HIDALGO2
CENTRE OF EXCELLENCE

Urban Air Project

Castiel 2 – Code of the month presentation

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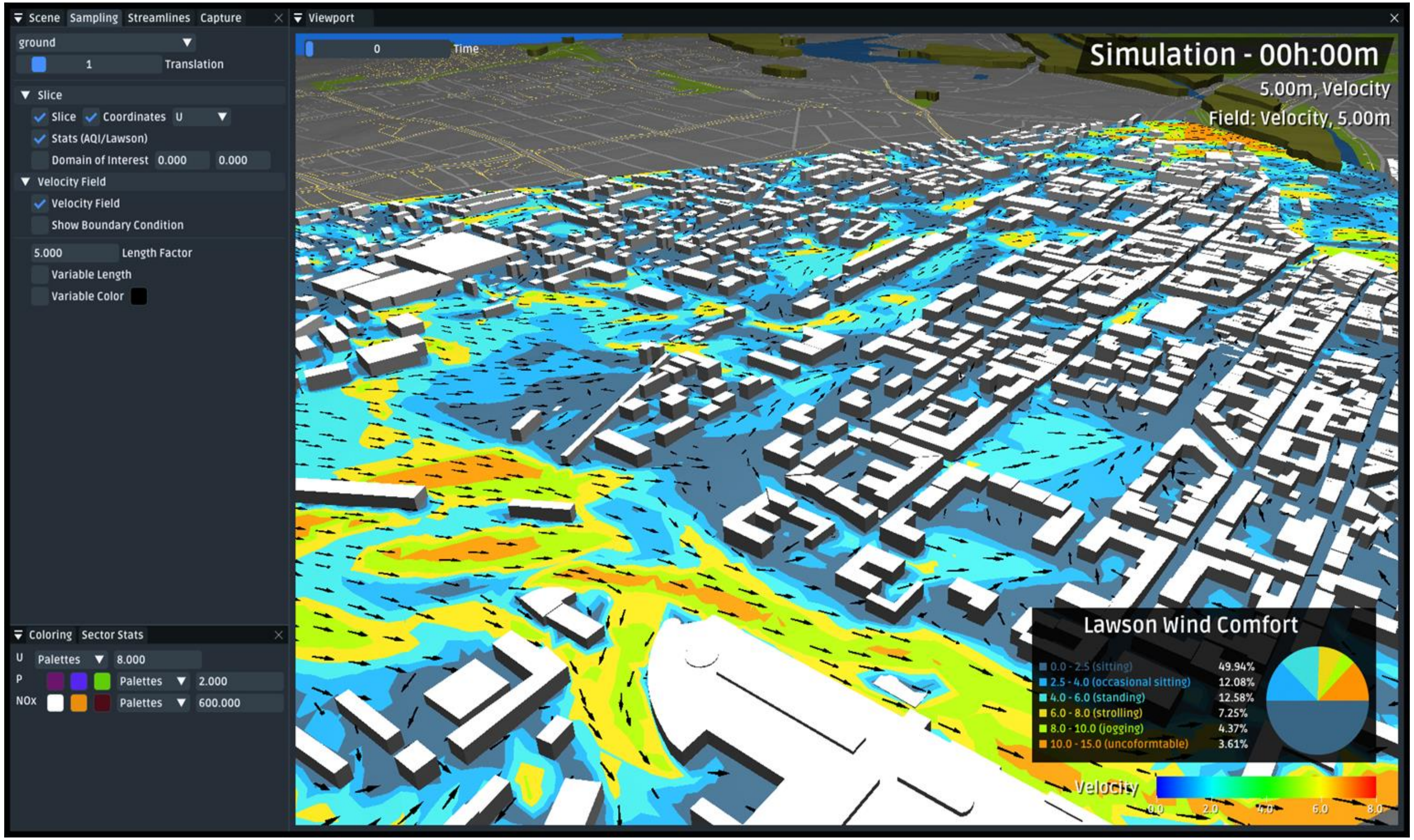
Preface


Scene
Sampling
Streamlines
Capture
ground
1
Translation
Slice
Slice
Coordinates
U
Stats (AQI/Lawson)
Domain of Interest
0.000
0.000
Velocity Field
Velocity Field
Show Boundary Condition
5.000
Length Factor
Variable Length
Variable Color
Coloring
Sector Stats
U
Palettes
8.000
P
Palettes
2.000
NOx
Palettes
600.000
Viewport
0
Time
Simulation - 00h:00m
5.00m, Velocity
Field: Velocity, 5.00m
Lawson Wind Comfort
0.0 - 2.5 (sitting) 49.94%
2.5 - 4.0 (occasional sitting) 12.08%
4.0 - 6.0 (standing) 12.58%
6.0 - 8.0 (strolling) 7.25%
8.0 - 10.0 (jogging) 4.37%
10.0 - 15.0 (uncoformtable) 3.61%
Velocity
0.0
2.0
4.0
6.0
8.0

Contents

1.1 Global challenges of urban air

Air pollution is above health limits in many cities, due to traffic, or factory emissions (NOx, PM)

- EU regulations
- Current services only at a very coarse resolution

https://www.thelocal.de/20171115/eu-planning-to-sue-germany-over-dirty-air-in-cities-report

Accidental/intentional toxic gas **release** (e.g. from batteries) in cities is a major concern

- A very fast operation is needed e.g. for an evacuation

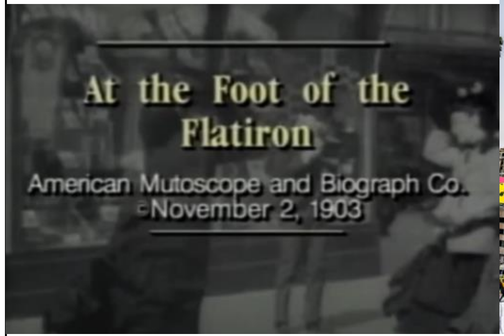
Germany: toxic fumes alert after massive warehouse fire in Hamburg

Police have warned people in the Hamburg to close their windows after a large fire that engulfed several warehouses sent black, chemical-laden smoke drifting over the city.

https://www.euronews.com/2023/04/09/germany-toxic-fumes-alert-after-massive-warehouse-fire-in-hamburg

Pedestrian **wind discomfort** or danger near tall buildings, due to corners' amplification or the channel effect mainly

- E.g. Flatiron Building, NYC
- Standards for building design, e.g. by Lawson, or the NL-standard NEN 8100:2006 - Wind Comfort and Wind Danger in the Built Environment



https://www.youtube.com/watch?v=iZDE73cjaC8

1.2 Solution-methodologies and their requirements

1. Computational tools for the **analysis** of a design: high-resolution (1 meter at ground level) simulation
2. **Reporting tool** according to the EU regulations (e.g. full-year simulation and assessment of air quality)
3. **Decision-making or risk analysis** computational tools for scenario analysis: simulate several options fast
4. **Real-time digital twin** for the airflow / air quality / pollutant concentration (i.e. live simulation that assimilates sensor data continuously to simulation)
5. **Design tool** for urban building planning

1.3 The UAP solution for the societal problem and its codes

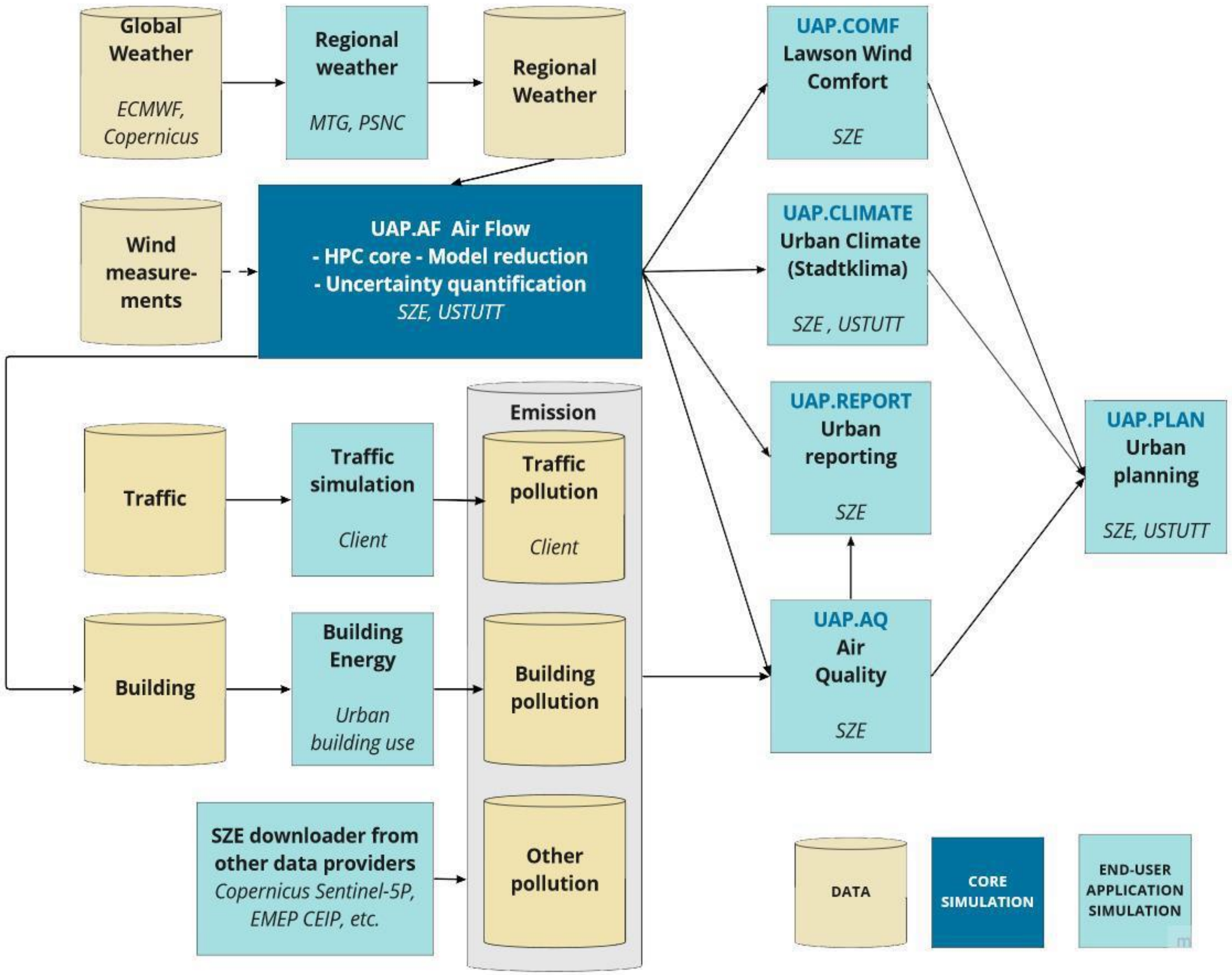
According to the requirements, we need:

→ HPC-solutions that can be run by non-HPC-experts as well → **Urban Air Project (UAP)**

→ **General, scalable** UAP-components, which can serve arbitrary CFD HPC applications, e.g. in industry

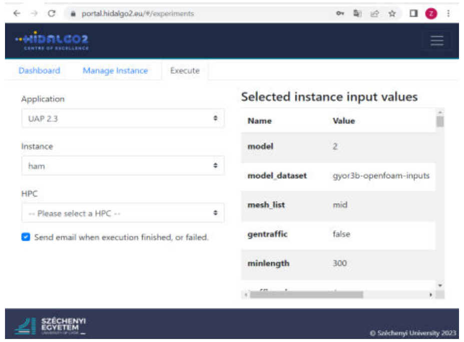
1. **MathSO-Portal**, i.e. a web-interface for HPC-job configuration, execution, postprocessing
2. CFD (computational fluid dynamics) solvers for airflow and dispersion computations
    1. **OpenFOAM**-based solution UAP-Foam
    2. **RedSim**: our native multi-GPU and multi-CPU CFD solver for complex geometries
        1. Exactly the HPC code runs on PCs as well (N.B. the consumer PCs are quite strong, often with some GPUs)
        2. Uses mathematical technologies for model order reduction
    3. **CFDR**: our HPC-visualizer in-the-web

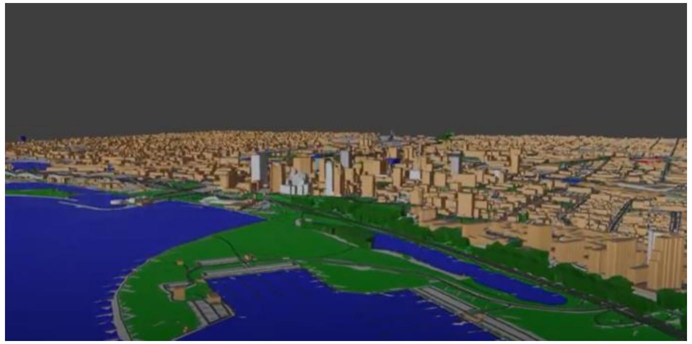
2.1 The UAP workflow

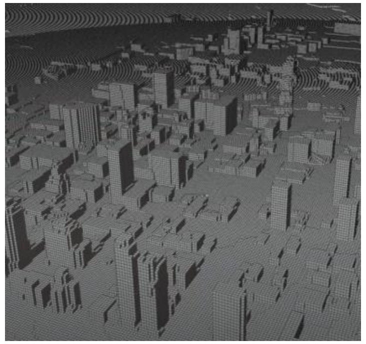


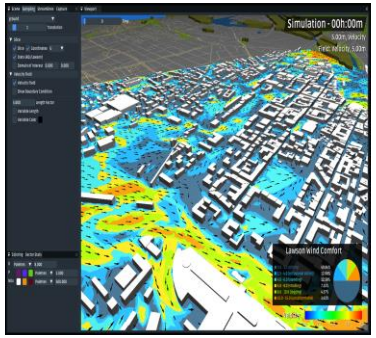
2.1 Overview of the UAP application from the portal

- **MathSO-portal: Automated deployment of containerized solutions to HPC platforms** with
  - Configuration (on the web application)
  - Preprocessing (geometry from OpenStreetMap, meshing),
  - Simulation (OpenFOAM, RedSim), and
  - Visualization (with CFDR).



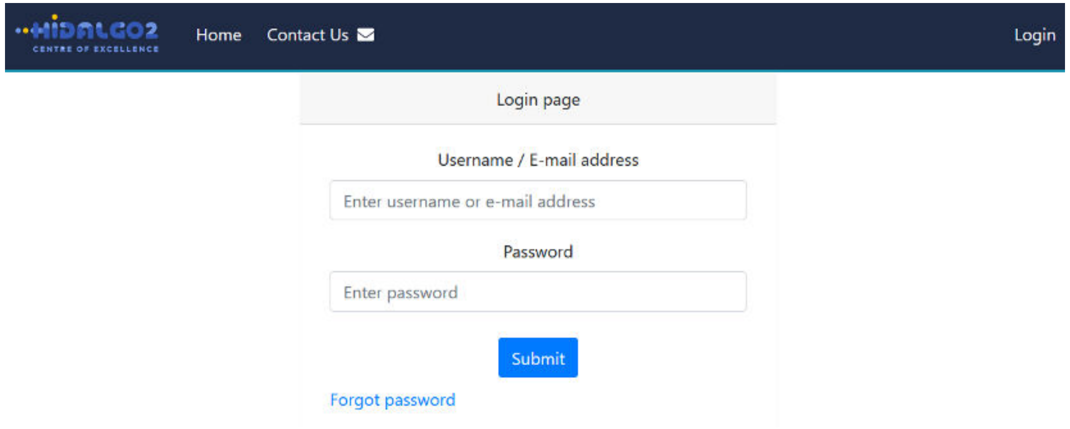


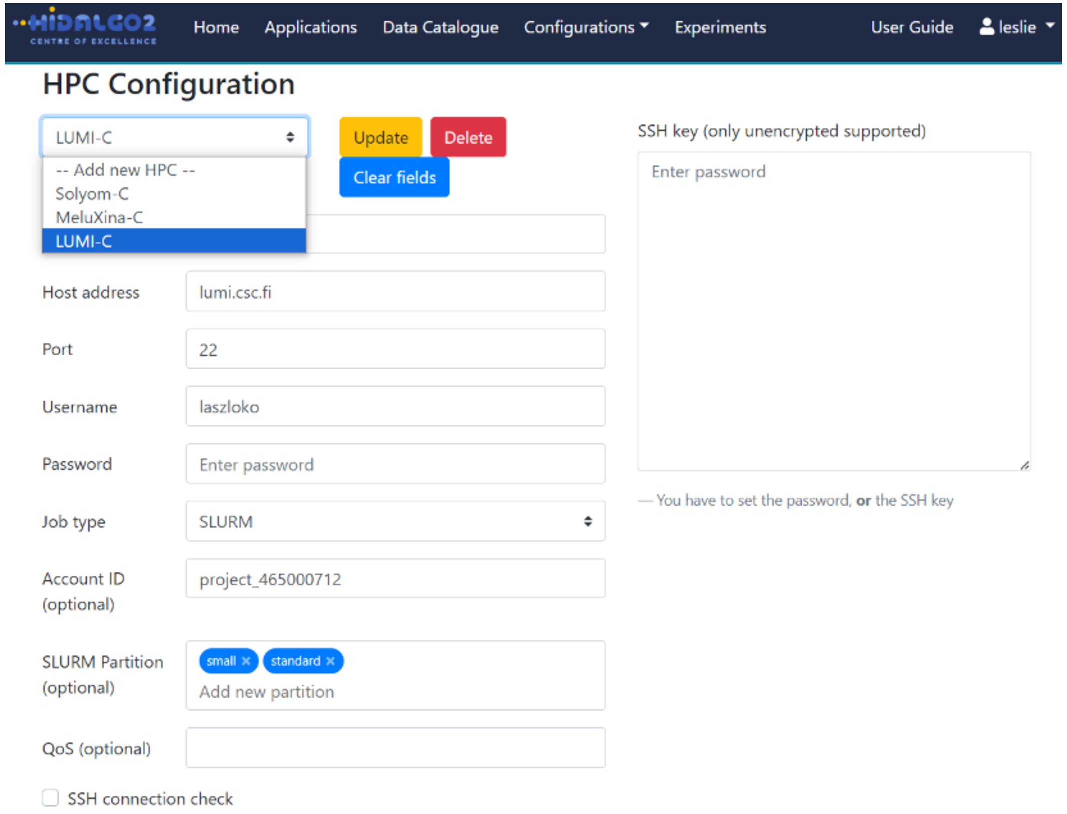


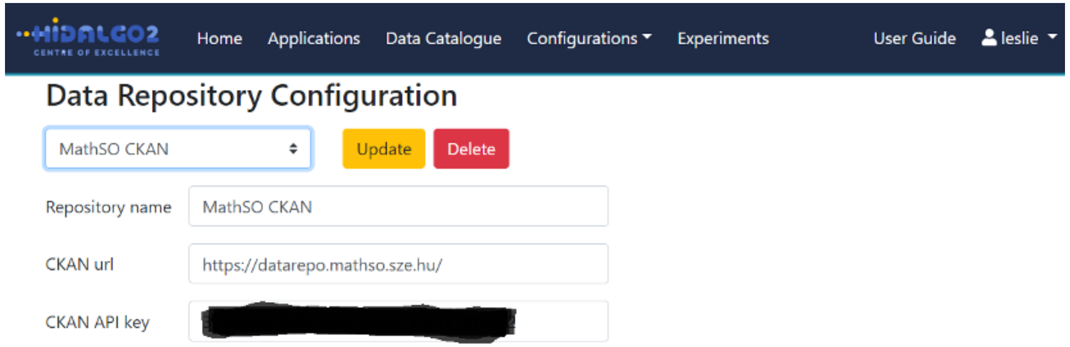


Details will be demonstrated in a couple of minutes!

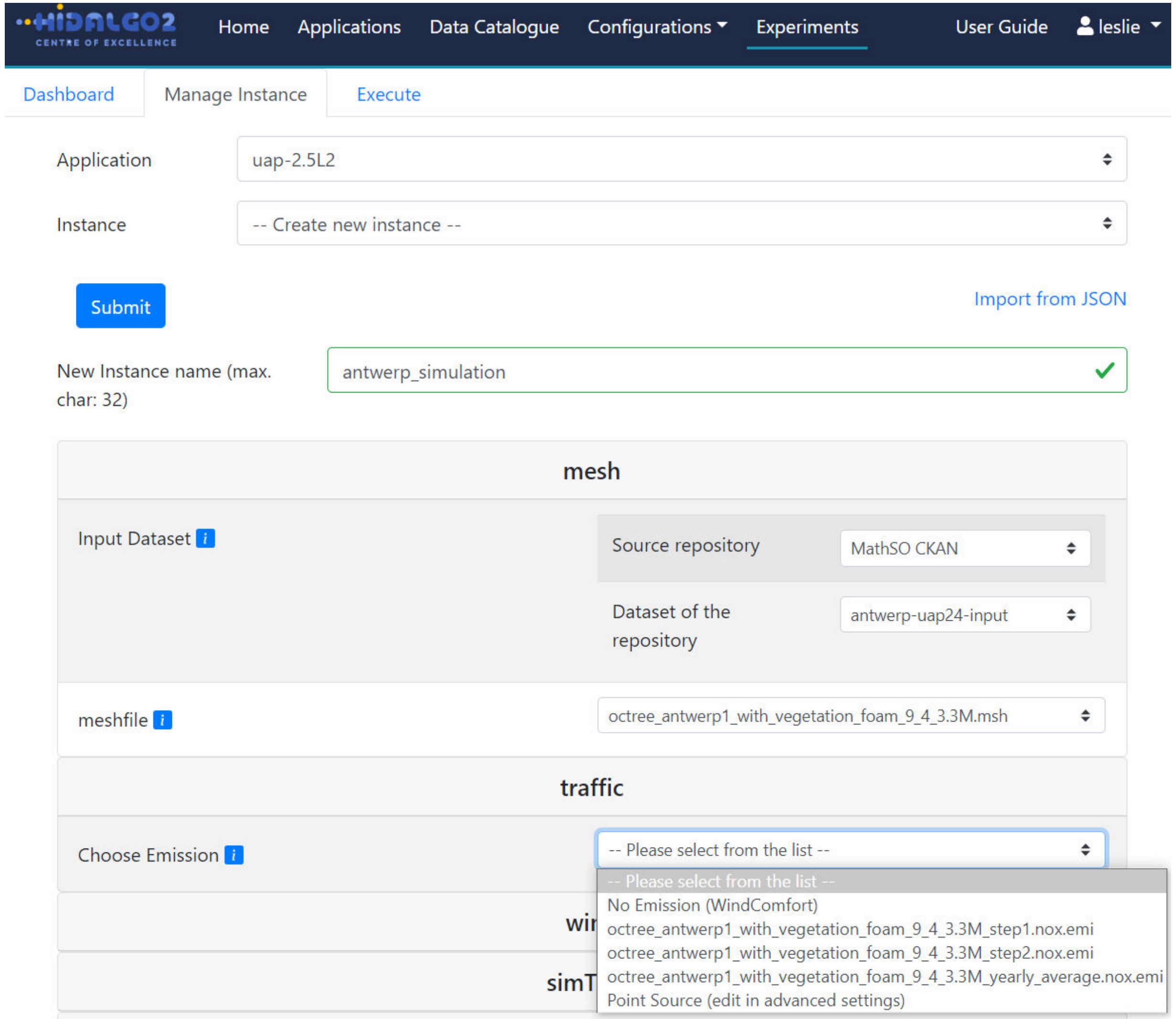
2.2 Overview of the HiDALGO2 Portal - Configuration and Features

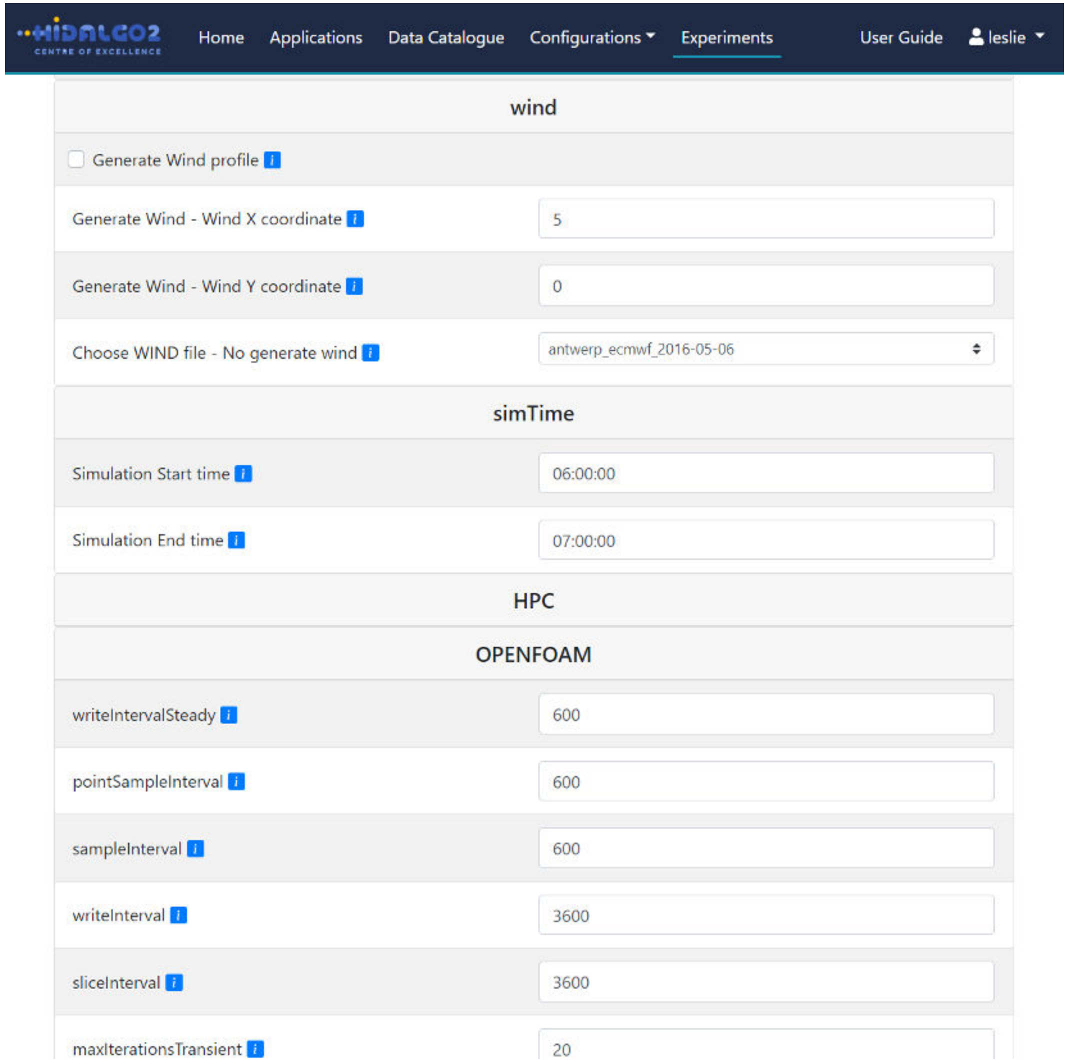




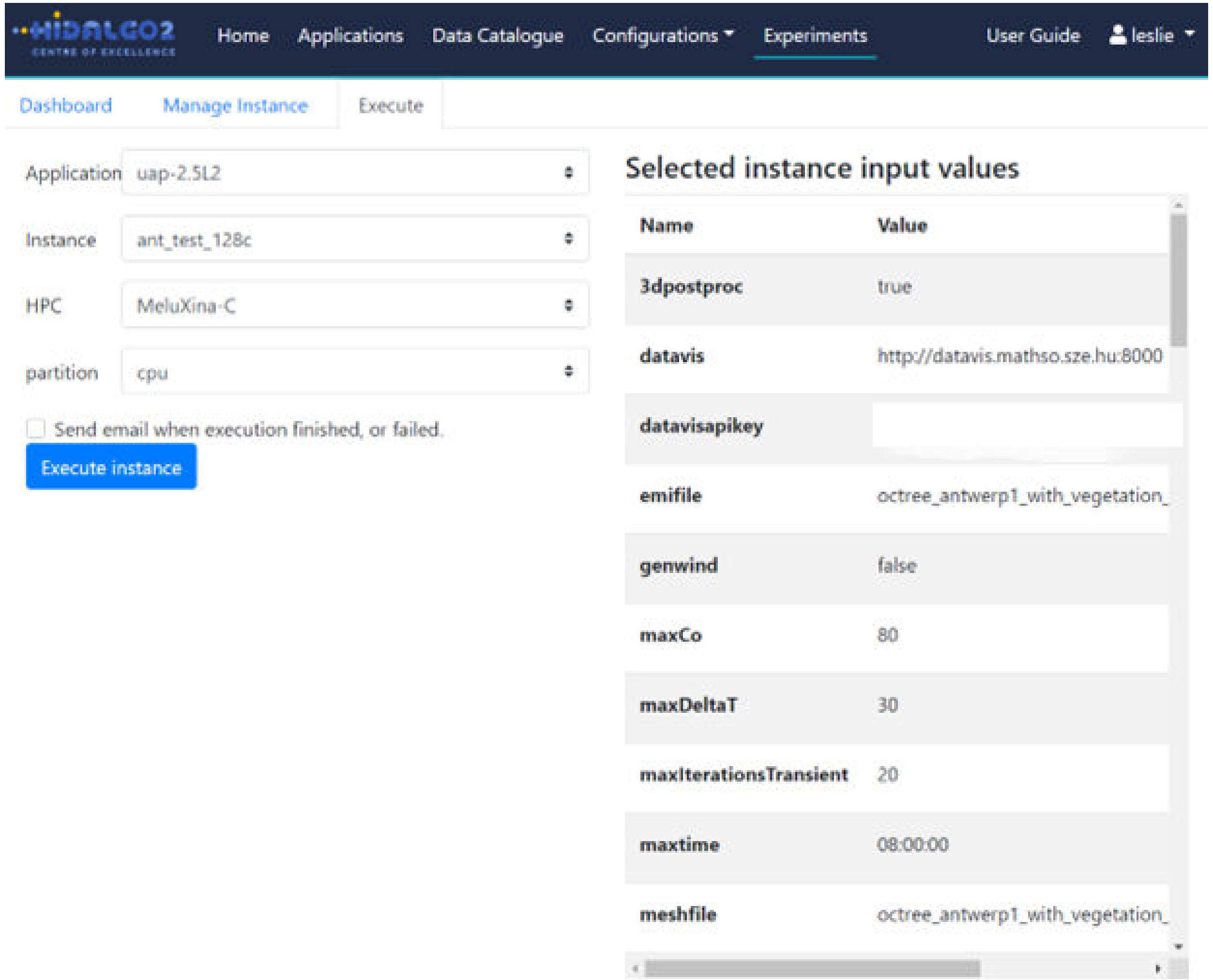


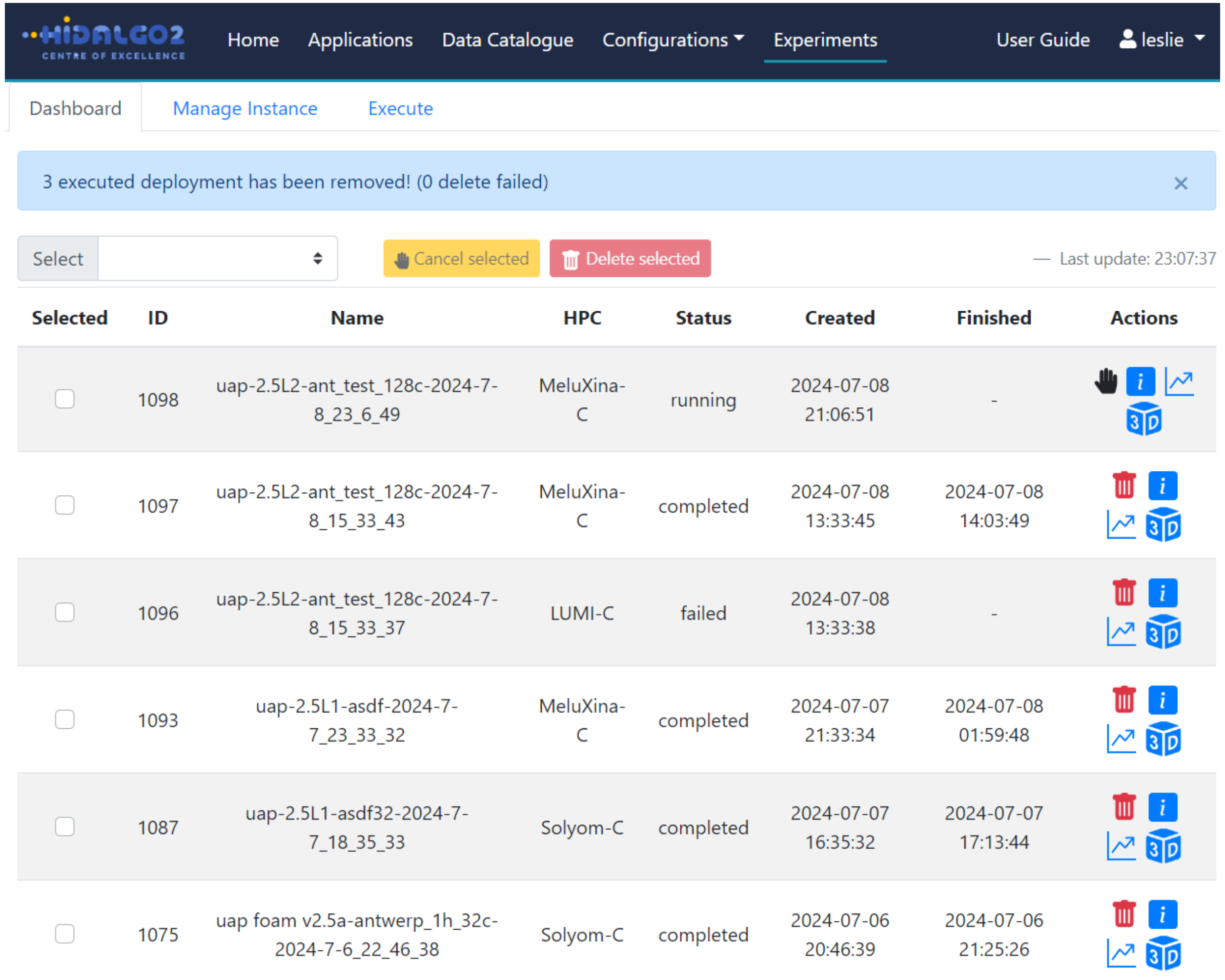
2.2 Overview of the HiDALGO2 Portal - Configure simulation for the UAP-FOAM



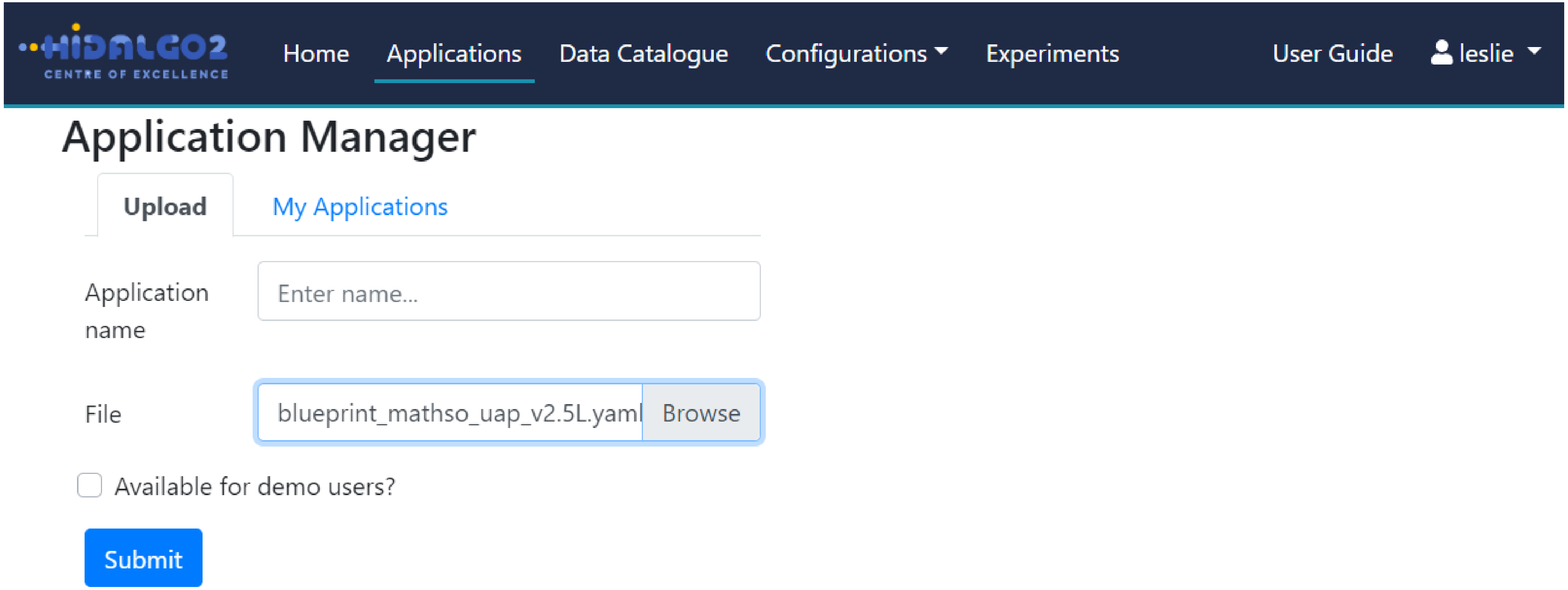


2.2 Overview of the HiDALGO2 Portal - Submit and Monitor

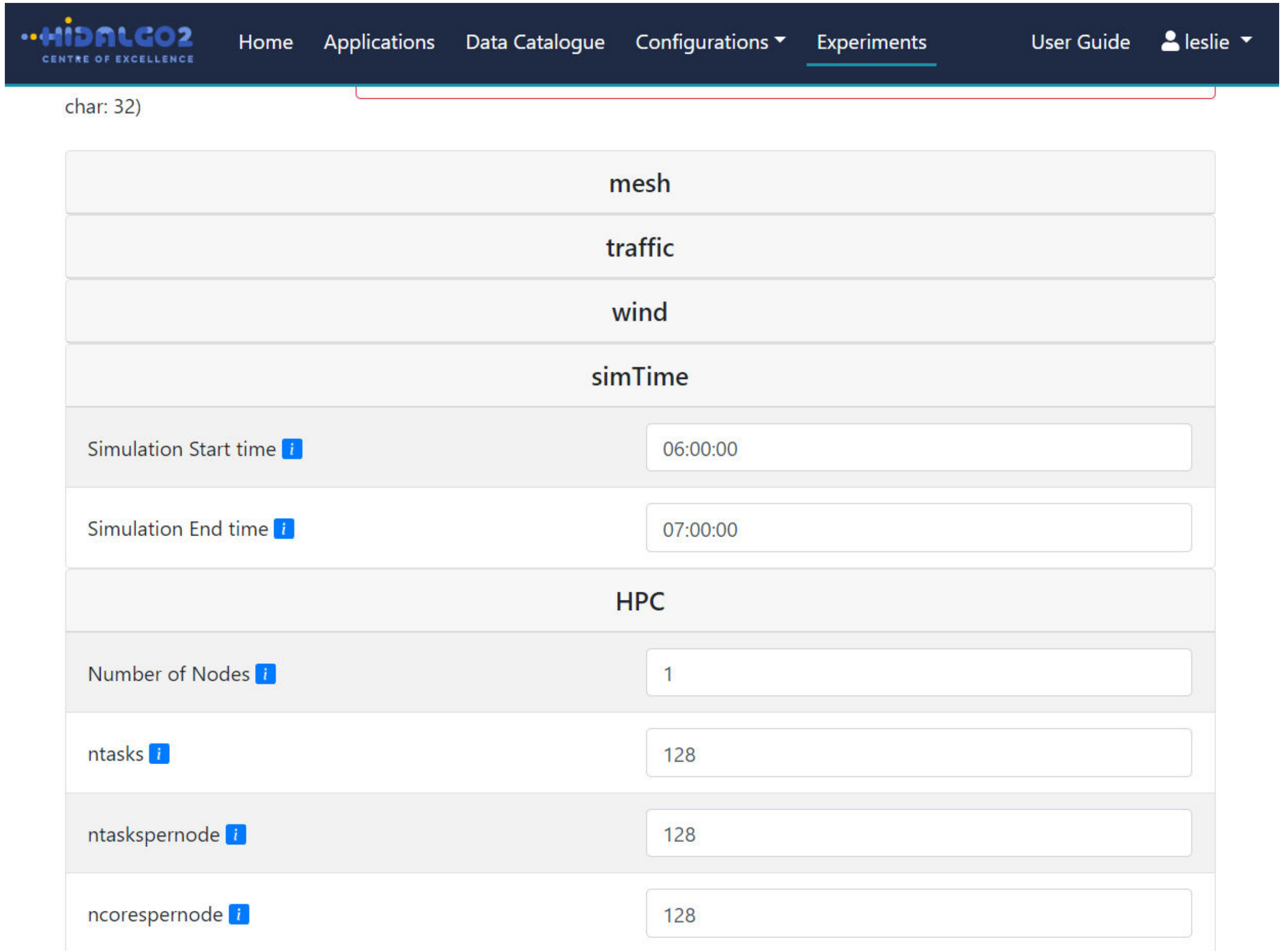




2.2 Overview of the HiDALGO2 Portal - Portal Application Manager



2.2 Overview of the HiDALGO2 Portal – Blueprint input fields

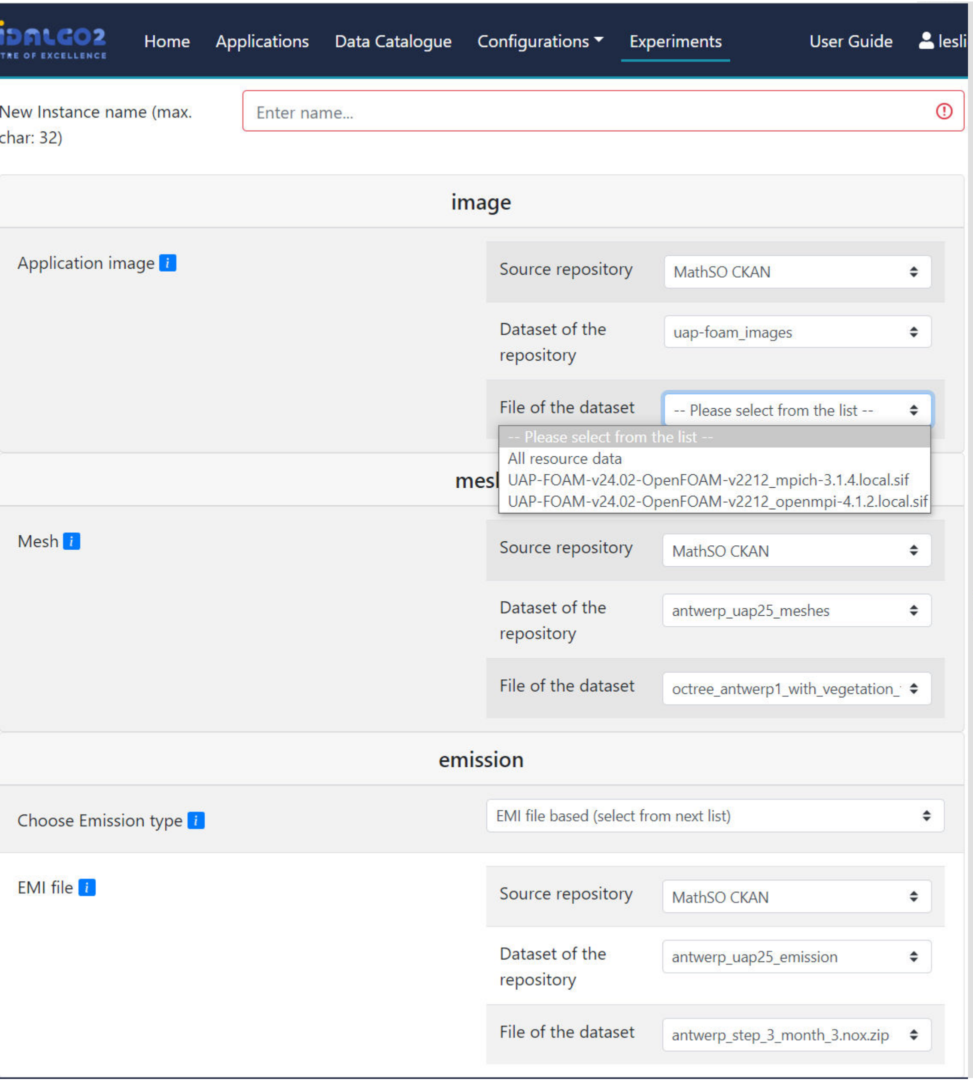



```yaml
simstarttime:
  name: Simulation Start time
  description: "Simulation Start time"
  default: "00:00:00"
  type: text
  group: simTime
  order: 9
  optional: false

simendtime:
  name: Simulation End time
  description: "Simulation End time"
  default: "23:59:00"
  type: text
  group: simTime
  order: 10
  optional: false


jobmanager_list:
  name: Jobmanager
  description: "Choose the used JobManager"
  type: hidden
  default: "SLURM"
  group: HPC
  order: 11
  optional: false

nnodes:
  name: Number of Nodes
  description: "Number of Nodes"
  default: "2"
  type: text
  group: HPC
  order: 40
  optional: false
```

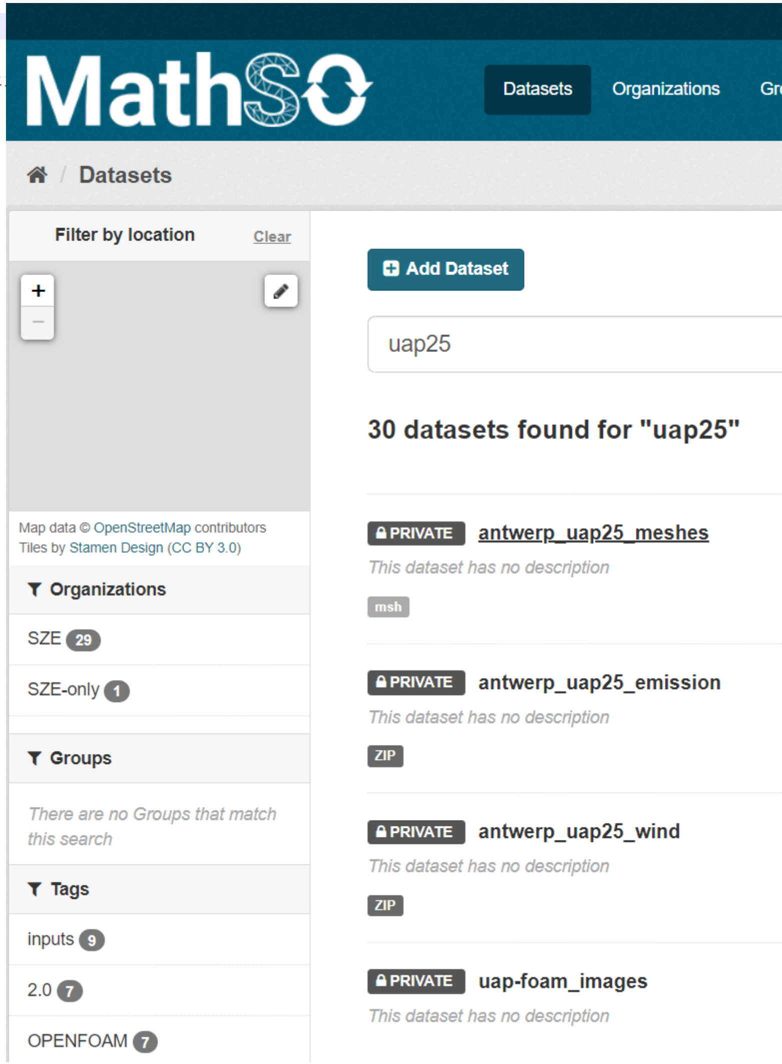
2.2 Overview of the HiDALGO2 Portal – Workflow in TOSCA

```yaml
copying:
        type: hpc.nodes.Job
        properties:
            job_options:
                type: 'HEAD'
                command: { concat: [ 'wget ', { get_input: pilot_url }
            deployment:
                #bootstrap: 'scripts/bootstrap_traffic.sh'
                #revert: 'scripts/revert_traffic.sh'
            skip_cleanup: true

sim_conf:
        type: hpc.nodes.Job
        properties:
            job_options:
                type: 'HEAD'
                command: { concat: [ 'sleep 15 && ./mathso-gencfg.sh '
        relationships:
            - type: job_depends_on
              target: copying
preproc:
        type: hpc.nodes.Job
        properties:
            job_options:
                type: 'SRUN'
                command: './run.sh'
                nodes: '1'
                tasks: '1'
                cpus_per_task: '12'
                max_time: 01:00:00
            deployment:
                #bootstrap: 'scripts/bootstrap_traffic.sh'
                #revert: 'scripts/revert_traffic.sh'
            skip_cleanup: true
        relationships:
            - type: job_depends_on
              target: sim_conf

simu:
        type: hpc.nodes.Job
        properties:
            job_options:
                type: 'SBATCH'
                command: './cfd/simulate.job'
                max_time: '48:00:00'
                std_out: 'slurm_out'
                err_out: 'slurm_err'
            deployment:
                #bootstrap: 'scripts/bootstrap_traffic.sh'
                #revert: 'scripts/revert_traffic.sh'
            skip_cleanup: true
        relationships:
            - type: job_depends_on
              target: preproc

upload:
        type: hpc.nodes.Job
        properties:
            job_options:
                type: 'HEAD'
                command: './upload.sh'
                std_out: 'upload_out'
                err_out: 'upload_err'
            deployment:
            skip_cleanup: true
        relationships:
            - type: job_depends_on
              target: simu

expected_results:
  - type: 2D
  - type: 3D
```

2.2 Overview of the HiDALGO2 Portal - CI/CD from the portal, incl. container integration




```yaml
app_image:
  name: Application image
  description: Singularity image for UAP-FOAM applicat
  default: ""
  type: ckan_file
  ckan_tag: uap25 image
  group: image
  order: 2
  optional: false
  dataset_optional: false

model_mesh:
  name: Mesh
  description: Mesh dataset and mesh.
  default: ""
  type: ckan_file
  ckan_tag: uap25 mesh
  group: mesh
  order: 3
  optional: false
  dataset_optional: false

emitype:
  name: Choose Emission type
  description: "Choose Emission Type Source"
  type: list
  choices:
    - first:
      text: No Emission (WindComfort)
      value: noemission
    - second:
      text: EMI file based (select from next list)
      value: emiemission
    - fifth:
      text: Point Source (edit in advanced settings)
      value: pointsource
  group: emission
  order: 11
  optional: true
```

2.3 CFD codes in UAP

Overview

1. **OpenFOAM**
    1. 3D incompressible Navier-Stokes, FVM on unstructured meshes, RANS and URANS, (pimpleFOAM, simpleFOAM), passive scalar (for pollutant dispersion)
    2. Optimized code for CPU (OpenMPI)
        1. **Parallel efficiency: >80% (#cells=10M)**
    3. Participated in the FAIRMODE-hackathon: simulation and assessment for Antwerp 2016

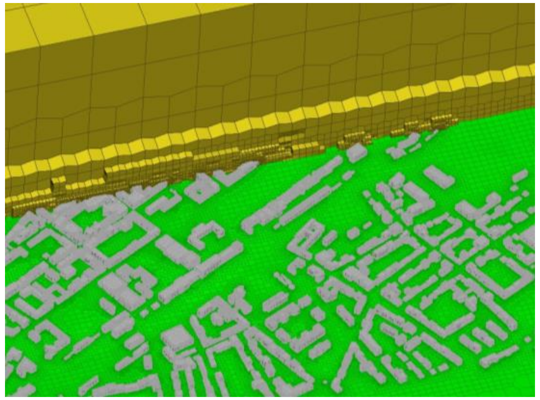
2. **RedSim**
    1. Native C/C++/CUDA code for the 2D/3D Euler and Navier-Stokes, compressible, 1st & 2nd order FVM, unstructured polyhedral meshes, reduced order mode (POD, POD-DEIM)
    2. Optimized for multi-GPU (CUDA, NVLINK), and CPU (OpenMPI, cray-mpich on LUMI) randomized SVD
        1. **Parallel efficiency > 85% with 8 GPUs (KAROLINA) and #cells = 30M**
    3. Compact, expressive Lua-API
    4. Exactly the HPC code runs on PCs (under Linux/MacOS/MS Windows) as well

3. **CFDR**
    1. CFD Rendering: data preprocessing on the HPC, visualization on the web
    2. Lua-API

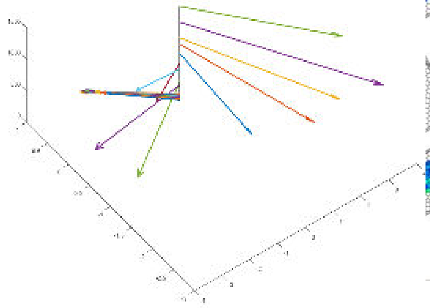
2.3.1 UAP-FOAM

- Input
  - 3D Mesh City Model
  - Weather-based boundary, ECMWF coupled
  - Traffic or point-based pollution source
- Equations and solution
  - Incompressible URANS solved with k-e turbulence model
  - NOx Pollution s calculated with scalar transport with volumetric source S_s.
  - Transient simulation with PIMPLE method, initialized with SIMPLE method

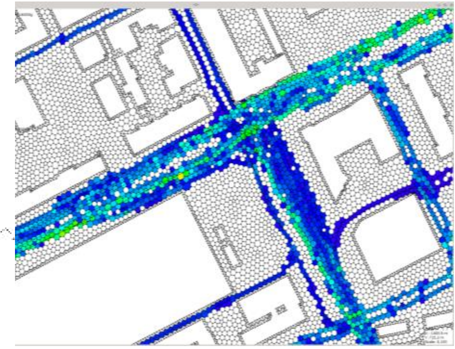
Model



Boundary



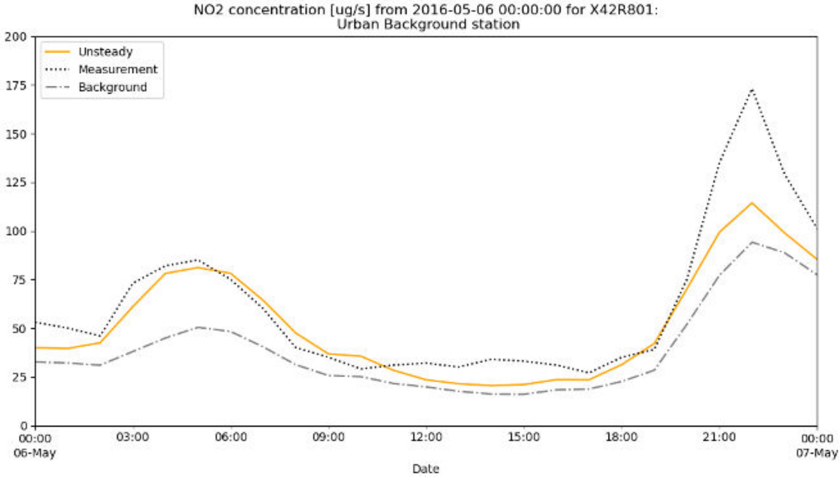
Traffic

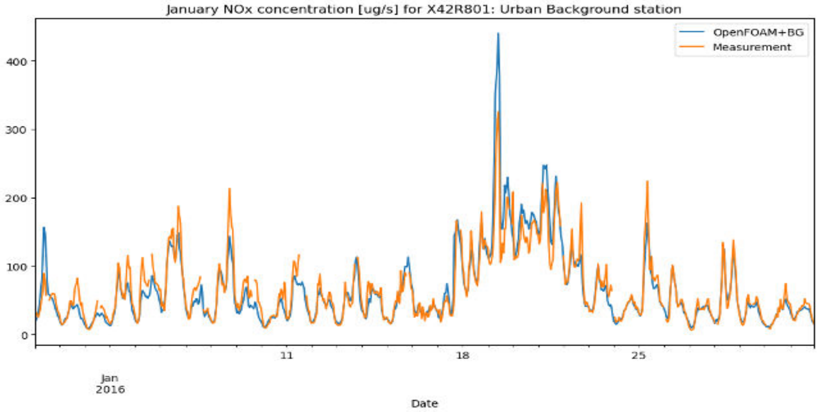


3D Result

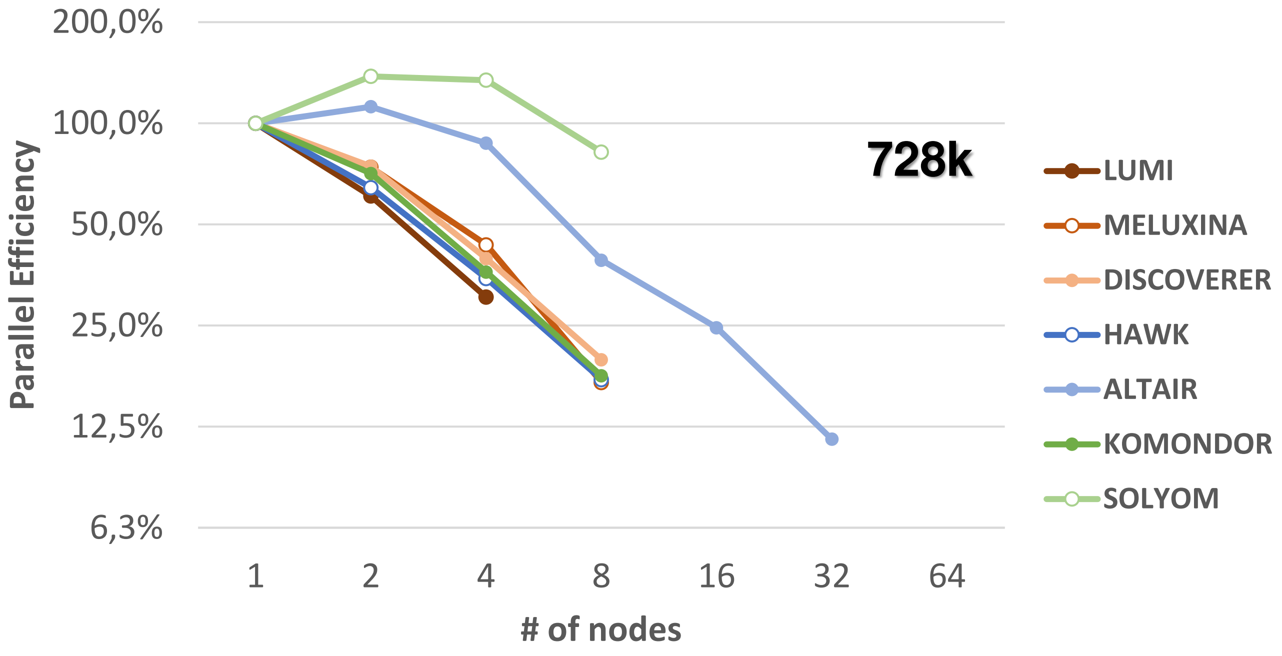
2.3.1 UAP-FOAM Validation

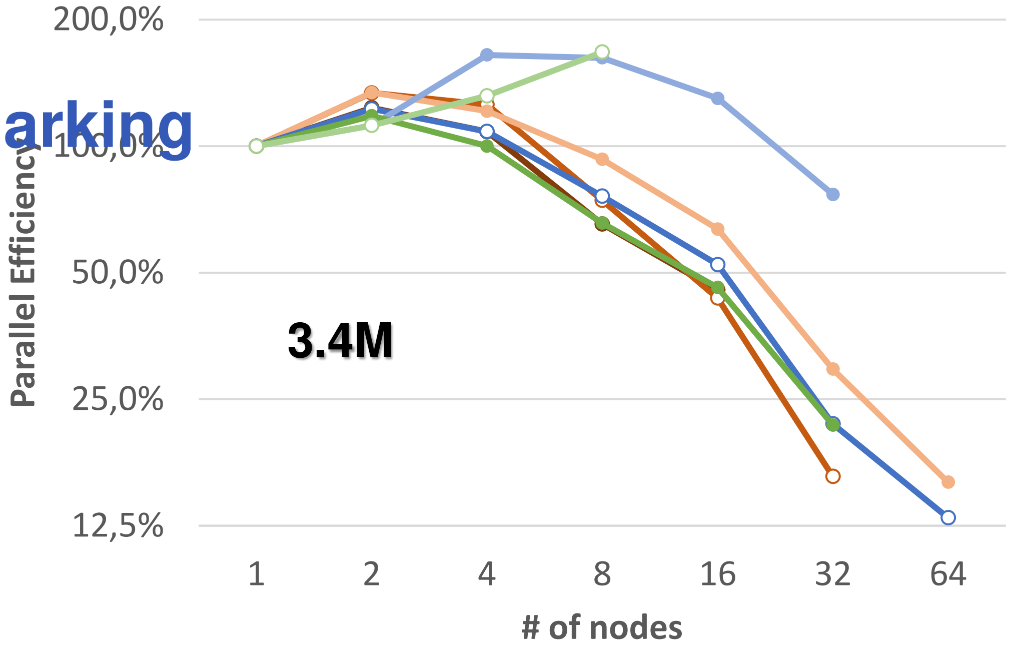
- FAIRMODE-hackathon
  - Simulation data: Antwerp, 2016, full-year simulation, measured wind, yearly average traffic
  - Measurements: 2 EU measurement stations and several passive samplers
  - Computational time with UAP-FOAM: 19 days on Solyom (SZE local cluster) on 12x 32 cores
  - Comparison with several modeling groups in FAIRMODE, paper in the journal STOTEN 171761

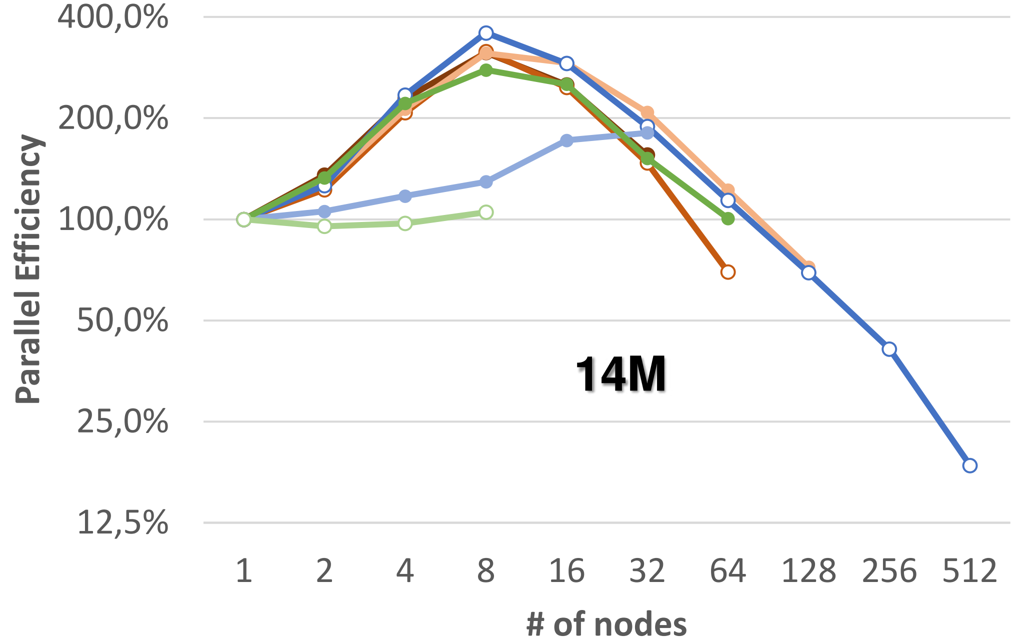




2.3.1 UAP-FOAM Benchmarking







- Győr City geometry with mesh sizes 728k, 3.4M, 14M
- Testruns on 7 architectures incl. LUMI, MELUXINA, DISCOVERER of the EuroHPC JU
- Parallel efficiency with regard to 1 node

2.3.2 The RedSIM and CFDR software

https://redsim.mathso.sze.hu/

RedSim:

- Native multi-GPU CFD-solver to simulate compressible fluids on unstructured, polyhedral meshes.
- The same code runs on HPC and PC (under Linux/MacOS/MS Windows)

CFDR:

- Visualization software for CFD running on HPC and to visualize data on your web browser live.

API:

- Expressive, compact API written in Lua, helps the users to write their applications with RedSim and CFDR.

2.3.2 The RedSIM and CFDR software

Licenses

All codes were developed at the Széchenyi István University, Győr, Hungary (SZE) by Zoltán Horváth (RedSim algorithm, project lead) and Mátyás Constans (programming).

RedSim and CFDR will have multiple licenses, to be released in July 2024:

`testing` : access to the APIs and executable files of the solvers on 1 CPU node for testing purposes

`academic` : access to the APIs and executable files of the solvers with full functionality for academic research

`commercial closed source` : access to the APIs and the executable files of the solvers for any use

`commercial open source` : access to the APIs and the source code of the solvers for any use.

RedSim uses LUA, Eigen, OpenMPI, the CUDA toolkit.

CFDR uses Emscripten, SDL2 and OpenGL ES 3. Some other libraries are used for loading 3D models/data.

If you want to use RedSim, send an email to math@sze.hu.

Testing license is free (for academic use).

2.3.2 The RedSIM software: The FOM algorithm

Algorithms and data structures

1. Solves the compressible Euler and Navier-Stokes equations with the ideal equation of states (EOS)
2. Uses finite volume method for the spatial (semi)discretization
    1. Control volumes = unstructured polyhedra
    2. Upwinding with the Vijayasundaram flux-vector splitting
    3. 2nd order scheme with averaging to vertices and linear reconstruction on faces
3. (Yet) Explicit time-stepping with the Euler and optimal TVD schemes
4. One single algorithm for 2D/3D computations
5. Input/Output data formats: industrial standards, e.g. Ensight Gold, Nastran.

2.3.2 The RedSim software: the reduced order algorithm

Algorithms

- Basic method: the POD – proper orthogonal decomposition method
  - Snapshot collection from the representative states and the SVD to define the projections
- Several variants of DEIM (discrete empirical interpolation methods) are implemented for numerical performance purposes
- For the snapshot collection the RedSim FOM multi-GPU version was applied
- For the SVD computations
  - From the Eigen library, and
  - the RedSVD randomized numerical solver, see https://github.com/cequencer/redsvd

2.3.2 The RedSIM software: Code features

Coding style

- Developed from scratch by the authors (algorithms: ZH, programming: MC)
- Written in C99-style, compiled as C++, avoids C++ features (RAII, reflections, exceptions, ...)
- Custom memory allocators, such as Linear Arena, Heaps, or Pools when appropriate; no use of new
- ”Data Oriented Approach” (cf. Mike Acton), SOA paradigm
- One single algorithm and one source file, runs easily on each platform
- Parallel:
    - CPU (OpenMPI + OpenMP)
    - Multi-GPU (with CUDA)
- One single algorithm and code for handling 2D/3D
- Integrated in-house real-time 3D visualizer
- Reconfigurable during running, due to suitable lua-scripts
- Highly optimized code for data size, data copy, and computations

2.3.2 RedSim benchmarks

Benchmark architectures

1. Solyom local cluster
   1. 1x FAT node, #CPU-cores = 80, RAM = 3TB
   2. 1x V100s NVIDIA GPU
2. Komondor HPC-machine of the EuroHPC Hungarian National Competence Center KIFÜ
   1. 1x GPU-node with 8x A100 NVIDIA

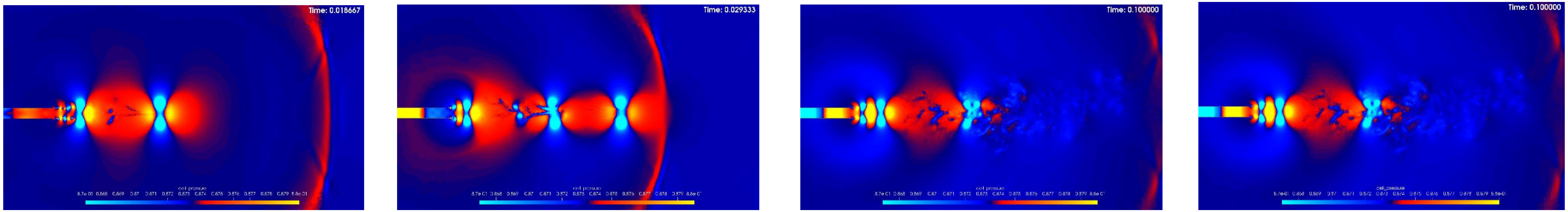
Benchmark problems

1. Exhaust pipe acoustics problem – for FOM
   1. Origin: industrial problem from automotive industry
   2. #cells = 70M, d.o.f. = 350M
   3. Simulated time (physical time): 1.0 sec
2. Urban air flow computation for the city of Gyor – for FOM and ROM
   1. Small mesh: #cells = 1.4M (d.o.f. = 7M) (spatial resolution: 5 m) (Remark: 1 state vector = 100 MB)
   2. Medium mesh: #cells = 18M (d.o.f. = 90M) (spatial resolution: 2 m) (Remark: 1 state vector = 1 GB)

2.3.2 RedSim benchmarks

Benchmark problem 1: Exhaust pipe acoustics problem

1. Runtime: 6 hours with the multi-GPU version, video: https://www.youtube.com/watch?v=rAKsChm9-b8



2. Validation to measurements

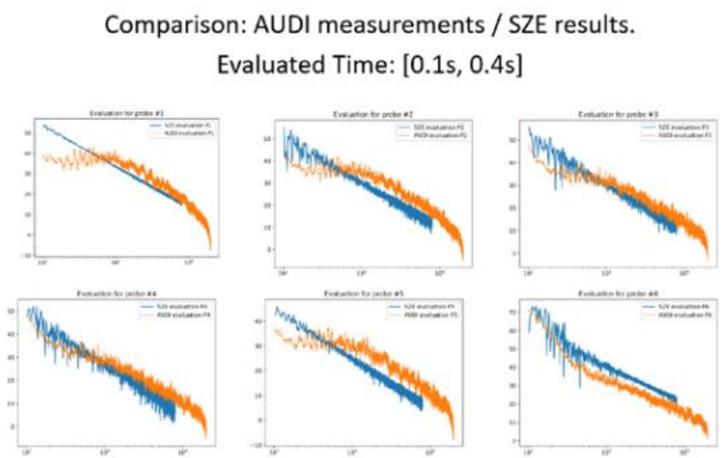
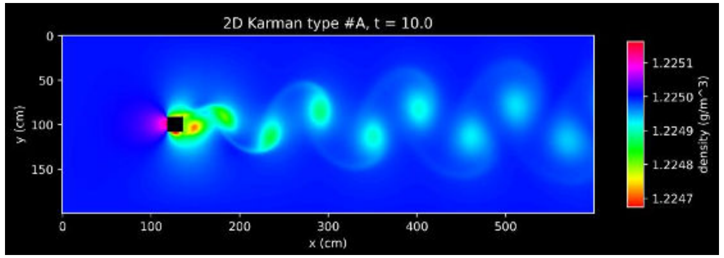


Figure 5: Comparison between the measured SPL values for the straight-pipe provided by the industrial partner (see [3]), and the simulated SPL values by SZE.

2.3.2 RedSim benchmarks

2D Karman vortex

efficiency	3 747 336 cells	33 726 456 cells	59 959 102 cells	183 623 998 cells	374 742 956 cells
1 GPU	100.0%	100.0%	100.0%	*out of VRAM*	*out of VRAM*
2 GPUs	89.3%	98.6%	98.9%	100.0%	*out of VRAM*
4 GPUs	67.5%	83.1%	84.0%	85.2%	100.0%
8 GPUs	45.6%	75.5%	79.3%	83.1%	98.5%



Urban airflow, for the city of Győr

efficiency	2 149 800 cells	10 058 445 cells
1 GPU	100.0%	100.0%
2 GPUs	87.1%	96.7%
4 GPUs	63.7%	85.1%
8 GPUs	34.2%	61.0%

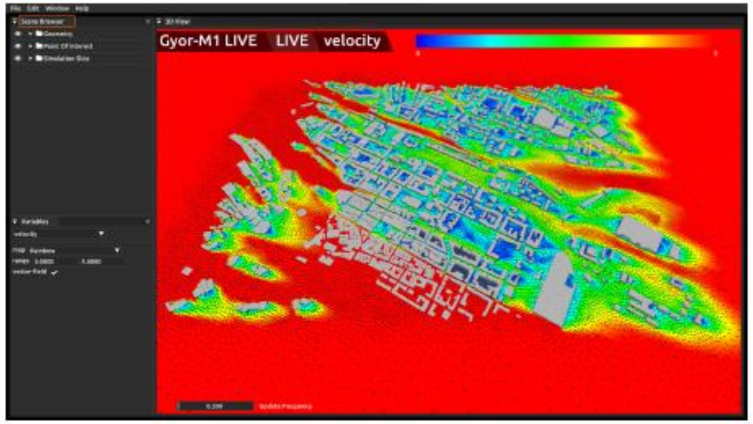
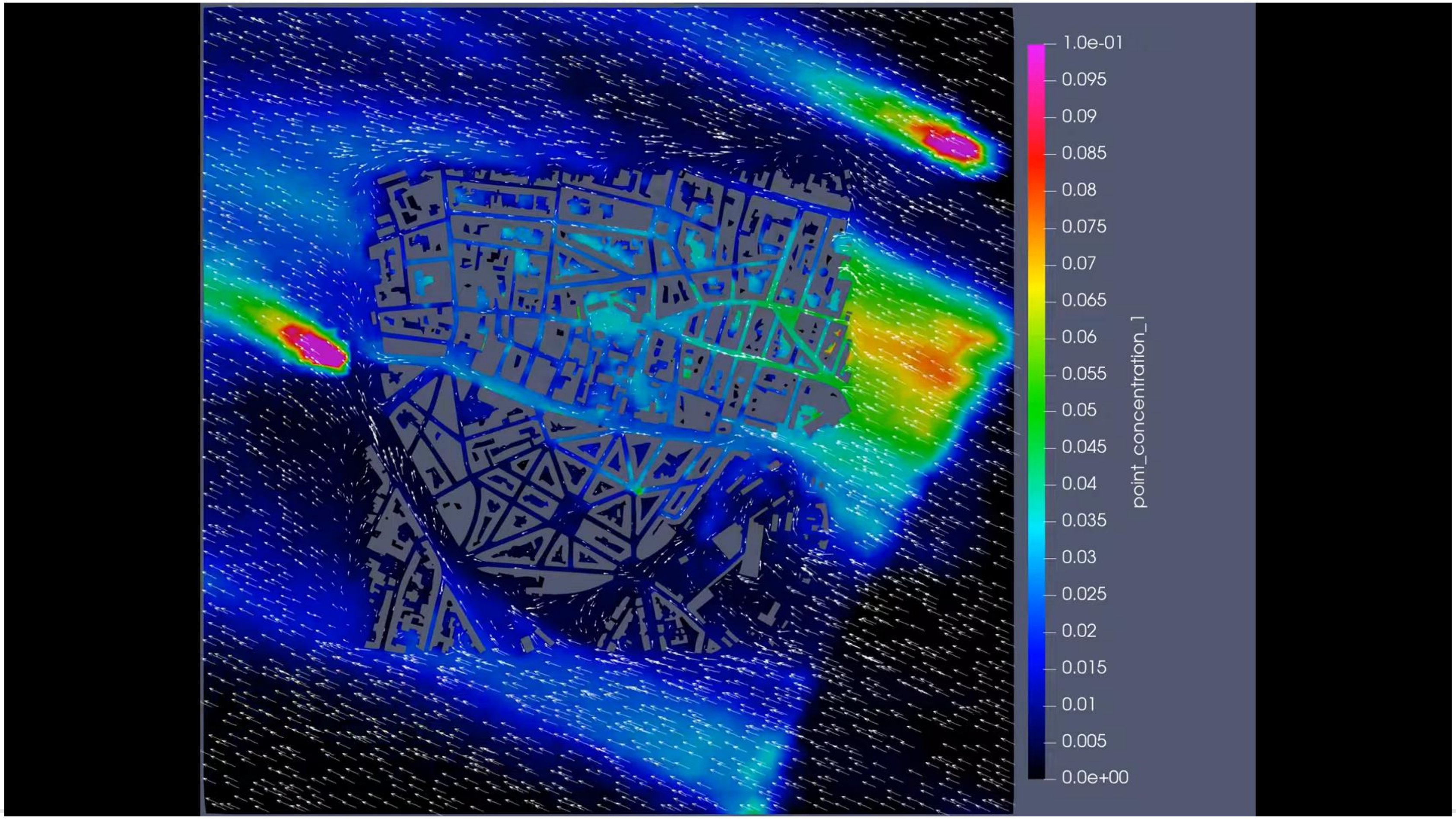


Fig. 1. Live visualization of the HPC-computations.

3. Conclusions 1

NOx concentration propagation in Antwerp for **1 full year**, within 19 days on <400 cores in the FAIRMODE intercomparison exercise.

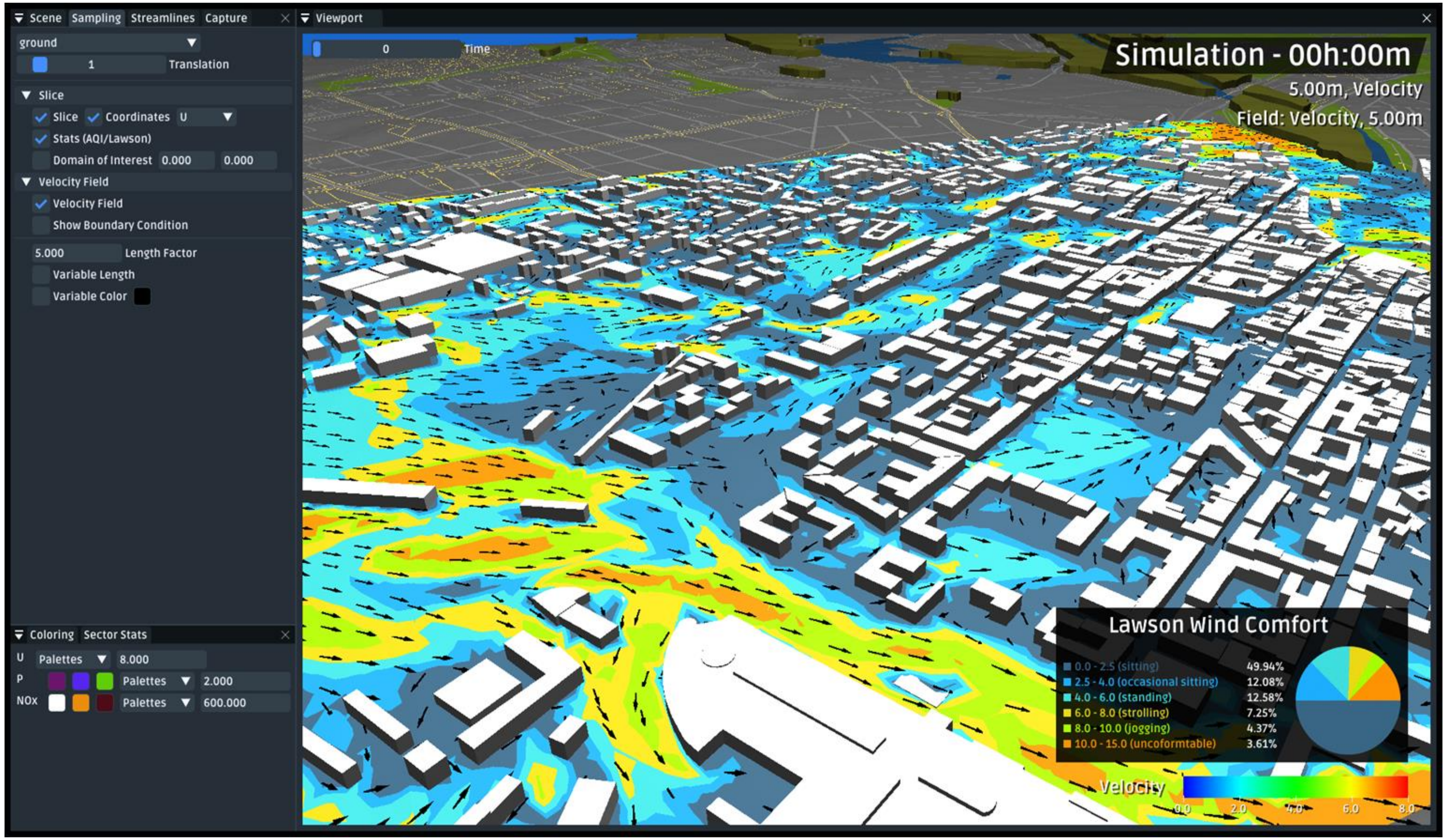


3. Conclusions 2

Real-time digital twin prototype for the airflow for the city of Győr

3. Conclusions 3

Real-time HPC + HPDA (Lawson wind comfort)



3. Conclusions 4: UAP runs from the portal

https://portal.hidalgo2.eu/

portal.hidalgo2.eu/#/experiments

Home | Applications | Data Catalogue | Configurations | Experiments | User Guide | horvathz

203	UAP 2.4 EuroHPC-FOAM-Pointsource short-2024-2-21_12_12_55	solyom.mathso.sze.hu	completed	2024-02-21 11:12:55	2024-02-21 11:41:34
202	UAP 2.4 EuroHPC-FOAM-Pointsource short-2024-2-21_11_37_58	solyom.mathso.sze.hu	completed	2024-02-21 10:37:58	2024-02-21 11:07:32
201	UAP 2.4 EuroHPC-FOAM-EMI short-2024-2-21_11_17_10	lumi.csc.fi	completed	2024-02-21 10:17:10	2024-02-21 10:47:52
200	UAP 2.4 EuroHPC-FOAM-EMI short 4n32c-2024-2-21_11_14_29	solyom.mathso.sze.hu	completed	2024-02-21 10:14:30	2024-02-21 10:44:57
190	redsim v2.0 VALIDATION-val5-2024-2-21_8_18_34	solyom.mathso.sze.hu	completed	2024-02-21 07:18:41	2024-02-21 07:25:54
189	redsim v2.0 VALIDATION-val6-2024-2-21_8_6_5	solyom.mathso.sze.hu	completed	2024-02-21 07:06:06	2024-02-21 07:09:26
186	UAP 2.4 EuroHPC-test-EC-2024-2-20_22_0_50	karolina.it4i.cz	running (on pending by hpc)	2024-02-20 21:00:52	-

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3. Further work for the next year

1. RedSim
    1. Co-design: Optimization of RedSim for special hardware (e.g. support tetrahedral mesh only) – we expect significantly (maybe 100x) faster code than the current multi-GPU code for polyhedral meshes
    2. MPI + Multi-GPU with CUDA and then with OpenCL
    3. Develop implicit time-stepping and an operational real-time digital twin for urban airflow
2. More physics
    1. A more detailed atmosphere model, coupled with WRF
    2. Couple with other HiDALGO2 use-cases
        1. Urban Building Model
        2. waLBerla for small particle propagation
        3. WildFIRES
3. Couple with the Destination Earth platform
4. Collaborations with UAP in EuroHPC: GPU-porting,
5. Services with UAP for the environmental sector and the general industry

4. Demonstrations

Demonstrations

1. UAP from the HiDALGO2 Portal with OpenFOAM, by László

2. RedSim, CFDR: for urban airflow and as a general solver, by Mátyás

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KIFÜ

Thank you for your attention

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