Training on HiDALGO urban air pollution application

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ENCCS (online), 27 April 2021

HiDALGO – EU founded project #824115

Introduction of the instructors

Zoltán Horváth:

prof. of maths and comp. sci., algorithm developer

Ákos Kovács:

PhD student in the field of network and computer science

Mátyás Constans:

programmer, data scientist

Urban Air Pollution (UAP) Training - details

1. UAP overview - 30 min, Zoltán Horváth
   1. Global challenge and the UAP application
   2. UAP workflows (simulation, digital twin)
2. Workflow automation – hands-on, 50 min, Ákos Kovács
   1. Modelling, implementation (TOSCA, yaml)
   2. Deployment, execution (Croupier / Cloudify)
   3. Data management (CKAN)

3. HPDA1: Model order reduction (MOR) with POD – 20 min, Zoltán Horváth
   1. CFD, numerical method → FOM (full order method)
   2. MOR with proper orthogonal decomposition (POD) → ROM (reduced order model)
4. HPDA1: Model order reduction with POD – hands-on, 50 min, Mátyás Constans
   1. Components: CFD solver: Fluid-Solver, Visualization: Paraview, SVD solvers
   2. FOM, ROM in action
5. HPDA2: Postprocessing – 30 min, Mátyás Constans
   1. Components: Pvpython, City-viewer (interactive visualization)
   2. HPDA for visualization and evaluation

6. UAP Demonstration on HPC and Q&A – 50 min, Zoltán Horváth, Ákos Kovács, Mátyás Constans

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6. UAP Demonstration – 50 min, Zoltán Horváth, Ákos Kovács, Mátyás Constans
   1. Demonstration on HPC
   2. Q & A

Course conditions

1. Licenses
    1. Course materials are copyrighted to SZE and provided for the participants of the ENCCS training only
        1. Fluid-Solver , City-Viewer and UAP-Preprocessor are developed from SZE TKP-IKP-project’s Digital Twins subproject.
    2. Some materials are unpublished yet →before further use, consult the SZE team coordinator
2. Moderation
    1. For questions, remarks: participants should
        1. use the HackMD file,
        2. ask immediately short questions any time, or
        3. ask longer questions in the last session.
3. Further collaboration
    1. SZE and HiDALGO is open to discuss any kind of collaboration

1. UAP Overview - 30 min, Zoltán Horváth
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Global challenge: improve urban air quality

- **3 million deaths** attributable to ambient air pollution, by WHO
  | https://www.who.int/phe/health_topics/outdoorair/databases/en/
- Traffic is emitting >40% of several contaminants (e.g. NO2)


EU planning to sue Germany over dirty air in cities: report

DPA/The Local
news@thelocal.de
@thelocalgermany

15 November 2017
10:36 CET+01:00

eu
ecj
diesel
pollution
air quality

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Photo: DPA

The European Commission (EC) is to sue Germany over the poor quality of air in its cities, the Stuttgarter Zeitung reported on Wednesday.

DPA/The Local, 15 November 2017


News > World > Europe

UK could face court action over air pollution after EU warning: 'We can delay no more'

Proposals made on Tuesday are 'not substantial enough to change the big picture'

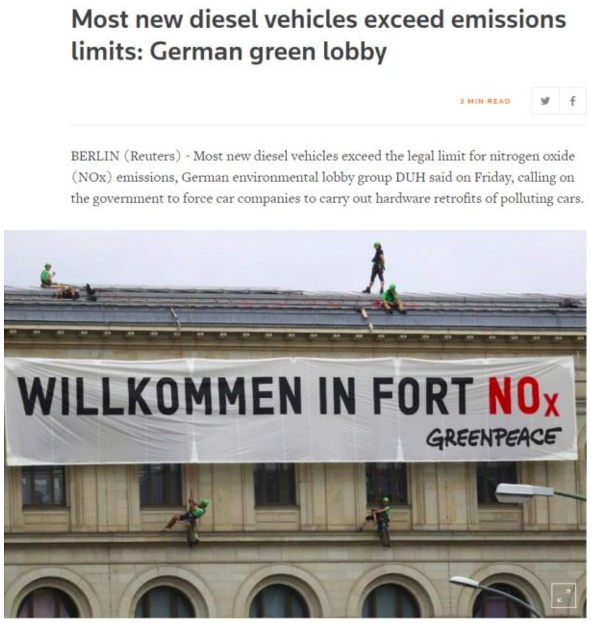
Judith Vonberg | Tuesday 30 January 2018 19:04 | 3 comments |
0 shares

Poor air quality in countries across Europe is believed to cause around 400,000 premature deaths every year (Reuters/Ognen Teofilovski)

Nine European countries including the UK could face legal action if they fail to make progress on reducing air pollution, the EU's top environment official has warned.

The intervention came as legal air pollution limits for the whole year were

Independent, 30 January 2018

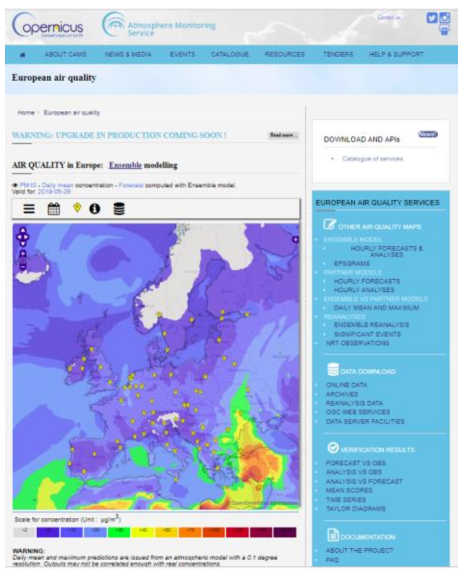

Most new diesel vehicles exceed emissions limits: German green lobby

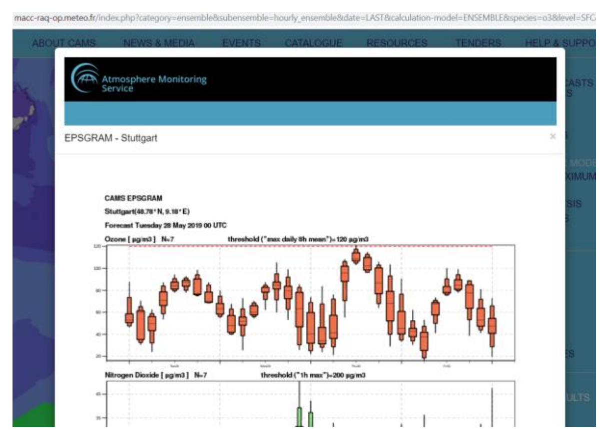
BERLIN (Reuters) - Most new diesel vehicles exceed the legal limit for nitrogen oxide (NOx) emissions, German environmental lobby group DUH said on Friday, calling on the government to force car companies to carry out hardware retrofits of polluting cars.

Reuters, 14 September 2018

Global challenge: improve urban air quality

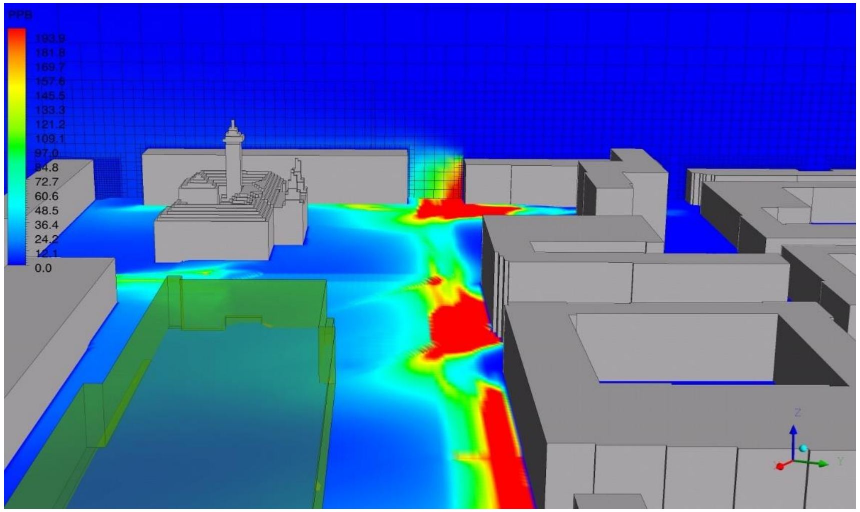
- EC regulates air quality management and allows the use of **computational models** for reporting (see Directive 2008/50/EC).
- EC provides forecasts for air quality from Copernicus AMS:
  - European AQ – Ensemble hourly forecasts and analyses
  - AQI for every 3 hours, for several cities**, now: one value for the whole town**





Global challenge: improve urban air quality

- Example: Győr, Hungary. NO_2 simulation with 3D geometry
  - Hot spots (above limit areas) occur locally while overall values are OK
  - → One pollution concentration cannot be valid for the whole city
  - → High resolution validated simulation is needed



→ **need of CFD & HPC** (for 10km x 10km x 1 km domain, 1m resolution at street level, aimed simulation time: 1 year: #variables: 10^9-10^{10} in each time step, #steps:10^6, #operations: 10^{11}-10^{12} in each step)

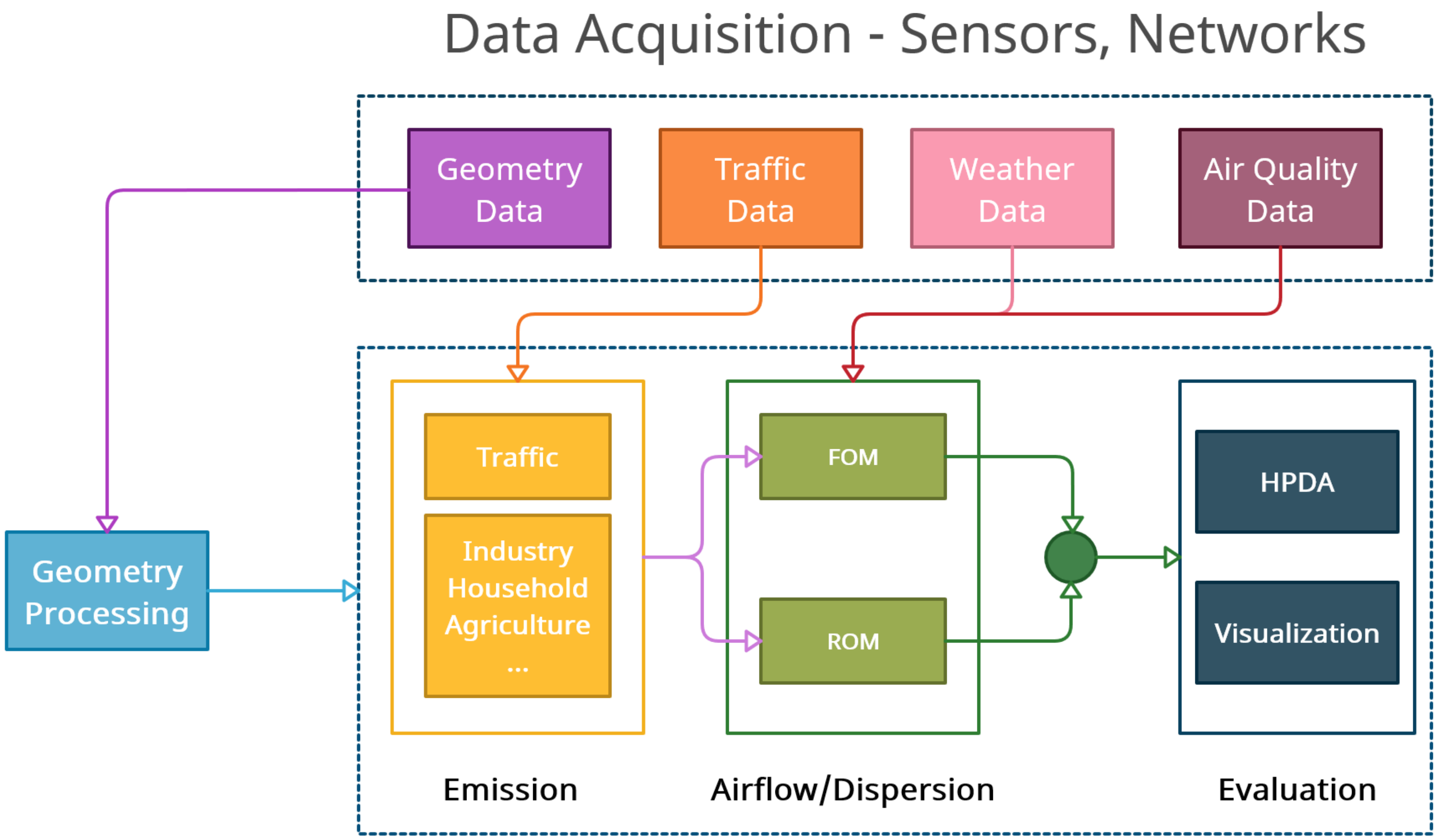
SZE urban air pollution simulation and control

Vision:

provide microscale simulation of air pollution in cities
and traffic control based on microscale simulation
in very high resolution (1m at street level)
by coupling
weather and climate macroscale forecasts/reanalysis data and
traffic sensor streaming data with
simulations on
supercomputers and on
edge online / (faster than) real time simulations,
configured, preprocessed, run, evaluated easily on web
in production mode!

Implementation (TRL 6/7 product), example for Graz, Austria

HiDALGO workflow for urban air pollution modelling



HiDALGO workflow for urban air pollution modelling – relation to other workflows

- SZE UAP workflow, a physical model based digital twin, might be considered as a realization of the „typical mixed simulation and machine learning workflow" of SRA4 of ETP4HPC, see p. 18.
- https://www.etp4hpc.eu/pujades/files/ETP4HPC_SRA4_2020_web.pdf
- SZE UAP is a use case for the Transcontinuum Initiative

THE NEW PARADIGM: HPC IN THE DIGITAL CONTINUUM

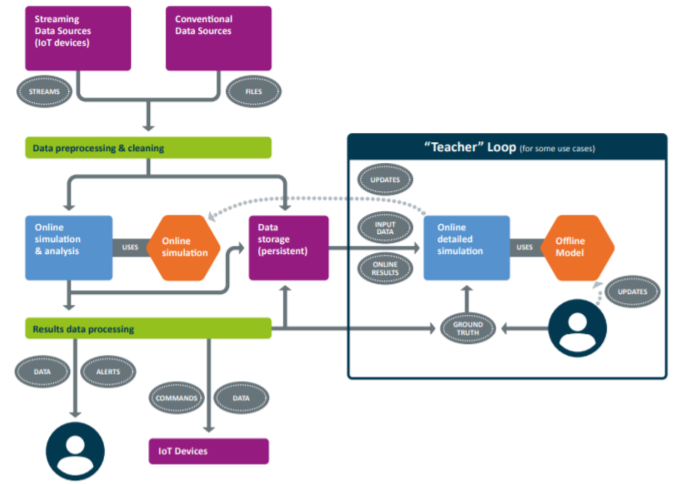


Figure 5: A typical mixed simulation and machine learning workflow

HiDALGO workflow for urban air pollution modelling

Modules:

0: Preprocessing

1-5: Data acquisition and coupling

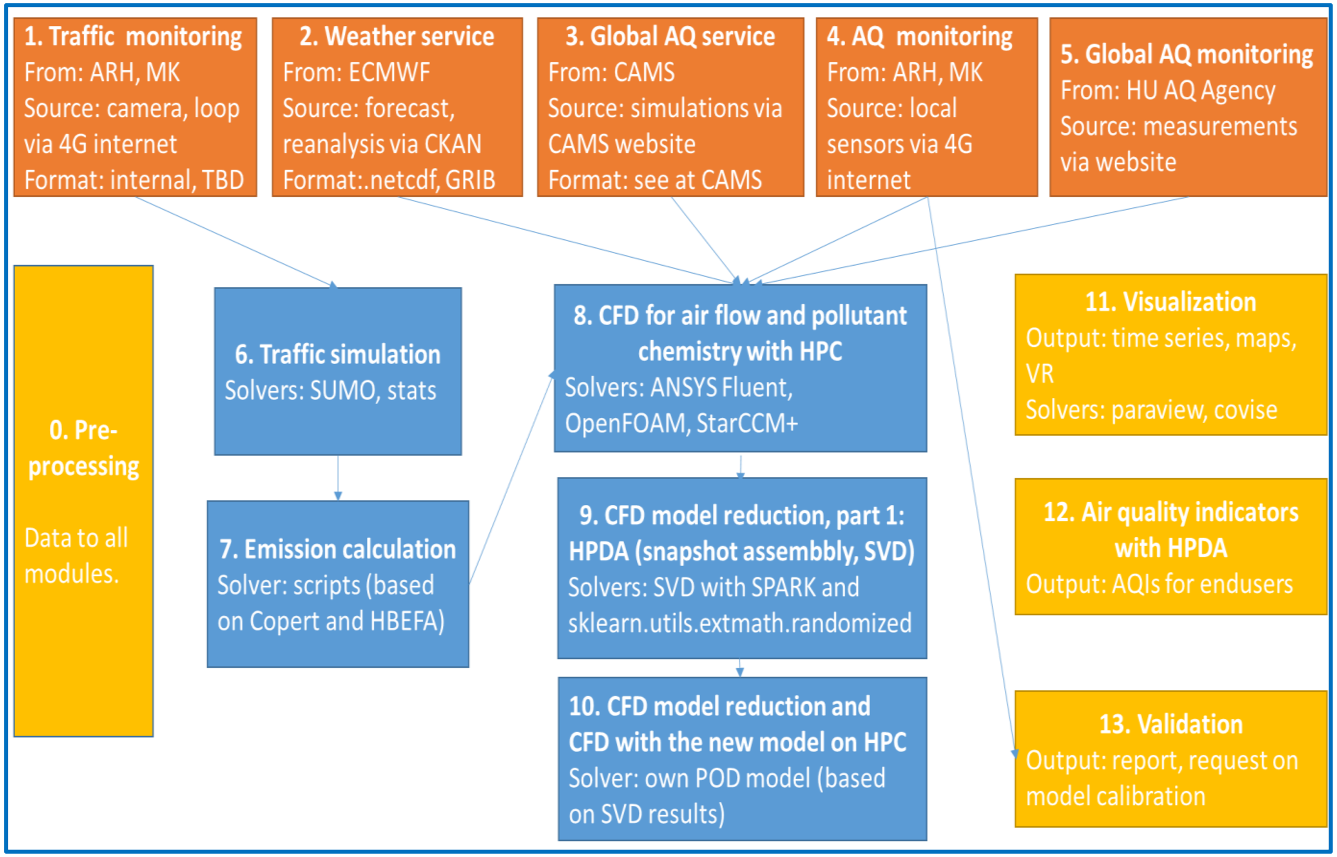
6-7: Traffic simulation and emission computation

8: Air flow simulation

9-10: Model reduction

11: Visualization

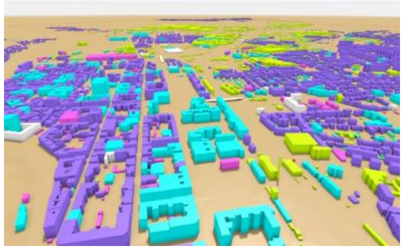
12-13: Postproc., validation

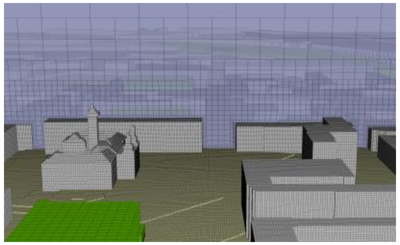


Each module has a standardized input-output format.
To apply a solver in a module, interfaces have to be written and applied.

0. Preprocessing – main steps

Creation of the 3D geometry of the air flow domain creation from OpenStreetMap	Mesh generation to the air flow domain	Traffic network generation (compatible to the air flow mesh)	Set up interfaces for data coupling, set up parameters

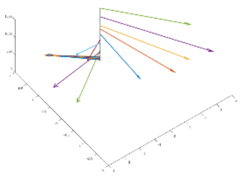




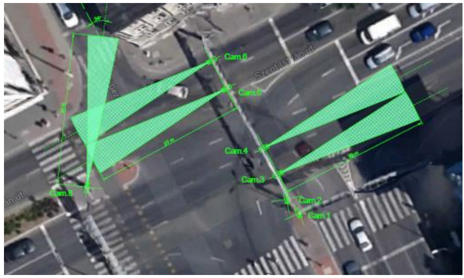
Preprocessing for Milwaukee, WI (here), or Graz here.

1-5. Data coupling

- Wind data
  1. ECMWF data: now from data files. Rest API is under developme
  2. User genarated data (meteorologically correct)



- Traffic data:
  - Implementation of the sensor network is ongoing by Adaptive Recognition Hungary (ARH) and Hungarian Public Road Ltd (MK)
  - Plate number recognition and loop detector data



- Global AQ data from the Copernicus Atmosphere Monitoring Service
- Local AQ monitoring network is under development

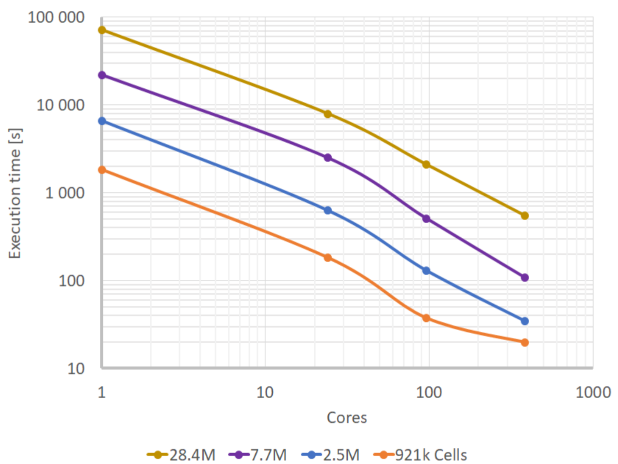
HiDALGO workflow for urban air pollution modelling

6-7. Traffic simulation and emission computation

- Solvers for the traffic simulation: SUMO (main), PTV's VISUM
- Emission is computed by applying standard models (Copert, HBEFA)

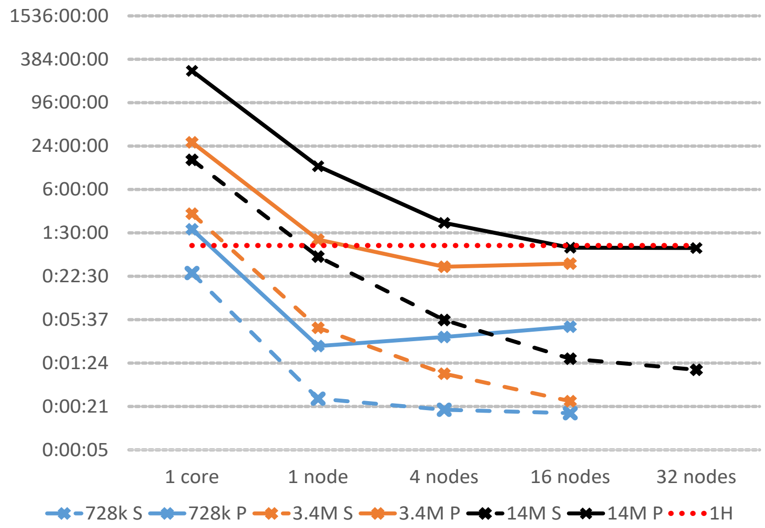
8. Air flow simulation with CFD

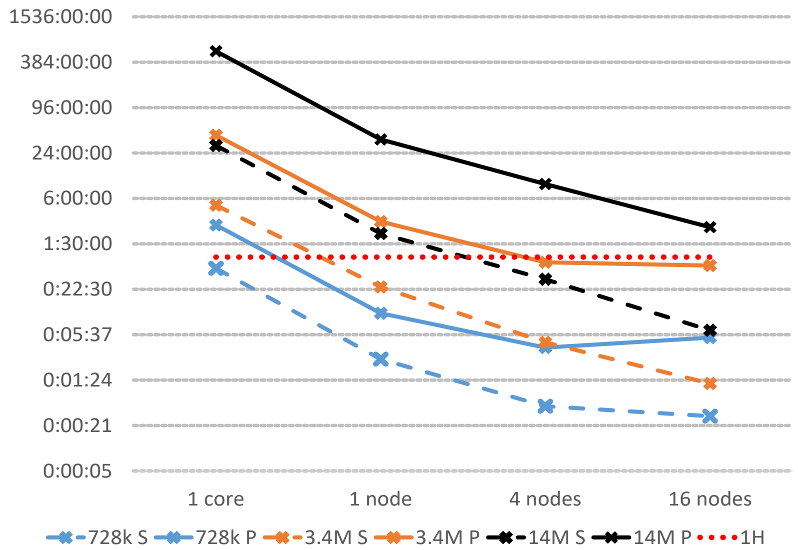
- Solvers: ANSYS Fluent, OpenFOAM, Fluid-Solver (ongoing)
- Physics: transient Navier-Stokes with turbulence modelling, pollutants: passive scalars; transient boundary conditions
- Scalability of OpenFOAM: see the graphs



- Simulations to Graz: here.

Scalability of the UAP air flow + dispersion simulation





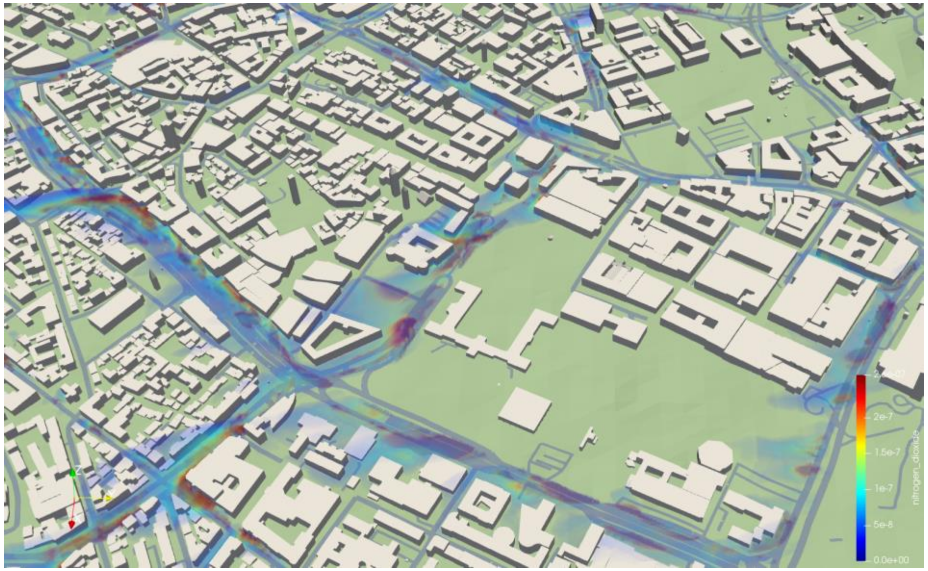
- Hawk, HLRS (left, 1 node = 2x128 cores) and Eagle, PSNC (right, 1 node = 2x14 cores)
- Runtime scaled to 1 hour simulated time.

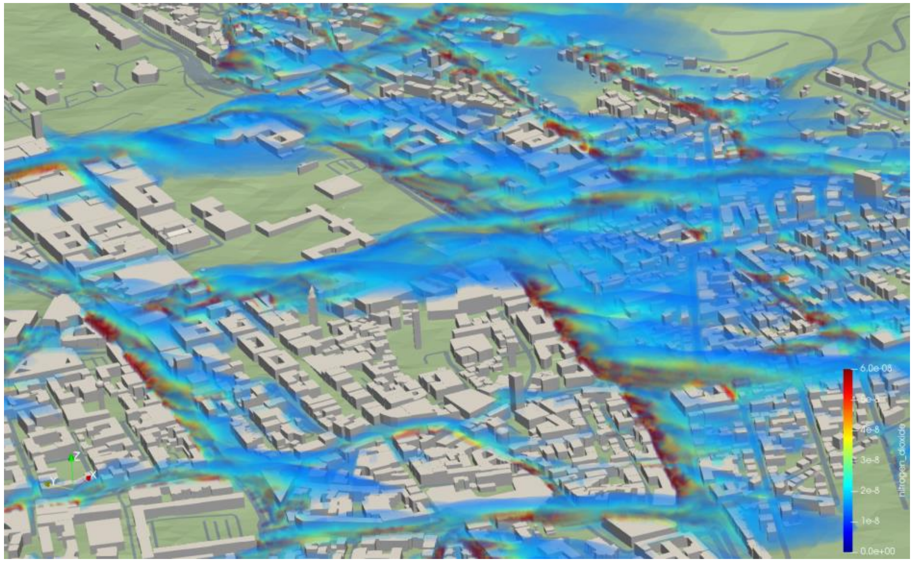
Környei, Horváth, Ruopp, Liszkai, Kovács; HPC Asia 2021 Companion, online, January 20–22, 2021.

Application to Stuttgart (test of the HiDALGO urban air pollution pilot)

- All preprocessing steps took 5 person days
- 3D geometry is generated from Open Street Map
- Meshing is done via in-house octree-mesher
- Traffic is simulated with SUMO based on synthetic data
- Weather data are from ECMWF forecast to 2019-05-25
  - Northern wind of 2 m/s, in most of the day

HiDALGO workflow for urban air pollution modelling

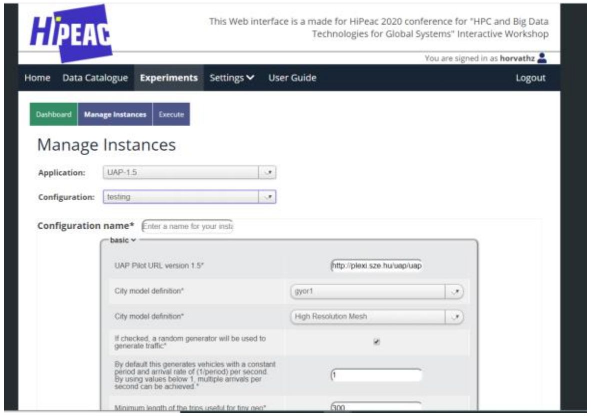


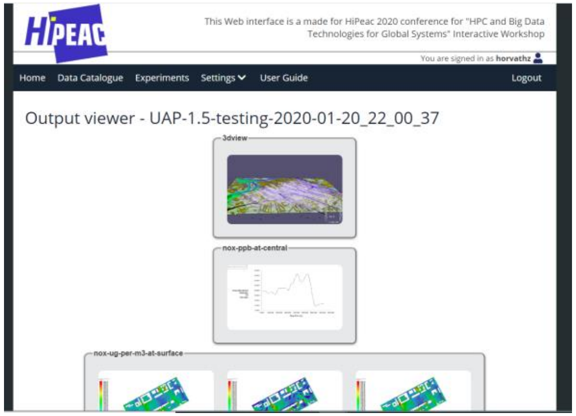


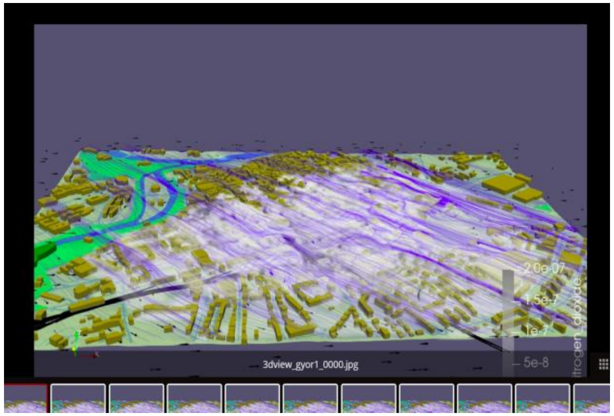
Hot spots (red areas) occur while the overall NOx values are OK (blue or not colored areas). To see this we need high resolution simulation with HPC.

Automated execution for easy access

- Usability: run the simulation on HPC from simple, webinterface → HPC is reachable for policy makers easily!
  - https://webint.hidalgo-project.eu/
- Demonstration from the HiDALGO webinterface!





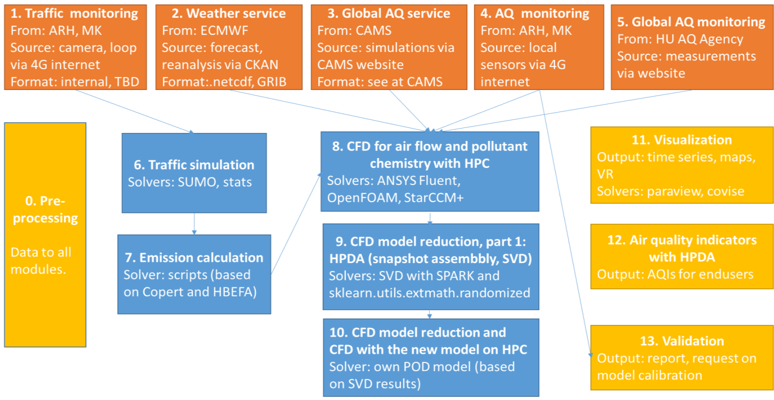


Automated execution for easy access

Methodology

1. **Workflow modelling**
   Mapped in TOSCA - Topology and Orchestration Specification for Cloud Applications → TOSCA blueprint in a yaml file
2. **Execution**
   with Cloudify using a HPC-plugin (Croupier)
3. **Web interface**
   dynamic portal in Python Django

→ Next session of the training



THANK YOU !

QUESTIONS ?

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3. HPDA1: Model order reduction (MOR) with POD

3. HPDA1: Model order reduction (MOR) with POD – 20 min, Zoltán Horváth

1. CFD, numerical method → FOM (full order method)
2. MOR with proper orthogonal decomposition (POD) → ROM (reduced order model)

Literature

1. CFD, numerical method → FOM (full order method)
   - Plenty of books and papers, e.g.
     - M. Feistauer, J. Felcman, I. Straskraba: Mathematical and Computational Methods for Compressible Flow. Oxford University Press (2003). ISBN 0-19-850588-4/hbk
     - A. Horváth, Z. Horváth: Application of CFD numerical simulation for intake port shape design engine. J. Comput. Appl. Mech. 4 (No 2), pp. 129-146 (2003). Link.
2. MOR with proper orthogonal decomposition (POD) → ROM (reduced order model)
   - Number of papers, e.g.
     - S. Chaturantabut, D. Sorensen: Nonlinear Model Reduction via Discrete Empirical Interpolation. SIAM J. Sci. Comput., 32(5), 2737–2764. https://doi.org/10.1137/090766498

3. HPDA1: Model order reduction (MOR) with POD: The full order method (FOM)

Physical problem:

- compute the variables (density, velocity, energy, pressure) of the fluid in a flow domain under given boundary conditions (inlet, outlet, wall) and initital data

Assumption during the HPDA1 part of the training:

- We consider the air flow computation only (and do not consider e.g. thermal effects (radiation), traffic modelling, emissions, and dispersion of the pollutants)

Complexity:

- Large domain, typically 5km x 5km x 1km
- Reynolds number: around 10^9 → turbulent flow

3. HPDA1: Model order reduction (MOR) with POD: The full order method (FOM)

Mathematical model: the compressible Navier-Stokes equations

- Physical laws: Conservation of mass, momentum, energy of the fluid →
  - 5 (scalar) time dependent partial differential equations for the variables
  - 1 algebraic equation of states (EOS): p = (gamma-1) (e – 0.5 rho*v^2)

Complexity:

- Exact ”analytical” solution of the equations is impossible → we need approximation of the variables
- Physical and computational requirements: density, energy, pressure > 0

  (Note: speed of sound c = sqrt(gamma * pressure / density) appears in the algorithm explicitely → NaN in the code if density / pressure < 0.)

3. HPDA1: Model order reduction (MOR) with POD: The full order method (FOM)

Numerical method to get approximations of the variables

1. Divide the fluid flow domain into small pieces (cells) (mesh size: 1-10 m at streets)
2. Divide the considered time interval into subsequent small time intervals adaptively, driven by stability and accuracy requirements
3. Approximate the flow variables by constants (or linear functions) on each cell during each time interval, according to the NS equations, as follows:
    1. Initialize the cell-variables from the given initial conditions
    2. In each time interval, one after the other (”in subsequent time steps”)
        1. compute the fluxes between cells and then the cell values

Complexity

1. Data: #cells = 1-10-100 * 10^6, N = #unknowns per time step = 5 * #cells
2. Computations:
    1. Explicit methods: c1 * N flops (c1 is a large constant) per time step, # time steps is large (10^6), easy parallelization
    2. Implicit methods: larger number of flops per time step, # time steps is moderate (10^3), difficult parallelization

3. HPDA1: Model order reduction (MOR) with POD: The reduced order method (ROM)

FOM (full simulation model):

x = state vector of t (time), components are cell variables, x is in R^N

f = sum of fluxes through cell faces

$$x'(t) = f(x(t))$$

$$x(0) = x_0$$

Time stepping with the Explicit Euler method:

$$x_{n+1} = x_n + \tau_n * f(x_n), \quad n = 0,1,\ldots, M-1$$

3. HPDA1: Model order reduction (MOR) with POD: The reduced order method (ROM)

ROM (reduced simulation model):

1. Approximate, under a threshold for the approximation, the span of x_i s from several offline FOM running (”training”, exploration of typical simulation results)

   $< x_0, x_1, \ldots, x_M, x_0, x_1, \ldots, x_M, \ldots > \approx < u_1, \ldots, u_r >$

   where the u-vectors form an orthonormal system in R^N

2. Approximate the exact solution of the FOM, x, in the lower dimensional space

   $x = x(t) \approx U_r * alpha = sum(\, alpha_i(t) * u_i, i=1..r)$

   where $U_r = [u_1, \ldots, u_r]$, $alpha = [alpha_1; \ldots; alpha_r]$

3. Substitute it to the FOM and equate the two sides:

   $U_r * alpha(t)' = f(\, U_r * alpha(t)\,)$, i.e.

   $alpha(t)' = U_r^T * f(\, U_r * alpha(t)\,)$

4. Solve it for alpha via the Explicit Euler method:

   $alpha_{n+1} = alpha_n + tau_n * U_r^T * f(\, U_r * alpha_n\,)$

5. Project $alpha_n$ back to x values:

   $x_n = U_r * alpha_n$

3. HPDA1: Model order reduction (MOR) with POD: The reduced order method (ROM)

ROM (reduced simulation model):

x = x(t) ≈ U_r * alpha

alpha(t)’ = U_r^T * f(U_r * alpha(t))

alpha_{n+1} = alpha_n + tau_n * U_r^T * f(U_r * alpha_n)

x_n = U_r *alpha_n

Optimal U_r selection from the SVD (singular value decomposition) of

X = [x_0, x_1, …, x_M , x_0, x_1, …, x_M, …] : snapshot matrix

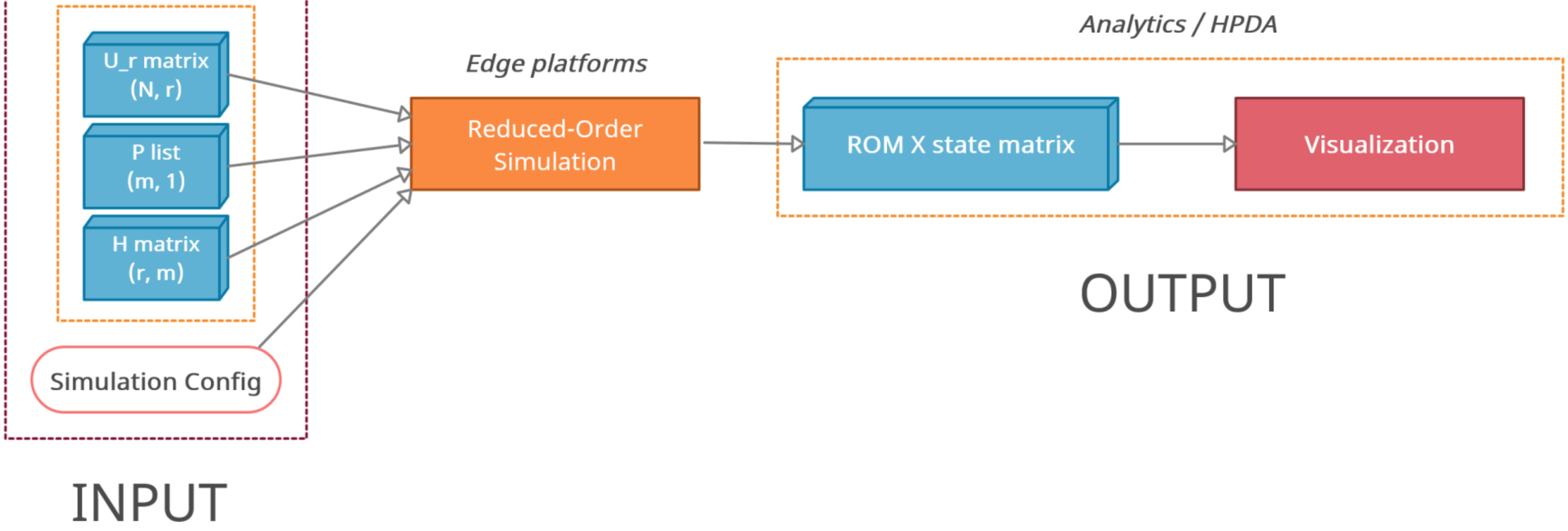
X = U * S * V^T ,

U = [u_1, …], U, V orthonormal, S = diag(s_1,…, s_R), s_1 ≥ s_2 ≥ …

Error of POD: proportional to

sum (s_i, i=r+1, R)

3. HPDA1: Model order reduction (MOR) with POD: The reduced order method (ROM) – online phase



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