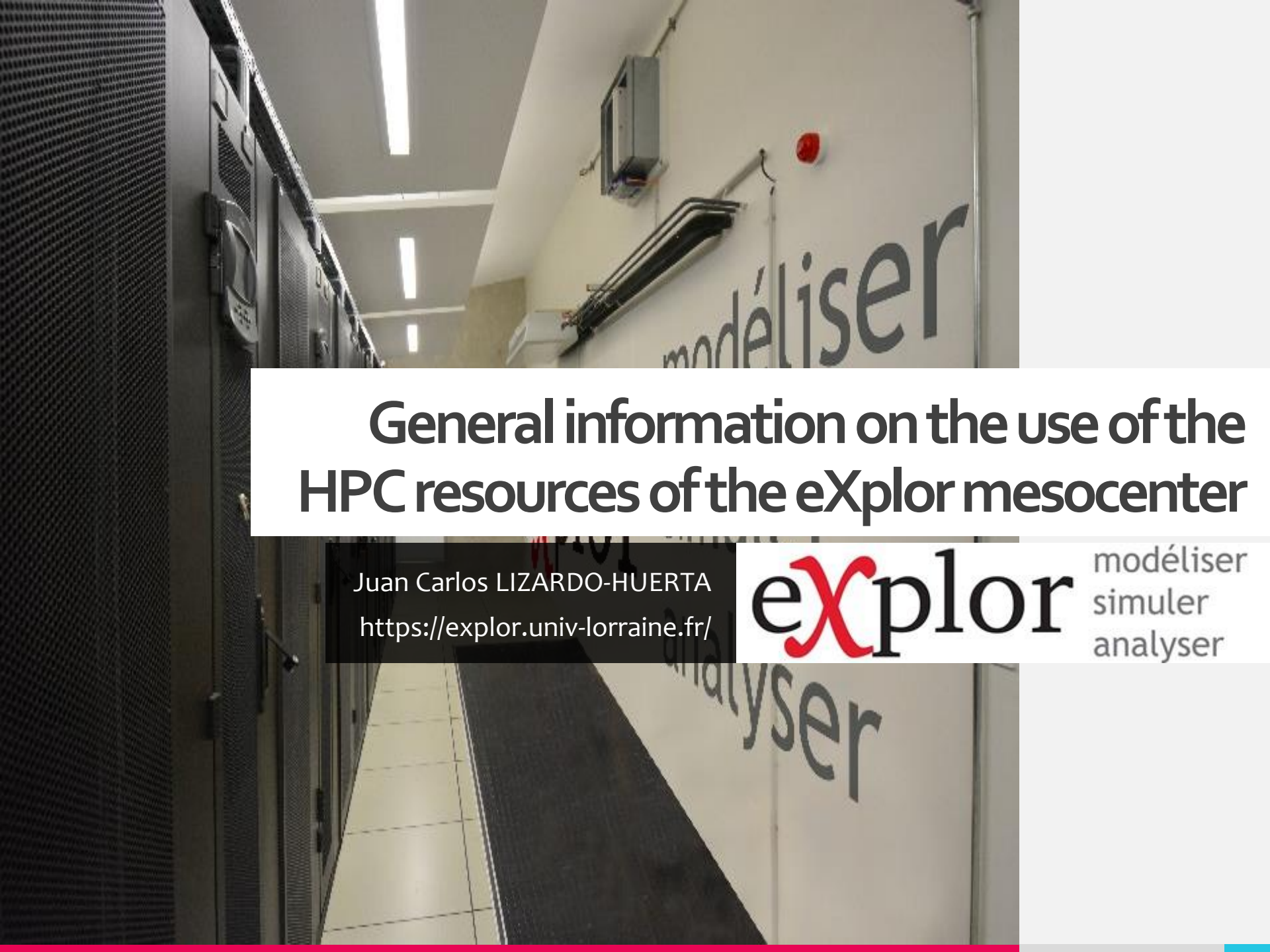




General information on the use of the HPC resources of the eXplor mesocenter

Juan Carlos LIZARDO-HUERTA
<https://explor.univ-lorraine.fr/>

eXplor modéliser
simuler
analyser

What is an HPC mesocenter?

- ❑ Infrastructure dedicated to providing high-performance computing resources for scientific research and innovation



Our missions

- ❑ Provision of HPC computing resources
- ❑ Promotion of high-performance and parallel computing techniques
- ❑ Tailored training provided by eXplor support
- ❑ User community

Team

❑ Emilie Gaudry

- ❖ Directrice du mésocentre

❑ DN université (2 ETPs parmi Florian Audinot, Stéphane Dugravot, Benoît Marchal et Doru Mihalachi)

- ❖ Administration réseau et systèmes

❑ Juan Carlos Lizardo Huerta

- ❖ Gestion du catalogue des applications
- ❖ Support aux utilisateurs
- ❖ Formations

❑ Francis Kosior

- ❖ Chef du projet déploiement eXplor v.2

Material

- ❑ **343 computing nodes (Omnipath and Infiniband)**
 - ❖ Intel and AMD processors
- ❑ **Over 11,000 computing cores**
 - ❖ 4 – 16 GB per core
 - ❖ 8 – 64 cores per node
 - ❖ 60 – 512 GB per node
- ❑ **760 TB of fast storage**
- ❑ **450 TB of persistent storage**
- ❑ **16 GPU nodes for a total of 45 GPU cards**
 - ❖ Nvidia: P100, GTX1080, T4, RTX600, L40

More details: <https://explor-tech.univ-lorraine.fr/fr/materiel/>



Application examples

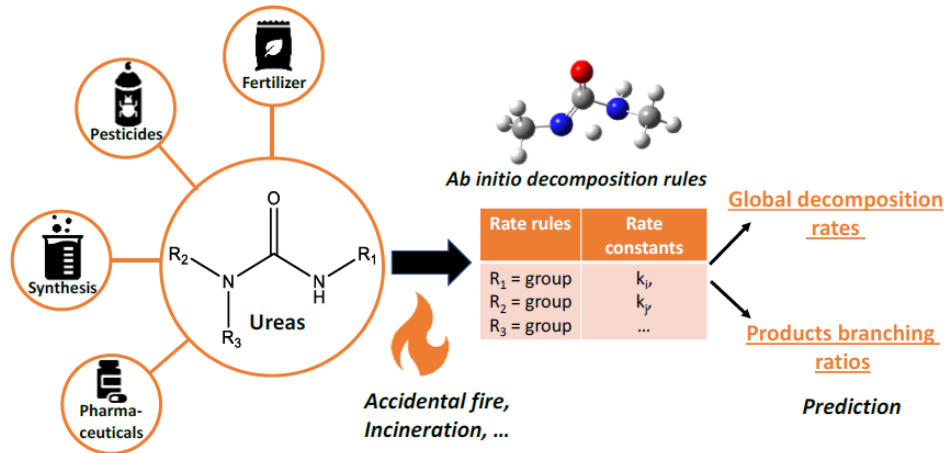
more examples on https://explor.univ-lorraine.fr/files/2024/06/synthese-rapports-explor_2022-24-1.pdf



Energy

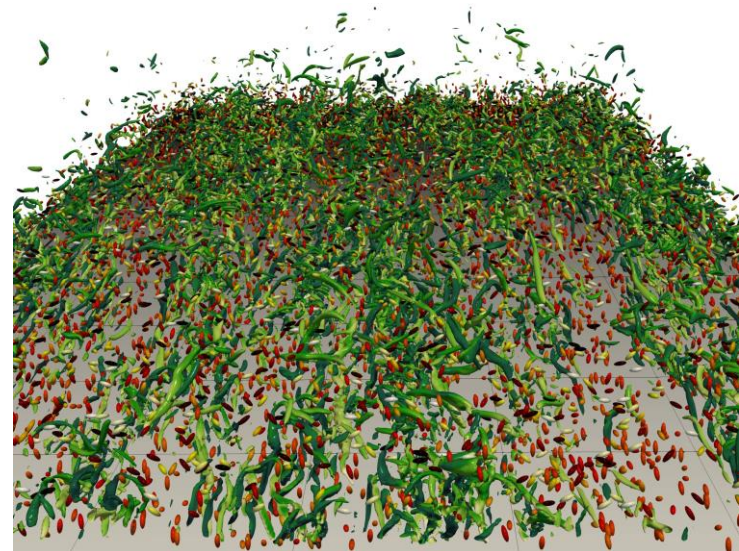
Detailed kinetic modeling of thermal reactions in the gas phase

J. Honorien, R. Fournet, P.-A. Glaude, B. Sirjean, J. Phys. Chem. A 126 (2022) 6264-6277



DNS simulation of turbulent flows laden with ellipsoidal solid particles

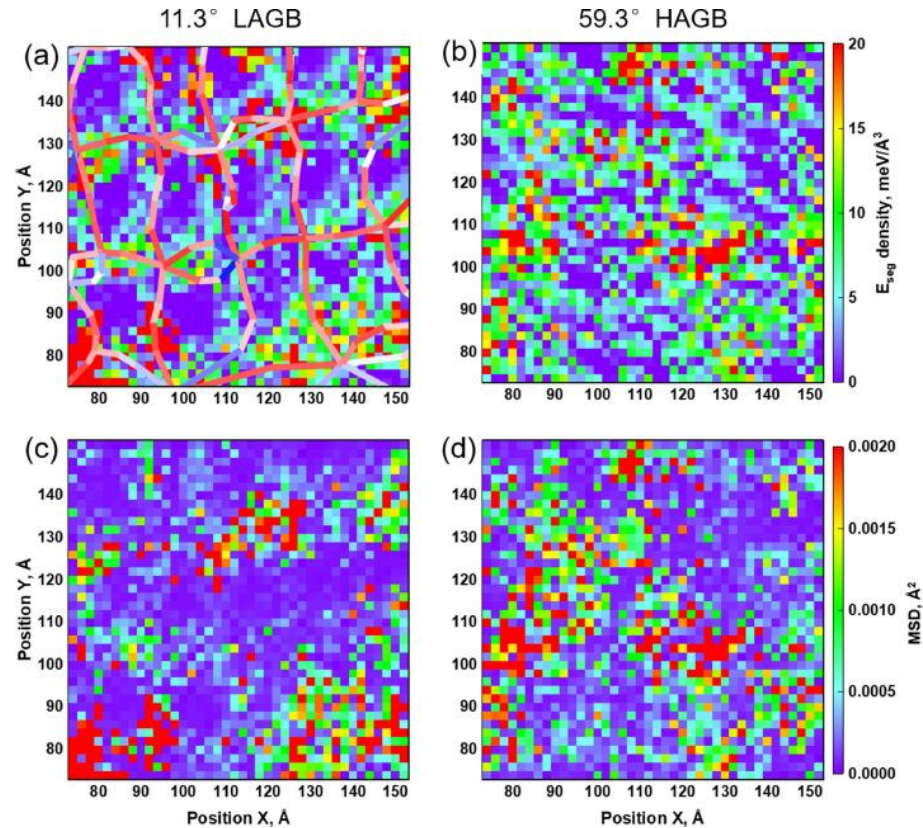
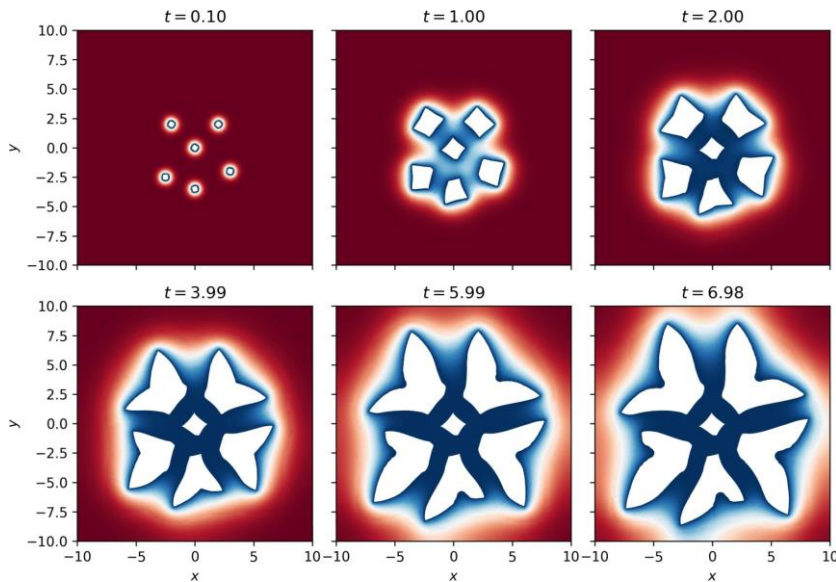
A. Michel and B. Arcen. Translational and angular velocities statistics of inertial prolate ellipsoids in a turbulent channel flow up to $Re \tau = 1000$ ". Journal of Fluid Mechanics , 966, 2023. Doi 10.1017/jfm.2023.420.



Materials

Mesososcopic modeling of dendritic solidification

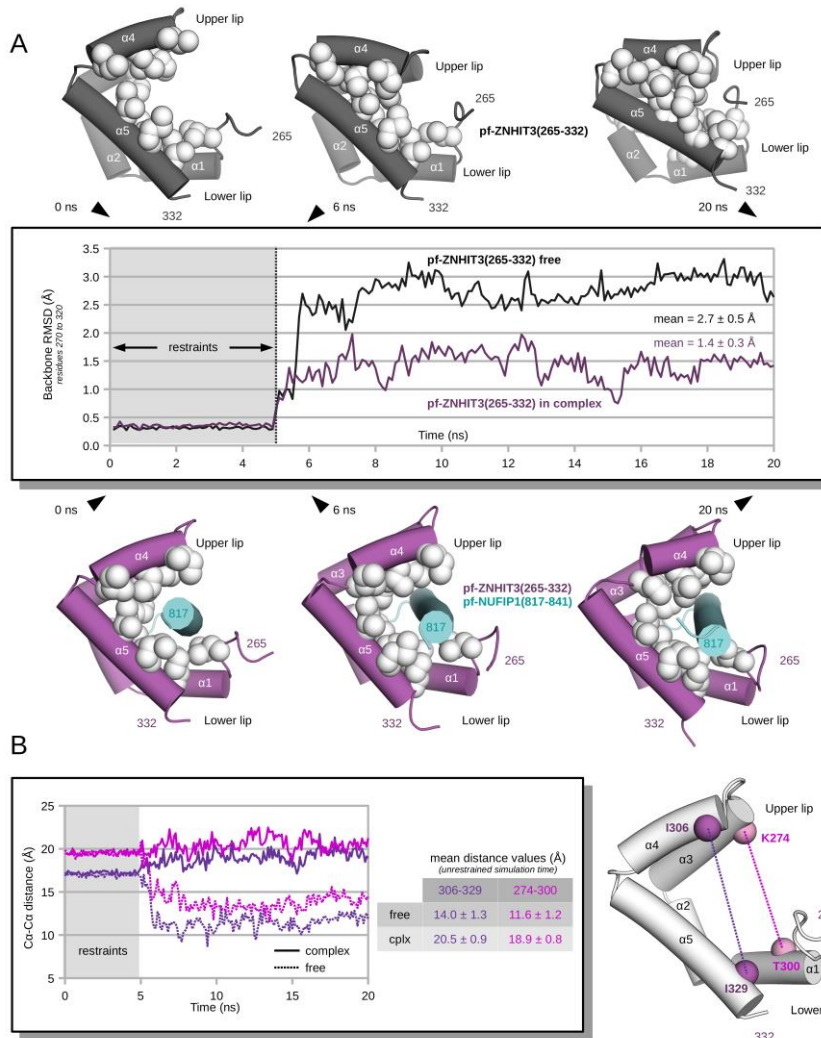
Jančič, M., Založnik, M., Kosec, G., Meshless interface tracking for the simulation of dendrite envelope growth. Journal of Computational Physics 2024, 507, 112973.



Atomic study of defects in crystals

Atomistic insights into the inhomogeneous nature of solute segregation to grain boundaries in magnesium, R Pei, Z Xie, S Yi, S Korte-Kerzel, J Guénolé, T Al-Samman, Scripta Materialia 230 (2023) 115432

Biology



Structural analysis of the TPR1 domain of the human SPAG1 protein

Chagot, M.-E., Boutilliat, A., Kriznik, A., Quinternet, M., Structural Analysis of the Plasmodial Proteins ZNHIT3 and NUFIP1 Provides Insights into the Selectivity of a Conserved Interaction. *Biochemistry* 2022, 61, 479–493.



Access

Access conditions

- ❑ Staff from UL and associated EPST, working in a UL entity or an EPST associated with UL
- ❑ With authorization from the management board for individuals outside of UL and associated EPSTs
- ❑ PhD students
- ❑ Postdocs
- ❑ Students as part of an internship

Access request

- ❑ It is necessary to submit a project via a project submission form

<https://enquetes.univ-lorraine.fr/index.php/327599?lang=fr>

- ❑ Validation of the project by the Explor scientific committee.
- ❑ User account openings are done through an account creation form using a UL email address. Without a UL email address, authorization from the management board is required

<https://enquetes.univ-lorraine.fr/index.php/434841?lang=fr>

- ❑ Each project manager provides a report on their activities during the report feedback campaign launched by the mesocenter, approximately once every two years

- ❑ **Pricing: 0 €**

Shared resources

The eXplor mesocentre offers a resource pooling solution, allowing partners to acquire computing nodes integrated into eXplor. The ASR team of the mesocenter is responsible for the installation, configuration, and maintenance of these nodes. Thanks to these initiatives, the resources that have been acquired since 2020 are :

- ❖ 154 CPU nodes
- ❖ 6 GPU nodes for a total of 17 GPU cards

Les laboratoires participants

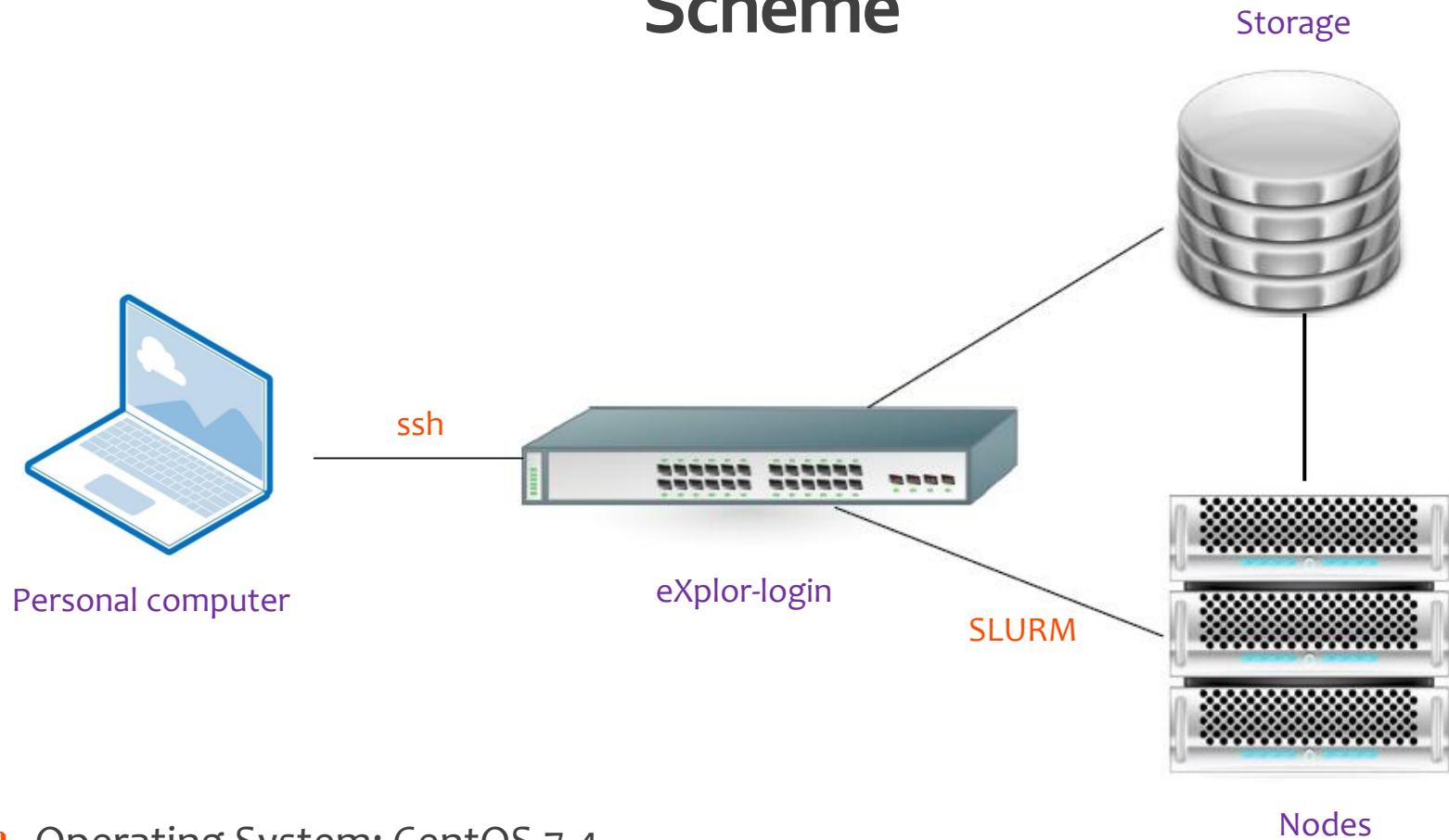


<https://explor.univ-lorraine.fr/explor/mutualisation/>



Getting started

Scheme



- ❑ Operating System: CentOS 7.4
- ❑ Scheduler: SLURM
- ❑ Environment Module Manager: LMOD 7.4

Connection

❑ In console mode:

```
ssh -p <N°-port projet> login@193.54.9.82
```

❑ In graphics mode:

- ❖ **X2GO** : compatible with windows, mac os and linux
- ❖ **MobaXterm** : windows, linux
- ❖ PuTTY
- ❖ autres

Configuration of X2Go

Paramétrage de la session - Nouvelle session

Session Connexion Entrées/Sorties Media Dossiers partagés

Nom de la session : Nouvelle session

 << changer d'icône

Chemin : /

Serveur

Hôte : 193.54.9.82

Identifiant: votreidentifiant

Port SSH : votreport

Utiliser une clé RSA/DSA pour la connexion SSH: /home/c /ssh/id_rsa (FACULTATIF)

☐ Essayer l'authentification automatique (via l'agent SSH ou la clé SSH par défaut)

☐ Authentification Kerberos 5 (GSSAPI)

☐ Délégation de l'identification GSSAPI au serveur

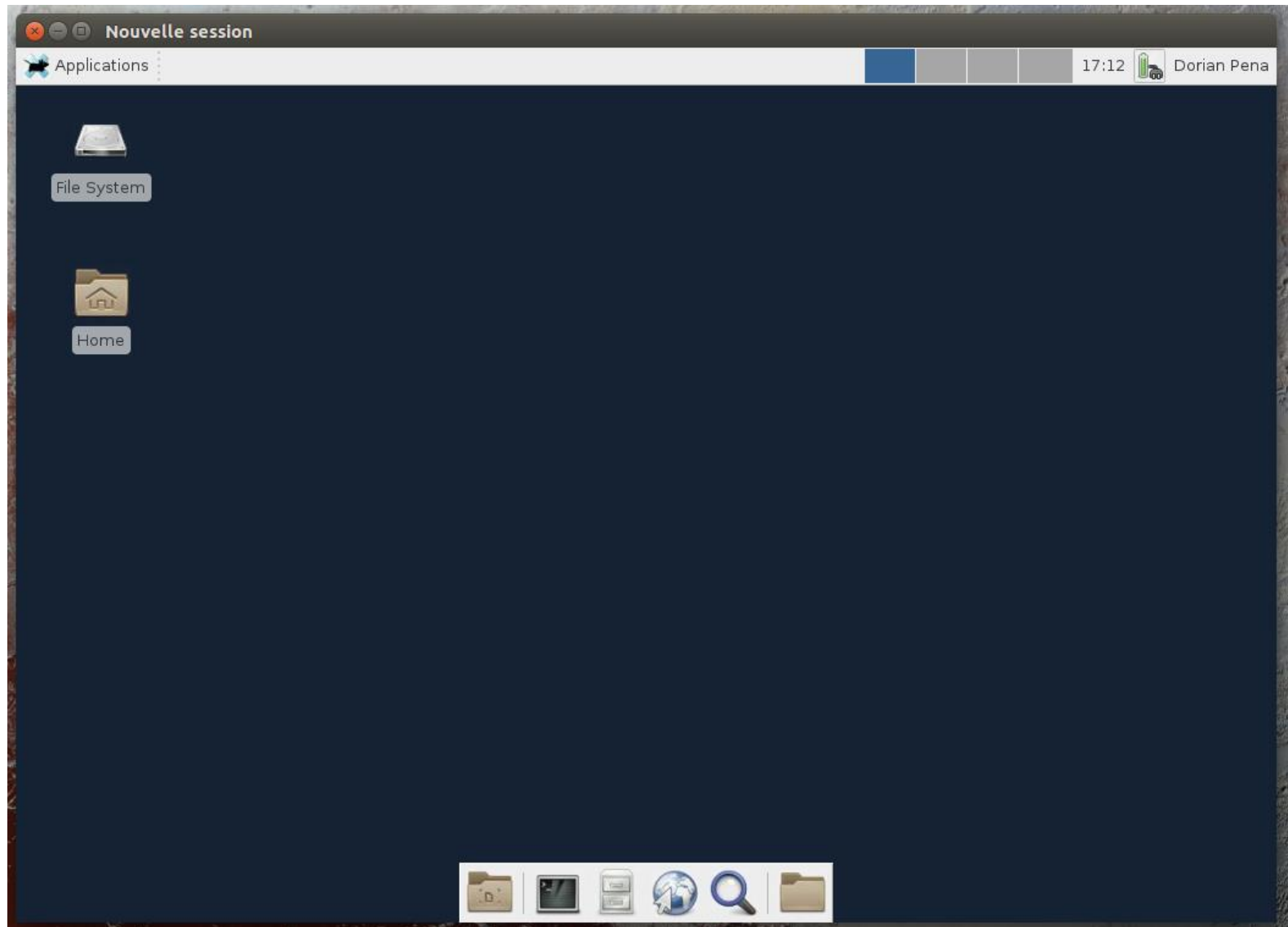
☐ Utiliser un serveur mandataire pour la connexion SSH

Type de session

XFCE Commande

Ok Cancel Défauts

You're now on your personal eXplor desktop!



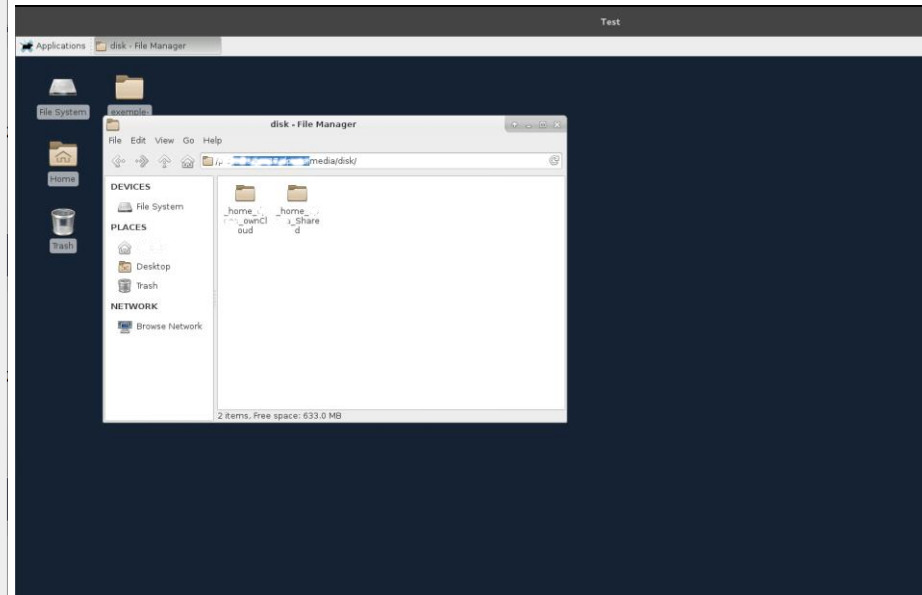
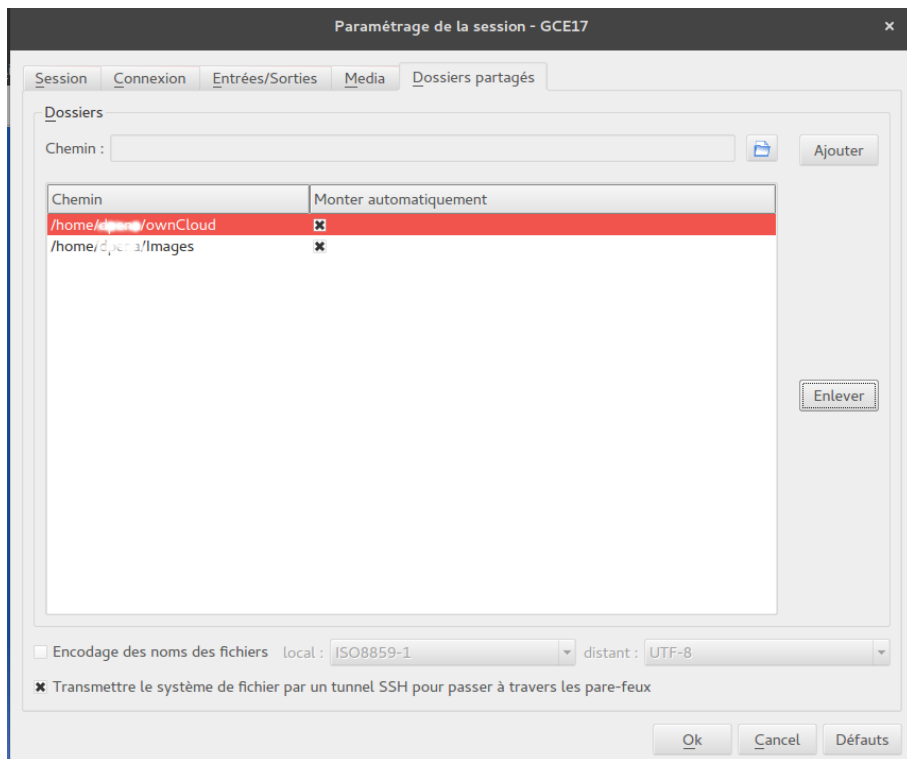
Data transfer

❑ In console mode:

`scp -r -P xxxx <dossier> votre_identifiant@193.54.9.82:chemin`

❑ In graphics mode:

❖ Avec WinSCP, MobaXterm ou X2Go



Environment modules

- ❑ The eXplor mesocenter has several applications available in the form of modules.
- ❑ It allows you to set environment variables according to your needs (PATH, LD_LIBRARY_PATH, ...)
- ❑ List of modules: <https://explor-tech.univ-lorraine.fr/fr/applications/#>
- ❑ To access this list on the cluster:
 - ❖ `$ module avail`
 - ❖ `$ module avail <nom_du_module>`
- ❑ Some operations on modules:
 - ❖ `$ module load <nom_du_module>` → to load a module
 - ❖ `$ module list` → to get the list of loaded modules
 - ❖ `$ module unload <nom_du_module>` → to unload a specific module
 - ❖ `$ module purge` → to unload all loaded modules

Environment modules

Structure arborescente

❑ **/opt/modulefiles/compiler**

- ❖ Compilateurs: Intel, gcc, cuda, ..

❑ **/opt/modulefiles/libraries**

- ❖ Libraires mathématiques: mkl, mpi, openmpi, ...

❑ **/opt/modulefiles/apps**

- ❖ Logiciels installés au mésocentre

❑ **/opt/modulefiles/tools**

- ❖ outils:, applications graphiques

❑ **\$SHARED/modules**

- ❖ Installation en local sur les projets (licence spécifique, code propre)

Environment modules

Modules installed on the cluster:

```
[cal01@vm-support01 ~]$ module avail
```

/opt/modulefiles/compilers									
cuda/6.5	cuda/7.5	cuda/9.0	cuda/9.2	gcc/5.4.0	gcc/7.1.0	intel/2017.4.196 (D)	intel/2018.4	intel/2019.4_fixed	intel/2019.4
cuda/7.0	cuda/8.0	cuda/9.1	gcc/4.9.4 (D)	gcc/6.3.0	intel/2017.1.132	intel/2018.3	intel/2018.5	intel/2019.4-full	pgi/17.10

/opt/modulefiles/mpi				
intelmpi/2017.1.132	intelmpi/2018.5.274	openmpi/2.1.1/gcc-4.9.4 (D)	openmpi/2.1.1/gcc/7.1.0	openmpi/3.0.1/gcc/5.4.0
intelmpi/2017.4.196 (D)	intelmpi/2019.4	openmpi/2.1.1/gcc/5.4.0	openmpi/2.1.1/intel	openmpi/3.0.1/gcc/6.3.0
intelmpi/2018.0.128	openmpi/2.1.0/intel	openmpi/2.1.1/gcc/6.3.0	openmpi/3.0.0/intel18	openmpi/3.0.1/gcc/7.1.0 (D)
				openmpi/4.0.0/gcc/7.1.0
				openmpi/4.1.0rc5-mlnx/gcc/4.8.5

/opt/modulefiles/libraries						
atlas/3.10.3	fftw/3.3.7/intelmpi17-intel17	hypre/2.10.0b	metis/4.0.3	mkl/2017.4.196 (D)	mkl/2018.5.274	nfft/3.4.0/intel17
boost/1.64.0	hdf5/1.10.1/intelmpi/intel17	hypre/2.11.2	mkl/2017.1.132	mkl/2018.0.128	mkl/2019.4	plumed/2.3.1

/opt/modulefiles/apps			
FDS/6.7.0/intel.2017.4	amber/16/std-intel.2017.4 (D)	foam-extend/4.0/openmpi-2.1.1-gcc-4.9.4	siesta/4.0.1/intel17-2
FEFF/9.0	ansys/17.2	gaussian/03_REV_B05/intel17	siesta/4.0.1/intel18 (D)
NAMD/CPU/2.14	ansys/18.0	gaussian/09/pgi	uspex/9.4.4
NAMD/GPU/2.15	ansys/19.1	gaussian/09/pgi-17.10	vasp/5.4.1/5.4.1/intel17
R/3.5.2	ansys/24.2 (D)	gromacs/2016.3/gcc-6.3.0	vasp/5.4.4/gpu
abaqus/2017	caffe/2.0 (D)	gromacs/5.1.4-plumed/gcc-6.3.0	vasp/5.4.4/hf
abinit/8.10.2	caffe1/cpu-only	intel/runme_xeon64	vasp/5.4.4/sky
abinit/9.10.3 (D)	caffe1/gpu	lammps-2018/lammps_2018_INTELMPI	vasp/5.4.4/std (D)
amber/16/hf-intel.2017.4	caffe1/18-09 (D)	lammps/11Aug17/intel_cpu_intelmpi	
amber/16/intel17	cp2k/4.1/intel17	matlab/r2017b	
amber/16/ivy-intel.2017.4	crystal/14	matlab/r2019b	
amber/16/k20	firefox/65	matlab/r2024a (D)	
			siesta/4.0.1/gcc-4.9.4
			siesta/4.0.1/intel17

/opt/modulefiles/tools			
Boltz2/20.2.1	anaconda/3/5.1	idb/2018	inspector/2019 (D)
advisor/2018.4.0	cmake/3.10.2	idb/2019 (D)	libtool/2.4.6
advisor/2019 (D)	git/2.15.1	inspector/2018	mmg/5.4.3
anaconda/2/5.1	gmsh/3.0.6	inspector/2018.4.0	mumax/3.10b
			paraview/4.4.0
			paraview/5.10.1 (D)
			python/3.6/anaconda
			python/intel/2017.3/2.7
			python/intel/2017.3/3.5 (D)
			python/intel/2019/2
			python/intel/2019/3 (D)
			tbb/2018.5.274
			tbb/2019
			vtune-amp/2018
			vtune-amp/2018.4.0
			vtune-amp/2019 (D)

```
[cal01@vm-support01 ~]$
```

List of modules: <https://explor-tech.univ-lorraine.fr/fr/applications/#>

SLURM

- ❑ SLURM is the resource manager used in the eXplor mésocentre
- ❑ Allows resources to be reserved as required
- ❑ A submission script is used to submit a job:

```
#!/bin/bash

#SBATCH --account=<your-group>
#SBATCH --partition=std
#SBATCH --job-name=job_name
#SBATCH --nodes=1           # 1 node
#SBATCH --ntasks=32        # 32 CPUss
#SBATCH --time=12:00:00    # the job will killed after 12h
#SBATCH [...]

module purge
module load <nom_du_module>

./my_code
```

- ❑ Job soumission
 - ❖ `$ sbatch scrip.sh`
- ❑ Monitoring job status
 - ❖ `$ squeue -u <login>`
- ❑ Cancelling a job
 - ❖ `$ scancel <jobid>`



eXplor v.2

eXplor v.2

- ❑ Replacement
 - ❖ management servers
 - ❖ storage servers (/home, /sharedir, scratch)
- ❑ Updating of operating systems and applications
- ❑ Shutdown of computing nodes on the Omnipath network outside of warranty and addition of computing nodes
- ❑ Modification of project, account, and partition management..

eXplor v.2

New Features

- ❑ Open on demand (Web-based computing interface)
- ❑ Visualisation

Expected implementation date: September 2025

eXplor v.2

Survey - Hardware Needs for EXPLOR

<https://enquetes.univ-lorraine.fr/index.php/317257?lang=fr>





Questions



Chiffres clés

11000+

CŒURS CPU

490

TFLOPS

90+

PROJETS

400+

UTILISATEURS

Notre vision

Le Mésocentre eXplor est la plateforme de calcul mutualisé de l'Université de Lorraine, dédiée à soutenir la recherche dans tous les domaines nécessitant des capacités de calcul intensif.

Nous contacter

IJL – Campus Artem - Bureau 1.A004

2 Allée André Guinier, 54011 Nancy

Tel. 03 72 74 26 63

explor-contact@univ-lorraine.fr

eXplor modéliser
simuler
analyser

Un ensemble de calculs scientifiques
pour la Lorraine

Project partners

