

OPTIMIZATION OF INDUSTRIAL CODES

Kick-Off Webinar

December 13, 2024













Daniel Verwaerde

Teratec Chairman













Agenda

4:00 PM: Welcome Address – *Daniel Verwaerde, Teratec*

4:10 PM: Presentation of Codes and Industrial Challenges:

4:10 PM: Code Aster – Cyril Baudry, EDF

4:25 PM: Code Serial – Patrick Demichel, Viridien

4:40 PM: Presentation of the Platform and Support:

Conrad Hillairet, ARM

Gilles Tourpe & Arthur Petitpierre, AWS

Benjamin Depardon, UCIT

5:15 PM: Q&A Session

5:30 PM: Webinar Closing













2024

Teratec HACKATHON HPC 2025

Timeline

Machine access and technical support Monday, January 20, 2025, 9 AM to Friday, January 25, 2025, 7 PM



September to November 25, **December 13, 2024**

1 week virtual competition

Monday, January 20, 2025, 9 AM to Monday, January 27, 2025, 9 AM

Awards Ceremony

May 22, 2025 @ FORUM **TERATEC**













Communication



- Linkedin post
- Twice a week, starting from December 16
- Focus on teams and Schools











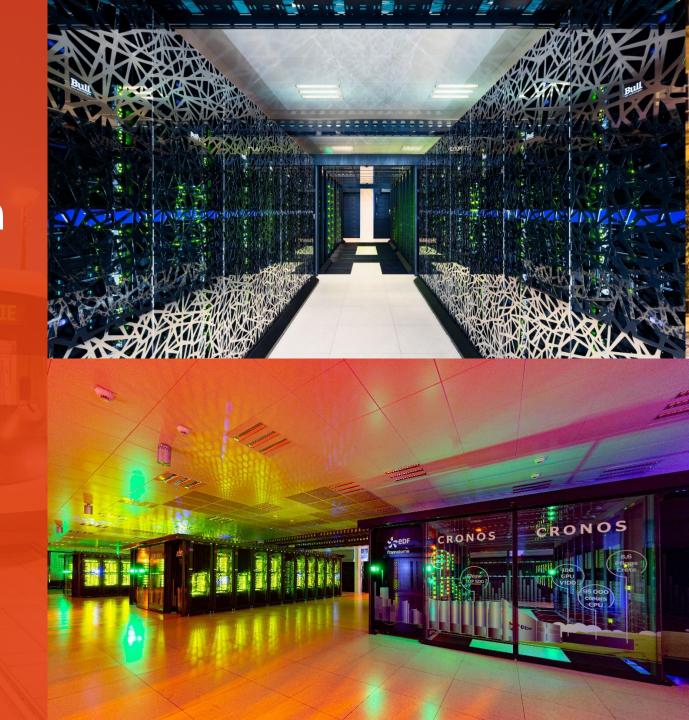


Hackathon HPC 2025: Code_aster presentation

Cyril BAUDRY

Scientific Information System Architect, EDF R&D HPC senior expert

2024/13/12



EDF IN BRIEF



EDF GROUP PRESENTATION

OUR raison d'être

EDF adopted its raison d'être in 2020 :

Building a net zero energy future with electricity and innovative solutions and services, to help save the planet and drive wellbeing and economic development.

KEY FIGURE!



40.3 million customers around the world

143.5 billions euros of sales 171 490 employees throughout the world

22

431.7 TWh electricity generated by EDF Group

649 million
euros
research and develoment
budget

90 % production free from CO2 emissions

The Group integrates all activities between upstream and downstream.

As a major player in the energy transition, EDF is present in production, transport, distribution, trading, energy sales and energy services...

Electricity generation

EDF produces safe, affordable and carbon-free electricity in power plnats which it designs and operates.

Energy supply

The EDF Group sells energy and energy services to nearly 40 million client sites around the world.

Transmission and distribution

The transmission and distribution networks carry electricity to the end customer while balancing supply and demand.

Optimisation and trading

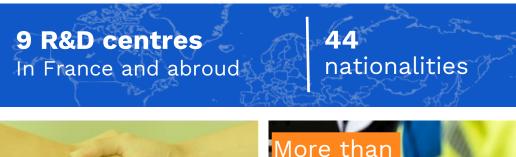
This activity allows EDF to fulfil the energy supply commitments made to its customers by choosing between available resources.



R&D IN FIGURES (2023)













2 178 patents



11 petaflopsComputing capacity



21 joint laboratoires



EDF POLICY: SOME CONTEXTUAL ELEMENTS TO INTEGRATE

Plants operated over 40 – 100 years

- · Guarantee safety, minimize environmental footprint
- Maintain assets

Fast changing operating conditions

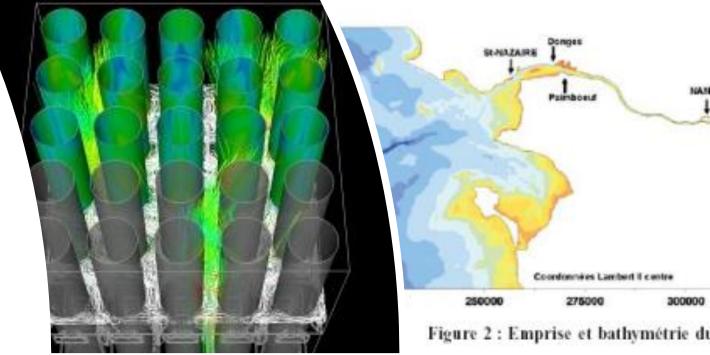
- More competitive markets,
- Tougher regulations, ageing, environment

New business models and services

- Data science, Open Data, Artificial Intelligence, Blockchain,
- Cloud computing
- Smart meters

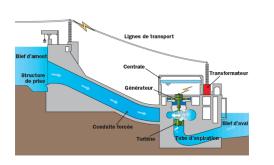
Energy Transition

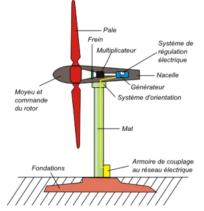
- Diversified energy mix (nuclear, renewables,...)
- Products and services, energy-saving solutions, help customers to manage their consumption
- A dual digital and energy transition for both society and the economy





Main domains of HPC applications (both Physical Simulation and Data Analysis)





ENERGY PRODUCTION (Nuclear, Renewable, Hydraulic, Thermal, Environment)







Network / Smarties (smart-grids, smart-cities)



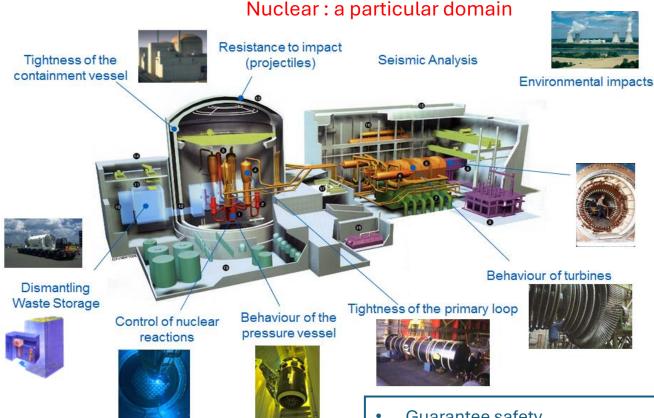
Marketing



Energy Management

Benefits of the HPC:

- Less simplifying assumptions
- More information
- More calculation scenarios
- Take into account incertainties



- Guarantee safety
- Improve performances/costs
- Maintain assets
- Face unexpected events
- Ageing issues...

Simulation at EDF: a key element to support studies for their operation

Codes developed at EDF R&D

... a know-how in the state of international art and accessible by all thanks to the Open Source!

- Code Saturne ((i.e. SALOME-CFD)
 - general usage single phase CFD, plus specific physics
 - property of EDF, open source (GPL)
 - http://www.code-saturne.org





- multiphase CFD, esp. water/steam
- property of EDF/CEA/AREVA/IRSN DUPTUDE



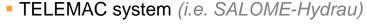
SYRTHES

- n thermal diffusion in solid and radiative transfer
- property of EDF, open source (GPL)
- https://www.syrthes-software.org/

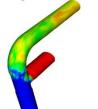


- Code_Aster (i.e. SALOME-MECA)
 - general usage structure mechanics
 - property of EDF, open source (GPL)
 - http://www.code-aster.org





- ☐ free surface flows
- Many partners, mostly open source (GPL, LGPL)
- http://www.opentelemac.org



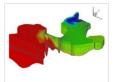
SALOME platform

- integration platform (CAD, meshing, post-processing, code coupling)
- property of EDF/CEA/OpenCascade, open source (LGPL)
- http://www.salome-platform.org



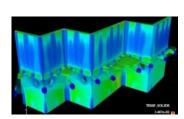
Open TURNS

- tool for uncertainty treatment and reliability analysis
- property of EDF/CEA/Phimeca, open source (LGPL)
- https://openturns.github.io/www/



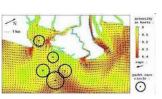
and many others...

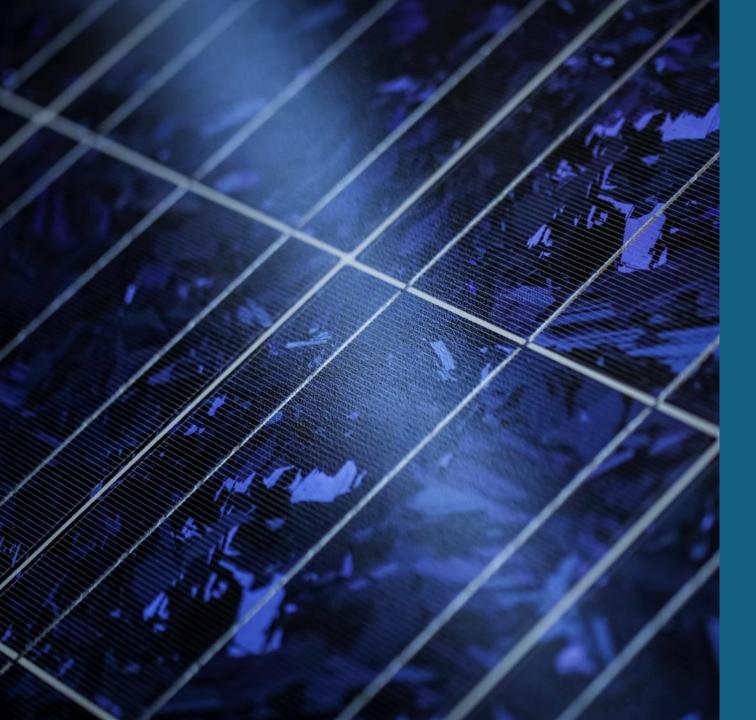
- Neutronics, electromagnetism
- Component codes, system codes
- Optimization codes....











salome_meca:
EDF R&D simulation
platform for structural
mechanics

CODE aster



A SIGNIFICANT RANGE OF STUDIES

- Licenses are expensive
- Dependent on the software provider for specific applications
- Sometimes you don't find the advanced method you need on the simulation market
- ☐ The workflow of study changes from a tool to another
- Different simulation environments generate compatibility issues
- Ensuring a 100 years-old archive of the numerical studies may be complicated

- □ Civil engineering□ Fracture mechanics□ Seismic analyses□ Soil mechanics
- Metallurgy
- ☐ Fuel Assemblies
- □ Rotation machines
- □ Vibrations and acoustics,
- □ .. And much more

Every field has specific and different needs: functionalities, ergonomic, performance, etc.

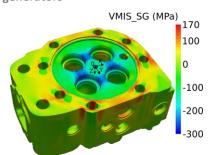
Thus, *many* simulation softwares are employed

But...

FROM RESEARCH TO TECHNOLOGY TRANSFER

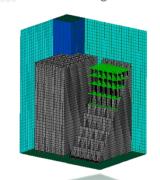
Cylinder heads cracking of 900 MWe reactors back-up diesel generators



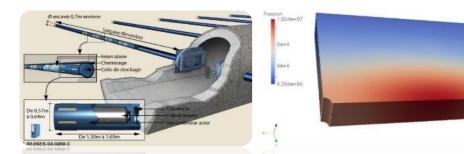


Behaviour of fuel racks under seismic loading



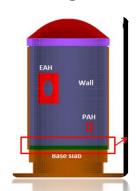


Optimization of sub-surface storage site for nuclear waste



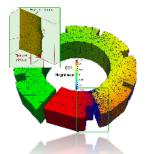
Behaviour of containment buildings



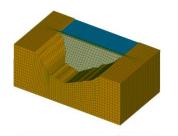


Analysis of cracking in graphite bricks (UK)





Civil structures subjected to earthquakes





QUALITY INSURANCE



1M source code lines



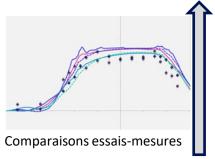
25 000 documentation pages



4 200 verification testcases

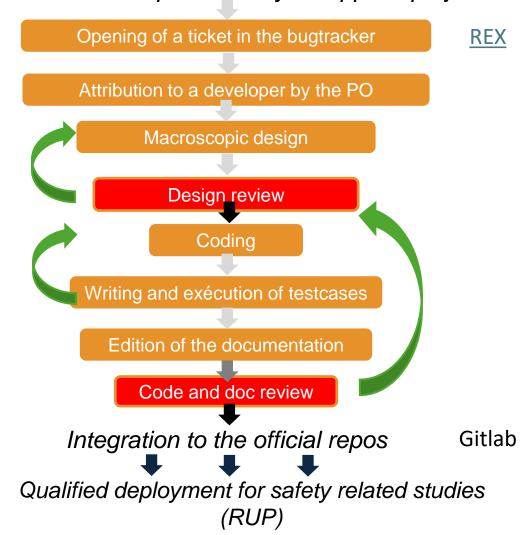


420 validation tests

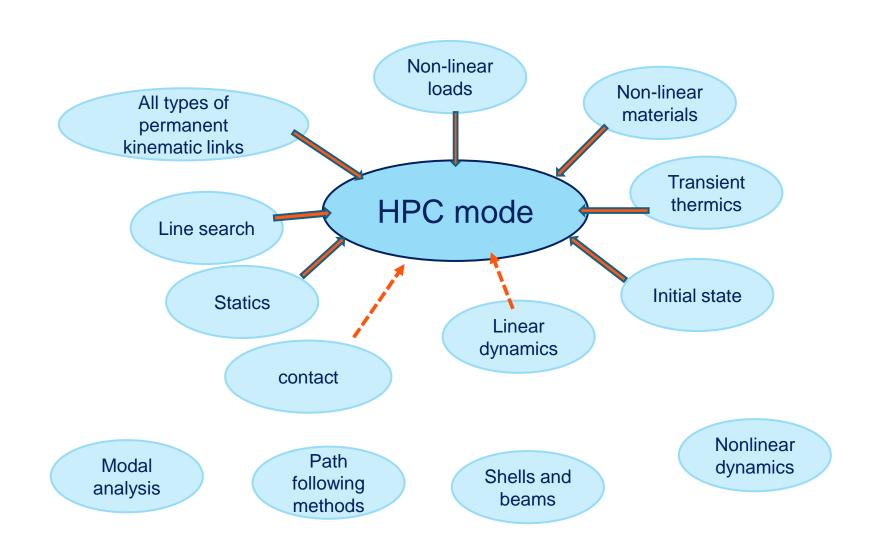


Specific facility or equipment project

Statement of need by an engineering unit Technical requirement by an applied project



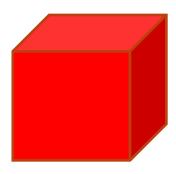
HPC COMPUTATIONS: SUPPORTED ANALYSES



HPC FUNCTIONALITIES: EXAMPLES AND RESULTS

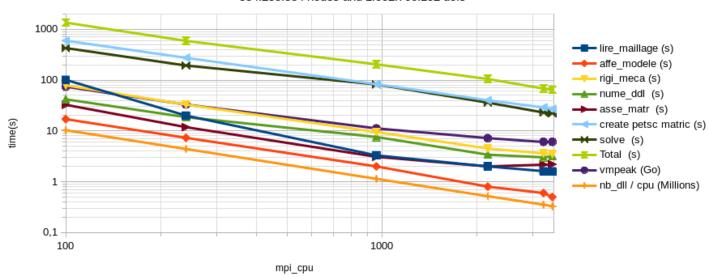
Elastic cube over 1Md Dofs

- Demonstrates the efficience of data distribution
- And scalability of all operations for a linear problem



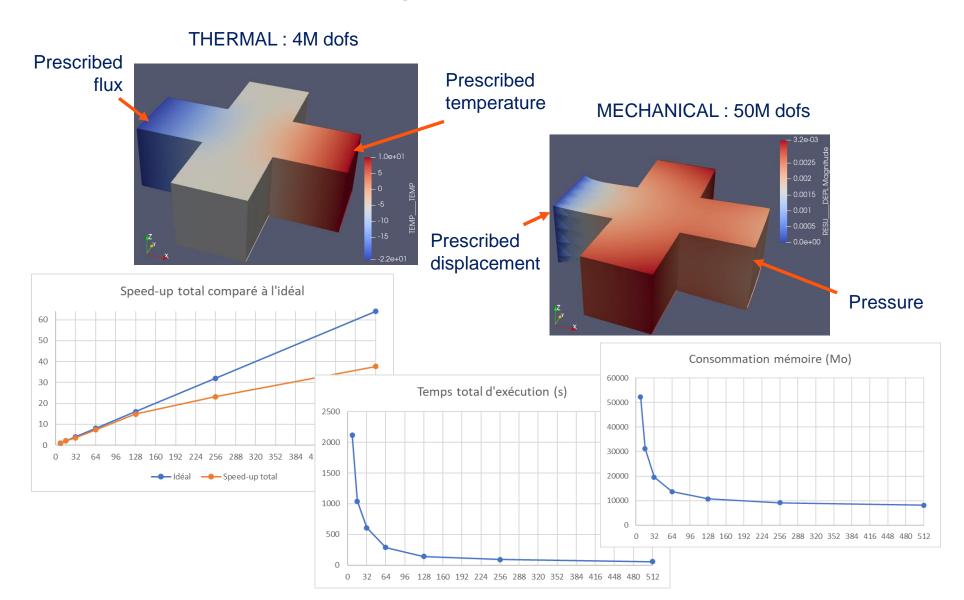
Cube694 (mpi gcc + gaia)

334.255.384 nodes and 1.002.766.152 dofs



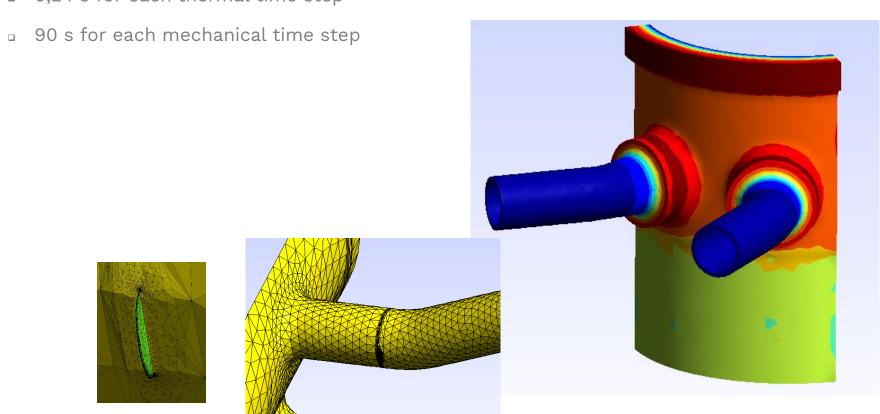
HPC FUNCTIONALITIES: EXAMPLES AND RESULTS

Linear thermomecanic computation

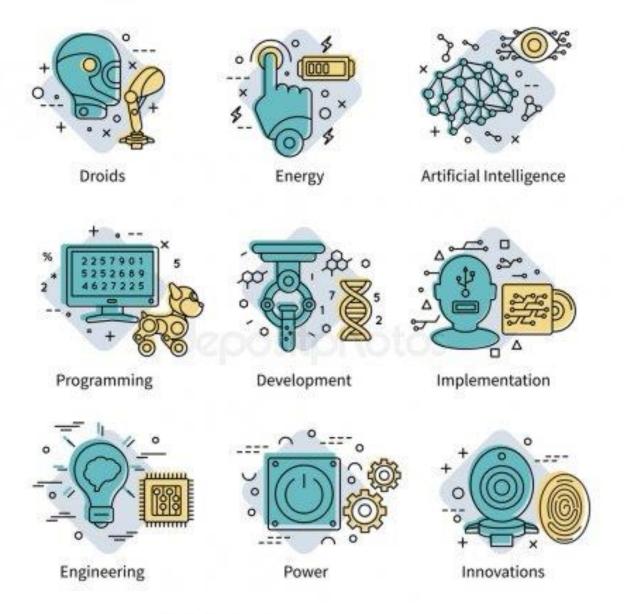


HPC FUNCTIONALITIES: EXAMPLES AND RESULTS

- Thermal shock (elasto-plasticity) on a portion of vessel
 - Transient linear thermics, then statical elastoplastic computation
 - 5M dofs thermics, 127M dofs mechanics
 - 1920 MPI processes
 - 0,24 s for each thermal time step

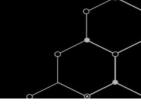


Energy needs modelization, simulation ... and more and more artificial intelligence!



Thanks you for your attention





OPTIMIZATION OF INDUSTRIAL CODES

Black-Scholes Tuning

Hafsa Demnati **Patrick Demichel**

December 13th, 2024





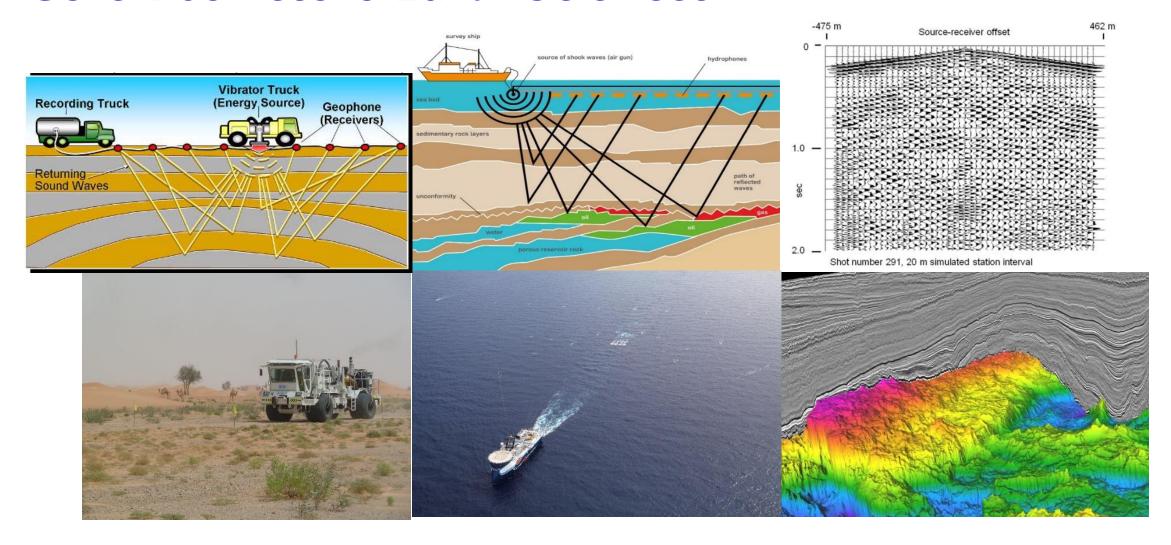








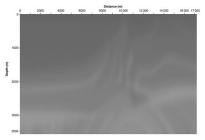
Core Business is Earth Sciences



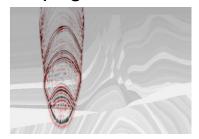
What is seismic imaging? Why the HPC is so critical

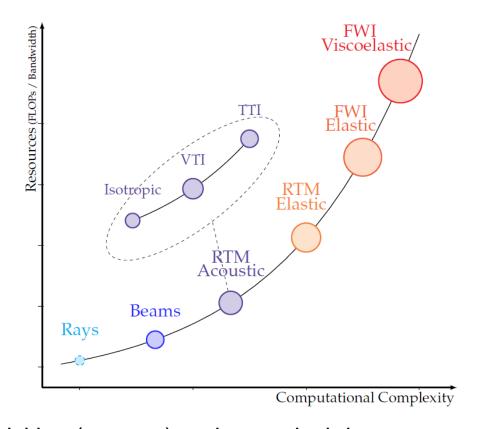
Inversion algorithms RTM,FWI...

Start with initial velocity/density model

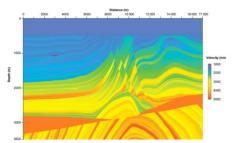


Propagate waves and record data « numerically »

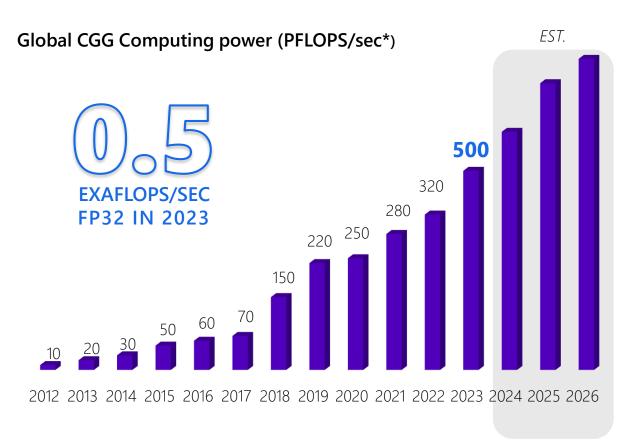




Compute differences between data acquisition (surveys) and numerical data + Compute gradient + update velocity/density model



High Performance Computing – a core industrial asset in CGG

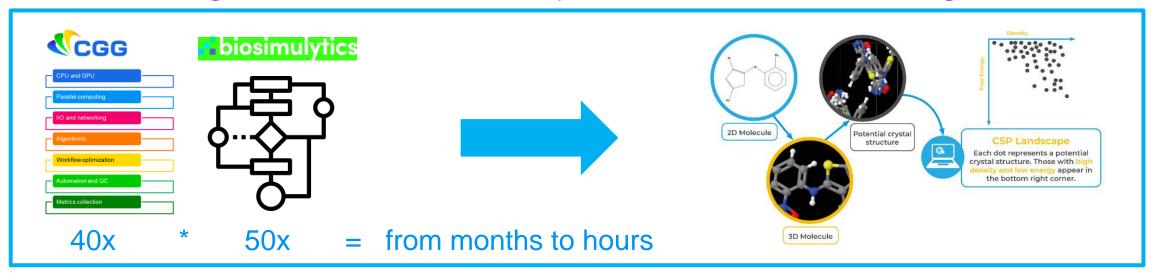






- The largest compute power in Energy running the worlds most advanced algorithms for seismic data
- Highly-optimized HPC resources and digital platform

New business: Viridien now helps other customers to make breakthrough on extreme compute intensive challenges



Extreme-scale AI and HPC computations require achieving significant leaps in performance, which can only be realized through the collaboration of experts from various fields.

Our partnership with **CGG** has proven to be a game-changer, thanks to the substantial enhancements we've made to our codes. This marks just the initial stages of our exciting journey.

Peter Doyle: CEO and cofounder of hiosimulytics



15mn at 4:25 PM: Code Serial – *Patrick Demichel, Viridien*

The 2025 challenge is a classical algorithm used by banks and insurance companies to protect enterprises from the risk of price fluctuations of the core resources they need to purchase during long-term projects.

The code mimics real-world usage but has been adapted specifically for this Hackathon. It reflects exactly what an HPC expert would do if tasked with optimizing a production code.

We expect participants to focus on parallelization and tuning on the ARM architecture. The objective is not only to achieve high performance but also to reach a precise quality objective.

More details are provided in two documents that will be distributed at the start of the Hackathon. We will also be available to assist throughout the week.











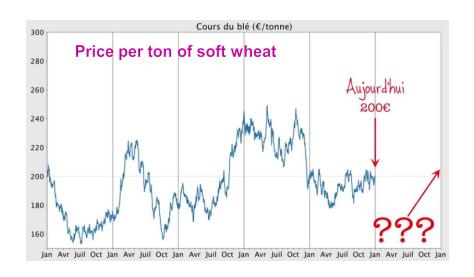
Basic products

Large fluctuations observed on commodity products

e.g: Order of 10K croissants to be delivered in 1 year for a reception.

How to guarantee a price without losing money?

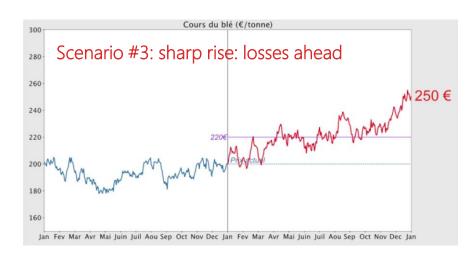


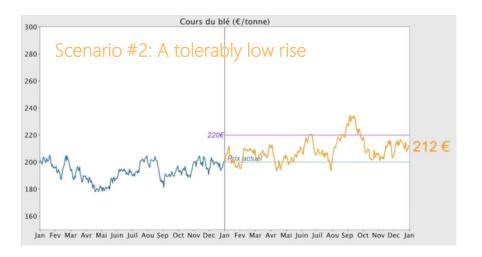




Several possible scenarios

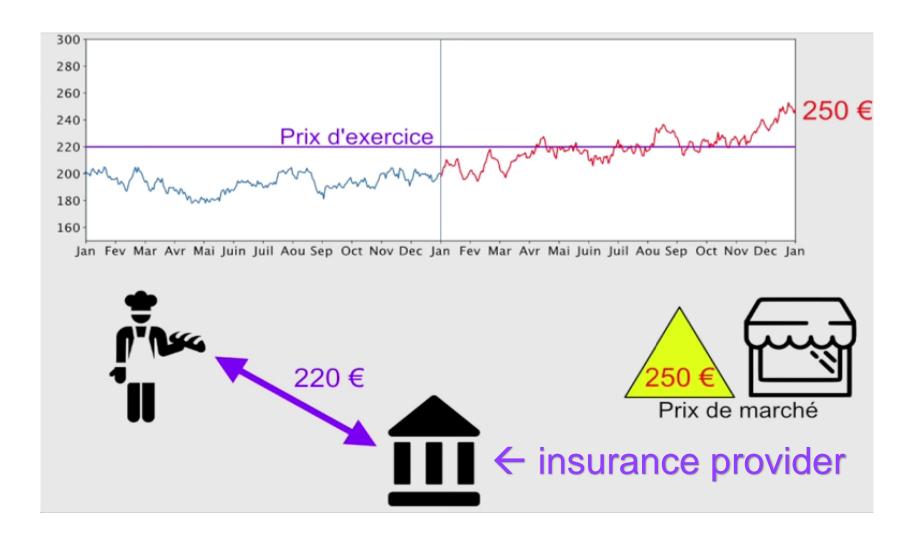




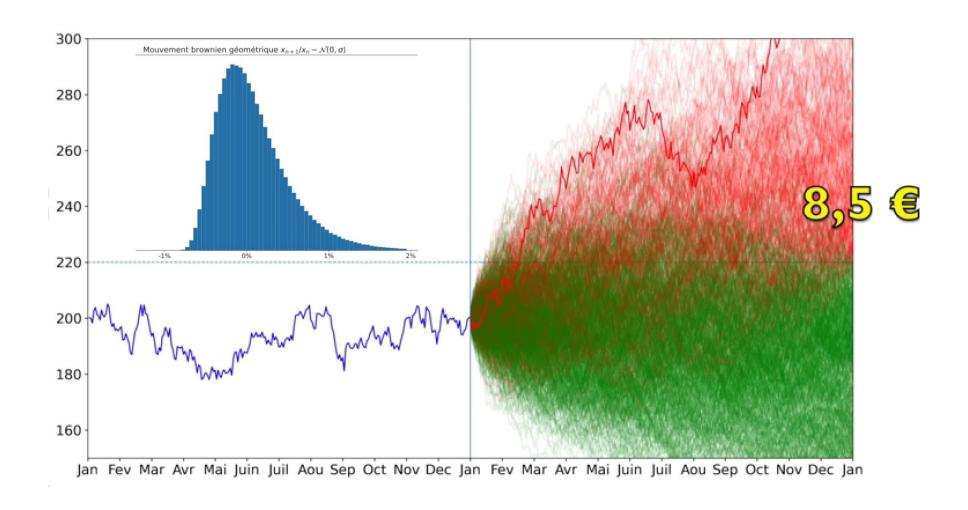




Call option exercised: price paid €220



Example: option price for 220 euros



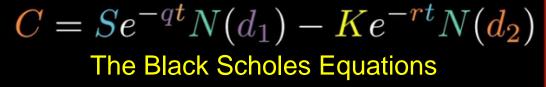
Can we eliminate the risk of waiting for the deadline?



In 1997, Robert Merton and Myron

Scholes were awarded the Nobel Prize in

Fisher Black (who died in 1995), on the



$$P = Ke^{-rt}N(d_2) - Se^{-qt}N(d_1)$$

the Black-Scholes model

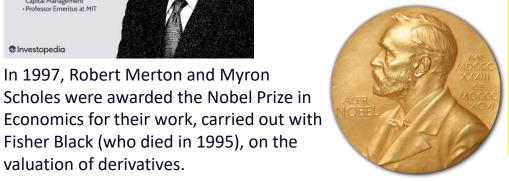
valuation of derivatives.

- Former principal of Long-Term
- Capital Management Professor Emeritus at MIT

Investopedia



- S = Underlying price (\$)
- K = Strike price (\$)
- = Volatlity (% p.a.)
- Continuously compounded interest rate (% p.a.)
- = Continuously compounded dividend yield (% p.a
- t = Time to expiration (% of year)



$$N(\mathbf{x}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\mathbf{x}} e^{\frac{-t^2}{2}dt}$$

$$d_1 = \frac{\ln \frac{S}{K} + t(r - q + \frac{\sigma^2}{2})}{\sigma \sqrt{t}}$$

$$d_2 = d_1 - \sigma \sqrt{t}$$

Expected performances for error reduction

Main goal: Analyze and tune the Black-Scholes application given to get the best precision.

Average error	Time expected (Arm)
0.001	10 hours
0.01	10 minutes
F .:	

<u>Estimated Time Based on Computed Error for Optimized Code</u>

For safety, we propose two error thresholds to aim for:

- 0.005
- 0.002

arm

Teratec Hackathon Edition #3

Conrad Hillairet – Staff HPC Engineer conrad.hillairet@arm.com

13th December 2024





Arm Compute Platform is the Most Pervasive in History

5
4
3
2
1
0
(Millions of Chips)
Legacy PC Orm Open Source

Arm Technology

280+ Billion

Arm-based chips shipped to date.

30.6 Billion

Arm-based chips shipped in FYE23.

18M+

Software developers on Arm.

The global leader in the development of licensable compute technology

R&D excellence for semiconductor companies and large OEMs.

Arm's power-efficient processor designs and software platforms enable advanced

Our technologies securely power products from the sensor to the smartphone and the supercomputer.

Arm delivers the foundational building blocks for trust in the digital world

Arm provides enhanced system-level security technologies such as Arm TrustZone and Arm Confidential Compute Architecture (CCA).



Arm HPC Ecosystem

Hardware

Benefit from the various solutions of all the partners of the Arm HPC Ecosystem

Azure Cobalt 100 **AWS Graviton Google Axion NVIDIA Grace**



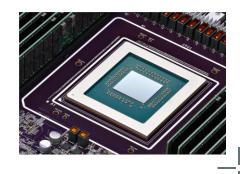














Google Cloud



AWS Graviton 4 Processor

Based on Arm Neoverse V2









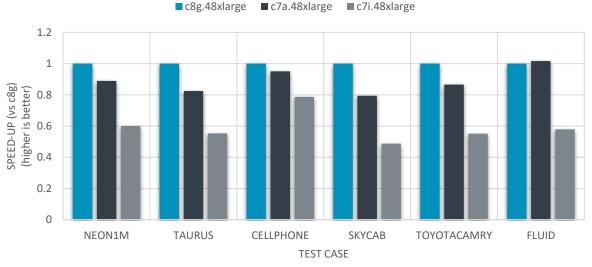


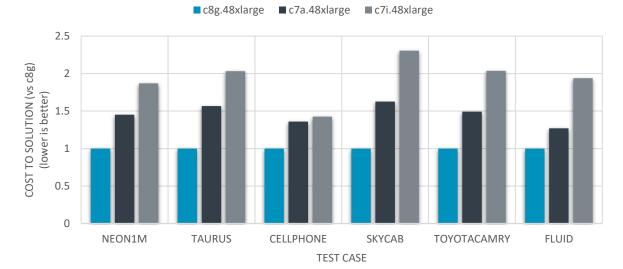


Altair OpenRadioss

AWS EC2 Instances benchmark







Competitive performance

Arm Neoverse V2-based AWS Graviton 4 processors gives competitive performance against AMD Genoa-based and Intel Sapphire Rapids-based instances.

Leading cost to solution

Graviton 4 shows great benefits in terms of price-performance compared to x86 instances.



I have no experience with Arm

Should I be worried?



Overthinking:

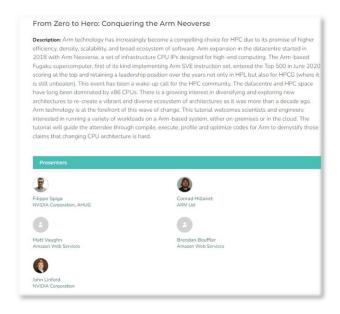
The art of creating problems that weren't even there.



Most applications compile on Arm architecture with little to no modification

- All major Linux distributions support Arm, with extensive library of common packages (AArch64).
- Upgrading to newer library / software versions might be needed.
- GNU Compiler Collection (GCC) and LLVM are fully supported.
- Commercial compilers for Arm are available.





https://github.com/arm-hpc-user-group/sc23-tutorial-neoverse



arm COMPILER

Arm provided C/C++/Fortran compiler with best-in-class performance



Compilers tuned for Scientific Computing and HPC



Latest features and performance optimizations



Freely available

Tuned for Scientific Computing and HPC workloads

- Processor-specific optimizations for Neoverse-based platforms
- Optimal shared-memory parallelism using latest Arm-optimized OpenMP runtime

Linux user-space compiler with latest features

- C++ 17 and Fortran 2003 language support with OpenMP 4.5
- Support for Armv8-A and SVE architecture extension
- Based on LLVM and Flang, leading open-source compiler projects

Freely available on leading Linux distributions

Documentation

- Fortran: https://developer.arm.com/documentation/101380/latest
- C/C++: https://developer.arm.com/documentation/101458/latest



arm Performance libraries

Optimized BLAS, LAPACK and FFT for HPC applications







Arm provided 64-bit Armv8-A math libraries

- Optimized BLAS, LAPACK, FFT and math.h routines
- FFTW compatible interface for FFT routines
- Sparse linear algebra and batched BLAS support

Best-in-class serial and parallel performance

- Generic Armv8-A optimizations by Arm
- Tuned for Arm Neoverse family of processors

Validated by Arm Engineers

- Validated with NAG's test suite, a de-facto standard
- Community supported

Documentation

https://developer.arm.com/documentation/102620/latest



GNU compilers are a solid option

- With Arm being significant contributor to upstream GNU projects
- GNU compilers are first class Arm compilers
 - Arm is one of the largest contributors to GCC
 - Focus on enablement and performance
 - Key for Arm to succeed in Cloud/Data center segment
- GNU toolchain ships with Arm Allinea Studio
 - Best effort support
 - Bug fixes and performance improvements in upcoming GNU releases
- GCC 14.2.0





MPI

+ Parallel Programming



- Supported since 3.1.2 (currently 4.1.7 & 5.0.6)
- Provided by default on AWS EC2
 Graviton instances
- + Upstream contributions
- → Used inhouse
- Active development from Arm and Arm partners



Support

→ How can I get some help during the event ?

- → Via Slack
 - 1. Join the AHUG Slack Workspace
 - + You may receive an invitation prior to the event
 - + Link available here https://a-hug.org/contact/
 - 2. Join the **teratec-hackathon-hpc** slack channel
 - + Send a private message to Conrad Hillairet
 - 3. Ask your questions:
 - In the slack channel
 - Using private message to Conrad Hillairet
 - + Email
 - conrad.hillairet@arm.com







Thank You
+ Danke
Gracias

Grazie 谢谢

ありがとう

Asante

Merci

감사합니다

धन्यवाद

Kiitos

شکرًا

ধন্যবাদ

תודה ధన్యవాదములు



Graviton4 introduction

Arthur Petitpierre

Graviton Principal SA Amazon Web Services



Graviton4

96 Neoverse V2 Cores

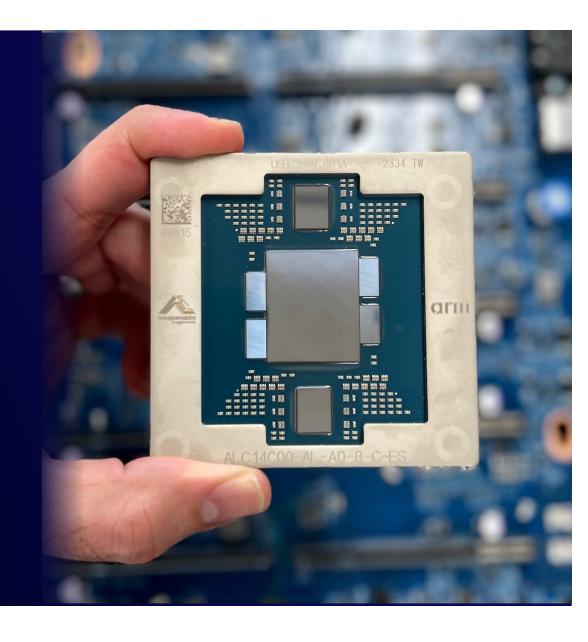
2M L2 cache per-core

Seven chiplet design

12 DDR5-5600 channels

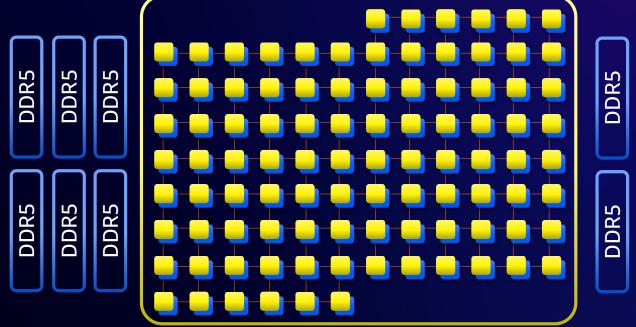
Up to 96 lanes of PCIe gen5





Graviton4 – Chip

PCle gen5



DDR5 DDR5

DDR5

DDR5

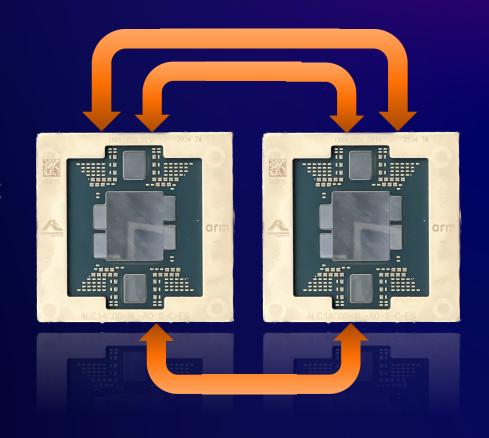
PCle gen5



Graviton4 Scale Up

EXPANDING WORKLOADS GRAVITON APPLIES TO

- Single socket 24xl (96 vCPUs)
 - 50% more cores-per-socket than Graviton3
- Support for coherent multi-socket
- Single systems with up to:
 - 3x more cores than Graviton3
 - 3x more DRAM than Graviton3





Flexible Dual-Socket Configurations

Four operating modes enabled by Nitro

- Two non-coherent virtual
- One coherent virtual instance
- Two metal instances
- One coherent metal instance

Save power when not operating in coherent mode





Focusing on Real Workload Optimization

	Graviton3 (V1)	Graviton4 (V2)	
Caches			
L2 Cache per core	1MB	2MB	
Branch Prediction			
NanoBTB	96	1k	
ВТВ	8k	4k+12k	
Fetch Queue	16 entries	32 entries	
Fetch Buffer	12 entries	16 entries	
Architecture Features			
SIMD	SVE	SVE2	
Control flow integrity	PAC	PAC+BTI	
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Thank you!

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Teratec Hackathon HPC

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one thing is sure... **Hybrid** is the future of HPC



The question is **HOW TO GET THERE?**



Your key partner for Hybrid HPC





















HPC Cloud Journey

Consulting

Build

Run



Identify HPC Workloads and their On-Premises Behaviour



Understand the appropriate Move to Cloud Strategy



HPC Reference Architecture



Prototype / Test / Benchmark Integration & Move-to-Cloud



CCME Support & Professional Services





Storengy Moves HPC to AWS, Runs Geoscientific Simulations 2.5 Times Faster

2021

Storengy, a subsidiary of the ENGIE Group, is a leading supplier of natural gas. The company offers gas storage, geothermal solutions, carbon-free energy production, and storage technologies to enterprises worldwide. To ensure its products are properly stored, Storengy uses high-tech simulators to evaluate underground gas storage, a process that requires extensive use of high-performance computing (HPC) workloads. The company also uses HPC technology to run natural gas discovery and exploration jobs.

For many years, Storengy ran its HPC workloads in an on-premises IT environment, but it struggled to manage an increase in jobs. "Our HPC environment was not designed to scale easily. We had to do larger simulations in a very short time as our business grew, and we lacked the ability to support the gas exploration workloads," says Jean-Frederic Thebault, engineer at Storengy.

Storengy also sought to accelerate the deployment of HPC clusters for its engineers. "It typically took weeks or sometimes months to provision server clusters for a new project," says Thebault. "We wanted our engineers spending their time on research, not provisioning."





Using the CCME tool on AWS, we can deploy HPC resources in 30 minutes, compared to the weeks or months it would take to procure servers and provision compute in our on-premises environment."

Jean-Frederic Thebault
Engineer, Storengy



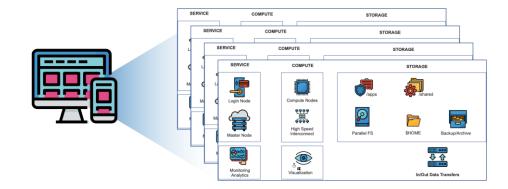


What is CCME?

Solution to transparently **build customizable HPC clusters in AWS**



Match workloads' needs: adapt the type and number of compute resources, provision a high-performance network and file system, automatically scale in and out...



adaptability simplicity
data management
heterogeneity publish services
remote visualization

standard jobs scheduler accessibility
web interface user management security
cost management



Cluster-in-a-Box: For An easy AWS Cloud Journey

UCit manages it for You

Cost & Budget under Control

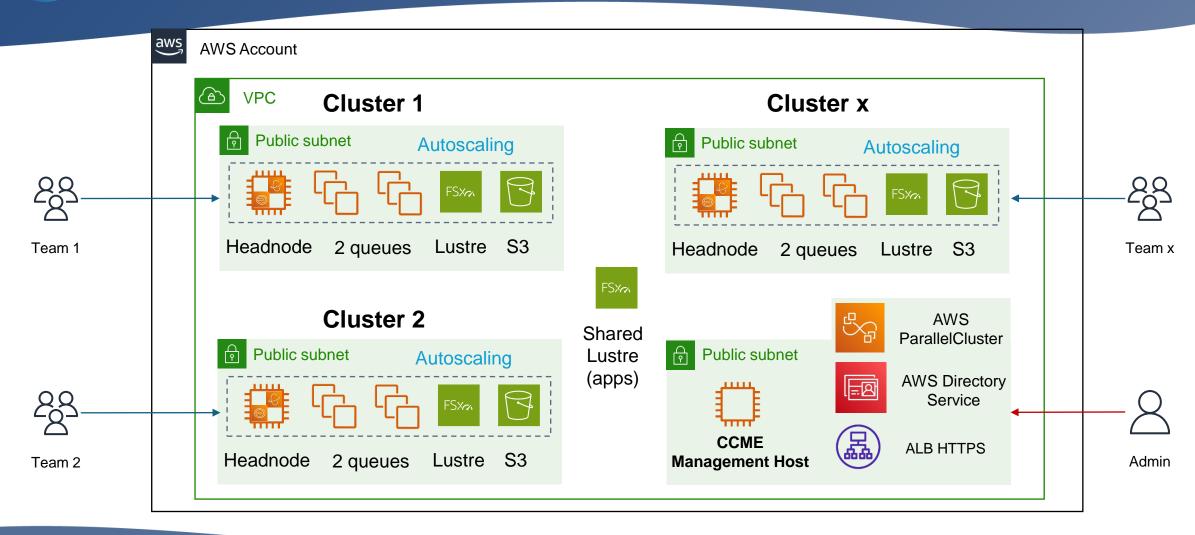


Your HPC Cluster of CHOICE on AWS...

Simple Access through SSH or a Web Portal



Hackathon Architecture





Cluster available for each team

- Each cluster is fully isolated from the others (network, accounts...)
- Job scheduler: SLURM
- Headnode: c8g.4xlarge (16 vCPUs, 32 GiB)
- Compute, 2 queues
 - c8g.24xlarge (96 vCPUs, 192 GiB) 1 instance
 - c7g.16xlarge (64 vCPUs, 128 GiB) 1 instance
- Storage
 - Shared NFS 500GiB (/home)
 - FSx for Lustre 1.2TB (/fsx)
 - S3 for results
- Remote access
 - SSH connection to frontend node through login/password
 - Web portal EnginFrame



The Hackathon Box

Available from Monday 9AM to Friday 7PM



Learn more at

www.ucit.fr



Teratec HACKATHON HPC 2025

THANK YOU **GOOD LUCK!**









