URBAN ATMOSPHERIC BOUNDARY LAYER DYNAMICS AND POLLUTION PATTERNS: OBSERVATIONS AND MODELLING

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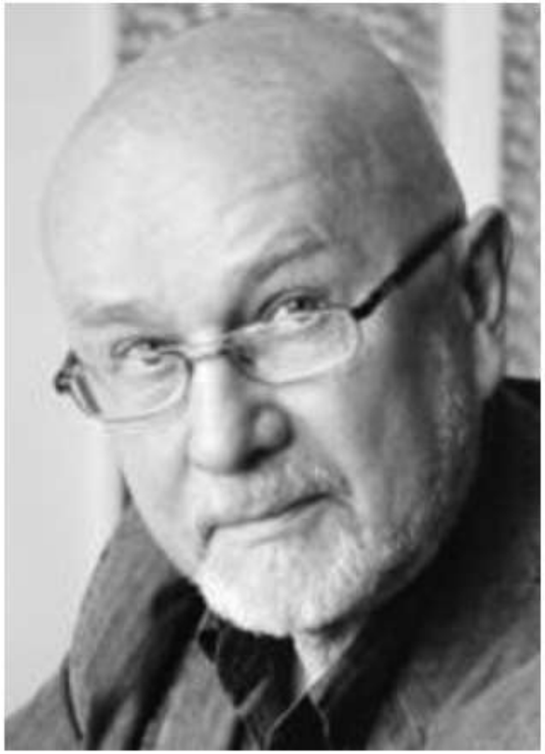
Workshop on Russian MegaGrant "Megapolis – heat and pollution island", Faculty of Geography, Moscow State University, 23 March 2021

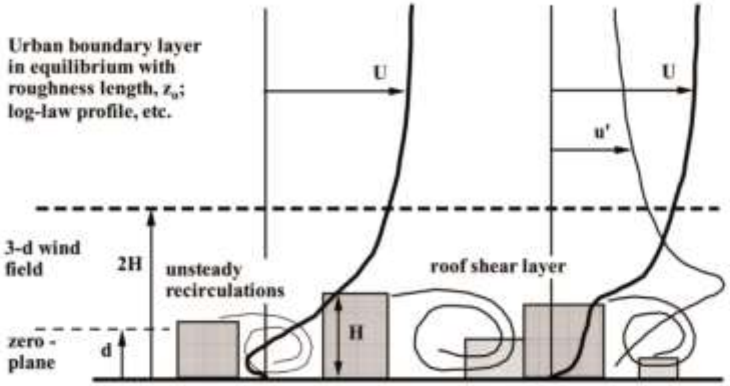


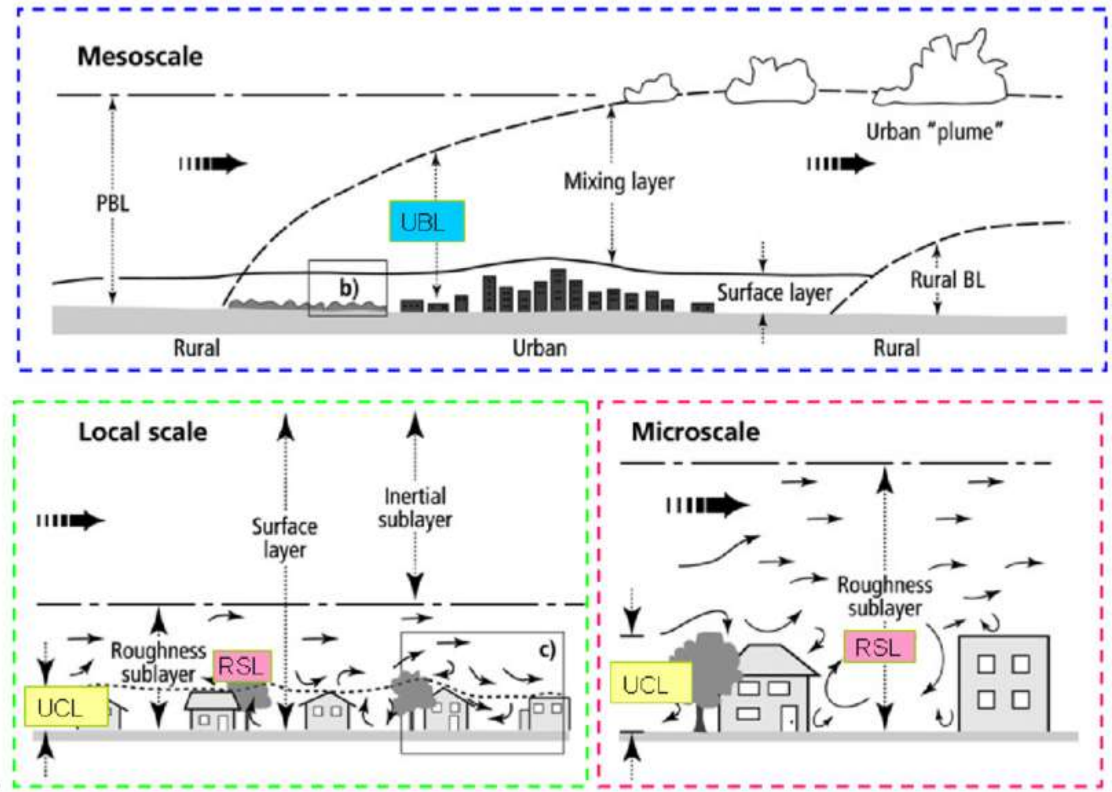
Sergej Zilitinkevich
(1936 - 2021)

“Turbulence is ever produced in the low-viscosity/large-scale fluid flows by the velocity shears and, in unstable stratification, by buoyancy forces. … in fact buoyancy produces chaotic vertical plumes, merging into larger ones and making inverse cascade towards their conversion into **self-organized regular motions**.”

(Zilitinkevich et al., 2021)

Coherent dynamics and pollution patterns: from microscale to mesoscale





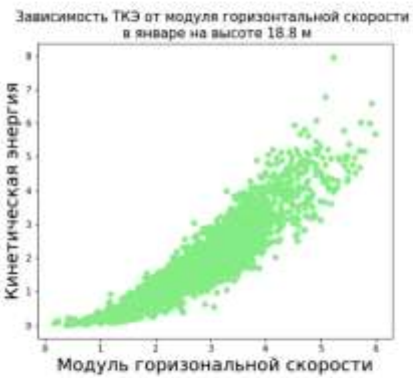
- Coherent structures in ABL mix pollution in vertical
- <u>Hypothesis</u>: coherent flow structures are important for gas and aerosol transformations of the same time scale

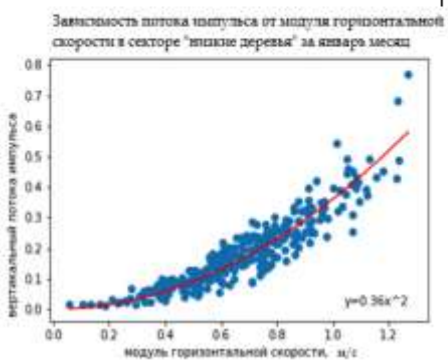
<u>Tasks:</u>

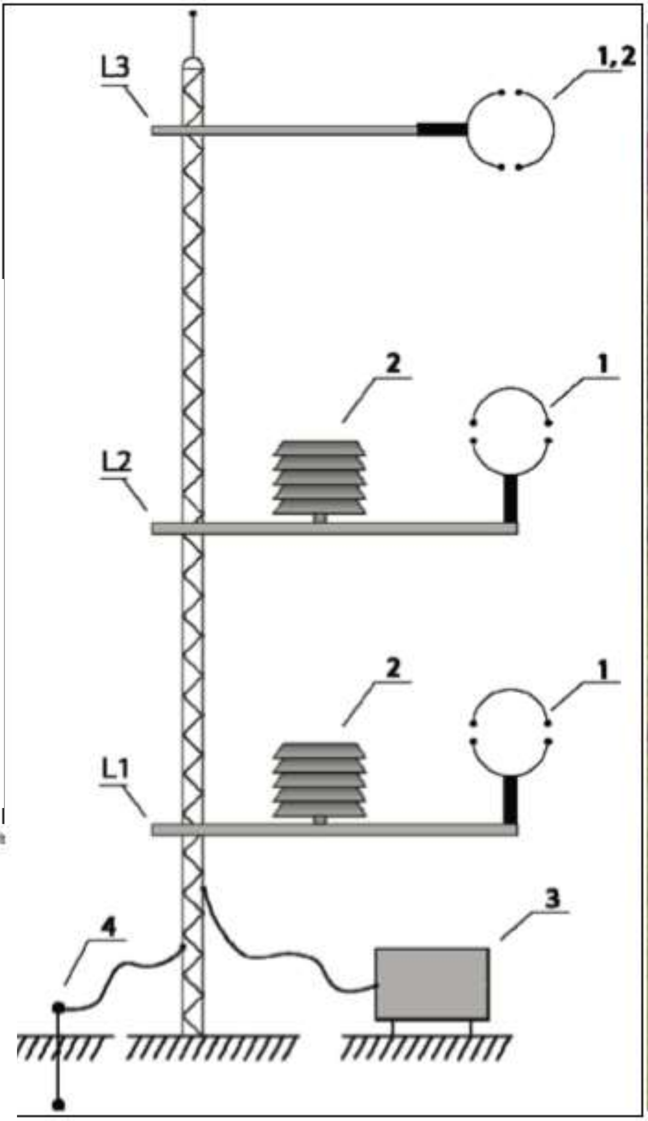
- The study of long-lived circulation patterns dynamics in the urban ABL: from coherent vortices induced by surface heating and complex morphometry to megacity-scale breeze and plume structures
- Assessment of implications of long-lived circulation patterns for aerosol and gas transport and transformations

Existing EC tower in MSU campus

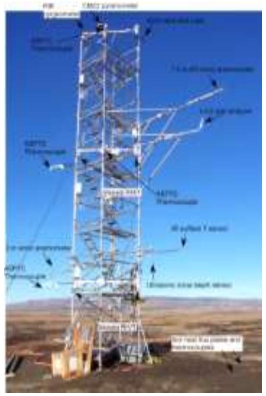
- Since the fall of 2019, a 22 m high eddy covariance tower
- 2 m, 11 m and 19 m of METEK sensors for momentum and heat







Verification and validation of the ABL theory with long-lived dynamics based on experimental data in urban conditions

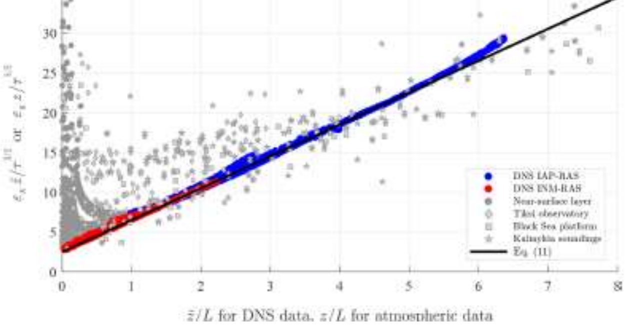


Eureka
10 m

Tiksi 20 m

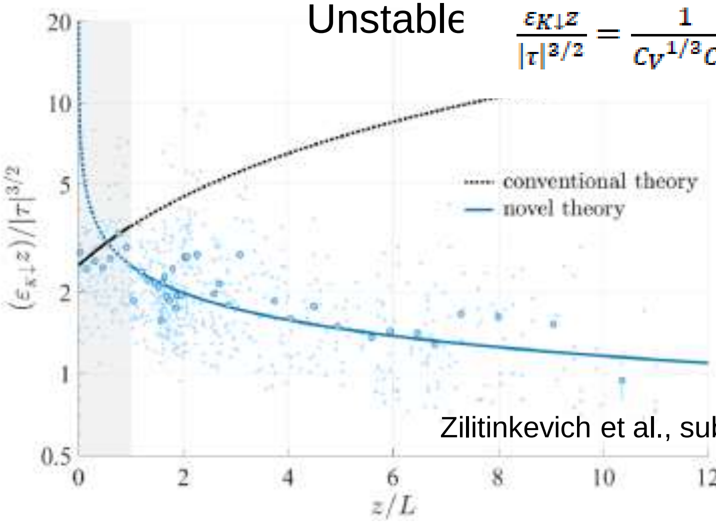
Stable

Zilitinkevich et al., 2019

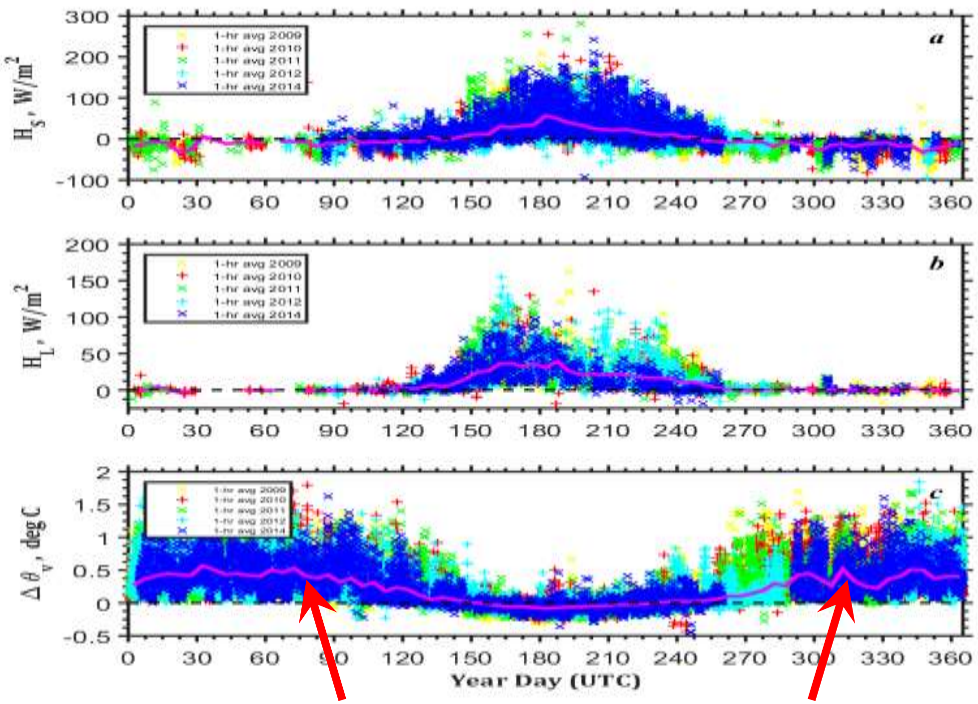


Unstable

$$\frac{\varepsilon_{K\downarrow}z}{|\tau|^{3/2}} = \frac{1}{C_V^{1/3} C_K}\left(\frac{z}{L}\right)^{-1/3}$$

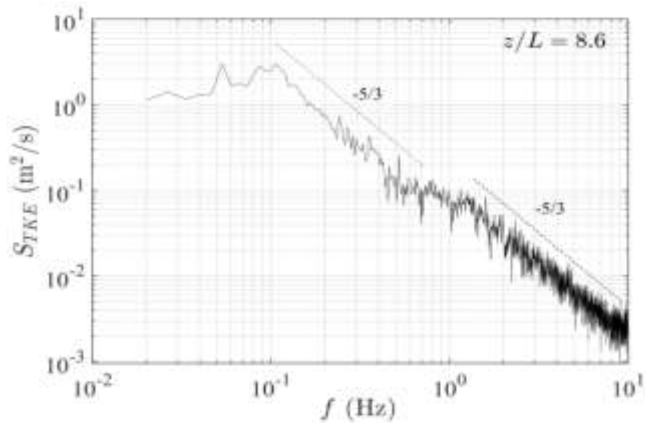


Zilitinkevich et al., submitted



Long-lived SBL

<u>Hypothesis</u>: urban boundary layer possesses some features of long-lived convective BLs



Contribution of coherent structures to vertical turbulent exchange in the urban boundary layer

Third-order moments

Zilitinkevich et al., 1999

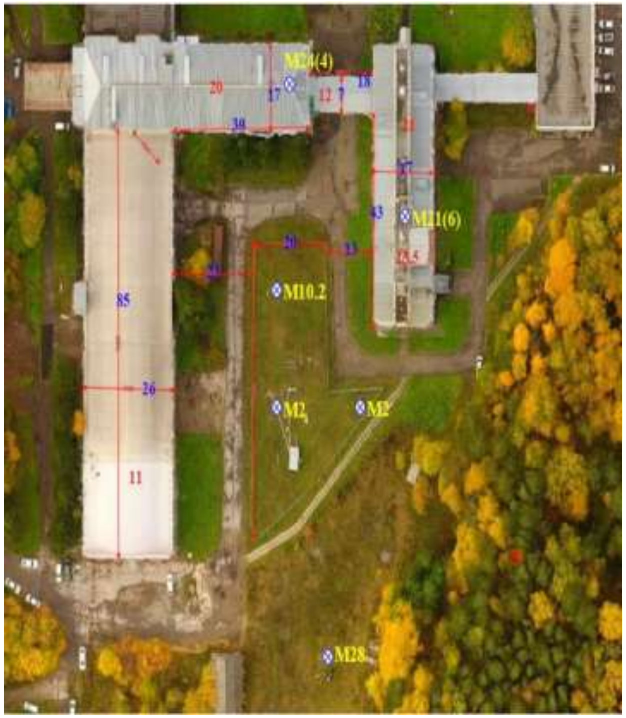
$$\overline{w'\theta'\theta'} = C_\theta S_\theta \left(\overline{\theta'^2}\right)^{\frac{1}{2}} \overline{w'\theta'}$$

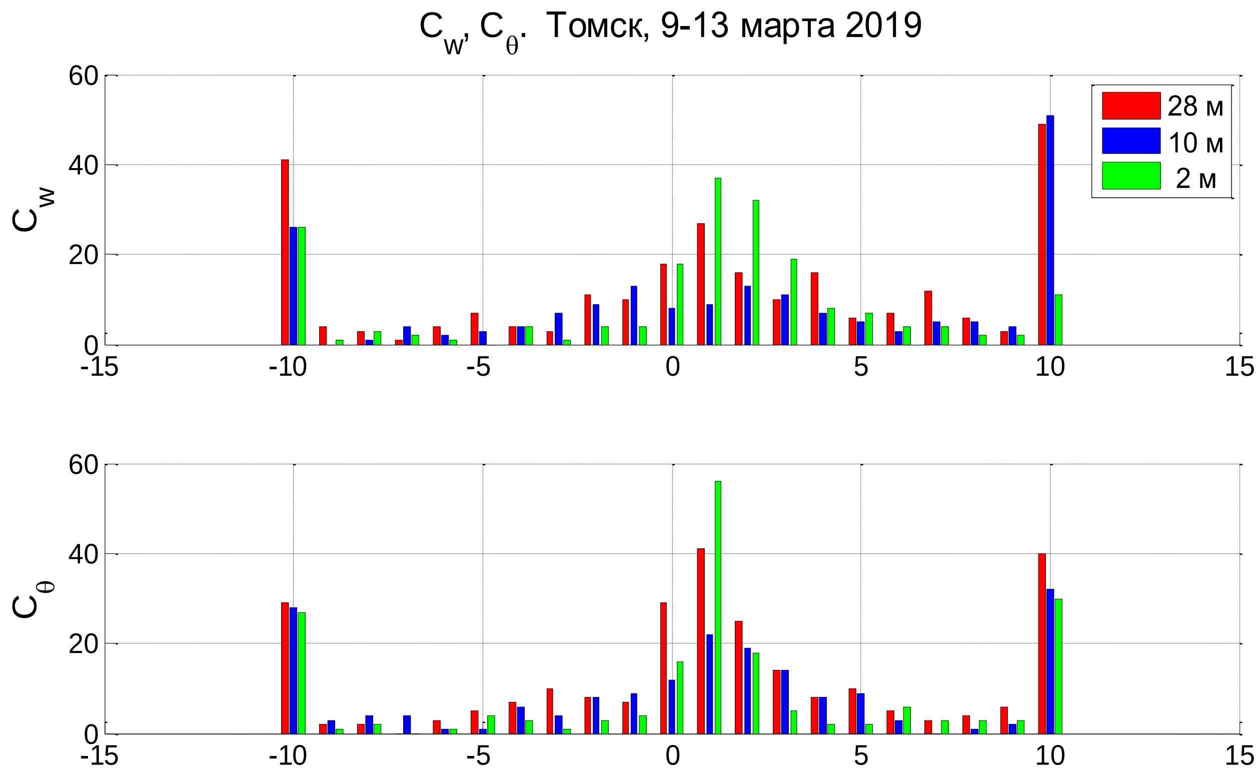
$$\overline{w'w'\theta'} = C_w S_w \left(\overline{w'^2}\right)^{\frac{1}{2}} \overline{w'\theta'}$$

$$H_{CS} = -C_p \rho \overline{w'\Theta'} = -C_P \rho \frac{\overline{w'w'\Theta'}}{S_w \left(\overline{w'^2}\right)^{\frac{1}{2}}}$$

Contribution of coherent structure to the heat flux

Tomsk experimental site





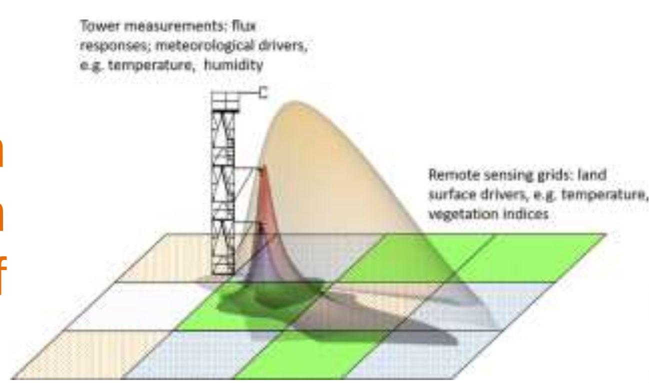
Task: identify background flow (synoptic) conditions where coherent structures dominate the vertical heat and pollution flux

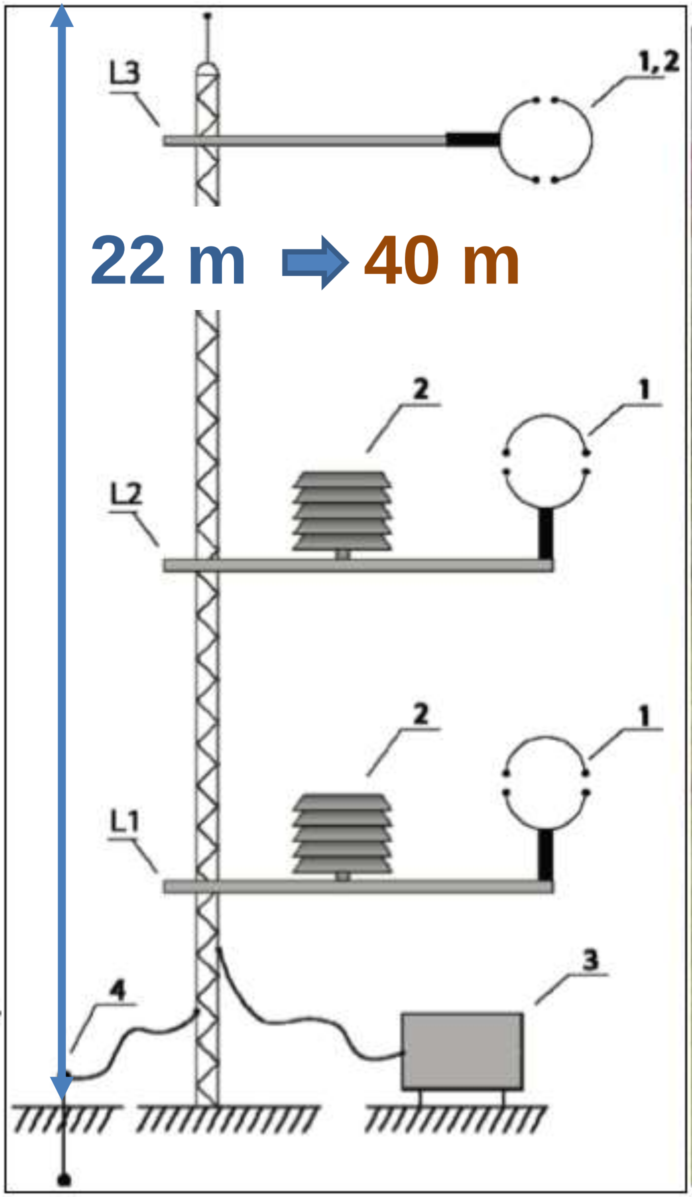
A prospect for a new tower in MSU campus

(towards FLUXNET and SMEAR standards), planned for 2022

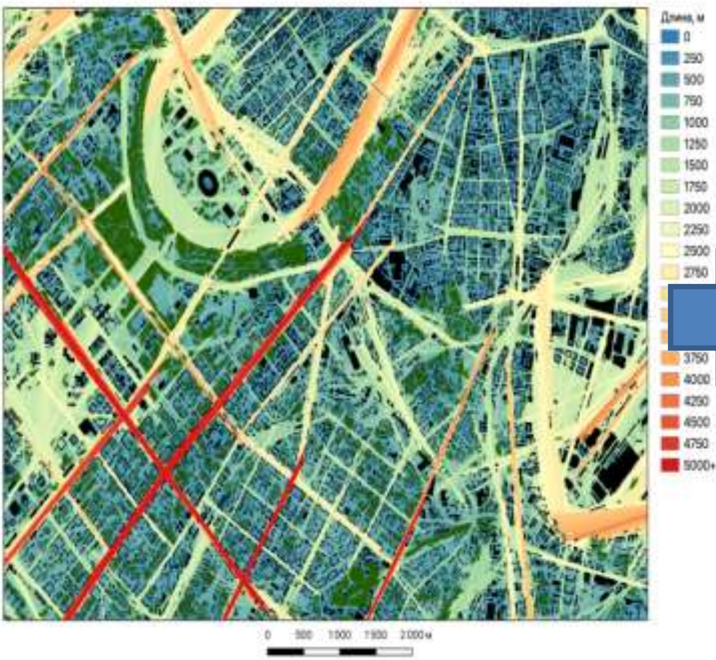
- New tower of **~40 m** height (2-times higher than closest buildings)
- 3 levels of heat and momentum eddy covariance measurements
- 2-3 levels **PM10, PM2.5, PM1 concentration**
- Optimal choice of aerosol sensors on tower compliant to that used in MO MSU aerosol complex
- Optimal choice of mast construction and location in order not to disturb ongoing measurements
- Flux footprint analysis

A postdoc visit to Helsinki in 2021, ca. 2 weeks, to learn state-of-the-art practices of urban EC measurements

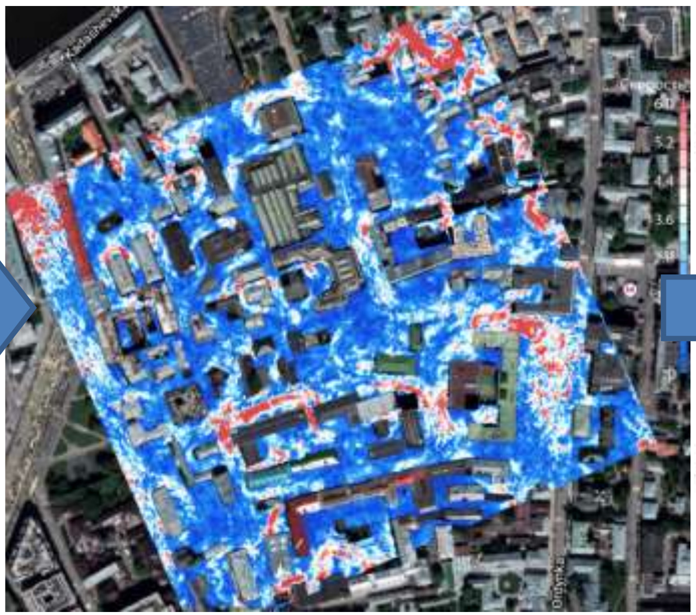




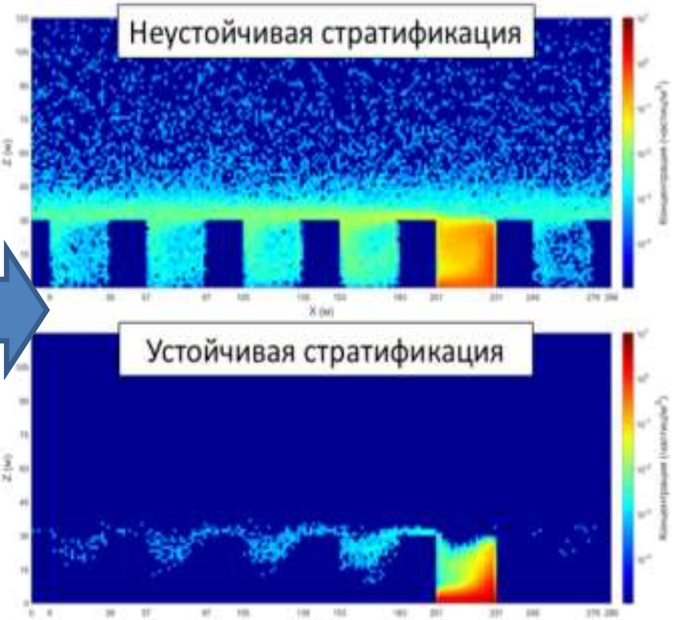
Computation and data-flow framework for modeling micrometeorological regime and aerosols on a scale from district to streets



GIS DATA
(color – the length of urban canyon)



Wind speed distribution in Moscow district



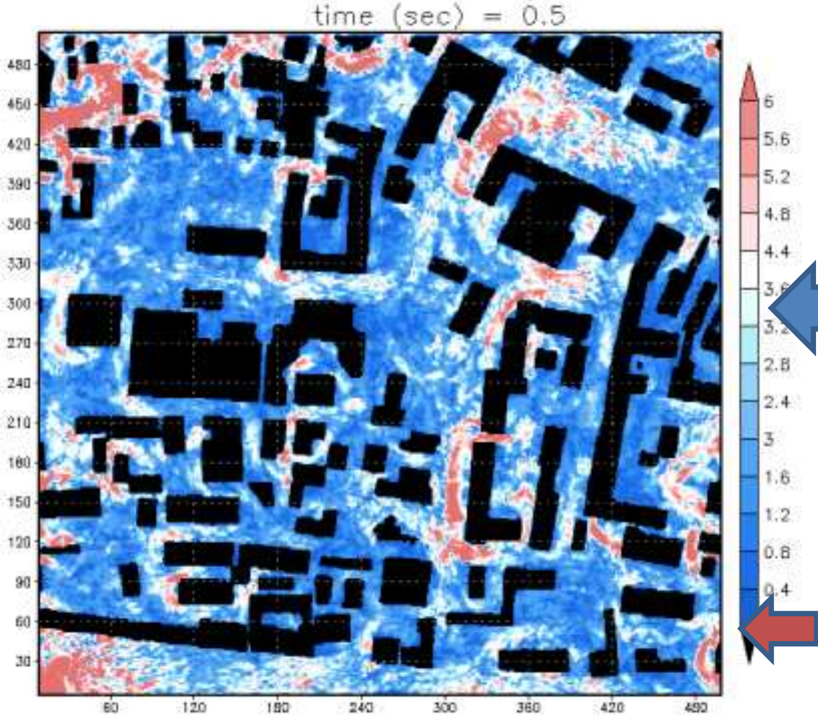
Aerosol concentration in a series of city canyons

Small-scale simulation of the urban boundary layer

DNS – Direct Numerical Simulation,
LES – Large Eddy simulation,
RANS – Reynolds-averaged Navier–Stokes

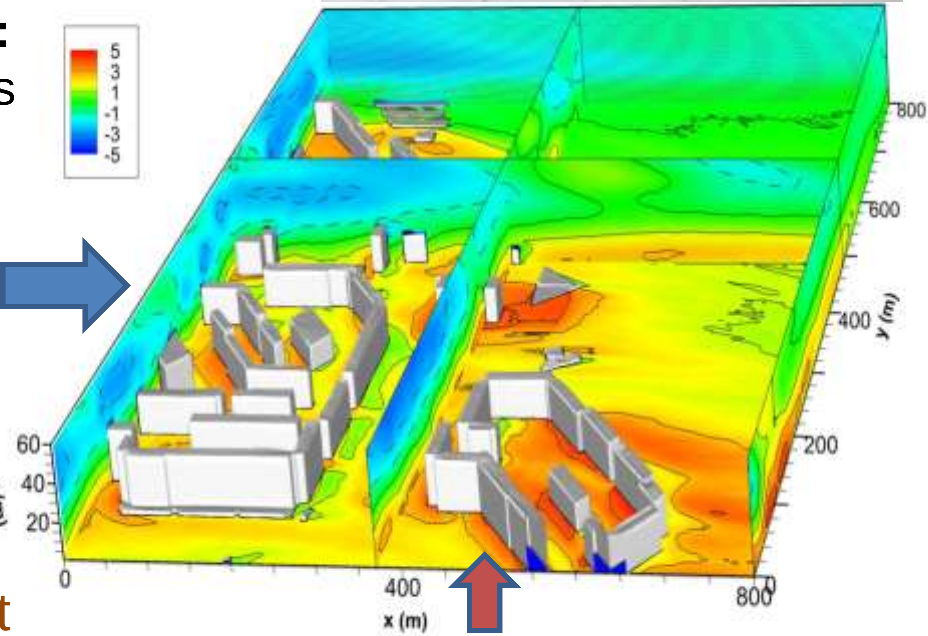
- Immersed boundary method
- Unstructured grids (permitting the local grid refinements)
- Parallel realization on CPU and GPU
- Original subgrid models for LES
- Transport of heavy suspended particles and tracers

Lomonosov-2 supercomputer (MSU)



Moscow district

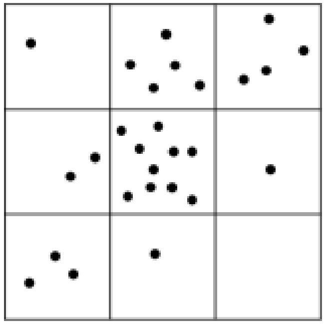
Applications: turbulent flows and pollution above different landscapes, especially **urban environment**



Nadym city

Largangian stochastic models

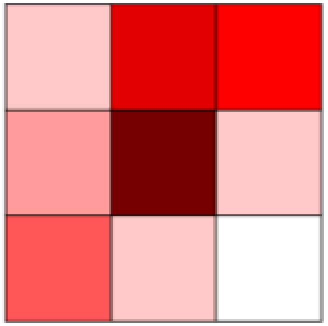
Largangian approach



Trajectories of **individual particles** are tracked.

Computationally expensive, but provides more information

Eulerian approach



Advection and diffusion of **concentration** is computed

$$\frac{\partial\langle s\rangle}{\partial t} + \langle u_i\rangle\frac{\partial\langle s\rangle}{\partial x_i} = \frac{\partial}{\partial x_i}K_s\frac{\partial\langle s\rangle}{\partial x_i} + Q_s$$

Equation of motion for each particle:

$$\frac{\mathrm{d}X_i}{\mathrm{d}t} = V_i \quad \text{and} \quad \frac{\mathrm{d}V_i}{\mathrm{d}t} = \frac{1}{\tau_p}\left[u_i(X_i) - V_i\right] - \delta_{i3}(1-\rho_0/\rho_1)\,g_i$$

Ambient velocity is decomposed in mean, simulated by LES/RANS, and subgrid-scale fluctuation:

$$u_i = \bar{u}_i + u_i'$$

where fluctuation is simulated using one of stochastic equation systems (Durbin, 1983; Thomson, 1987):

$dx_i' = \alpha_i dt + b_{ij} d\xi_j$ - zero-order model, equivalent to Eulerian equation for $\langle s\rangle$

$du_i' = a_i dt + B_{ij} d\xi_j$ - first-order Langevin model

$dx_i^i = u_i' dt$

New particle formation and growth

(Kerminen et al., 2018)

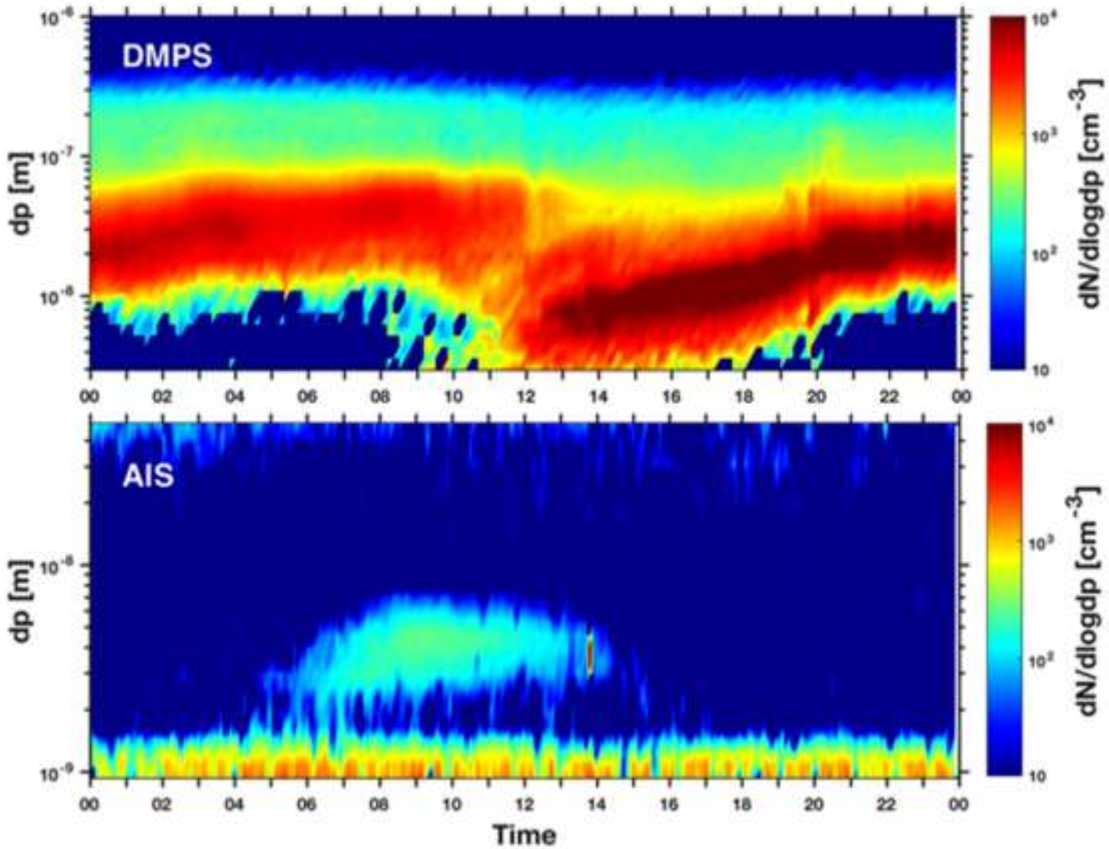


Figure 1. (Top) An example of a regional NPF event day, as measured by a differential particle mobility sizer (DMPS) in Hyytiälä, Finland, on 8 April 2017. The data is presented in UTC + 2 (Finnish winter time). The time in the *x*-axis refers to the time of day, whereas the color indicates the number density of particles of different size (particle diameter, *y*-axis). One may see that the newly-formed particles appear into the measured size distribution at around the noon, after which they grow in size reaching diameters between about 15 and 50 nm by midnight. (Bottom) An example of a local NPF event day, as measured by an air ion spectrometer (AIS) at Dome C, Antarctica, on 19 March 2011. The data are presented in UTC (local time in UTC + 8). Unlike the feature in the regional NPF event, no clear growth in size is observed in the local NPF event after the appearance of a new mode between 2 and 10 nm in the measured size distribution. The presence of this new mode lasts for several hours.

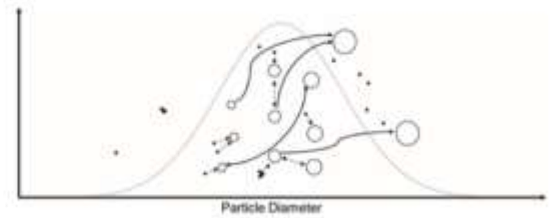


Figure 2. Growth of individual aerosol particles (open circles) and a particle population (all open circles inside the dashed region). Individual particles grow by the net flux of vapor molecules (black small circles) or their clusters into them, illustrated by thin one-headed arrows. Thick one-headed arrows represent the coagulation scavenging of particles in this population onto larger particles. The two-headed arrows represent self-coagulation within this particle population.

Table 1. Statistics (median, 5th and 95th percentiles) of the particle formation rates (J) and growth rates (GR) based on literature data. Mountain sites include studies conducted in China. For each site type, N refers to the number of sites from which the median values of J and GR were determined. As an example, the median GR of 2.7 nm h^{-1} for boreal forest sites is the median value of the 17 study-average (or median if mean was not reported) values of GR reported in each individual study. It should be noted that the size range used in calculating J and GR varied from study to another (e.g. J could refer to J_3, J_{10} etc), and we had no way of harmonizing the results in this respect.

		J (cm^{-3} s^{-1})				GR (nm h^{-1})		
Site type	N	5th	Median	95th	N	5th	Median	95th
Boreal	12	0.13	0.4	0.92	17	0.49	2.7	5.3
Remote and rural	6	0.59	4.1	11.0	22	2.0	3.5	9.6
Urban	17	1.2	2.9	13.7	26	4.0	5.9	12
Arctic	2	—	0.51	—	6	0.23	2.3	4.1
Antarctica	2	—	0.05	—	4	1.4	4.5	5.5
Mountain	10	0.2	0.79	3.9	11	1.2	4.0	13
China: rural	11	1.8	4.9	19.7	13	3.8	6.2	9.8
China: suburban	4	1.4	3.3	3.6	9	3.5	7.4	13
China: urban	8	1.8	7.9	12.9	16	4.1	6.4	12
China: marine and coastal	1	—	0.3	—	5	2.9	4.5	7.1

New particle formation and growth: key processes and parameterizations

(Kerminen et al., 2018; Riechelmann et al., 2012)

$$\frac{dm_p}{dt} = \frac{d(\rho_p V_p)}{dt} = V_p \frac{d\rho_p}{dt} + \frac{1}{2}\pi \rho_p \mathrm{dp}^2 \times \frac{d\mathrm{dp}}{dt} \approx \frac{1}{2}\pi \rho_p \mathrm{dp}^2 \mathrm{GR}_{\mathrm{ind}}.$$

The growth of particles due to condensation of non-volatile organic compounds, H_2SO_4 other precursors, and collision with small molecular clusters

Example of similar parameterization in PALM Largangian cloud model:

$$r\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{S-1}{F_k + F_d} \quad \text{with} \quad S = \frac{e_v}{e_s}, \quad F_k = \left(\frac{L_e}{R_v T - 1}\right)\frac{L_e \rho_l}{KT} \quad \text{and} \quad F_d = \frac{\rho_l R_v T}{D e_s(T)},$$

The growth of large particles with radius R using a concept of collision kernel *K(R,r)*:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \frac{1}{3R^2}\int_0^R r^3 K(R,r) n(r)\, \mathrm{d}r$$

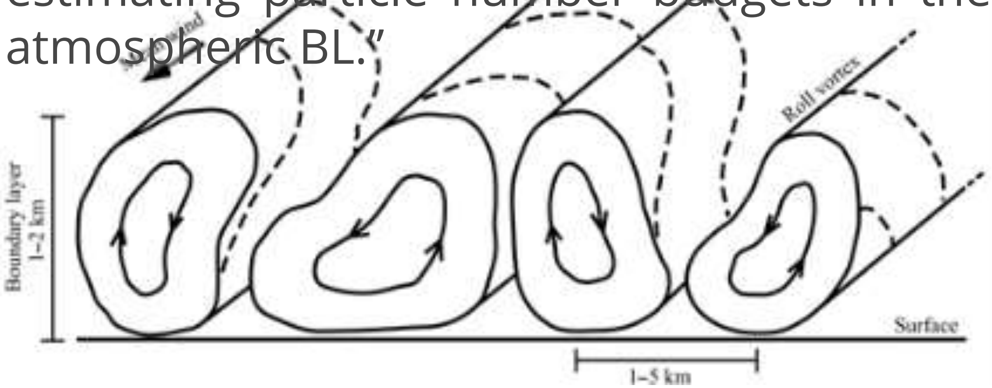
There is a number of parameterizations for collision kernel *K(R,r),* including that for inertial subrange turbulence (e.g., Ayala et al., 2008), which are suitable for LES simulations.

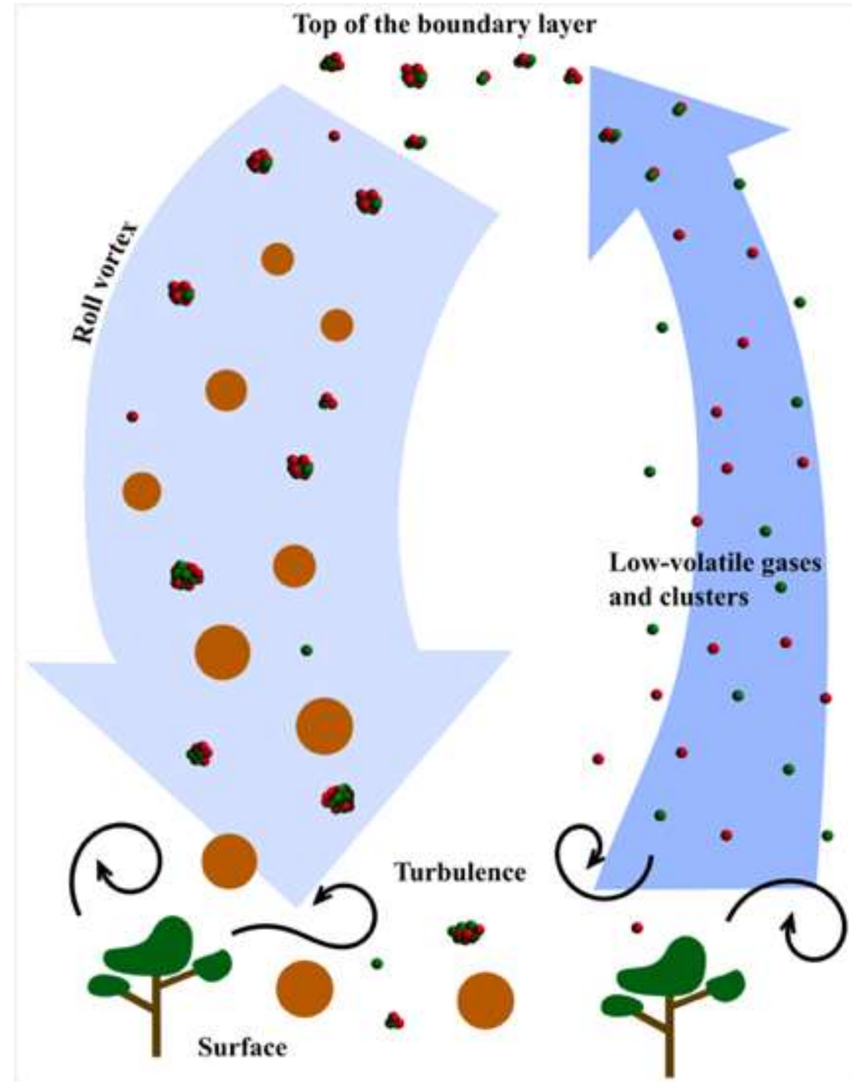
Gaseous precursors of particles are simulated in framework of Eulerian approach.

Roll vortices induce new particle formation (NPF) bursts in the planetary boundary layer

(Lampilahti, …, Zilitinkevich … et al., 2020;)

"… Here we show that rolls frequently induce NPF bursts along the horizontal circulations and that the small clusters and particles originating from these localized bursts grow in size … We … estimate the impact of roll vortices on the overall aerosol particle production due to NPF at a boreal forest site (83 % ± 34 % and 26 % ± 8 % overall enhancement in particle formation for 3 and 10 nm particles, respectively). We conclude that the formation of roll vortices should be taken into account when estimating particle number budgets in the atmospheric BL."





For the project research plan

- Development of a new aerosol block including particles growth and collisions in LES/RANS codes developed in INM RAS/MSU
- The study of the role turbulent regime in the urban boundary layer on the *new particle formation and growth*, especially the role of large long-lived coherent structures
- The data on typical particles sizes, particle compositions, precursor concentrations are taken from Finnish sites and Meteorological observatory in MSU

A master student visit to Helsinki in 2021, ca. 2-3 months.

The task: formulate a subset of gas/aerosol species, processes and parameterizations to be included in LES (microscale) model

Collaboration groups:

- Markku Kulmala group
- SILAM
- Enviro-HIRLAM

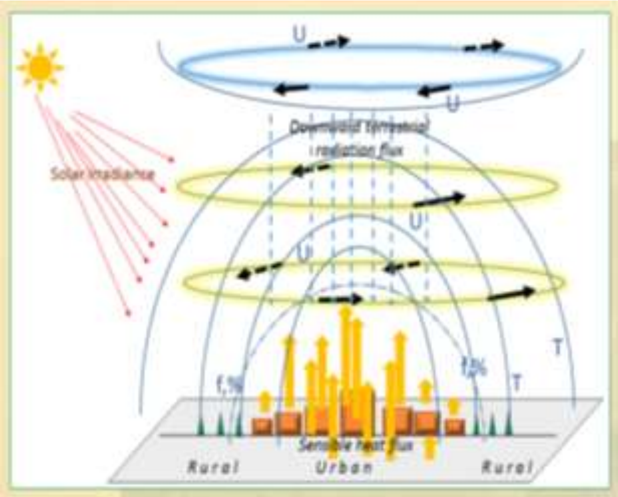
Urban boundary layer on mesoscale

Research questions:

- Urban-induced effects in the lower atmosphere (ABL heat/dry islands, urban circulation…) according to detailed mesoscale modelling and observations
- Focus on long-living ABL effects (e.g. in winter conditions)
- Concepts of “urban islands” and “urban circulation” as self-sustained systems
- Feedbacks between urban-induced ABL effects, radiation and aerosols
- Interaction between local-scale and mesoscale factors shaping UHI and urban-induced ABL effects
- Extreme precipitation and wind events in urban atmosphere

Research tools:

- Mesoscale models with urban parameterizations (COSMO + TERRA_URB, COSMO-ART + TERRA_URB, possibly other models), including evaluation and development of urban parameterizations
- Boundary-layer observations (MTP-5 profilers, SODARs)
- Surface-layer observations (Roshydromet, Moseconitoring, crowdsourcing)



Synthesized picture of Moscow UHI, developed based on ground measurements, satellite MetOP A B profiles and model simulations

Sections of the plan:
1.12, 1.14, 2.6*, 2.13, 3.13, 3.6*
* Interaction with WP3

3D urban heat (moisture, pollution) island as self-sustained system

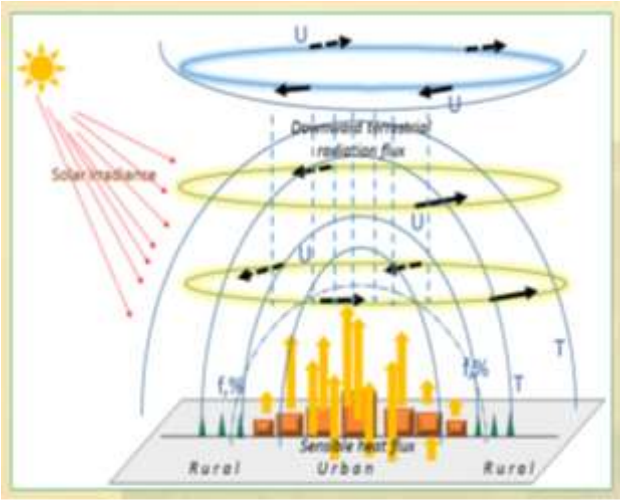
- **Towards concepts of "urban islands" and "urban circulation" as self-sustained systems**
- **Feedbacks between urban-induced ABL effects, radiation and aerosols**

Important peculiarity of the heat budget in Moscow is an increase in the downward long-wave radiation flux that has been observed in the recent decades (δ*F*). It was manifested in the growth of annual net radiation roughly by **10** W/m^2 from the 1970s till now. This effect may be interpreted as a feedback: the UHI formed due to additional heat influx, favored the heating of the city environment and intensified atmospheric downward radiation flux. Actually, using the well-known Brent formula for the calculation of downward longwave radiation flux, we get that its increase (δ*F*) is connected with the temperature anomaly (δ*T*) by the relationship

$$\delta F \sim 4\sigma T^3 \delta T (D + G\sqrt{e})(1 + Cn)$$

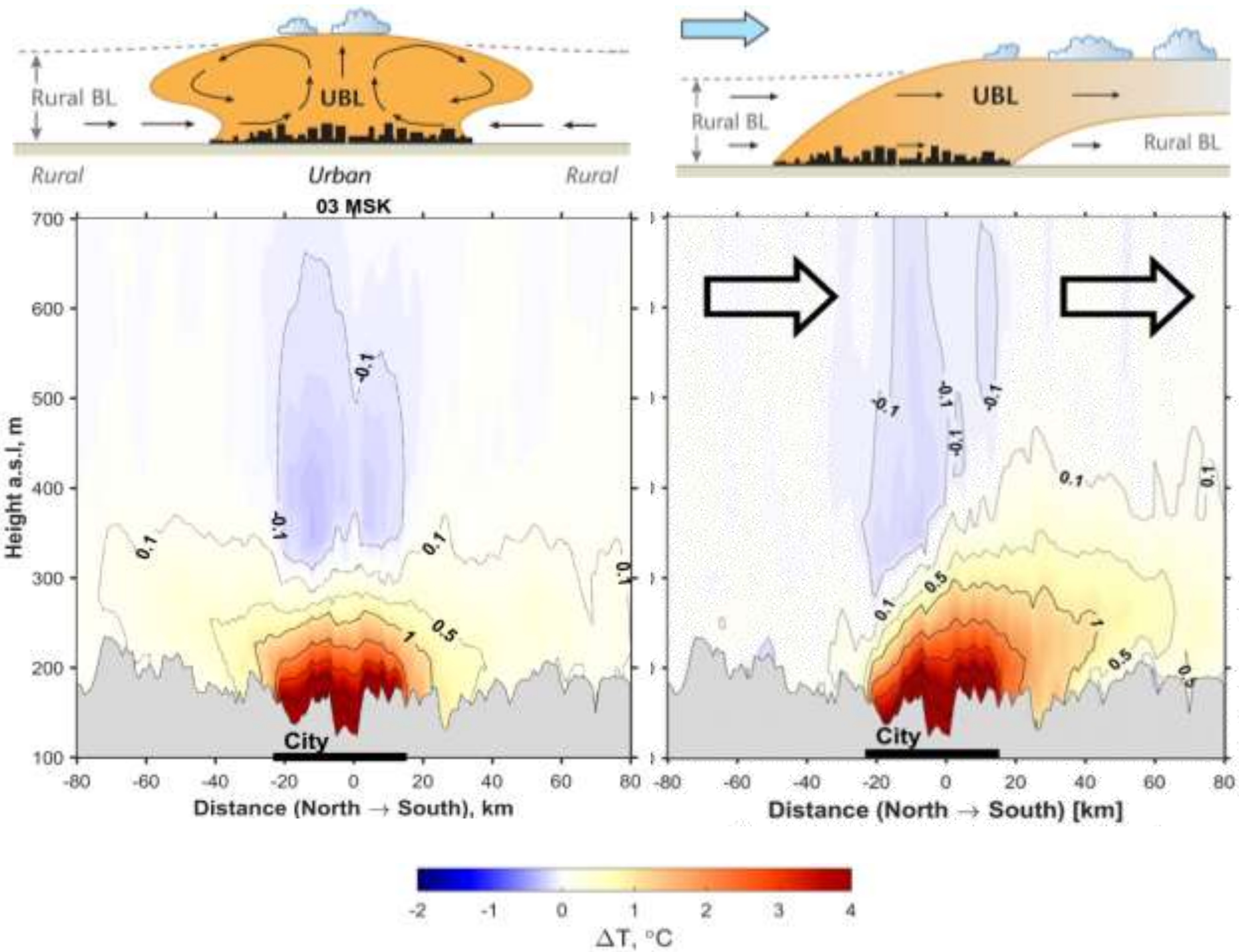
where σ is the Stefan's constant; *D* = 0.61; *G* = 0.05; the cloud coefficient *C* = 0,76. Assuming that partial water vapor pressure *e* = 6 hPa, *n* = 0.5, and δ*T* = 2 K, we get the estimate for δ*F*= **9.5** W/m^2.

The heat island is to some extent a self-sustained system due to a feedback (providing about 10% of the effect created mostly due to the transformation of heat budget and permanent anthropogenic heat emissions) between temperature and downward longwave radiation flux.



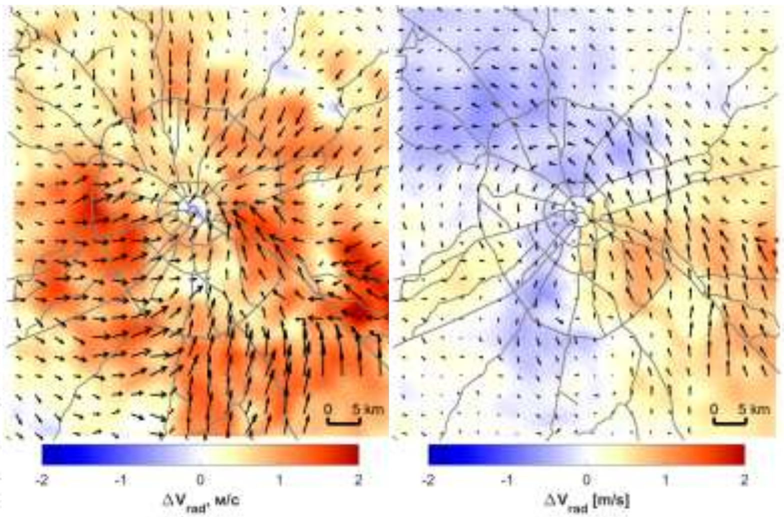
Synthesized scheme of Moscow UHI, developed based on ground measurements, satellite MetOP A B profiles and model simulations

3D structure of the "island": domes and plumes



Cross-section of the nocturnal UHI over Moscow:
mean conditions and cases with southern/northern winds

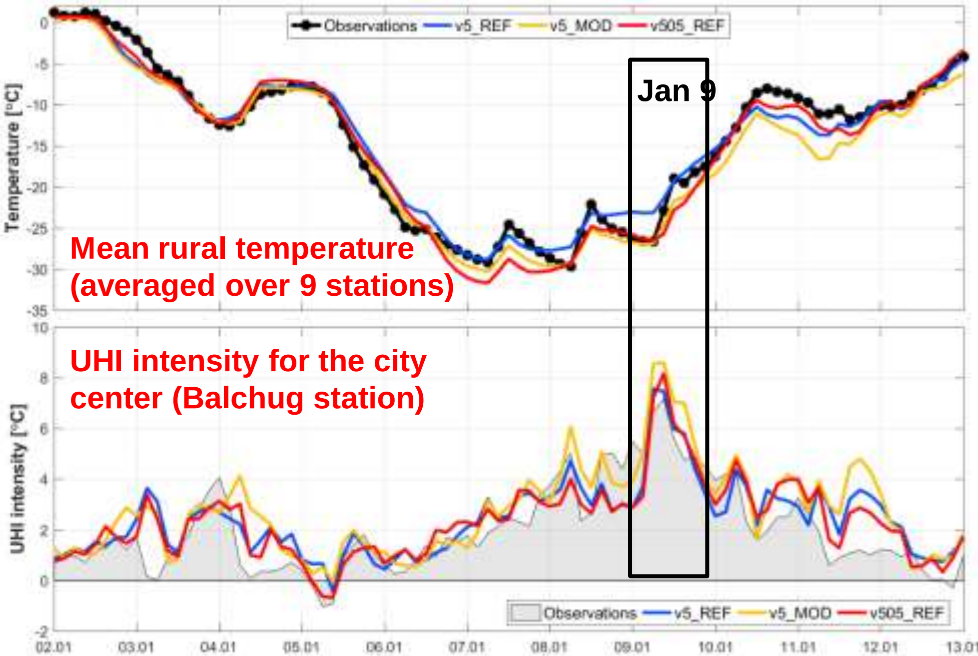
"urban breeze" in evening | cyclonic vorticity at night



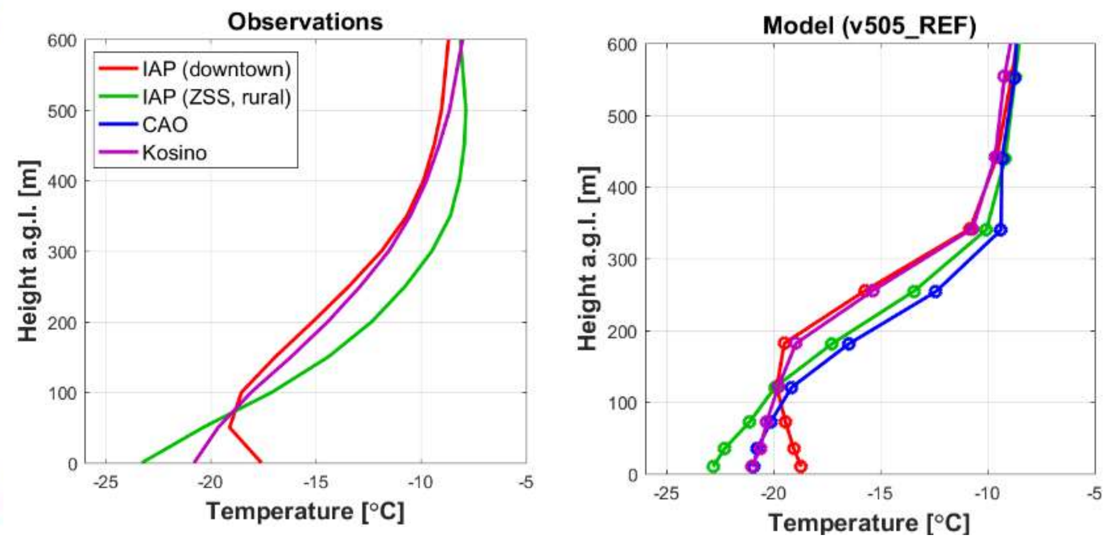
Urban-induced circulation component at the height aprox. 120 m above the surface

Results are based on numerical simulations with COSMO&TERRA_URB for summer 2014 (Climate of Moscow…, 2017; Varentsov et al., 2018; Kislov 2020)

Long-living urban-induced ABL effects in winter *(absent or weak diurnal cycle)*



Modelled and observed temperature profiles on 9th January 2017



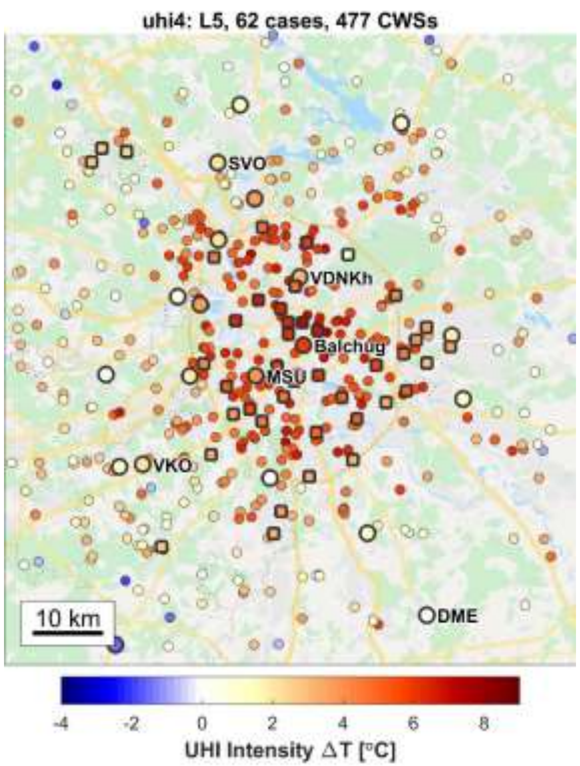
Mean vertical temperature profiles for 9th of January, modelled and observed by MTP-5 profilers. The model captured the vertical UHI extent and a so-called cross-over effect. (PT AEVUS report, 2019; Rivin et al., 2020)

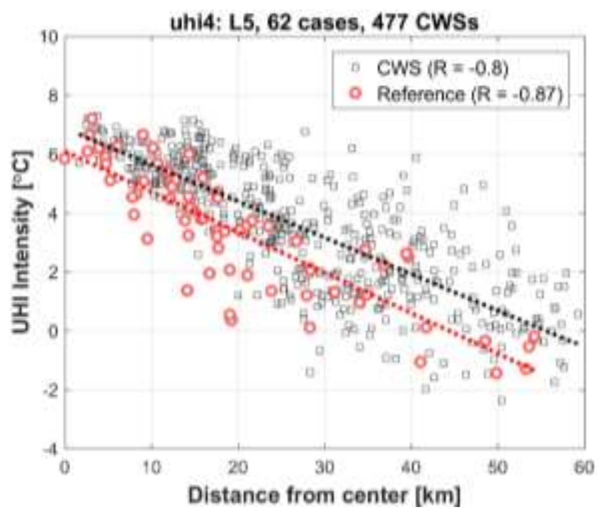
MTP-5 profiler at the top of Institute of Atmospheric Physics roof at the city center

<u>Task:</u> the study of vertical ABL structure and near-surface thermal regime under weak diurnal cycle

Local-scale and mesoscale drivers shaping UHI

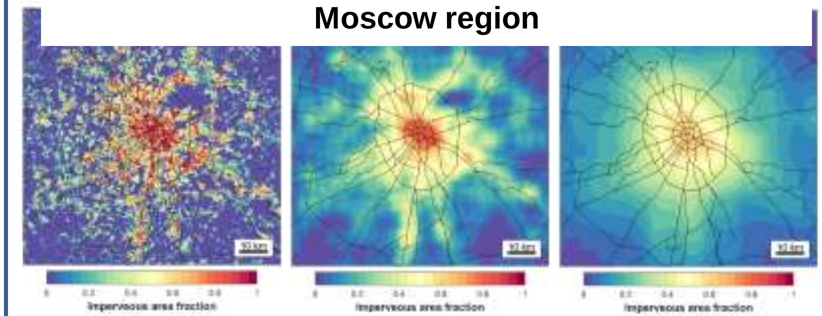
… deriving fine-scale structure of the urban heat island using crowdsourcing data

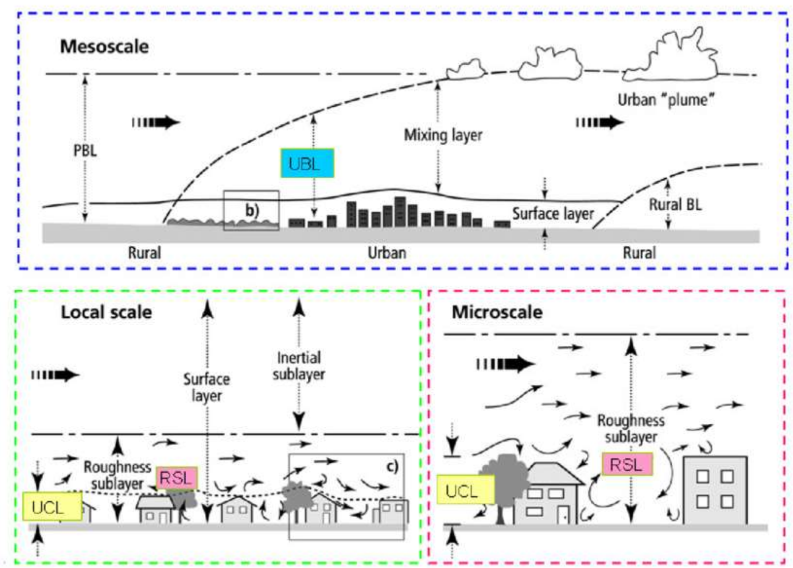




Decreasing UHI intensity with a distance from city center indicates contribution of the mesoscale processes

Local-scale to mesoscale heterogeneity of Moscow region



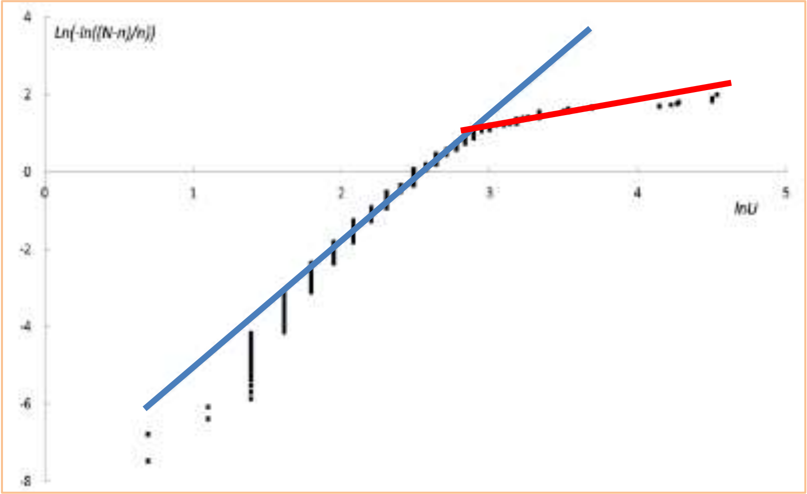


Task: the study of links between surface properties and local UHI intensity under different synoptic conditions

Extreme coherent structures: hazardous weather

Classification of extreme weather conditions

Using cumulative distribution functions (CDF) we can detect anomalies (velocity, precipitation) adhering to different weather events. For example, on the Figure below the wind speed outliers belong both to base CDF and another CDF joining mostly important anomalies.



Empirical CDF of wind speed maxima (station observations, Teriberka) straightening on the coordinate axis of the Weibull distribution, and linear regression lines corresponding to the Weibull functions.

Numerical simulation of detected weather events in the framework of the COSMO&TERRA_URB.

- Assessment of model data quality
- Study the structure of meteorological fields (using additionally atmospheric sounding data)

Mesoscale convective system in Moscow

Task: estimate the effect of UHI on extreme weather

MSU RCC MOSCOW STATE UNIVERSITY RESEARCH COMPUTING CENTER 1

ГЕОГРАФИЧЕСКИЙ ФАКУЛЬТЕТ МГУ имени М.В. Ломоносова 2

3

ИФА 4

ИВМ 5

6

URBAN ATMOSPHERIC BOUNDARY LAYER DYNAMICS AND POLLUTION PATTERNS: OBSERVATIONS AND MODELLING

Victor Stepanenko

Alexander Kislov

Irina Repina

Andrey Glazunov

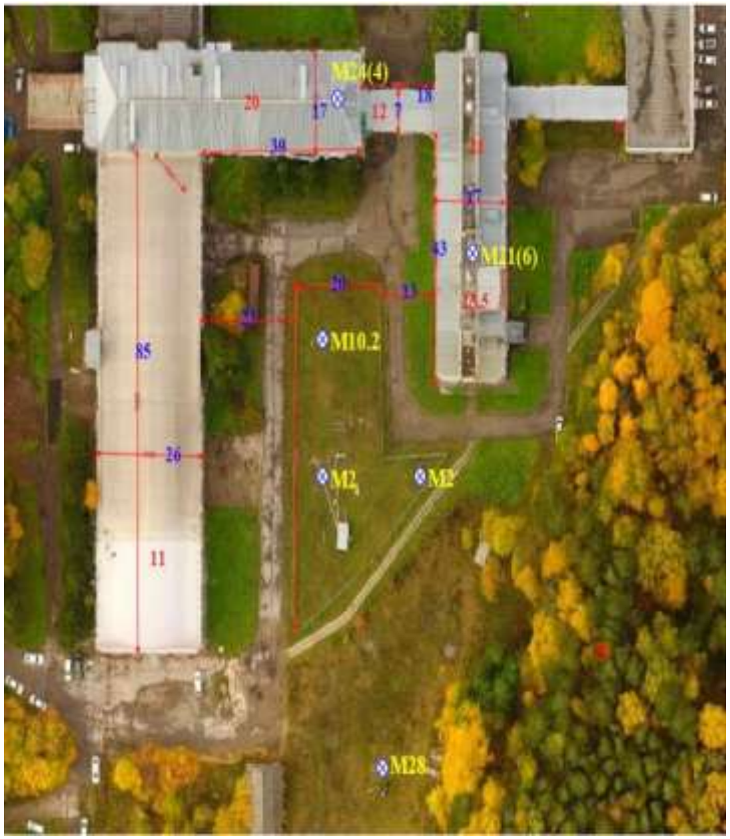
Mikhail Varentsov

Thank you!

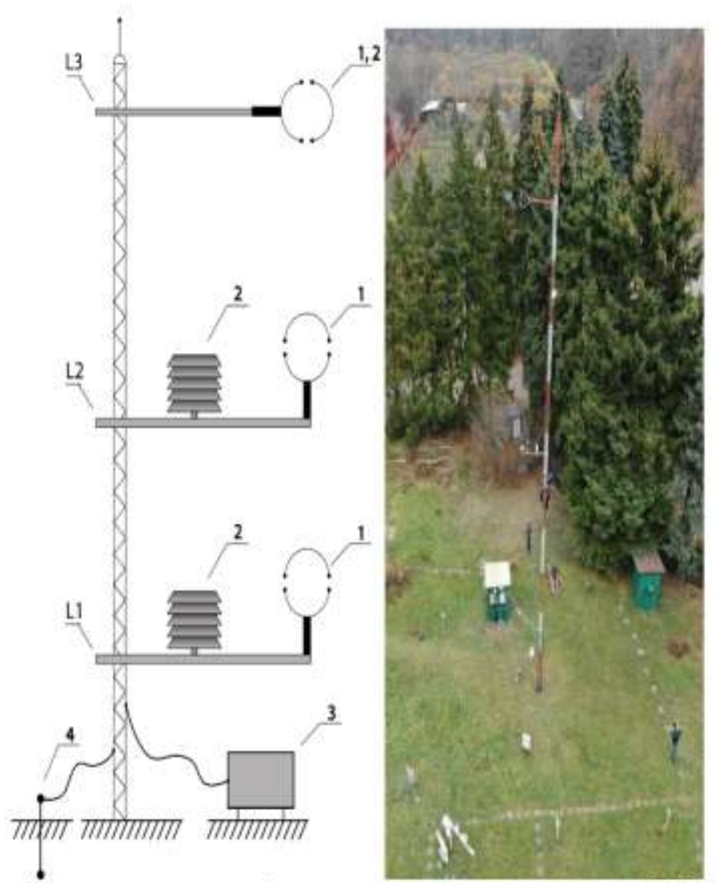
Workshop on Russian MegaGrant "Megapolis – heat and pollution island", Faculty of Geography, Moscow State University, 23 March 2021

Data sets to test the theory of long-lived planetary layers, including in urban conditions

Tomsk



Moscow

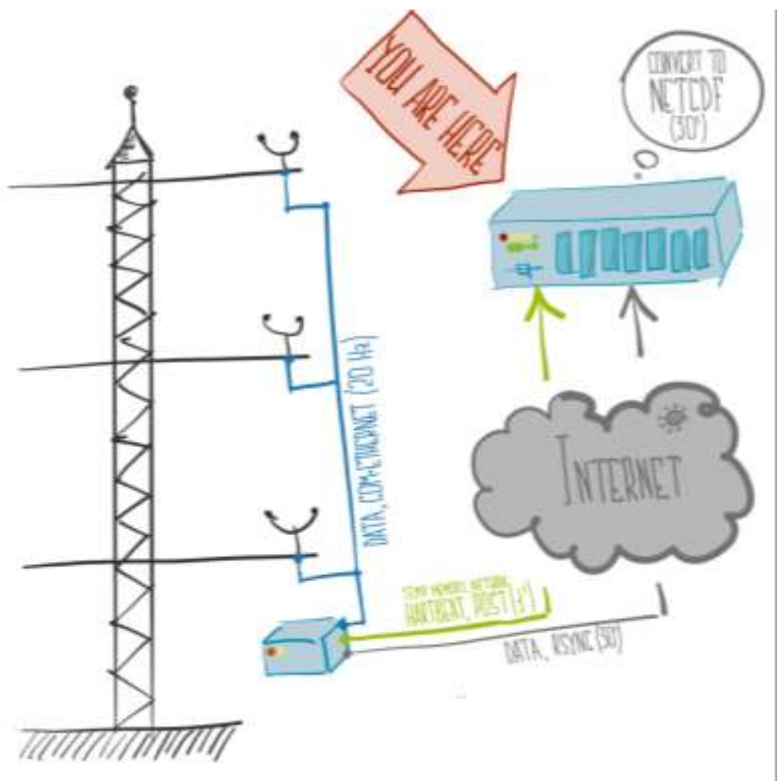


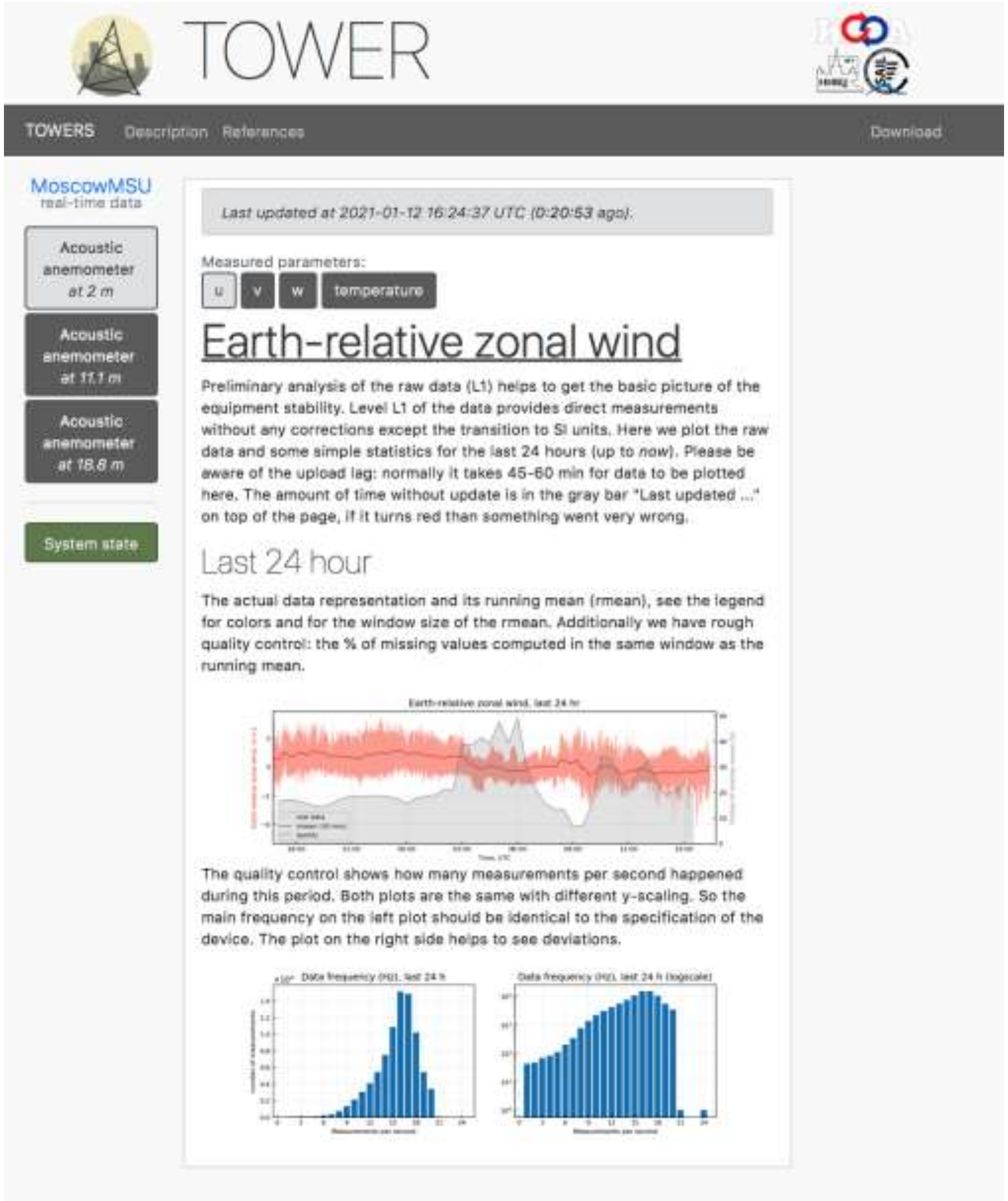
Helsinki, SMEAR III

Website of the MSU tower

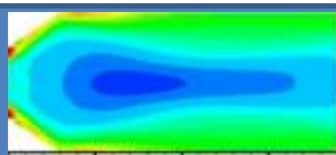
https://tower.ocean.ru/rtdata?tower=MSU&city=Moscow

- ❑ real-time online monitoring of system state
- ❑ online display of the latest 24 h data
- ❑ online screening of the latest data quality
- ❑ downloading of the raw data by registered users





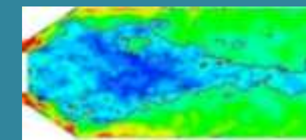
Interaction of modeling techniques



Reynolds-Averaged Navier-Stokes (ENVI-met, RCC MSU)

Largangian particles simulator

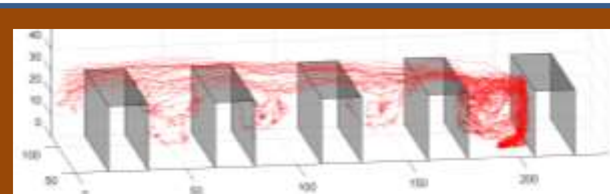
Validation of RANS by LES for typical and extreme synoptic conditions



Large Eddy Simulation (RCC MSU, INM RAS)

Largangian particles simulator

Fields of velocity and turbulence quantities for simulations of different aerosol types

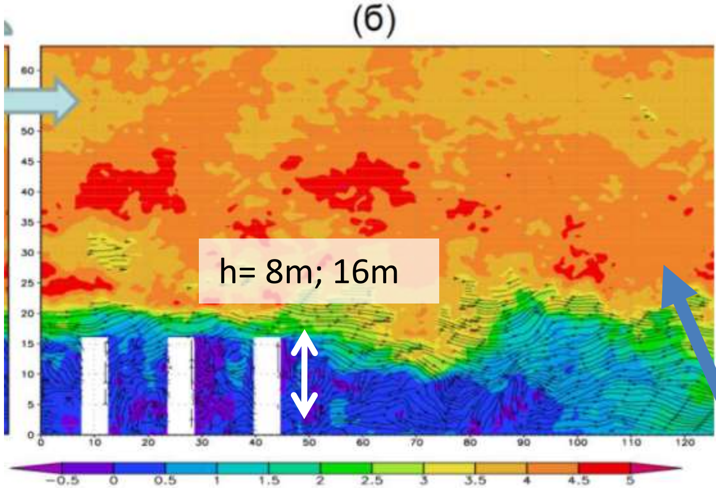


Largangian particles simulator (RCC MSU)

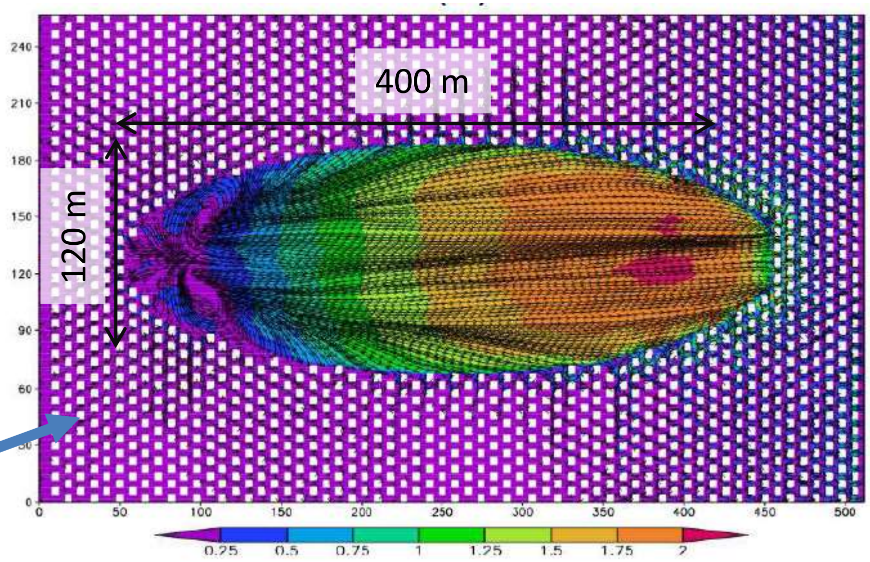
Computing resources are a bottleneck!

Aerosol transport modeling using Large Eddy Simulation

(Glazunov and Stepanenko, 2015; Glazunov et al., 2016, 2018)

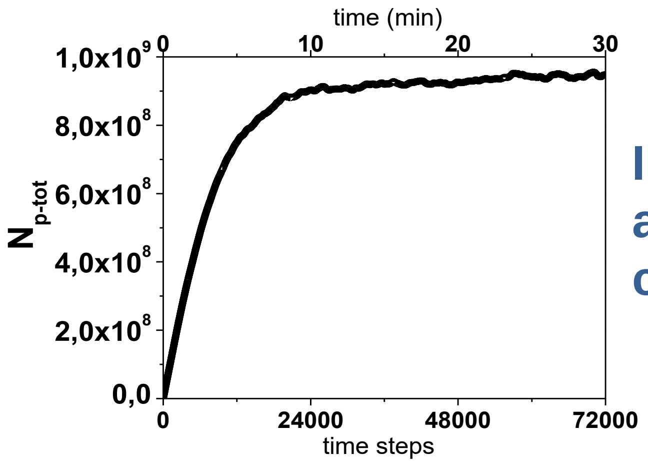


Velocity and streamlines over a clearing

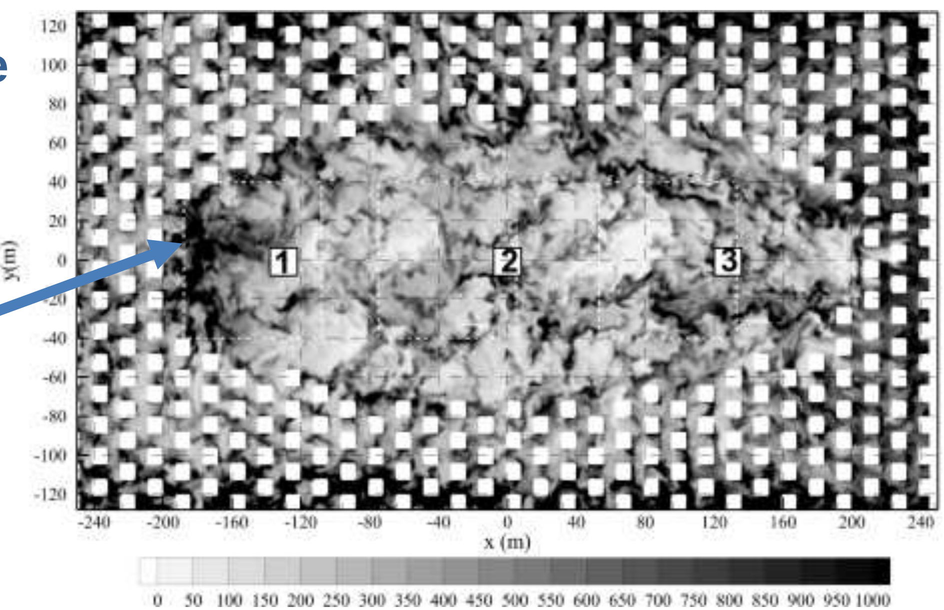


Mean velocity at the height z=0.25 m

Number of particles during model runtime



Instantaneous aerosol concentration



Possible collaboration with other Tasks and WPs

- **WP2, Task 1, “Measurement of the physical-chemical properties of urban aerosols”**: the data on measured physical and chemical properties of aerosols, especially those of interest, will be used to setup numerical experiments;
- **WP3, Task 3.2**, **“Atmospheric urban aerosols in the city environment with account of its morphology, and their relationship with solar radiation and the urban heat island”**: numerical experiments allow to obtain fine scale spatial distribution of *different* aerosols in complex urban geometry, under contrasting background meteorological conditions, both typical and extreme in terms of wind and stratification;
- **WP4, “Creation of concept and methods of calculation of the mega-urban planetary boundary layer (PBL)”**: validating the newly developed theories for urban PBL development and their implications for aerosol distribution and transformations;
- **WP 6, “Interrelations and chemical (microparticles) transfer between urban atmosphere, soils and surface water”**: simulations of deposition of *different* aerosols on the soil and water surface in urban canopy under *different* background conditions.

Outline

- ❑ Objectives, tasks, deliverables
- ❑ Background
- ❑ Research questions
- ❑ Numerical techniques and facilities
- ❑ EC and aerosol monitoring tower in the MSU campus
- ❑ Collaboration with other Tasks and WPs

Objectives, tasks, deliverables

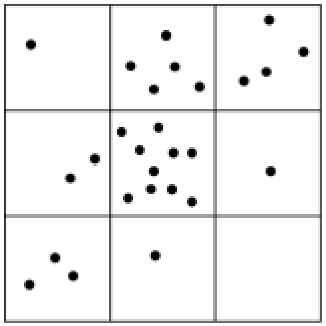
<u>Objective 3.</u> Assessing the links and consequences of spatial and temporal variability of urban pollution in various spheres (atmosphere, hydrosphere and pedosphere) and find out proper feedback loops to quantify formation and **urban heat island – air pollution – boundary layer dynamics interactions and feedbacks, as well as for prediction and diagnosis of pollution and aerosol dispersion having various origin with spatial resolution down to the scale of individual streets and buildings**

<u>Deliverable 2.</u> Patterns of transportation and accumulation of aerosols of various origin, in a wide range of sizes from nano- to microparticles in the urban canopy depending on background meteorological conditions

<u>WP2. Task 2.2</u> Study of aerosols formation and transport in urban boundary layer based on hydrodynamic turbulence-resolving models

Aerosol transport modeling

Largangian approach



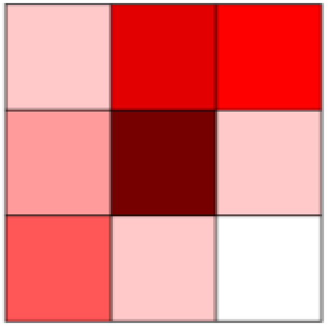
Trajectories of **individual particles** are tracked

$$\frac{\mathrm{d}\boldsymbol{x}_p}{\mathrm{d}t} = \boldsymbol{u}_p, \frac{\mathrm{d}\boldsymbol{u}_p}{\mathrm{d}t} = \sum \boldsymbol{F}$$

$\boldsymbol{x}_p$ – particle location,
$\boldsymbol{u}_p$ – particle velocity

+: explicit solution of particles motion

Eulerian approach



Advection and diffusion of **concentration** is computed

$$\frac{\partial\langle s\rangle}{\partial t} + \langle u_i\rangle\frac{\partial\langle s\rangle}{\partial x_i} = \frac{\partial}{\partial x_i}K_s\frac{\partial\langle s\rangle}{\partial x_i} + Q_s$$

$\langle s\rangle$ – Reynold-averaged particle concentration

+: low computational cost

Largangian approach contains more information, because concentrations can be computed from particles trajectories, but not *vice versa*

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t – time
$\boldsymbol{F}$ – external forces

$\langle u_i\rangle$ – *i*-th Euleran velocity component
K_s – turbulent diffusivity
Q_s – sources and sinks

Research questions

- How the locally measured concentrations of *different* aerosols of *various* origins are related to concentrations over the city regions under *different* synoptic conditions?
- What is the vertical distribution of *different* aerosols of *various* origins under *different* synoptic conditions inside an urban canopy and above?
- What is the deposition of *different* aerosols of *various* origins on the soil surface in urban canopy under *different* synoptic conditions?
- What is the role of aerosol particles *dynamics* in their *interactions* in convective and stable boundary layers?
- Are there indices which may diagnose on a routine basis the vertical spread of surface-originated aerosols?