EuroHPC PL


Narodowa Infrastruktura Superkomputerowa dla **EuroHPC**

# National Supercomputing Infrastructure for EuroHPC – EuroHPC PL

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Rzeczpospolita Polska
Unia Europejska Europejski Fundusz Rozwoju Regionalnego

# EuroHPC JU – how did it all start

| | 2017 | 2020 |
|---|---|---|
| 1 | Sunway TaihuLight, China | Supercomputer Fugaku, Japan |
| 2 | Tianhe-2A, China | Summit, United States |
| 3 | **Piz Daint, Switzerland** | Sierra, United States |
| 4 | Gyoukou, Japan | Sunway TaihuLight, China |
| 5 | Titan, United States | Selene, United States |
| 6 | Sequoia, United States | Tianhe-2A, China |
| 7 | Trinity, United States | **JUWELS Booster Module, Germany** |
| 8 | Cori, United States | **HPC5, Italy** |
| 9 | Oakforest, Japan | Frontera, United States |
| 10 | K computer, Japan | Dammam 7, Saudi Arabia |
| 11 | Mira, United States | **Marconi-100, Italy** |
| 12 | Stampede2, United States | **Piz Daint, Switzerland** |
| 13 | TSUBAME3, Japan | Trinity, United States |
| 14 | **Marconi, Italy** | AI Bridging Cloud Infrastructure, Japan |
| 15 | **Cray XC40, United Kingdom** | **SuperMUC-NG, Germany** |

# EuroHPC JU

European funding entity

- Created in 2018, members:
  - The European Union
  - 34 Member States and Associated Countries
  - 3 Private partners
- Budget: around EUR 7 billion for the period 2021-2027, funded by its members

Aim:

- Deploy top-of-the-range supercomputing infrastructures across Europe to support European HPC users whereve they are in Europe,
- Implement an ambitious research and innovation agenda to develop a competitive HPC ecosystem and supply chain in Europe, which includes hardware, software, applications but also training and skills.

EuroHPC Joint Undertaking

# Towards EuroHPC PL

EuroHPC JU approach:

- Pre-exascale resources:LUMI, Leonardo, Marenostrum 5
- Mid-range systems: Meluxina, Karolina, Deucalion, Vega, Discoverer
- R&D in the area of HPC

PLGrid approach

- Past experience of joint projects: PL-Grid, PLGrid Plus, PLGrid NG and PLGrid Core
- All HPC centres on TOP500 list in 2011 and 2015
- R&D within “domain grids”

# Polish Map for Research Infrastructures

- 2019: National Supercomputing Infrastructure for EuroHPC
  - Program awarded for PL-Grid Consortium
- 2020: 4th call within Measure 4.2 of the Smart Growth Operational Programme
  - Project: National Supercomputing Infrastructure for EuroHPC – EuroHPC PL
  - Extended consortium, partners:
    - Academic Computer Centre Cyfronet AGH (coordinator)
    - Poznan Supercomputing and Networking Centre
    - Centre of Informatics Tricity Academic Supercomputer and network
    - Wroclaw Centre for Networking and Supercomputing
    - National Centre for Nuclear Research
    - Institute of Theoretical and Applied Informatics
    - Center for Theoretical Physics PAS

# An idea – support for multiscale computations

- Users and Customers require more than just bare CPU/GPU cycles and/or data storage
- We provide deep understanding of the workflow
  - Tailored software solutions like HPC codes, science gateways, data management
  - Attention to performance and optimisation
  - State-of-the art technologies
  - Multiple level security features optimized for the given scenario
- Common denominator:
  - Infrastructure, software, data & simulation models
- Know-how: we support it all: modelling, data analysis, Machine Learning…
- So, let’s use Polish HPC resources as accelerator to European ones

# EuroHPC PL

Project aim:

- Development of a specialized, general-purpose infrastructure for multiscale computations, enabling to undertake research challenges in key areas from the point of view of Polish society, the scientific community and the economy

Major components:

- HPC infrastructure
- HPC software
- Domain specific applications
- Quantum computing and services

# The Hybrid Computing Platform

- Laboratory for modelling and parallel data processing in a pre-exascale environment
- Laboratory of the hybrid computing applications
  - Quantum Machine Learning e-Platform
  - Platform for supporting quantum computing with classical algorithms
  - Certification and error mitigation platform for quantum computers
  - Platform for quantum operational research and discrete optimisation
- Laboratory of application of supercomputers in medicine
  - Modelling platform for personalized medicine
  - Simulation platform for radiotherapy
  - Quantum simulation and medical imaging platform for PET scanners
- HPC software energy and computational efficiency lab

# Hardware

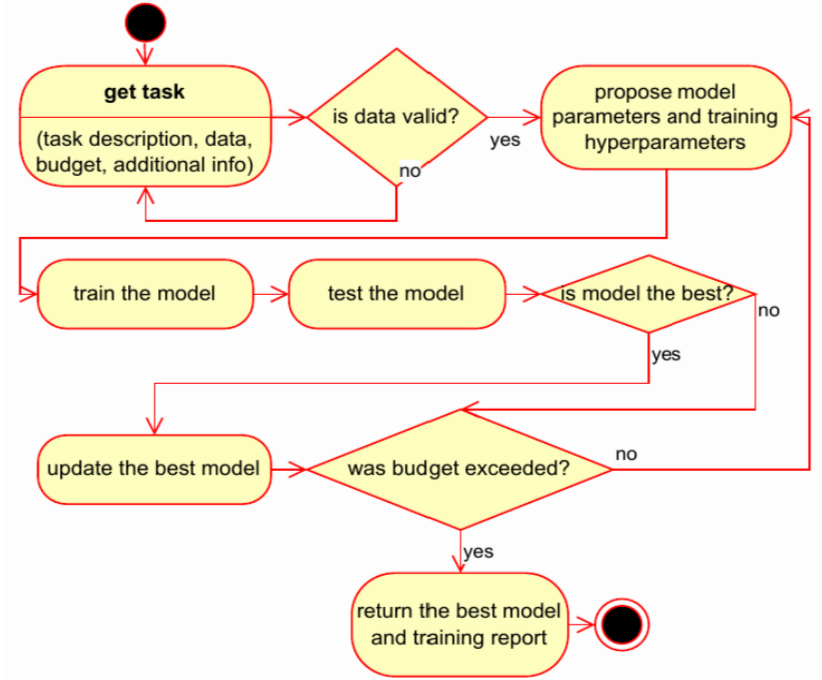
- Helios (Cyfronet, 30+ PFlops)
- Faeton (specialised platform)
- Lem (WCNS, 10+ PFlops
- Cloud access to the quantum computing resources (D-Wave) in Cyfronet and PSNC
- ORCA PT1 photonic system (PSNC)

# Pilot platform of high-performance domain applications

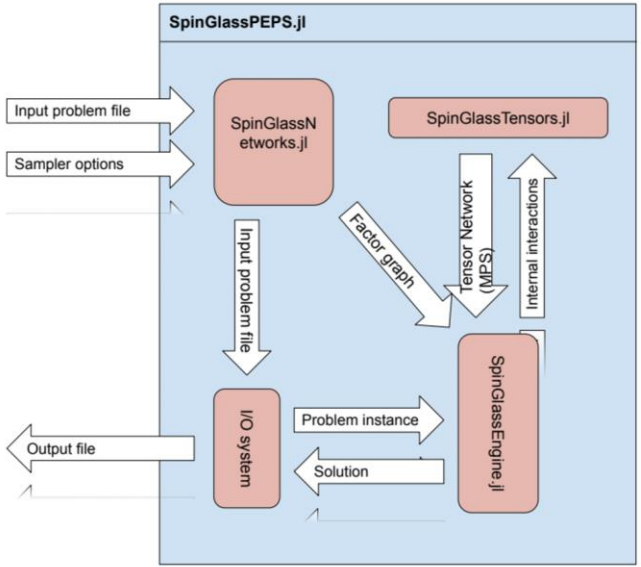
- Air quality forecasting
- Meteorology
- Astrophysics
- Solid state chemistry and physics
- Structural study at the nanoscale
- Discrete optimization in production and logistics systems
- Numerical simulations of thermal-flow processes
- Computer-assisted molecular testing in cancer treatment

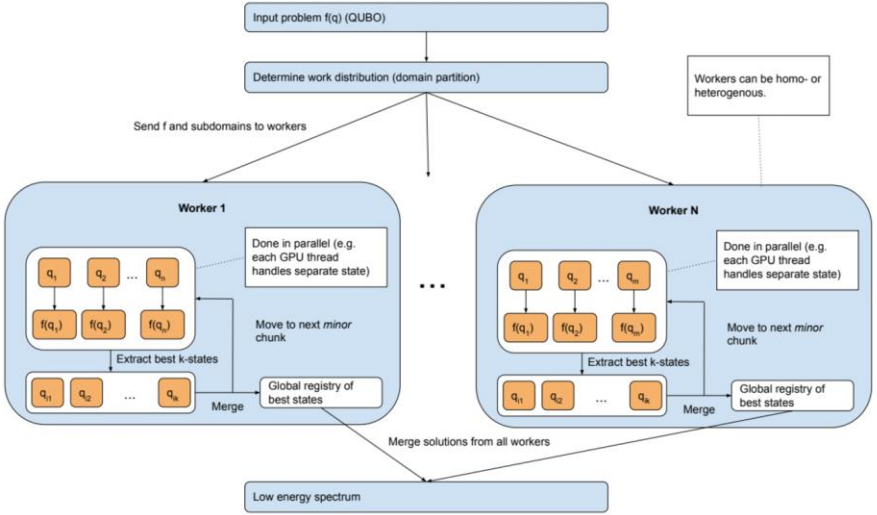
# Quantum Machine Learning e-Platform

- Facilitating the use of Quantum Machine Learning (QML) techniques by those without knowledge of quantum data processing.
- To develop an Auto Quantum Machine Learning (AQMLator) platform that automatically generates QML models from provided data.
- Proposing an auto-ML solution that enables integration of QML techniques into existing machine learning pipelines



# Simulating quantum annealing

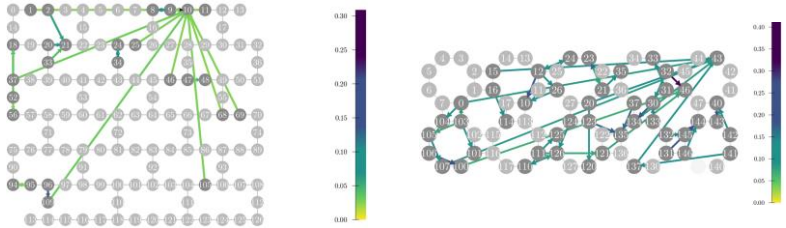


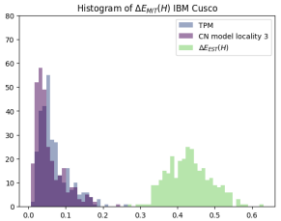
# Platforma charakteryzacji i mitygacji błędów pomiaru

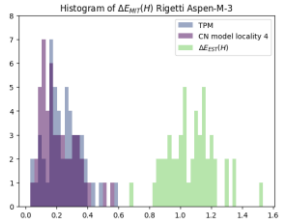
Moduł charakteryzacji błędów pomiarowych

Moduł mitygacji błędów pomiaru








**Zastosowanie pakietu pozwoliło na uzyskanie ok 25% poprawy dokładności wyników problemów MAX-2-SAT na urządzeniach Rigetti i IBM**

# Platforma kwantowych badań operacyjnych i optymalizacji dyskretnej

Rosnący poziom abstrakcji dla użytkownika

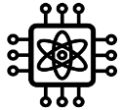
- Zastosowania i zdalny dostęp do platformy W PCSS
- Wybrane klasyczne i referencyjne problemy OR (np. JSSP*, Max-Cut, …)
- Algorytmy i struktury danych (QUBO)
- Różne paradygmaty obliczeń hybrydowych (kwantowe wyżarzanie, fotoniczne obliczenia kwantowe i bramki kwantowe)

QCG QA-API jupyter KEYCLOAK PIONIER.id

Rozwój i wdrożenie nowych narzędzi w ramach EuroHPC PL

**Kwantowo-klasyczna infrastruktura obliczeniowa w PCSS (sprzętowo-programowa)**





Optyczne komputery kwantowe i wyżarzanie



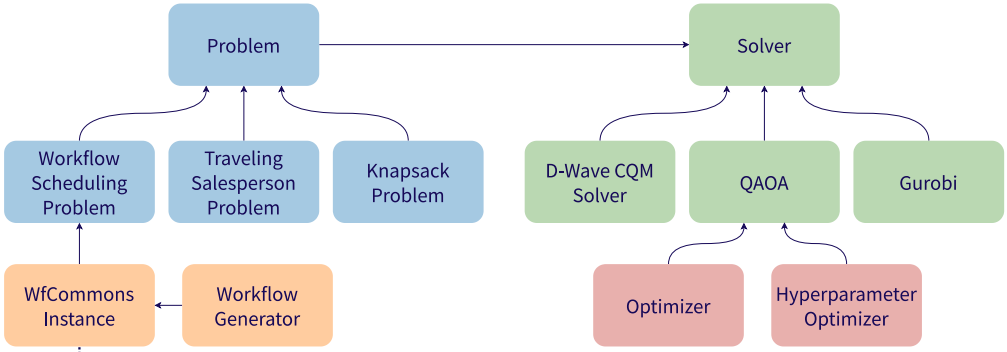
Symulatory kwantowe

pracelab 2

Programowalne i nadprzewodzące kubity


* *Krzysztof Kurowski, Jan Weglarz, Marek Subocz, Rafał Różycki, Grzegorz Waligóra: Hybrid Quantum Annealing Heuristic Method for Solving Job Shop Scheduling Problem. ICCS (6) 2020: 502-515*

# QHyper - hybrid optimization software




```
"workflow": {
        "machines": [{
            "nodeName": "",
            "cpu": ["speed": "", "count": ""] }],
        "tasks": [{
            "name": "",
            "runtime": "",
            "children": []
            }] }
```

Selected WfFormat fields.

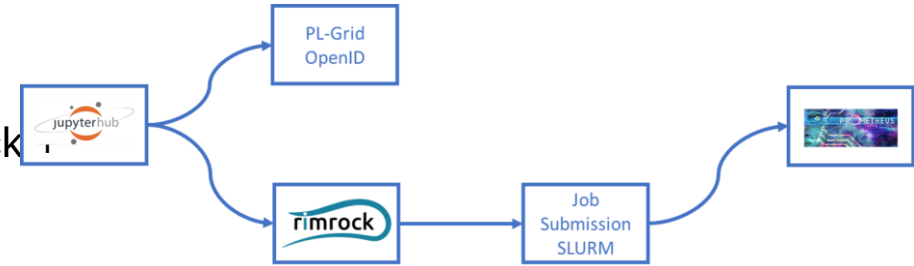
Optimization across domains with quantum-classical solvers.

Unified framework offering an easy interface combining:

- **problems**;
- **solvers** (gate-based, quantum annealing, classical);
- **optimization methods**.

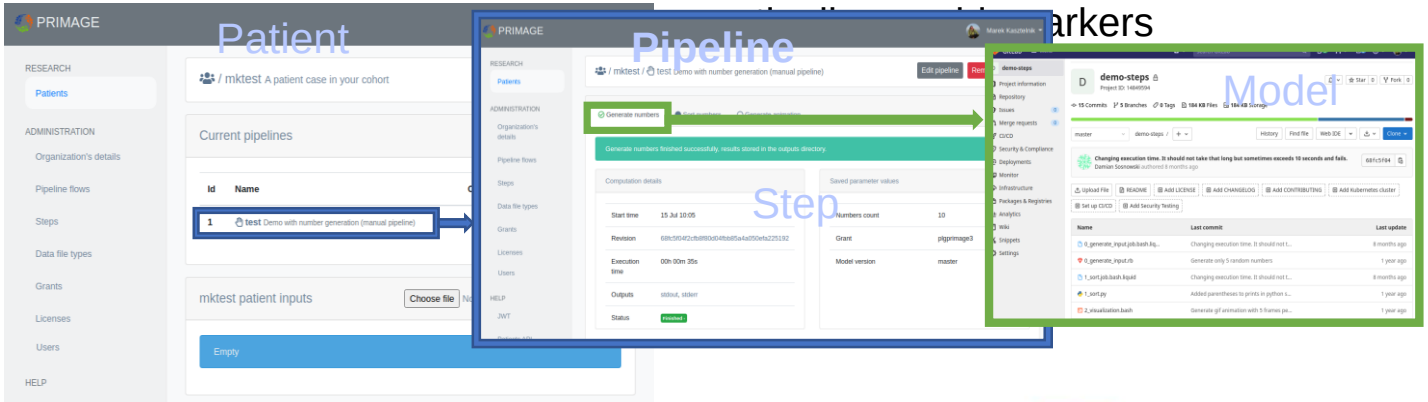
# Personalised medicine - JupyterHub for computational medicine

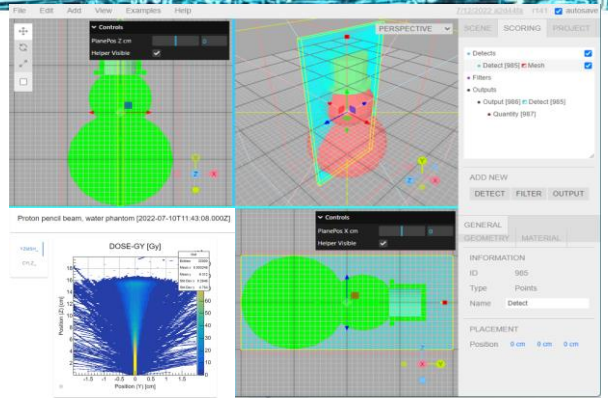
- Popular interface for data analysis, visualization and ML/AI applications
- Highly demanded by biomedical community
- Approach:
  - Develop a central JupyterHub at Cyfronet
  - Provide a set of kernels, modules, extensions and examples for biomedical applications
- From requirements to implementation:
  - Gathering typical requirements
  - Designing a solution based on Rimrock custom spawner
  - Integration with PL-Grid security
  - Implemented



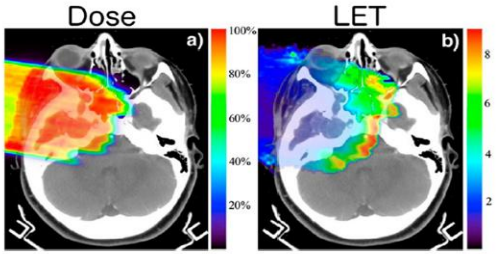
# Model Execution Environment extended for EuroHPC Community

- Each pipeline (workflow) is a well-defined set of computations (sequential or parallel)
- Each computation (a pipeline step) is an execution, on the HPC cluster, of a specific model, in a specific version (selected from the GIT repository)
- Pipelines can also be executed automatically, provided input data constraints are satisfied
- Used for running several scenarios: biomechanical system/organ 3D/4D simulations with CFD or FEM, medical imaging analysis, patient diagnostic time-series analysis with [illegible]arkers






View of the yaptide user interface with 3D geometry editor and simulation result presentation




Physics model allows to predict dose and linear energy transfer distribution in the patient. High LET values correlate with healthy tissue damage.

# Yaptide – simulation platform for radiotherapy

Aim: Simulations of particle interaction with matter for radiotherapy treatment plans

Pushing forward research: optimized radiotherapy plans, rich model of particles interaction leads to plan with better sparing of healthy tissues

- Evaluation of treatment plan quality
- In-silico studies for design of experiments
- Applications in other areas: space industry, radiation shielding
- Technically: platform with web interface, allowing user to execute simulations on HPC

Achievements:

- Used for simulation of the treament plans in the experimental campaign guiged by the European Radiation Dosimetry Group, several publications ongoing
- demo version of application deployed at https://yaptide.github.io/
- PLGrid service in proces of deployment for early users, should be available in PLGrid apps catalogue this year

# Quantum simulations and medical imaging software platform

**Common API**

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

**Group:**
- Wojciech Krzemień
- Konrad Klimaszewski
- Mateusz Bała
- Oleksander Fedoruk
- Lech Raczyński
- Aldona Spirzewska
- Damian Trybek
- Dawid Meleszczuk

**Services**

Quatum emulators/ Quantum computer

**Libraries**

**Simulators**

**Quantum simulations**

**Standard simulations**

**PET Image Reconstructor**

**Image reco.**

**Quantum Imaging**

**Phantom generator**

**GAN networks**

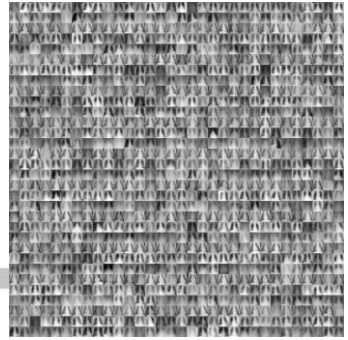
Qiskit

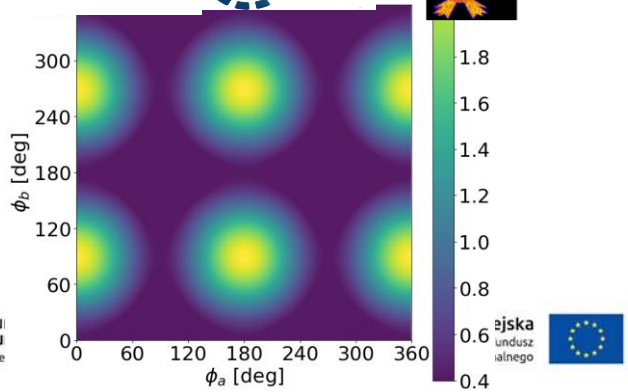
GEANT4

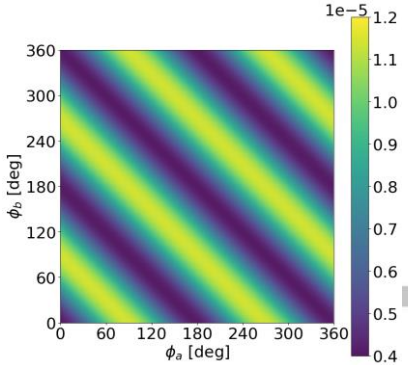
GATE

TensorFlow

PYTORCH





# Urgent Computing Platform

Urgent computing provisioned with native, built-in mechanisms of Slurm Workload Manager

- Easy access and fast approval path
- Based on job preemption
- Developed multiple procedures and recommendations for implementation of Urgent Computing
- Example configurations in order to allow quick and easy implementation

# Computing Energy Efficiency Platform

Improvement of Energy Efficiency through managing idle CPU states and performance states

- Based on widely available and common tools such as RAPL, IPMI, cpupower, likwid
- Possible **energetic savings** through frequency scaling for scientific software such as Gaussian16
- Largest possible savings: 30% in energy consumption and 40% in average power, with approx. 30% penalty in computing time
- Analysis extendable to other (scientific) software

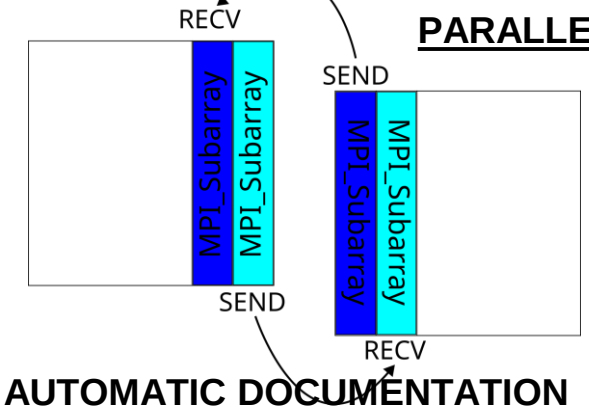
# Pilot doman applications

# THATMPI

Particle-In-Cell (PIC) code that models astrophysical plasma systems

We prepare the THATMPI code with upgrades and new features for the new exa-scale supercomputing era.

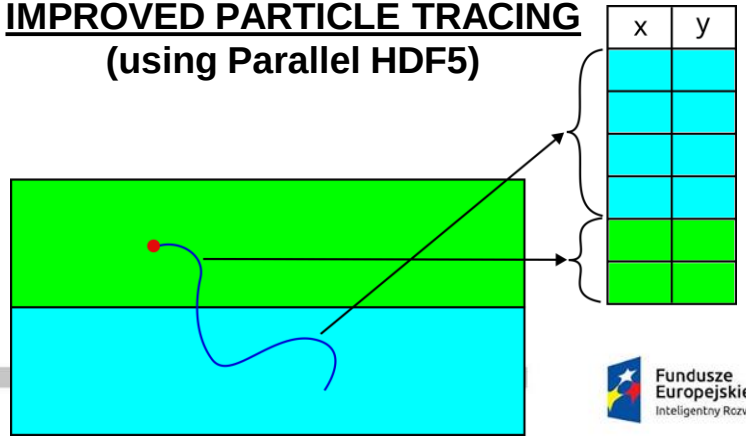
## IMPROVED FIELD PASSING (using MPI Subarrays)



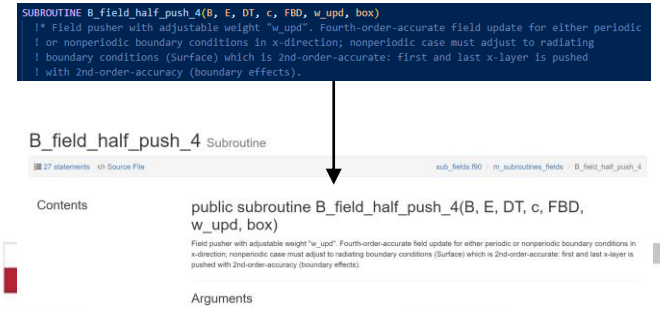

## PARALLEL POST-PROCESSING (using MPI)

MORE CPUS
↓
FASTER POST-PROCESSING!

## IMPROVED PARTICLE TRACING (using Parallel HDF5)




## AUTOMATIC DOCUMENTATION (using FORD)



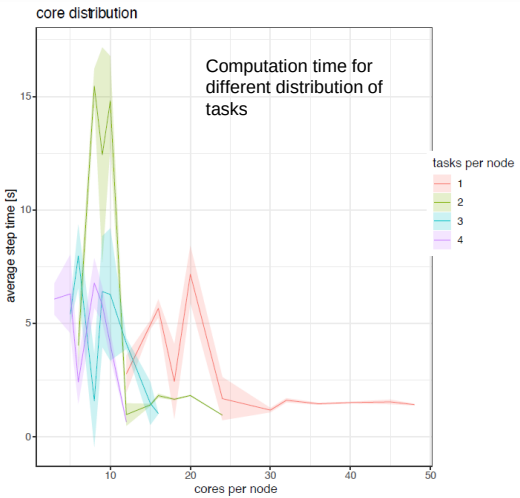

- Parallel HDF5 output
- New particle pusher
- Restructuration of the whole code

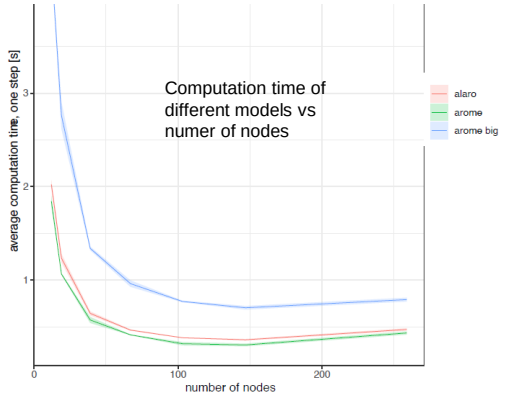
# Meteorology

- **Aladin Models on Supercomputers:**
- Tested Arome and Alaro models on Ares supercomputer.

- **Optimization Results:**
  - Compilation: Best performance with specific compilation flags.
  - Data Input: GROUP_STORAGE volume slightly outperformed SCRATCH.
  - Parameter Tuning: Identified optimal grid shape and NPROMA
  - I/O Nodes: Too many nodes slow down computations; optimal number identified.
  - Core Utilization: Full core utilization per node is most efficient.

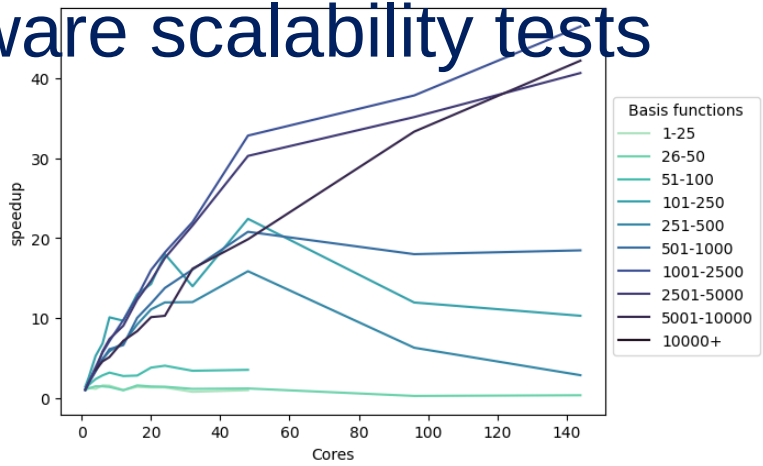
- **ML Models Testing:** Successful performance of Fourcast and PanguWeather models on ACK Cyfronet supercomputers. Detailed evaluation still under investigation.

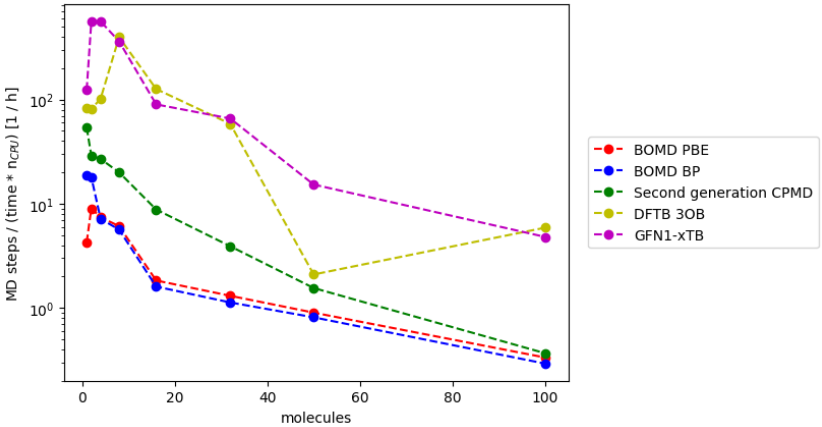


# Quantum chemistry and MD software scalability tests

- Tests of scaling for static and dynamic calculations in a range of software packages, with the use of broad array of different systems and methods.
- Comparison of different MD approaches in terms of speed and demand for computational resources.
- Detection and description of common problems in routine usage of tested software; preparation of best practices for users.



# Thank you for your Hard Work!

I am much obliged to:

- Managements of our Units
- Tasks leaders and project employees
- Project's Offices
- National Information Institute
- All other employees of our Units not directly involved in project but without whom we would not deliver project results

# Future steps:

- EU & EuroHPC JU funding projects
- European Funds for Smart Economy, 2021-27
  - New call in 2024