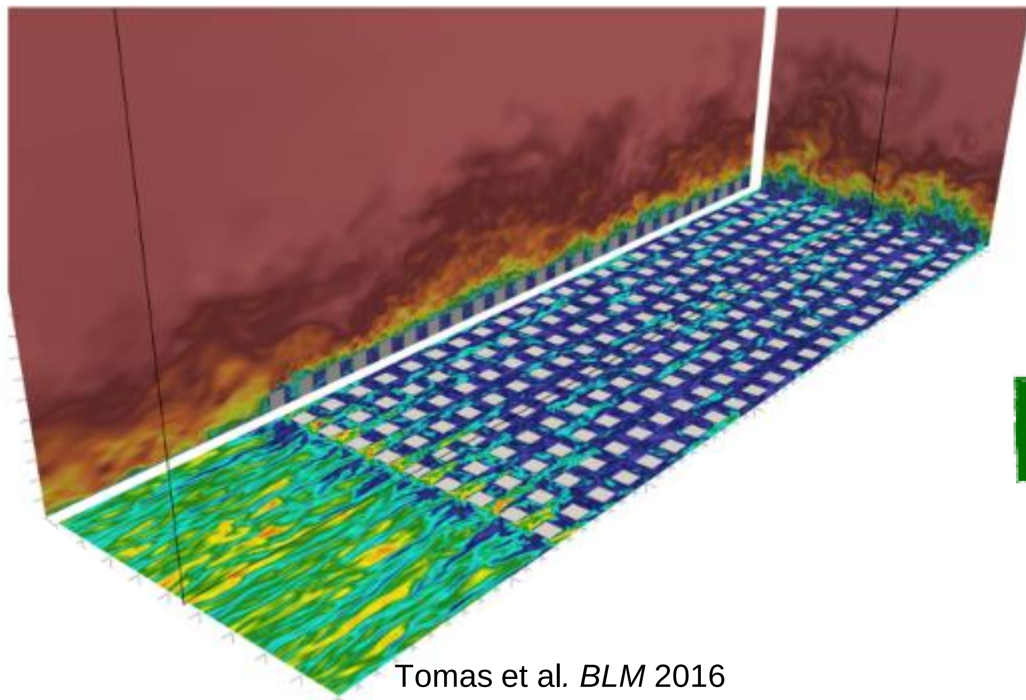
bringing our high-resolution urban microclimate models to the exascale



Tomas et al. *BLM* 2016

artstation.com

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TU Delft, 3ME, Process & Energy Dept.

TU Delft

Climate Action Lunch Lecture | TU Delft | 14 Sep 2023

outline

- **motivation**

  urban flows

  why bothering about speeding-up our numerical solvers

  high-performance computing and the exascale milestone

- **efficient high-resolution simulations of the air flow through a city**

  recipe to achieve this efficiently while securing the solution fidelity

  computational tools @ TU Delft and their extreme-scale computing readiness

  ongoing projects

- **summary & outlook**

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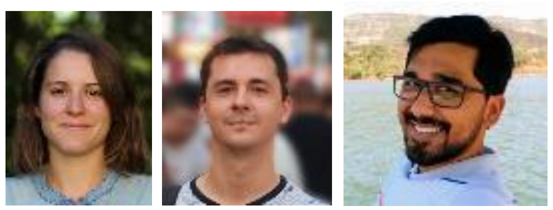

BK – 3D Geoinformation

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Stephan de Rhode
Fredrik Jansson
Caspar Jungbacker

CiTG – Atmospheric Sciences

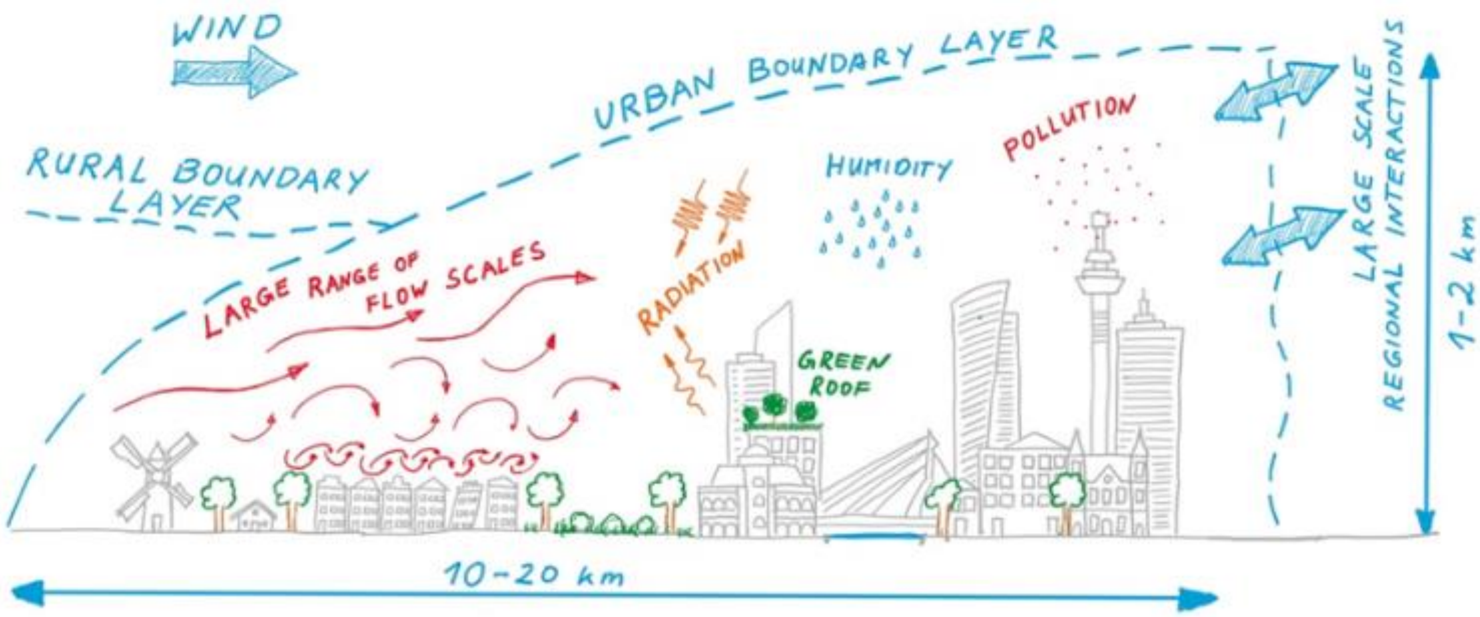
TU Delft

NVIDIA

motivation

(Lapalissade)

transport phenomena in urban areas



recurrent issues:

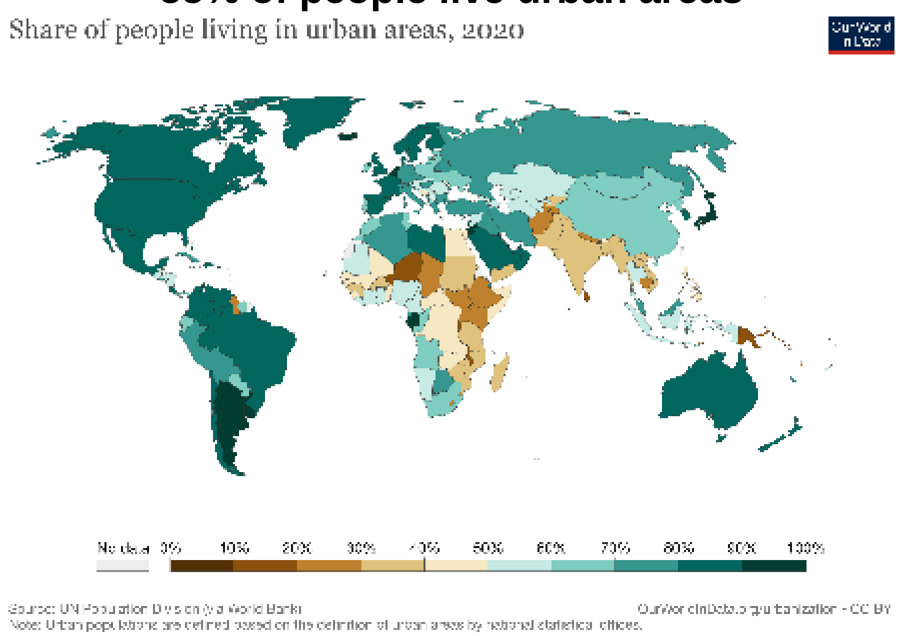
- higher emissions of pollutants & green house gases
- 'urban heat island'
- increased energy consumption
- poorer comfort and health
- ecosystem & surrounding climate disruption
- …

and all exacerbated by climate change!

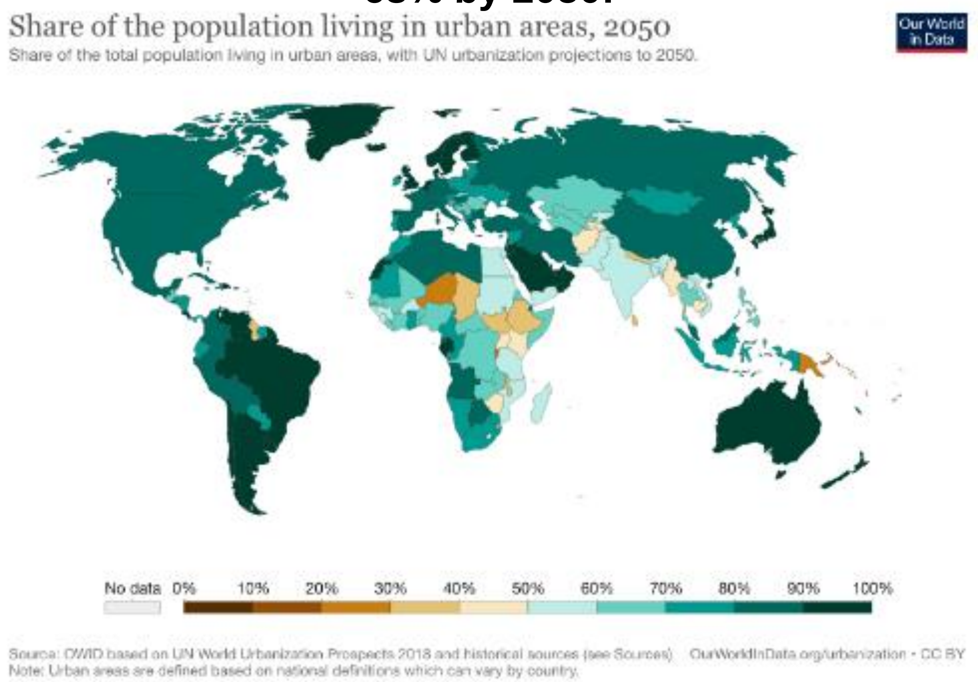
we ***cannot*** thrive sustainably without adapting to and mitigating (if not minimising) these issues

… and for that we need to understand and predict the transport dynamics of an urban system

55% of people live urban areas

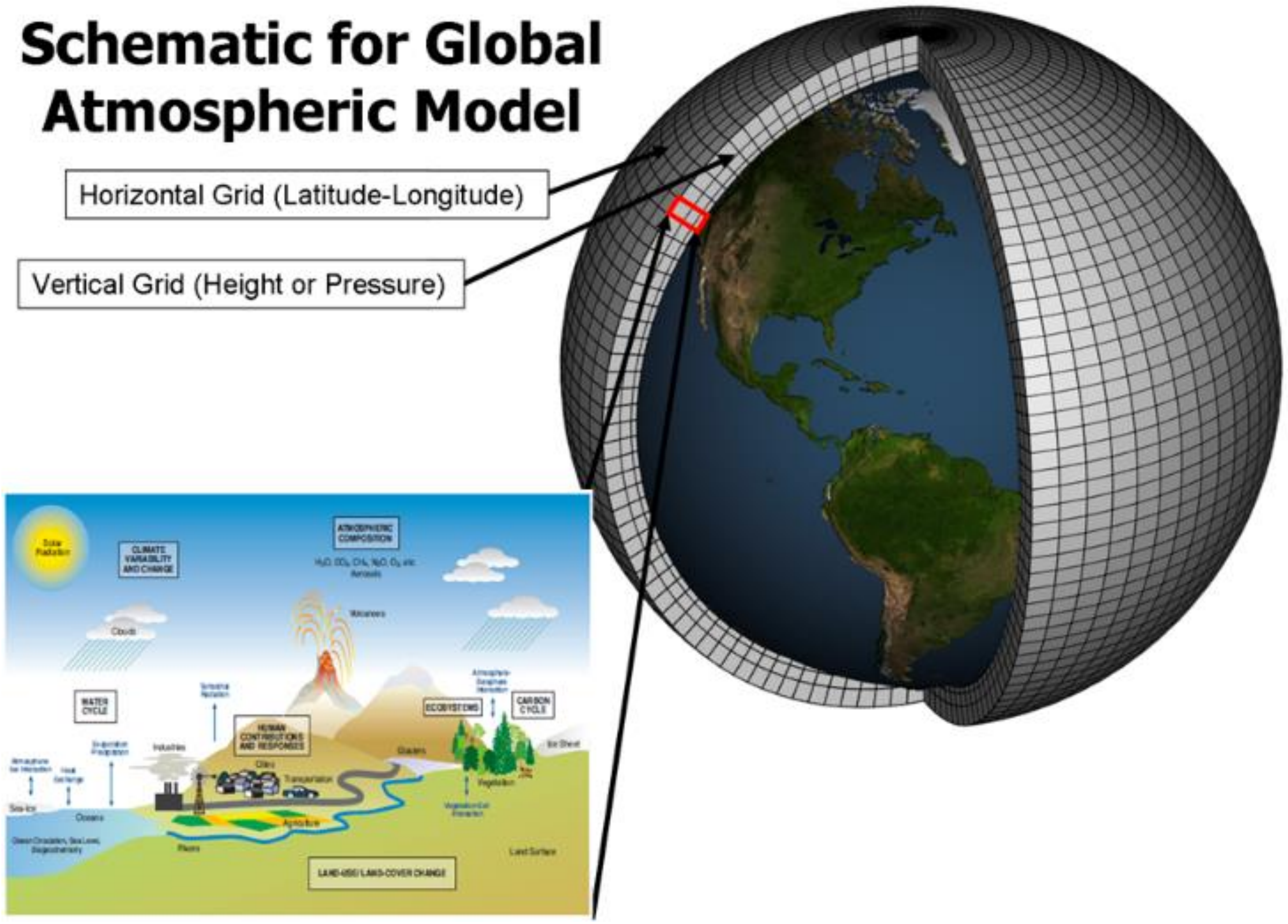


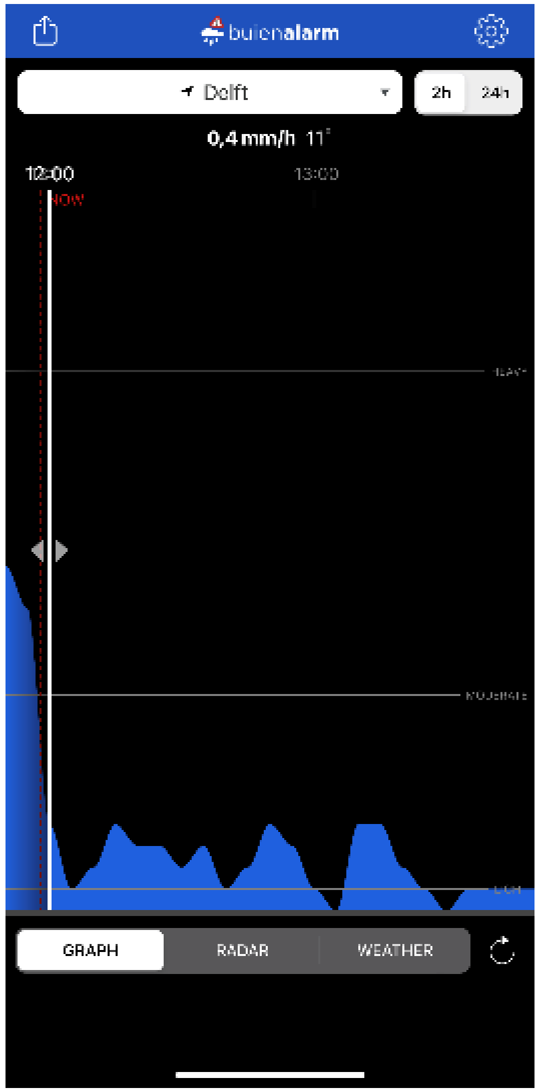
68% by 2050!



- **more urban area** (~ 1 South Africa by 2030)
- **more people in urban areas** (~2.4 billion people by 2050)
- **higher urban population density**

why do we need high-performance computing?



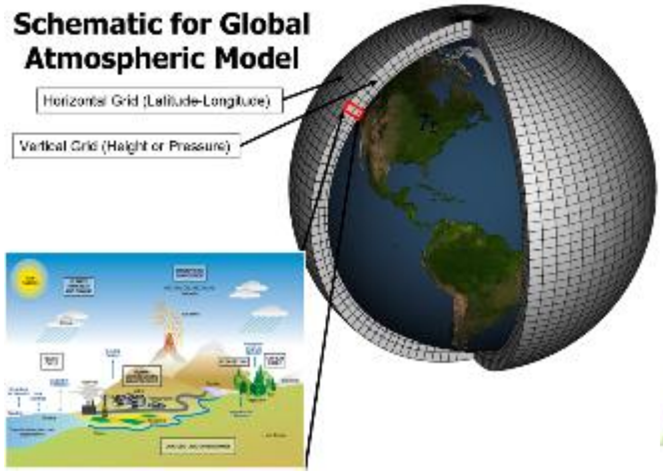


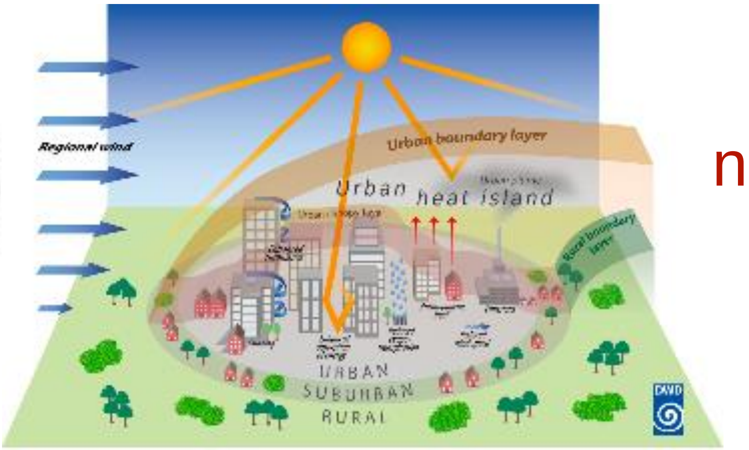
weather & climate

we need to simulate <u>big systems</u>, <u>fast</u>!

motivation

more broadly, why keep pushing the limits of our numerical solvers?

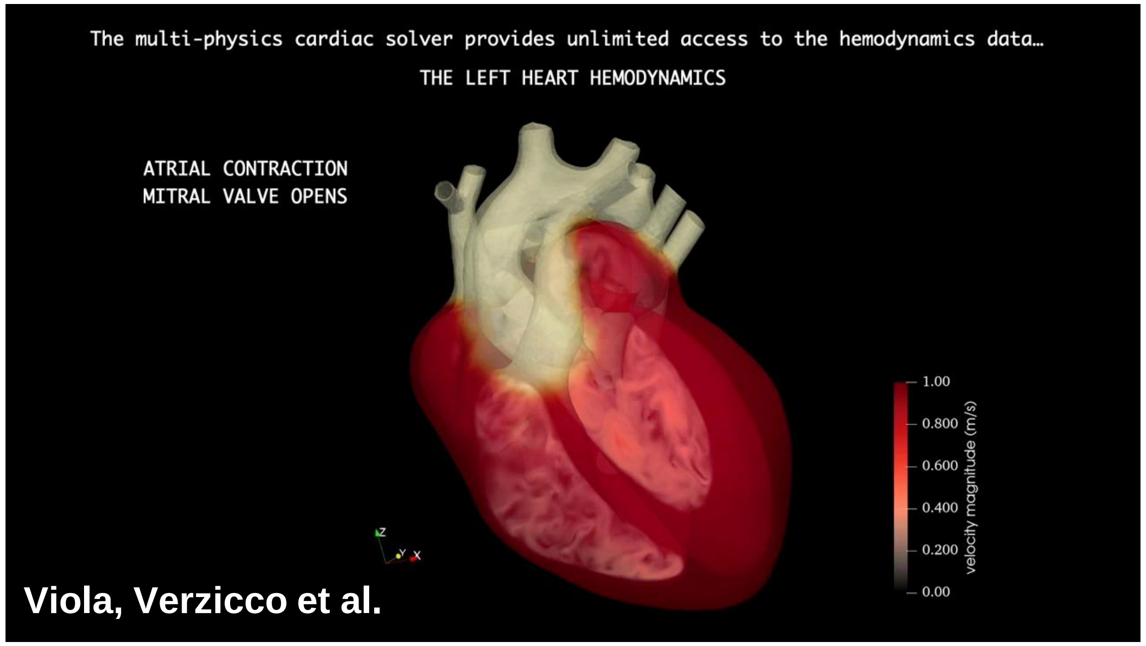




dwd.de

climate / energy

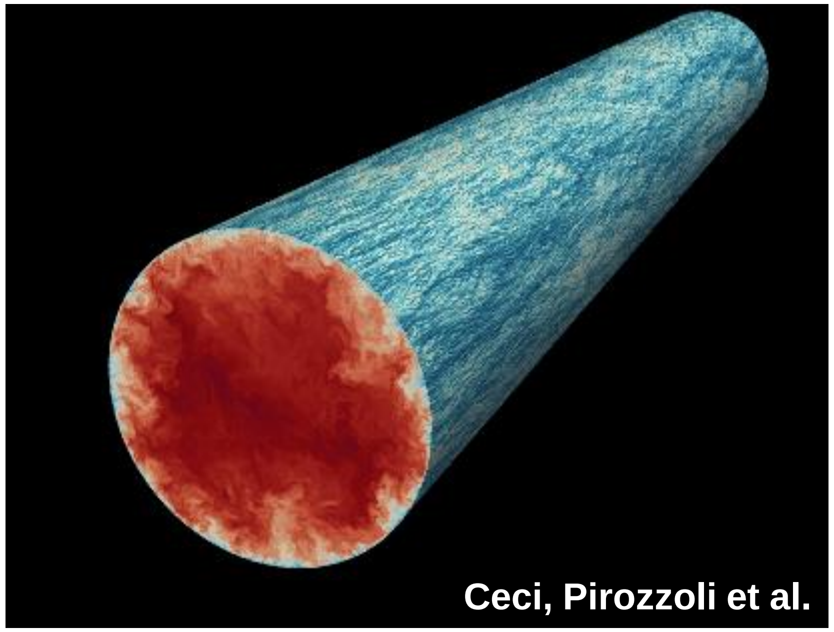
need to **increase resolution**!



Viola, Verzicco et al.

health

need for **fast** predictions and U.Q. in digital twins



Ceci, Pirozzoli et al.

fundamentals of turbulent fluid transport

need to understand the flow of water at high flow speeds

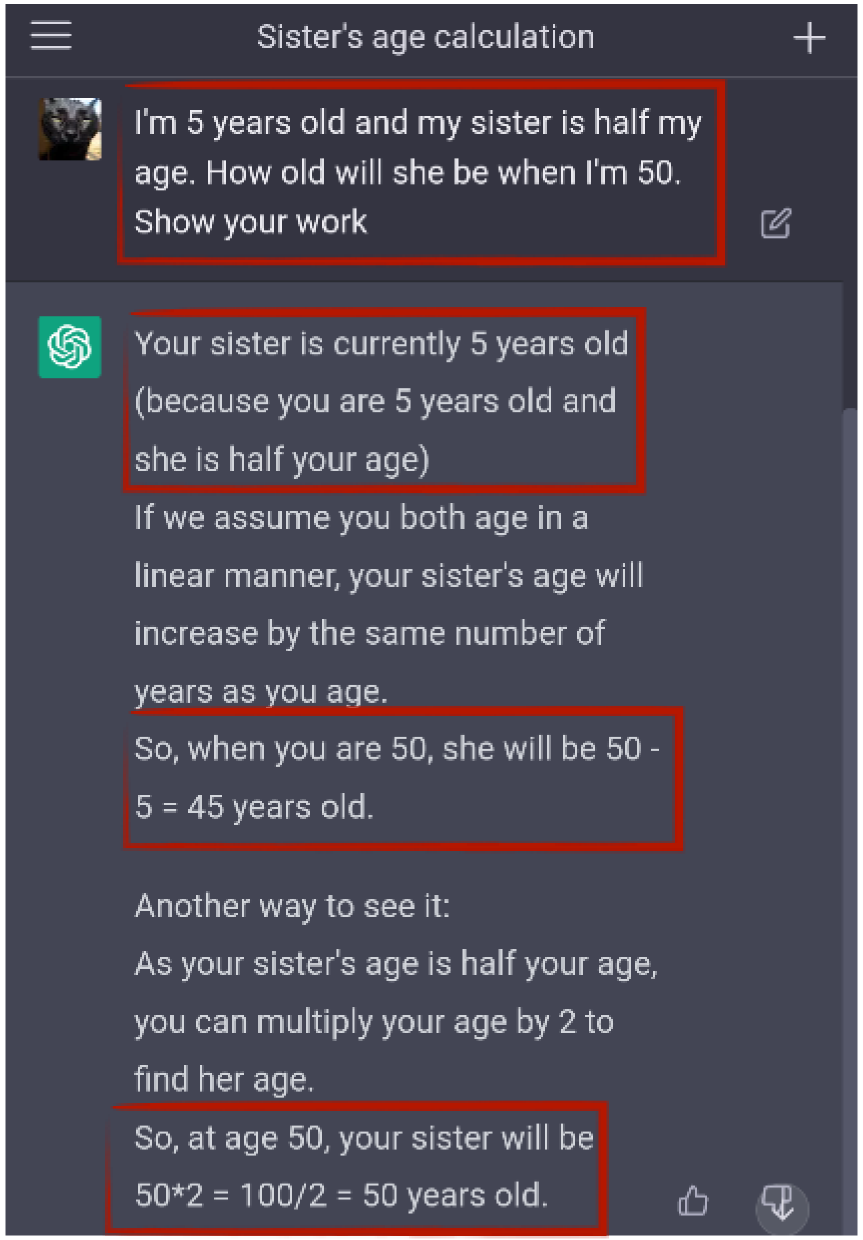
all these important applications and many more require solving the equations governing an incompressible fluid flow — the Navier-Stokes equations

the exascale computing milestone

log scale!

10^{18}FLOPS/s

change in paradigm



HPC systems not anymore driven by engineering applications, but by AI!

turns out that adapting to this change is annoyingly hard, though the benefits are extremely compelling!

parallel simulation of an incompressible flow

challenges

- air modelled as <u>incompressible</u>, — speed of sound is infinite!

- in the simulation, a sneeze in the sports center will change the wind velocity *everywhere*

- unlike in AI applications, in this problem the GPUs need to talk *a lot* to each other during a calculation like this — a so-called all-to-all communication pattern
- different vendors provide different approaches for GPU programming — performance is not necessarily portable!

- **motivation**

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obstacle-resolving simulations of turbulent wind flow through the urban built environment

ingredients

- fast solver for the Navier-Stokes equations
- immerse city while retaining a simple computational grid
- efficient parallelization of the numerical algorithm
- versatility (handle city heterogeneity)
- sub grid-scale models for the turbulent transport
- closures for land surface fluxes (friction, heat, humidity)
- uncertainty quantification

Pađen et al.
Frontiers in Built Environment (2022): 141.

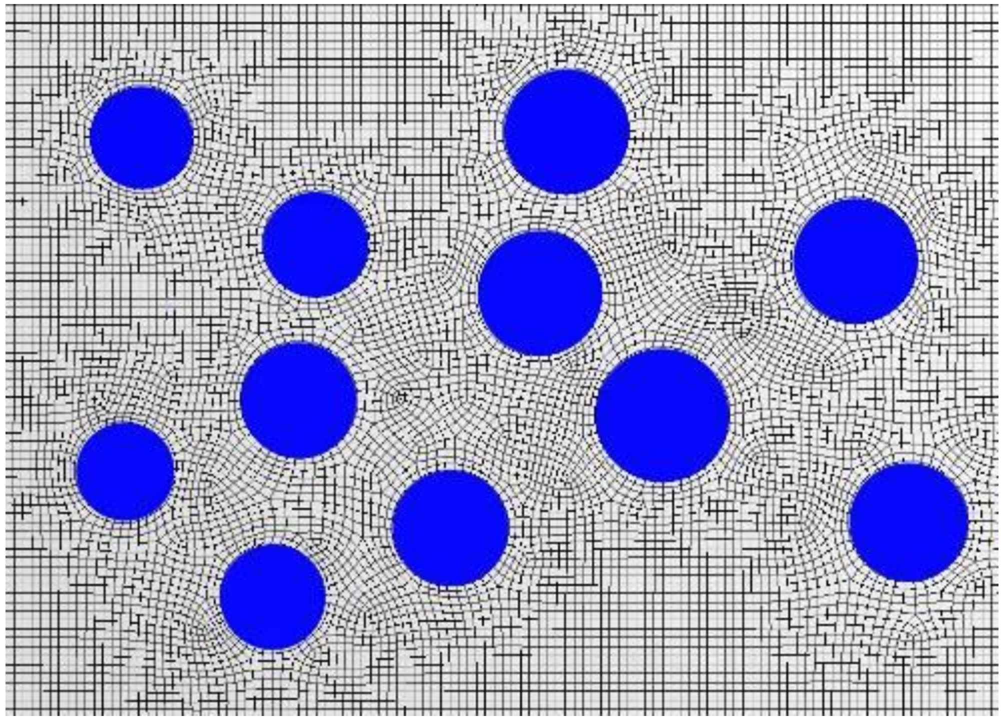
“solving the equations *right*”

“solving the *right* equations”

“solving the equations *enough*”

immersing a city in our solvers: immersed-boundary method

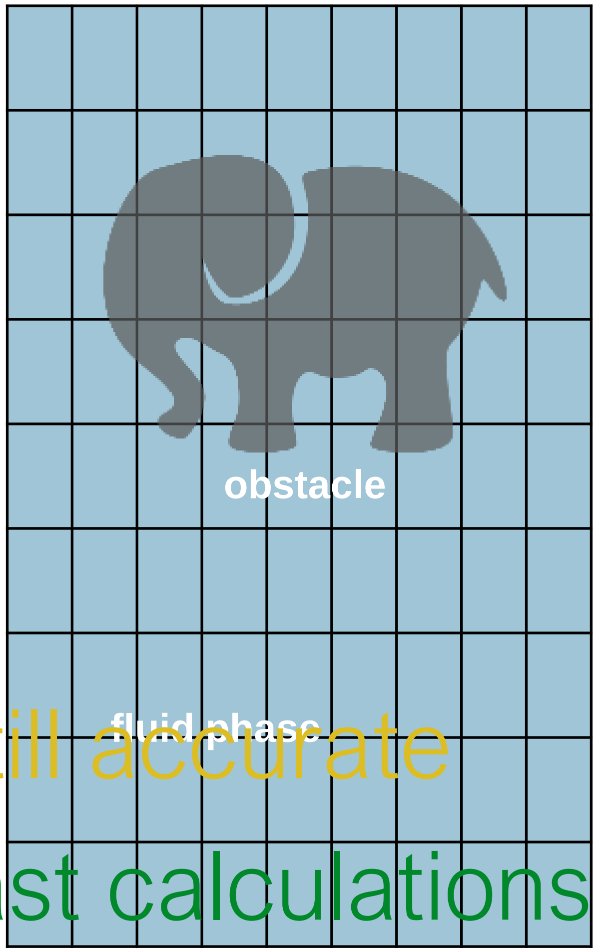
body-fitted **vs** **immersed-boundary**



accurate

very expensive

difficult implementation



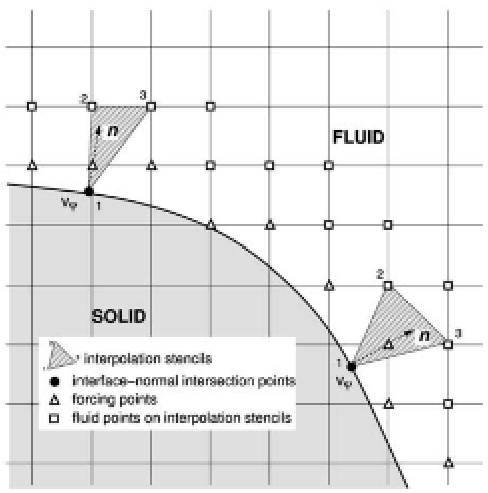
still accurate

fast calculations

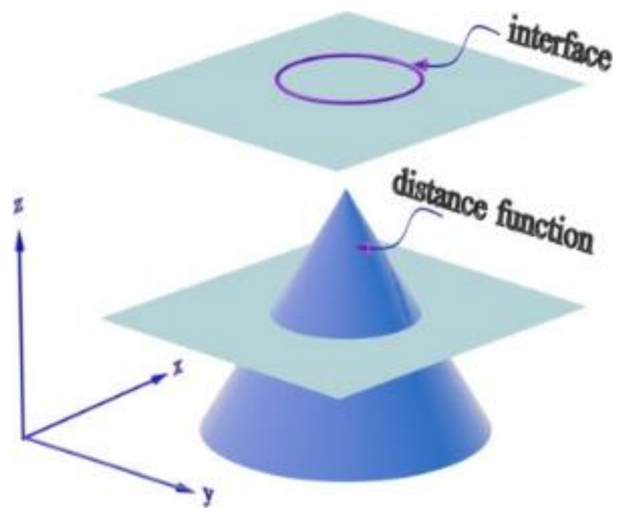
easy to implement

versatile boundary immersion

use signed-distance fields!



Yang & Balaras JCP 2006



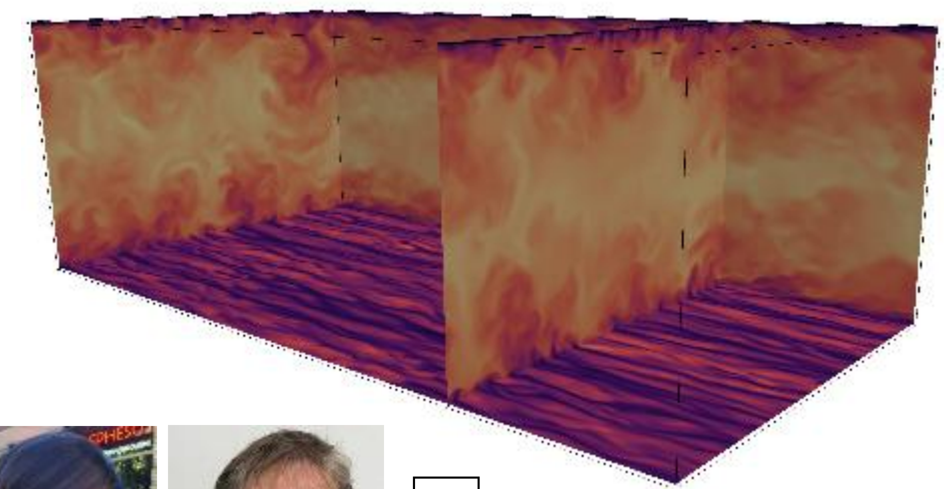
- simple
- versatile (complex geometries & BCs)
- compact stencils (computational efficiency)
- straightforward GPU acceleration
- implicit interface representation on our underlying Cartesian grid (avoid Lagrangian markers) — geometry naturally downsampled to our desired resolution

the backbone — fast incompressible finite difference solver

GitHub.com/CaNS-World/CaNS

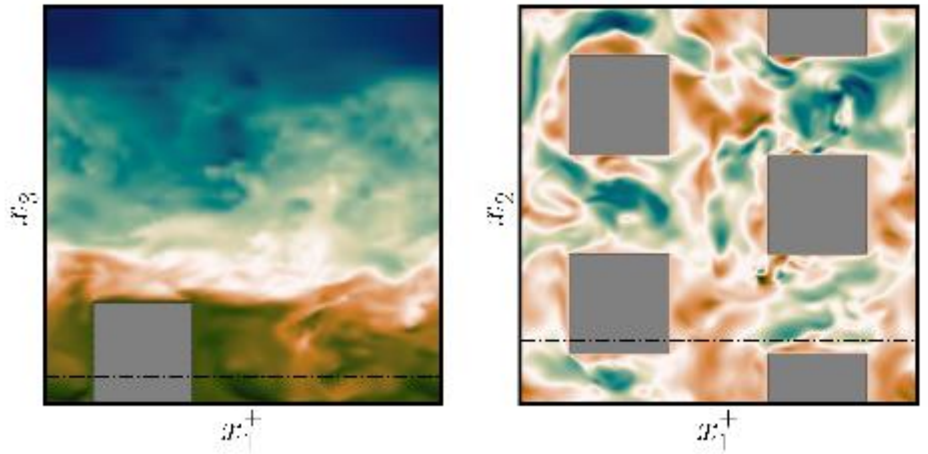
- old school, simple but versatile solver exploiting very fast numerical methods
- **runs efficiently up to ~10,000 GPUs** in parallel, leveraging an hardware-adaptive implementation
- tailored numerical method allowing for high-fidelity simulations of flows bounded by solid walls

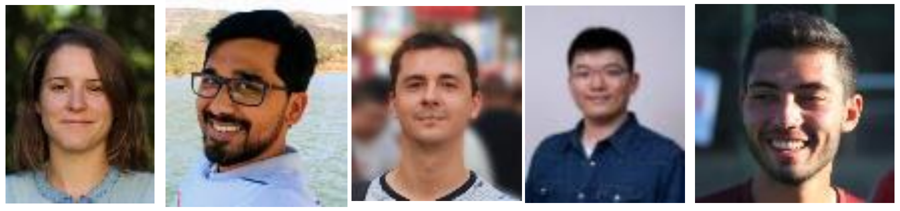
domain corresponding to a ***10 km^2 city with 1m resolution*** *in reach for CaNS 2.0 on O(100) A100 GPUs*



- Swarztrauber. ***Siam Review*** **19.3 (1977): 490-501**
- Costa. ***CAMWA 76 (2018) 1853–1862***
- Romero et al. **PASC22**

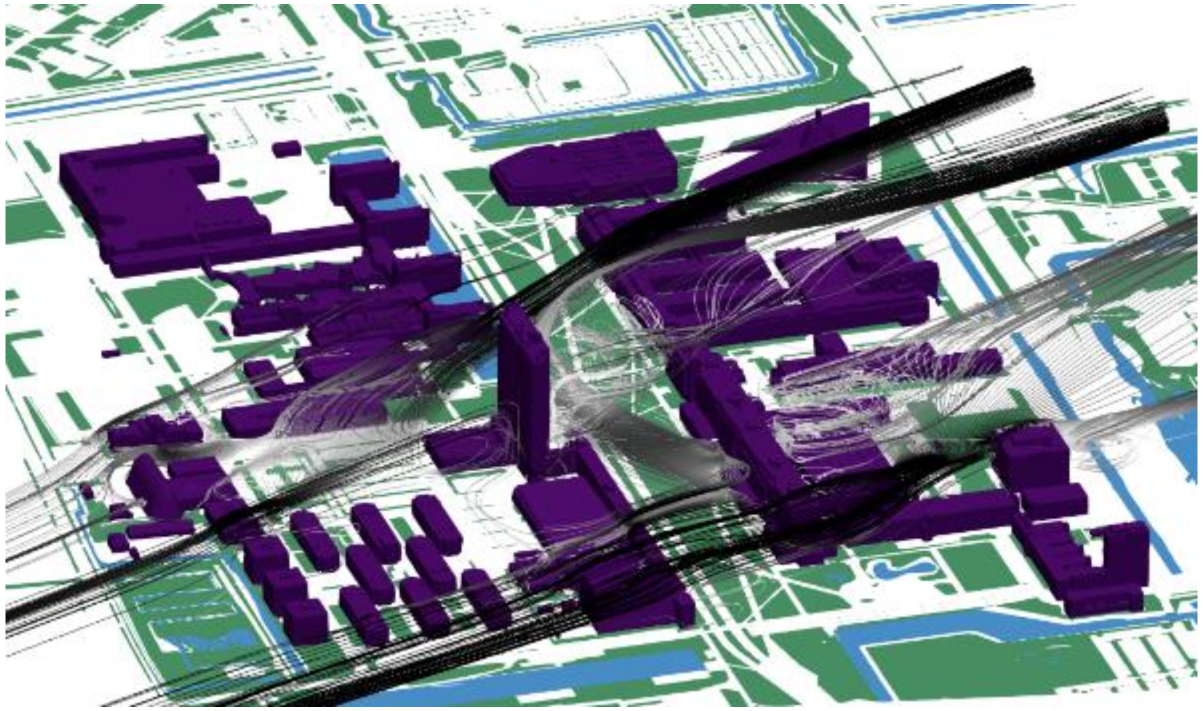
ongoing work — `urban-CaNS`





ongoing efforts

low-hanging fruit:
TUDFlow — the fluid dynamics of our campus
(CA Research and Education Seed Funding Grant)



Pađen et al.
Frontiers in Built Environment (2022): 141.

assessment “pedestrian”-level (dis)comfort

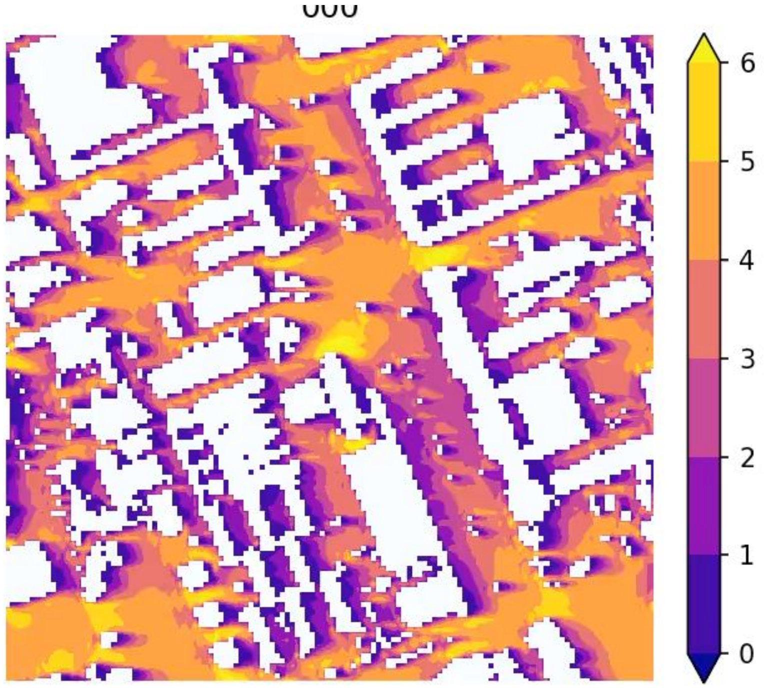
Dutch Atmospheric LES model (DALES)

- DALES is a complete and widely used high-resolution atmospheric model

- extended in 2016 to solve the flow over immersed obstacles (buildings)

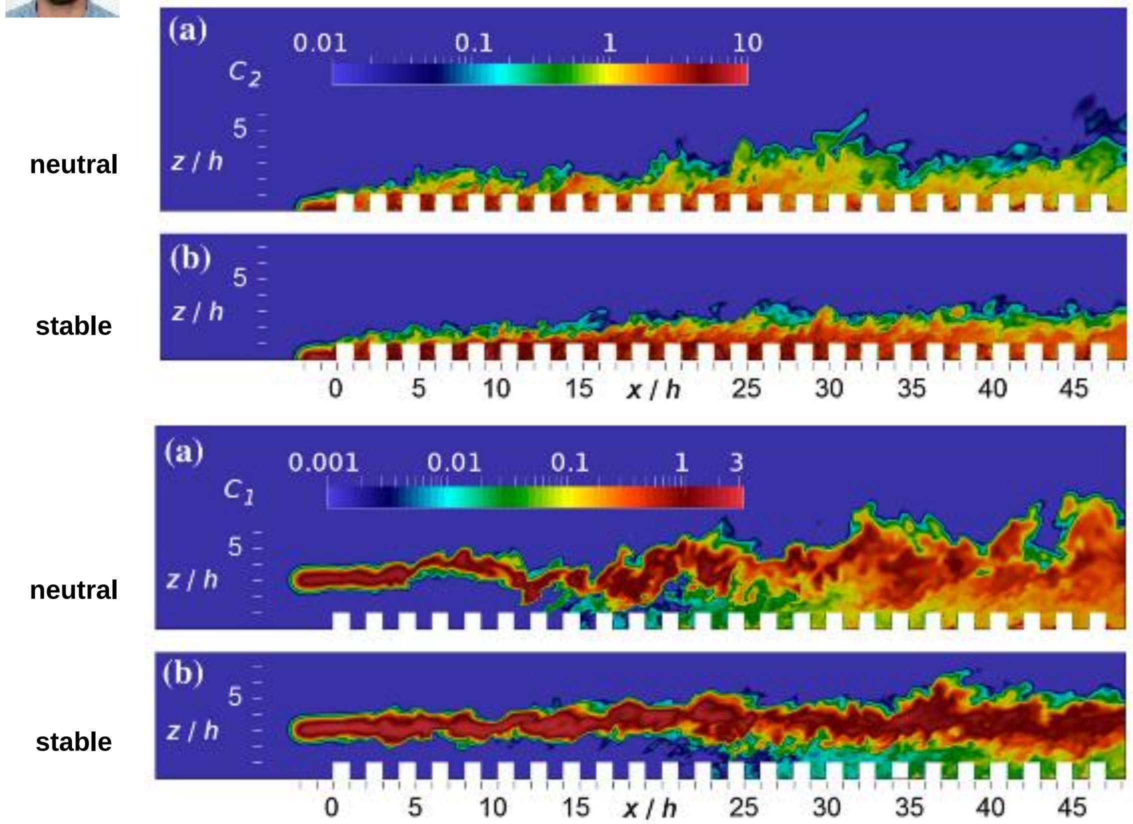
- fortunately, the base of CaNS and DALES is similar, which facilitates exchanges in features
- porting DALES for GPUs is hard, however:

Casper Jungbacker working on its porting using OpenACC, and making great progress: <u>about 2.5x speedup overall compared to the CPU version, w/ some parts featuring almost 10x speedups 🚀</u>

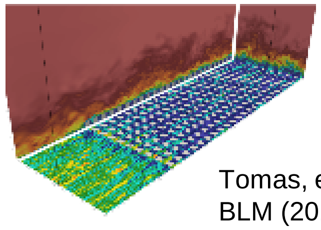


DALES simulation of a familiar site by Stephan de Roode & Fredrik Jansson

spatially-developing flow over a rural—urban roughness transition



- Stress IBM
- Vreman LES model
- 70M points
- Driver LES + Developing BL



Tomas, et al. BLM (2016)

CaNS ↔ DALES

ongoing work and outlook

fundamental studies at the microscale

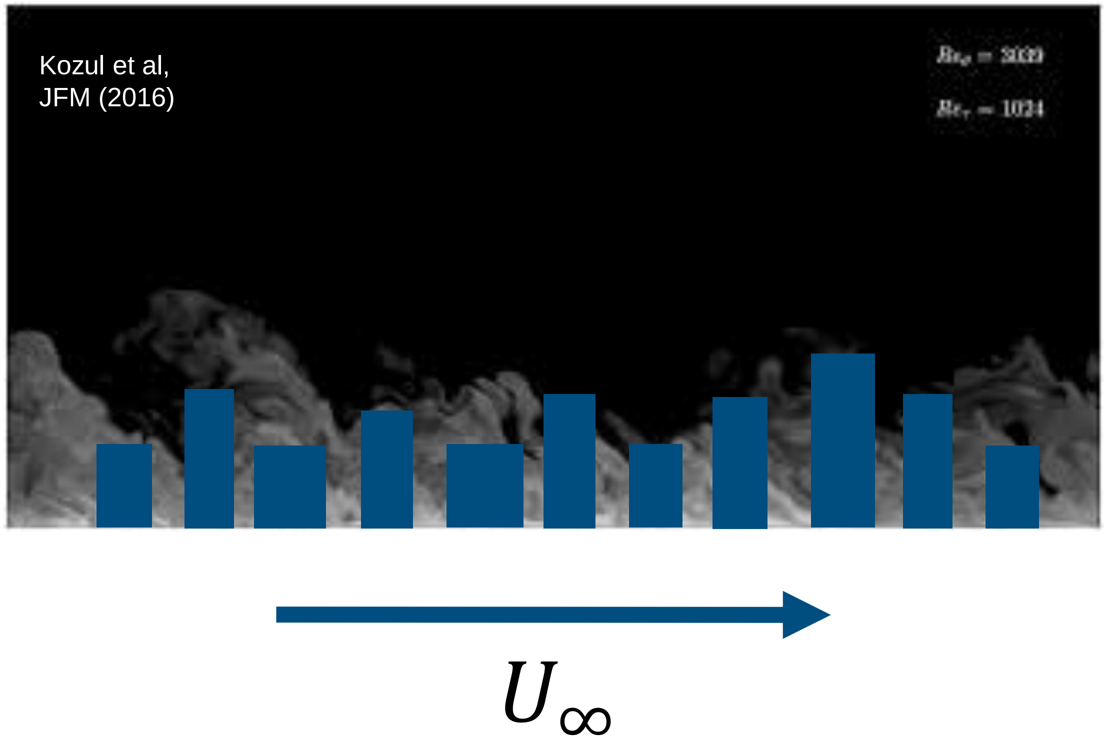
PhD project of Bartu Fazla, starting in October

science begins by asking simple questions about complex phenomena, but advances by asking more penetrating questions about simpler systems, whose solution could be obtained with rigour and explained with clarity.

— Stanley Corrsin

periodic roughness temporal boundary layer

- **features all transport dynamics** while allowing many fast insightful calculations with varying parameters
- **upscaling** — e.g., applicability of MOST within the internal BL?
- *Eulerian-eulerian & Eulerian-Lagragian **pollutant transport varying stability conditions & canopy layout***
- investigate the effectiveness of turbulence in the transport dynamics under **conjugate heat transfer**, **evapotranspiration** (grassland, then ideal trees), and **radiation** in non-participating and participating media — which remain elusive



mid-term outlook — predictive efforts

towards a high-resolution urban climate digital twin which allows to predict the effectiveness of adaptation/mitigation strategies

CaNS ↔ DALES

summary & outlook

- leveraging exascale computing is hard, since we do not do AI or other embarrassingly-parallel problems, but we are ready to exploit it!
- ideas from image processing and numerical modelling of multiphase flows are very useful for obstacle-resolving simulations of urban flows
- immersed-boundary methods provide simple and — for the right problems — powerful approaches for extreme-scale simulations of flows over complex topologies
- ongoing work
  - urban CaNS
  - TU Delft Campus Simulation effort
  - CaNS ↔ DALES
  - fundamental studies at the microscale
- outlook — high-resolution predictive efforts and converge towards an urban digital twin

thank you for your attention!