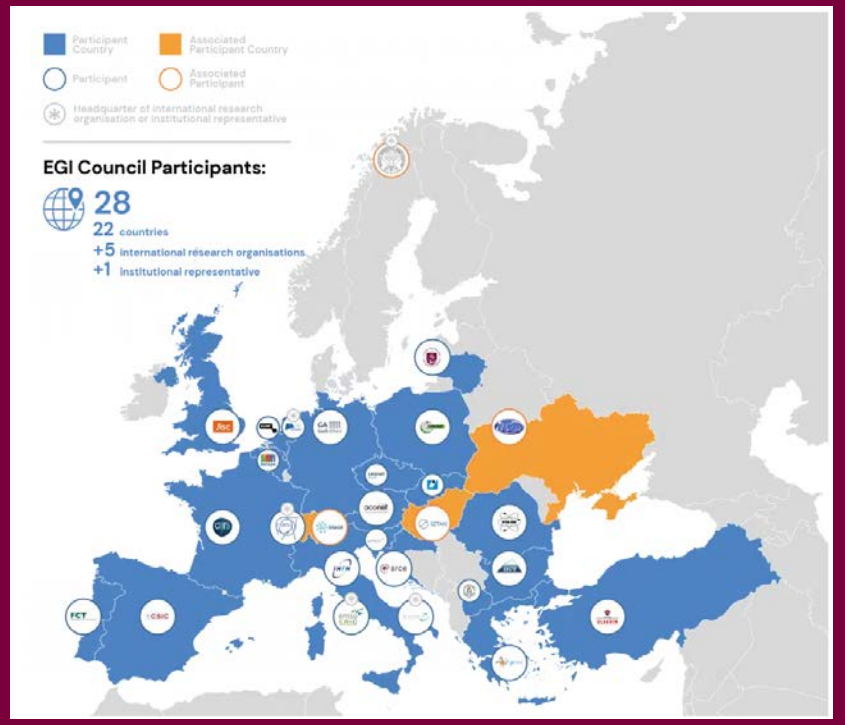
Vilnius University

Vilnius University contributions to scientific computing

Asoc. Prof. Mindaugas Mačernis
Vilnius University, Lithuania
2022



Vilnius University

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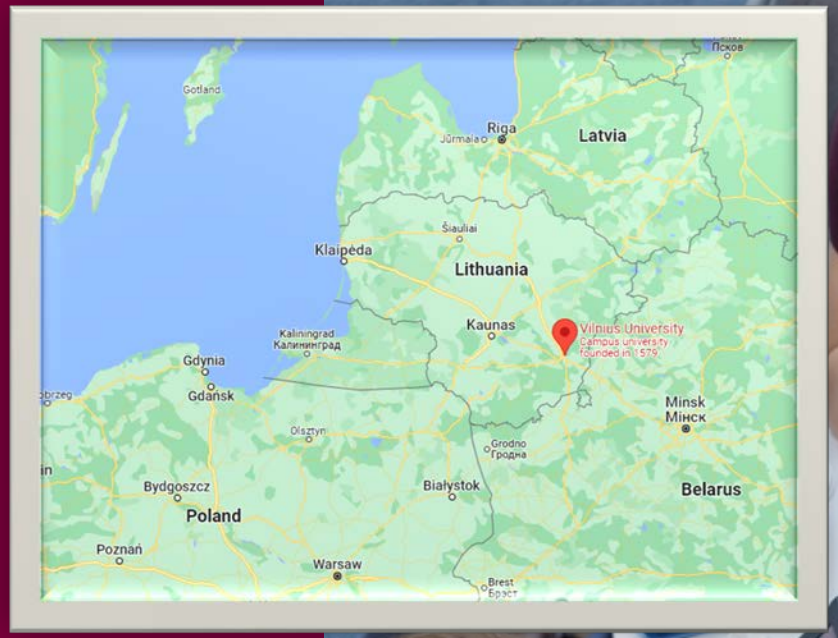
2. Computing infrastructures available nationally
3. Important research communities in Lithuania
4. EGI & Lithuania

Vilnius University

Some facts about about Vilnius University

VU

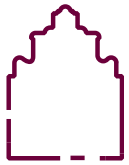


Vilnius University – the first and largest university in Lithuania, one of the oldest and most prominent higher education institutions in Central and Eastern Europe, established in 1579 in Lithuania's capital city Vilnius, with a faculty in the second largest city, Kaunas.

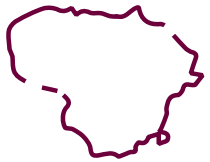
Website: www.vu.lt

Facts and Figures

Vilnius University



Founded in 1579 m.



#1 in Lithuania*

400 in the world*

189 study programmes offered

~1 500 scientific publications annually

~25 000 students

*QS World University Rankings

Vilnius University

Studies

76 Bachelor and integrated study programmes

106 Master study programmes

29 Fields of doctoral studies

63 Medicine and dentistry residency programmes

Vilnius University

Membership in international networks:

- ERASMUS
- NORDPLUS
- UTRECHT, MAUI, AEN
- BSRUN
- CREPUQ
- UNICA
- ISEP
- Scholars at Risk/New York University
- EUA
- IAU
- EAIE
- ALTE
- BUP
- Magna Charta Observatory
- COIMBRA Group

Vilnius University

International projects

Educational Erasmus projects:

- Knowledge alliances
- Capacity building
- Strategic partnerships

Scientific projects:

- ES Horizon 2020
- NATO Science programmes
- Frameworks 5, 6, 7
- Others (CERN, EUROSTAT, etc.)

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Cooperation with business:

- Barclays Technologies
- Sensor Electronics Technology Inc.
- Huawei Technologies Co.
- IBM
- TELE2
- CERN

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Computing infrastructures available nationally

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Supercomputer „VU HPC“ & Open Access Center (OAC) for HPC

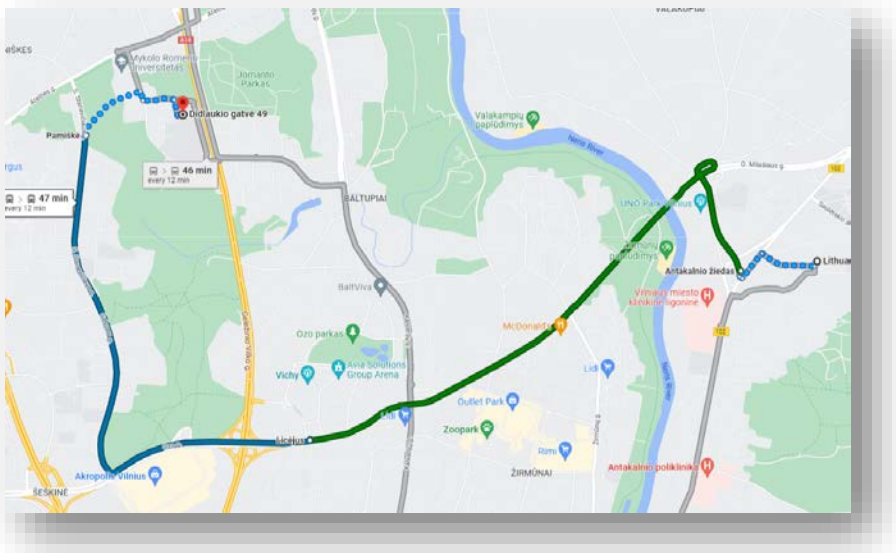
Vilnius University

Lithuanian Open Access National Computational Center

Lithuanian Open Access National Computational Center is located in Vilnius university over two faculties: Faculty of Physics (Saulėtekis) and Faculty of Mathematics and Informatics.

The supercomputer “VU HPC” has over 0.5 Pflops infrastructure while its Sauletekis location achieved 0.25 PFlops real HPLinpack speed up.

Faculty of Mathematics and Informatics



Faculty of Physics

Institute of Chemical Physics

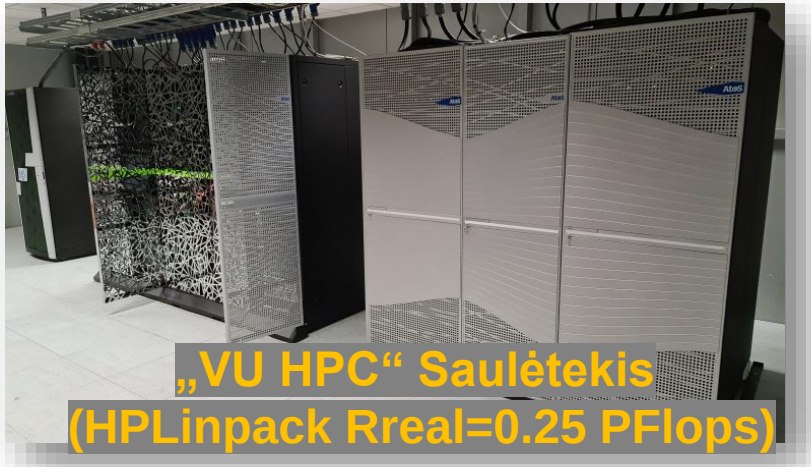
What has happened

Asoc. Prof. Mindaugas Macernis, Vilnius University

Vilnius University

„VU HPC“ (HPLinpack Rpeak > 0.5 PFlops)

„VU HPC“ ITOAC



„VU HPC“ Saulėtekis
(HPLinpack Rreal=0.25 PFlops)

Supercomputer „VU HPC“

Staff: about 11-15 active HPC experts

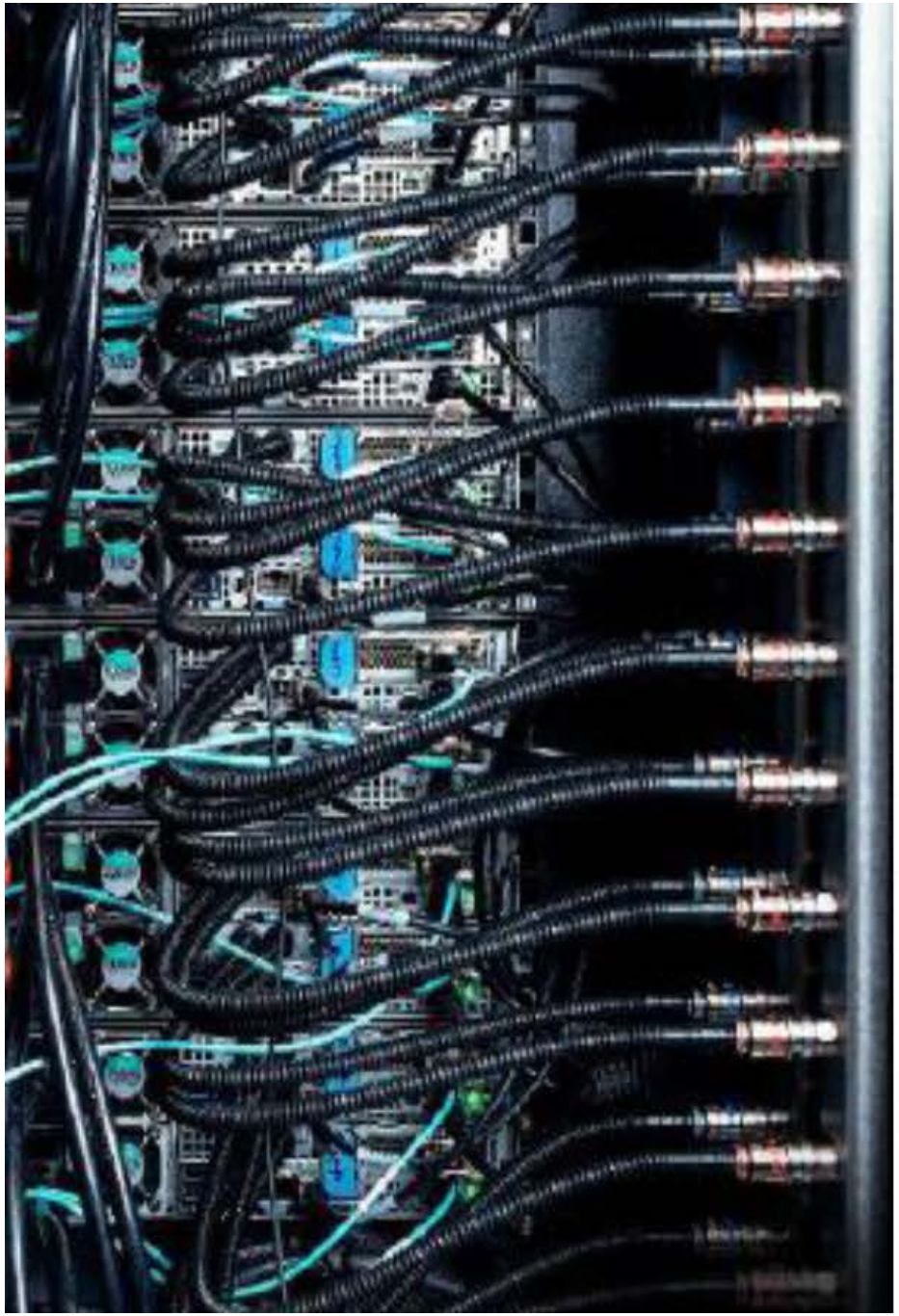
Mapping
- Competence mapping (over CASTIEL project)

Training
- Bachelor and Master studies in Vilnius University
- Activity on site trainings in Lithuanian and English
- Documentation/Tutorials (Lithuanian and English)

Interaction with industry
- EuroCC (NCC Lithuania) activity
- Trainings (important in Lithuanian language)

Communication
- Websites,Social media
- Initial articles with success stories

Management
- Working plans
- Periodical training activities
- collaborations



IT Open Access Center

Solution from Dell Technologies and Novian Technologies is a prime example of carefully selected and powerful hardware technologies.

The proposed solution provides the faculty with more than 750 TB of storage 17 TB RAM, 1,728 computing cores and 32 NVIDIA GPUs.

The total theoretical performance of the installed system is 112 TFLOP DP CPU and 3 PFLOP DL GPU respectively.

DELL Technologies

NOVIAN | Technologies

- Dell EMC PowerEdge R640 servers
- Dell EMC PowerEdge C6420 servers with NVMe drives and NVIDIA GPUs
- Dell EMC PowerVault ME4024 and ME4084 storage arrays
- Dell EMC PowerVault ME484 storage expansion with HDD drives
- Dell EMC PowerSwitch S4048-ON, S3048-ON and Mellanox InfiniBand Switches

Faculty of Physics

Institute of Chemical Physics

Vilnius University

Supercomputer „VU HPC“ Saulėtekis

1. Solution from Atos (Bull) and Bull Baltic: BullSequana X1000

2. The solution with more than 350 TB of storage, 53 TB RAM,
9152 computing Cores* and 8 NVIDIA GPUs **

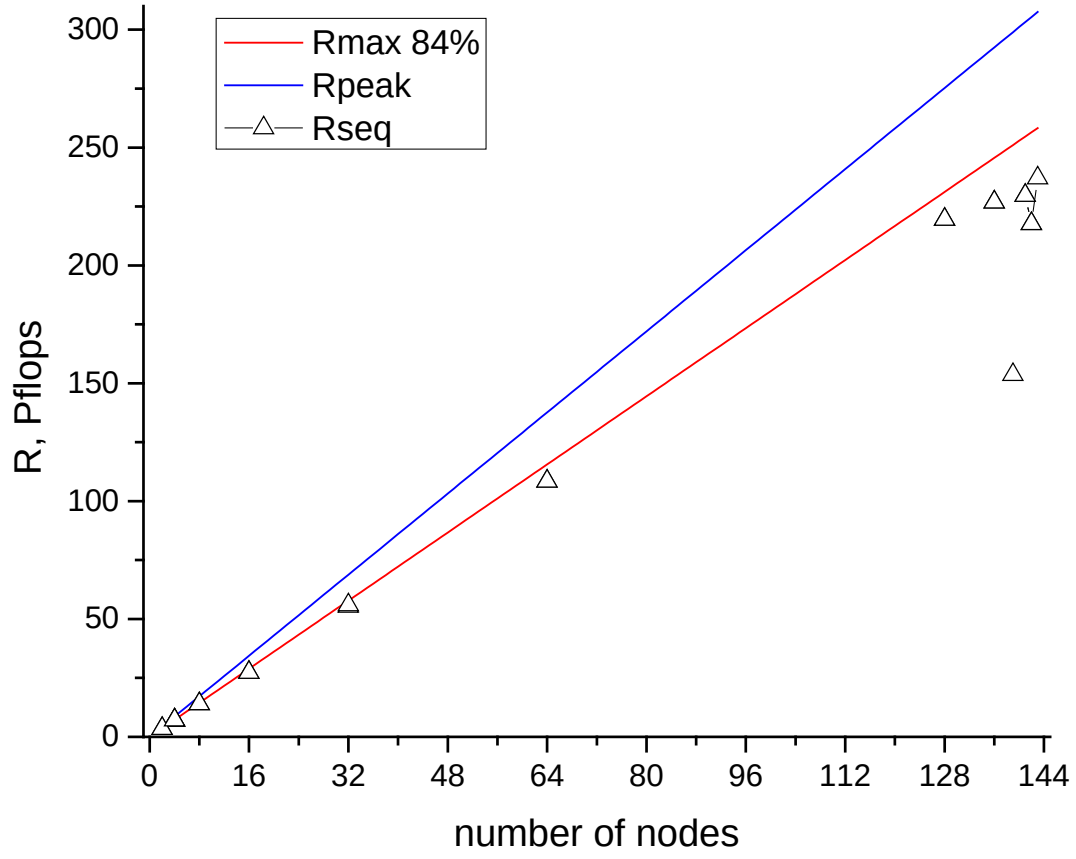
* Intel(R) Xeon(R) Gold 6130 CPU @ 2.10GHz

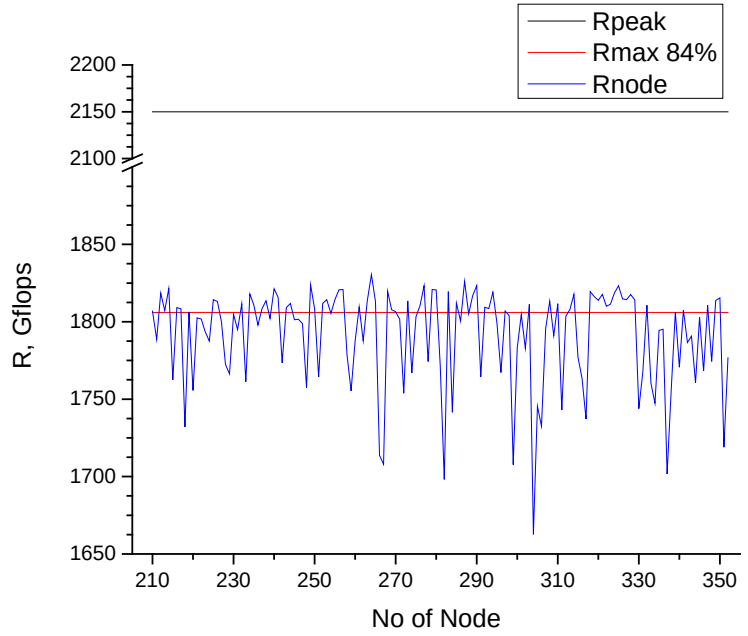
** Tesla V100-SXM

Supercomputer „VU HPC“ Saulėtekis

Vilnius University

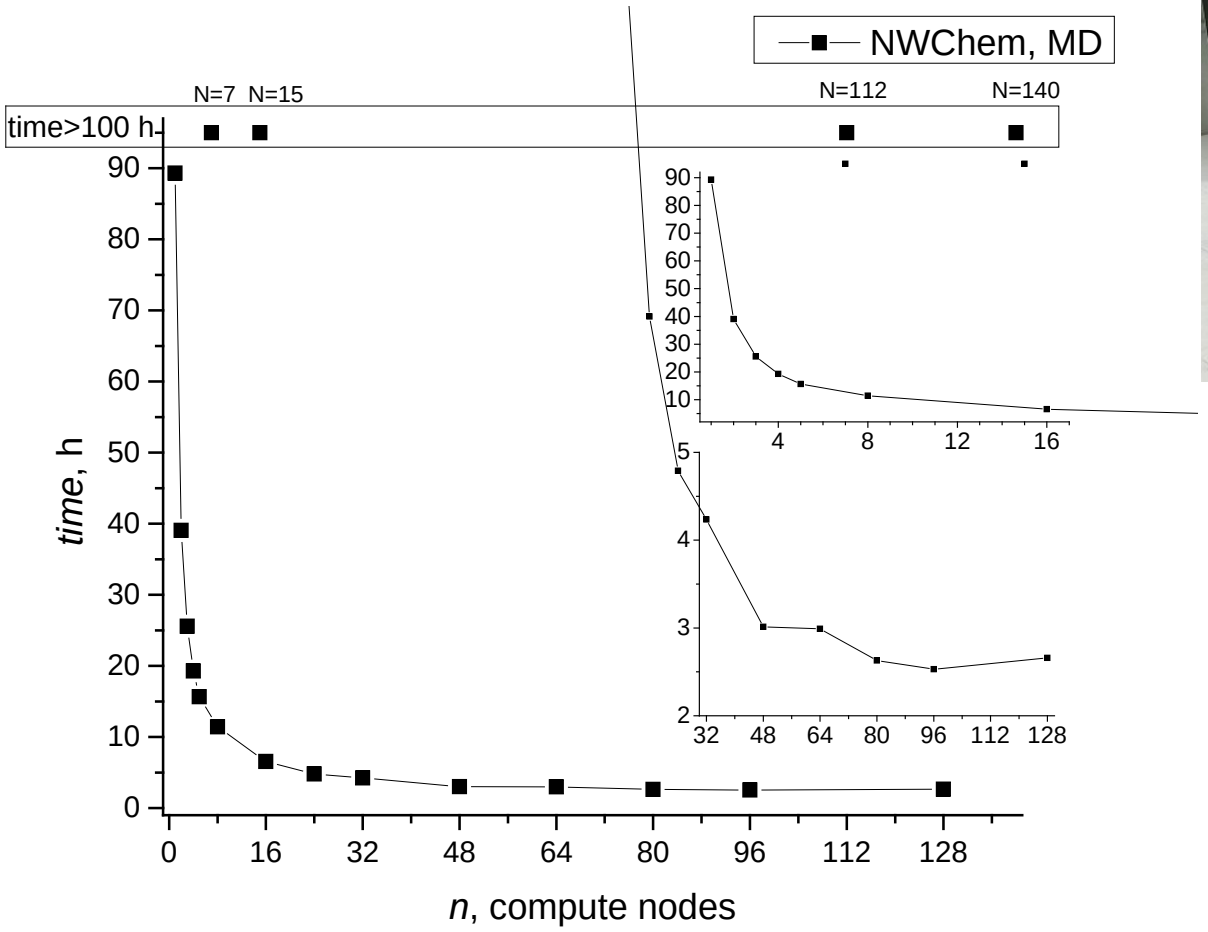
0.31 PFlops homogeneous hardware
HPLinpack: R=0.25 Pflops



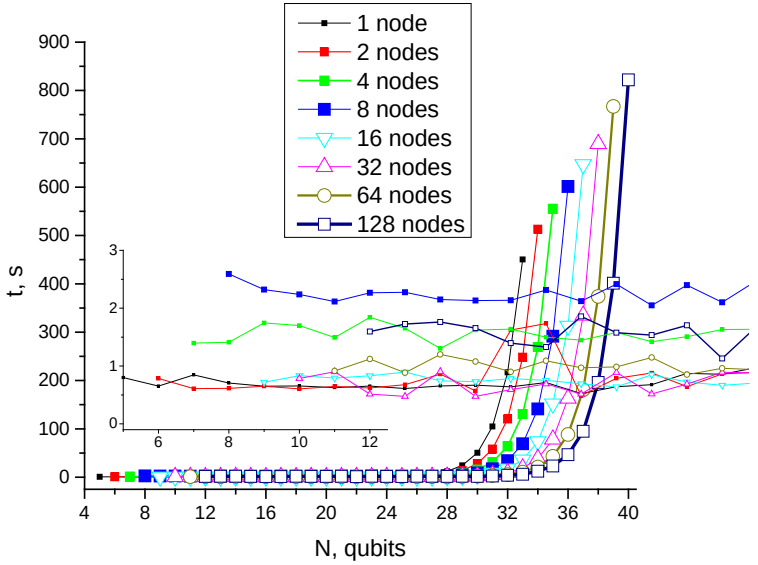


Supercomputer „VU HPC“ Saulėtekis

Vilnius University



Quantum Molecular dynamics (NwChem)



Quantum Computer Simulators

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Important research communities in Lithuania

Vilnius University supercomputing centre activities

Vilnius University

EGI Federation (*now*)

BUX member

EuroHPC and EuroCC member
(NCC Lithuania – HPC competence center in Lithuania)

RedHat Academia

MATLAB Academia

Cisco Networking Academy

Collaboration with LitNET (part GÉANT network)

HPC Competences

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Several examples

SMEs needs for specific problems

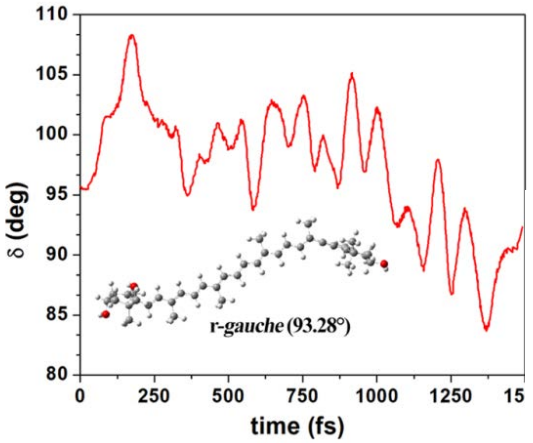
Quantum computing

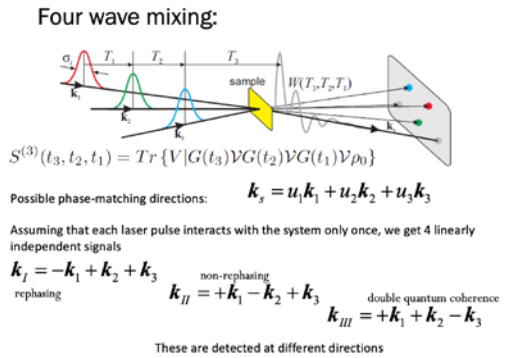
Material & Life sciences

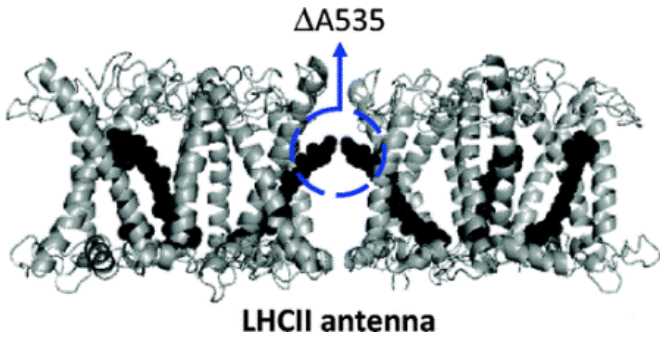
Scientific software adaptation for HPC and SMEs

Astrophysics

Cybersecurity







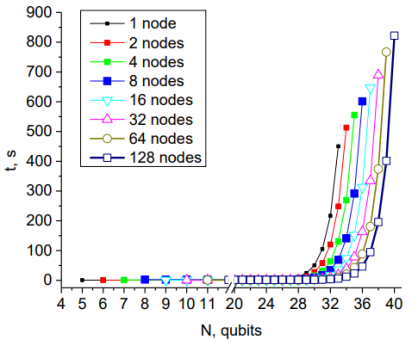


Figure 6. Simulations for maximum qubit number by changing the computing node number.

Material & Life sciences

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Standard packages for HPC:

- Gaussian
- NwChem
- Gamess
- WebMO integration

- AMBER
- Q-Chem
- Dalton
- Vasp
- Gromacs
- etc

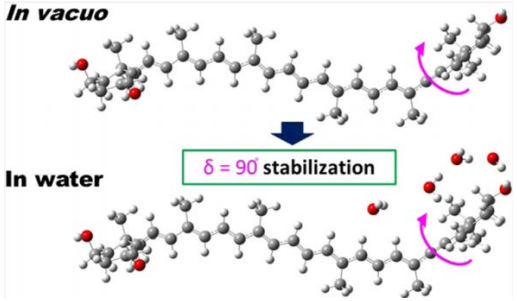
NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

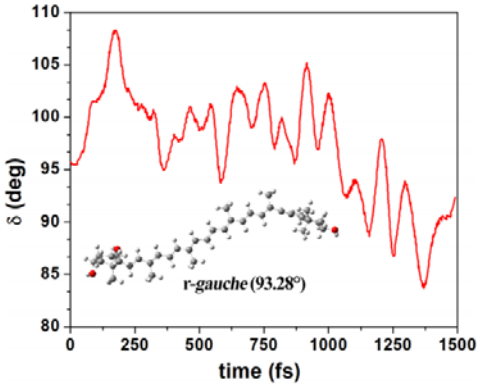
Expanding the limits of computational chemistry

WebMO .net

GAMESS

Dalton and LSDalton
Two powerful molecular electronic structure programs.





Universal tool for nonlinear spectroscopy

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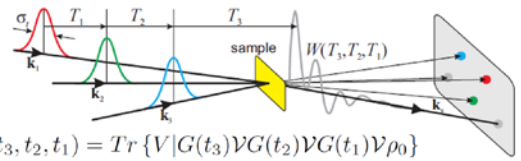
QCFP - universal tool for nonlinear spectroscopy simulations

- Parallelization
- Direct reading of structure files (PDB)
- Frequency domain techniques
- 2-nd order nonlinear techniques
- SHG, SFG, DFG

Four wave mixing:



$$S^{(3)}(t_3,t_2,t_1) = Tr\{V|G(t_3)\mathcal{V}G(t_2)\mathcal{V}G(t_1)\mathcal{V}\rho_0\}$$

Possible phase-matching directions: $\boldsymbol{k}_s = u_1\boldsymbol{k}_1 + u_2\boldsymbol{k}_2 + u_3\boldsymbol{k}_3$

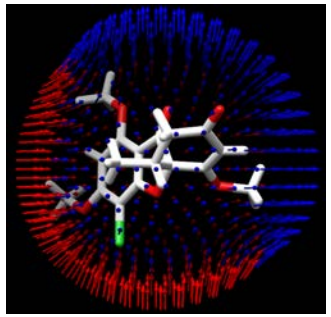
Assuming that each laser pulse interacts with the system only once, we get 4 linearly independent signals

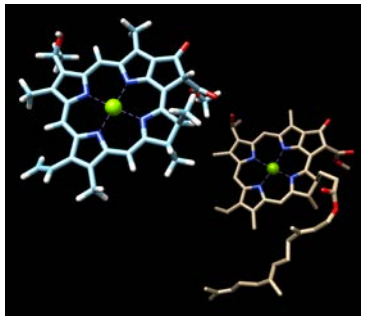
$\boldsymbol{k}_I = -\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3$ rephasing

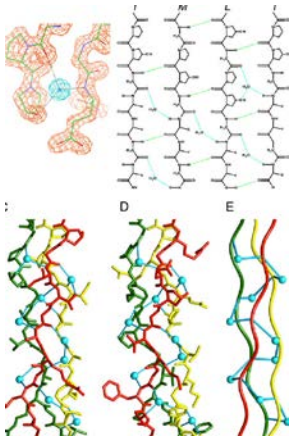
$\boldsymbol{k}_{II} = +\boldsymbol{k}_1 - \boldsymbol{k}_2 + \boldsymbol{k}_3$ non-rephasing

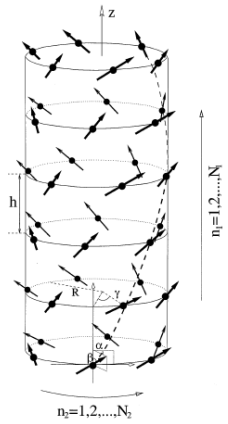
$\boldsymbol{k}_{III} = +\boldsymbol{k}_1 + \boldsymbol{k}_2 - \boldsymbol{k}_3$ double quantum coherence

These are detected at different directions





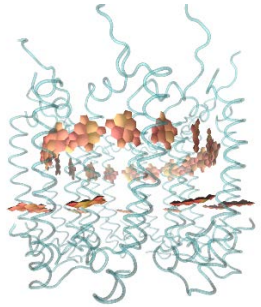


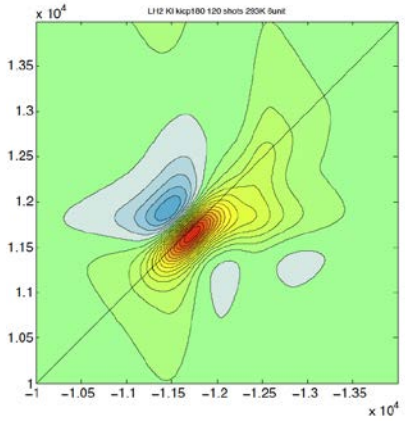


QCFP

Quantum Correlation Functions and Propagators

Combine coherent and stochastic propagation approaches





HPC ready

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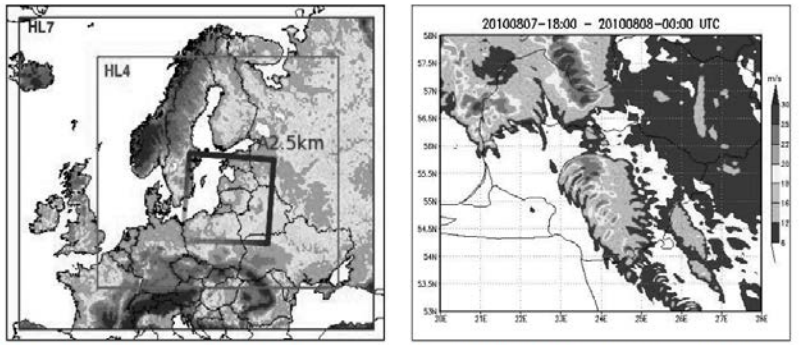
Various packages for HPC or adaptation for HPC related to SMEs requirements:

- MATLAB
- The R Project for Statistical Computing
- ANSYS
- COMSOL
- CUDA, CUDNN
- etc.



1 pav. Lietuvoje naudojamų skaitmeninių orų modeliavimo sistemų HIRLAM (HL7, HL4) ir HARMONIE (A 2,5 km) operatyvinės skaičiavimo teritorijos

2 pav. HARMONIE maksimalių vėjo gūsių prognozė 2010 m. rugpjūčio 7 d. (18 UTC) – 2010 m. rugpjūčio 8 d. (00 UTC)

- Competences providing and adaptation meteorology HARMONY, video processing, etc.

Services at Disposal

IT Open Access Center offers for **business** + **scientific** + **study** commutnity:

- *IaaS* (Infrastructure as a Service) – bare metal
- *PaaS* (Platform as a Service) –VU MIF HPC ready infrastructure
- *SaaS* (Software as a Service) – problem centric HPC solution

Resources and Identity management:

OpenNode

Waldur as a platform for managing hybrid cloud resources used for both for controlling internal enterprise IT resources and for selling cloud services to customers.

LITNET Lietuvos mokslo ir studijų institucijų kompiuterių tinklas FEDI

Litnet FEDI identity service for research and education institutions in Lithuania.

eduGAIN

eduGain interfederation service that connects identity federations around the world.

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Main research areas in Computer Sciences

- Computational modelling
- Complex graphs and networks, combinatorics
- Formal modelling and verification of software
- Cognitive computing
- Global optimization
- Blockchain technologies
- Image and signal analysis
- Operations research
- Cyber social systems engineering
- Education systems
- Cybersecurity

Communities in Lithuania

Vilnius University

Universities and Research centers

- Vilnius university (VU);
  - CERN
- Vilnius Gediminas Technical University (VILNIUS TECH);
- Kaunas University of Technology (KTU);
- Vytautas Magnus University
- State research institute Center for Physical Sciences and Technology
- etc.

Public sector & SMEs

- Lithuanian Hydrometeorological Service (LHMT).
- over Open Access Center
- over collaborations with Faculty of Physics
- over collaboration with Faculty of Mathematics and Informatics

Vilnius
University

EGI & Lithuania

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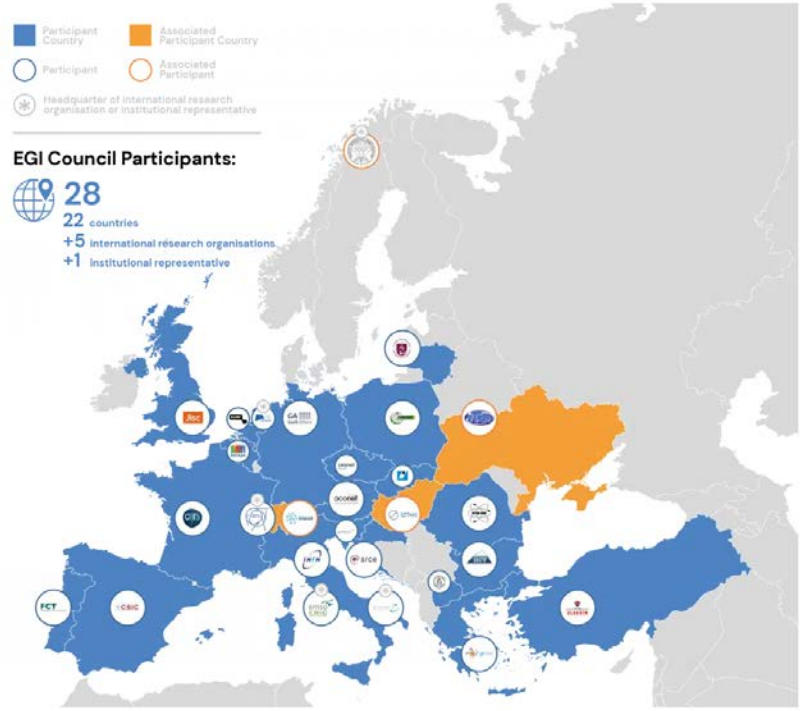
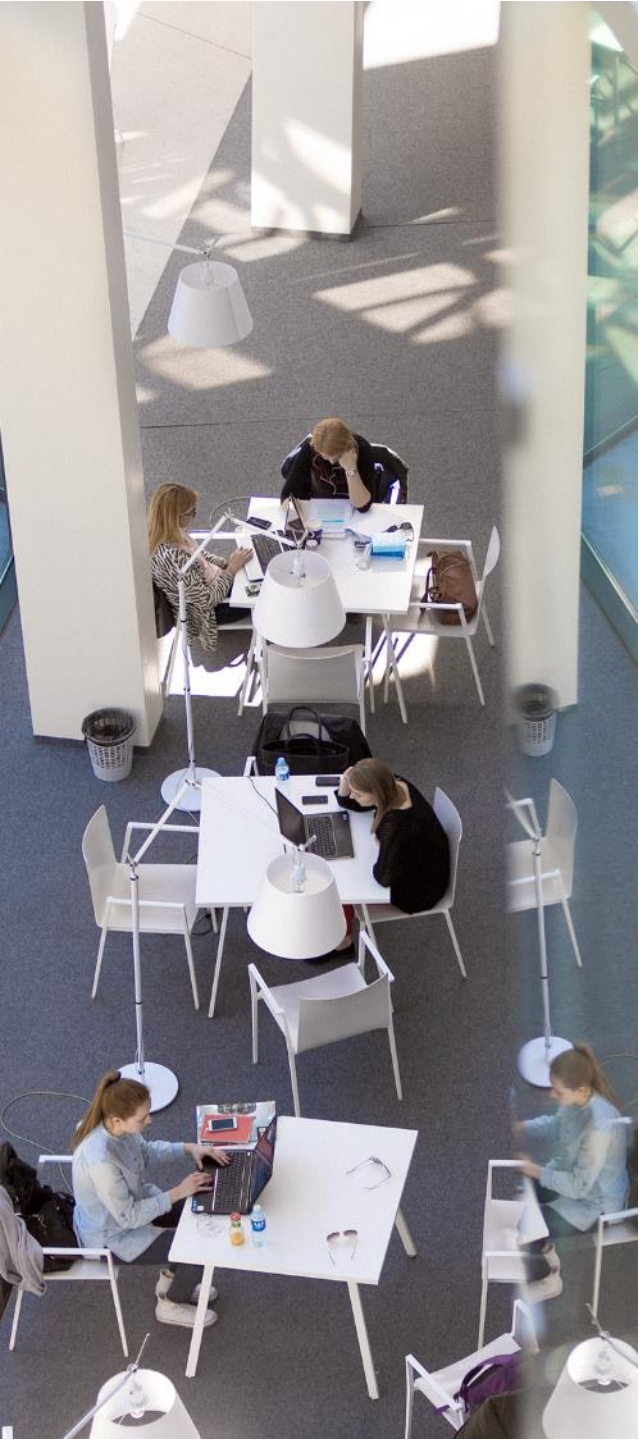
What was the reason for Lithuania to join EGI?

- Become EU level HPC infrastructures by adapting local HPC infrastructures and providing HPC knowledge and international experience locally.
  - Be part of HPC community where local scientific communities and SMEs could benefit of it also
  - The local users could easer access the EGI federated infrastructures from HPC competences point of view;
  - Local communities better understand the HPC computing possibilities;
  - Local SMEs and public sector could have easier access to larger HPC resources where both sides could benefit;





How EGI can help supporting Lithuanian national strategy and reference user communities?

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- Helping providing higher level HPC access;
- gathering and sharing the HPC related information;
- Exchange of know-how in HPC field
- Be ready for upcoming new HPC technologies

Vilnius University

Thanks

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