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## *New Trends and Challenges for Air Quality Control*

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# On a Multilevel Parametric CFD Model for Urban Air Pollution Modelling


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# Overview of models for urban air quality

- Main components:
  - Geometry (street, buildings, plants, …)
  - Emission (traffic + vehicle emission, …)
  - Weather
  - Dispersion
  - Reaction, deposition
  - …
- Type of models
  - ”Parametric”: components from a given set of simplified, preprocessed physical submodels
  - ”Direct physical”: solves the (almost whole) physical model approximately

# Overview of models for urban air quality

- There exist plenty of urban AQ models…

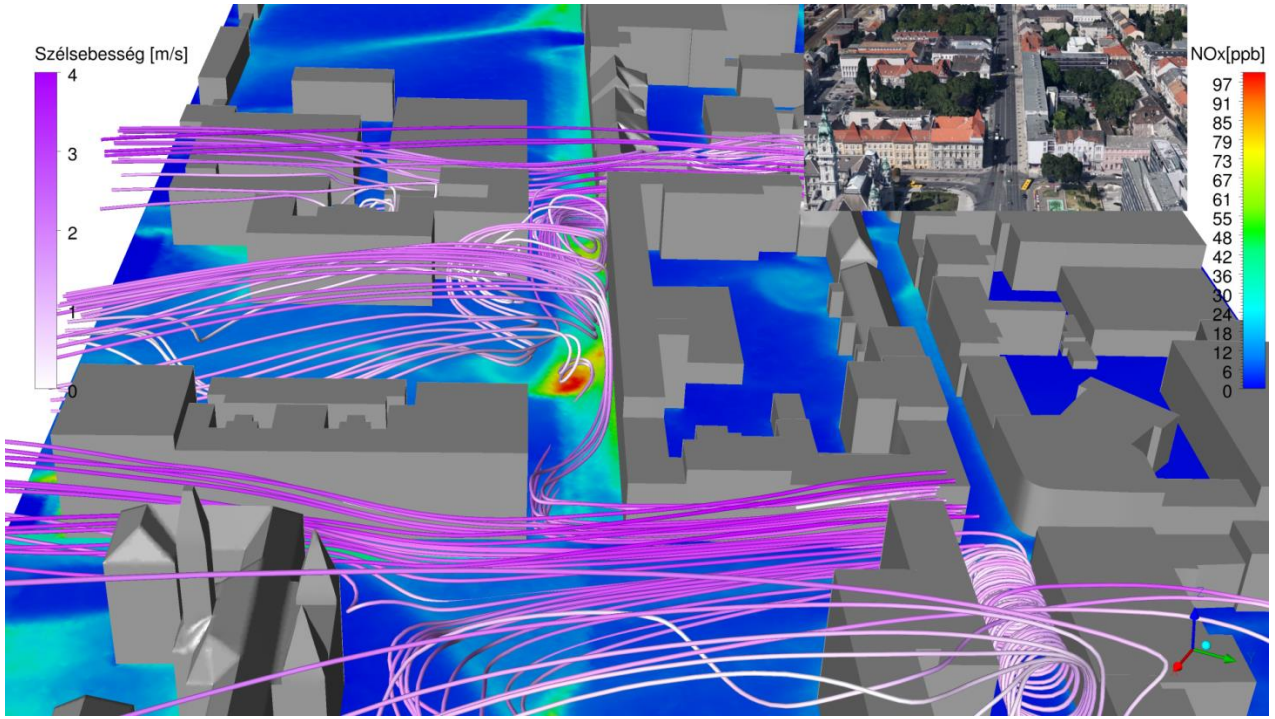
| | Parametric | Direct physical |
|---|---|---|
| **comp. time** | short | long |
| **accuracy** | high/moderate/low | high |
| **usage** | easy | difficult |
| **cost (SW/HW)** | cheap | expensive/cheap |
| **flexibility** | no | yes |
| **support policy** | yes | rarely |
| **applicable for real time control** | yes | no |

- **Our motivation: develop a direct physical model with many good properties of the parametric models**

# Overview of models for urban air quality

- Do we need direct physical models?

  Example: simulation and measurements $NO_x$ in Győr

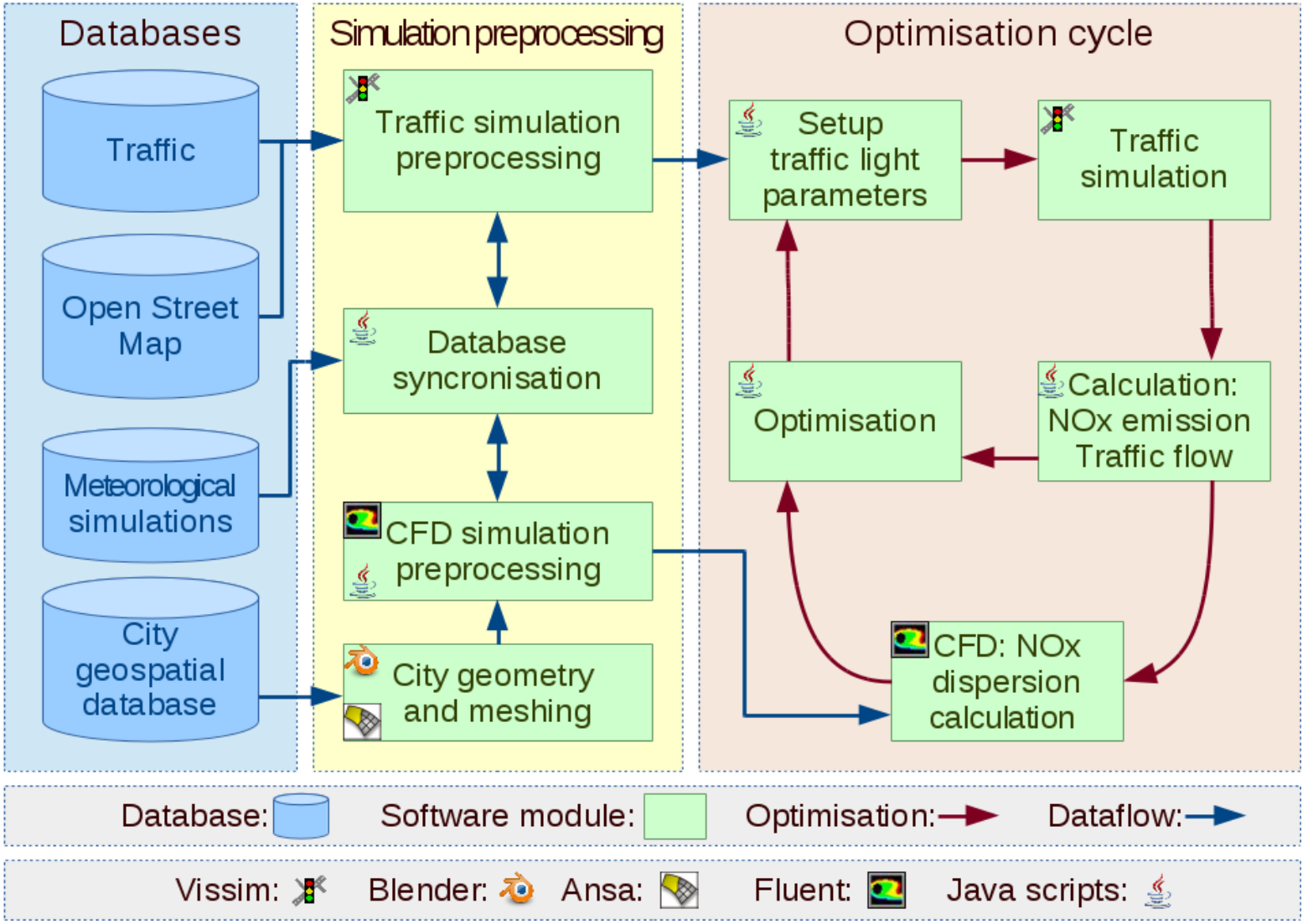



Prediction with parametric models:

Globally? OK
Locally and in short term? difficulties

➔ **Multilevel models with switches governed by measurements**

# 2.1. 3DAirQC - Framework of the control scheme



# Overview of models for urban air quality

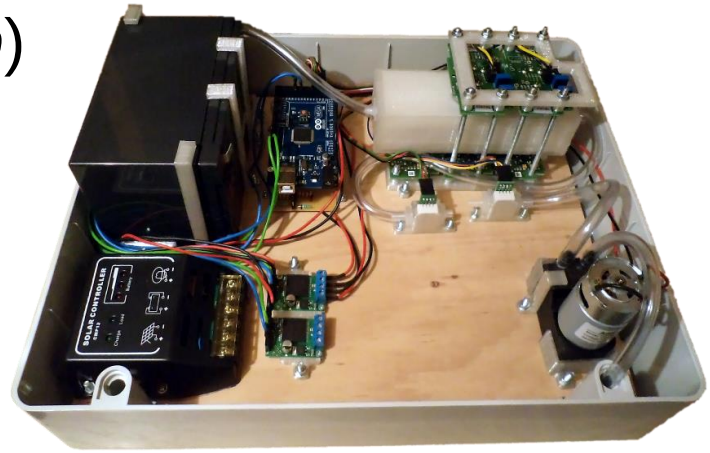
- Direct physical multilevel model in 3DAirQC: Multilevel model with switches governed by measurements

**Sketch**:

1. Initialize a simple model
2. Perform the actual model
3. Measure and validate
4. Good fit? Go to 2. else
    5. Go back in simulation time
    6. Refine actual model and go to 2

# Emission module: measurements

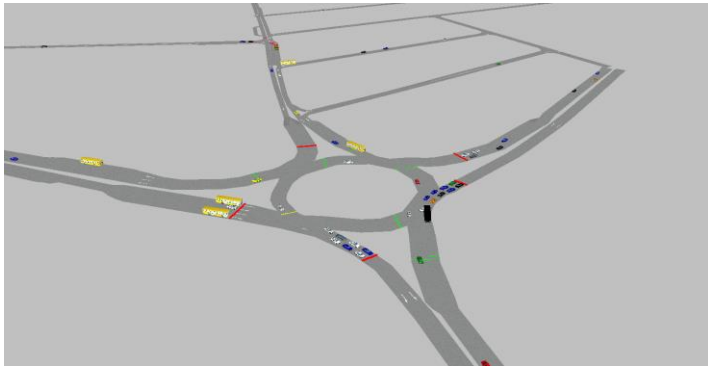
- **Air quality sensor modules** - under development:
  - Electrochemical sensors for NO, $NO_2$, $O_3$, CO, $SO_2$ (from *Membrapor AG*)
  - Optical sensor: $PM_{10}$, $PM_{2.5}$ (from *Sharp*)



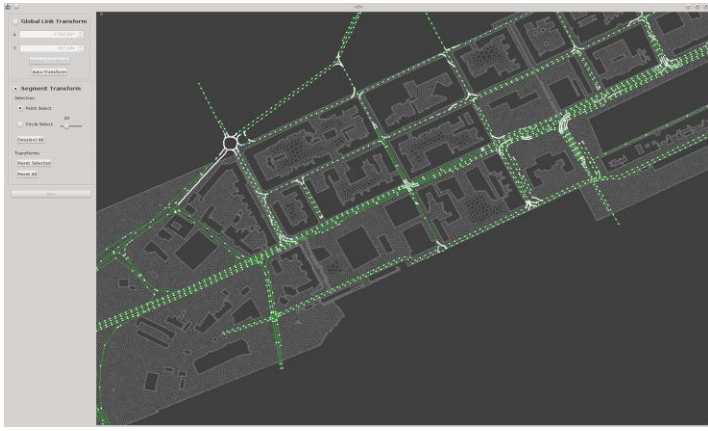
- **Automatic monitoring network**
  - Hungarian Air Quality Network
  - Two AQ containers in Győr
  - $SO_2$, NO, $NO_2$, CO, $O_3$; $PM_{10}$, $PM_{2.5}$

# Emission module: traffic simulation

- Microscopic traffic simulation with PTV Vissim
- Modelling:
  - Traffic input and flow
  - Signal control (fixed-time)
  - Measurements



- Compatibility between CFD mesh and traffic simulation segments
  - Developed software in Java
  - Transform traffic network to CFD mesh:
    - Global transformation
    - Segment transformation

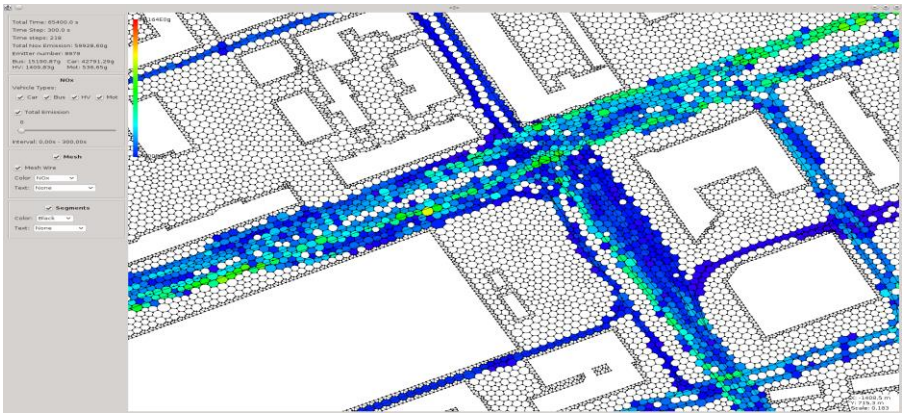


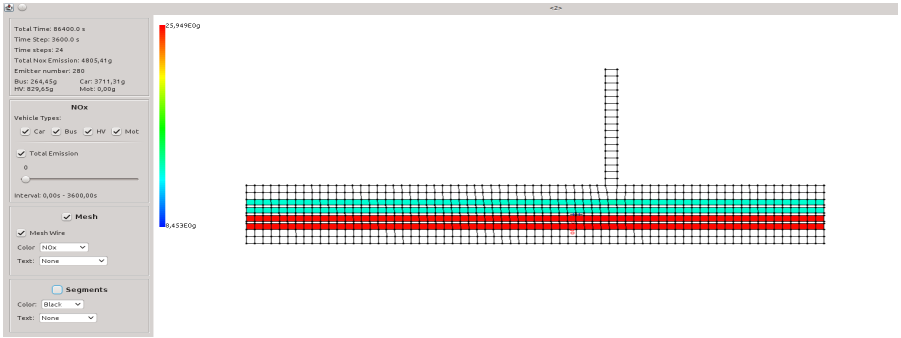
# Emission module: emission models

- Emission model
  - Copert 4 implemented in Java based on real fleet data
  - Emission source location
    - Based on traffic model and CFD mesh, calculated with own java program

    or

    - Parametric
      Lanes defined by some measures (distances) and emitted values by given (statistical) data or by model





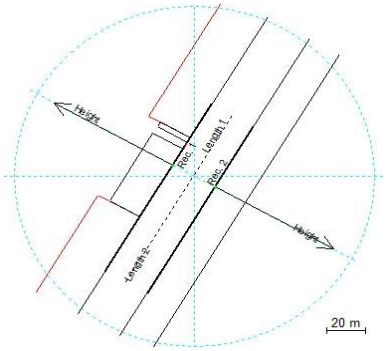
# Dispersion module

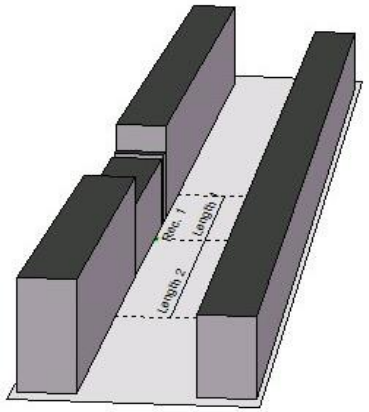
- CFD features are set up automatically with integrated scripts and configuration files

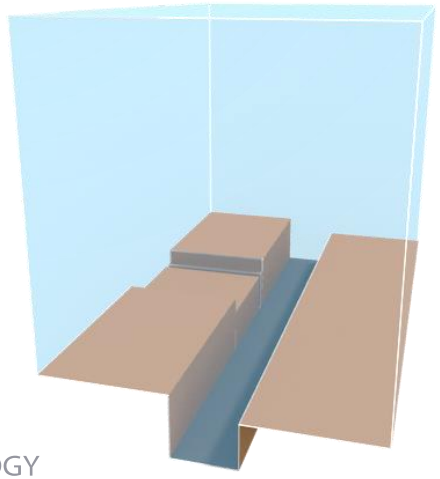
- CFD model components:
  - 3D RANS k-ε turbulence model
  - Air mixture of 8 gaseous materials
  - Humidity usage
  - Parks and groves as porous zones
  - Meteorological wind data as inlet boundary condition
  - Initialized with wind and temperature profiles
  - Polyhedral and hex core meshes, with/without boundary layer resolutions
  - Mesh and geometry independent model building, connection by zone name matches

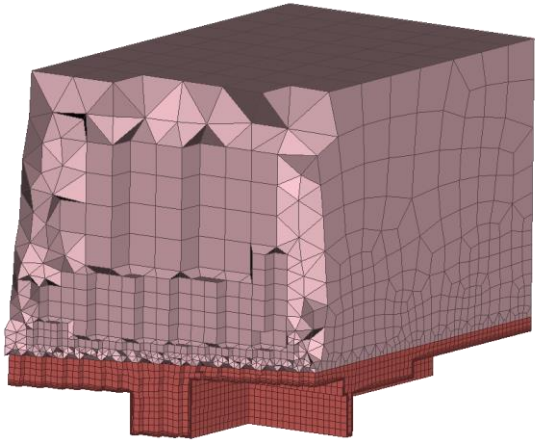
# Application: simple geometry

- Validation against OSPM on Jagtvej street example
- Model geometry, weather, traffic, emission based on OSPM database
  - Geometry:
    - OSPM street configuration converted to CAD geometry by script using some additional parameters (for the 3D model size)
  - CFD compatible mesh generated from CAD geometry
    - Element number: 90,000 (tetra+hexa+penta+pyramid)



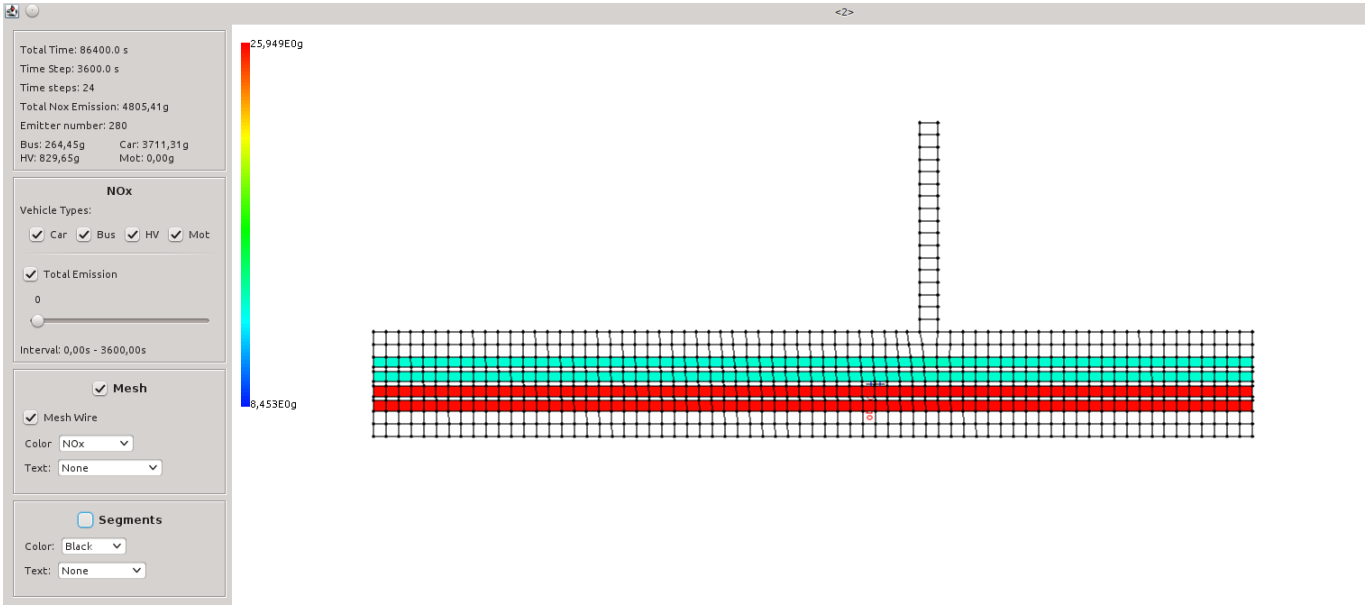


# Application: simple geometry

Two scenarios for $NO_x$ emission

1. Calculated as in OSPM
2. Traffic sources exported from OSPM, simulated with Vissim, emission calculated with Copert 4 model

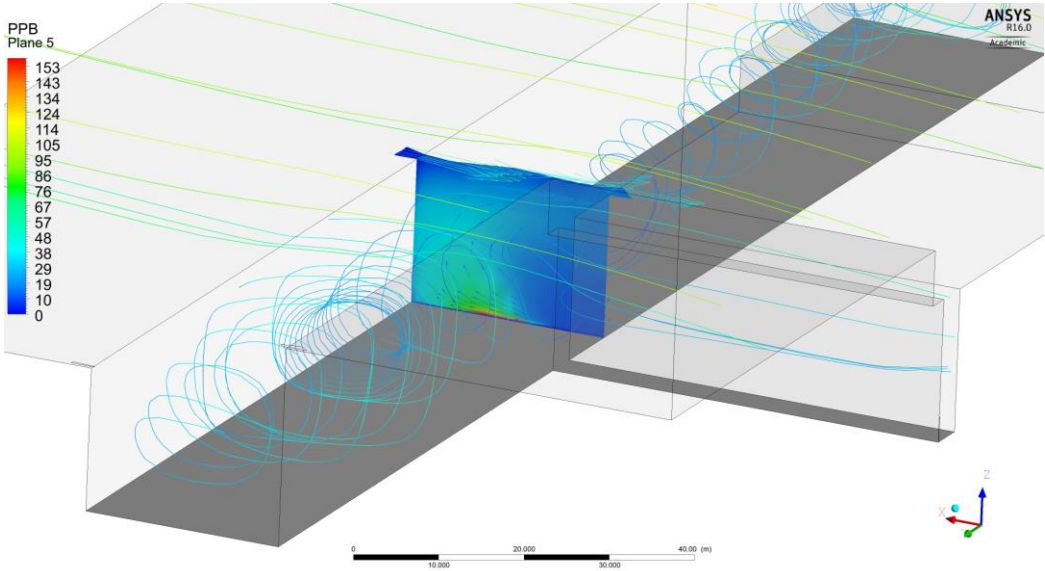
Emission locations calculated automatically, based on road lanes

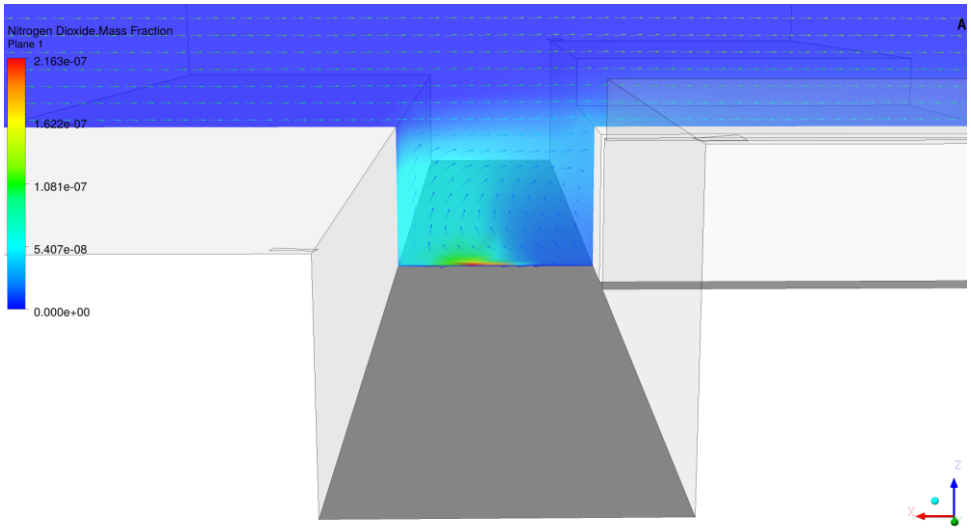


# Application: simple geometry

## CFD simulation results

- 24 h transient calculation
- SW: Ansys Fluent
- CPU: intel i7@3.2GHz 4 core
  (modern laptop)
- Simulation time: 30 min on 4 cores



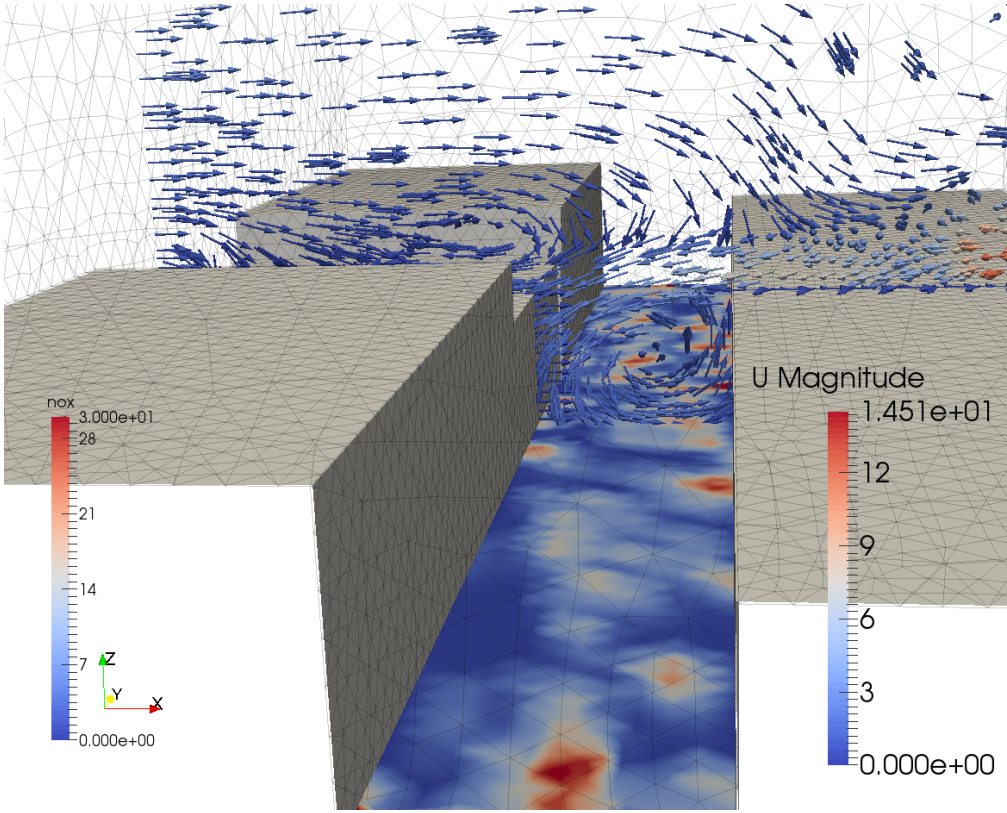



# Application: simple geometry

CFD simulation results

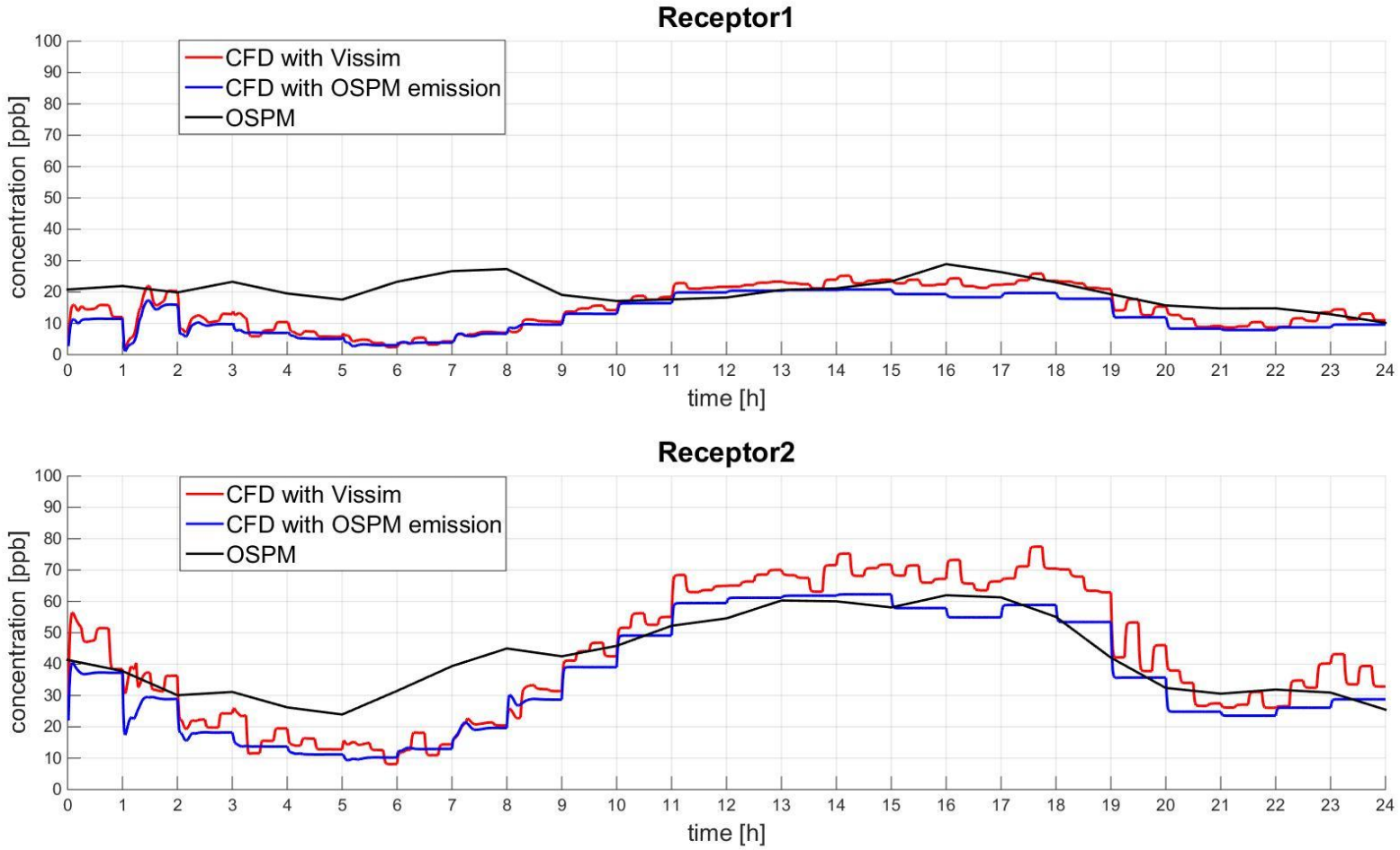
- steady state windfield and 15 min transient dispersion calculation
- SW: OpenFOAM
- HW: 8x8 core@2.27GHz Intel i7 SMP
- Physics: RANS for windfield + linear diffusion-advection for NOx dispersion

- **Simulation time:**
  **45 sec for windfield on 32 cores,**
  **15 sec for dispersion on 1 core**



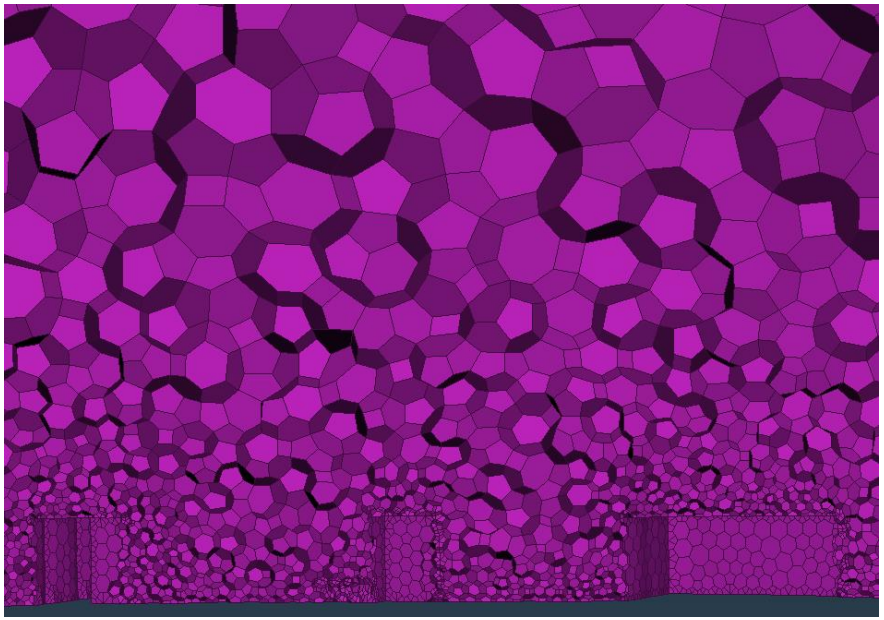
# Application: simple geometry

Simulation results compared with OSPM calculated values



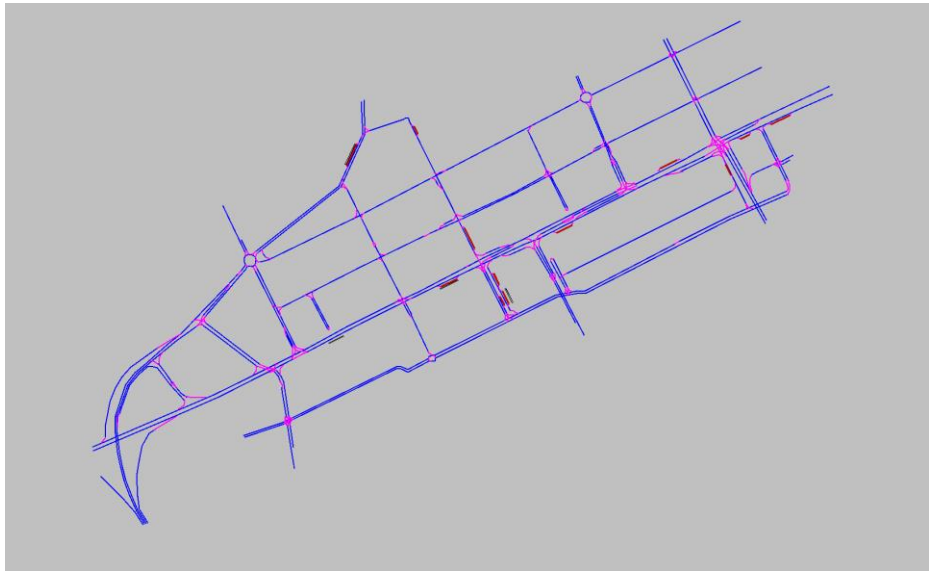
# Application: complex geometry

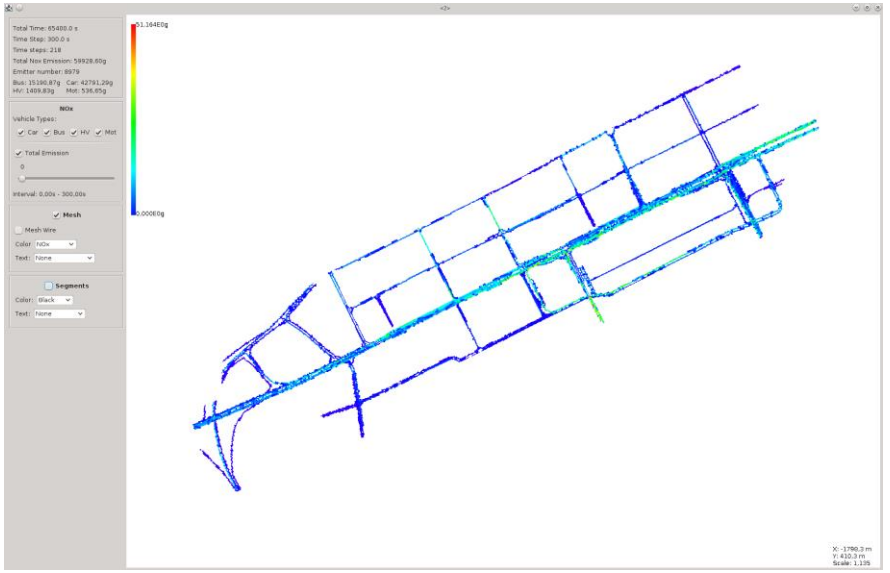
- Full 3D geometry of the city was generated from a geospatial database, with python script
- Part of the geometry (city center) was prepared for full CFD simulation, the rest is simplified strongly
  - Layered mesh with 3.300.000 polyhedral elements
  - Mesh without layer 1.260.000 polyhedral elements

# Application: complex geometry

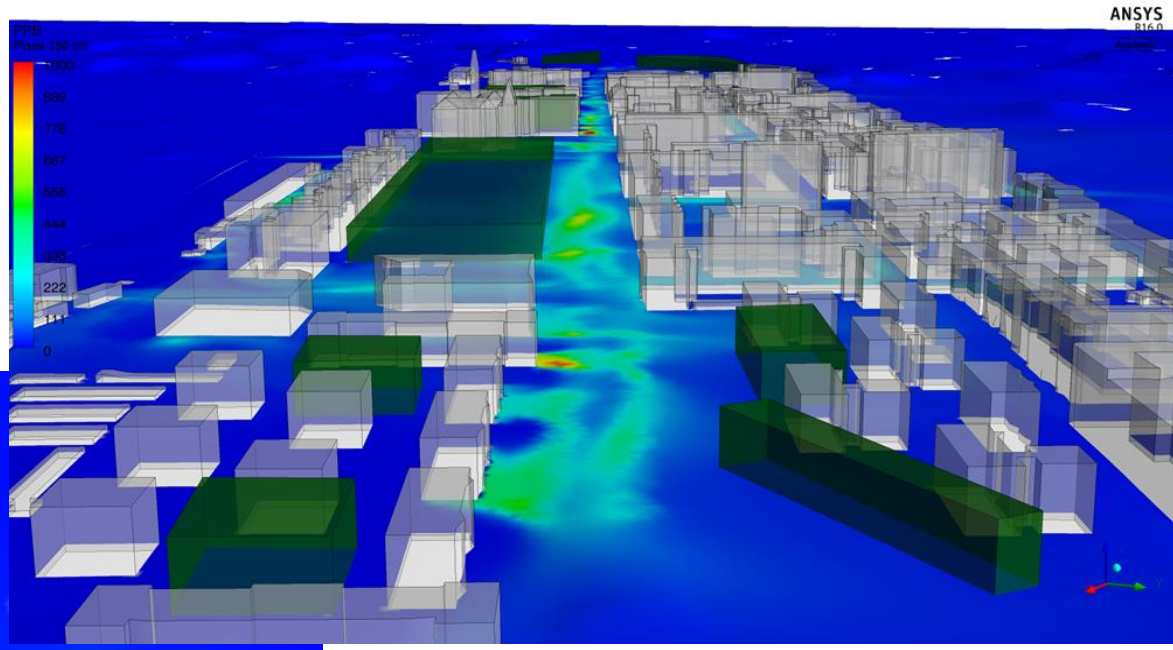
- Validated traffic simulation with PTV Vissim
- $NO_x$ calculation with Copert 4 model, fitted to the fleet of Győr

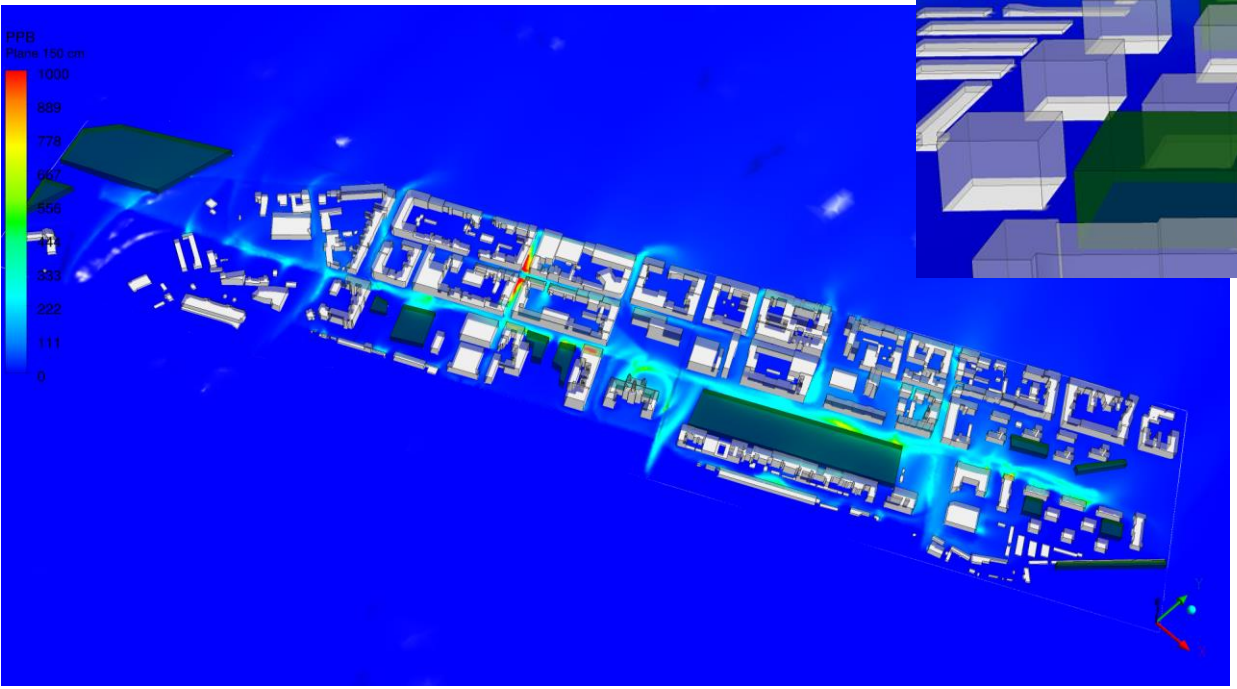




# Application: complex geometry

Simulation results of the full transient 24h calculation: $NO_x$ concentration at 1.5m and peak hour



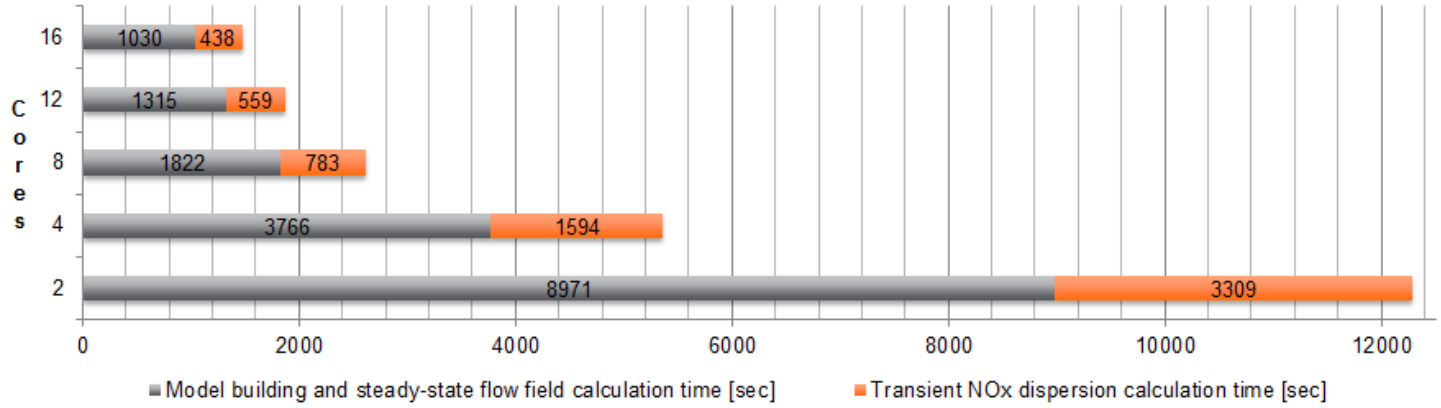



# Application: complex geometry

Geometry of size 4000x4000x400m with detailed 2000x460x400m

**Simulation time** for scenarios on CPUs 16 core@2.27GHz

1. Full transient simulation of 1 day (wind, $NO_x$)
    1. Layered mesh: **7 hours**
    2. Mesh without layer: **5 hours**
2. Frozen flow field (steady state air flow)
    1. Transient pollutant dispersion simulation on the saved flow field for 1h, without flow calculating: 17+7=**24min**



# CONCLUSIONS

- **Main achievements**
  - **Detailed physical model (coupled traffic+emission+3D dispersion) has been developed**
    - **Portable, easy-to-use due to integrated scripts**
    - **Interfaces exist from some parametric models, e.g. OSPM**
    - **Runs fast on simple HW for moderate size problems**
    - **Runs pretty fast on moderate cluster for large scale problems (of 2km x 0.5 km)**
    - **Preliminary validation to measurement sexists**
- **Open problems**
  - **Further integration and automation of modules with scripts to be tuned**
  - **Integration to a sensor network needed**
    - **Work to develop own sensor module is under progress but tests/integration to some existing network would be nice to try**