

romeoLAB, le portail web HPC : cas d'utilisation pour la pédagogie et les logiciels à la demande



Dr Arnaud RENARD - HPC CTO & Research Engineer


Dr Jean-Mathieu ETANCELIN - HPC Research Engineer

Pr Michael KRAJECKI - HPC Center Director



romeolab@univ-reims.fr

<http://romeo.univ-reims.fr>

 @HPCromeo
#romeoHPC







University of Reims

Université de Reims Champagne-Ardenne (URCA)

Multidisciplinary university

- about 27 000 students
- 5 campus : Reims, Troyes, Charleville-Mézières, Chaumont et Châlons-en-Champagne
- a wide initial **undergraduate** studies program
- **graduate** studies and **PhD** program linked with **research labs**





HPC Center
ROMEO
Centre de Calcul Régional



ROMEIO HPC Center for Grand-Est region

Its **mission** is to deliver, for both **industrial and academic** researchers :

CLASSICAL MISSIONS

- **high performance** computing **resources**,
- **secured storage** spaces,
- specific & **scientific softwares**,
- **advanced user support** in exploiting these ressources,
- in-depth **expertise** in different engineering fields: HPC, applied mathematics, physics, biophysics and chemistry, ...



SPECIFIC MISSIONS

- promote and diffuse HPC and **simulation** to companies / **SMB**
- identify, experiment and master **breakthrough technologies**
 - which give new **opportunities** for our user
 - from **technology-watching** to **production**
 - for all **research domains**



GPU, DL, Quantum



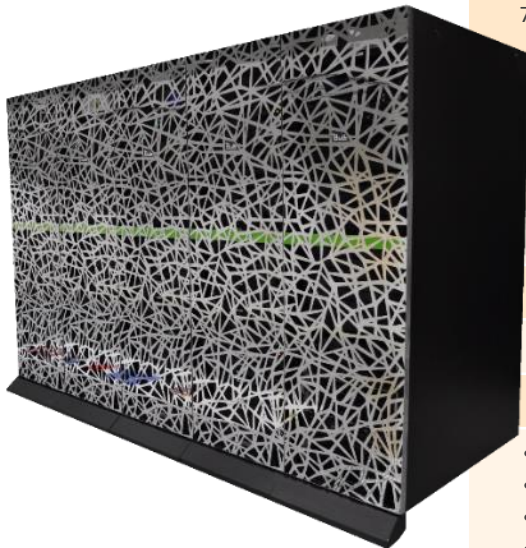
- **Teaching High Performance Computing to Researchers and Students**



ROMEO

Principales machines de production

2013 / Bull	Année / Constructeur	2018 / Bull-ATOS
2,5 M€	Investissement	6,5 M€
2 080 cœurs 700 000 cœurs GPU (260 K20X)	CPU	3 220 cœurs (skylake @2,6 GHz) 1 000 000 cœurs GPU (280 P100)
254,0 Tflops	Puissance	1,022 Pflops x 4
70 KW	Energie	120 KW
4 To	Mémoire	15 To
200 To (//)	Stockage	600 To (//)
130	Serveurs	115
40 Gb/s IB	Interconnexion	100 – 200 Gb/s BXI
<ul style="list-style-type: none"> • GPU • romeoLAB • TOP500 #151 • GREEN500 #5 • GRAPH500 #105 		<ul style="list-style-type: none"> • DLI & DL • TOP500 #254 • GREEN500 #20 • HPCG #63 • GRAPH500 #??



Motivation: romeoLAB must be *powerfull*

Necessity of computer science courses dedicated to parallel programming on heterogeneous architectures. (Students, Reserchers, European & French projects)

- HPC is more and more complex (different processors, memory, network, ...)
- Hardware specific phenomenon (bandwidth bottleneck, cache page issues, ...)
- We want to execute code on a real HPC facility.

Romeo works perfectly, got software already installed and supported.



As an example, we organized a 5 days event dedicated to GPU technologies in 2016

[Arnaud Renard, Jean-Matthieu Etancelin, Michaël Krajecki: romeoLAB: A High Performance Training Platform for HPC, GPU and DeepLearning. CARLA2017: 55-67]





Motivation: romeoLAB must be *powerfull*

But using HPC supercomputer is difficult :

- Ssh, Sftp (+installing clients),
- Password, login, account opening account process,
- Load module environment,
- Deal with Slurm,
- Xserver or VNC client for Graphical interface (profiler, debugger, viewers, ...),

Using those tools

- is time-consuming;
- is not pedagogic objectives of courses;
- are obstacles to the pedagogical process efficiency;



Motivation: romeoLAB must be *easy*

A web-based solution is the most easy-to-use solution.

- Users already have a browser
- Lot of references / other experiences
- HTML5 allow almost everything
- Multi-device
- Poor internet connections

User management

- Simple registration process
- Disposable accounts
- Access to session with access code
- Start and Stop labs thru SLURM jobs / reservation



Fonctionnalités :

- romeoLAB
 - Orienté HPC
 - Execution sur notre cluster de prod (2500 coeurs / 260 GPU), slurm (reservation)
 - Cours (session, via token, persistance) = $n * \text{exercice (Lab)} = n * \text{notebook}$
 - Contenus dans GIT
 - Interface Enseignant

-  UTP 2017 (started)
✓ valid session • 📅 from 01/06/2017 16:51 → 31/08/2017 16:51 • 🗑️ All labs datas will be deleted after this date.



- **Mpi Beginner**
Introduction to MPI
Message Passing Interface Standard (MPI) is a specification for the developers and users of message passing libraries. Simply stated, the goal of the Message Passing Interface is to provide a widely used standard for writing message passing programs over distributed systems. The interface attempts to be:
 - Practical
 - Portable**Lab Started**
- **Introduction to CUDA**
Introduction to CUDA C
CUDA is a parallel computing platform and application programming interface (API) model created by Nvidia to generate kernels for his GPU. [Plus d'information](#)
Content of this course:
 - Execution model (CUDA threads and blocks)
 - Unified memory
 - Shared memory**Lab Off**
- **IntroductionOpenMP**
« Open Multi-Processing » API (Application Programming Interface) is an industrial standard for parallel programming in shared memory.
The Programming model is based on pthreads.
Lab Started
- **Introduction to OpenACC and MPI**
lab 2.2 : Multi GPU Programming with OpenACC and MPI
OpenACC is a portable, high-level, domain-specific language for GPU communication with OpenACC
MPI+OpenACC applications
Communication times
Lab Off

ROMEOLab features examples

Notebook developed by [Jean-Matthieu Etancolin](#) (ROMEOLab).
The complete documentation can be found here: [Documentation](#)

1 Jupyter Notebook cells

```
In [4]: %bash
hostname
uname -a
nvidia-smi

romeo00
Linux romeo00 2.6.32-504.23.4.el6.bull.75.x86_64 #1 SMP Thu Jun 18 23:11:50 CEST 2015 x86_64 x86_64 x86_64 GNU/Linux
Sat Aug 5 01:16:29 2017
-----
| NVIDIA-SMI 367.48             Driver Version: 367.48             |
|-------------------------------|-----|-----|-----|
| GPU Name      Persistence-M| Bus-Id  Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|  Memory-Usage | GPU-Util  Compute M. | |
|---|---|---|---|
| 0.  Tesla K20Xm    On      | 00000:02:00:0  Off |                    |
| N/A   24C    P8   18W / 235W |  0MiB / 6003MiB |    0%   E. Process |
|-----|-----|-----|-----|
| 1.  Tesla K20Xm    On      | 00000:03:00:0  Off |                    |
| N/A   26C    D8   19W / 235W |  0MiB / 6003MiB |    0%   E. Process |
|-----|-----|-----|-----|
```

3 Embedding videos

Here the ROMEOLab HPC Center youtube video:

```
In [7]: from IPython.display import IFrame
IFrame("https://www.youtube.com/embed/o3QtClx1e8k", width=900, height=720)
```

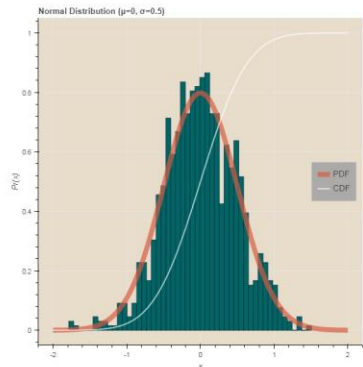


5 Files edition

The cell below shows a remote text file editor:

```
In [9]: editor('exercice1')
```

```
Out[9]: Files Term Ctrl. helloworld.c
Debug
exercice1 save reload open Folder open in Browser Hex-Editor Settings syntax check comment wrap
1 #include <stdio.h>
2
3 int main (int argc, char **argv) {
4     printf("hello world ! \n");
5     return 0;
6 }
```



Motivation: romeoLAB must be *Pedagogic*

In romeoLAB, (like modern MOOC - Massive Open Online Course), development environments is completely integrated into pedagogical content.

➤ We use Jupyter Notebook



The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and explanatory text. Uses include: data cleaning and transformation, numerical simulation, statistical modeling, machine learning and much more.





Motivation: romeoLAB must be *Pedagogic*

On the same web-page :

- development environments
 - File browser & Editors (native & NodeMirror)
 - Compilation, command lines & modules loading (native)
 - Execution live (native)
 - Execution in batch for large runs (in-house Ipython-batch-execution-magics) :
24 students can each run a 32-nodes MPI runs with 32 nodes in total
- Desktop access to run Graphical software
 - Profilers, Debuggers, Graphical interfaces like Paraview
(in-house integration with VNC + x11vnc + VirtualGL)
- Pedagogical content
 - Pdf, Video, content, images, iframed web pages ... (native or in-house)

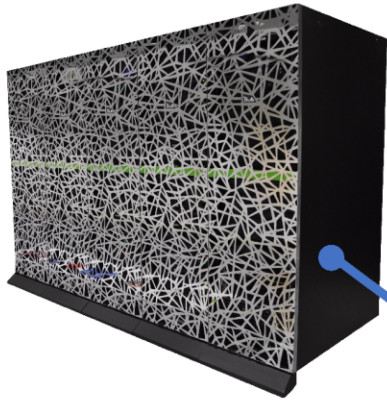




romeoLAB : a High Performance Training Platform for HPC, GPU and DeepLearning

Dr Jean-Matthieu ETANCELIN - jean-matthieu.etancelin@univ-reims.fr
Dr Arnaud RENARD - arnaud.renard@univ-reims.fr
University of Reims Champagne-Ardenne - CReSTIC EA3804 - <http://romeo.univ-reims.fr>

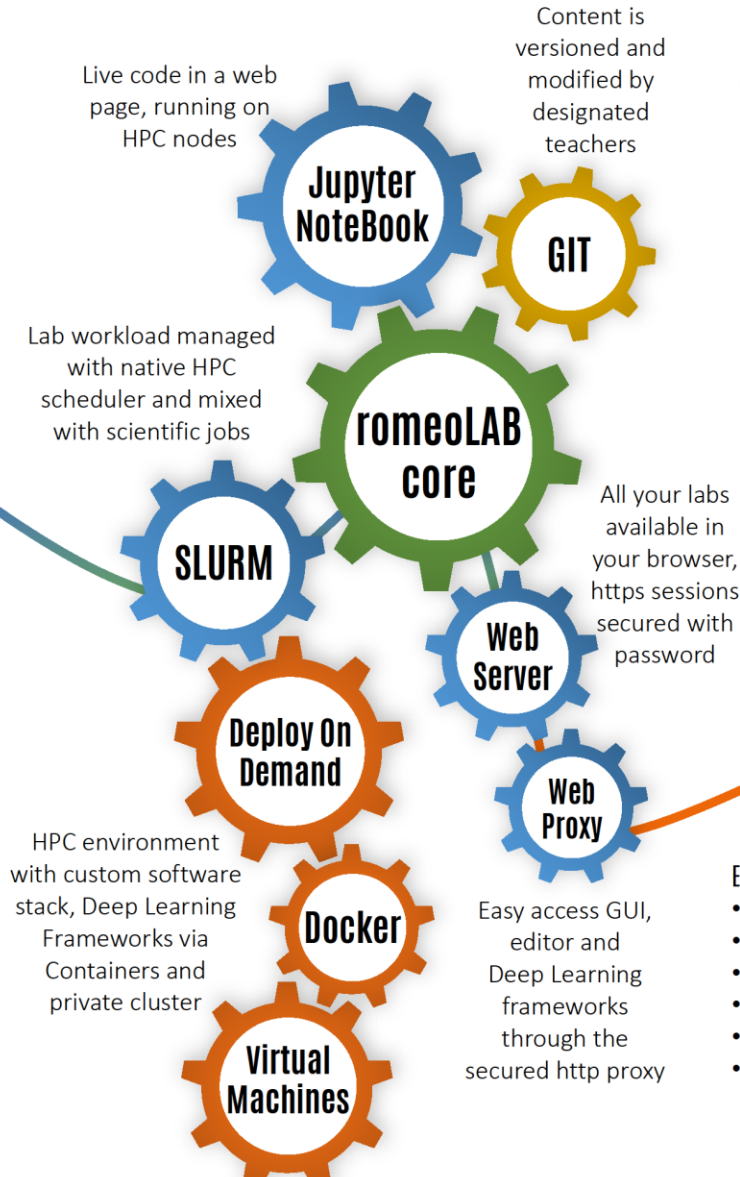
“ Romeo : THE MOST AMAZING GPU CLUSTER IN EUROPE ”
Pr Krajecki - GTC2016





Hosted at University of Reims
Champagne-Ardenne.
Designed by Atos-Bull.
Powered by 260 GPU Tesla Cards
Ranked 151@Top500 in Nov. 2013

Romeo is dedicated to research,
professional services and
education,
in the GrandEst Region, France

2,5 M€, funded by



EXAMPLE OF TEACHING SESSIONS :

- Master courses
- Reims GPU Spring School 
- GTC2016 and GTC2016-Eu Hands-on Labs
- DeepLearning Schools 2017 

EXAMPLE OF EXISTING LABS :

- GPU Accelerated Libraries (cuBLAS, cuFFT, cuRand, ...)
- Multi-GPU Programming with OpenACC
- Advanced Multi-GPU: rCUDA and GPU Direct RDMA
- OpenFoam Tutorial
- OpenMP for HPC, Python programming
- Caffe for DeepLearning

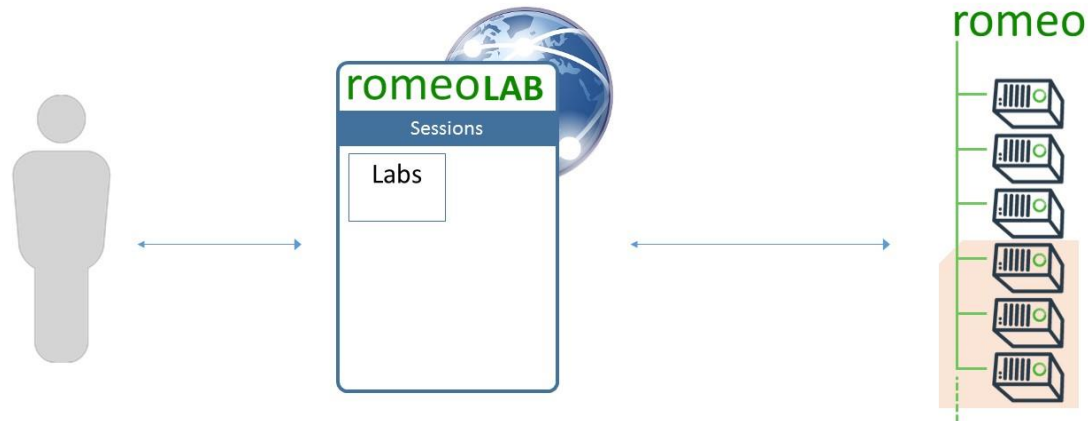


romeoLAB Big Picture 1/3

The Jupyter Notebook is running on the compute node (protected mode)

All the management of *romeoLAB* is made on the web server (FrontEnd)

We need to develop our own server because existing one (like jupyterHub) do not correspond to our needs of customization, integration, evolutivity, dedicated to teaching ... Written in PHP + MVC + RedBean + MariaDb + ...

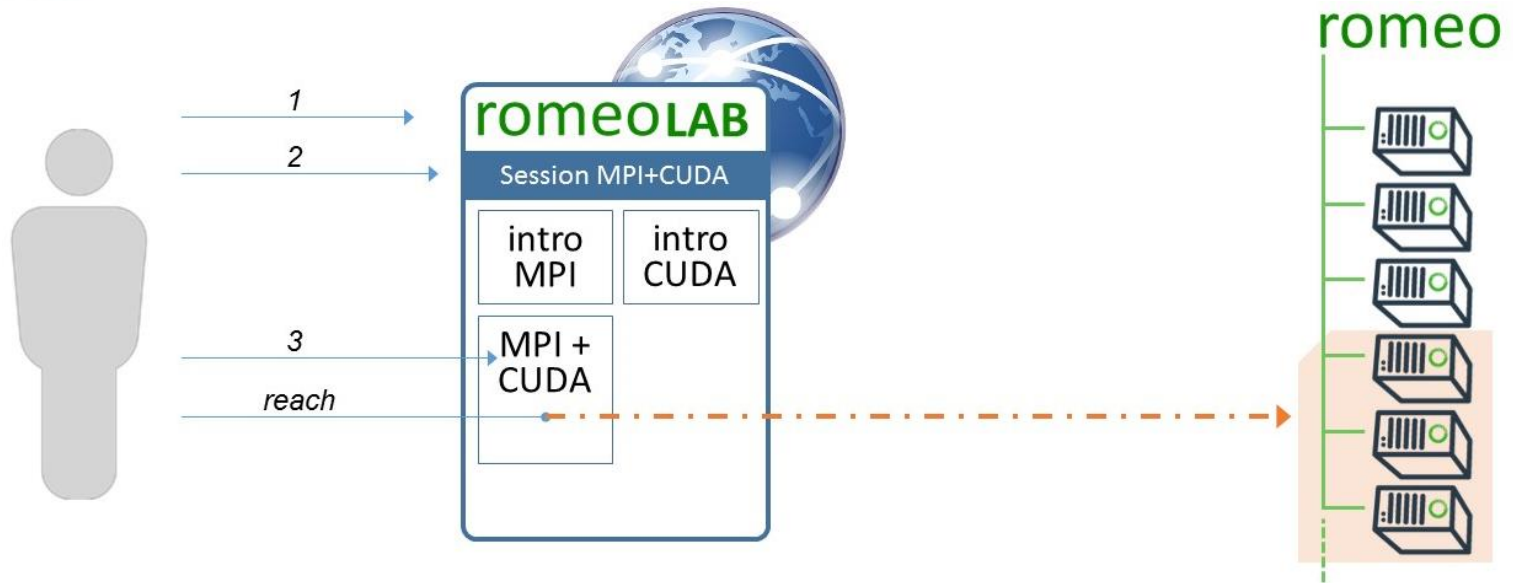


Users can reach and leave sessions, start and stop labs, ...

Teachers can create sessions or labs, update labs contents, and manage students.



romeoLAB Big Picture 2/3

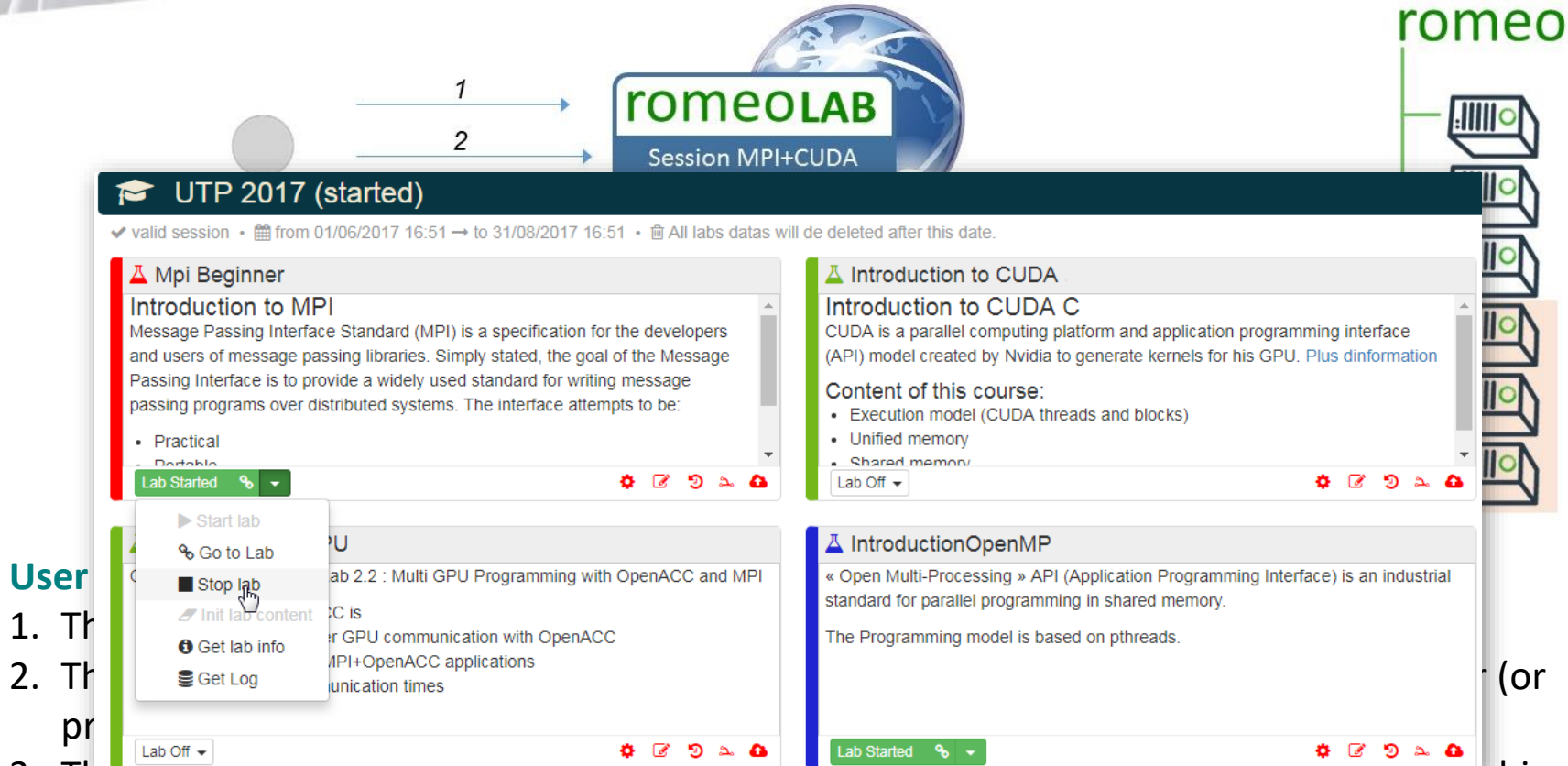


User view of accessing an interactive content in *romeoLAB*:

1. The user **creates an account**, and log in to the platform
2. The user **reach an active Session (=classroom)** with the access code given by teacher (or provided by an activation link, provided by email, on a webpage or Paypal)
3. The user can **list available labs** and their description to finally start one lab and reach his IPython Notebook running on one compute node. He can watch videos and documents, fill table with performance results, edit, compile and also profile code via a remote desktop.



romeoLAB Big Picture 2/3

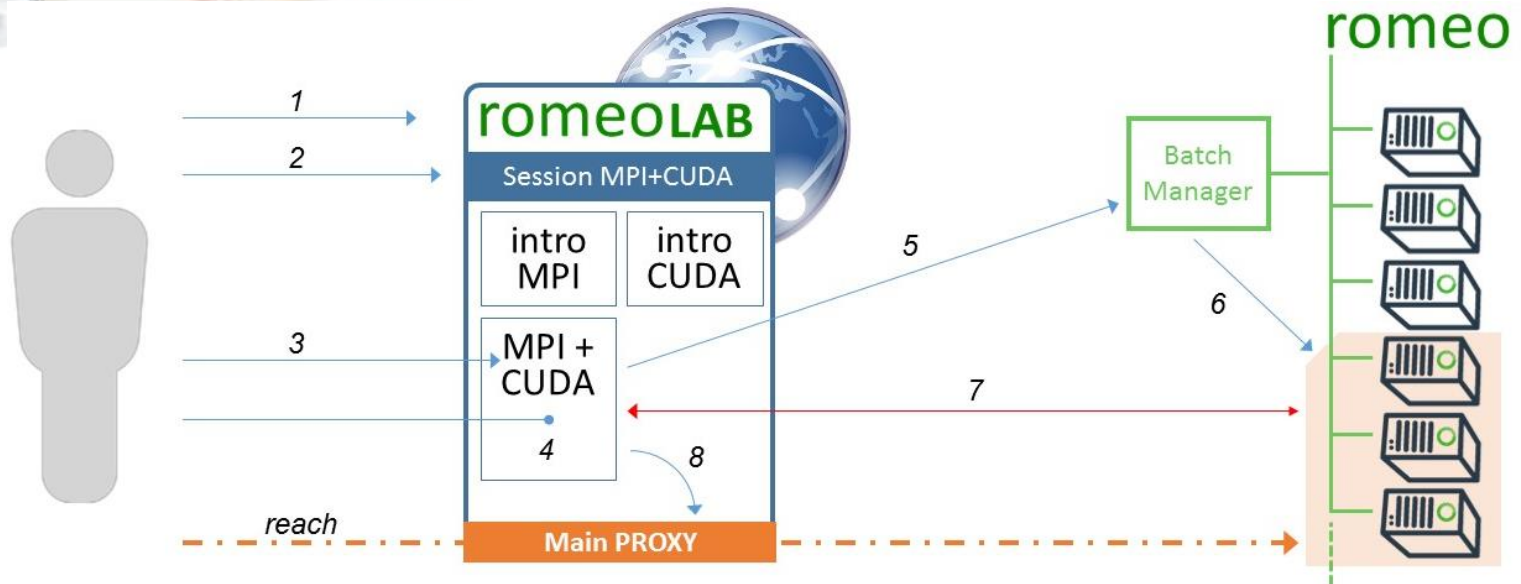


User

1. The user can list available labs and their description to finally start one lab and reach his IPython Notebook running on one compute node. He can watch videos and documents, fill table with performance results, edit, compile and also profile code via a remote desktop.
2. The user can watch videos and documents, fill table with performance results, edit, compile and also profile code via a remote desktop.
3. The user can watch videos and documents, fill table with performance results, edit, compile and also profile code via a remote desktop.



romeoLAB Big Picture 3/3



Internal behavior when a user starts a lab:

4. Server assign a **temporary cluster-user** to the user and dynamically load initial lab content (from the lab repository with GIT protocol).
5. It launches a job through the workload scheduler (and possibly via reserved dedicated resources).
6. This job setting up all resources parameters (available ports), starts all services (notebook, editors, VNC server, ...)
7. romeoLAB is waiting / probing the start of those services
8. **Proxy routes** are setup (Main proxy) to provide direct access to these services (we use “Configurable HTTP Proxy”, which is a NodeJS tool)





Email address

Password

Je ne suis pas un robot 
Confidentialité - Conditions

[Log in](#) [Forgotten password](#)
[Create your Account](#)



This site is the lab platform for the [University of Reims Champagne-Ardenne](#) computer science courses. The site is used to facilitate the hands-on lab and is developed by [ROMEO HPC Center](#).



Labs are powered by ROMEO HPC Cluster which is the largest GPU Cluster in France. Courses are provided by ROMEO HPC Center, University of Reims Champagne-Ardenne, and partners worldwide. You are welcome to contribute.



ROMEO HPC Center is dedicated to teaching and research in French Grand-Est region and offers computational resources, storage, expertise and services for companies. Please contact us for any request : romeo@univ-reims.fr.





USAGE: Previous events and Sessions

Name	Attendees	Duration	Courses
<i>2017:</i>			
JDEV2017	24	4 days	GPU programming
Groupe Calcul	38	3 days	Advanced Python for HPC
Profiler Days	17	3 days	Profiling tools for parallel codes
<i>2016:</i>			
Master Courses	40	4 months	GPU programming and HPC ←
OpenFOAM School	20	3 days	OpenFOAM software
10th LoOPS day	60	2 days	C++ (HPX) vs Python (DSLs)
GTCEU2016	55	90 minutes	MPI and OpenACC
GPU Spring School	36	1 week	GPU programming
GTC2016	60	90 minutes	Advanced tools for hybrid cluster ←

2017/2018 :

linux / Gaussian / Molden / OpenFOAM / industriels / VI-HPS / Abaqus



USAGE: Available content

romeoLAB is addressing a wide range of technologies and audience levels. As we encourage mutualization, this list is growing :



Beginner :

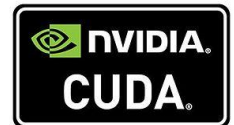
- Introduction to : Python, OpenMP, MPI , CUDA, OpenACC, ...
- GPU accelerated applications : CUDA, OpenACC, Python, ...
- GPU accelerated libraries : cuBLAS, cuRand, cuFFT, ...

OpenFOAM

The Open Source CFD Toolbox

Intermediate

- OpenFOAM
- Gaussian / Molden
- OpenCL, CUDA Asynchronism



Advanced

- Profiling : TAU, MAQAO
- Advanced Python : Cython, Numba, Pythran
- CUDA Optimizations
- Multi-GPU with CUDA
- Multi-GPU with OpenACC and MPI
- Multi-GPU with rCUDA & GPU-Direct RDMA



OPEN MPI





Conclusion

Powerfull : we want to execute code on a real HPC facility, because ours works perfectly and we've got all the software already installed and supported. Where're using a proxy for external users to access to compute nodes.

Easy : romeoLAB is a modern MOOC platform making it possible to run HPC in a simple web browser.

Ssh, ftp and job managers (Slurm) are not part of courses educational objectives nor prerequisites.

Pedagogic : on the same web page, student must find lessons (video, pdf, images, ...) and the edition / compilation / execution interfaces. Jupyter Notebook is our solution for strong interactivity.

Teacher can create his courses on the same platform and manage attendees to his courses,

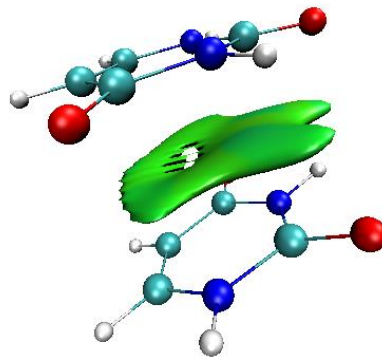
Multi-Application : Compiling and executing code is not enough. We must run profilers, GUIs, and other scientific software.



IGMPlot On-demand

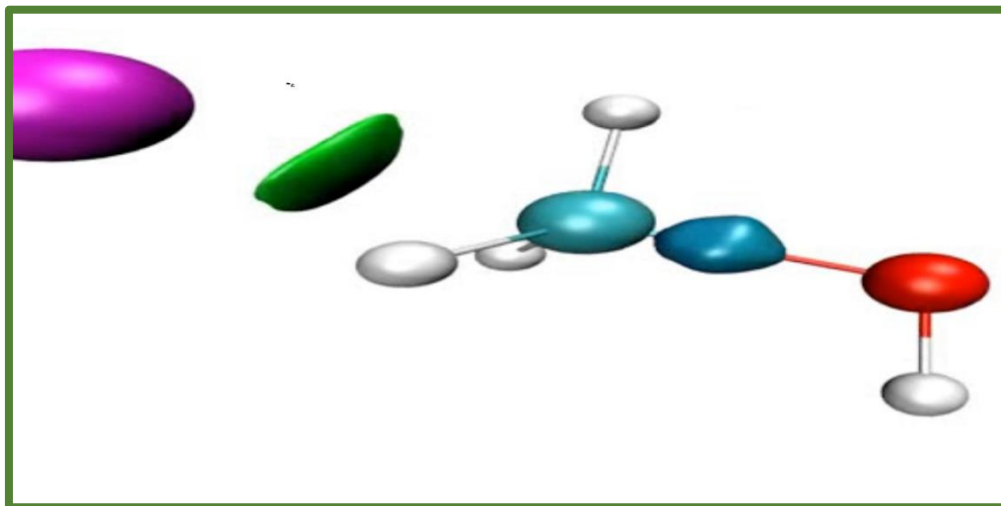


romeoLAB
on-demand

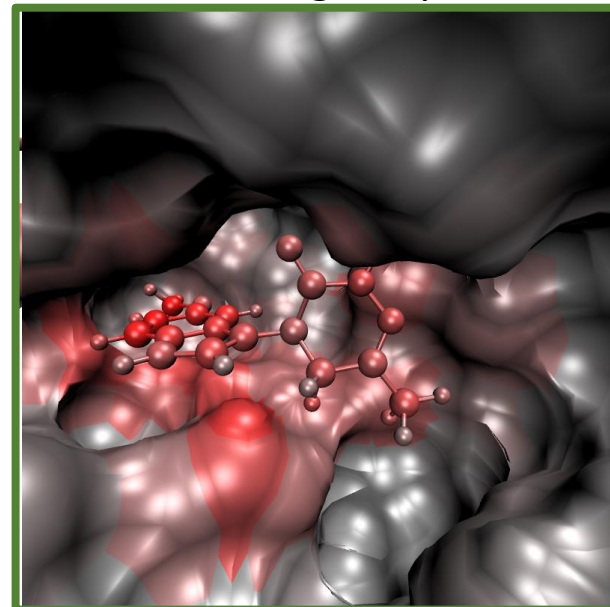


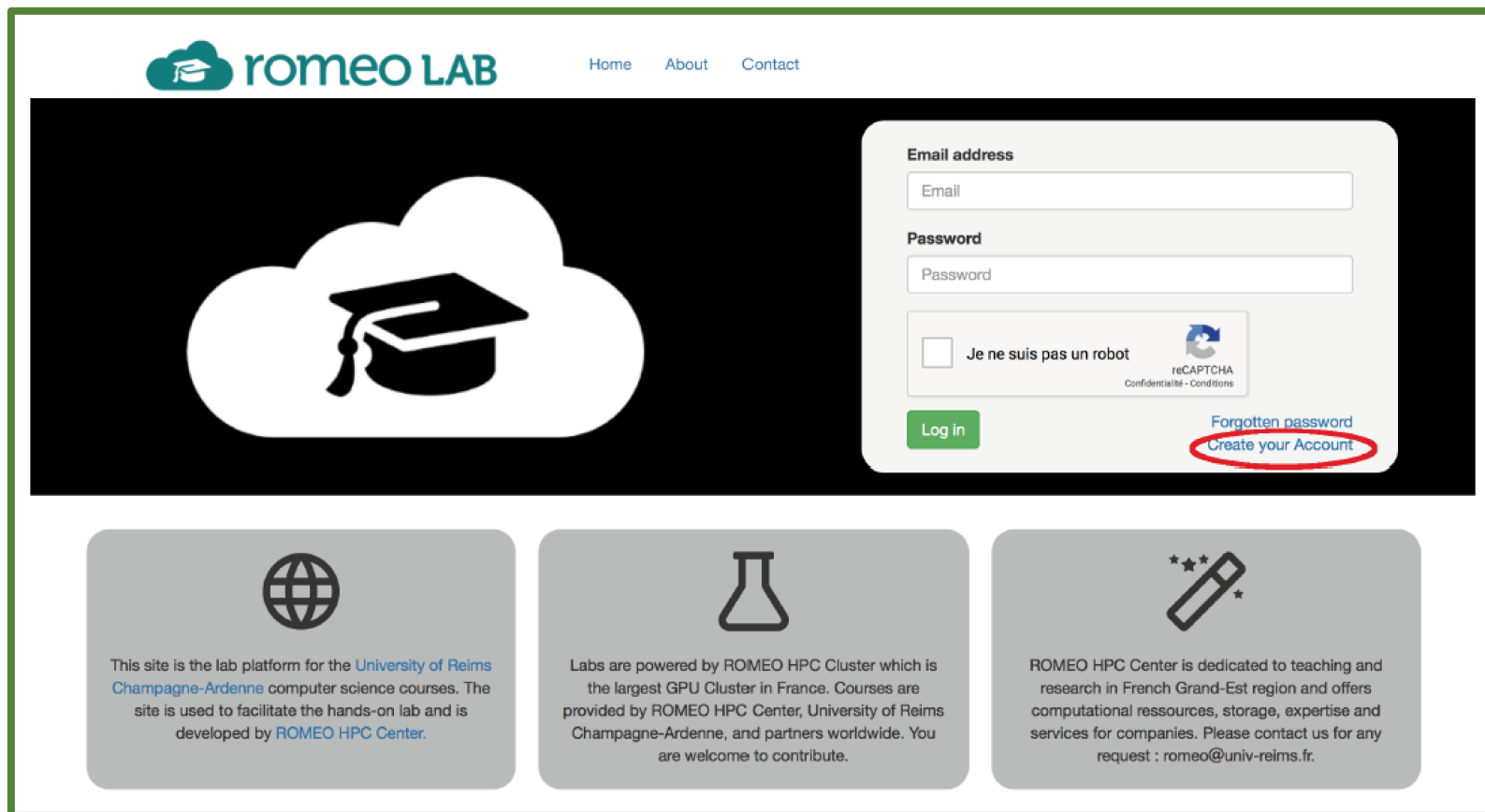
<http://igmplot.univ-reims.fr>

Réaction chimique SN_2



Interaction ligand-protéine






The screenshot shows the login page for romeo LAB. The header includes the romeo LAB logo and navigation links for Home, About, and Contact. The main content area features a large graphic of a graduation cap inside a cloud on the left, and a login form on the right. The login form has fields for Email address and Password, a checkbox for "Je ne suis pas un robot" (I am not a robot) with a reCAPTCHA logo, and a green "Log in" button. Below the form, there are links for "Forgotten password" and "Create your Account", with the latter circled in red. The footer consists of three grey boxes with icons and text: a globe icon for the lab platform, a flask icon for the HPC cluster, and a test tube icon for the HPC center's services.


romeo LAB Home About Contact


Email address
Email


Password
Password

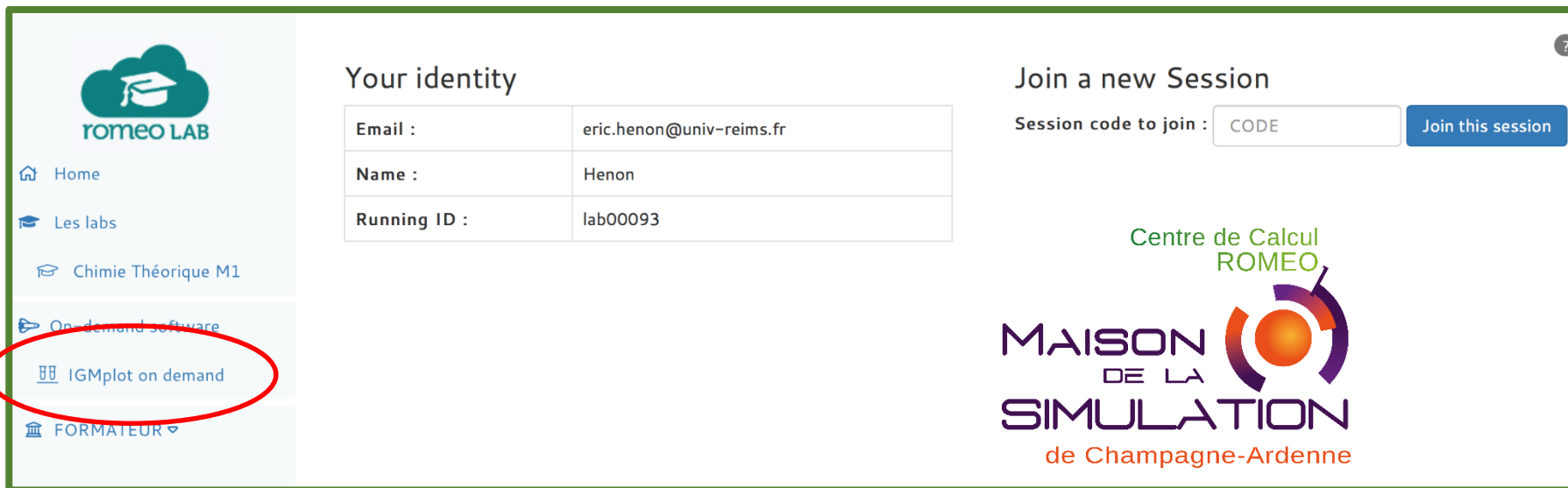
Je ne suis pas un robot 
reCAPTCHA
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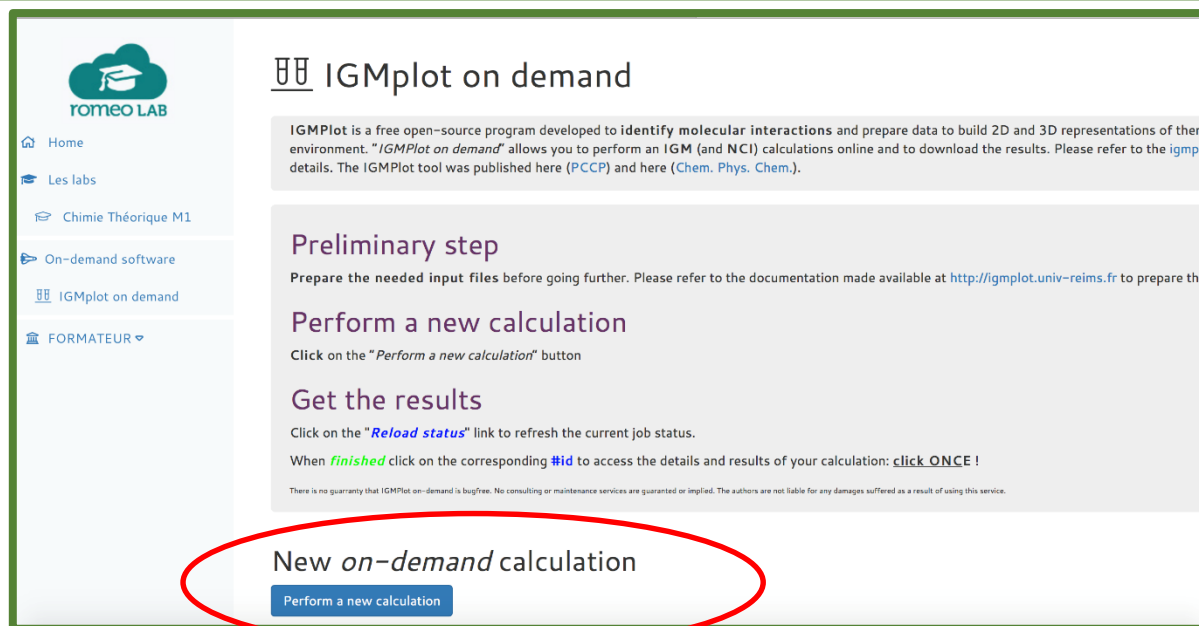
The screenshot shows the Romeo Lab dashboard. On the left is a navigation menu with the following items: Home, Les labs, Chimie Théorique M1, On-demand software, **IGMplot on demand** (circled in red), and FORMATEUR. The main content area is divided into three sections: 'Your identity' with a table, 'Join a new Session' with a form, and a logo for 'Centre de Calcul ROMEO MAISON DE LA SIMULATION de Champagne-Ardenne'.

Your identity	
Email :	eric.henon@univ-reims.fr
Name :	Henon
Running ID :	lab00093

Join a new Session

Session code to join :

Centre de Calcul ROMEO
MAISON DE LA SIMULATION
de Champagne-Ardenne



The screenshot shows the 'IGMplot on demand' page. The left navigation menu is identical to the dashboard, with 'IGMplot on demand' selected. The main content area contains the following sections:

IGMplot on demand

IGMPlot is a free open-source program developed to identify molecular interactions and prepare data to build 2D and 3D representations of them in a virtual environment. "IGMPlot on demand" allows you to perform an IGM (and NCI) calculations online and to download the results. Please refer to the [igmplo](#) details. The IGMPlot tool was published here ([PCCP](#)) and here ([Chem. Phys. Chem.](#)).

Preliminary step

Prepare the needed input files before going further. Please refer to the documentation made available at <http://igmplo.univ-reims.fr> to prepare these files.

Perform a new calculation

Click on the "Perform a new calculation" button

Get the results

Click on the "Reload status" link to refresh the current job status.

When **finished** click on the corresponding **#id** to access the details and results of your calculation: **click ONCE !**

There is no warranty that IGMPlot on-demand is bug-free. No consulting or maintenance services are guaranteed or implied. The authors are not liable for any damages suffered as a result of using this service.

New on-demand calculation

IGMPlot On-demand



DEMO

romeoLAB : actualités

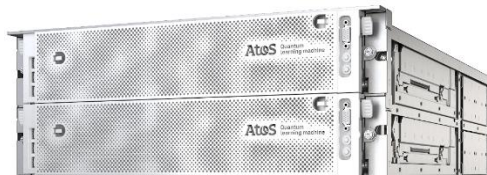


15 – 19
octobre



Open **FOAM**
formation
19-21 octobre 2016, REIMS
Programme / Informations / Inscriptions limitées
<https://romeo.univ-reims.fr/OpenFOAMSchool>

2 – 4
février



19 – 20
septembre

ECOLE D'AUTOMNE DGX-1 CENTRE DE CALCUL ROMEO
DEEP REIMS
LEARNING 24/25 OCT
<https://romeo.univ-reims.fr/DeepLearning>

8
novembre



DEEP
LEARNING
INSTITUTE



DEEP
LEARNING
INSTITUTE

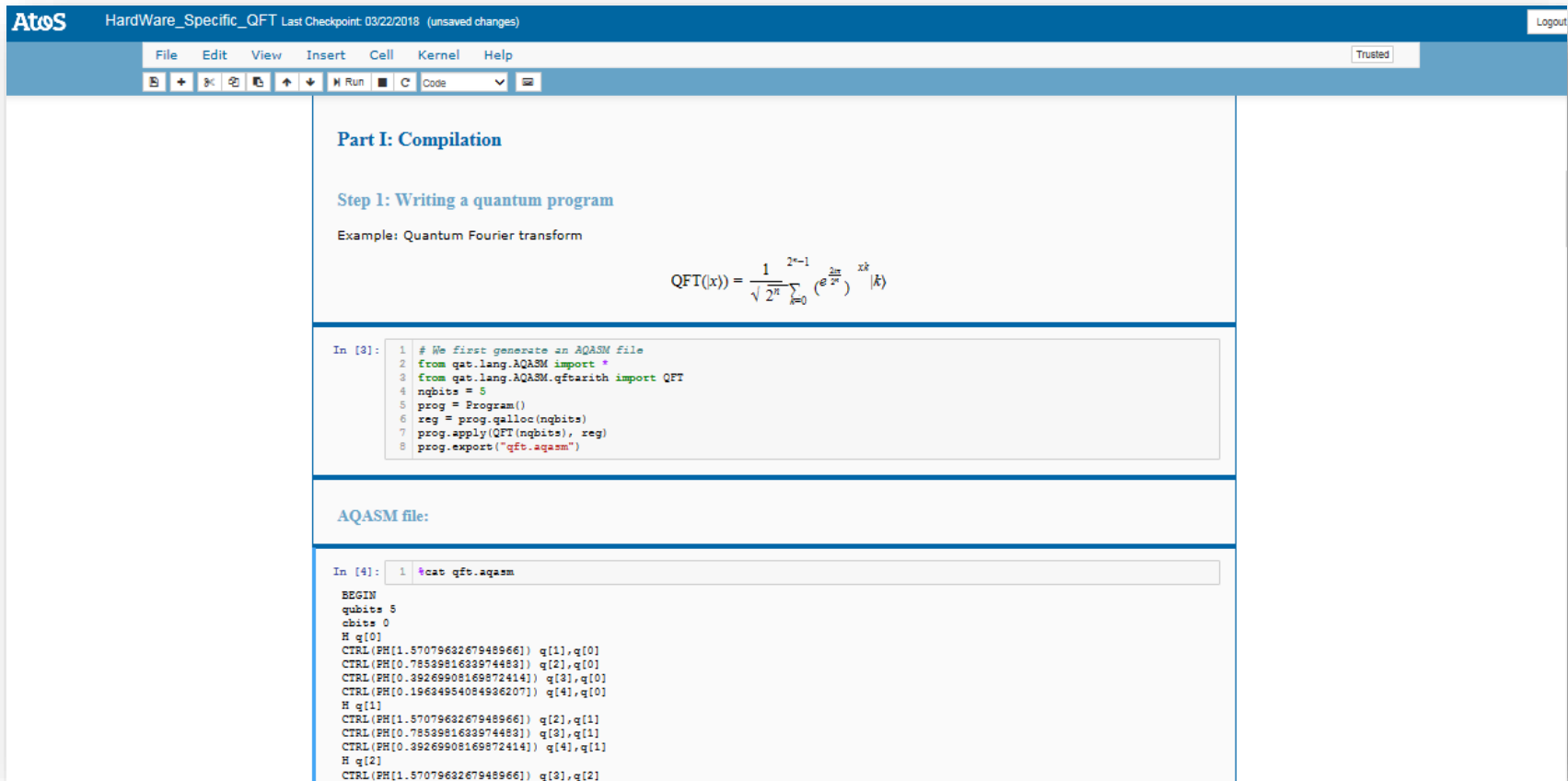
UNIVERSITY
AMBASSADOR



Université de Reims Champagne-Ardenne



romeoLAB : access single nodes (DGX - QLM - ...)



The screenshot displays the Atos QuantumLab web interface. At the top, the title bar reads "Atos HardWare_Specific_QFT Last Checkpoint: 03/22/2018 (unsaved changes)" and includes a "Logout" button. Below the title bar is a menu bar with "File", "Edit", "View", "Insert", "Cell", "Kernel", and "Help". A toolbar contains icons for file operations and a "Code" dropdown menu.

The main content area is titled "Part I: Compilation" and "Step 1: Writing a quantum program". It provides an example of a Quantum Fourier transform (QFT) and includes a mathematical formula:

$$\text{QFT}(x) = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} \left(e^{2\pi i \frac{xk}{2^n}} \right) |k\rangle$$

Below the formula, there are two code blocks. The first, labeled "In [3]:", shows a Python script for generating an AQASM file:

```
In [3]: 1 # We first generate an AQASM file
2 from qat.lang.AQASM import *
3 from qat.lang.AQASM.qftarith import QFT
4 nqubits = 5
5 prog = Program()
6 reg = prog.qalloc(nqubits)
7 prog.apply(QFT(nqubits), reg)
8 prog.export("qft.aqasm")
```

The second code block, labeled "In [4]:", shows the execution of the generated AQASM file:

```
In [4]: 1 %cat qft.aqasm

BEGIN
qubits 5
obsts 0
H q[0]
CTRL (PH[1.57079632679489666]) q[1],q[0]
CTRL (PH[0.7853981633974483]) q[2],q[0]
CTRL (PH[0.39269908169872414]) q[3],q[0]
CTRL (PH[0.19634954084936207]) q[4],q[0]
H q[1]
CTRL (PH[1.57079632679489666]) q[2],q[1]
CTRL (PH[0.7853981633974483]) q[3],q[1]
CTRL (PH[0.39269908169872414]) q[4],q[1]
H q[2]
CTRL (PH[1.57079632679489666]) q[3],q[2]
```





Perspectives *romeoLAB*

- Maintenir
- Version distribuable
 - nouveau supercalculateur
 - partenaires / opensource
 - rename
- Sécurité
- OpenStack & Single machie



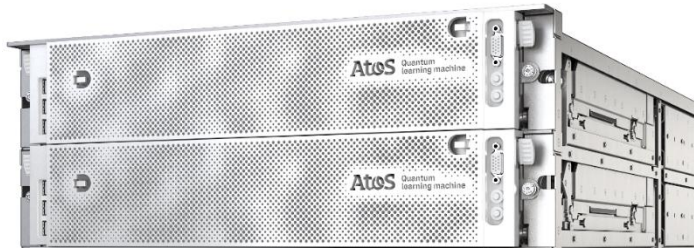


romeolab@univ-reims.fr



Quantum computing

- Solve difficult problems
 - Classical bit VS Qubits



- QLM Group (partners on right)
 - Quantum simulator platform
 - Develop new algorithms (BD, AI, SC, Cyber security)
 - Designing computing architectures
 - Quantum safe cryptography algorithms

