HIDALGO2
CENTRE OF EXCELLENCE

The Urban Air Project pilot

Z. Horváth, L. Környei, M. Constans, Á. Kovács, T. Budai, J. Bakosi
Széchenyi István University (SZE)

Workshop with the NCCs, 15 June 2023

EuroHPC Joint Undertaking
Grant number: 101093457

HiDALGO2 CENTRE OF EXCELLENCE

Contents

1. Global challenges with the urban air flow: urban air pollution

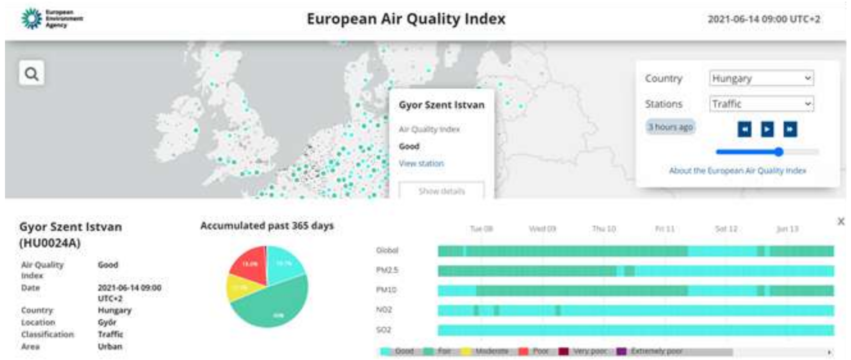
1. Importance of urban challenges: 55% of the world's population lives in urban areas now, and 68% by 2050, says UN, see UN DESA at https://population.un.org/wup/.
2. Challenge 1: Air quality
   - WHO: 6.7 million deaths are attributable each year to exposure to ambient and household air pollution, see https://www.who.int/data/gho/data/themes/air-pollution.
   - Many cities are polluted (air quality values are above health-critical values)
     → Protests by citizens and new, stricter regulations by policymakers
3. Challenge 2: Wind comfort and safety
   - Urban wind can cause discomfort for pedestrians and even critical safety situations in particular near high buildings
4. Challenge 3: Urban planning
   - How can urban policymakers mitigate or cease the negative effects of urban challenges?

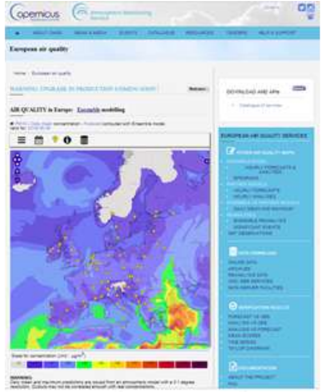
Reuters

Freepik

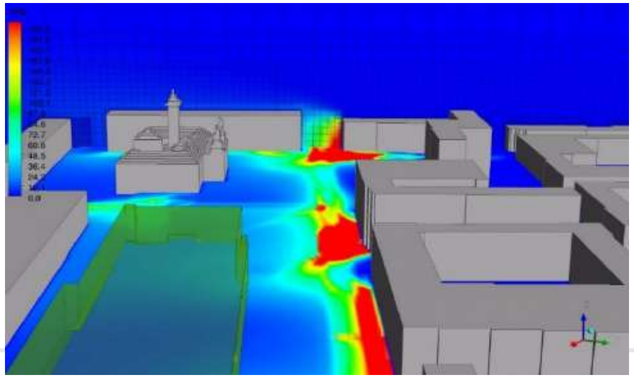
1. The global challenge: existing tools and missing properties

- EU Ambient Air Quality Directive: each EU country reports annual measures of air quality
- Current services of the European Commission: Monitoring, forecasts, and reanalysis for air quality of several cities on a coarse mesh (10 km x 10 km) by Copernicus, see e.g.: https://airindex.eea.europa.eu/Map/AQI/Viewer/.



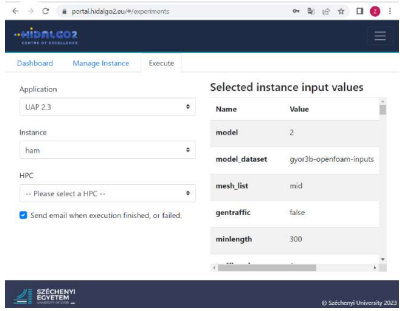


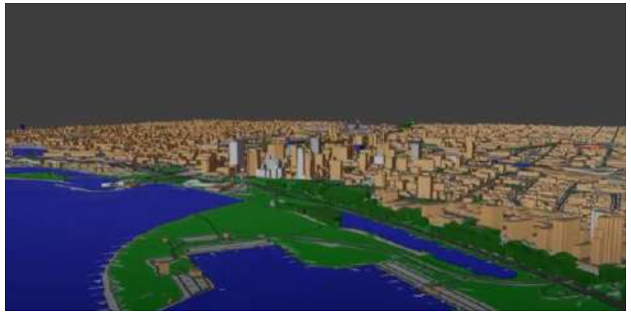
- However: in cities there can be permanent local hot-spots, significantly effecting health conditions. Detecting, evaluating health effects of hot-spots are impossible with coarse simulations → **need of fast simulation for a city at 1-5 meter resolution, for a full year** → large scale problem.

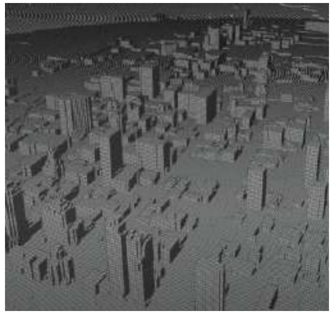


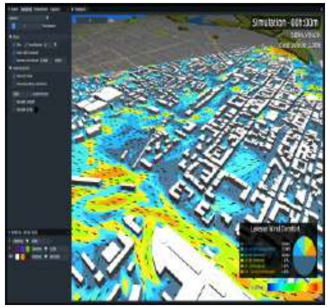
2. The goals of the research in HiDALGO

- In HiDALGO1 and local SZE projects (FIEK, TKP), SZE has developed and optimized a workflow with automated deployment of containerized solutions to HPC platforms with preprocessing (OpenStreetMap), simulation (OpenFOAM – scales up to 100k CPU cores, and Fluid-Solver (GPU)), and visualization.





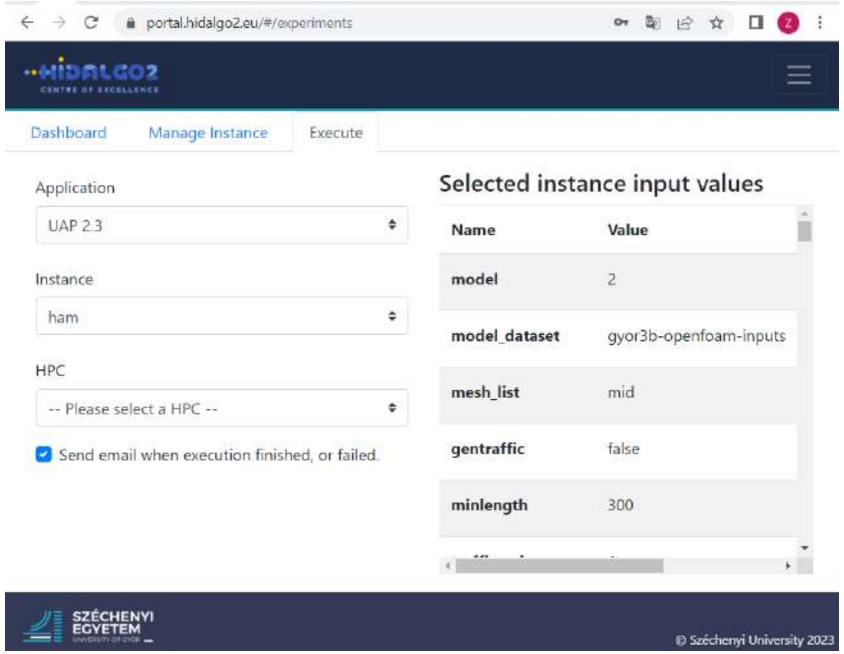




- Main requirements and software features:
  - Process 3D urban geometries → handle **unstructured meshes, 1-10-100 millions of cells**
  - **On-the-fly assimilate data** from external sources (operational meteo prediction/reanalysis simulation data, or sensor measurements) and **visualize results**
  - Be capable to run large scale simulations fast:
    - High spatial resolution (1 meter at ground level)
    - Full year, under medium precision (say <10% relative accuracy)
    - Exploit machine learning

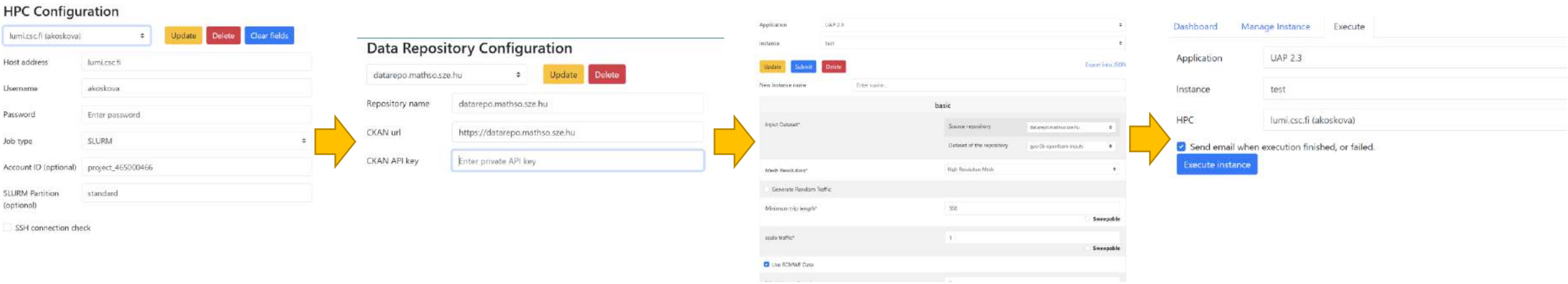
- **In HiDALGO2: Use the EuroHPC ecosystem, both machines and community to develop the solutions further! Use the synergies of HiDALGO2 to couple pilots!**

3. HiDALGO2 HPC tools:
3.1: The HiDALGO2 portal

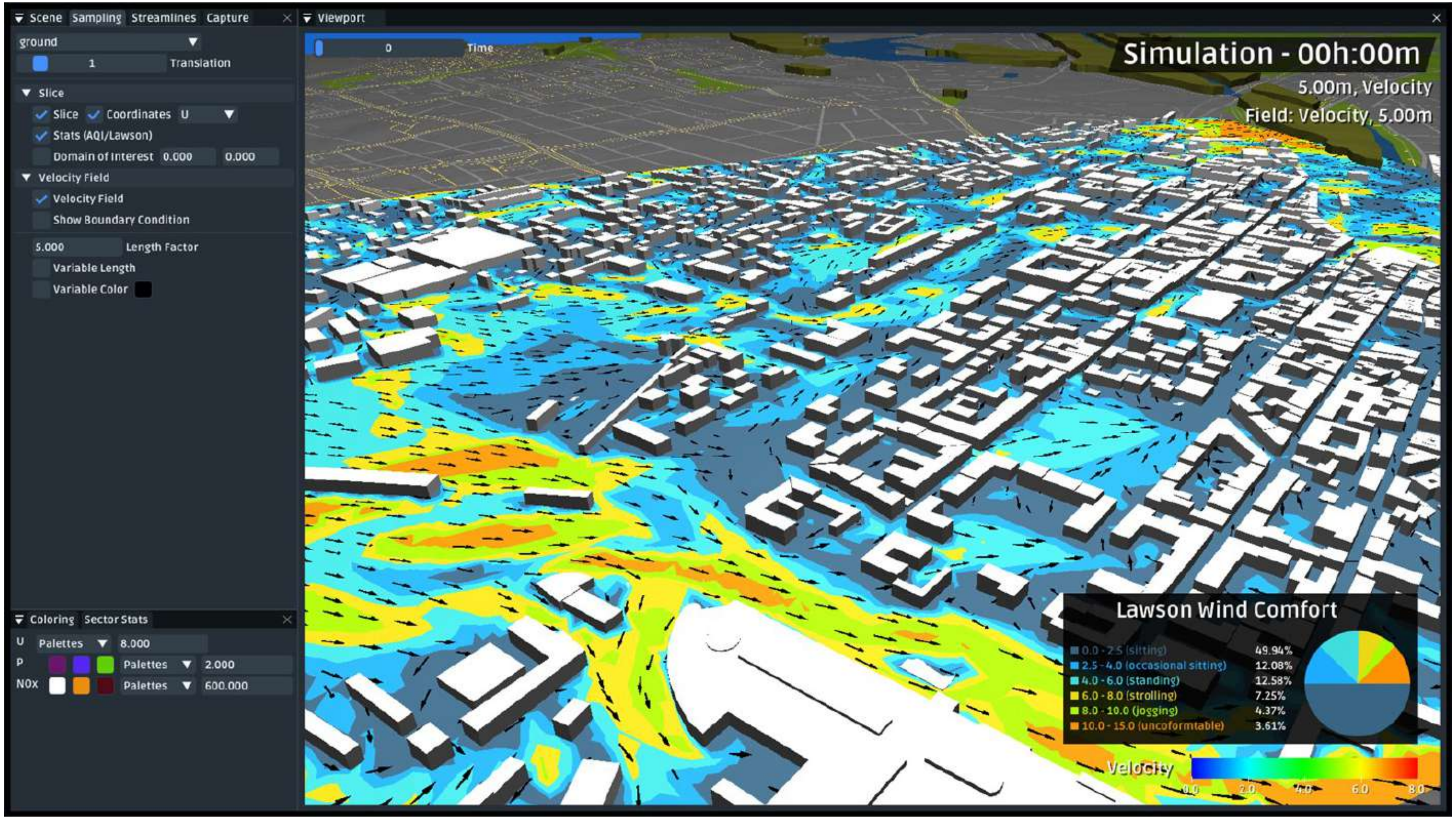


Portal:

- Manage, execute, monitor, and post-process HPC jobs
- Data repository: CKAN
- Own orchestrator (predecessor: Cloudify)
- Deployment and execution: LUMI, Altair (PSNC), Solyom (SZE)



3.3 Visualization and HPDA postprocessing



3.2.1 CFD Module with OpenFOAM

- Incompressible URANS solved with k-e turbulence modell

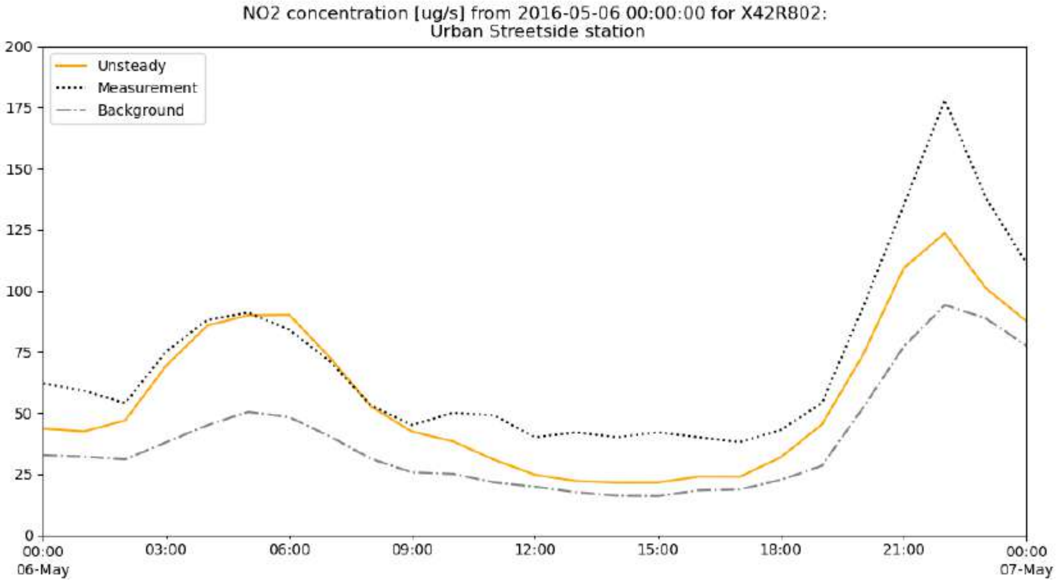
$$\nabla \cdot (\rho \mathbf{u}) = 0$$
$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \mathbf{g} + \nabla \cdot \overline{(\tau)} - \nabla \cdot (\rho \mathbf{R})$$
$$\frac{D}{Dt}(\rho k) = \nabla \cdot (\rho D_k \nabla k) + P - \rho \epsilon$$
$$\frac{D}{Dt}(\rho \epsilon) = \nabla \cdot (\rho D_\epsilon \nabla \epsilon) + \frac{C_1 \epsilon}{k}\left(P + C_3 \frac{2}{3} k \nabla \cdot \mathbf{u}\right) - C_2 \rho \frac{\epsilon^2}{k}$$

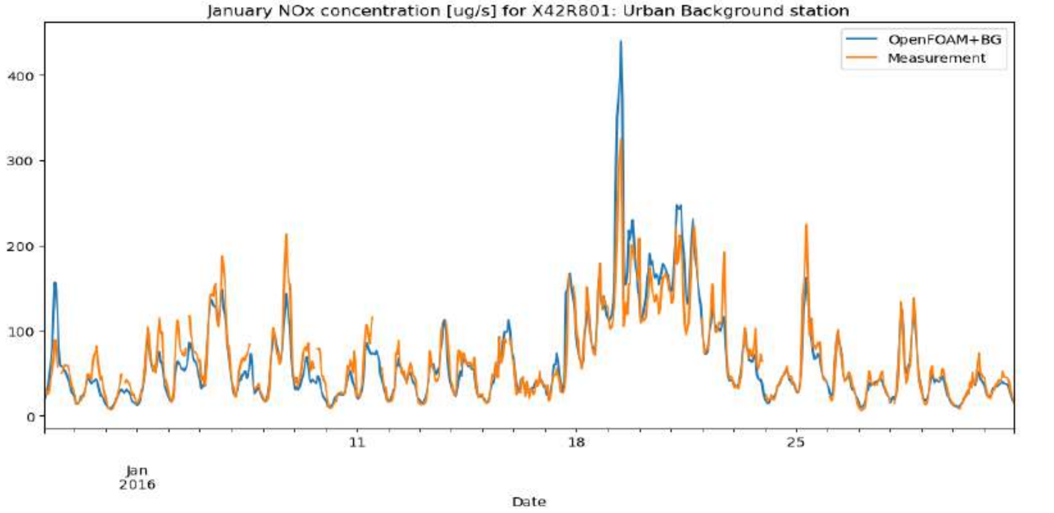
- NOx Pollution s calculated with scalar transport with volumetric source S_s.

$$\frac{\partial}{\partial t} s + \nabla \cdot (\mathbf{u} s) - \nabla \cdot (D_s \nabla s) = S_s$$

- Transient simulation with PIMPLE method, initialized with SIMPLE method

3.2.1 CFD Module with OpenFOAM
Validation on FAIRMODE Intercomparison exercise on Antwerp





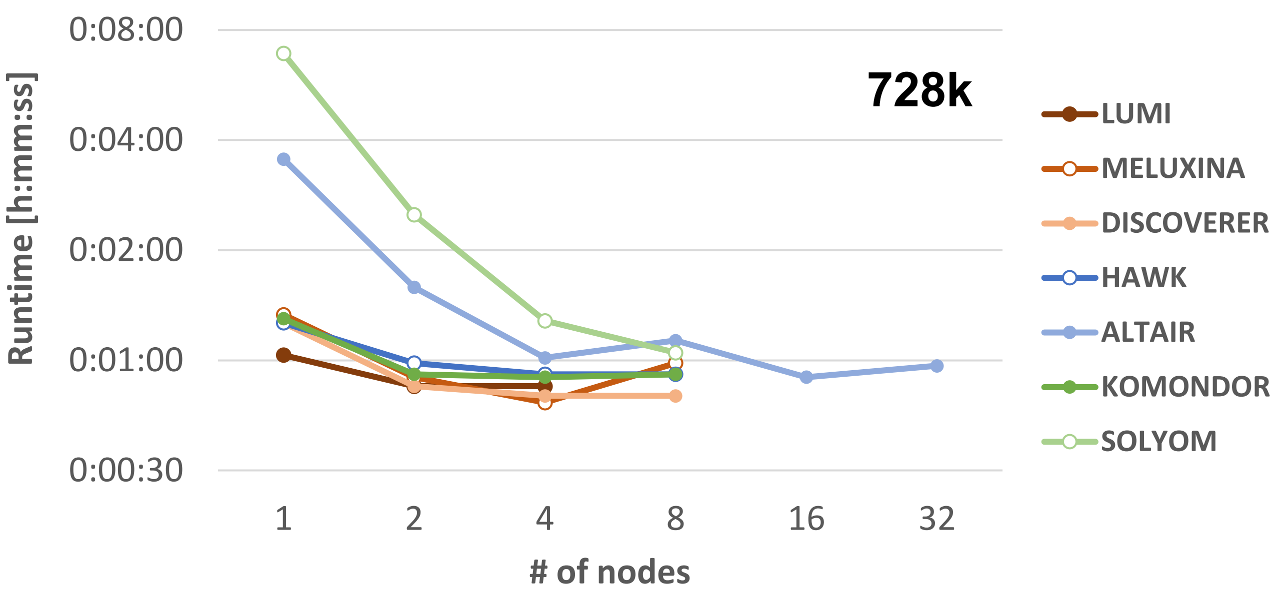
HiDALGO2 CENTRE OF EXCELLENCE

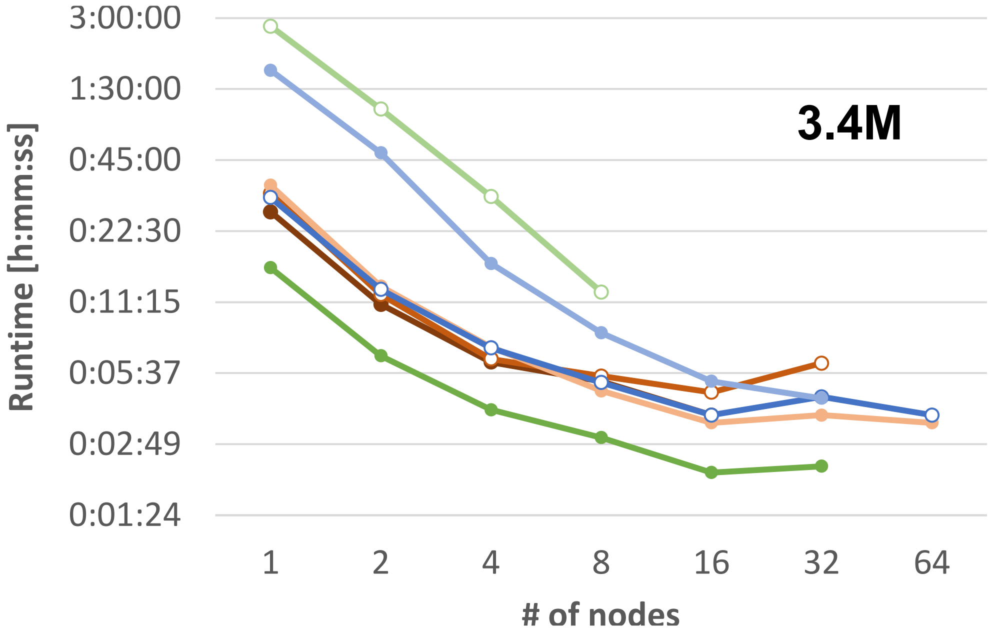
3.2.1. UAP OpenFOAM Benchmark Hardware Overview

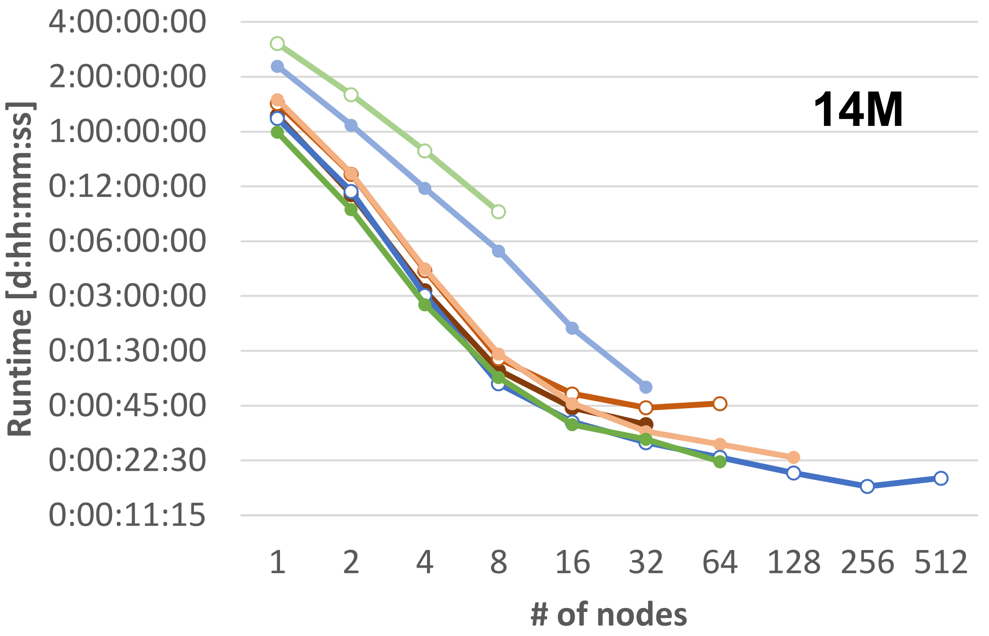
		LUMI	MELUXINA	DISCOVERER	HAWK	ALTAIR	KOMONDOR	SOLYOM
Location		Finland	Luxembourg	Bulgaria	Germany	Poland	Hungary	Hungary
# of CPU nodes available		1022	573	1110	5632	1321	184	12
# of sockets per node		2	2	2	2	2	2	2
# of cores per socket		64	64	64	64	24	64	16
# of cores total		130816	73344	142080	720896	63408	23552	384
CPU	*vendor*	AMD	AMD	AMD	AMD	INTEL	AMD	INTEL
	type	EPYC 7763	EPYC 7H12	EPYC 7H12	EPYC 7742	XEON 8268	EPYC 7763	XEON 6226R
RAM per node		256 GB	512 GB	256 GB	256 GB	192 GB	256 GB	192 GB
Interconnect	*type*	Slingshot	Infiniband	Infiniband	Infiniband	Infiniband	Slingshot	Infiniband
	card	SS11	MT4123	MT4123	HDR	MT4119	SS11	MT4123
	BW	200 Gbit/s	200 Gbit/s	200 Gbit/s	200 Gbit/s	100 Gbit/s	200 Gbit/s	100 Gbit/s
Compiler		cray clang	gnu gcc	gnu gcc	gnu gcc	gnu gcc	gnu gcc	gnu gcc
	version	14.0.2	11.3.0	11.3.0	9.2	10.2	12.2.0	9.4.0
MPI		cray-mpich	openmpi	openmpi	hpe mpt	openmpi	cray-mpich	openmpi
	version	8.1.18	4.1.4	4.1.4	2.23	4.1.0	8.1.24	4.1.2
OpenFOAM	*version*	v2112	v2206	v2206	v2012	v2012	v2112	v2112

LUMI MELUXINA DISCOVERER HAWK ALTAIR KOMONDOR SOLYOM

Benchmarking: Runtime

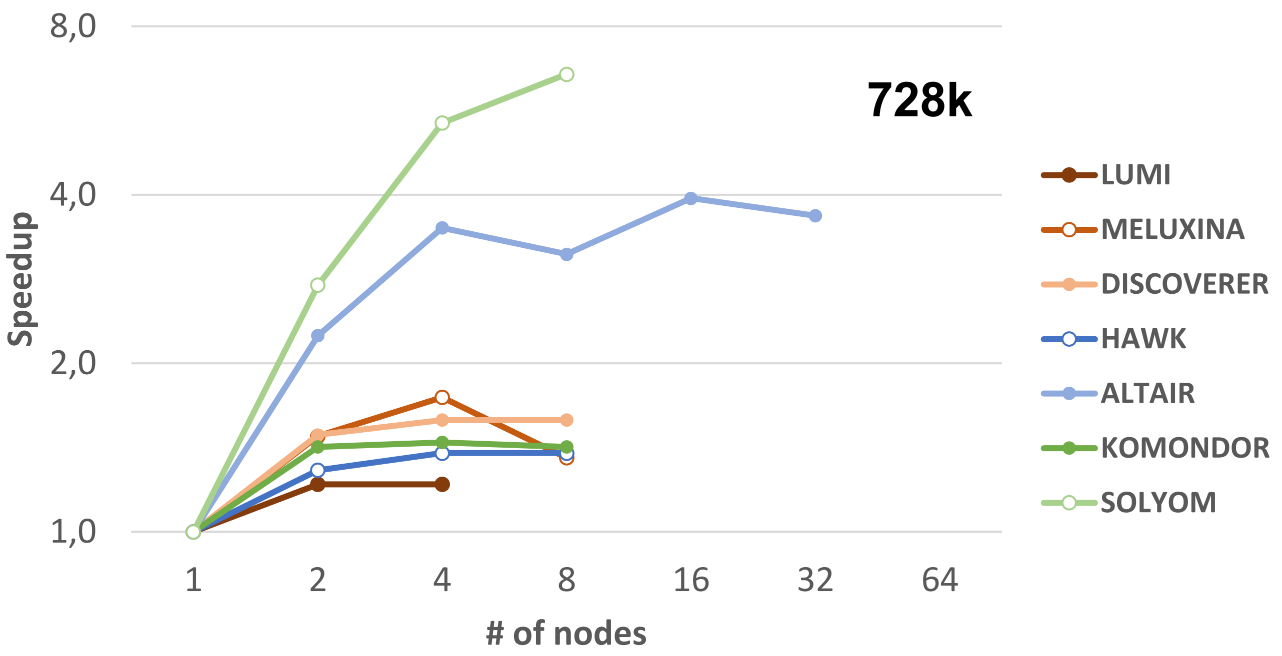


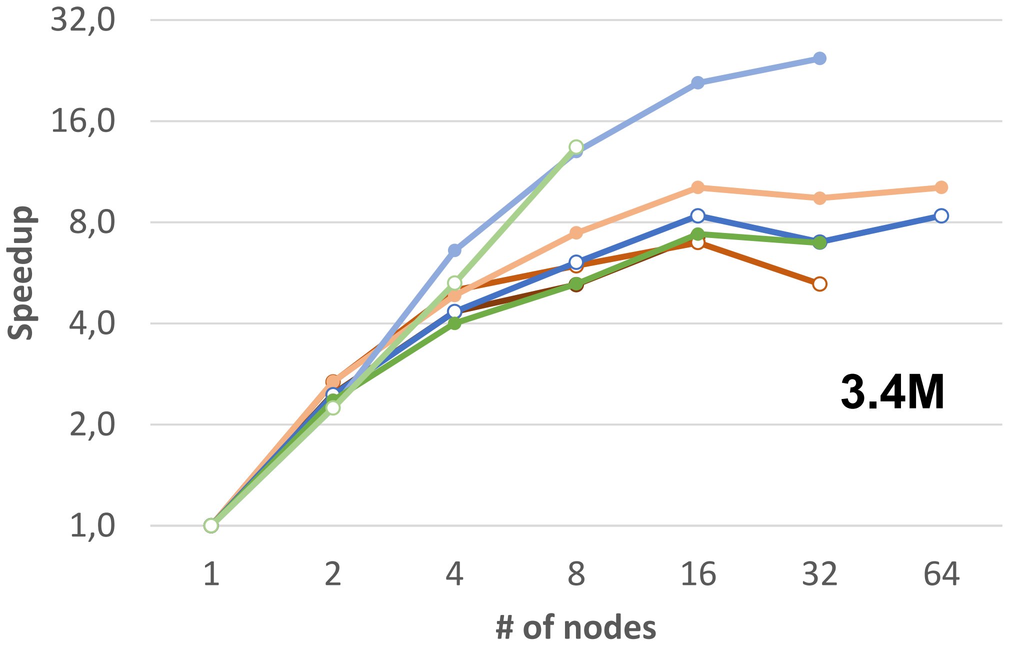


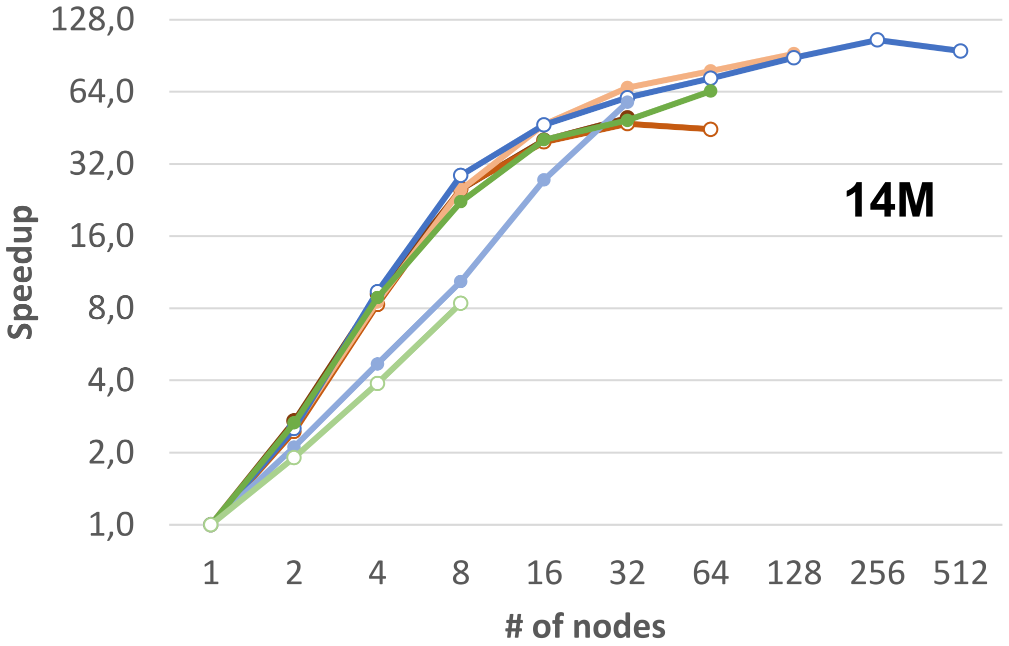


- Győr geometry with mesh sizes 728k, 3.4M, 14M
- Testruns on 7 architectures
- Runtime estimation [hh:mm:ss] for 1h simulated time

Benchmarking: Speedup

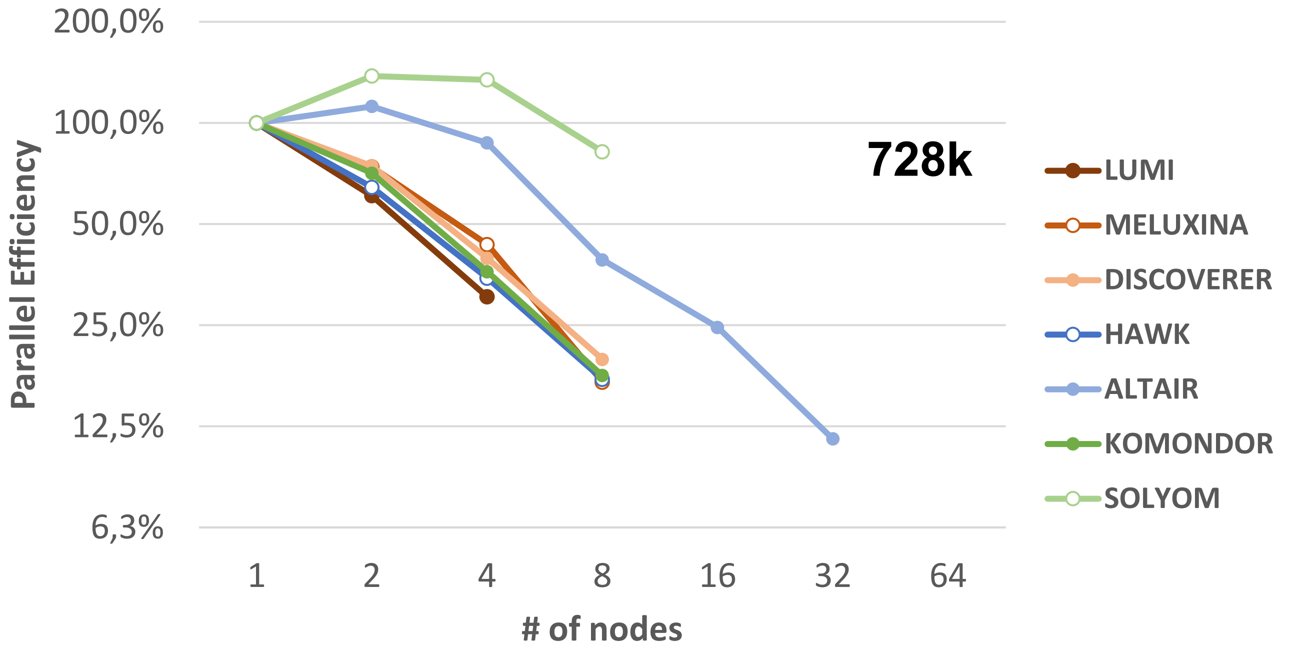


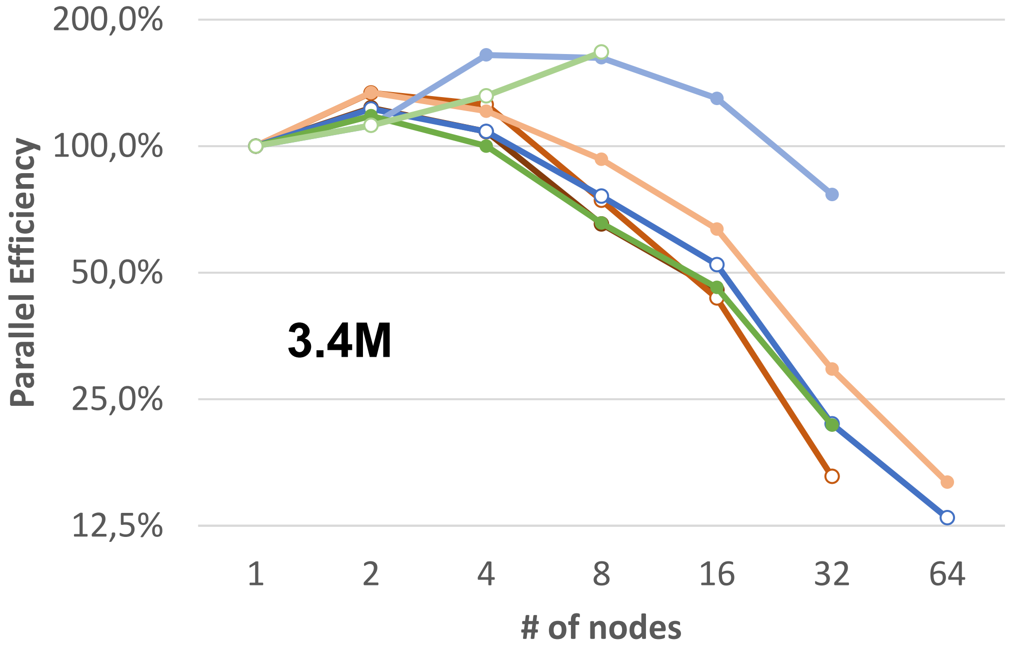


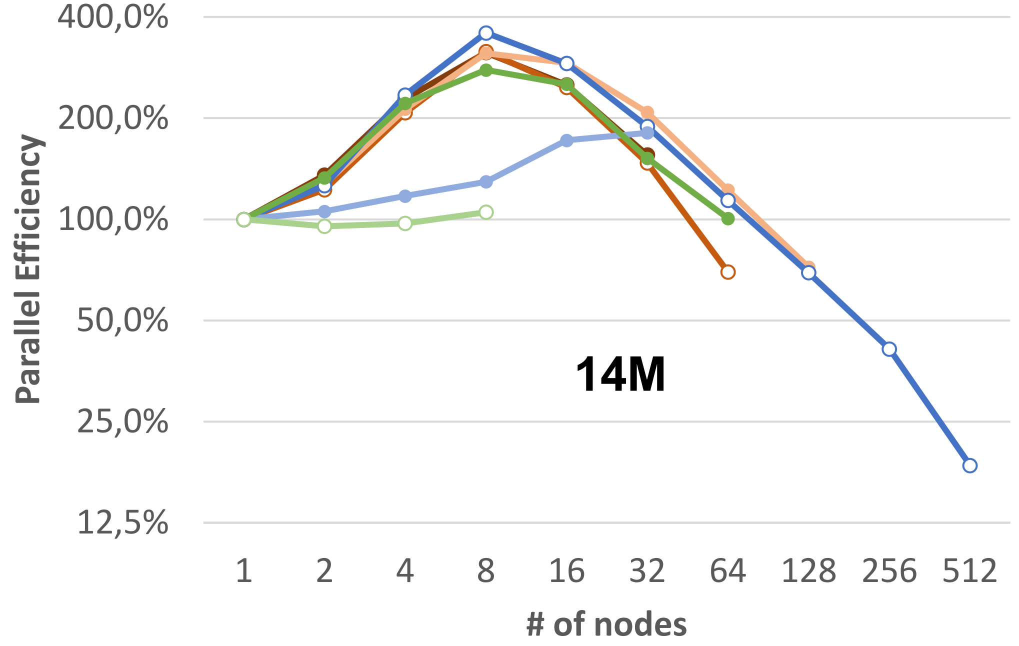


- Győr geometry with mesh sizes 728k, 3.4M, 14M
- Testruns on 7 architectures
- Speedups with regard to 1 node

Benchmarking: Parallel Efficiency







- Győr geometry with mesh sizes 728k, 3.4M, 14M
- Testruns on 7 architectures
- Parallel efficiency with regard to 1 node

Conclusions on the benchmarking

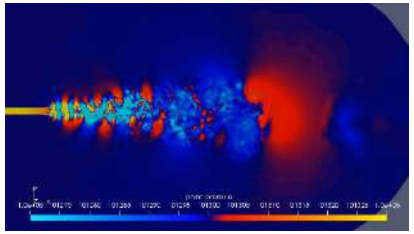
Conclusions for the OpenFOAM scaling

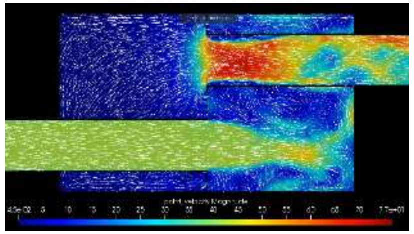
- Testruns on 7 architectures incl. 3 EuroHPC machines
- Efficiency is already the same as was on the Hawk (in HiDALGO1) up to # nodes = 128
- On small/medium scale problems the local cluster with INTEL CPUs performs very well

3.2.2 CFD Fluid-Solver GPU for the compressible Euler and Navier-Stokes equations

Overview:

- Own, **general purpose code for compressible flows** from industry with validated results to measurements in, e.g.:
    - Acoustics (pressure oscillation) of exhaust pipe with muffler flow (2nd order NS with 70M cells),
    - Diesel engine flow (oscillating),
    - High-Voltage Circuit Breaker (3-Mach, with A. Horváth).





- Numerical methods:
    - Based on flux-vector splitting scheme for the compressible Euler and Navier-Stokes equations, 2nd order accurate on unstructured meshes. Ongoing activity: implementation of a Low-Mach solver
    - Operational hybrid AI/ML module (model-order-reduction module with POD)

3.2.2 CFD Fluid-Solver GPU for the compressible Euler and Navier-Stokes equations

Code features

- Written in C99-style, compiled as C++, avoids C++ features (STL, templates, exceptions, ...)
- Parallel:
    - multicore CPU (via OpenMP)
    - **Multi-GPGPU (with CUDA)**
- Optimized code, with no dependency, runs easily on each platform we tried (HPC, ...)
- One single algorithm and thus code for handling 1D, 2D, 3D
- Integrated in-house real-time 3D visualizer (with paraview features)

3.2.2 CFD Fluid-Solver GPU for the compressible Euler and Navier-Stokes equations

Scalability results

- Parallel efficiency

Efficiency: Urban Airflow, Gyor. **N = 30,291,099**		
efficiency	**KOMONDOR**, 4x NVIDIA A100-SXM4-40GB	**VEGA**, 4x NVIDIA A100-SXM4-40GB
P = 1	1	-
P = 2	0.9449242544	-
P = 4	0.8752212861	-

Efficiency: Urban Airflow, Gyor. **N = 18,342,623**		
efficiency	KOMONDOR, 4x NVIDIA A100-SXM4-40GB	VEGA, 4x NVIDIA A100-SXM4-40GB
P = 1	1	1
P = 2	0.9225121646	0.9742910708
P = 4	0.8208693259	0.4716167595

Efficiency: Urban Airflow, Gyor. **N = 3,154,126**		
efficiency	KOMONDOR, 4x NVIDIA A100-SXM4-40GB	VEGA, 4x NVIDIA A100-SXM4-40GB
P = 1	1	1
P = 2	0.7968193341	0.9222091521
P = 4	0.5919466096	0.4022917729

3.2.2 CFD Fluid-Solver GPU for the compressible Euler and Navier-Stokes equations

Scalability results

- Computational time

Wall-Clock Time: Urban Airflow, Gyor. **N = 18342623**			
wall-clock (s)	ONDOR, 4x NVIDIA A100-SXM4-4	, 4x NVIDIA A100-SXM4-	SOLYOM, 1x NVIDIA Tesla V100S-PCIE-32GB
P = 1	2781.590725	2783.904732	2127.01869
P = 2	1507.617369	1428.682257	NO DATA
P = 4	847.147846	1475.724026	NO DATA
Wall-Clock Time: Urban Airflow, Gyor. **N = 3154126**			
wall-clock (s)	**KOMONDOR**	**VEGA**	**SOLYOM**, 1x NVIDIA Tesla V100S-PCIE-32GB
P = 1	432.583269	433.15866	276.966294
P = 2	271.443758	234.848385	NO DATA
P = 4	182.695222	269.181903	NO DATA

4. Demonstration

1. Demonstrations from the HiDALGO2 portal: https://portal.hidalgo2.eu/

2. **Request demo access if you want to have a try!**

5. Possible collaborations with NCCs

1. Application to Urban Air Pollution, Urban Wind Comfort to the NCC stakeholders
2. OpenFOAM application on HPC
   1. Consultation/Solution to bring your OpenFOAM solution to HPC
   2. Improve the scalability of your solution
3. Host your applications in HiDALGO2-Portal or create a similar platform for them
4. Visualize your simulation data on EuroHPC
5. …

Acknowledgments

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Poland, Germany, Spain, Hungary, France, Cyprus under grant agreement number: 101093457.

This publication expresses the opinions of the authors and not necessarily those of the EuroHPC JU and Associated Countries which are not responsible for any use of the information contained in this publication.

Co-funded by the European Union

EuroHPC Joint Undertaking

Disclaimer

Further acknowledgments

SZE acknowledges KIFÜ, the Hungarian NCC for providing HPC resources and support.

KIFÜ

Thank you for your attention

www.hidalgo2.eu

e-mail: office@hidalgo2.eu

Zoltán Horváth

Széchenyi István University (SZE)

Egyetem tér 1.
9026 Győr, Hungary

phone: (+36 96) 613-657
e-mail: horvathz@math.sze.hu