A Practical guide to HPC

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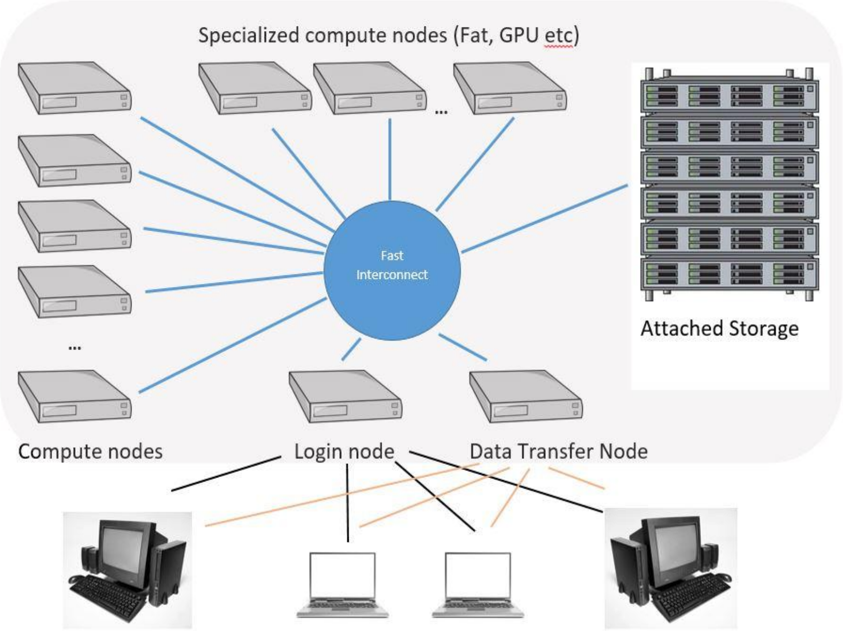
What is a cluster? (1)

- A **computer cluster** is a group of tightly coupled computers (**nodes**) that work together closely
- They can be seen as a **single computer**
- Clusters are commonly connected through **fast local area network**
- Clusters have evolved to support various applications:
    - **Ecommerce**
    - **High performance database** applications
- Clusters are usually deployed to improve **speed** and **reliability** over that provided by a single computer

What is a cluster? (2)

- In cluster computing each node (within a cluster) is an **independent system**
  - Has its own **operating system**
  - **Private** memory
  - Its own **file system** (in some cases)
- Programs or software run on clusters usually employ a procedure called "***message passing***" (memory is not shared)
- Cluster computing can also be used as a **low-cost** form of **parallel processing** for scientific applications

What is a cluster? (3)



History

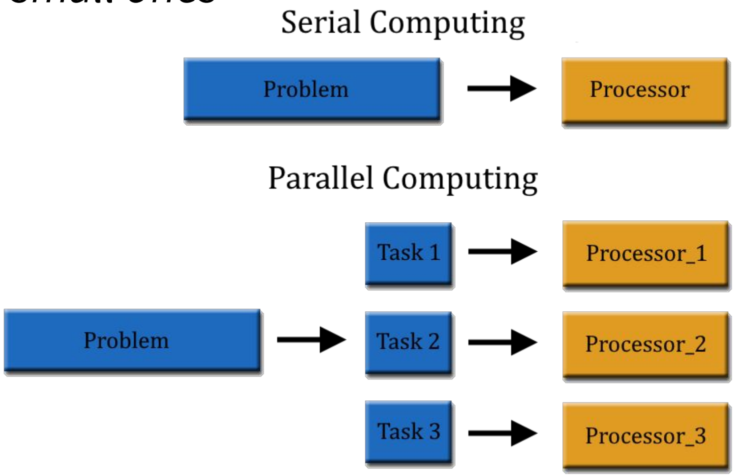
- The first clustering product was **ARCnet**, distributed and developed by Datapoint in **1977**
- Then in **1980 VAXcluster** produced a new product
- **Sun Microsystem**, **Microsoft** and other leading hardware and software companies offer clustering packages

Serial computing

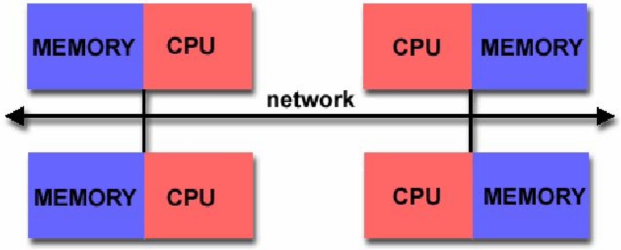
- **Serial computing**
  - Based on Von Neumann architecture, it have to process data and instructions respecting a sequential order
  - Limits:
    - Need **high speed** cpu
    - **Light** speed
    - **Heat**
    - **VLSI** (very large scale integration) is not infinite

Parallel computing

- **Parallel computing**
  - “*Big problems can be often divided into small ones*”
  - Problems can be solved simultaneously
  - Advantages:
    - Improve computing speed
    - Break memory limits
    - Exploit non-local resources



Distributed Memory



- Distributed memory requires a communication network for the information exchange:
  - Each **processor** has its own **local memory**.
  - Each **memory** has a **separate**, **independent** address space.
  - **Read**/**write** operations are local
  - To allow a task to **access remote data**, the programmer must explicitly **manage** the **communication** among tasks.
  - The corresponding programming model is called **message passing**

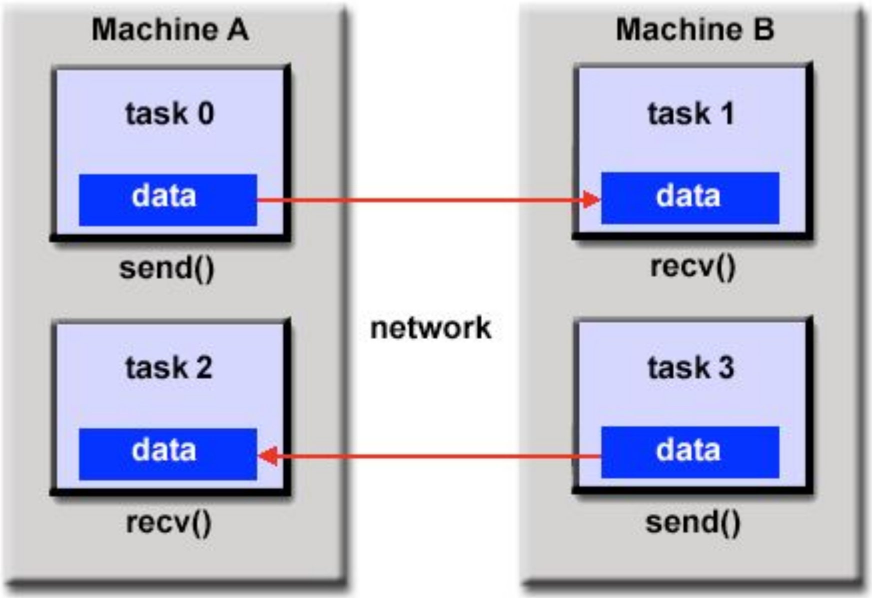
MPI

- **Message passing Interface**:
    - Communication protocol for **message exchanges**
    - There are **multiple** implementations of MPI
    - It is **not** a **language**
    - The standard has been defined through an **open process** by **community** of parallel computing vendor, computer scientists, nd application developers
    - It does not have a debugging facility and this make MPI **lightweight**
    - Several MPI implementations: **MPICH**, **Open MPI** (best overall), **Intel MPI Library**

MPI

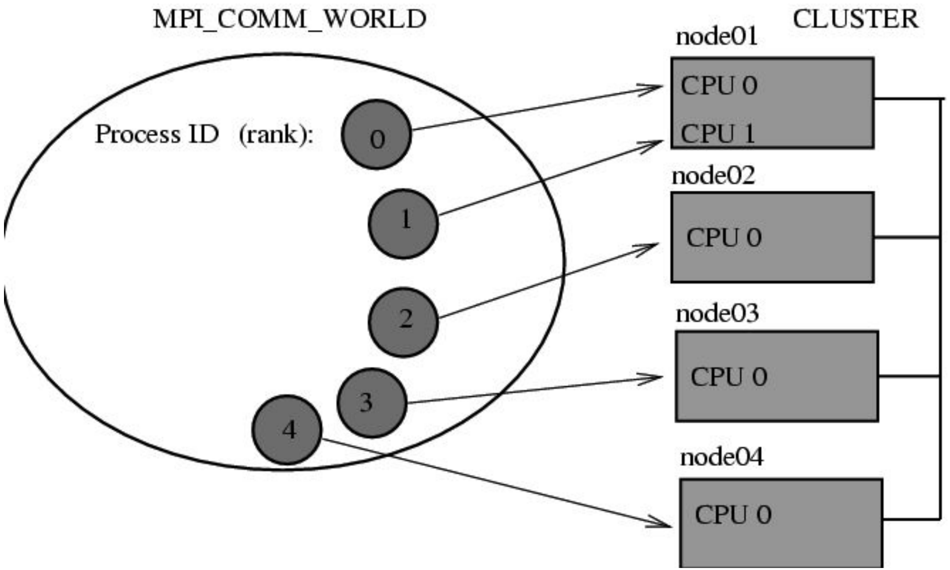
- Cooperation among processes is based on **explicit communication**
- A **sender** process and a **receiver** process exchange messages
- Each process is an **instance** of running sub-program.

- Each process is identified by an integer number, called **rank**, ranging from **0** to **n-1**, where n (size) is the total number of processes.



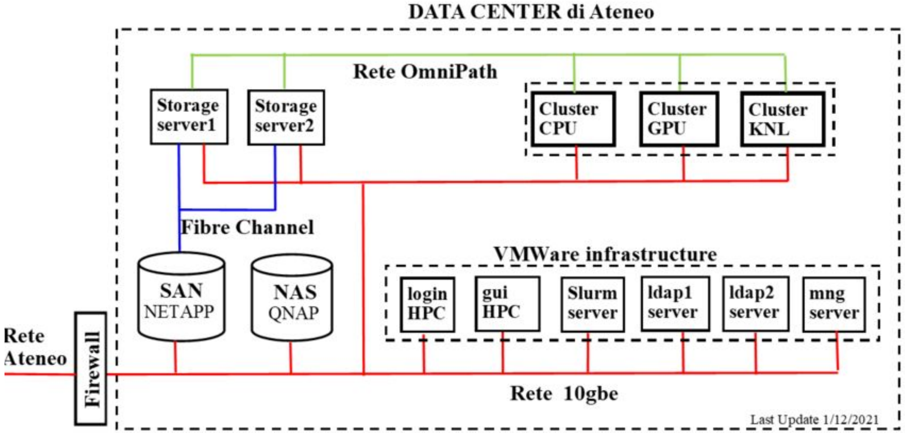
Finire con le ultime specifiche di MPI

- MPI allows you to create logical **groups** of processes
  - In each **group**, a process is identified by its **rank**.
- **Communicators** are **objects** that handle communication between processes.
  - **intra-communicator** handles processes within a single group
  - **inter-communicator** handles communication between two distinct groups.
- By default, there is a single group that contains all your processes, and the intra-communicator **MPI_COMM_WORLD**

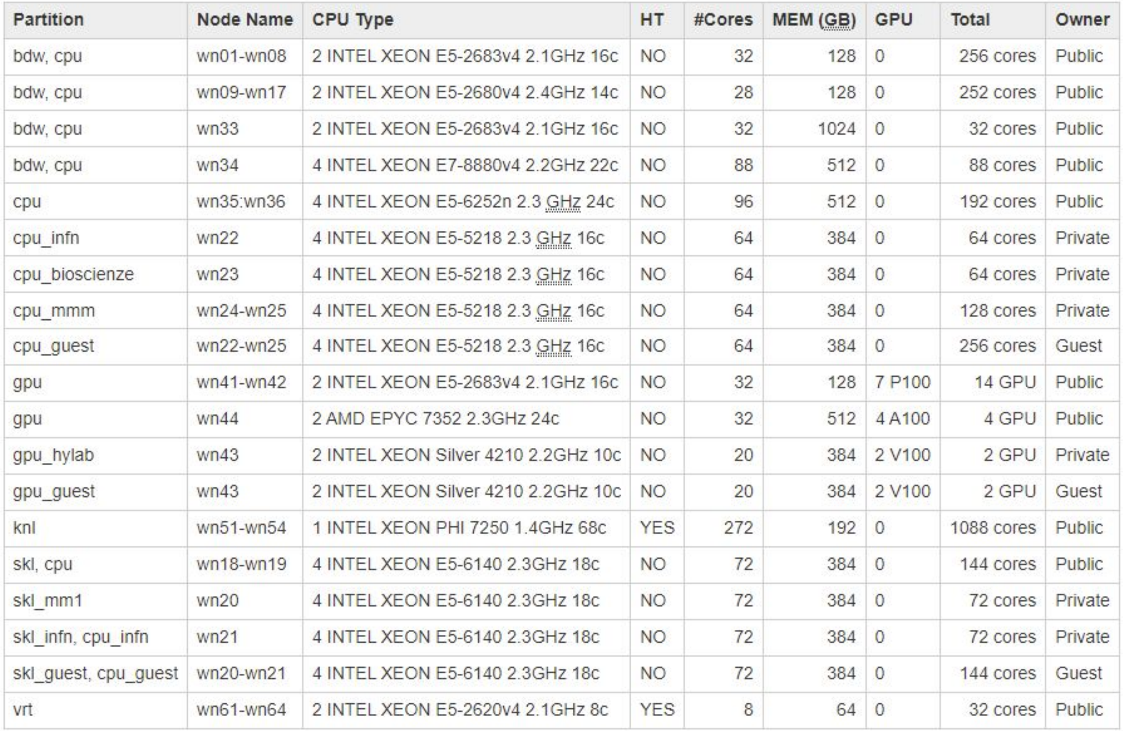


Unipr - HPC

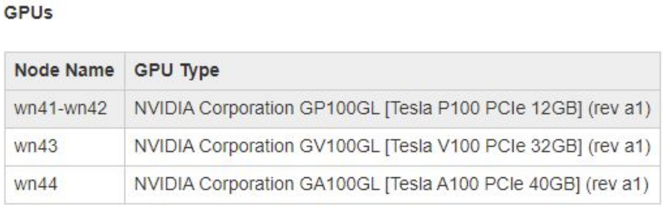
- **Website**:
  - https://www.hpc.unipr.it
- **Project Description:**
  - https://www.hpc.unipr.it/dokuwiki/doku.php?id=calcoloscientifico:progetto
- **User Guide:**
  - https://www.hpc.unipr.it/dokuwiki/doku.php?id=calcoloscientifico:userguide



Unipr - HPC - Nodes



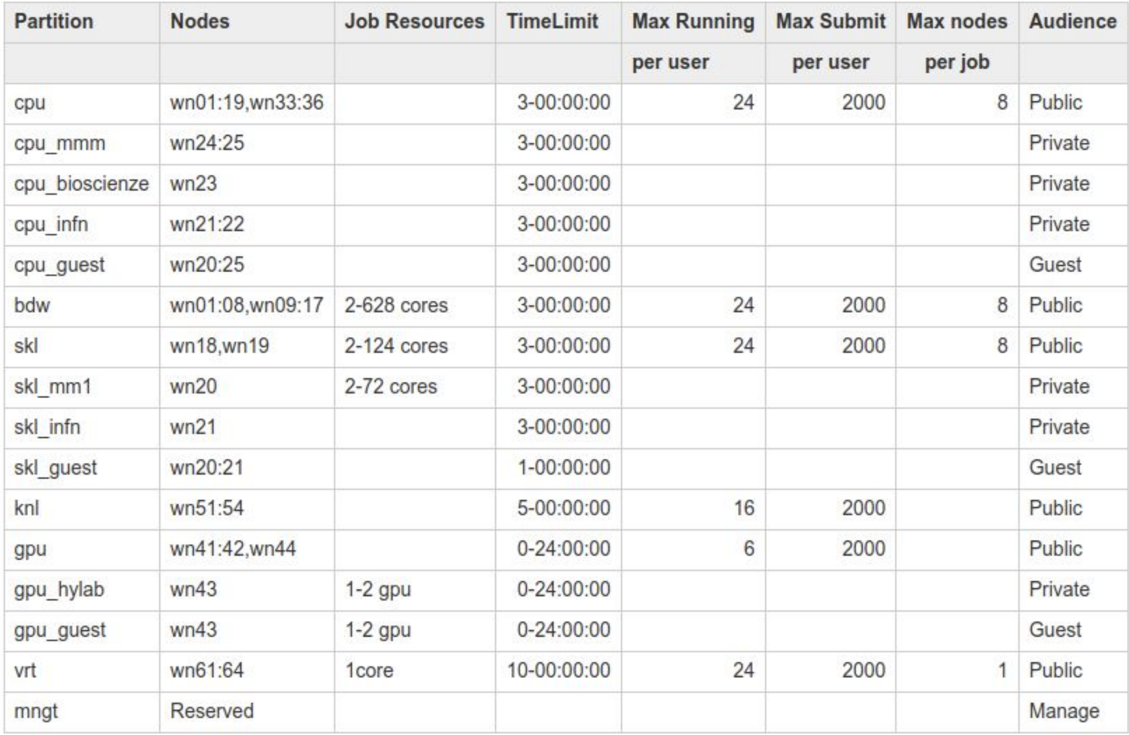
Partition	Node Name	CPU Type	HT	#Cores	MEM (GB)	GPU	Total	Owner
bdw, cpu	wn01-wn08	2 INTEL XEON E5-2683v4 2.1GHz 16c	NO	32	128	0	256 cores	Public
bdw, cpu	wn09-wn17	2 INTEL XEON E5-2680v4 2.4GHz 14c	NO	28	128	0	252 cores	Public
bdw, cpu	wn33	2 INTEL XEON E5-2683v4 2.1GHz 16c	NO	32	1024	0	32 cores	Public
bdw, cpu	wn34	4 INTEL XEON E7-8880v4 2.2GHz 22c	NO	88	512	0	88 cores	Public
cpu	wn35:wn36	4 INTEL XEON E5-6252n 2.3 GHz 24c	NO	96	512	0	192 cores	Public
cpu_infn	wn22	4 INTEL XEON E5-5218 2.3 GHz 16c	NO	64	384	0	64 cores	Private
cpu_bioscienze	wn23	4 INTEL XEON E5-5218 2.3 GHz 16c	NO	64	384	0	64 cores	Private
cpu_mmm	wn24-wn25	4 INTEL XEON E5-5218 2.3 GHz 16c	NO	64	384	0	128 cores	Private
cpu_guest	wn22-wn25	4 INTEL XEON E5-5218 2.3 GHz 16c	NO	64	384	0	256 cores	Guest
gpu	wn41-wn42	2 INTEL XEON E5-2683v4 2.1GHz 16c	NO	32	128	7 P100	14 GPU	Public
gpu	wn44	2 AMD EPYC 7352 2.3GHz 24c	NO	32	512	4 A100	4 GPU	Public
gpu_hylab	wn43	2 INTEL XEON Silver 4210 2.2GHz 10c	NO	20	384	2 V100	2 GPU	Private
gpu_guest	wn43	2 INTEL XEON Silver 4210 2.2GHz 10c	NO	20	384	2 V100	2 GPU	Guest
knl	wn51-wn54	1 INTEL XEON PHI 7250 1.4GHz 68c	YES	272	192	0	1088 cores	Public
skl, cpu	wn18-wn19	4 INTEL XEON E5-6140 2.3GHz 18c	NO	72	384	0	144 cores	Public
skl_mm1	wn20	4 INTEL XEON E5-6140 2.3GHz 18c	NO	72	384	0	72 cores	Private
skl_infn, cpu_infn	wn21	4 INTEL XEON E5-6140 2.3GHz 18c	NO	72	384	0	72 cores	Private
skl_guest, cpu_guest	wn20-wn21	4 INTEL XEON E5-6140 2.3GHz 18c	NO	72	384	0	144 cores	Guest
vrt	wn61-wn64	2 INTEL XEON E5-2620v4 2.1GHz 8c	YES	8	64	0	32 cores	Public



GPUs

Node Name	GPU Type
wn41-wn42	NVIDIA Corporation GP100GL [Tesla P100 PCIe 12GB] (rev a1)
wn43	NVIDIA Corporation GV100GL [Tesla V100 PCIe 32GB] (rev a1)
wn44	NVIDIA Corporation GA100GL [Tesla A100 PCIe 40GB] (rev a1)

Unipr - HPC - Limits



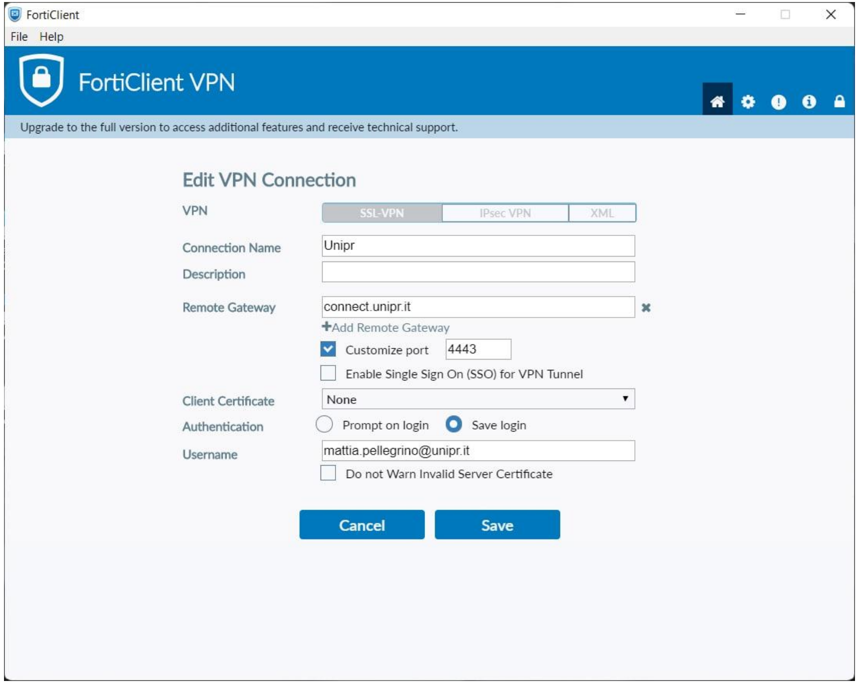
Partition	Nodes	Job Resources	TimeLimit	Max Running	Max Submit	Max nodes	Audience
				per user	per user	per job	
cpu	wn01:19,wn33:36		3-00:00:00	24	2000	8	Public
cpu_mmm	wn24:25		3-00:00:00				Private
cpu_bioscienze	wn23		3-00:00:00				Private
cpu_infn	wn21:22		3-00:00:00				Private
cpu_guest	wn20:25		3-00:00:00				Guest
bdw	wn01:08,wn09:17	2-628 cores	3-00:00:00	24	2000	8	Public
skl	wn18,wn19	2-124 cores	3-00:00:00	24	2000	8	Public
skl_mm1	wn20	2-72 cores	3-00:00:00				Private
skl_infn	wn21		3-00:00:00				Private
skl_guest	wn20:21		1-00:00:00				Guest
knl	wn51:54		5-00:00:00	16	2000		Public
gpu	wn41:42,wn44		0-24:00:00	6	2000		Public
gpu_hylab	wn43	1-2 gpu	0-24:00:00				Private
gpu_guest	wn43	1-2 gpu	0-24:00:00				Guest
vrt	wn61:64	1core	10-00:00:00	24	2000	1	Public
mngt	Reserved						Manage

SLURM

- Slurm is an open source, fault-tolerant, and highly scalable **cluster management** and **job scheduling system** for large and small Linux clusters
- SLURM manages user jobs with the following key characteristics:
    - set of requested resources:
        - X number of computing resources: **nodes** (including all their CPUs and cores) or **CPUs** (including all their cores) or cores
        - X number of accelerators (**GPUs**)
        - X **amount** of **memory**: either per node or per (logical) CPU
        - X the (wall)**time** needed for the user's tasks to complete their work
        - a set of **constraints** limiting jobs to nodes with specific features
        - a requested **node partition** (job queue)

PRACTICAL GUIDE

- First of all, you need to be connected to UNIPR wireless network, instead you must use a VPN in order to connect to the HPC facility



Upgrade to the full version to access additional features and receive technical support.

Edit VPN Connection

VPN: SSL-VPN | IPsec VPN | XML

Connection Name: Unipr

Description:

Remote Gateway: connect.unipr.it

+Add Remote Gateway

☑ Customize port 4443

□ Enable Single Sign On (SSO) for VPN Tunnel

Client Certificate: None

Authentication: ○ Prompt on login ● Save login

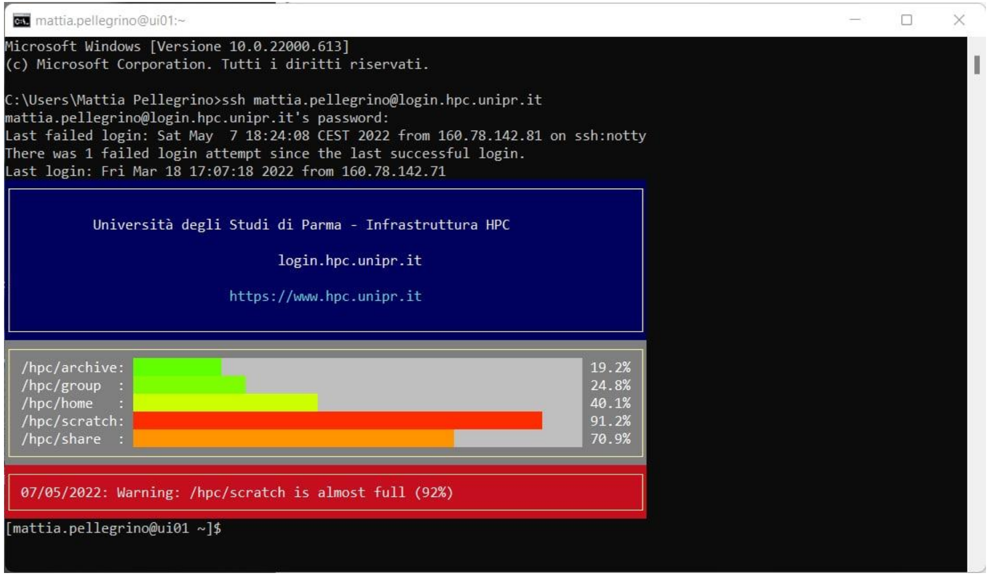
Username: mattia.pellegrino@unipr.it

□ Do not Warn Invalid Server Certificate

- **Steps**:
  - Download **FortiClient**: https://www.fortinet.com/it
  - Use this parameters to setting a new VPN connection:
    - Host: **connect.unipr.it**
    - Port: **4443**
  - Use you UNIPR credentials to login

PRACTICAL GUIDE

- In order to connect to the HPC Cluster, you must use an SSH protocol connection



```
Microsoft Windows [Versione 10.0.22000.613]
(c) Microsoft Corporation. Tutti i diritti riservati.

C:\Users\Mattia Pellegrino>ssh mattia.pellegrino@login.hpc.unipr.it
mattia.pellegrino@login.hpc.unipr.it's password:
Last failed login: Sat May  7 18:24:08 CEST 2022 from 160.78.142.81 on ssh:notty
There was 1 failed login attempt since the last successful login.
Last login: Fri Mar 18 17:07:18 2022 from 160.78.142.71

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                          login.hpc.unipr.it

                       https://www.hpc.unipr.it

 /hpc/archive:                                                 19.2%
 /hpc/group  :                                                 24.8%
 /hpc/home   :                                                 40.1%
 /hpc/scratch:                                                 91.2%
 /hpc/share  :                                                 70.9%

 07/05/2022: Warning: /hpc/scratch is almost full (92%)

[mattia.pellegrino@ui01 ~]$
```

- **Steps**:
  - Open the system terminal
  - **ssh <nomeutente>@login.hpc.unipr.it**
  - Password: your institutional password

FILE TRANSFER

- SSH is the only protocol for external communication and can also be used for file transfer.

- If you use a Unix-like client (Linux, MacOS X) you can use the command scp or sftp.

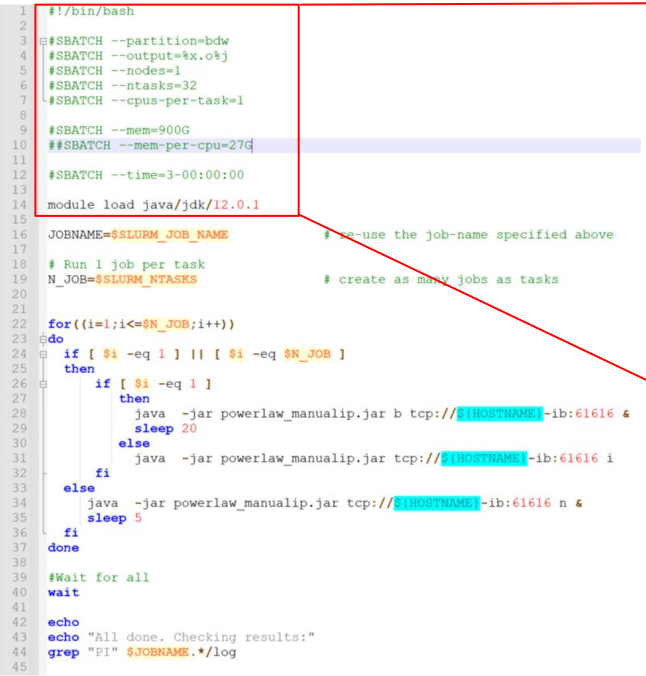
- On Windows systems, the most used tool is WinSCP (https://winscp.net/eng/docs/introduction).

scp example: **scp /path/to/local/file remote_user@remote_host:/path/to/remote/file**

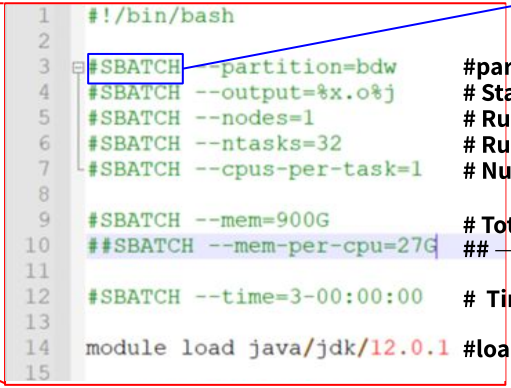
scp foo.file mattia.pellegrino@login.hpc.unipr.it:/hpc/group/G_SOWIDE/10-05-2022/python/NN/foo.file

PRACTICAL GUIDE

- To correctly launch a job on hpc you have to write an .sh script. This script is required to use SLURM functionalities



```bash
#!/bin/bash

#SBATCH --partition=bdw
#SBATCH --output=%x.o%j
#SBATCH --nodes=1
#SBATCH --ntasks=32
#SBATCH --cpus-per-task=1

#SBATCH --mem=900G
##SBATCH --mem-per-cpu=27G

#SBATCH --time=3-00:00:00

module load java/jdk/12.0.1

JOBNAME=$SLURM_JOB_NAME                    # re-use the job-name specified above

# Run 1 job per task
N_JOB=$SLURM_NTASKS                        # create as many jobs as tasks


for((i=1;i<=$N_JOB;i++))
do
  if [ $i -eq 1 ] || [ $i -eq $N_JOB ]
  then
      if [ $i -eq 1 ]
      then
        java  -jar powerlaw_manualip.jar b tcp://${HOSTNAME}-ib:61616 &
        sleep 20
      else
        java  -jar powerlaw_manualip.jar tcp://${HOSTNAME}-ib:61616 i
      fi
  else
     java  -jar powerlaw_manualip.jar tcp://${HOSTNAME}-ib:61616 n &
     sleep 5
  fi
done

#Wait for all
wait

echo
echo "All done. Checking results:"
grep "PI" $JOBNAME.*/log

```



```bash
#!/bin/bash

#SBATCH --partition=bdw
#SBATCH --output=%x.o%j
#SBATCH --nodes=1
#SBATCH --ntasks=32
#SBATCH --cpus-per-task=1

#SBATCH --mem=900G
##SBATCH --mem-per-cpu=27G

#SBATCH --time=3-00:00:00

module load java/jdk/12.0.1

```

This is not a comment!

#partition name

# Standard output and error log

# Run all processes on a single node

# Run a single task

# Number of CPU cores per task

# Total memory limit

## → comment

# Time limit hrs:min:sec

#load the desire module

module avail to see all module supported by the HPC

How to launch a script: sbatch <nomescript>.sh

Queue: squeue | grep <partition_name>

squeue | grep <username>

squeue | grep <job_id>

Delete a job: scancel <job_id>

Job's details: scontrol show jobid <job_id>

ACTODES

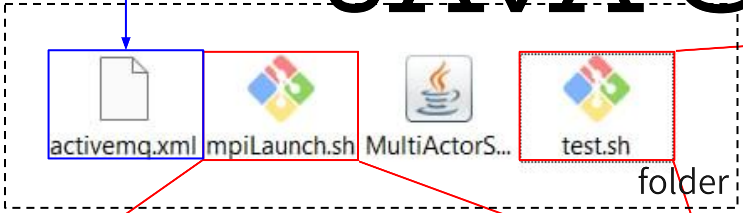
- Java **framework**

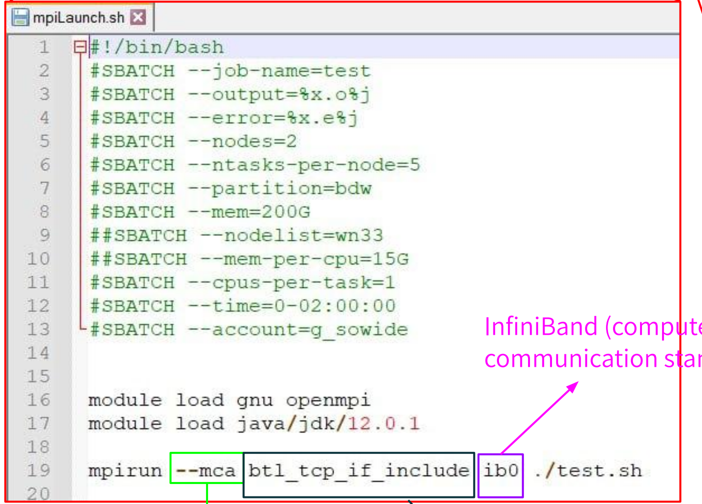
- Support the **actor** paradigm:
  - Simple and independent **agents**
  - Based on **message queue** and **exchange**

- It can be used in **distributed architecture**

JAVA ON HPC (actodes)

To ignore time limit!



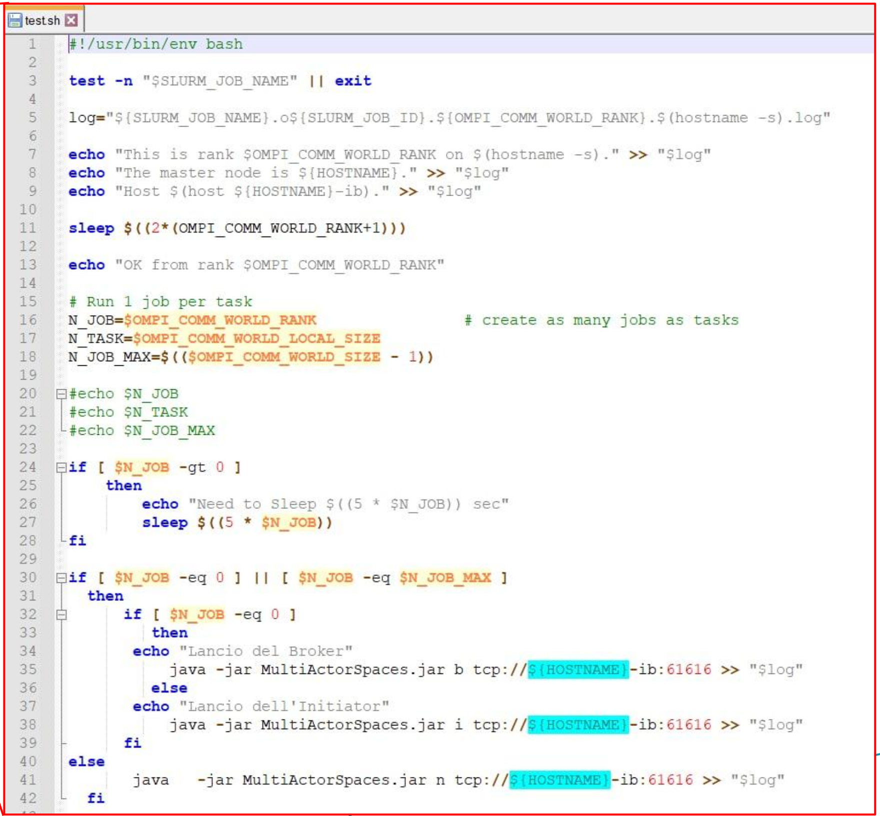


```
#!/bin/bash
#SBATCH --job-name=test
#SBATCH --output=%x.o%j
#SBATCH --error=%x.e%j
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=5
#SBATCH --partition=bdw
#SBATCH --mem=200G
##SBATCH --nodelist=wn33
##SBATCH --mem-per-cpu=15G
#SBATCH --cpus-per-task=1
#SBATCH --time=0-02:00:00
#SBATCH --account=g_sowide


module load gnu openmpi
module load java/jdk/12.0.1

mpirun --mca btl_tcp_if_include ib0 ./test.sh

```

InfiniBand (computer networking communication standard)

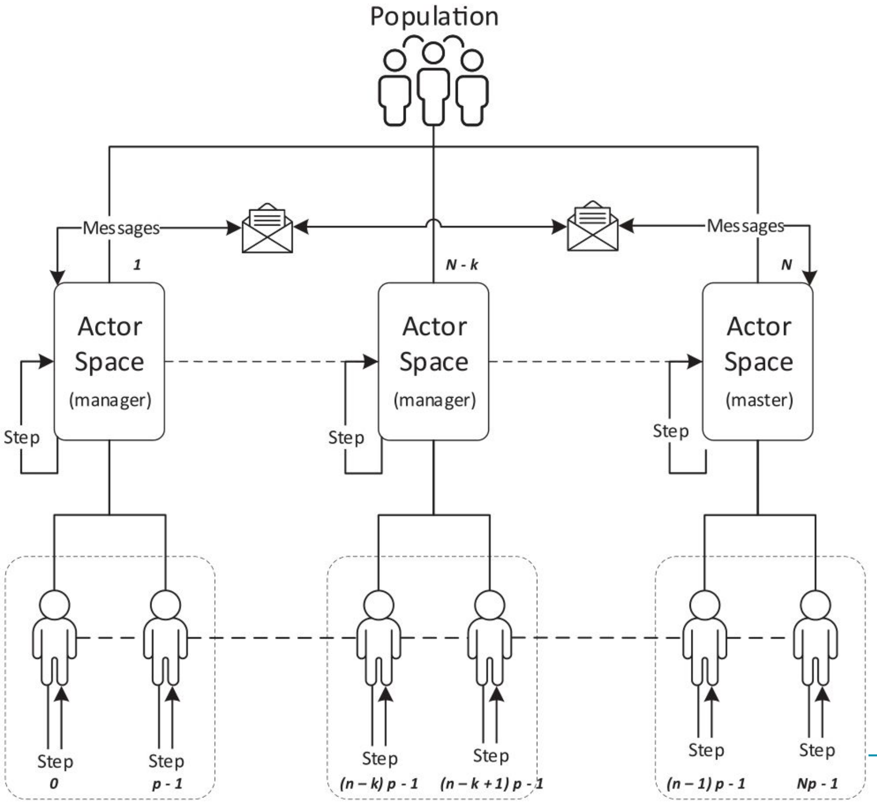
Modular component architecture

Use TCP protocol



```
#!/usr/bin/env bash

test -n "$SLURM_JOB_NAME" || exit

log="${SLURM_JOB_NAME}.o${SLURM_JOB_ID}.${OMPI_COMM_WORLD_RANK}.$(hostname -s).log"

echo "This is rank $OMPI_COMM_WORLD_RANK on $(hostname -s)." >> "$log"
echo "The master node is ${HOSTNAME}." >> "$log"
echo "Host $(host ${HOSTNAME}-ib)." >> "$log"

sleep $((2*(OMPI_COMM_WORLD_RANK+1)))

echo "OK from rank $OMPI_COMM_WORLD_RANK"

# Run 1 job per task
N_JOB=$OMPI_COMM_WORLD_RANK                # create as many jobs as tasks
N_TASK=$OMPI_COMM_WORLD_LOCAL_SIZE
N_JOB_MAX=$(($OMPI_COMM_WORLD_SIZE - 1))

#echo $N_JOB
#echo $N_TASK
#echo $N_JOB_MAX

if [ $N_JOB -gt 0 ]
    then
        echo "Need to Sleep $((5 * $N_JOB)) sec"
        sleep $((5 * $N_JOB))
fi

if [ $N_JOB -eq 0 ] || [ $N_JOB -eq $N_JOB_MAX ]
  then
      if [ $N_JOB -eq 0 ]
         then
     echo "Lancio del Broker"
         java -jar MultiActorSpaces.jar b tcp://${HOSTNAME}-ib:61616 >> "$log"
         else
     echo "Lancio dell'Initiator"
         java -jar MultiActorSpaces.jar i tcp://${HOSTNAME}-ib:61616 >> "$log"
      fi
else
       java   -jar MultiActorSpaces.jar n tcp://${HOSTNAME}-ib:61616 >> "$log"
  fi
```

ACTODES ON HPC

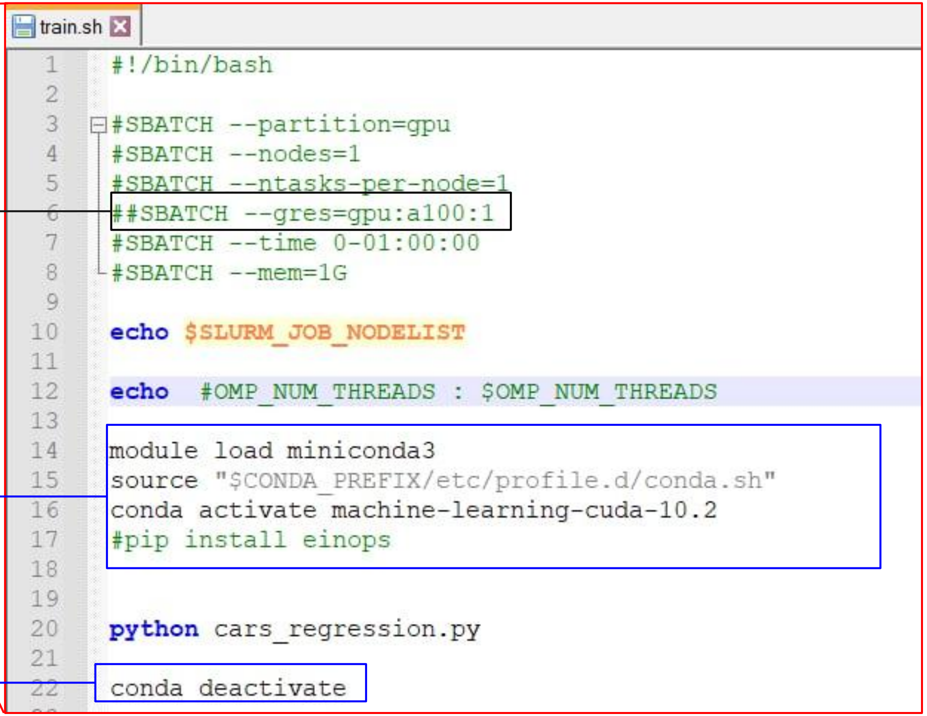


PYTHON for ML

You can select a specific GPU

Load ML resources

Release ML resources



```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
##SBATCH --gres=gpu:a100:1
#SBATCH --time 0-01:00:00
#SBATCH --mem=1G

echo $SLURM_JOB_NODELIST

echo  #OMP_NUM_THREADS : $OMP_NUM_THREADS

module load miniconda3
source "$CONDA_PREFIX/etc/profile.d/conda.sh"
conda activate machine-learning-cuda-10.2
#pip install einops


python cars_regression.py

conda deactivate
```

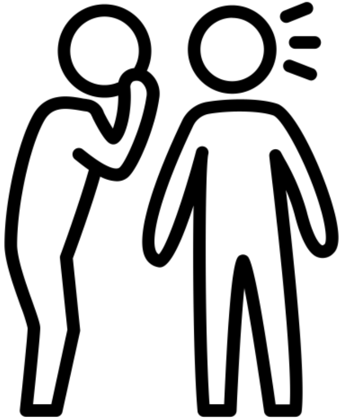
GOSSIP ALGORITHM

Exercise

- Systems-oriented **computational and communication paradigm** distributed on a **large scale** with high dynamic characteristics

- Probabilistic approach

- Main features:
  - **Simplicity**
  - **Scalability**
  - **Efficiency**
  - **Robustness**



EXERCISE

A Gossip Algorith

- Modify the source code available at the following address: https://github.com/Maegorn/HPC_practice
- Each agent involved in the simulation can be: **infected or healthy**
- Agents meet each other **randomly**
- Every time an **interaction** occurs, there is a chance that an **infected** agent **will infect** a **healthy** one

EXERCISE

- Classes and function to complete:
  - **Phases.class**
  - **PersonManager.class**:
    - BuildPopulation(), infectionInPartition(), setinfectedpeople(),saveMeasure()
  - **Manager.class**
    - messageDataHandler()

- When the simulator is done (test it locally) launch the simulator on the HPC with 1M of agents, utilizing 8 16,24,32 cores. Finally, measure the temporal perfomance

EXERCISE

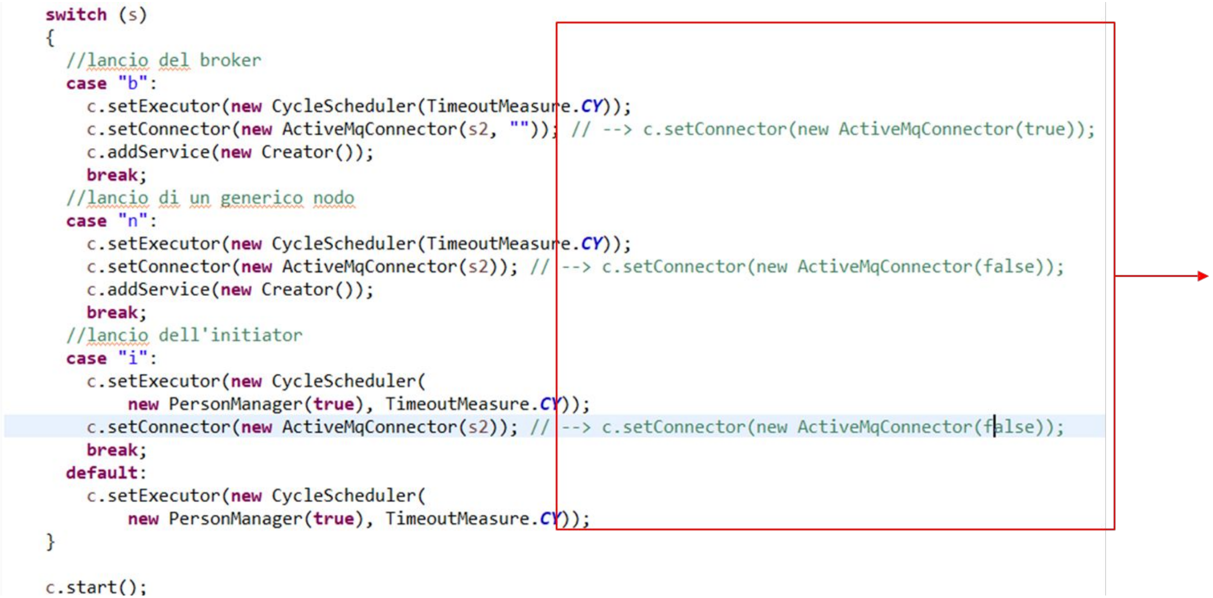
Login

- **Login and take reservation**:
  - ssh <nomeutente>@login.hpc.unipr.it
  - ssh-keygen -t rsa -P '' -f ~/.ssh/id_rsa
  - cat ~/.ssh/id_rsa.pub >> ~/.ssh/authorized_keys
  - chmod 0600 ~/.ssh/authorized_keys
  - newgrp T_2022_SISTEMI_DISTRIBUITI

  - **Aggiungere allo script mpiLunch.sh**:
    - #SBATCH --reservation=t_2022_sistemi_distribuiti-20230418
    - #SBATCH --account=t_2022_sistemi_distribuiti

Local Execution

Initiator Class



```
switch (s)
{
  //lancio del broker
  case "b":
    c.setExecutor(new CycleScheduler(TimeoutMeasure.CY));
    c.setConnector(new ActiveMqConnector(s2, "")); // --> c.setConnector(new ActiveMqConnector(true));
    c.addService(new Creator());
    break;
  //lancio di un generico nodo
  case "n":
    c.setExecutor(new CycleScheduler(TimeoutMeasure.CY));
    c.setConnector(new ActiveMqConnector(s2)); // --> c.setConnector(new ActiveMqConnector(false));
    c.addService(new Creator());
    break;
  //lancio dell'initiator
  case "i":
    c.setExecutor(new CycleScheduler(
        new PersonManager(true), TimeoutMeasure.CY));
    c.setConnector(new ActiveMqConnector(s2)); // --> c.setConnector(new ActiveMqConnector(false));
    break;
  default:
    c.setExecutor(new CycleScheduler(
        new PersonManager(true), TimeoutMeasure.CY));
}

c.start();
```

- **s2** is the string that contains the IP address of the broker: **tcp://x.x.x.x:port** (es. tcp://127.0.0.1:61616)
- To run the simulator on local machine you can also change the object argument **ActiveMqConnector**
- To launch the simulator correctly you need to:
  - Launch a broker instance **(b)**
  - Launch one or more generic instances **(n)**
  - Launch an initiator instance to start the simulation (master) **(i)**