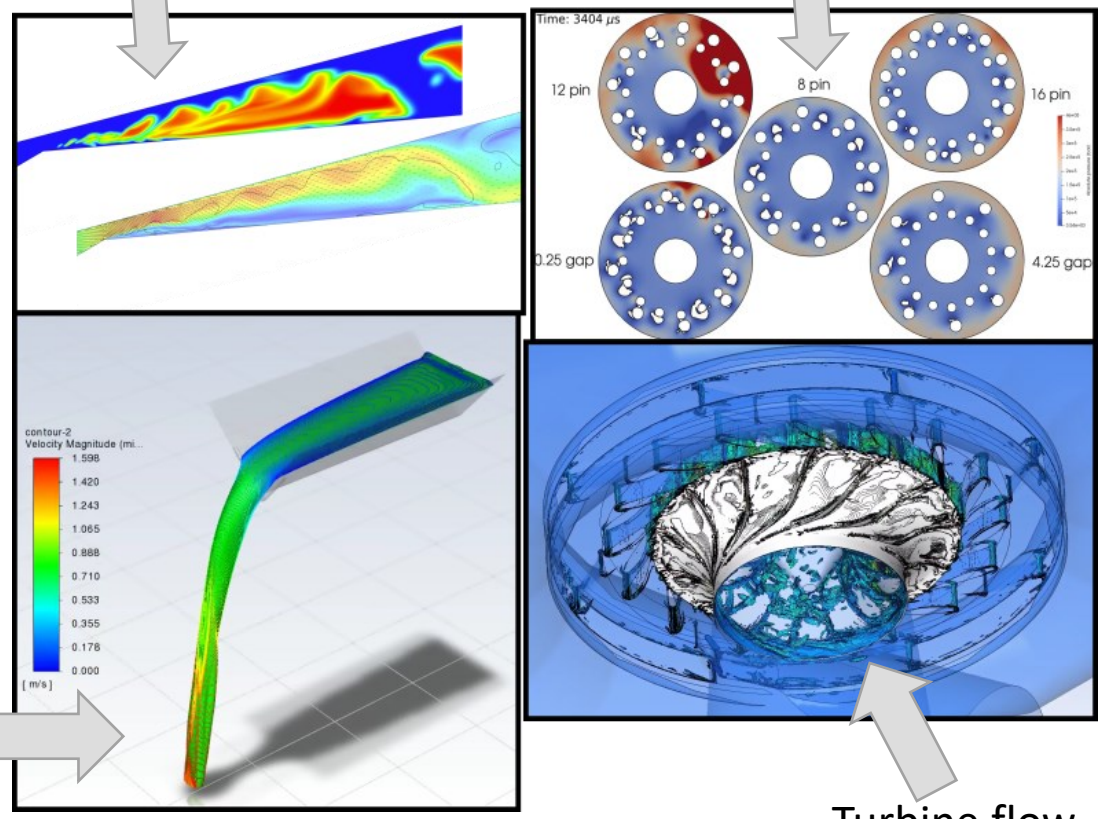
Laboratory for water and turbine machines (ULFME)

Area of usage:

- Computational Fluid Dynamics (CFD) in research and industrial projects
- Various flow simulations (free surface flows, multiphase flows, turbine flows, FSI, etc.)
- Numercial simulation are supplementing the experimental research work

Venturi channel flow

Cavitation generator

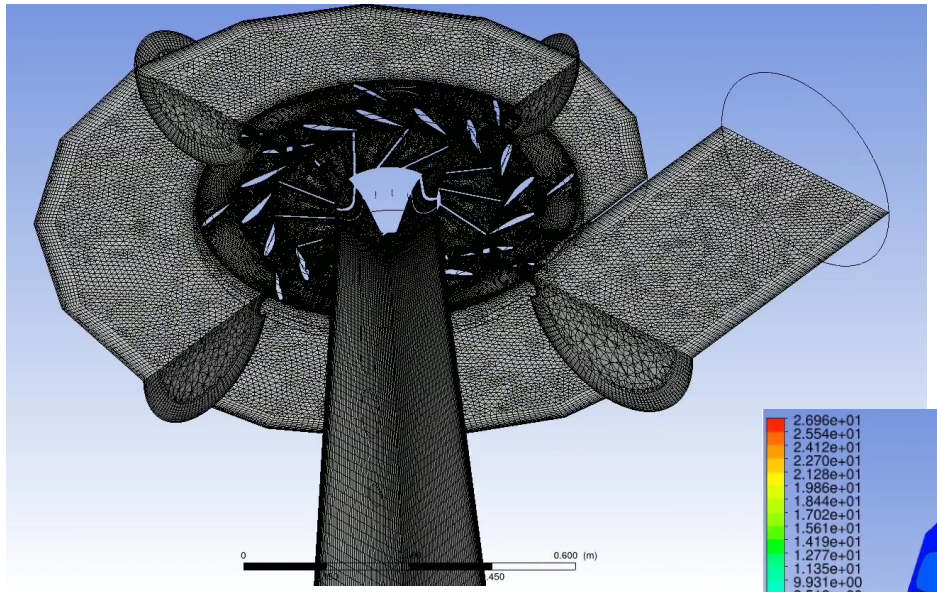


Free surface flow

Turbine flow

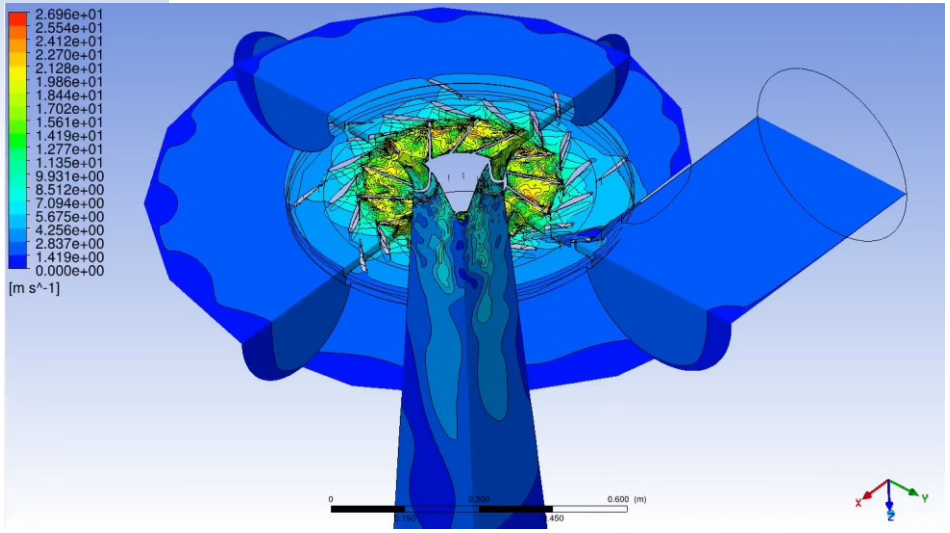
Current projects on HPCFS - LVTS

- **Usage of HPCFS (capacity for analyses)**



Case I: Francis turbine

- Solver: Ansys CFX
- Multi domain mesh (rotational-stationary domain interaction)
- ~40.000.000 numerical cells (hexa, some tetraheadrons)
- 2-3h on 96 HPC cores for 1000 iterations (stationary SST-kω)
- 5 days on local 16 cores PC for 1000 iterations (stationary SST-kω)
- 8 days to get solution on 240 HPC cores (unsteady SAS-SST) for ~15 000 timesteps (6-8 iterations/Ts)



Current projects on HPCFS - LVTS

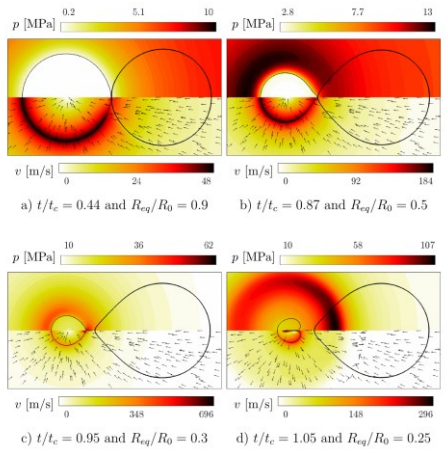
Advantages of HPC usage :

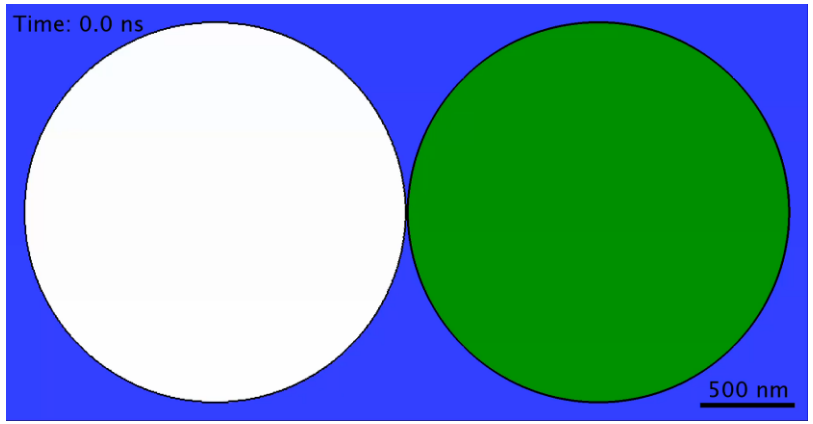
- Imensly shortenes time to get solution (unsteady, advanced turbulence models, multiphase models, etc.) in comparison to the local PC
- In some instances, it is almost impossible to solve large cases with complex geometry (wall bounded flow) without the HPC

Challenges of HPC usage:

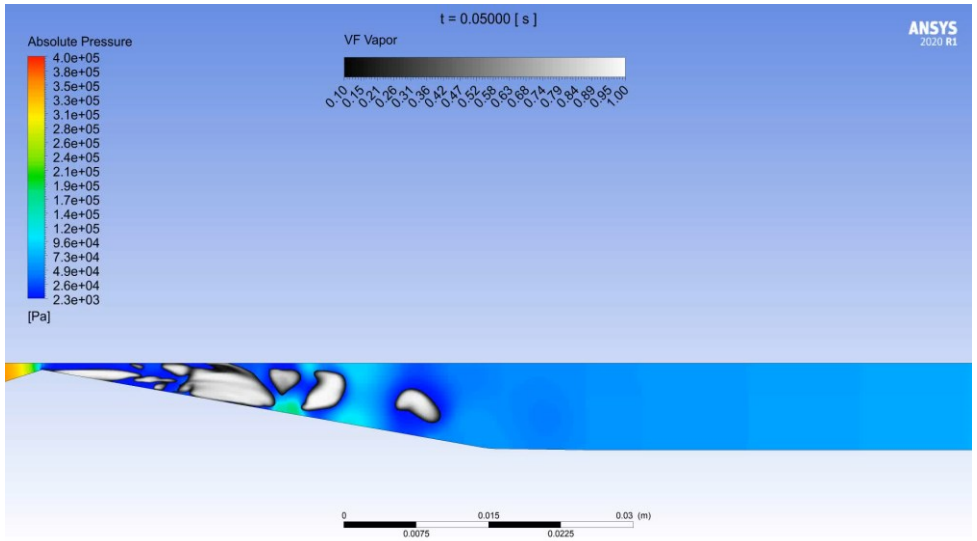
- The communication between user and HPC support (the collaboration between IT and other fields)
- Large result data, upload/download time

FSI case: an imploding bubble





Multiphase case: a venturi channel



EuroCC project

- National Competence Centres for HPC in 33 countries
- GOAL: fill the gaps in HPC knowledge in different areas:
  - Use in industry,
  - School education,
  - Higher education institutions and
  - Enthusiastic individuals.

EuroHPC Joint Undertaking

EuroCC trainings

- 18 May / Introduction to Linux for HPC
  https://indico.ijs.si/event/1491/
- 25 - 26 May / Neural Networks with TensorFlow
  https://indico.ijs.si/event/1489/
- 30 - 31 May / Upravljanje z velepodatki
  https://indico.ijs.si/event/1490/
- 07 Jun / Jupyter in Galaxy za analizo podatkov v odprti znanosti
  https://indico.ijs.si/event/1494/
- 13 - 15 Jun / CFD on HPC: OpenFOAM
  https://indico.ijs.si/event/1492/
- 20 - 21 Jun / GPU programming in CUDA
  https://indico.ijs.si/event/1488/

Presenter: Dr. Pavel Tomšič

Thank you for your attention :)

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