

Uni.lu HPC School 2019

PS5b: Scalable Science II: CFD / MD / Chemistry applications



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<http://hpc.uni.lu>



Latest versions available on Github:



UL HPC tutorials:

<https://github.com/ULHPC/tutorials>

UL HPC School:

<http://hpc.uni.lu/hpc-school/>

PS5b tutorial sources:

ulhpc-tutorials.rtf.d.io/en/latest/multiphysics/





Summary

1 Introduction

2 UL HPC software environment



Foreword

So we have some news...

Foreword



Foreword




Foreword



Foreword



Foreword



Donnerstag, 04. Juli 2019 10°

Luxemburger Wort


HOME RUBRIKEN INFO-SERVICE FAMILIENANZEIGEN ANZEIGENMARKT E-PAPER SUCHE

LOGIN ABONNEMENT

"Meluxina" unter den 25 schnellsten Supercomputern

Das LuxConnect Datenzentrum in Bissen (Pétus). Das Gebäude links wird neu errichtet.

WIRTSCHAFT / 12. Juli 2019 17:46/2019

 **Wirtschaftsminister Etienne Schneider stellte am Freitag Luxemburgs zukünftigen Hochleistungsrechner vor.**

Recht TREL

Zehn Petaflops Rechenleistung wird "Meluxina" bieten, wie der neue luxemburgische Hochleistungsrechner vom Betreiber Luxconnect getauft wurde. Das sind zehn Millionen Milliarden oder 10 hoch 18 Rechenoperationen

<https://www.wort.lu/de/ressources/meluxina-unter-den-25-schnellsten-supercomputern-5451842366301794634089> **30 Millionen Euro teuren Supercomputer weltweit**

Foreword



jeudi 30 juin 2016 20°

FR

ACCUEIL SECTIONS SERVICES ANNONCES FAMILIALES PETITES ANNONCES E-PAPER RECHERCHER

Meluxina, le nouveau superordinateur du Luxembourg

Le superordinateur de l'université à Bissen aux limites technologiques

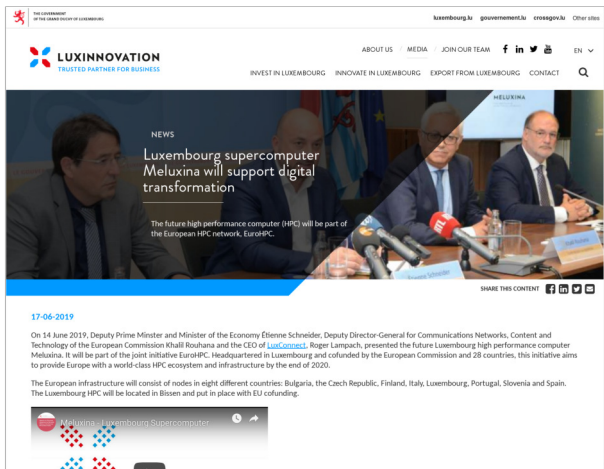
INTERNATIONAL / 14.06.2016

L'engin, d'une puissance de dix pétaflops, sera hébergé dans le datacenter de LuxConnect à Bissen. Dédié à la recherche, la médecine personnalisée et aux projets eHealth, il devrait à terme employer 50 personnes.

MARC AUBERTS

Le superordinateur n'a rien d'une sirène. Dévoilé sous le nom de Meluxina par le ministre de l'Économie Etienne Schneider (LSAP) ce mardi, il calcule cependant vite, très vite: à raison de 10.000.000.000.000.000 opérations à la

Foreword



The screenshot shows the Luxinnovation website with a news article titled "Luxembourg supercomputer Meluxina will support digital transformation". The article is dated 17-06-2019 and discusses the future high performance computer (HPC) Meluxina, which will be part of the European HPC network, EuroHPC. The article mentions that Meluxina is a joint initiative EuroHPC, headquartered in Luxembourg and cofunded by the European Commission and 28 countries. It also states that the European infrastructure will consist of nodes in eight different countries: Bulgaria, the Czech Republic, Finland, Italy, Luxembourg, Portugal, Slovenia and Spain. The Luxembourg HPC will be located in Bissen and put in place with EU cofunding.

NEWS
Luxembourg supercomputer Meluxina will support digital transformation

The future high performance computer (HPC) will be part of the European HPC network, EuroHPC.

17-06-2019

On 14 June 2019, Deputy Prime Minister and Minister of the Economy Étienne Schneider, Deputy Director-General for Communications Networks, Content and Technology of the European Commission Khallil Rouhana and the CEO of [LuxConnect](#), Roger Lampach, presented the future Luxembourg high performance computer Meluxina. It will be part of the joint initiative EuroHPC. Headquartered in Luxembourg and cofunded by the European Commission and 28 countries, this initiative aims to provide Europe with a world-class HPC ecosystem and infrastructure by the end of 2020.

The European infrastructure will consist of nodes in eight different countries: Bulgaria, the Czech Republic, Finland, Italy, Luxembourg, Portugal, Slovenia and Spain. The Luxembourg HPC will be located in Bissen and put in place with EU cofunding.

Meluxina - Luxembourg Supercomputer

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IN LUXEMBURG
14. Juni 2019 17:07, Akt: 14.06.2019 20:36

«Meluxina» soll Lücke zu China und USA schließen

BISSEN – Der Supercomputer, der bis Ende 2020 installiert wird, soll einer der 20 schnellsten Rechner der Welt werden. Das teilte Wirtschaftsminister Schneider am Freitag mit.



Mario Grotz, Étienne Schneider, Khalif Rouhana und Roger Lampech (v.l.) haben am Freitag den Supercomputer vorgestellt. (Bild: L'essentiel)

TIERISCHE FRACHT

Cargolux liefert die Beluga-Wale wohlbehalten ab



LUXEMBURG – In einer Bucht bei Island entsteht ein Freiwasserreservat für Wale und Delphine – als Alternative zu Freizeitparks. Zwei Beluga-Wale wurden nun aus China eingeflogen.

CHAMBER-PRÄSIDENT

Etgen zieht nach dem erstem Halbjahr Bilanz



LUXEMBURG – Vor einem halben Jahr hat Fernand Etgen das Amt des Parlamentspräsidenten übernommen. Zeit für eine Zwischenbilanz.

RADARE IN LUXEMBURG

Am Donnerstag heißt es wieder aufpassen!



LUXEMBURG – Die Police Grand-Ducale zeigt keine Gnade für Raser: Am Donnerstag hat sie sich dieserorts im Großherzogtum auf die Lauer gelegt.

IN LUXEMBURG



Thursday, 30 Jun 2019

Chronicle.lu

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HOME / NEWS / ECONOMICS / LUXEMBOURG MELUXINA SUPERCOMPUTER TO JOIN EUROPEAN EUROHPC NETWORK

Luxembourg Meluxina Supercomputer to Join European EuroHPC Network

Published on Friday, 14 Jun 2019 17:11 by BD

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On Friday 14 June 2019, Luxembourg's Deputy Prime Minister and Minister of the Economy, Etienne Schneider, together with the Deputy Director General of the Directorate General of Communication Networks, Content and Technologies (DG CNECT) at the European Commission, Khalil Rouhana, as well as LucConnect CEO, Roger Lampach, presented the future Luxembourg supercomputer, named 'Meluxina', which will join the European network of EuroHPC supercomputers.

The EuroHPC Joint Undertaking, headquartered in the Grand Duchy, is an initiative co-financed by the European Commission and 28 countries, including Luxembourg, which aims to provide Europe with an ecosystem and a computing infrastructure. By June 2019, following a call for projects, EuroHPC selected eight sites in different Member States to host supercomputers. The Luxembourg project to install the petascale supercomputer Meluxina at LucConnect in Bissen has

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TRENDING NEWS

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Abroad 16 Jun, 2019 09:59

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Nicolas Grass Formally Appointed Honorary Consul General of India in Luxembourg
Embassies & Consulates 17 Jun, 2019 20:05

Luxembourg-UK Agreement Guarantees Citizens' Voting Rights Post-Brexit
Politics 18 Jun, 2019 15:04

Grosbusch Introduces 100% Recyclable, Biodegradable Packaging
Environnement 17 Jun, 2019 10:10

Luxembourg, LU

https://Subject-Chronicle.lu/https://chronicle.lu/category/economy/2019/06/14/luxembourg-meluxina-supercomputer-to-join-european-eurohpc-network-high-performance

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DELANO

LUXEMBOURG IN ENGLISH

MEET MELUXINA, LUXEMBOURG'S NEW SUPERCOMPUTER

NEWS • BUSINESS • 17.06.2019 • DELANO STAFF

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Luxembourg's petascale supercomputer, planned to open in Bissen before the end of 2020, was presented to the public on Friday.

Industry and startups will be able to access Meluxina, as the computer has been dubbed, at the offices of LuxConnect in Bissen, where project will eventually generate up to 50 jobs. The Luxembourg supercomputer is one of eight to join the European network of supercomputers.

According to a government statement published on Friday, it will have a computing power of 10 petaflops/second, which corresponds to 10,000,000,000,000,000 computing operations per second.

Meluxina will be dedicated to applications in research, personalised medicine and eHealth projects, as well as the needs of companies, in



Meluxina will join the European EuroHPC network of supercomputers. Photo: Shutterstock

LATEST NEWS



Foreword



MELUXINA

HIGH PERFORMANCE
COMPUTING IN LUXEMBOURG



MeluXina National Supercomputer

MeluXina - coming in 2020

- 10 PetaFlop supercomputer
- Modular architecture covering a wide variety of needs
- High performance network & storage for HPC, BigData & AI

MeluXina National Supercomputer

MeluXina - coming in 2020

- 10 PetaFlop supercomputer
- Modular architecture covering a wide variety of needs
- High performance network & storage for HPC, BigData & AI

What this means for you

- Algorithms and applications must be run **at scale**
- **Code development** will play a large role
- Need to use different computing elements and memory hierarchy
 - ↪ will play a critical role in your **application performance**

Session Objectives

Practice utilization of parallel codes on UL HPC clusters

- Computational Physics
- Computational Chemistry
- Engineering

Application	Description
NAMD	Parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.
Quantum Espresso	Integrated suite of tools for electronic-structure calculations and materials modeling at the nanoscale .
ABINIT	Materials science package implementing DFT, DFPT, MBPT and TDDFT.
ASE	Atomistic Simulation Environment with the aim of setting up, steering, and analyzing atomistic simulations with the help of external codes.
NWChem	Computational chemistry tools scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources.
OpenFOAM	CFD package for solving complex fluid flows involving chemical reactions, turbulence and heat transfer.



Summary

1 Introduction

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Material Science & Engineering sw.

Software on UL HPC	In 2018 software set	In 2019 software set*
ABINIT	8.6.3	8.10.2
ASE	3.16.0	3.17.0
CRYSTAL	17.v1.0.1	17.v1.0.2
ESPResSo	3.3.1	TBA - latest
GROMACS	2016.5	2019.2
Meep	1.4.3	TBA - latest
NAMD	2.12	2.13
NWChem	6.8	6.8
QuantumESPRESSO	6.2.1	6.4.1
VASP	5.4.4.18Apr17	WIP - 5.4.4.18Apr17
Yambo	4.3.1	TBA - latest
OpenFOAM	v1712	WIP - v1812
Salome	8.5.0	TBA - latest
Gmsh	4.3.0	TBA - latest

*Being tested in development environment: `module load swenv/default-env/devel`
 List not exhaustive! More complete lists at <https://hpc.uni.lu/users/software/>



Quick Q&A

- 1 What particular software are you using?
- 2 Do you use it from the HPC global software sets?
- 3 Do you compile/install it yourself?
- 4 Would you like to have something added to the global set?
- 5 What computational patterns does it exhibit?
- 6 Is it scalable? What's the largest test that you've done?
- 7 Can we help you optimize your executions?

Questions?

<http://hpc.uni.lu>

High Performance Computing @ uni.lu

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1 Introduction

2 UL HPC software environment