



EXPLORING THE FRONTIERS OF DIGITAL INTELLIGENCE





Training Agenda

- *09h00 – 09h30 – Morning coffee*
- **09h30 – 10h30 – Introduction to MeluXina – HPC Infrastructure**
- **10h30 – 11h45 – Introduction to Quantum Computing**
- *12h00 – 13h00 – Lunch break*
- **13h00 – 15h00 – Quantum Computing in Action – Quantum Simulator on GPU**
- *15h00 – 15h30 – Coffee break*
- **15h30 – 17h30 – Introduction to SYCL for accelerator to Run Quantum Simulators**
- *17h30 – 17h35 – Conclusion*



Expectations

- This training is an introduction on “*how to use MeluXina for simulating quantum circuits/algorithms*”
- Quantum Computing is a vast and large topic encompassing many fields (quantum mechanics, complexity theory, computability theory...)
- Every topic we will cover deserves days/months/years on their own

LuxProvide's supercomputing platform unleashes the power of data through AI, advanced analytics and simulation to explore the frontiers of the digital intelligence.



EuroHPC
Joint Undertaking





EuroHPC
Joint Undertaking

European High Performance Computing Joint Undertaking

Over 8 billion Euro for cutting-edge supercomputing and quantum computing ecosystem in Europe



European Network of Competence Centers in HPC

United network of HPC actors in 33 European countries to foster adoption of HPC



European Master for HPC

Pan-European Master's program by leading educational institutions focused on HPC





WE SERVE

RESEARCH



PUBLIC



BUSINESS



>600 projects | >2100 users from Luxembourg, Europe and beyond



When it was launched in June 2021, the MeluXina accelerator module has been ranked:



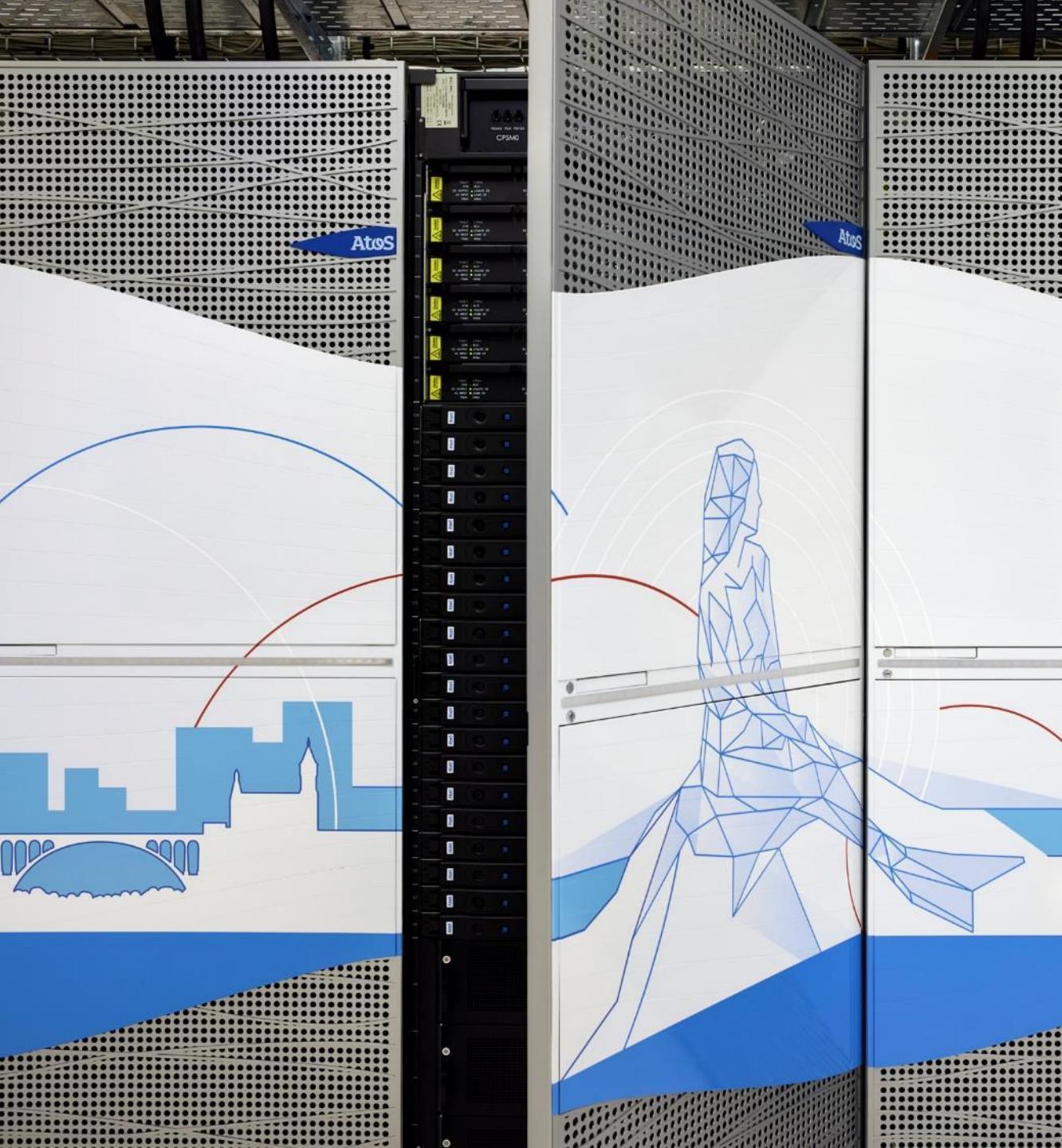
TOP500 in 2021

36th



GREEN500 in 2021

4th 1st
(world) (EU)





We guarantee **high-speed** and **low latency** connectivity, advanced applications, the easiest onboarding and the **highest quality** assistance, in a confidential, trusted, and cybersecured environment.



**DATA
SOVEREIGNTY**



**DATA CENTER
TIER IV**



ISO 27001

They have already trusted us





GREEN TIER IV DATACENTER

- PUE of the Data Centers constantly measured and monitored
- Continuous improvement plan for Energy Efficiency supervised by the government agency Klima-Agence
- Waste heat from servers used to heat office space and preheat diesel generators
- Certified 100% Green Electricity supplied from hydroelectric power sources
- Optimized use of Free Cooling
- Biomass recycling representing a yearly reduction in CO₂ in excess of 27,000 metric tons





MELUXINA

Atos

Atos

Atos

Atos

Atos

Atos

Atos

Atos

Atos



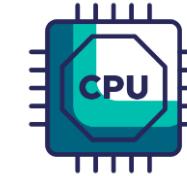
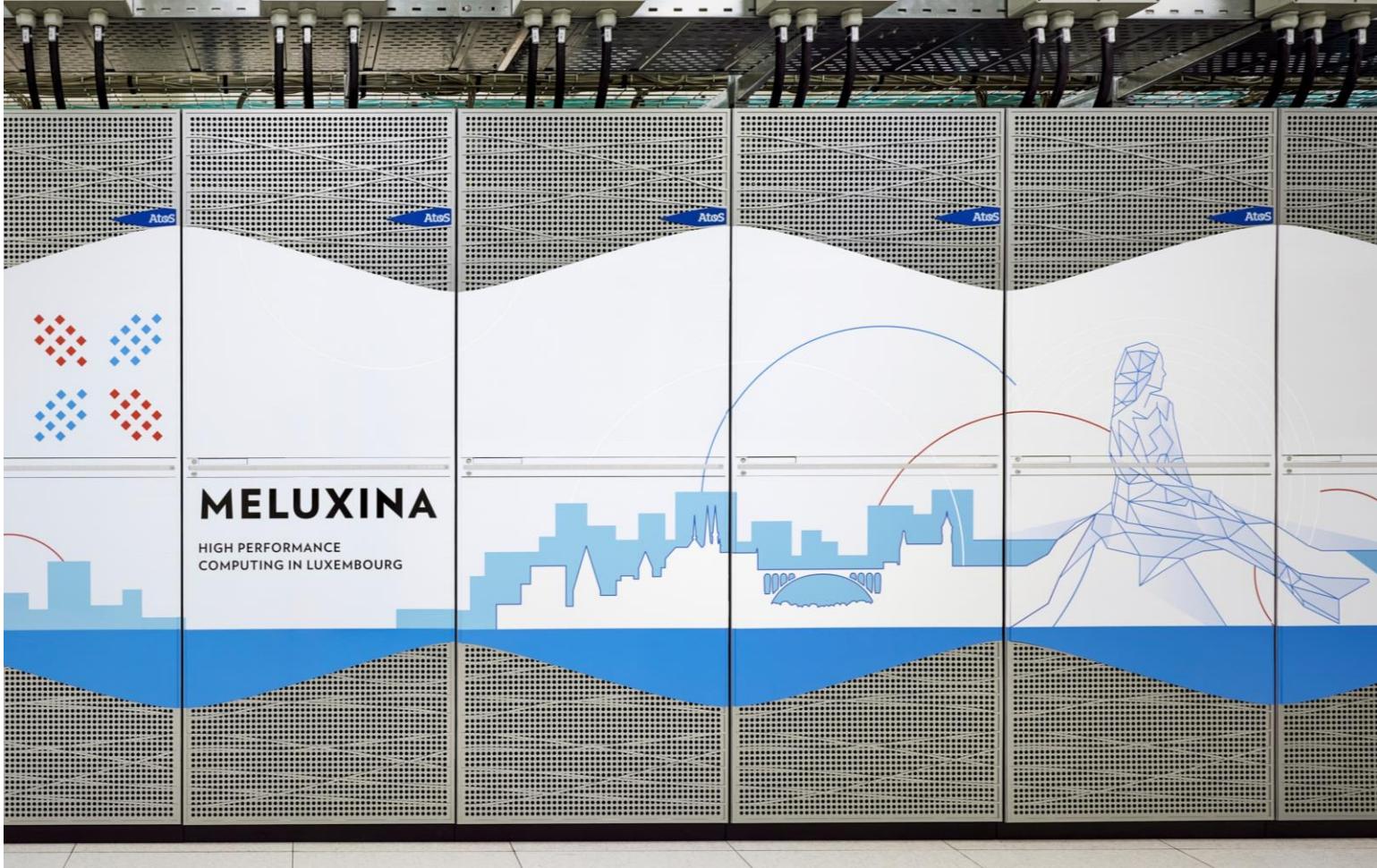
MELUXINA

HIGH PERFORMANCE
COMPUTING IN LUXEMBOURG



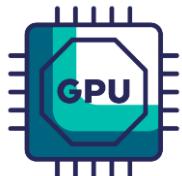


LUXEMBOURG'S NATIONAL SUPERCOMPUTER MELUXINA



90.000

HPC CPU cores



800

GPU-AI
accelerators



20

Petabytes high
performance storage



+450

TB RAM



400+

Tailored software
packages



INFRASTRUCTURE ESSENTIALS

573x CPU NODES

- 2x AMD Rome (64-core, 2.6 GHz)
- 512 GB RAM
- HDR 200Gb/s Infiniband

200x GPU NODES

- 2x AMD Rome (32-core, 2.35 GHz)
- 512 GB RAM
- 4x NVIDIA A100 (40GB HBM, NVlink)
- 1.92 TB SSD local storage
- 2x HDR 200Gb/s Infiniband

20x LARGE MEMORY NODES

- 2x AMD Rome (64-core, 2.6 GHz)
- 4 TB RAM
- 1.92 TB NVMe local storage
- HDR 200Gb/s Infiniband

20x FPGA NODES

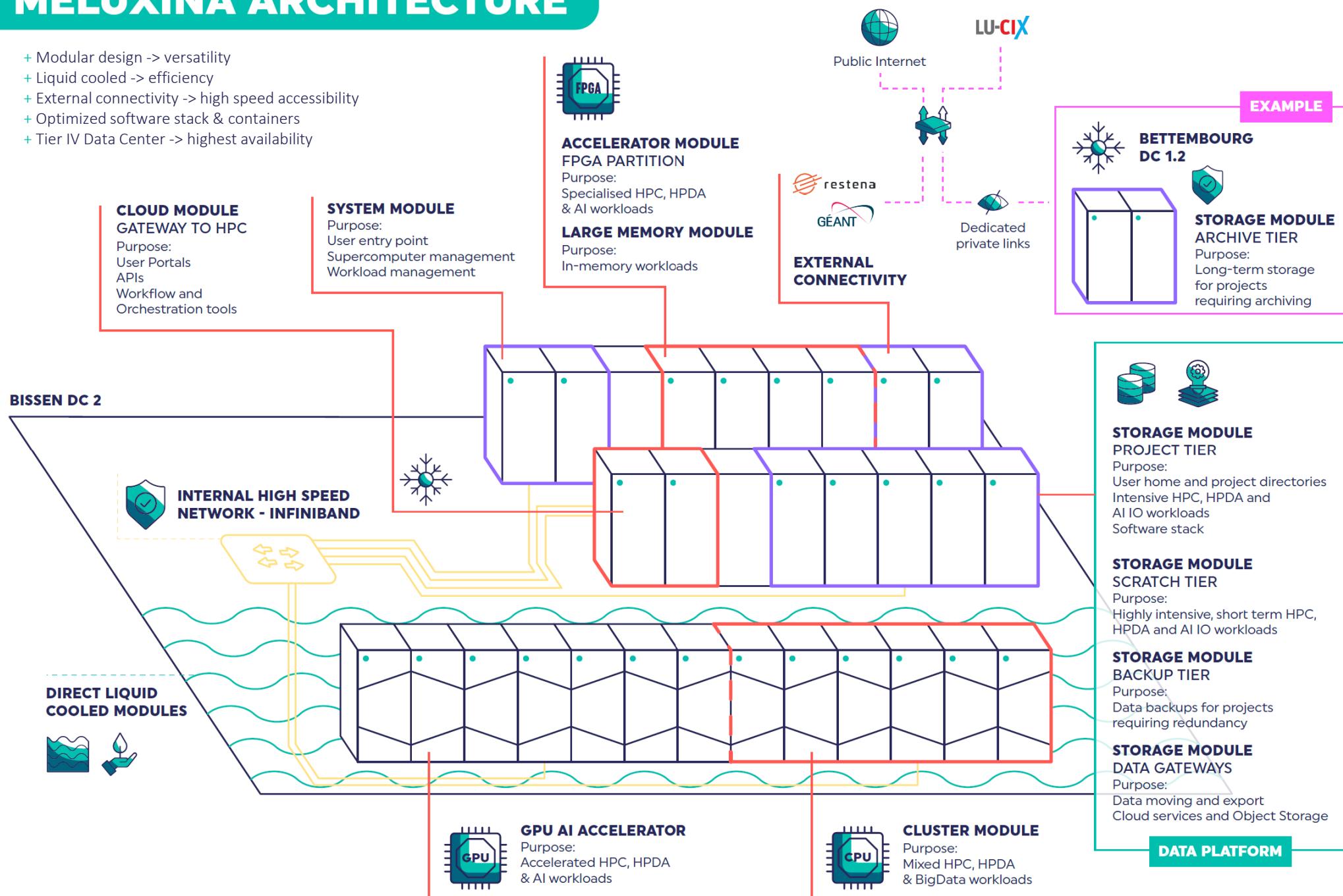
- 2x AMD Rome (32-core, 2.35 GHz)
- 512 GB RAM
- 2x BittWare520N-MX (Intel Stratix 10MX 16GB chip)
- 1.92 TB SSD local storage
- 2x HDR 200Gb/s Infiniband

DATA STORAGE

- Tier1 –Scratch
 - 0.6 PB, 400 GB/s, Lustre PFS
 - Self-Encrypting NVMe drives
- Tier2 -Home/Project
 - 13 PB, 190 GB/s, Lustre PFS
 - Self-Encrypting NVMe & HDD drives
- Tier3 –Backup
 - 7 PB, 30 GB/s, Lustre PFS
 - Self-Encrypting NVMe & HDD drives
- Tier4 –Archive
 - 5 PB
 - Tape-based Archival system

MELUXINA ARCHITECTURE

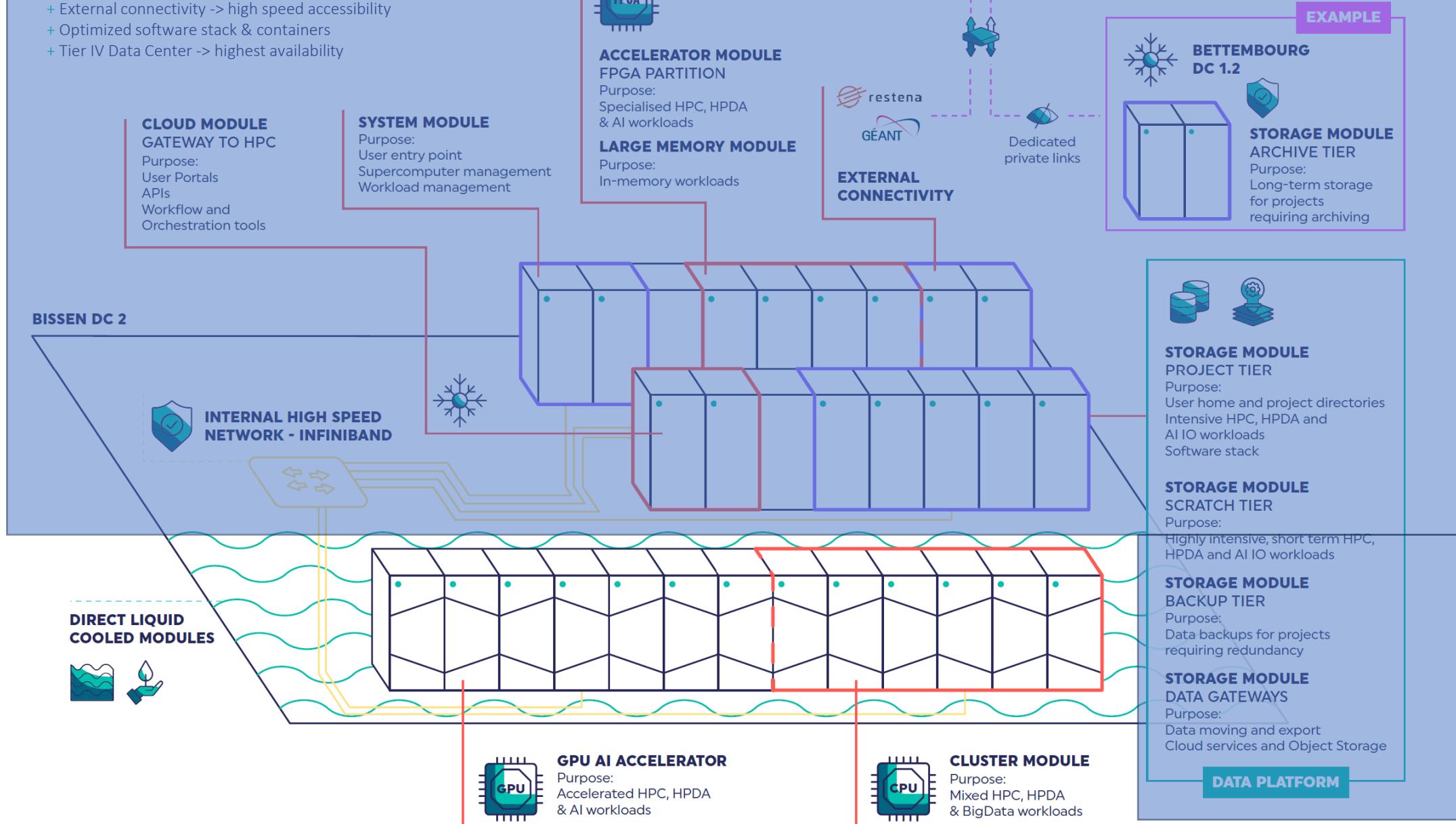
- + Modular design -> versatility
- + Liquid cooled -> efficiency
- + External connectivity -> high speed accessibility
- + Optimized software stack & containers
- + Tier IV Data Center -> highest availability



MELUXINA ARCHITECTURE

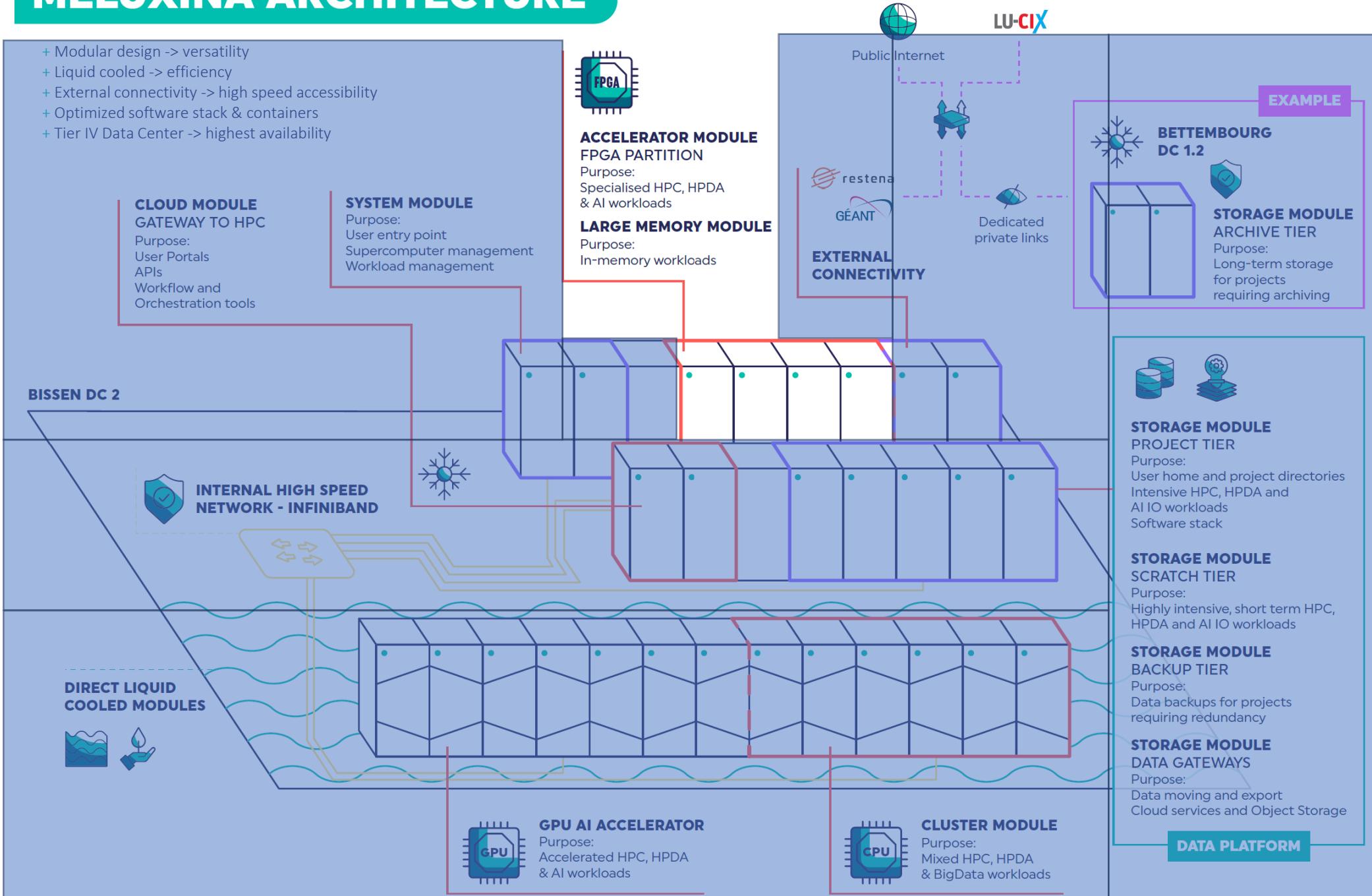
LU-CIX

- + Modular design -> versatility
- + Liquid cooled -> efficiency
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- + Tier IV Data Center -> highest availability



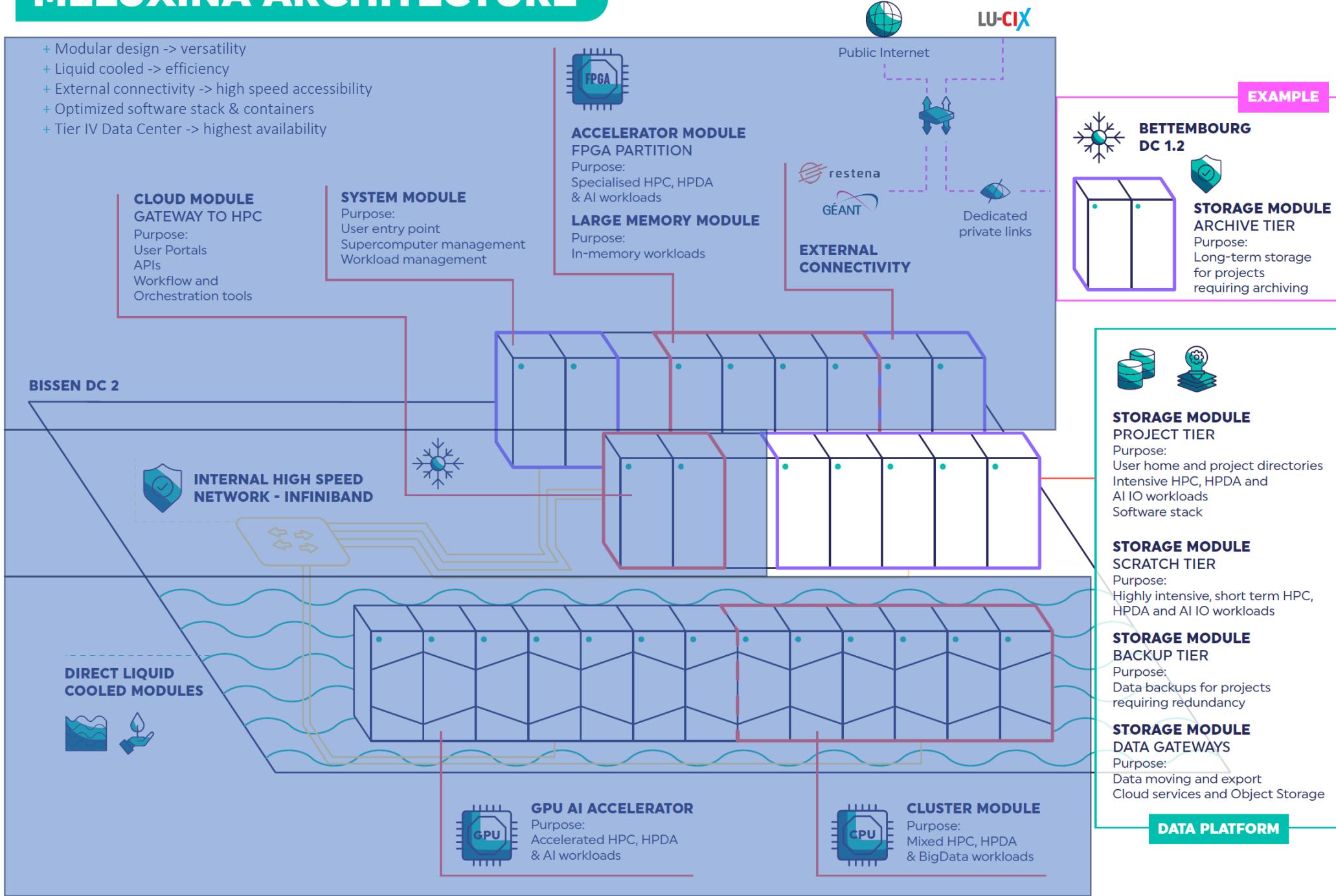
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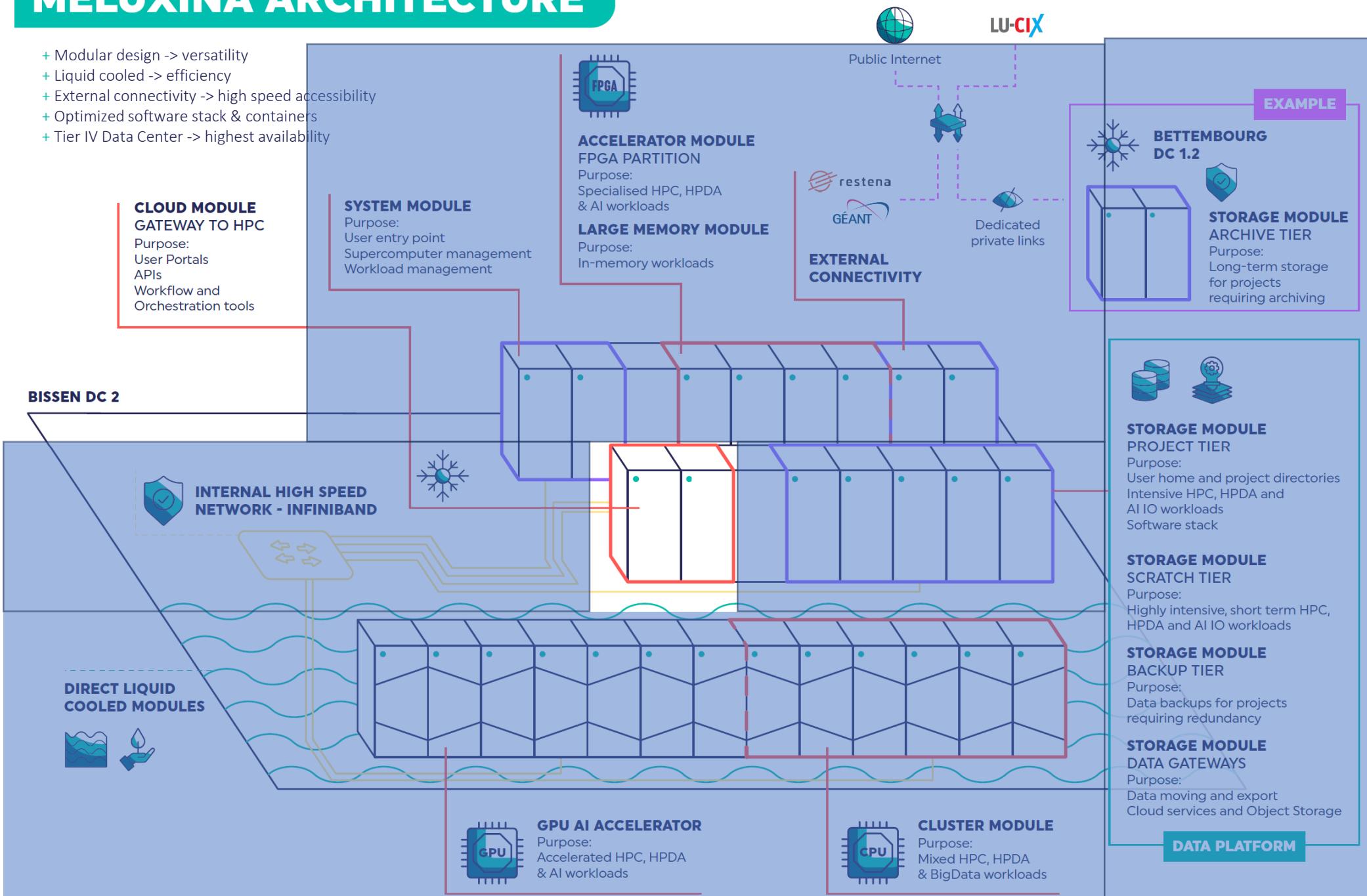
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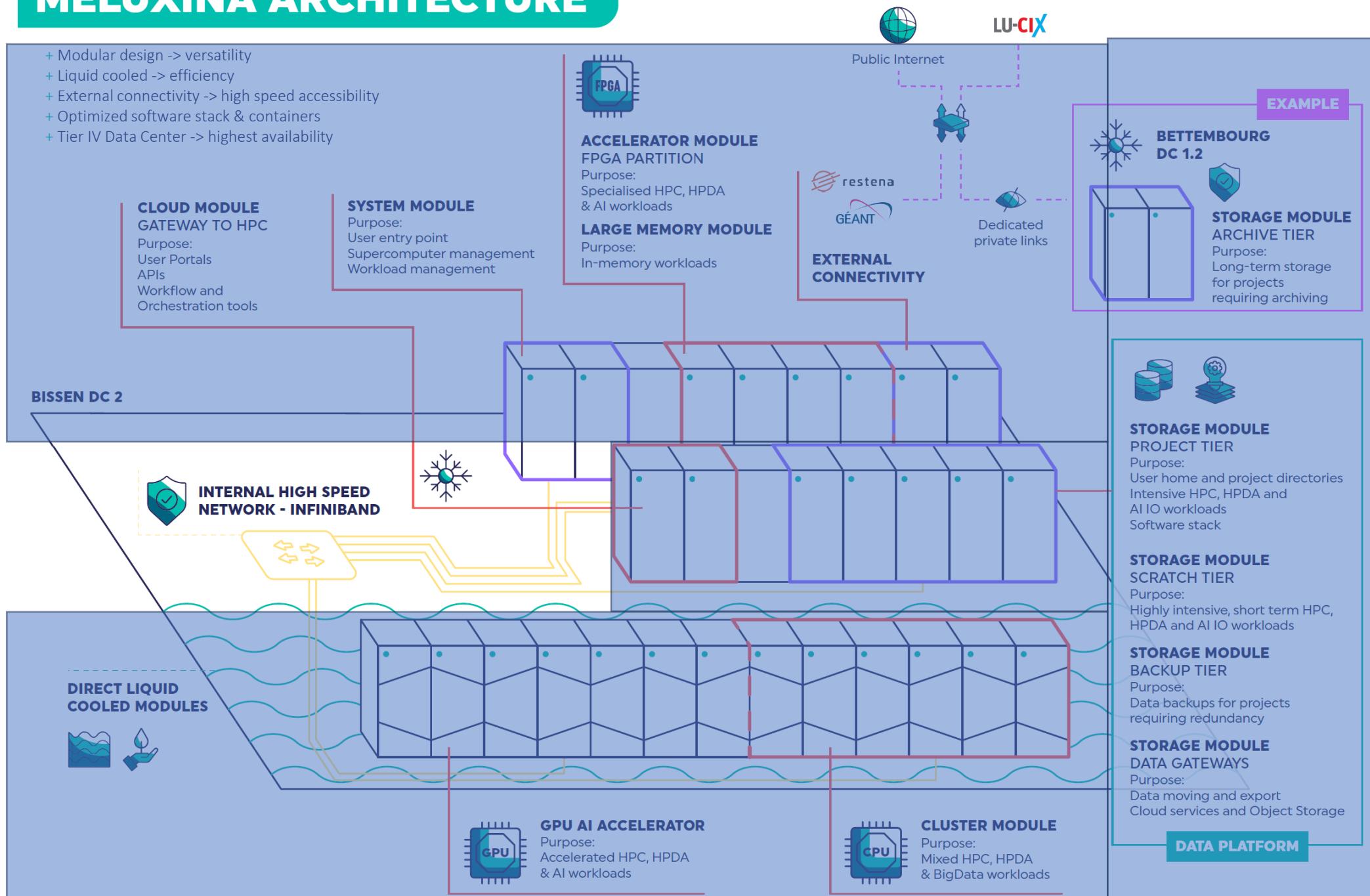
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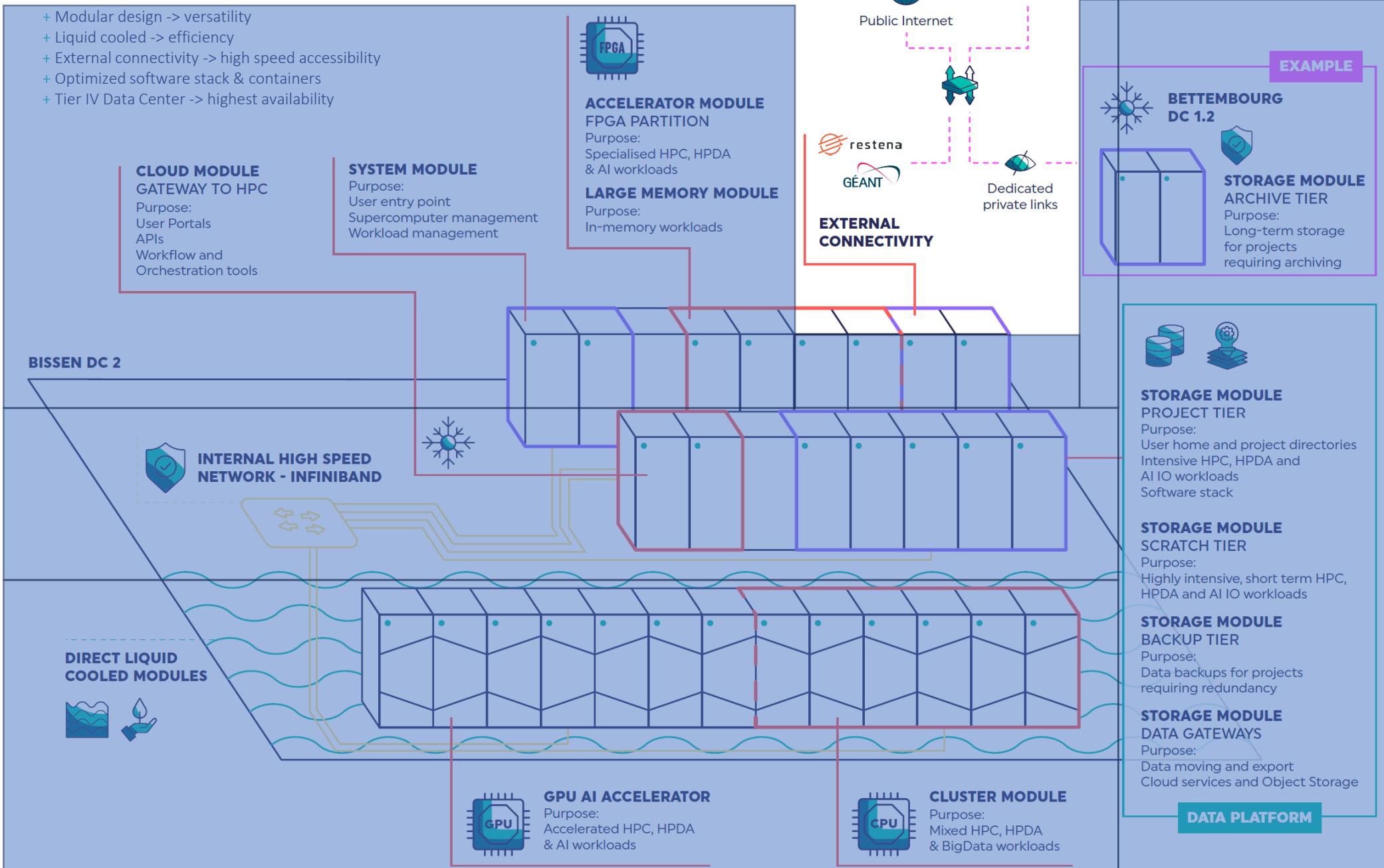
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ACCESSING AND USING MELUXINA



GETTING HELP

<https://docs.lxp.lu/>

The screenshot shows the homepage of the MeluXina User Documentation. At the top, there's a navigation bar with a "PROVIDE" button, the title "MeluXina User Documentation", and a search bar. Below the header, a sidebar on the left lists categories like "Welcome", "MeluXina supercomputer", "Gaining access", "First steps", "HPC", "HPDA", "Containerization", "Cloud", "What's new", and "FAQ". The main content area features a large heading "Welcome" and a sub-section titled "The MeluXina supercomputer" which includes a photograph of the server racks and some explanatory text.

Publicly available

<https://servicedesk.lxp.lu>

The screenshot shows the LXP Service Desk interface. At the top, it displays "MeluXina maintenance / events" with a single entry for "2023-10-30 09:00 CET (12h) MeluXina performance, reliability and security maintenance". Below this, there are sections for "LXP Service Desk" and "LXP Support". A central "Welcome! How may we help you today?" section encourages users to check the documentation or the weather report. To the right, there are several "Accounts & Projects" sections: "[Accounts] Add or update your SSH key", "[Accounts] Request information", and "[Accounts] Request changes to an existing Account or Project", each with a list of sub-topics. A search bar is also present at the bottom.

Requires existing user account



ACCESSING MELUXINA

- **ssh user@login.lxp.lu -p 8822**
 - 4 login nodes in total, at the moment round-robin between 2 login nodes
 - Login nodes directly accessible (not recommended)
 - Can switch between login nodes
- **Ed25519 key pair-based authentication**
 - Passphrase on private key highly recommended
- **Steps to generate appropriate key**
 - <https://docs.lxp.lu/first-steps/connecting/>

```
Welcome to Luxembourg - EuroHPC supercomputer
# Meluxina
You are on a MeluXina login node
System information: Compute
Nodes | CPU | RAM | Accelerator | Disk
573N | 2x AMD 7H12: 128c @2.6G | 512GB | - | -
200N | 2x AMD 7452: 64c @2.3G | 512GB | 4x NVIDIA A100-40 | 1.92G
20N | 2x AMD 7452: 64c @2.3G | 512GB | 2x Intel Stratix 10MX-16 | 1.92G
20N | 2x AMD 7H12: 128c @2.6G | 4096GB | - | 1.92G
System information: Data
Tier | Capacity | Speed | Type | Location on compute/login
Scratch | 0.6PB | 400GB/s | NVMe | /project/scratch
Home/Project | 12.5PB | 180GB/s | HDD | /home/users, /project/home
Backup | 7.5PB | 30GB/s | HDD | -
System information: Interconnect
Fabric: Infiniband HDR, 200Gbps, DragonFly+ topology
Links : 1x on CPU nodes, 2x on GPU, FPGA & LargeMemory nodes
System information: Software
Production software stack: 2021.3, current default and obsolete on
14 Jan 2023
Production software stack: 2022.1, default from 15 Jan 2023, use it
now with: module load env/release/2022.1
Center information
News & Events : luxprovide.lu
Documentation : docs.lxp.lu
System status : weather.lxp.lu
Support : servicedesk.lxp.lu, servicedesk@lxp.lu
LinkedIn & Twitter : @luxprovide #meluxina @EuroHPC_JU
#####
# System events, in-progress and upcoming
#
# * 2023-10-30 09:00 - 19:00 CET MeluXina update for performance, security
# and reliability. Contact our Service Desk in case of any observed issues.
#####
Last login: Thu Nov 16 17:01:41 2023 from 158.64.12.102
[fbongiovanni@login02 ~]$
```



ACCESSING MELUXINA

- **On-premise JupyterLab**
 - <https://jlab.lxp.lu/>
- **2FA authentication using KeyCloak**
- **Steps to setup KeyCloak 2FA**
 - <https://docs.lxp.lu/cloud/keycloak/>

The screenshot shows a web browser window with the URL <https://jlab.lxp.lu/hub/spawn>. The page title is "jupyterhub". Below the title, there are two tabs: "Home" and "Token". The main content area is titled "Server Options" and contains the following fields:

- Account name: (empty input field)
- Reservation name: (empty input field)
- Allocation time (HH:MM:SS): 01:00:00
- Partition: CPU (dropdown menu)
- Nodes count: 1
- QOS: Short | Small jobs for backfilling (dropdown menu)
- Job name: default
- Log file: /dev/null
- Tip: /mnt/tier2/users/username/jlab.log
- Profile: release/2023.1 | Latest software stack (dropdown menu)

At the bottom right of the form is a large orange button labeled "Start".



PGI

AMD



intel

ParaStation
MPI

TensorFlow

Apache
Spark

PyTorch

Keras



MELUXINA USER SOFTWARE ENVIRONMENT (MUSE)

Compilers, Languages & Performance Eng.
<ul style="list-style-type: none">• AICC• GCC• Intel• NVIDIA HPC SDK<ul style="list-style-type: none">✓ incl. PGI• Support for various programming languages<ul style="list-style-type: none">✓ Python✓ R✓ Julia✓ Go✓ Rust• Performance and debugging tools<ul style="list-style-type: none">✓ Intel✓ NVIDIA✓ ARM (Forge)✓ Scalasca✓ SCORE-P✓ Exrae✓ PAPI✓ Valgrind✓ GDB✓ AMD-uProf✓ Nsight-Systems✓ Nsight-Compute✓ Vtune✓ gperf✓ extrap✓ Inspector• Many build & support tools (Autotools, CMake, ...)

Parallelization tools, MPI suites & acceleration libraries
<ul style="list-style-type: none">• OpenMPI• Intel MPI• ParaStationMPI• NVHPC• TBB• PETSc• KOKKOS• cuBLAS• cuFFT• cuDNN• NCCL• TensorRT

Numerical & data libraries
<ul style="list-style-type: none">• BLIS• Intel MKL• FFTW• OpenBLAS• ScalaPACK• Boost• Eigen• ARPACK• HDF5• netCDF• OpenCV• CDO

Frameworks, runtime & platform tools
<ul style="list-style-type: none">• PyTorch• RAPIDS• Torch Text+Vision• TensorFlow + Hub• Horovod• Keras• Theano• Jupyter Lab• Apache Spark• Matlab Runtime• dotNET Core + SDK• Dakota• Quantum Computing/AI<ul style="list-style-type: none">• Cirq• QsimCirq• Qiskit• CuQuantum• PennyLane

End user applications
<ul style="list-style-type: none">• GROMACS• OpenFOAM• FOAM-Extend• CP2K• QuantumESPRESSO• NAMD• QMCPACK• NWChem• HOOMD-blue• Freud-analysis• DualSPHysics• POV-Ray• Blender• MDAnalysis• BioPython• QUDA• Visualisation<ul style="list-style-type: none">✓ ParaView✓ VMD✓ OVITO✓ NCO✓ NCView

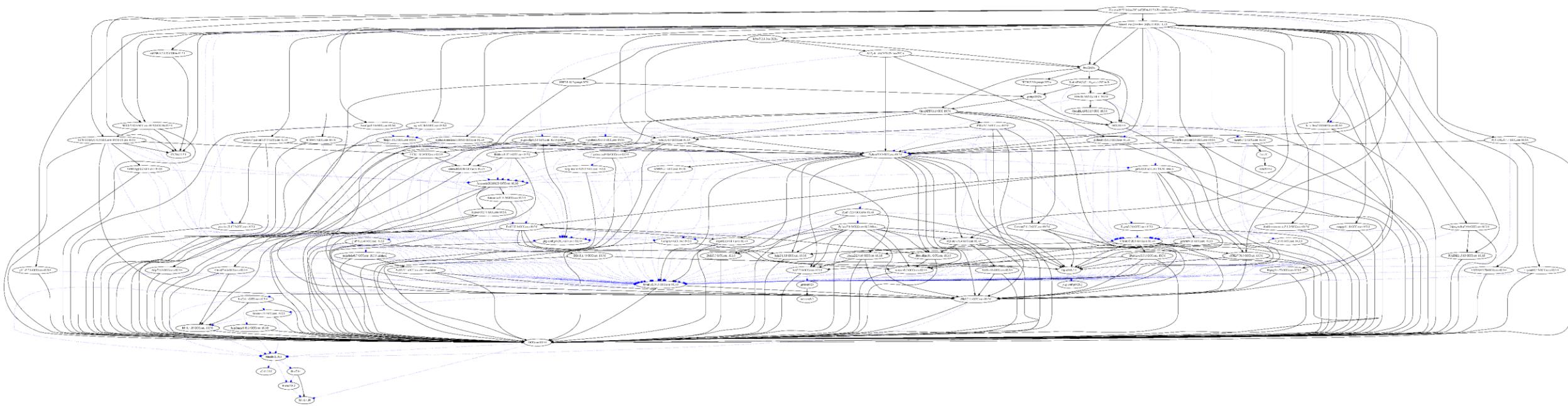
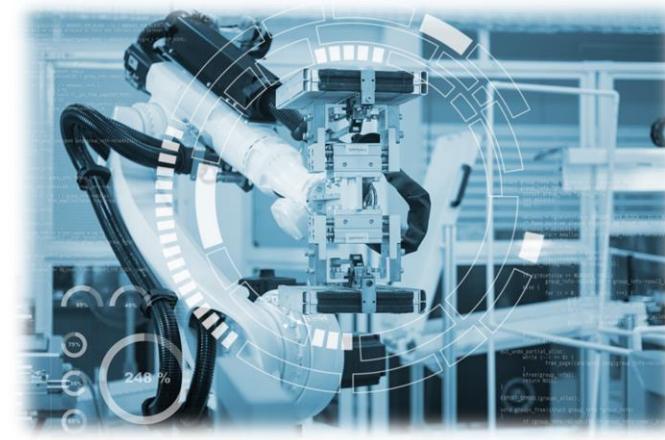
ISVs license can be implemented, we have 3
license servers dedicated for that



PRE-OPTIMIZED PACKAGES

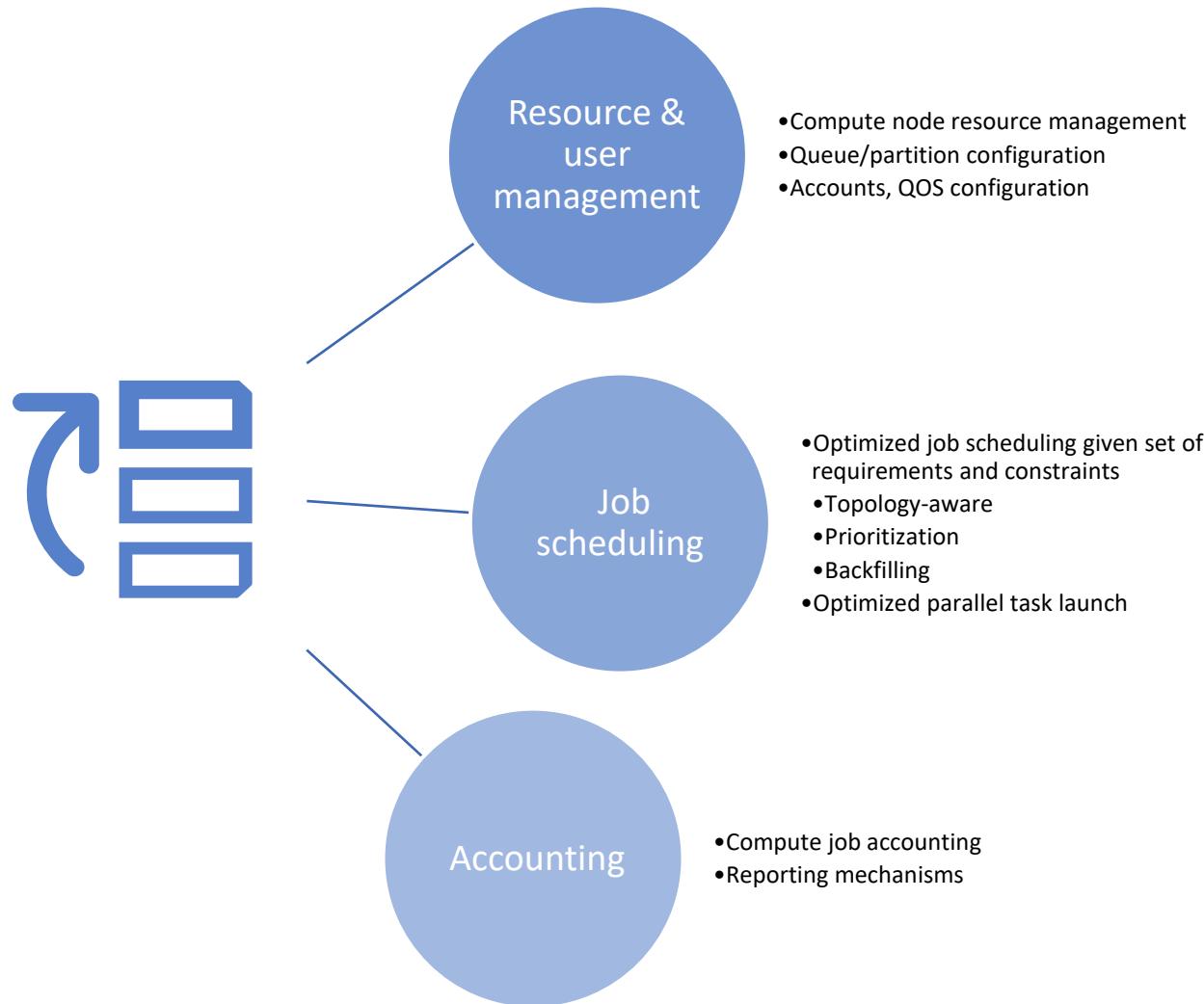
TensorFlow & Horovod packages

- Used for... scalable AI
- Many more dependencies..
- GPU-accelerated, MeluXina-optimized builds are essential





HPC SCHEDULER - SLURM



```
#!/bin/bash -l
#SBATCH --job-name=GROM_x100_t2
#SBATCH --account p200000
#SBATCH --partition gpu
#SBATCH --qos default
#SBATCH --nodes 64
#SBATCH --ntasks-per-node 4
#SBATCH --gpus-per-task 1
#SBATCH --cpus-per-task 8
#SBATCH --time 30:00
#SBATCH --output gromacs_%x_%j.out
#SBATCH --error gromacs_%x_%j.out

## Load software environment
module load GROMACS/2022.3-foss-2022a-CUDA-11.7.0

## Task execution
cd /project/home/p200000/x100_t2/
srun gmx_mpi mdrun -dlb yes -nsteps 500000 -ntomp 5 -pin on
-v -noconfout -nb cpu -s topol.tpr
```



SLURM partitions

- Node naming convention
 - CPU partition: mel0001-mel0573
 - GPU partition : mel2001-mel2200
 - FPGA partition : mel3001-mel3020
 - LargeMem partition : mel4001-mel4020
- Some nodes per partition always reserved for interactive jobs (*dev*)
- All QoS work across all partitions
- Limits enforced at QoS/account level

```
[fbongiovanni@login02 ~]$ sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
bench      up infinite   13  resv mel[0037,0061,0208,0382,0396,0550,2052,2062,2089,2096,2111,3013,4018]
bench      up infinite   247  alloc mel[0001-0003,0014-0015,0017,0026-0027,0029,0038-0040,0045-0046,0053-0055,0097-0099,0110-0111,0113-0114,0123,0125-0126,0128-0129,0131-0145,0149-0150,0169,0182,0193-01
95,0206-0207,0209-0210,0218-0219,0221-0222,0229-0233,0237-0248,0266-0267,0269-0270,0272-0273,0275-0276,0289-0292,0302-0303,0305,0314-0315,0317,0325-0327,0333-0335,0341-0344,0385-0395,0397-0399,0411,0413,0421
-0422,0428-0431,0437-0440,0470,0481-0484,0494-0495,0497,0506-0507,0509,0517,0525-0528,0533,0552,2001-2007,2009-2016,2021,2029,2033-2035,2037-2046,2057,2061,2065-2067,2069-2071,2073-2075,2078-2081,2098-2107,2
109-2110,2112,2117,2121,2129-2135,2137-2139,2141-2145,2161-2176,2181,2185,2189,2193-2197]
bench      up infinite   553  idle mel[0004-0013,0016,0018-0025,0028,0030-0036,0041-0044,0047-0052,0056-0060,0062-0096,0100-0109,0112,0115-0122,0124,0127,0130,0146-0148,0151-0168,0170-0181,0183-0192,01
96-0205,0211-0217,0220,0223-0228,0234-0236,0249-0265,0268,0271,0274,0277-0288,0293-0301,0304,0306-0313,0316,0318-0324,0328-0332,0336-0340,0345-0381,0383-0384,0400-0410,0412,0414-0420,0423-0427,0432-0436,0441
-0469,0471-0480,0485-0493,0496,0498-0505,0508,0510-0516,0518-0524,0529-0532,0534-0549,0551,0553-0573,2008,2017-2020,2022-2028,2030-2032,2036,2047-2051,2053-2056,2058-2060,2063-2064,2068,2072,2076-2077,2082-2
088,2090-2095,2097,2108,2113-2116,2118-2120,2122-2128,2136,2140,2146-2160,2177-2180,2182-2184,2186-2188,2190-2192,2198-2200,3001-3012,3014-3020,4001-4017,4019-4020]
cpu*      up infinite    6  resv mel[0037,0061,0208,0382,0396,0550]
cpu*      up infinite   148  alloc mel[0001-0003,0014-0015,0017,0026-0027,0029,0038-0040,0045-0046,0053-0055,0097-0099,0110-0111,0113-0114,0123,0125-0126,0128-0129,0131-0145,0149-0150,0169,0182,0193-01
95,0206-0207,0209-0210,0218-0219,0221-0222,0229-0233,0237-0248,0266-0267,0269-0270,0272-0273,0275-0276,0289-0292,0302-0303,0305,0314-0315,0317,0325-0327,0333-0335,0341-0344,0385-0395,0397-0399,0411,0413,0421
-0422,0428-0431,0437-0440,0470,0481-0484,0494-0495,0497,0506-0507,0509,0517,0525-0528,0533,0552]
cpu*      up infinite   419  idle mel[0004-0013,0016,0018-0025,0028,0030-0036,0041-0044,0047-0052,0056-0060,0062-0096,0100-0109,0112,0115-0122,0124,0127,0130,0146-0148,0151-0168,0170-0181,0183-0192,01
96-0205,0211-0217,0220,0223-0228,0234-0236,0249-0265,0268,0271,0274,0277-0288,0293-0301,0304,0306-0313,0316,0318-0324,0328-0332,0336-0340,0345-0381,0383-0384,0400-0410,0412,0414-0420,0423-0427,0432-0436,0441
-0469,0471-0480,0485-0493,0496,0498-0505,0508,0510-0516,0518-0524,0529-0532,0534-0549,0551,0553-0573]
gpu       up infinite    5  resv mel[2052,2062,2089,2096,2111]
gpu       up infinite   99  alloc mel[2001-2007,2009-2016,2021,2029,2033-2035,2037-2046,2057,2061,2065-2067,2069-2071,2073-2075,2078-2081,2098-2107,2109-2110,2112,2117,2121,2129-2135,2137-2139,2141-21
45,2161-2176,2181,2185,2189,2193-2197]
gpu       up infinite   96  idle mel[2008,2017-2020,2022-2028,2030-2032,2036,2047-2051,2053-2056,2058-2060,2063-2064,2068,2072,2076-2077,2082-2088,2090-2095,2097,2108,2113-2116,2118-2120,2122-2128,21
36,2140,2146-2160,2177-2180,2182-2184,2186-2188,2190-2192,2198-2200]
fpga      up infinite    1  resv mel3013
fpga      up infinite   19  idle mel[3001-3012,3014-3020]
largemem  up infinite    1  resv mel4018
largemem  up infinite   19  idle mel[4001-4017,4019-4020]
[fbongiovanni@login02 ~]$
```



Getting an allocation

- Example of getting an interactive allocation on 1 GPU node

```
[fbongiovanni@login02 ~]$ cat ~/.bashrc | grep giveme
alias givemegpu='srun -A lxp -q default -p gpu -N 1 -G 4 --time=02:00:00 --disable-perfparanoid --forward-x --pty /bin/bash -i'
alias givemecpu='srun -A lxp -q default -p cpu -N 1 --time=02:00:00 --disable-perfparanoid --forward-x --pty /bin/bash -i'
alias givemelarge='srun -A lxp -q default -p largemem -N 1 --time=02:00:00 --disable-perfparanoid --forward-x --pty /bin/bash -i'
alias givemefpga='srun -A lxp -q default -p fpga -N 1 --time=02:00:00 --disable-perfparanoid --forward-x --pty /bin/bash -i'
[fbongiovanni@login02 ~]$ givemegpu
srun: job 1381721 queued and waiting for resources
srun: job 1381721 has been allocated resources
[fbongiovanni@mel2174 ~]$ █
```

https://docs.lxp.lu/first-steps/quick_start/

MELUXINA USER SOFTWARE ENVIRONMENT (MUSE)

- Based on LMOD/EasyBuild
- Release and Staging stacks
- Stacks refreshed once a year
 - November: old release stack and future stack in staging coexist
 - Users can test it, transition their applications to the new stack
 - February: new release takes effect

```
[fbongiovanni@mel0237 ~]$ module available
```

Category	Module Name	Description
deploy/EasyBuild	4.7.0	(D)
	4.8.0	(D)
	2022.1	
deploy/deploy-apps	2023.1	
	2021.5	
	2022.1	(S,L,D)
deploy/deploy-user		
----- /apps/USE/system/modules -----		
env/release/2021.3		
env/release/2021.5		
env/release/2022.1	(S,L,D)	
env/staging/2021.5		
env/staging/2022.1		
env/staging/2023.1	(D)	
----- /apps/USE/easybuild/release/2022.1/modules/all -----		
SuiteSparse/5.13.0-foss-2022a-METIS-5.1.0		
Szip/2.1.1-GCCcore-11.3.0		
Tcl/8.6.12-GCCcore-11.3.0		
TensorFlow/2.9.1-foss-2022a		
Theano/1.1.2-foss-2022a-PyMC		
Tk/8.6.12-GCCcore-11.3.0		
Tkinter/3.10.4-GCCcore-11.3.0		
UCX-CUDA/1.12.1-GCCcore-11.3.0-CUDA-11.7.0		
UCX-CUDA/1.13.1-GCCcore-11.3.0-CUDA-11.7.0		(D)
UCX/1.12.1-GCCcore-11.3.0		
UCX/1.13.1-GCCcore-11.3.0		(D)
UDUNITS/2.2.28-GCCcore-11.3.0		
UnZip/6.0-GCCcore-11.3.0		
VMD/1.9.4a57-foss-2022a-CUDA-11.7.0		
VMD/1.9.4a57-foss-2022a		
VTK/9.1.0-foss-2022a		
VTune/2022.3.0		
Valgrind/3.19.0-gompi-2022a		
Voro++/0.4.6-GCCcore-11.3.0		
X11/20220504-GCCcore-11.3.0		

```
[fbongiovanni@mel0237 ~]$ module load Python
[fbongiovanni@mel0237 ~]$ module list
```

Currently Loaded Modules:

1) lxp-tools/myquota/0.3.1	(S)	5) binutils/2.38-GCCcore-11.3.0	9) Tcl/8.6.12-GCCcore-11.3.0	13) libffi/3.4.2-GCCcore-11.3.0
2) env/release/2022.1	(S)	6) bzip2/1.0.8-GCCcore-11.3.0	10) SQLite/3.38.3-GCCcore-11.3.0	14) OpenSSL/1.1
3) GCCcore/11.3.0		7) ncurses/6.3-GCCcore-11.3.0	11) XZ/5.2.5-GCCcore-11.3.0	15) Python/3.10.4-GCCcore-11.3.0
4) zlib/1.2.12-GCCcore-11.3.0		8) libreadline/8.1.2-GCCcore-11.3.0	12) GMP/6.2.1-GCCcore-11.3.0	

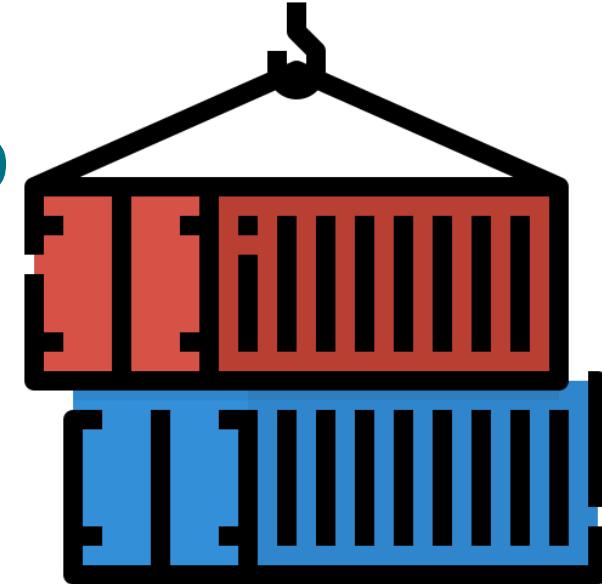
Where:
S: Module is Sticky, requires --force to unload or purge

Module Naming Scheme:

GROMACS/2022.3-foss-2022a

GROMACS/2022.3-foss-2022a-CUDA-11.7.0

MELUXINA AND CONTAINERIZED WORKLOAD



Singularity-CE / Apptainer

Container system on MeluXina



- Docker & OCI compatible
- Non-privileged mode for improved security
- Support for GPU accelerated applications
- Support for creating and running encrypted containers
- Support for trusted containers: PGP signed & verified



Bring-your-own software stack

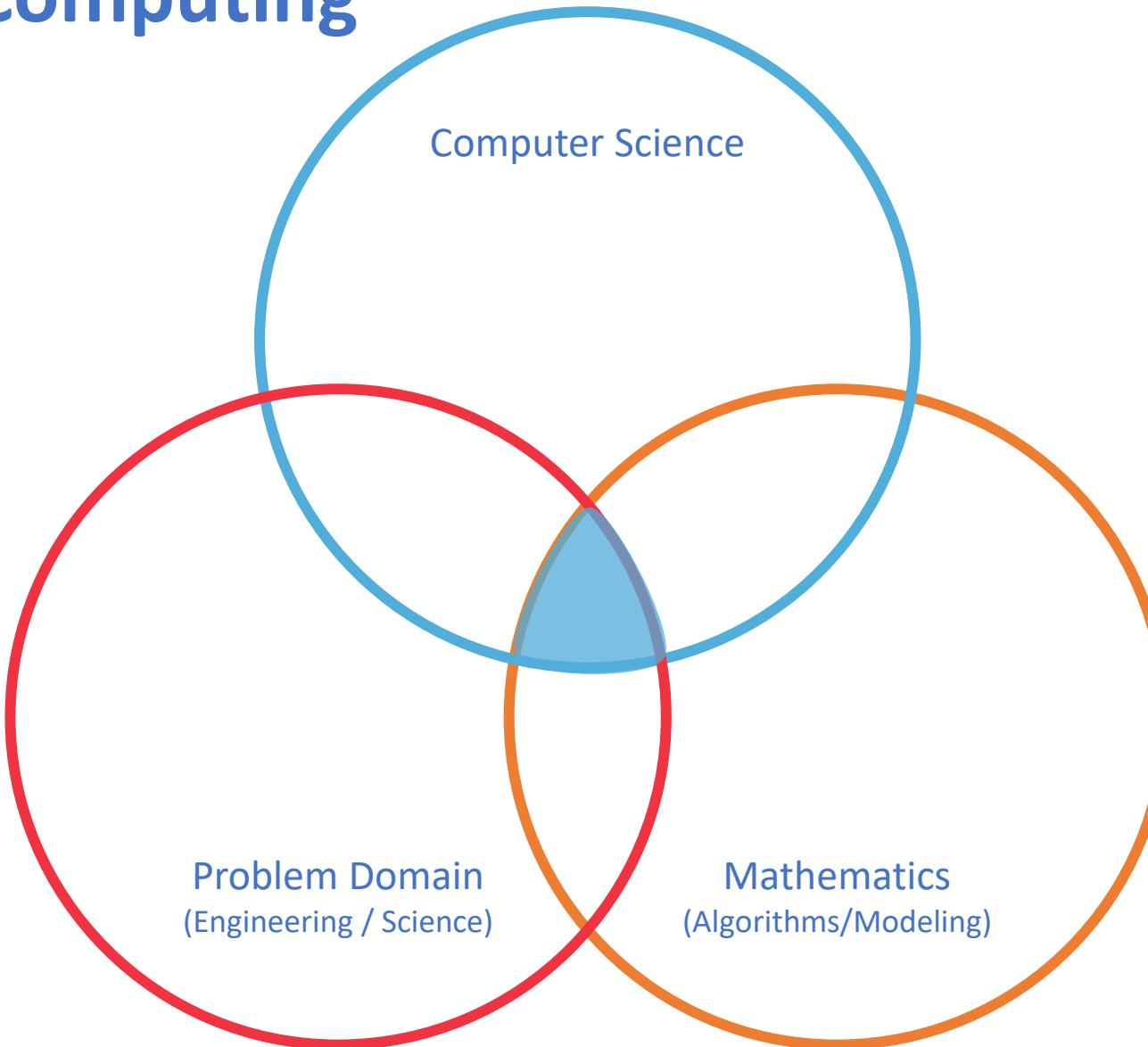
- Enable users to easily control complete stack --- REPRODUCIBILITY
- Users create tooling and pipeline on their infrastructure --- RUN PIPELINE ON MELUXINA



WHAT IS SCIENTIFIC COMPUTING ?

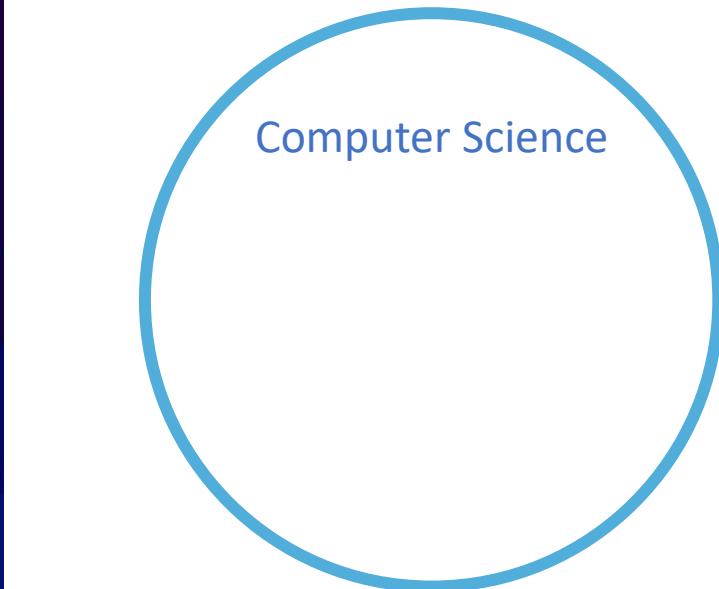
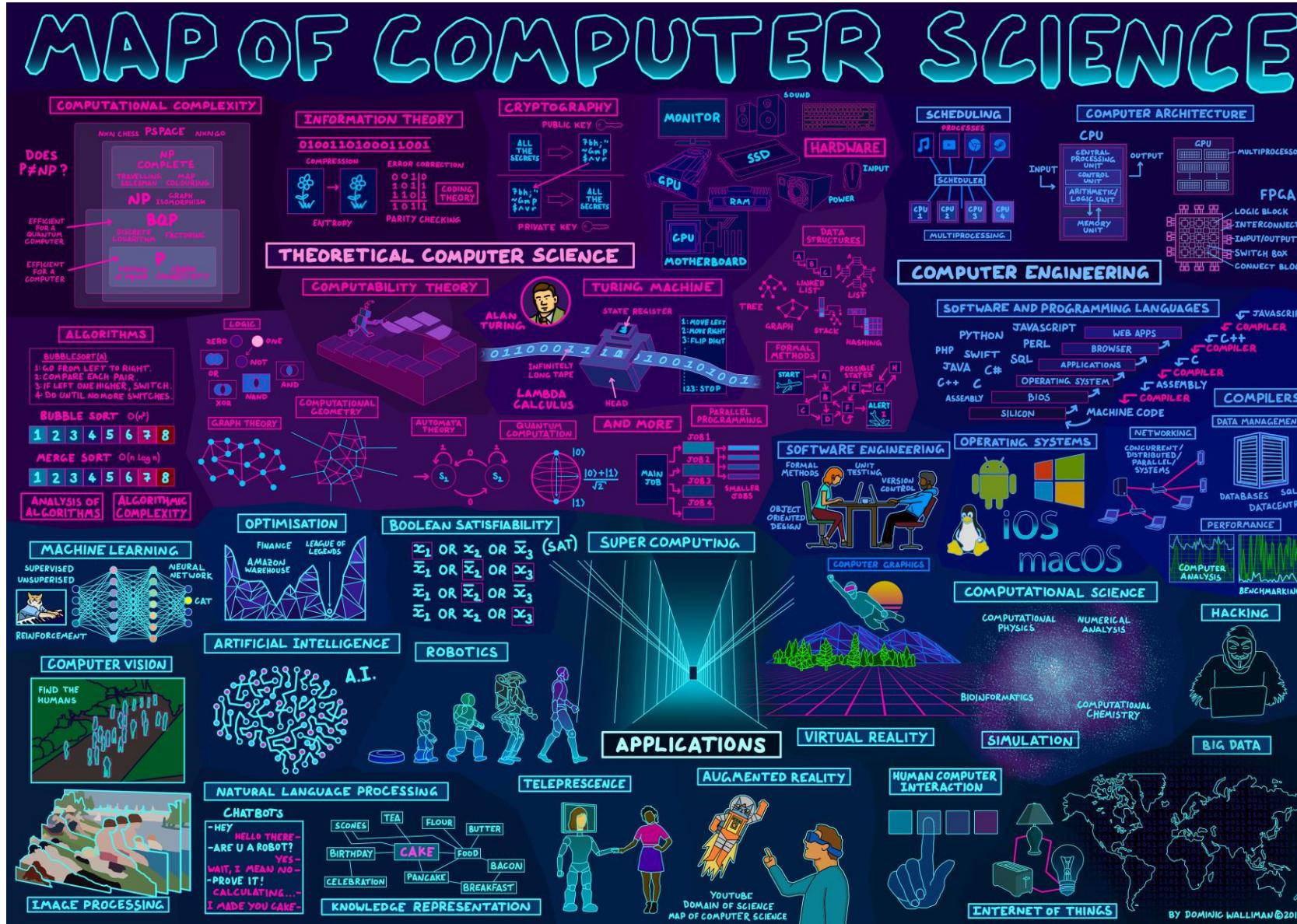


Scientific Computing





Scientific Computing



by Dominic Walliman



Scientific Computing



Navier-Stokes Equations 3 - dimensional - unsteady

Glenn
Research
Center

Coordinates: (x,y,z) Time : t Pressure: p Heat Flux: q
Velocity Components: (u,v,w) Density: ρ Stress: τ Reynolds Number: Re
Velocity Components: (u,v,w) Total Energy: Et Prandtl Number: Pr

Continuity: $\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$

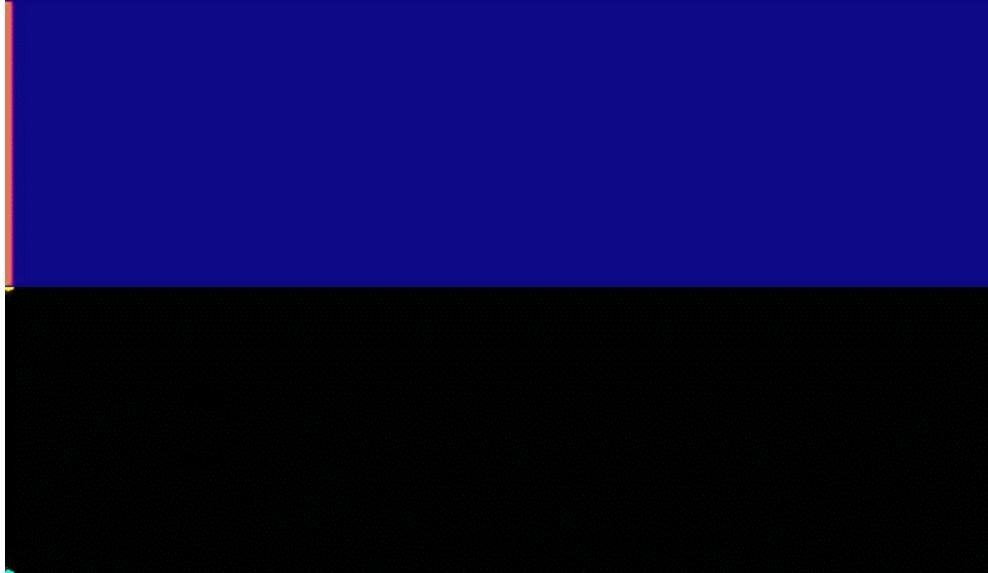
X - Momentum: $\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right]$

Y - Momentum: $\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right]$

Z - Momentum $\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right]$

Energy:

$$\begin{aligned} \frac{\partial(E_I)}{\partial t} + \frac{\partial(uE_I)}{\partial x} + \frac{\partial(vE_I)}{\partial y} + \frac{\partial(wE_I)}{\partial z} &= -\frac{\partial(uP)}{\partial x} - \frac{\partial(vP)}{\partial y} - \frac{\partial(wP)}{\partial z} - \frac{1}{Re_r Pr_r} \left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right] \\ &+ \frac{1}{Re_r} \left[\frac{\partial}{\partial x}(u \tau_{xx} + v \tau_{xy} + w \tau_{xz}) + \frac{\partial}{\partial y}(u \tau_{xy} + v \tau_{yy} + w \tau_{yz}) + \frac{\partial}{\partial z}(u \tau_{xz} + v \tau_{yz} + w \tau_{zz}) \right] \end{aligned}$$



Problem Domain
(Engineering /
Science)

Computational Fluid Dynamics - CFD



Scientific Computing



Navier-Stokes Equations 3-dimensional - unsteady

Glenn
Research
Center

Coordinates: (x,y,z) Time : t Pressure: p Heat Flux: q
Velocity Components: (u,v,w) Density: ρ Stress: τ Reynolds Number: Re
Velocity Components: (u,v,w) Total Energy: Et Prandtl Number: Pr

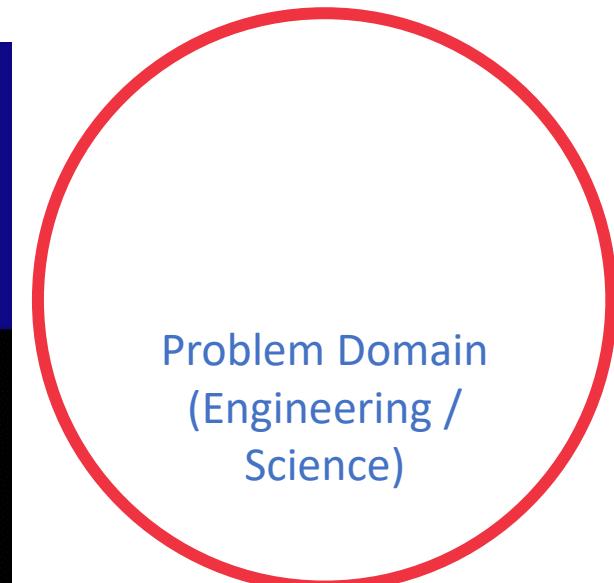
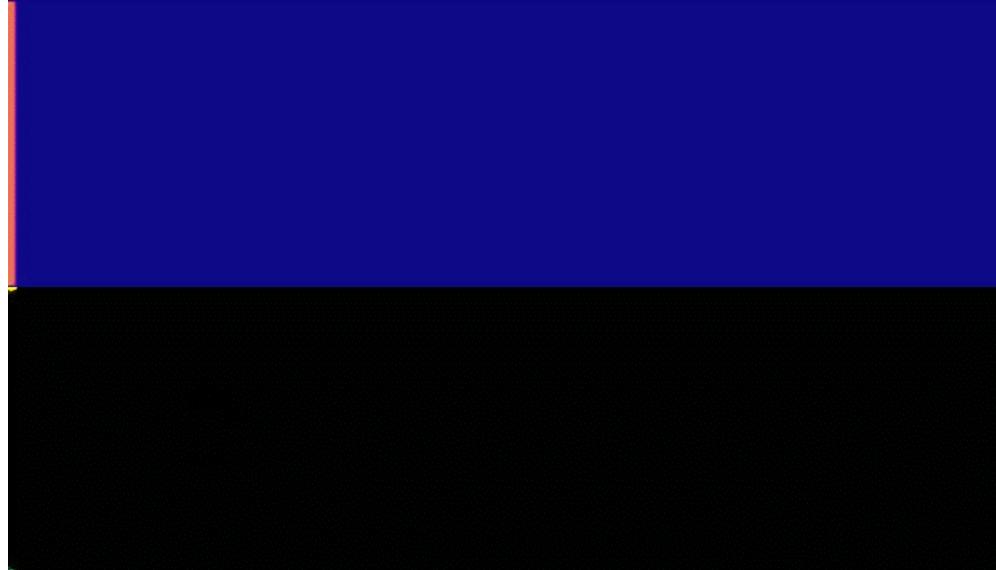
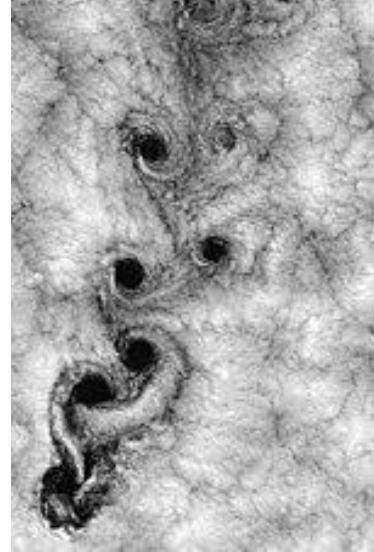
Continuity: $\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$

X - Momentum: $\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{Re} \left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right]$

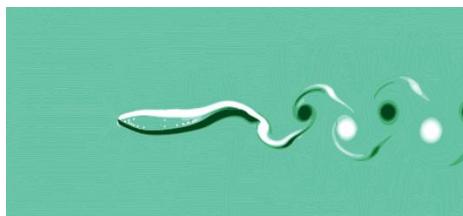
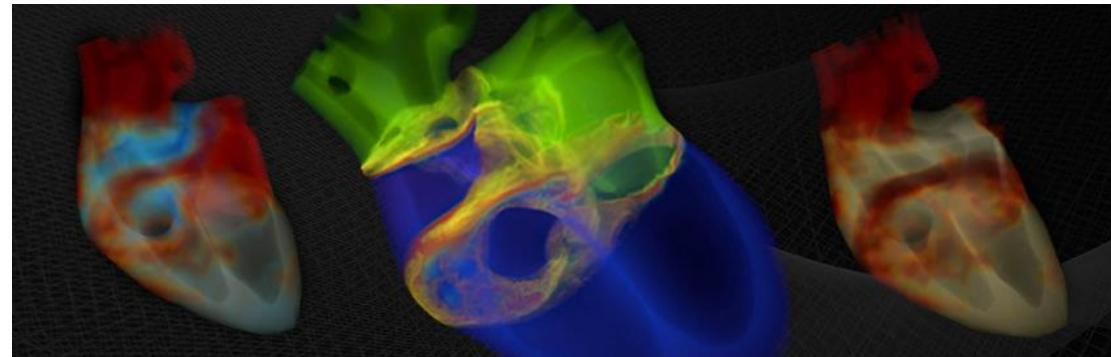
Y - Momentum: $\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{Re} \left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right]$

Z - Momentum $\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re} \left[\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right]$

Energy: $\frac{\partial(E_T)}{\partial t} + \frac{\partial(uE_T)}{\partial x} + \frac{\partial(vE_T)}{\partial y} + \frac{\partial(wE_T)}{\partial z} = -\frac{\partial(uP)}{\partial x} - \frac{\partial(vP)}{\partial y} - \frac{\partial(wP)}{\partial z} - \frac{1}{Pr} \left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right] + \frac{1}{Re} \left[\frac{\partial}{\partial x}(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}) + \frac{\partial}{\partial y}(u\tau_{xy} + v\tau_{yy} + w\tau_{yz}) + \frac{\partial}{\partial z}(u\tau_{xz} + v\tau_{yz} + w\tau_{zz}) \right]$



Problem Domain
(Engineering /
Science)





Scientific Computing

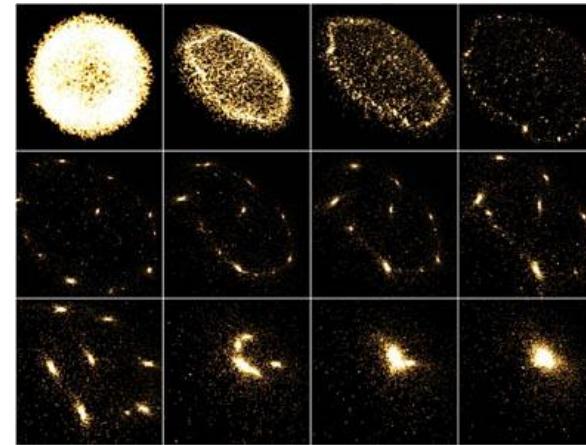
$$\mathbf{f}_{ij} = G \frac{m_i m_j}{\|\mathbf{r}_{ij}\|^2} \cdot \frac{\mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|},$$

$$\mathbf{F}_i = \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \mathbf{f}_{ij} = G m_i \cdot \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \frac{m_j \mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|^3}.$$

$$\mathbf{F}_i \approx G m_i \cdot \sum_{1 \leq j \leq N} \frac{m_j \mathbf{r}_{ij}}{\left(\|\mathbf{r}_{ij}\|^2 + \varepsilon^2\right)^{3/2}}.$$

$$\mathbf{a}_i \approx G \cdot \sum_{1 \leq j \leq N} \frac{m_j \mathbf{r}_{ij}}{\left(\|\mathbf{r}_{ij}\|^2 + \varepsilon^2\right)^{3/2}}.$$

All pairs N-Body simulation



Problem Domain
(Engineering /
Science)

Molecular Dynamics – MD



Scientific Computing

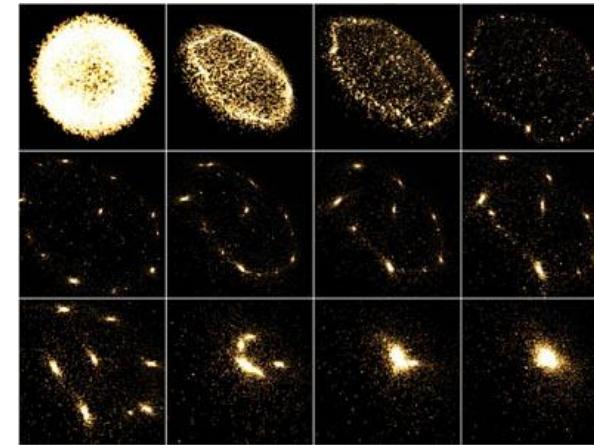
$$\mathbf{f}_{ij} = G \frac{m_i m_j}{\|\mathbf{r}_{ij}\|^2} \cdot \frac{\mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|},$$

$$\mathbf{F}_i = \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \mathbf{f}_{ij} = G m_i \cdot \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \frac{m_j \mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|^3}.$$

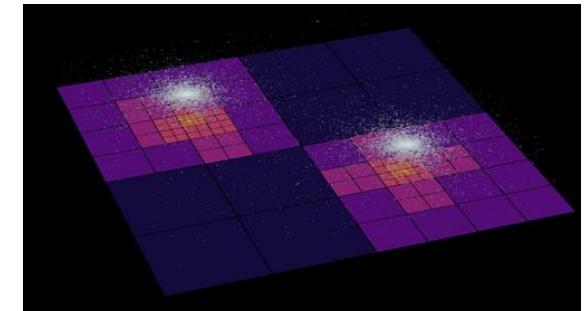
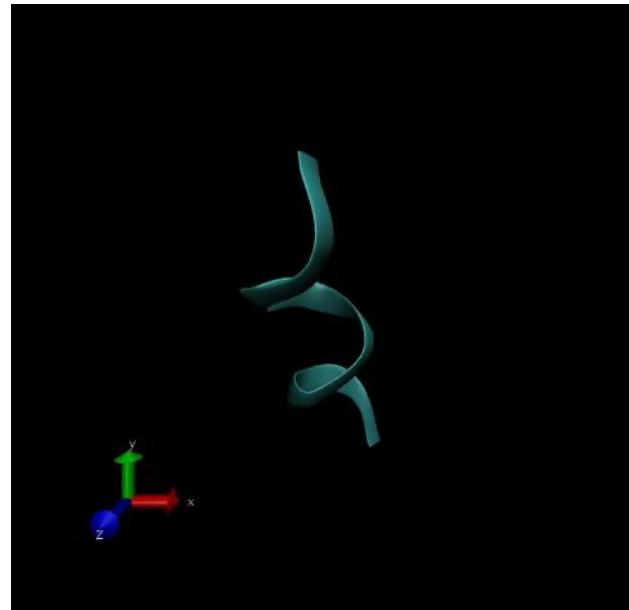
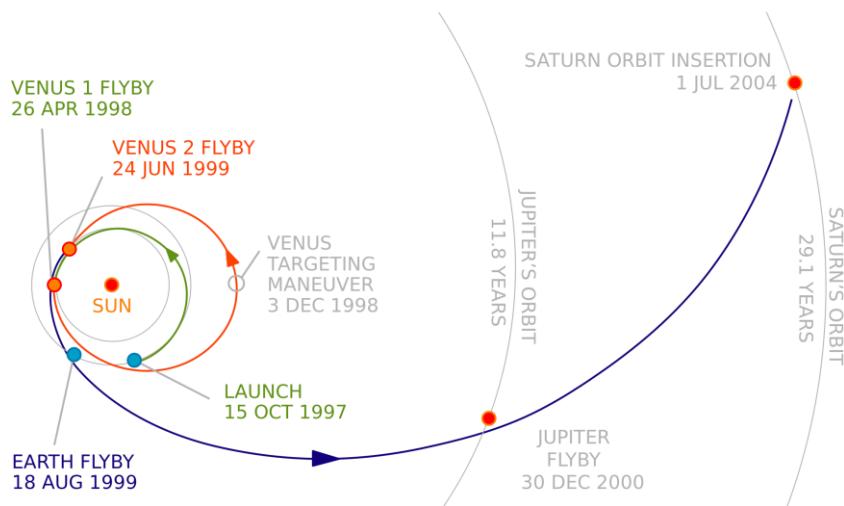
$$\mathbf{F}_i \approx G m_i \cdot \sum_{1 \leq j \leq N} \frac{m_j \mathbf{r}_{ij}}{\left(\|\mathbf{r}_{ij}\|^2 + \varepsilon^2\right)^{3/2}}.$$

$$\mathbf{a}_i \approx G \cdot \sum_{1 \leq j \leq N} \frac{m_j \mathbf{r}_{ij}}{\left(\|\mathbf{r}_{ij}\|^2 + \varepsilon^2\right)^{3/2}}.$$

All pairs N-Body simulation



Problem Domain
(Engineering /
Science)





Scientific Computing

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

Schrödinger's equation

Ab initio methods in Nuclear Physics

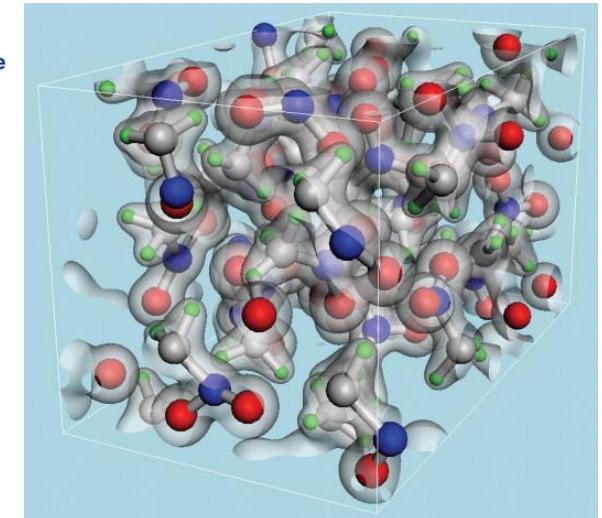
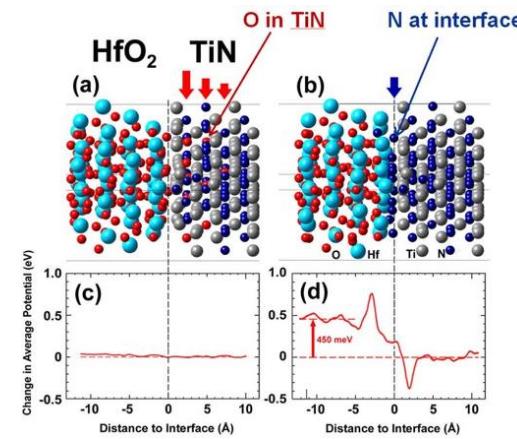
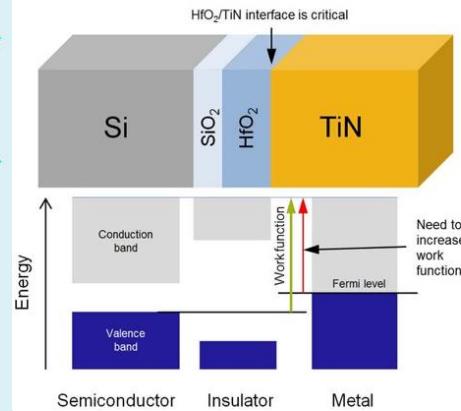
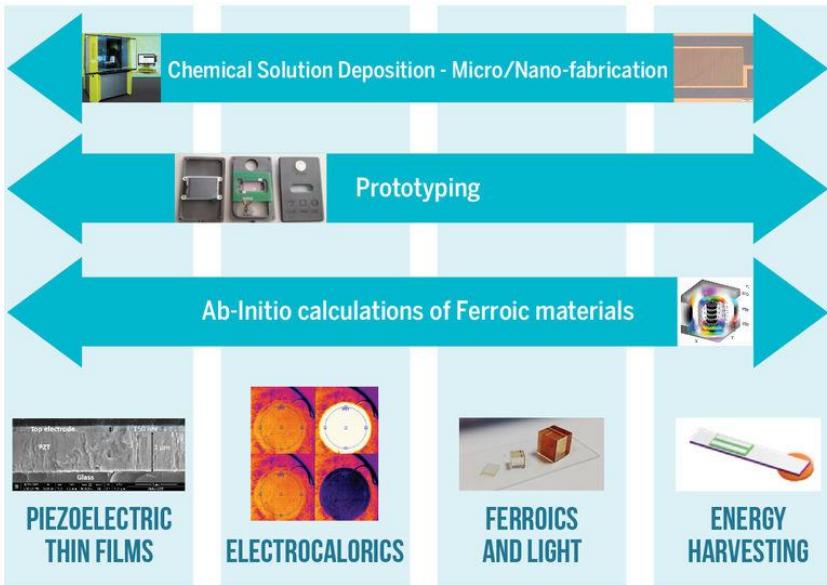
Density Functional Theory (DFT)

Material Science

Quantum Chemistry

Physics

Problem Domain
(Engineering /
Science)





Scientific Computing – *mathematical interlude*

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$



“What is unpleasant here, and indeed directly to be objected to, is the use of complex numbers. ψ is surely fundamentally a real function.”

Letter from Schrödinger to Lorentz. June 6th, 1926.

Problem Domain
(Engineering /
Science)



Scientific Computing – mathematical interlude

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

$$i = \sqrt{-1}$$

recall that $i^2 = -1$

On Complex numbers

- Origin: Italy, 14-15th century
- Reason of existence: to solve *depressed* cubic equations (e.g. $ax^3 + bx + c = 0$, without x^2 term)
- Main cast:
 - Scipione del Ferro, Antonio Fior, Niccolo Tartaglia, Gerolamo Cardano, Rafaelle Bombelli
- Second season:
 - Francois Viète (modern notation for symbolic algebra), Renee Descartes (coined *Imaginary Numbers*), Leonhard Euler (introduced the i in math notation)

Problem Domain
(Engineering /
Science)



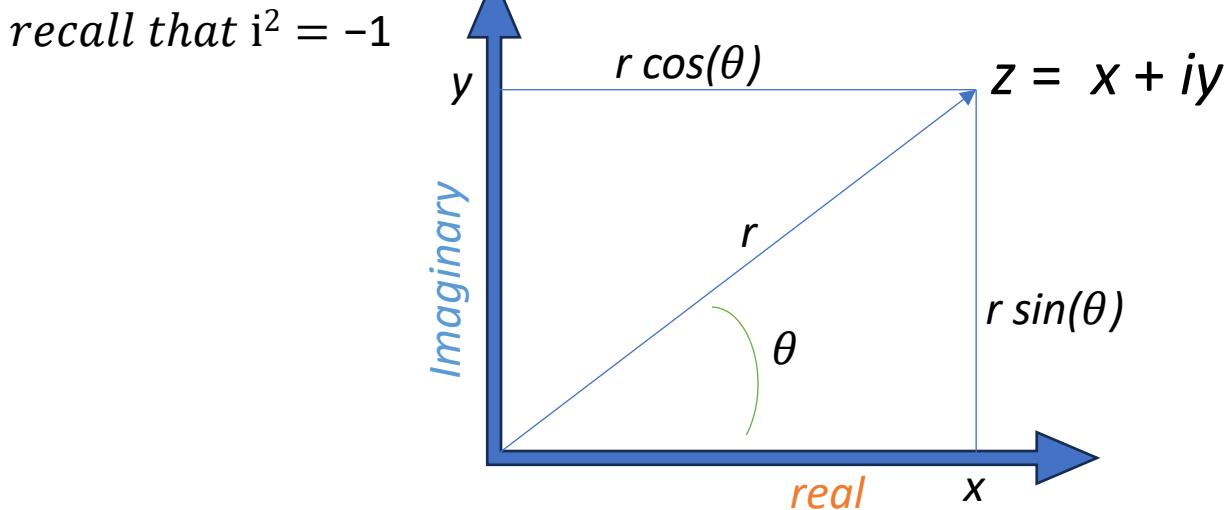
Scientific Computing – mathematical interlude

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

$i = \sqrt{-1}$

$z = x + iy$ with $x, y \in \mathbb{R}$

real *Imaginary*



Problem Domain
(Engineering /
Science)

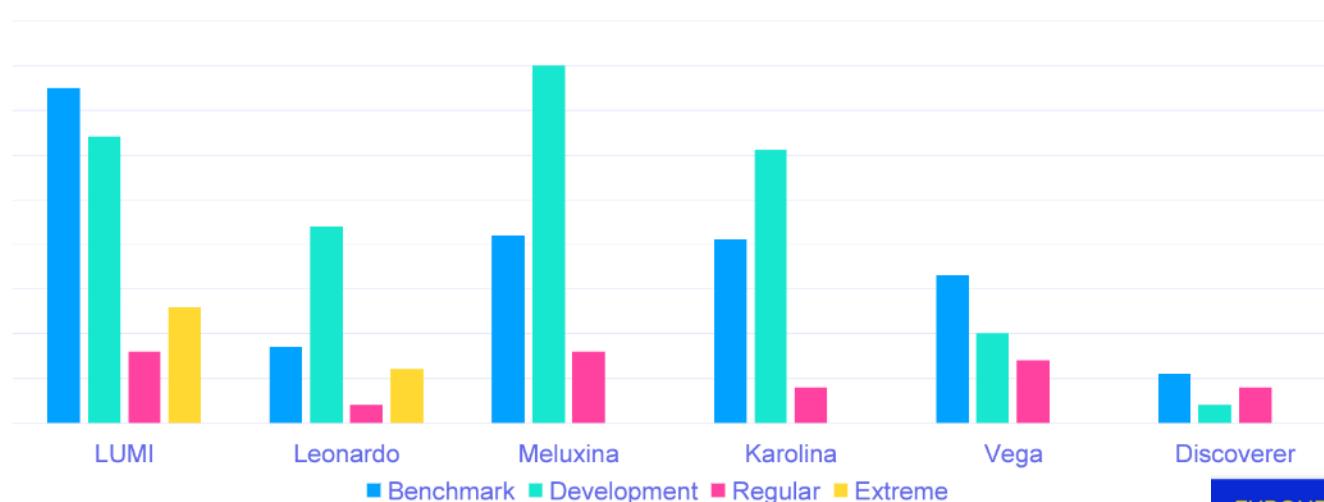
- Addition/multiplication/division follow algebraic rules
- In *polar* coordinates:
$$z = re^{i\theta} = r (\cos(\theta) + i \sin(\theta))$$
- Every complex number z has a complex conjugate z^* such that:
$$z^* = x - iy = re^{-i\theta}$$
$$z^* z = r^2$$



Use cases



596 active projects distribution per system per type of EuroHPC JU access modes

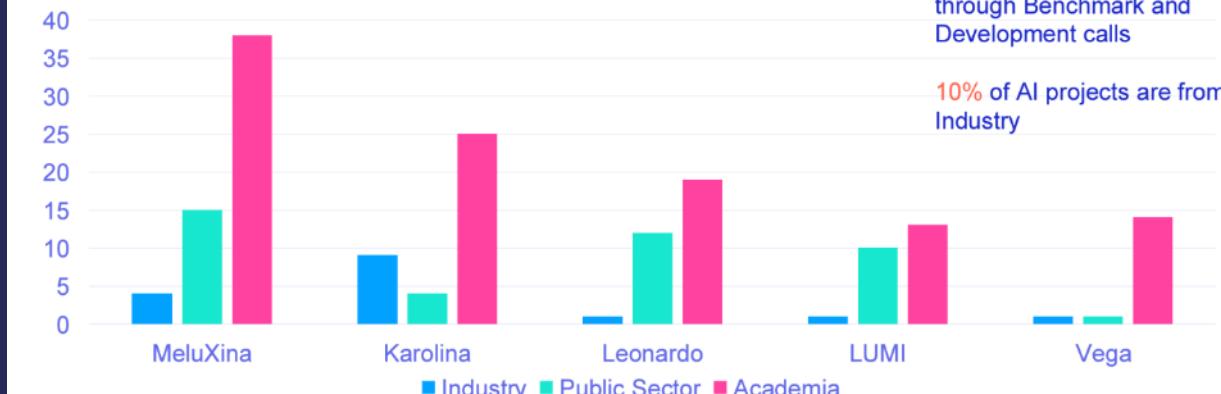


Meluxina runs
25% of all EuroHPC JU projects

Meluxina runs
35% of all EuroHPC JU AI projects

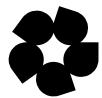


167 active AI projects distribution per system per type of applicant



(*) Leonardo was available for access since June 2023

(**) LUMI-G was on maintenances few times during the 2023 as it was newly installed



Hydrosat



SES[▲]



RSS-Hydro

WEC[○]



DESTINATION
EARTH
(DestinE)

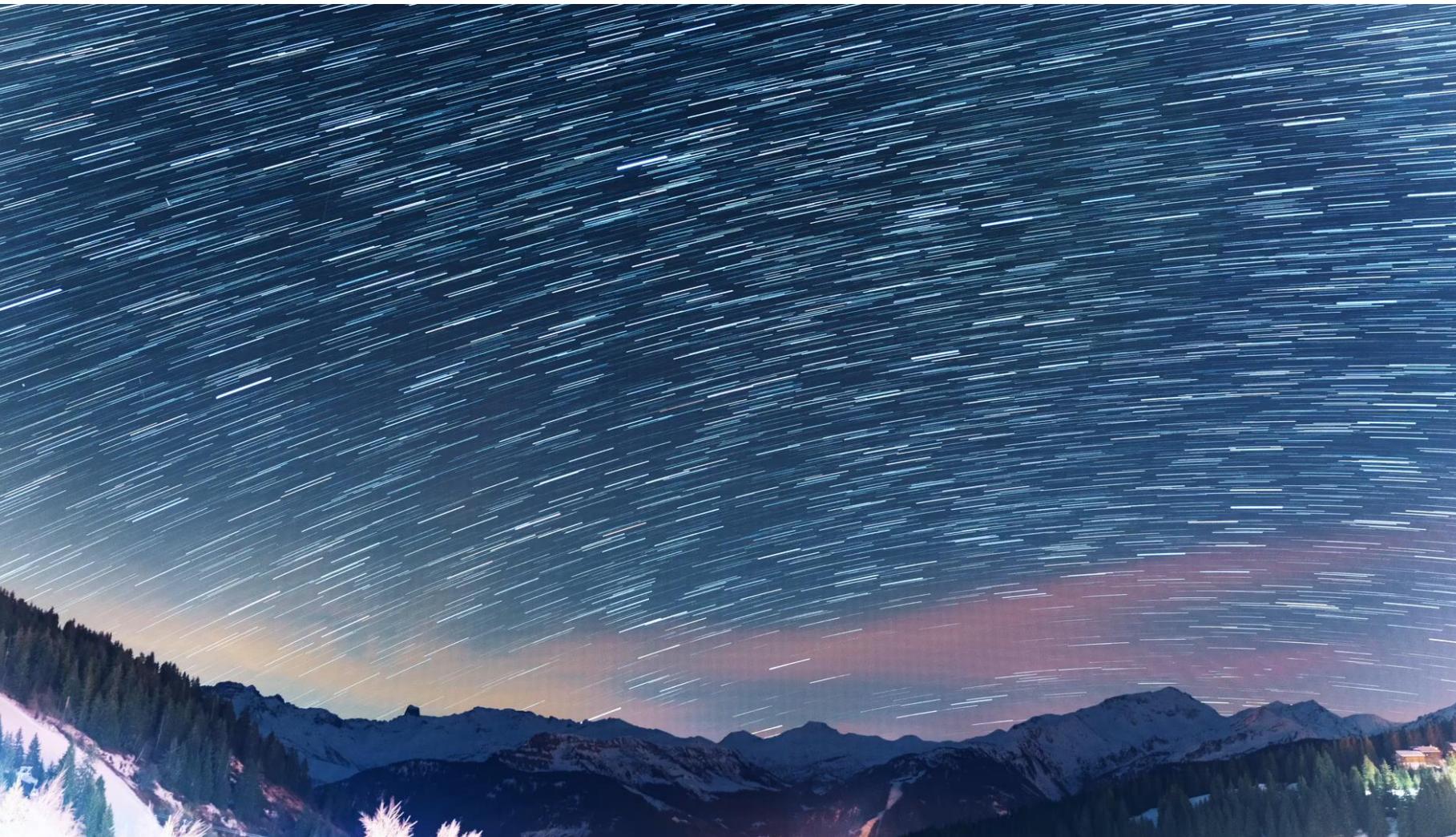


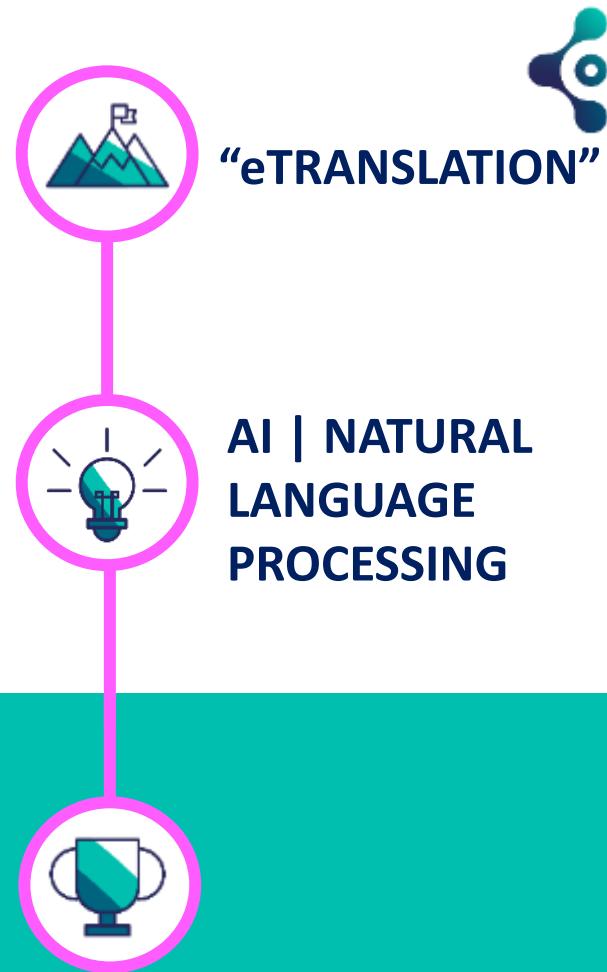
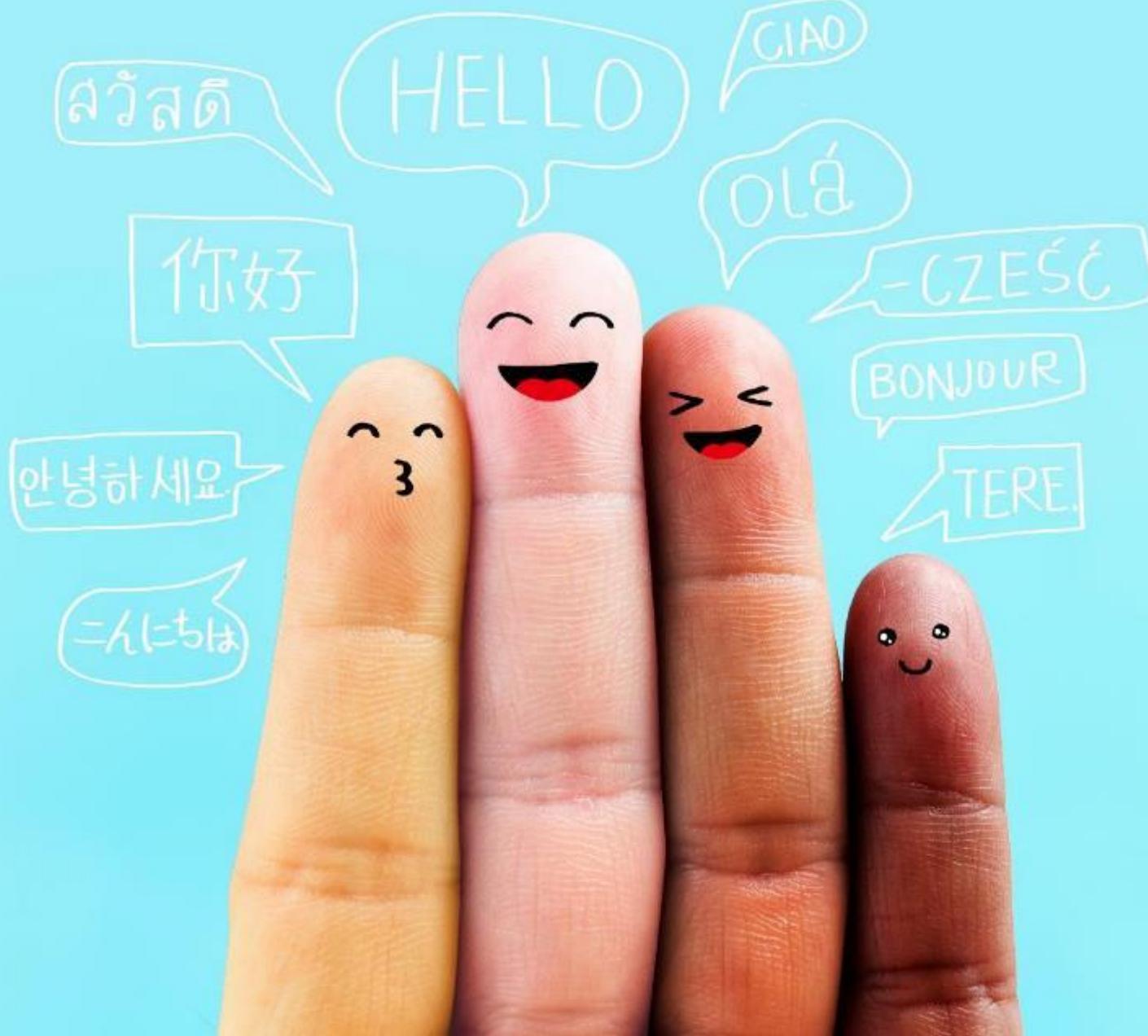
AI
& NUMERICAL
SIMULATIONS



DIGITAL TWIN OF THE
EARTH

UNDERSTAND THE PAST,
PREDICT THE FUTURE





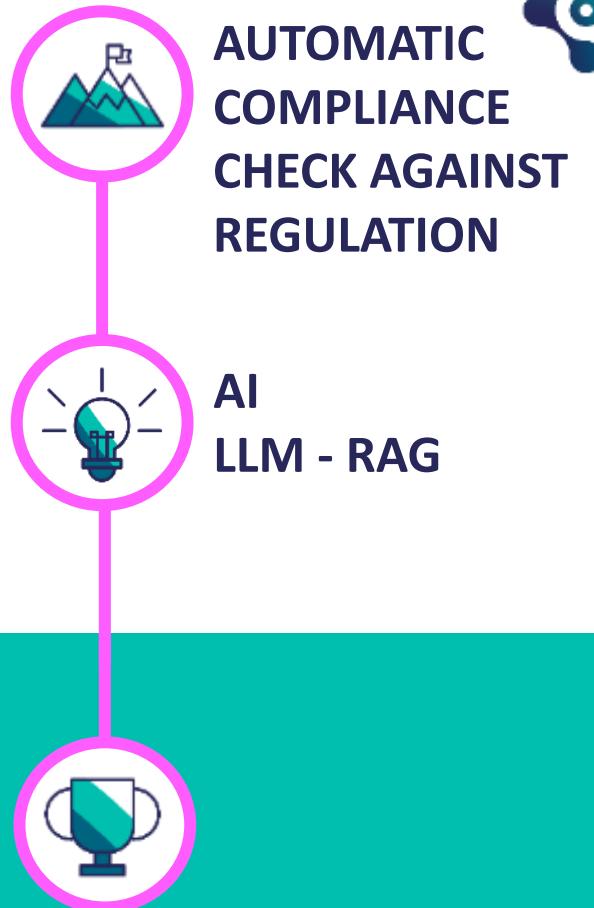


LuxProvide and ICHEC Forge Strategic Partnership to Advance High-Performance Computing in Europe

21 May 2024

[Luxembourg, May 21st] – In a pivotal development set to accelerate the adoption of HPC in Europe, LuxProvide, guardian of MeluXina, Luxembourg's state-of-the-art supercomputer, and the Irish Centre for High-End Computing (ICHEC), a leader in innovative HPC solutions and services, have entered into a strategic partnership. This alliance is aimed at bridging the transitional phase as ICHEC moves towards the decommissioning of its current platform and the establishment of a new, advanced HPC infrastructure with the support of the European High-Performance Computing Joint Undertaking (EUROHPC JU).

The Kay platform which supported the National HPC Service reached the end of its 5-year service life in late 2023 and an



AUTOMATIC
COMPLIANCE
CHECK AGAINST
REGULATION

AI
LLM - RAG



INCREASE PRODUCTIVITY
REDUCING ERRORS
INSTANT CHECKING



CoeFont



SPEECH
GENERATION



TTS / STT



GENERATION OF VOICES
FOR MANGAS/ANIMES
+
AUTO-TRANSCRIPTION
INTO TEXT FROM AUDIO



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The quantum transition of the two-dimensional Ising spin glass

[Massimo Bernaschi](#), [Isidoro González-Adalid Pemartín✉](#), [Víctor Martín-Mayor](#) & [Giorgio Parisi](#)

[Nature](#) **631**, 749–754 (2024) | [Cite this article](#)

15k Accesses | **59** Altmetric | [Metrics](#)



Acknowledgements

We thank A. Scardicchio for useful discussions. We also thank A. King for a most useful correspondence. We benefited from two EuroHPC computing grants. Specifically, we had access to the [Meluxina-GPU cluster](#) (Grant No. EHPC-REG-2022R03-182 for 158,306.5 GPU computing hours) and to the Leonardo facility (CINECA) through a LEAP grant (2×10^6 GPU computing hours). Besides, we received a small grant (10,000 GPU hours) from the Spanish Supercomputing Network (Contract No. FI-2022-2-0007). Finally, we thank Gianpaolo Marra for granting access to the Dariah cluster in Lecce. This work was partially supported by the Spanish Ministry of Science, Innovation and Universities, the Spanish Research Agency (10.13039/501100011033) and the European Regional Development Fund (A way of making Europe; Grant No. PID2022-136374NB-C21). This research has also been supported by the European Research Council under the European Union's Horizon 2020 research and innovation programme (Grant No. 694925-Lotglassy to G.P.). I.G.-A.P. was supported by the Spanish Ministry of Science, Innovation and Universities (FPU Grant No. FPU18/02665).



Quantum Spin Glasses



Study the critical phase transition of the quantum spin glass in two dimensions

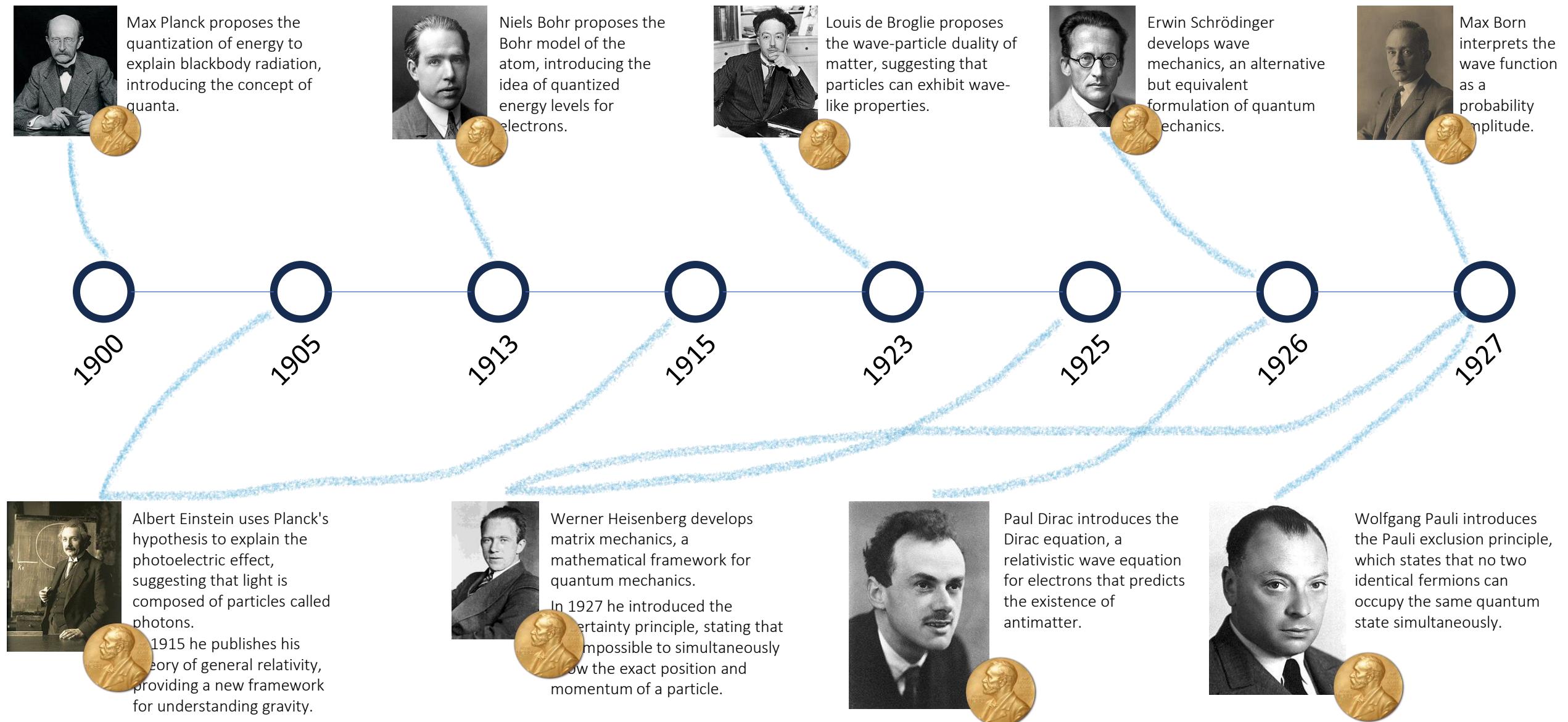


Improvement of the understanding of core physics inside Quantum Annealers

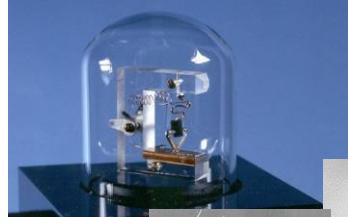


QUANTUM MECHANICS

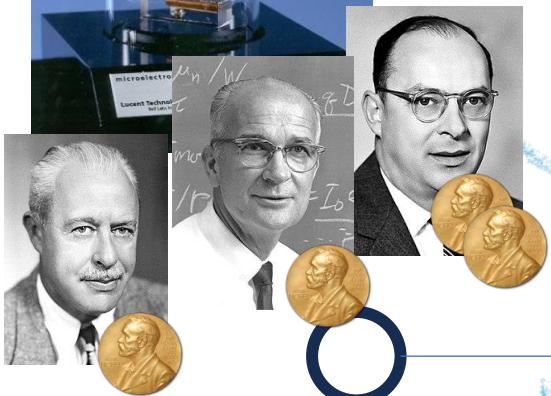
Quantum mechanics – theoretical foundations



Quantum mechanics – some initial applications



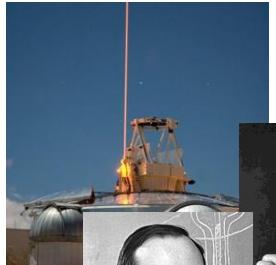
First transistor invented at Bell labs in 1947.



1930



An electron microscope uses a beam of electrons instead of light to create an image with a magnification factor of up to two million (compared to two thousand for a light microscope). The quantum mechanical principle on which the electron microscope is based is the wave-particle duality for electrons.



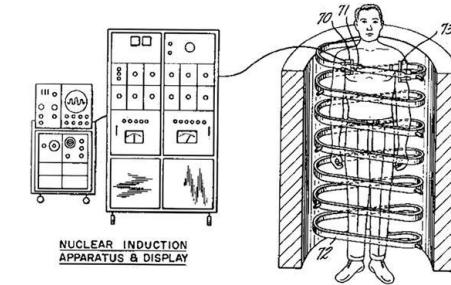
A laser is a quantum mechanical device that emits light with a well-defined wavelength in a very narrow beam.



Lasers were made in 1960 and since then have become widespread, for example in CD and DVD players, for cutting metals in industry, and in medicine.

1941

1950



First full-body Magnetic Resonance Imaging scan in 1977



1970



First nuclear power plant located near Arco, Idaho, that was activated on December 20, 1951

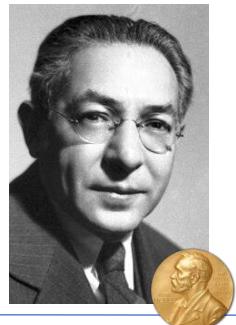


Calvin S. Fuller at work diffusing boron into silicon to create the world's first solar cell at Bell Labs in 1954.

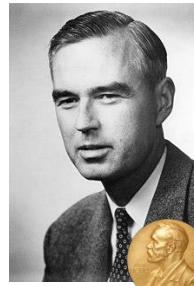
Quantum mechanics – some hidden applications



Hans Bethe made major contributions to nuclear physics, astrophysics, quantum electrodynamics, and solid-state physics.



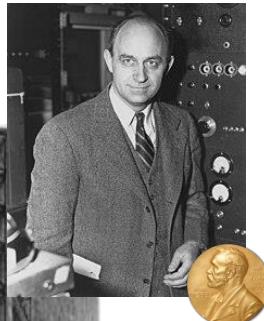
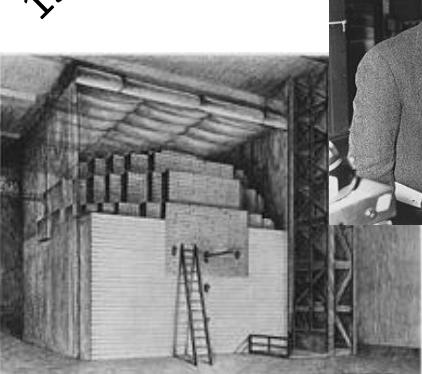
Isidor Isaac Rabi discovered nuclear magnetic resonance, which is used in magnetic resonance imaging (MRI)



Willis E. Lamb: Conducted experiments that led to the Lamb shift, a small difference in energy levels between two states of hydrogen.



1942



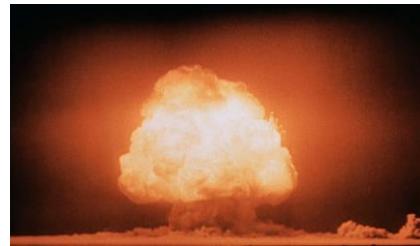
Enrico Fermi work on induced radioactivity by neutron bombardment and for the discovery of transuranium elements.



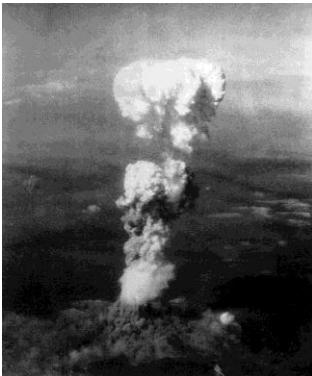
Richard Feynman known for his work in the path integral formulation of quantum mechanics, the theory of quantum electrodynamics, the physics of the superfluidity of supercooled liquid helium, as well as his work in particle physics for which he proposed the parton model.



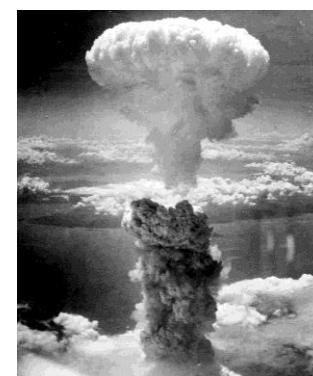
Chicago Pile-1 (CP-1) was the world's first artificial nuclear reactor. On 2 December 1942, the first human-made self-sustaining nuclear chain reaction was initiated in CP-1 during an experiment led by Enrico Fermi.



Trinity test



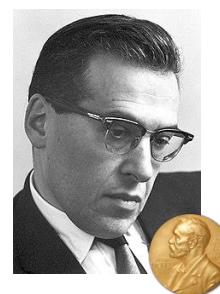
Hiroshima and Nagasaki



1945



Ernest Lawrence developed the cyclotron, a particle accelerator used in nuclear research.

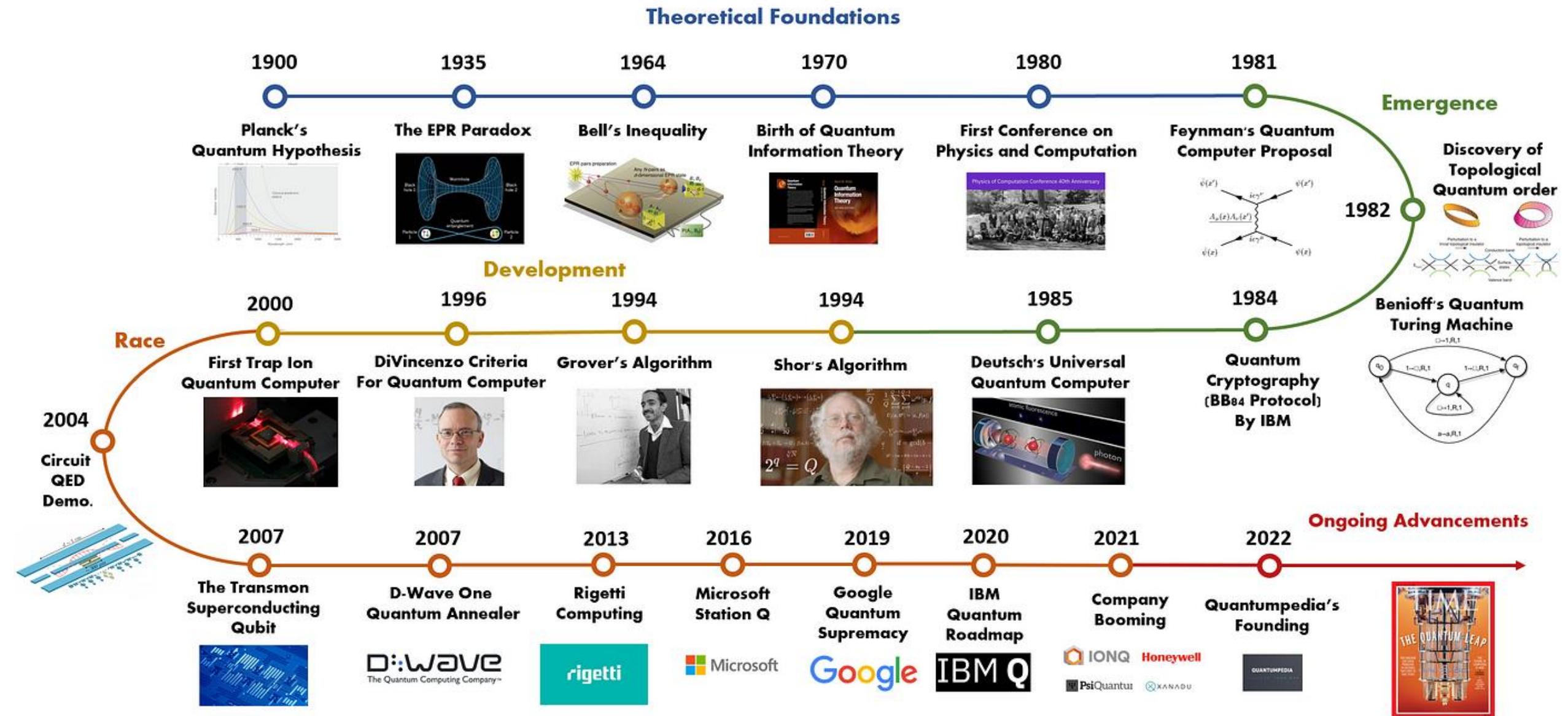


Julian Schwinger: Developed quantum electrodynamics (QED), a theory that describes the interaction between electrons and photons.



J. Robert Oppenheimer: Director of the Los Alamos Laboratory, where the atomic bomb was developed.

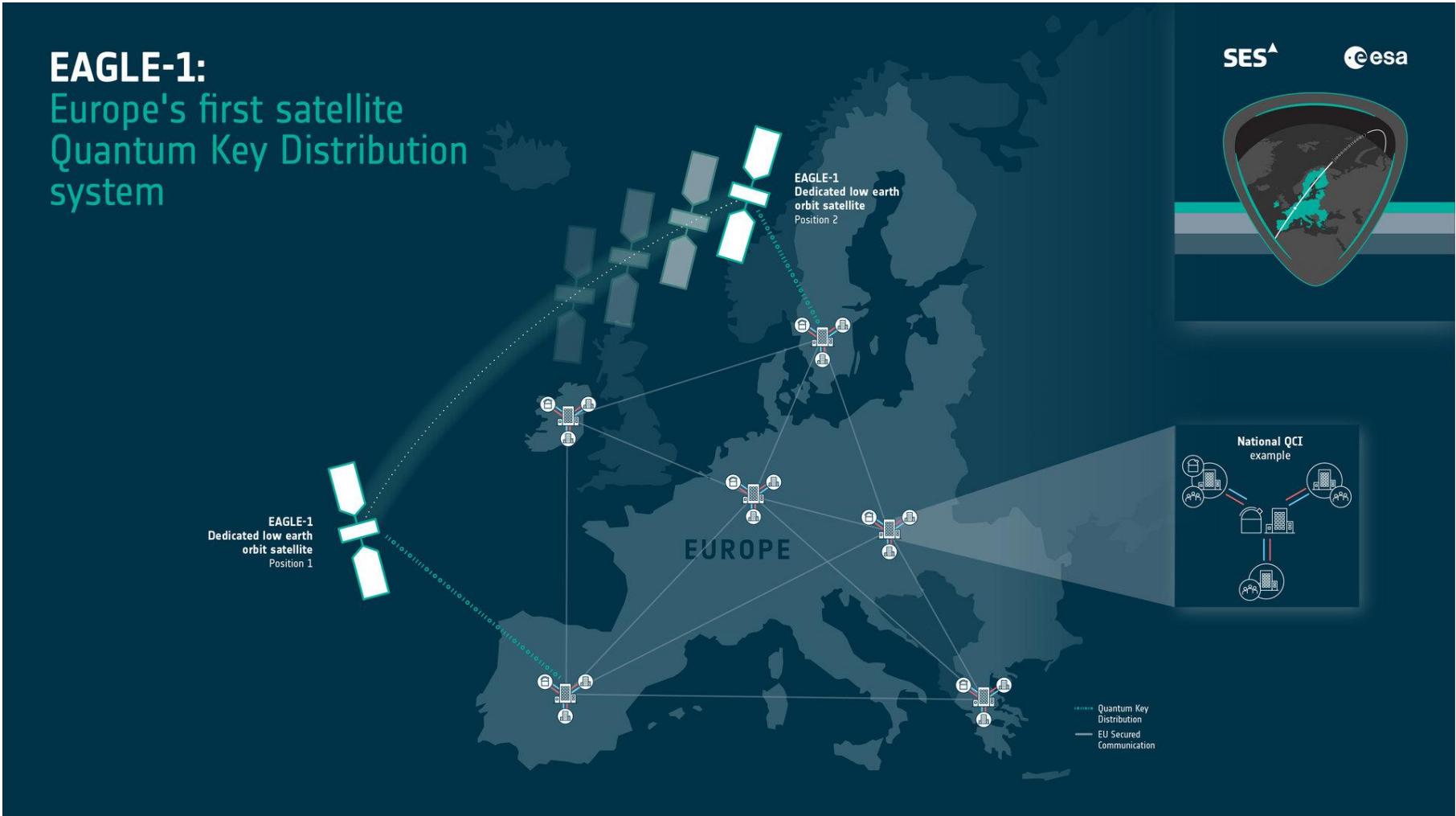
Quantum mechanics



Quantum mechanics – future application

The Eagle-1 satellite is due to launch in late 2025 to early 2026 and will then complete three years of in-orbit validation supported by the European Commission.

Eagle-1 will be operated by SES !



Quantum mechanics

102 companies shaping the quantum computing landscape

Quantum computer makers

Superconducting circuits

IQM
rigetti

seeqc
qci

SPINQ
XANADU
QUANDELÀ

Photonics

PsiQuantum
photonic
ORCA Computing
Quantum Source

OQC

pleximo
ATLANTIC QUANTUM
ALICE & BOB

QUANTWARE
Nord Quantique

Silicon, carbon, & helium

C12

equal 1
EeroQ

ARCHER
QUANTUM MOTION

Neutral atoms

PASQAL
ColdQuanta
planqc
atom computing

Trapped ions

QUANTINUUM
AQT
IONQ
eleQtron

Enterprise use cases

Cross-industry applications

ZAPATA
SandboxAQ
1QBit
qcWARE
MULTIVERSE COMPUTING
Jij
KIPU

Terra Quantum
PHASECRAFT

Drug discovery

POLARIS^{ab}
KUANO
ProteinDure
algorithmliq
QUBIT COMPUTING
menten.AI

Financial services

Quantum
QuantFi
QDT
QCLIQUE

Chemical & materials simulation

GOOD CHEMISTRY
QSIMULATE
BosonQ Psi
HQ5 QUANTUM SIMULATIONS
QuanSys
Quemix

Optimization & logistics

D-WAVE
Quantum-South
SAVANT X
ENTROPICA LABS
Light Solver
SolidStateAI
QUBIT COMPUTING

Developer & programming tools

STRANGE WORKS
MRS

CLASSIQ
blueqat

Quantagonia
π_u
HORIZON QUANTUM COMPUTERS

Quantastica
agnostiq
QbitSoft
QUANTUM FLYTRAP
AQUANTUM

Quantum hardware components

kiutra
BLUE FORS
Qubitekk

QUIX
AQUARK TECHNOLOGIES
QUANTOPTICON

aegiq
QPHOX
QANT

Qubit control & error correction

Q-CTRL
parityqc
Orange Quantum Systems
QBLOX

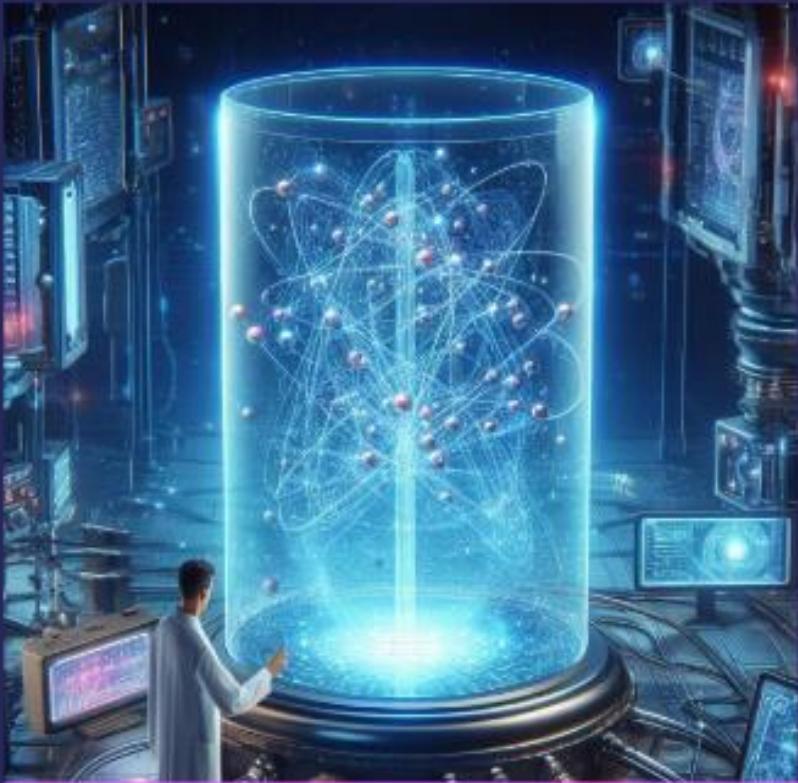


Deployment of 6 Quantum Computers

- 6 hosting sites
 - Czechia, France, Germany, Italy, Poland, Spain
- 4 different platforms
 - Trapped ions, Superconducting, Photonics, Rydberg atoms
- Call 2023-2024
 - At least 2 new hosts



WHAT'S NEXT?



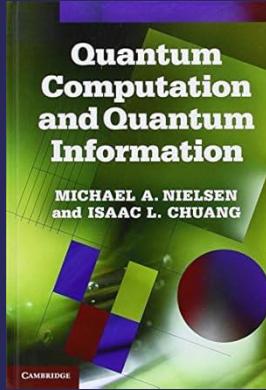
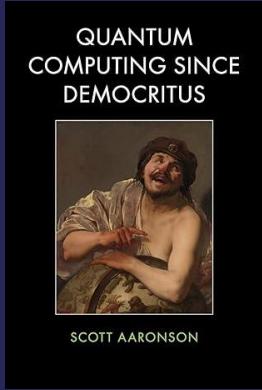
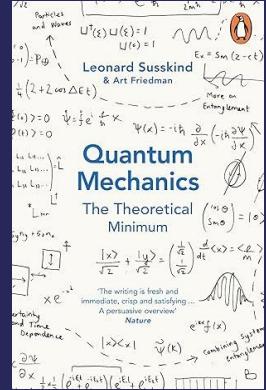
QUANTUM



MELUXINA 2.0

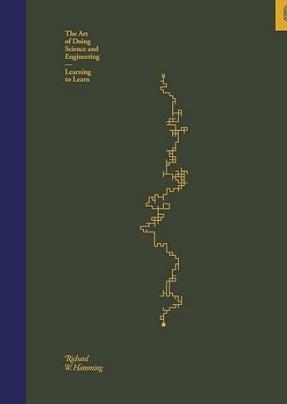
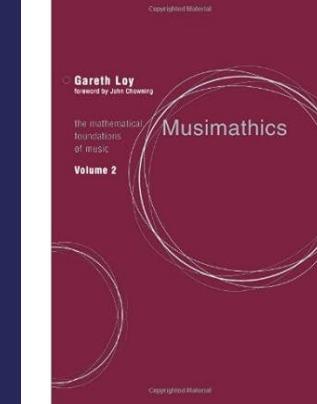
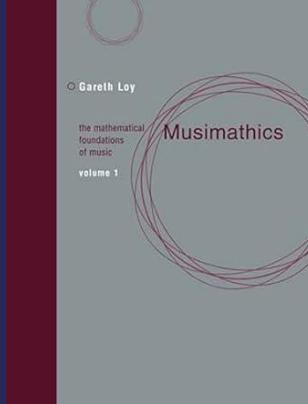
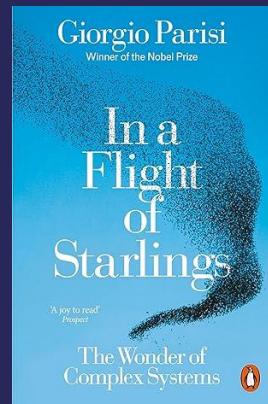


Good Literature



QC Quantum Country

<https://quantum.country/>





EXPLORING THE FRONTIERS OF DIGITAL INTELLIGENCE

Our mission is to fuse data science and supercomputing capabilities, ensuring accuracy, security, and sustainability for a thriving future.

