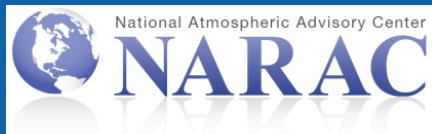


Development and Validation of a Fast CFD model for simulating flow and dispersion in urban areas and complex terrain

18th Joint Conference on the Applications of Air Pollution Meteorology with the A&WMA
Tuesday, 4th February 2014

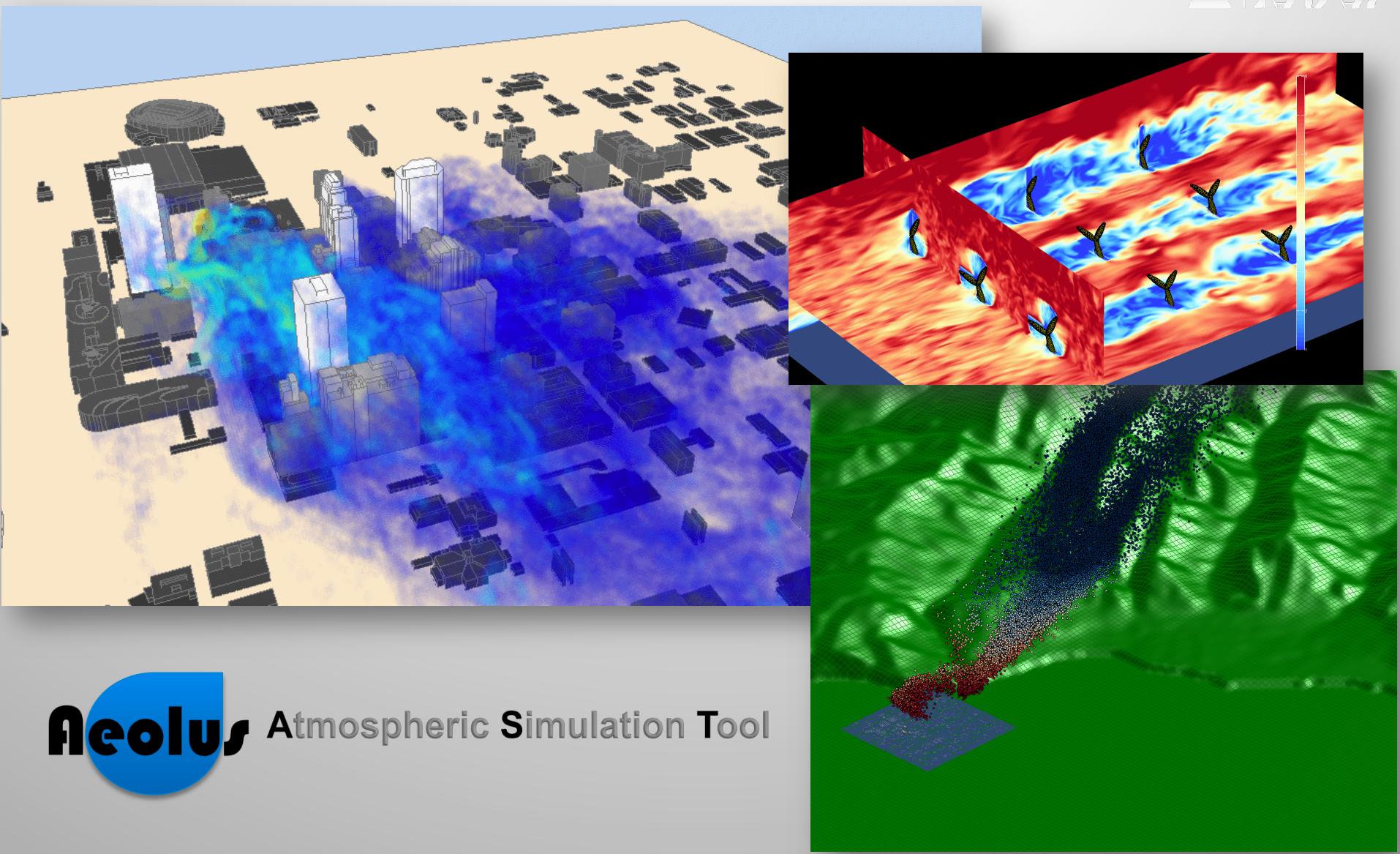
Akshay A. Gowardhan, LLNL



LLNL-PRES-648845

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC





Aeolus Atmospheric Simulation Tool

Aeolus Atmospheric Simulation Tool

- **Full physics atmospheric dispersion CFD model** developed for emergency planning and response applications in urban areas and complex terrain
 - Explicitly resolves buildings and terrain
 - Based on a **first principles physics solution of the** 3D Navier-Stokes equation (not a model based on simple empirical relationship and diagnostic parameterization that often **perform poorly** in complex urban scenarios)
- **Dual simulation modes**
 - Rapid assessment solution using **RANS** (dispersion simulation for a 2 km x 2 km urban area in minutes on a laptop)
 - Detailed dynamic high-resolution solution using **LES** (provides detailed turbulence analysis for complex dispersion scenarios)
- **Rapid fully-automated grid generation**
 - A grid for a 2km x 2km urban area can be generated from buildings shapefiles
 - Data available from 133-city NGA/USGS Dataset

Aeolus Atmospheric Simulation Tool

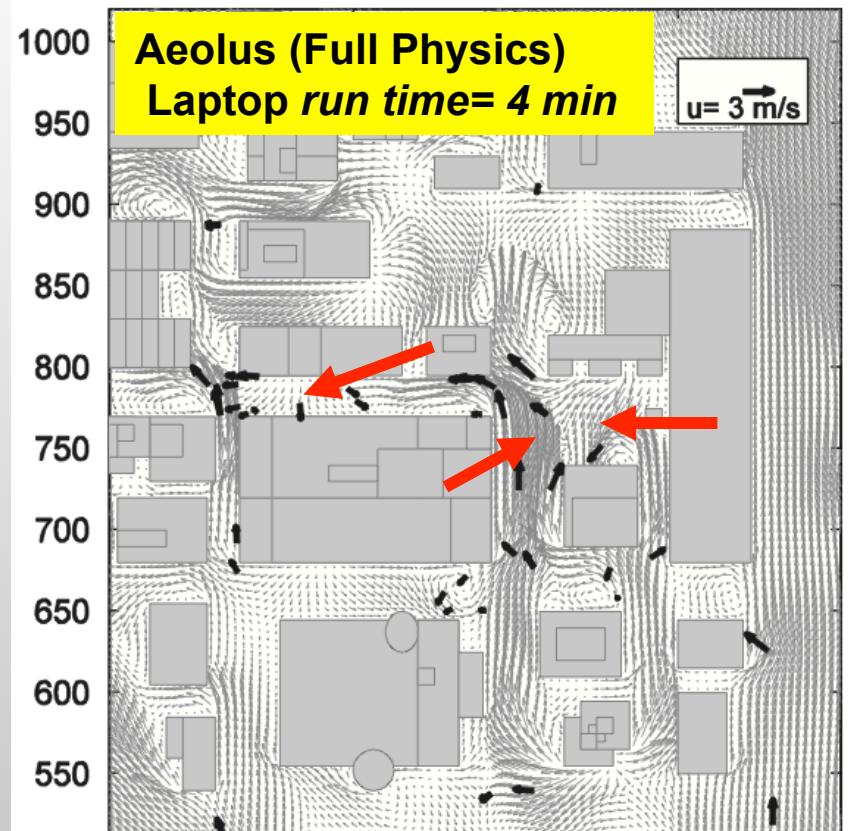
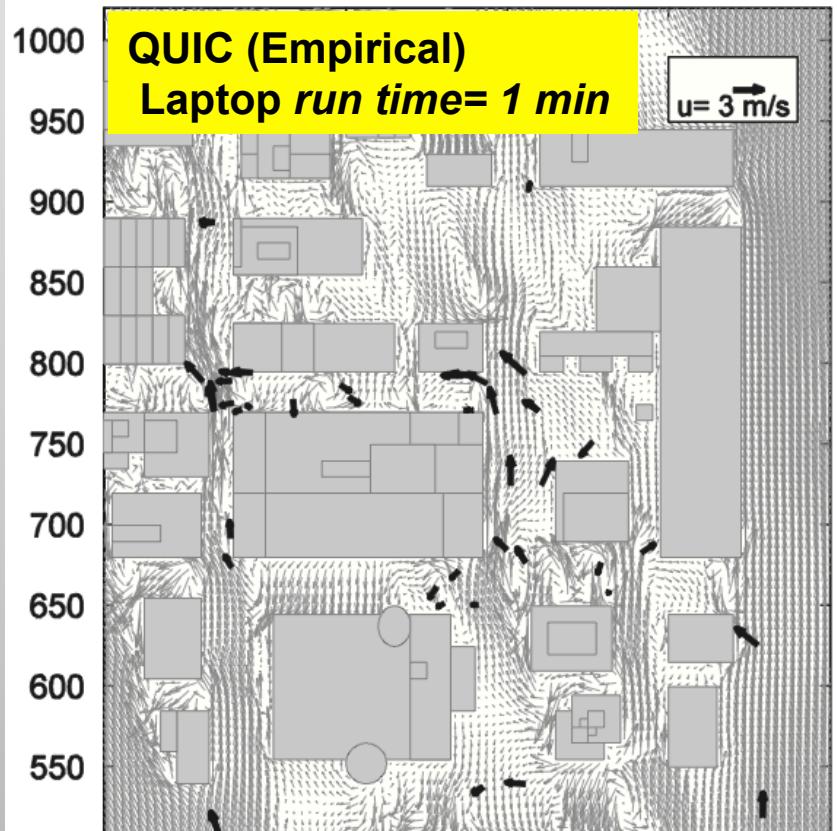
- Built-in **Lagrangian particle model** (no numerical diffusion)
 - Source types: neutrally buoyant gas, dense gas, buoyant releases, particulates
 - Dispersion model output:
 - 3D air concentration field
 - Detailed **3D deposition** patterns on ground and building surfaces
 - Dose calculations (based on toxic load model)
 - **3D pressure patterns** on buildings surfaces which can help drive indoor/outdoor infiltration models (e.g., CONTAM)
- Extensive validation against urban field study data, with demonstrated better performance than empirical models (*Gowardhan, A.A. and Brown, M.J., 2012: A Study of the Effects of Different Urban Wind Models on Dispersion Patterns Using Joint Urban 2003 Data, 17th Conference on Air Pollution Meteorology, New Orleans, Louisiana, USA, 22-26 January -26th, 2012*)

Technical Summary

Aeolus is a First-Principles Full-Physics Model

- Solves time dependent incompressible 3D Navier-Stokes equation
- Explicitly resolves complex terrain and buildings
- Produces 3D velocity, pressure, temperature, TKE, air concentration, and deposition fields
- Temperature effects incorporated using Boussinesq approximation
- High-fidelity Large Eddy Simulation model (Smagorinsky) or a fast response Reynolds Averaged Navier-Stokes model (Algebraic)
- Numerics: Uniform Cartesian mesh, second order accurate in space and time, pressure Poisson equation solved using a multigrid technique
- Dispersion modeled using a Lagrangian dispersion model
- Parallelized using OpenMP (Shared memory platform)

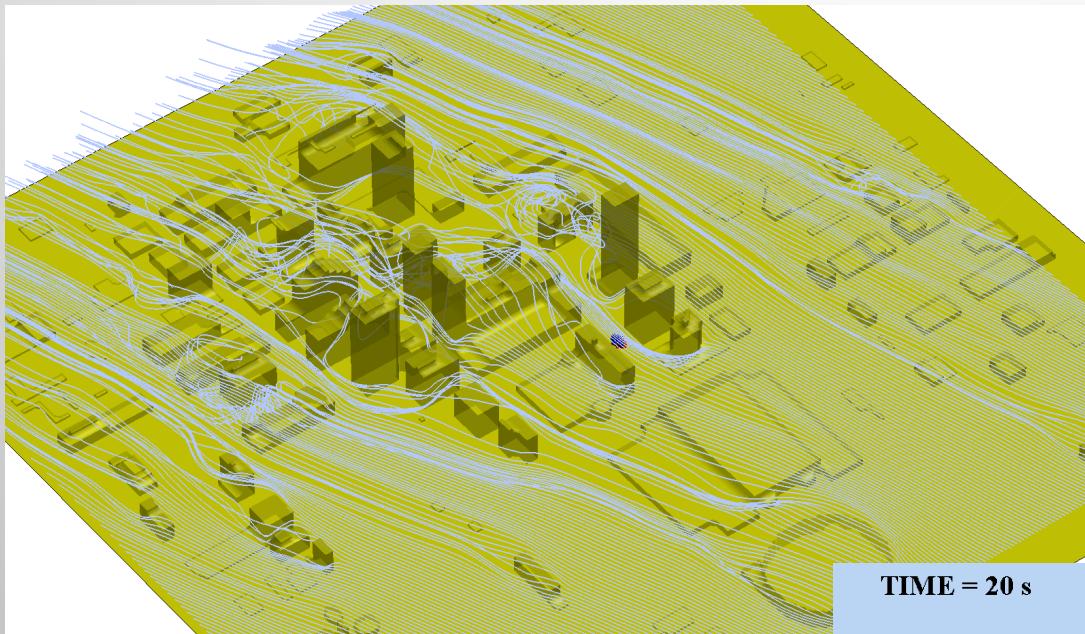
Aeolus Exhibits Better Performance Than Empirical Models in Complex Urban Environments



30 min. avg. velocity field: Measured (in black) and predicted (in gray) velocity field

Important features like **channeling**, **reversed flow**, **end vortex**, **divergence** etc. well predicted by Aeolus. Diagnostic models are unable to predict many of these features **from empirical relationships**.

Aeolus Provides Both Rapid Response and Detailed High-Resolution Capabilities



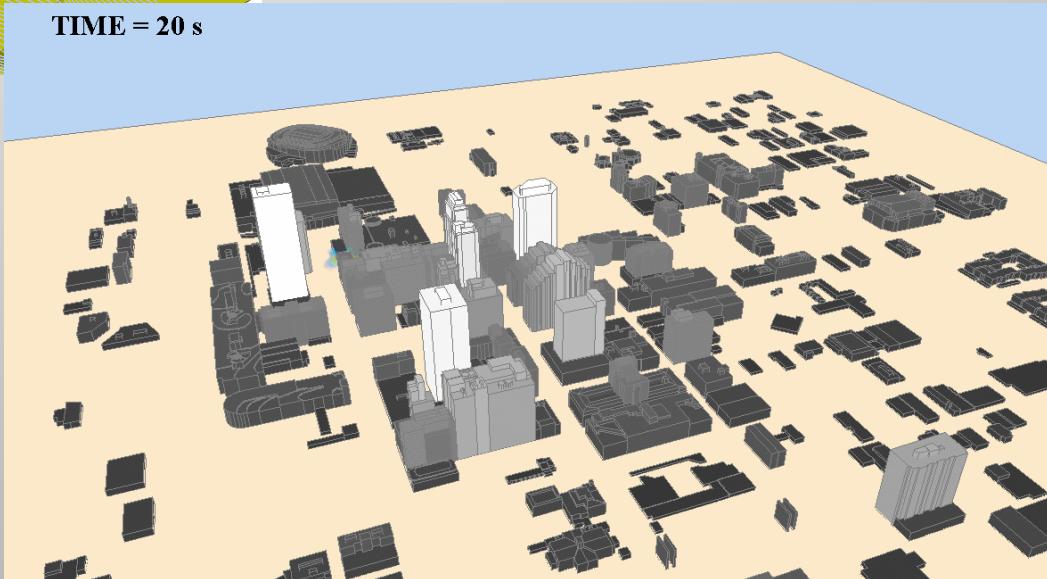
TIME = 20 s

(Bottom) Alternatively, it can be run in a *high fidelity Large Eddy Simulation* (LES) mode (~ hours) for a detailed analysis based on Smagorinsky model

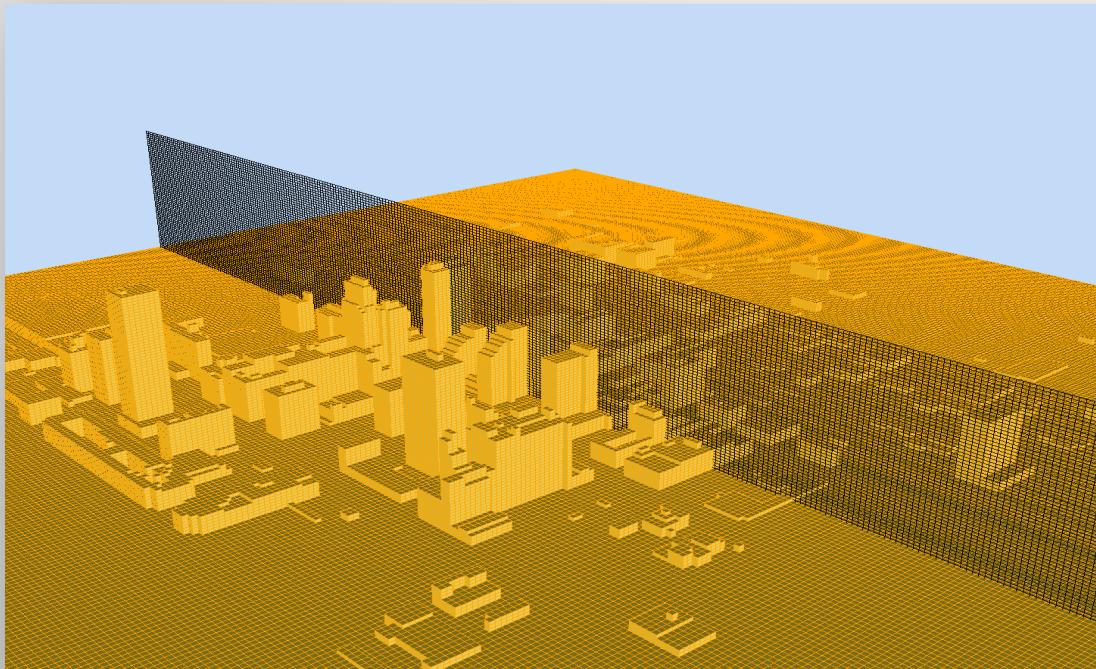
**LES simulation time =
several hours on a laptop**

(Top) The model can be run very efficiently (~5 min) using a Reynolds Averaged Navier-Stokes model (RANS) to produce a steady state solution for the 3D velocity, pressure and TKE field.

**RANS simulation time =
5 min on laptop**

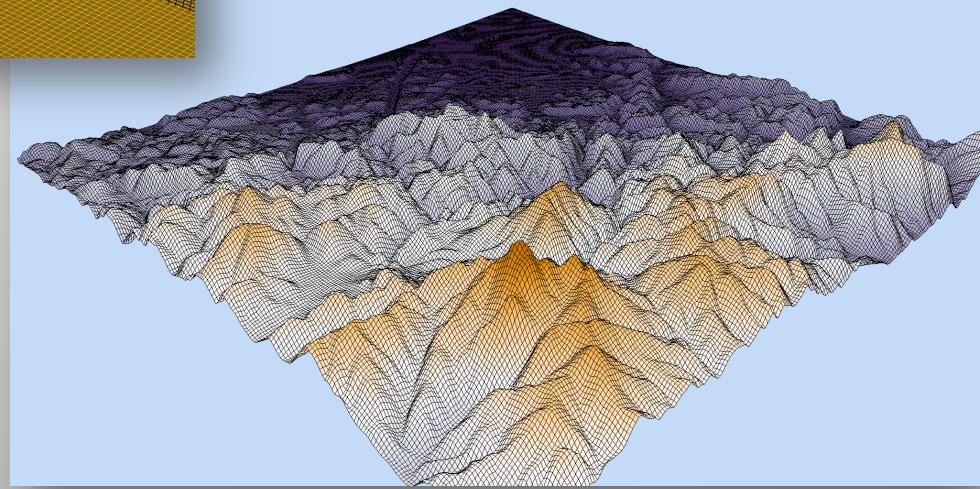


Grid Generation is Rapid and Fully Automated



Data available from 133-city
NGA/USGS Dataset

- Stair-stepped grid (3D matrix of 1s and 0s)
- Generated in seconds from shapefiles (few km) and/or USGS elevation data
- Same grid used for flow and dispersion



Aeolus Has Been Extensively Validated Against Urban Field Study Data Sets

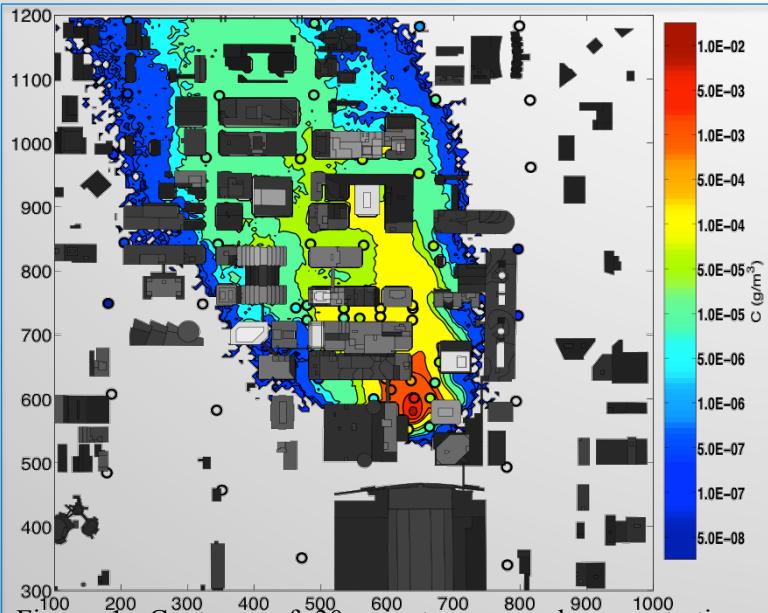


Figure 1: Contours of 30 minute averaged concentration overlaid with 30 min averaged field concentration data (color coded circle): horizontal slice (x - y plane) at 2 m AGL.

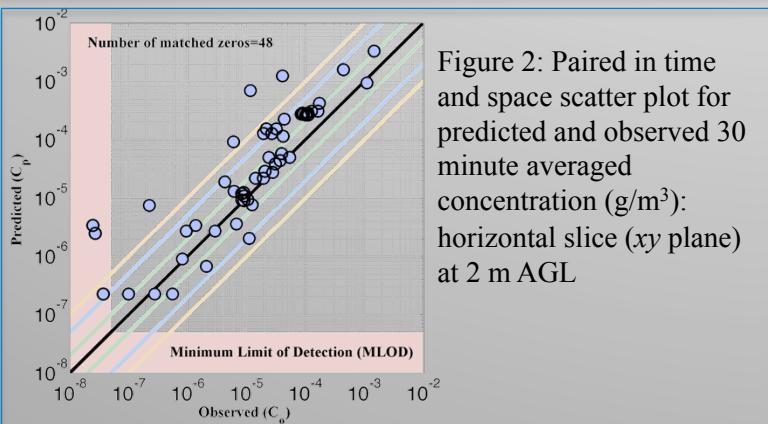


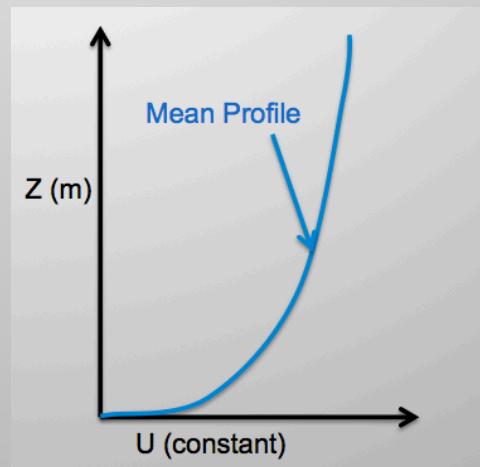
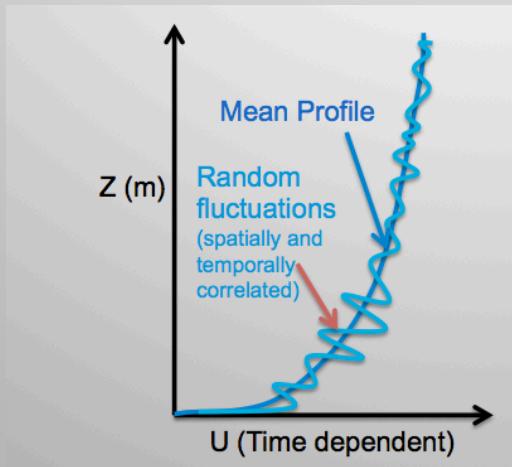
Figure 2: Paired in time and space scatter plot for predicted and observed 30 minute averaged concentration (g/m^3): horizontal slice (xy plane) at 2 m AGL

- The model was validated using data from 12 different trials during Joint Urban 2003 field campaign.
- The concentrations predicted by the model were found to be in **good agreement** with the field data (paired in time and space).
- ~50% were predicted within a factor of 2, ~70% within a factor of 5 and ~80% within a factor of 10.**
- The wind model (RANS) took ~200 sec for each of these cases (4.5 Million grid points) on a quad-core laptop.
- The Lagrangian dispersion model took ~80 sec (0.5 Million particles) on a quad-core laptop.

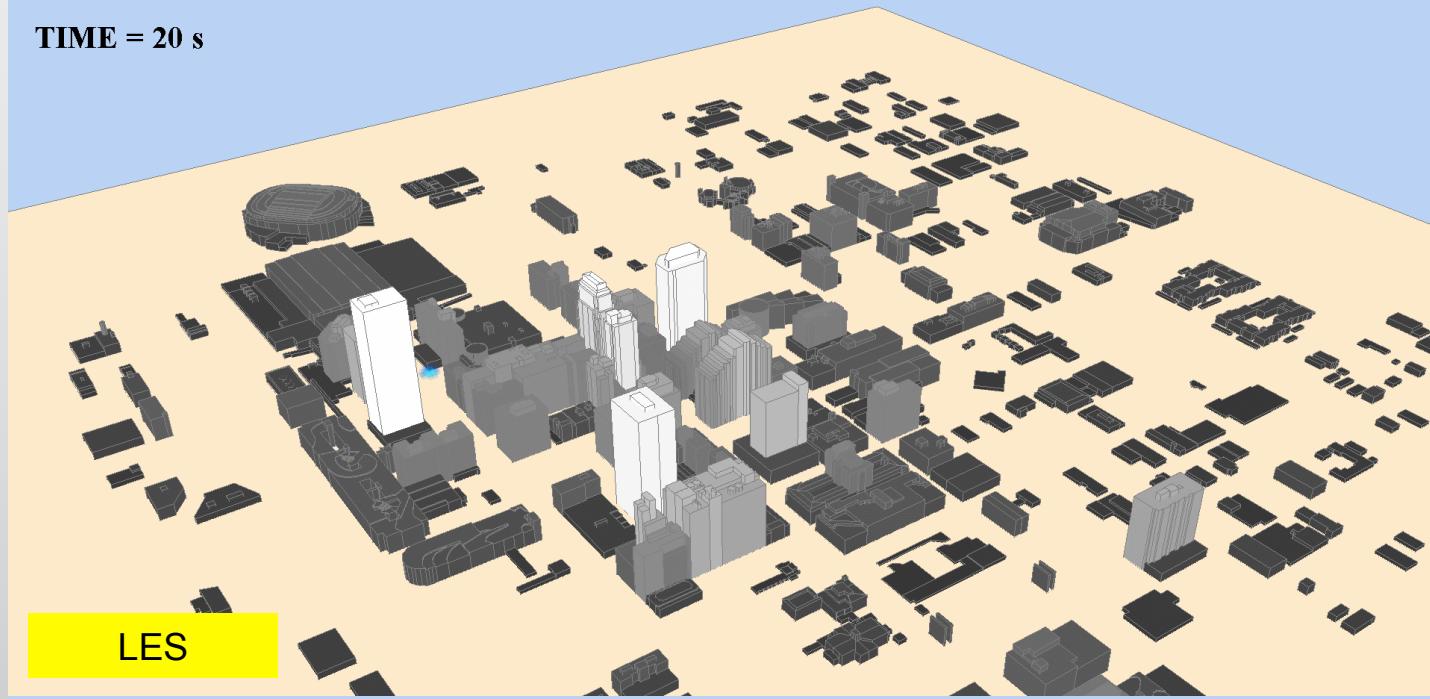
IOP#	FAC2 (%)	FAC5 (%)	FAC10 (%)	FB	Wind Model runtime (sec)	Plume Model runtime (sec)	Total runtime (sec)
IOP2, T3	46.67	61.67	70.00	-0.169	203.7	82.70	286.40
IOP3, T1	38.71	67.74	72.58	0.3770	202.7	67.10	269.80
IOP3, T2	53.33	70.67	86.67	0.0420	207.72	85.88	293.60
IOP3, T3	60.87	86.95	89.85	0.1477	203.53	78.93	282.46
IOP8, T1	35.41	60.41	79.16	-0.327	204.12	83.76	287.88
IOP8, T2	47.69	75.38	86.15	-0.486	211.17	82.14	293.13
IOP8, T3	45.45	68.18	71.21	-0.102	202.25	74.93	277.18
IOP9, T1	54.05	64.86	78.37	-0.201	204.23	83.54	287.77
IOP9, T2	60.41	79.16	85.41	-0.038	201.55	79.21	280.76
IOP9, T3	47.62	66.67	80.95	-0.017	198.62	72.33	270.95
IOP10, T1	46.67	68.89	82.22	0.1145	199.64	78.09	277.73
IOP10, T2	37.78	55.55	73.33	0.0777	208.27	84.62	292.89
Average	47.88	68.84	79.65	-0.048	203.95	79.43	283.38

LES vs. RANS

LES	RANS
• Time dependent 3D velocity field	• Steady state 3D velocity field
• Numerically resolves large energy containing eddies	• Numerically resolves only mean flow
• Smaller eddies (considered to be more universal) are modeled	• All of turbulence is modeled
• Needs more information to initialize	• Needs less information to initialize

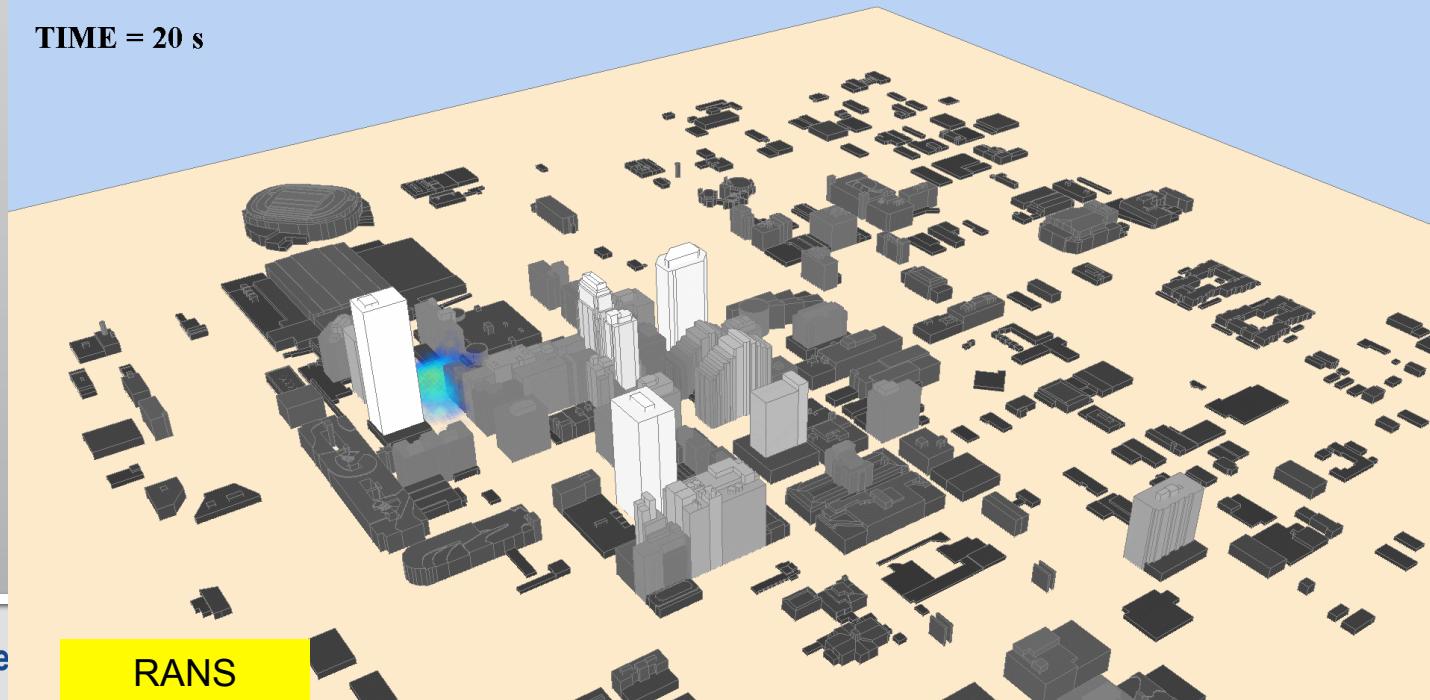


TIME = 20 s



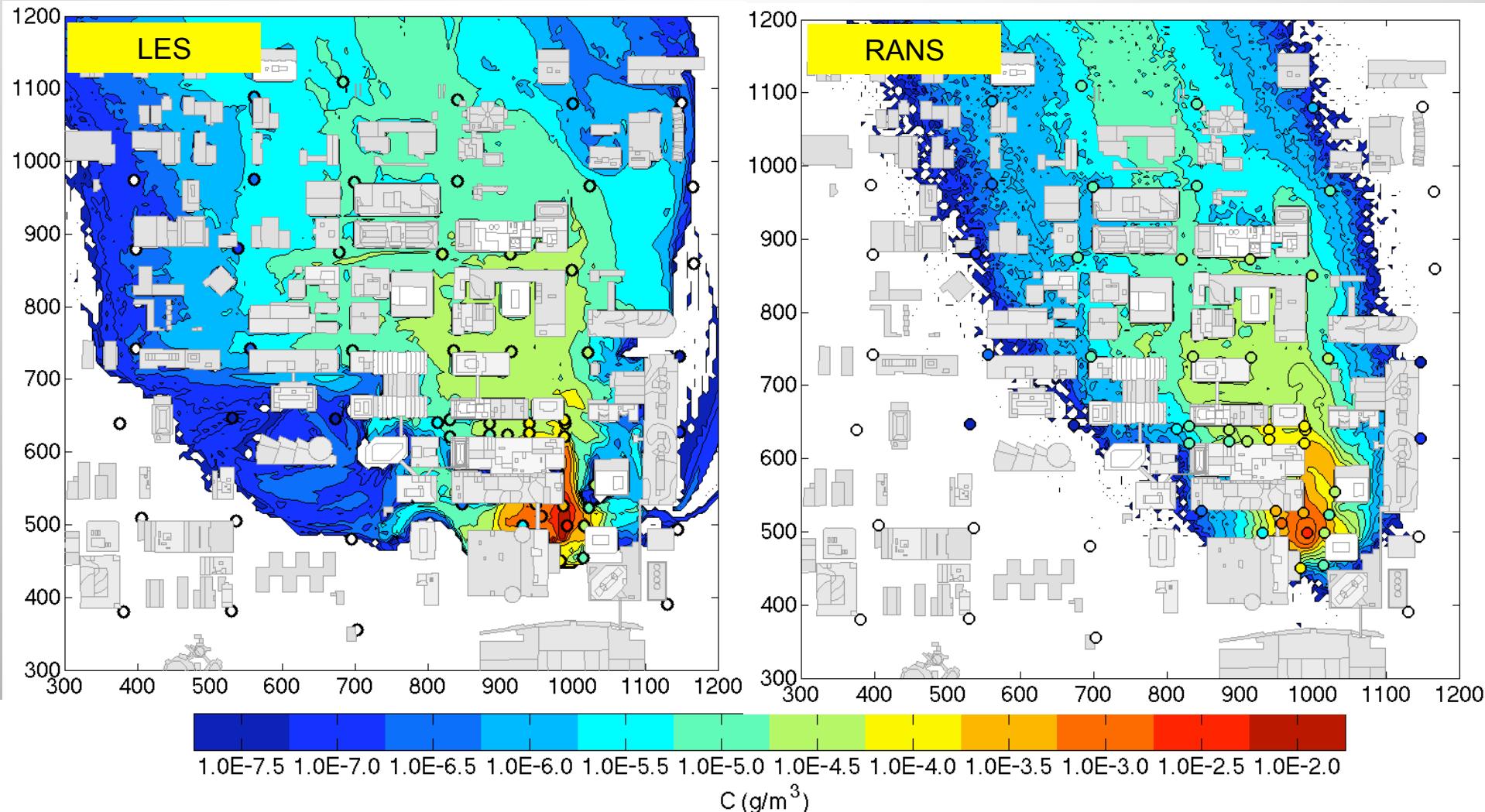
Runtime:
~6 hrs.
on Quad
core Laptop

TIME = 20 s



Runtime:
<5 min.
on Quad
core Laptop

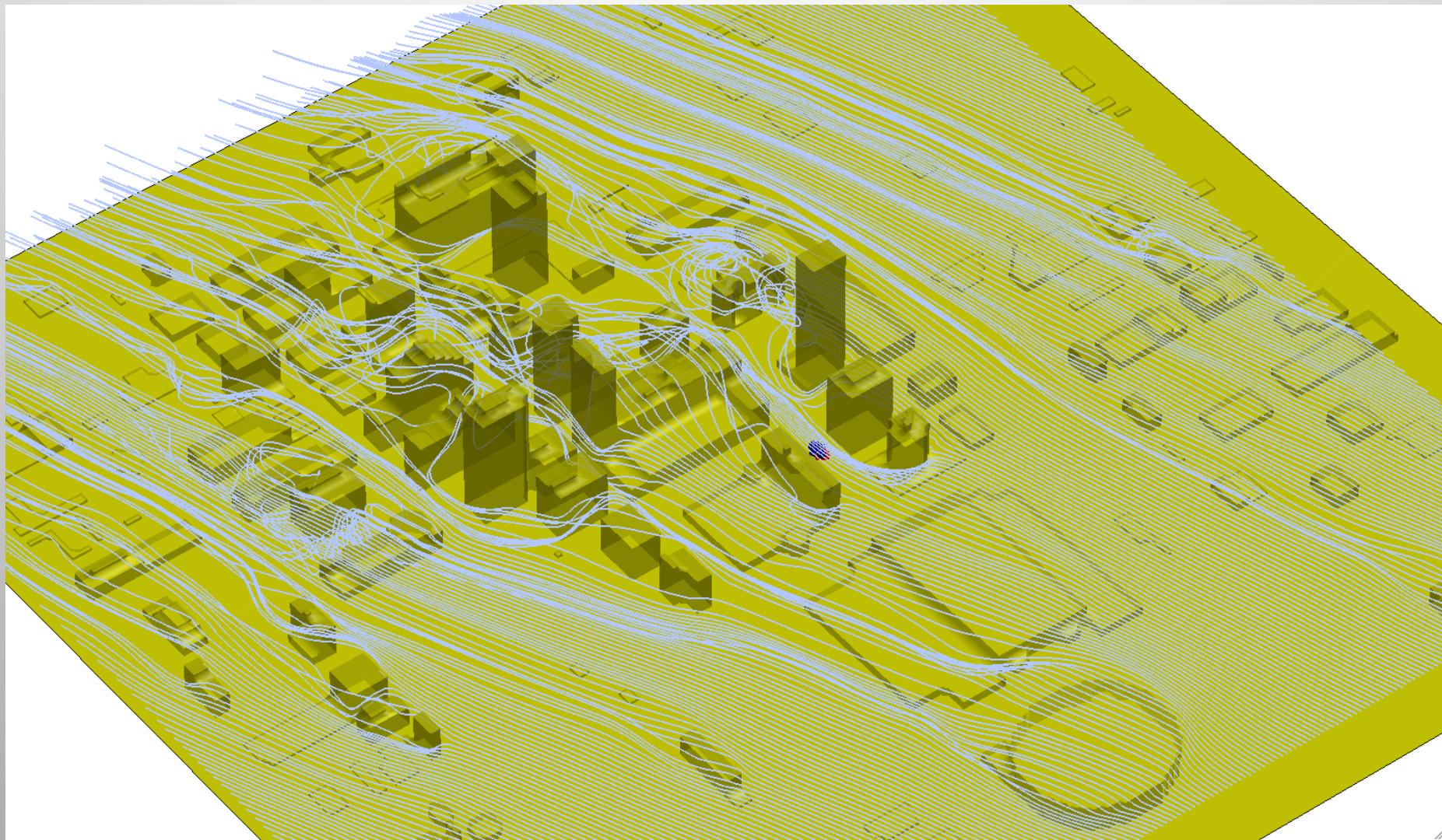
Results



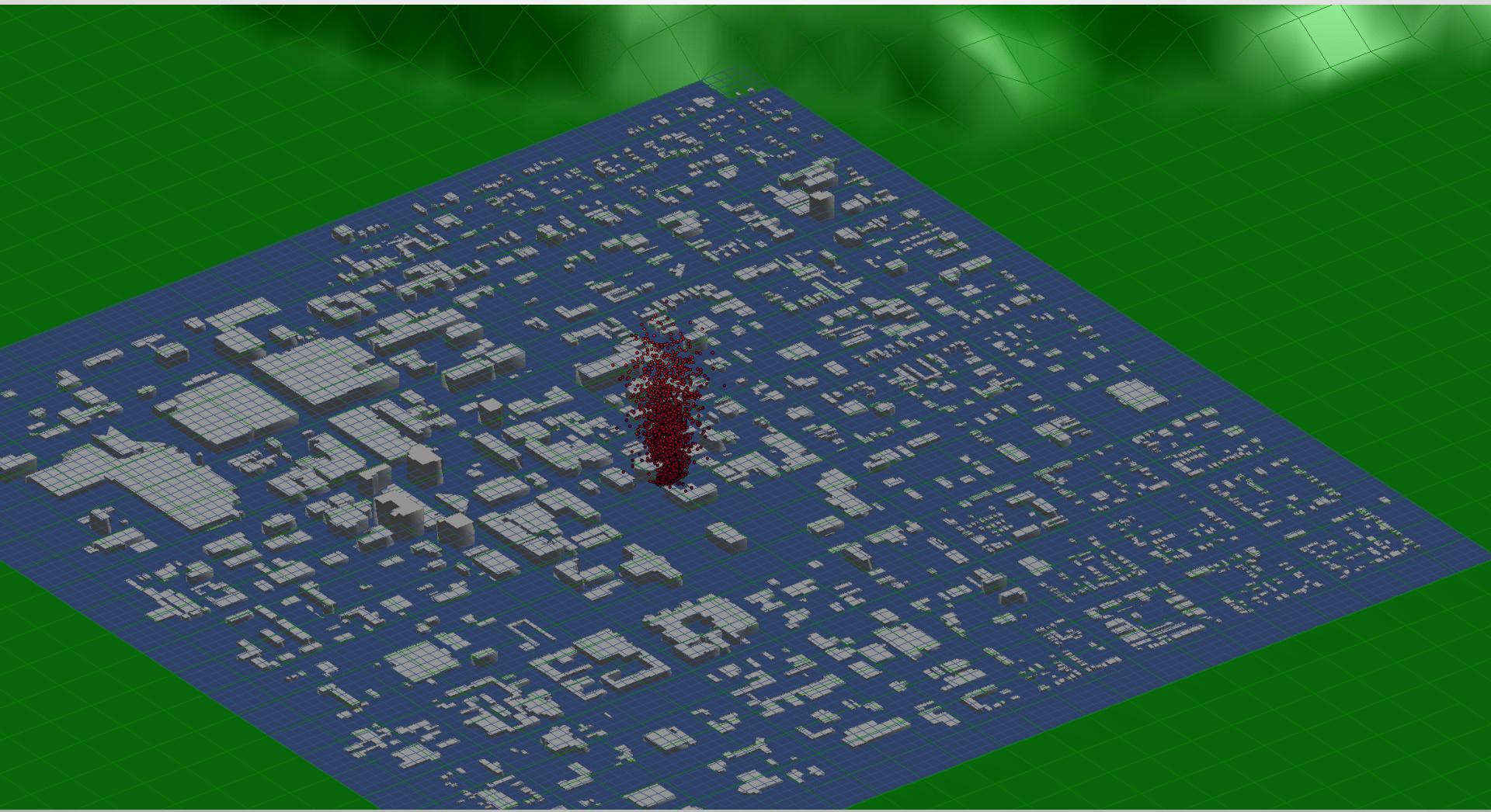
Contours of 30 minute averaged concentration overlaid with 30 min averaged field concentration data
 (color coded circle): horizontal slice (x - y plane) at 2 m AGL.

Example Results

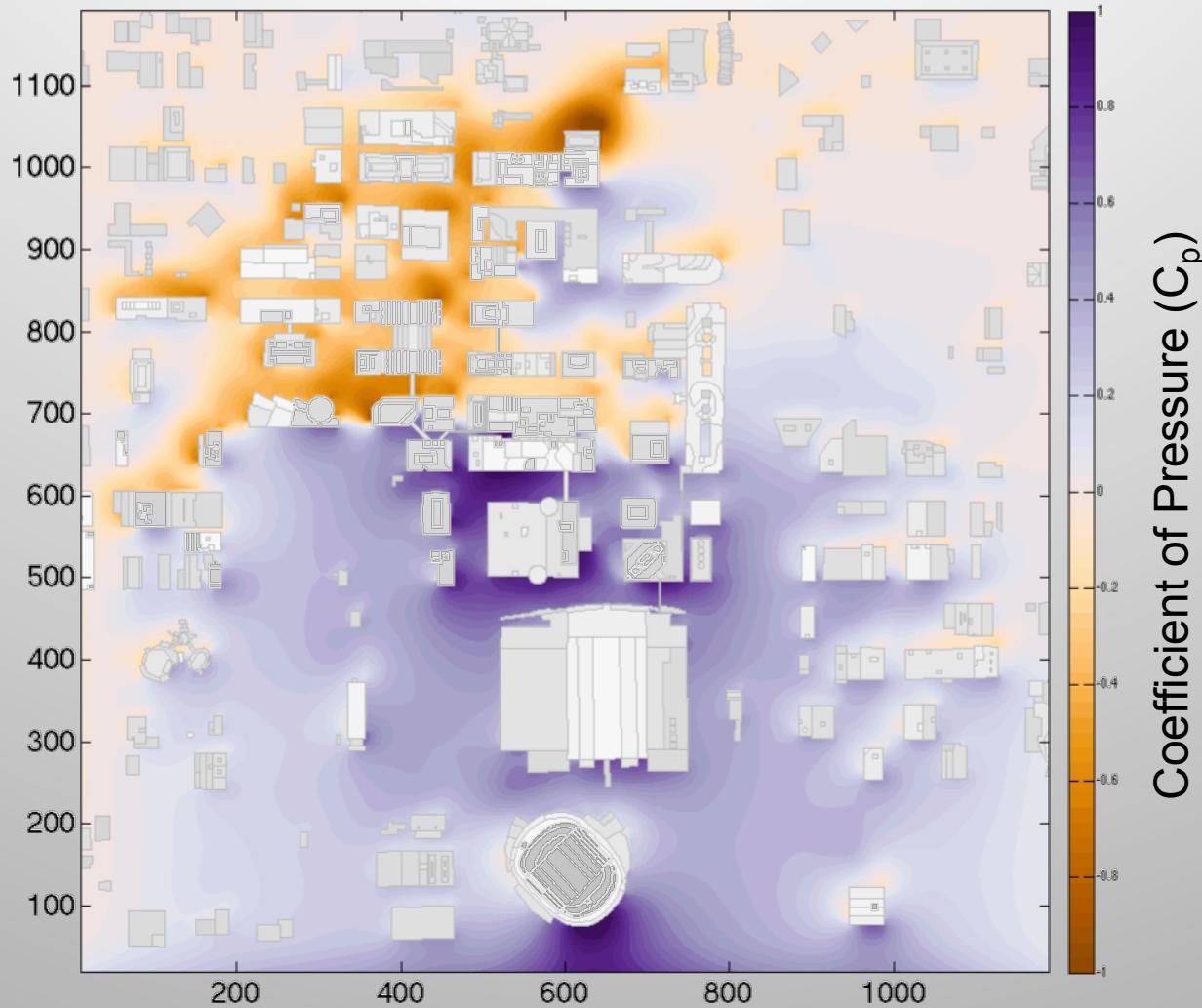
3D Velocity Field for Urban and Complex Terrain Environment



Example: Nesting of Complex Terrain and Urban Grids

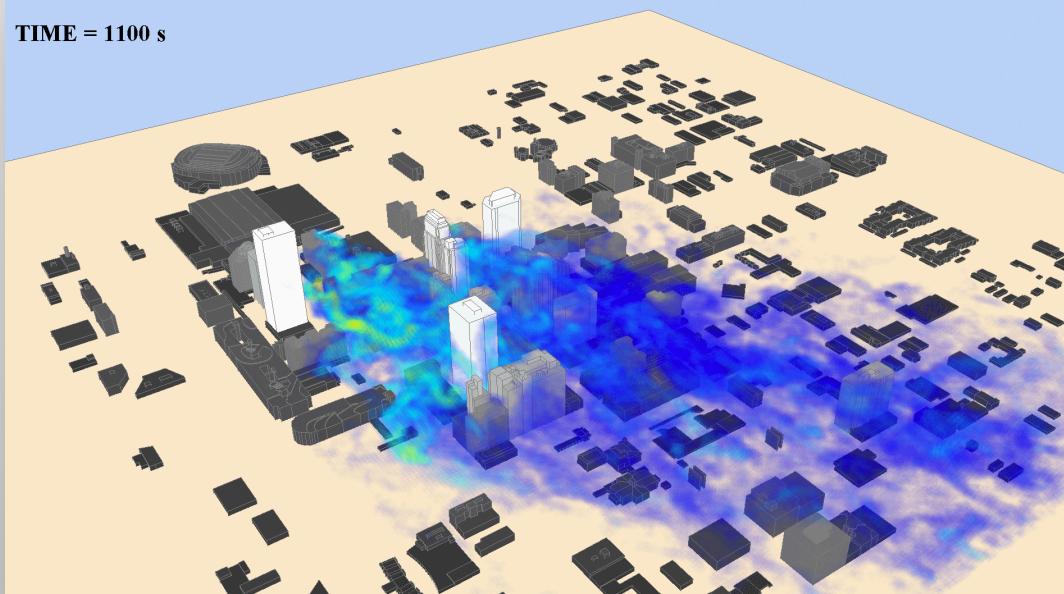


3D Pressure Field for Indoor/Outdoor Infiltration

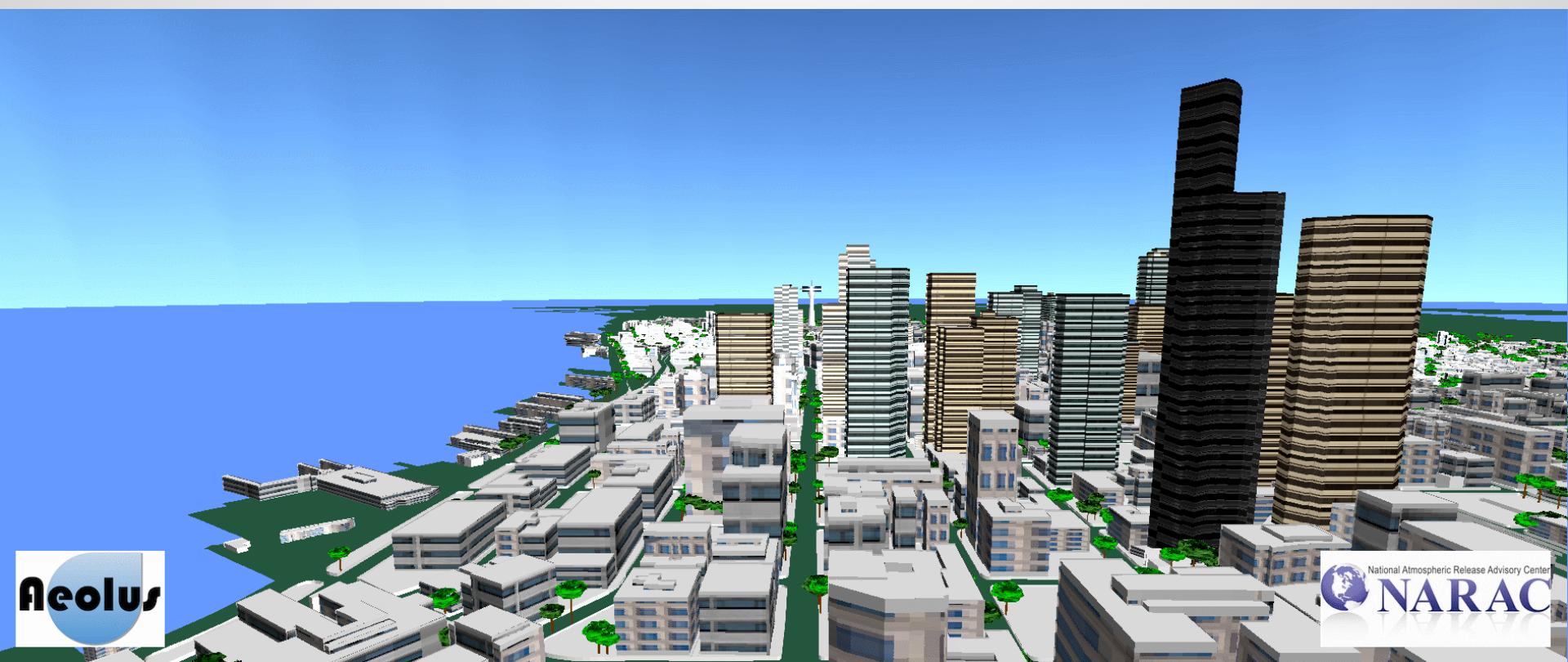


3D Concentration and Deposition Fields For Urban Scenarios

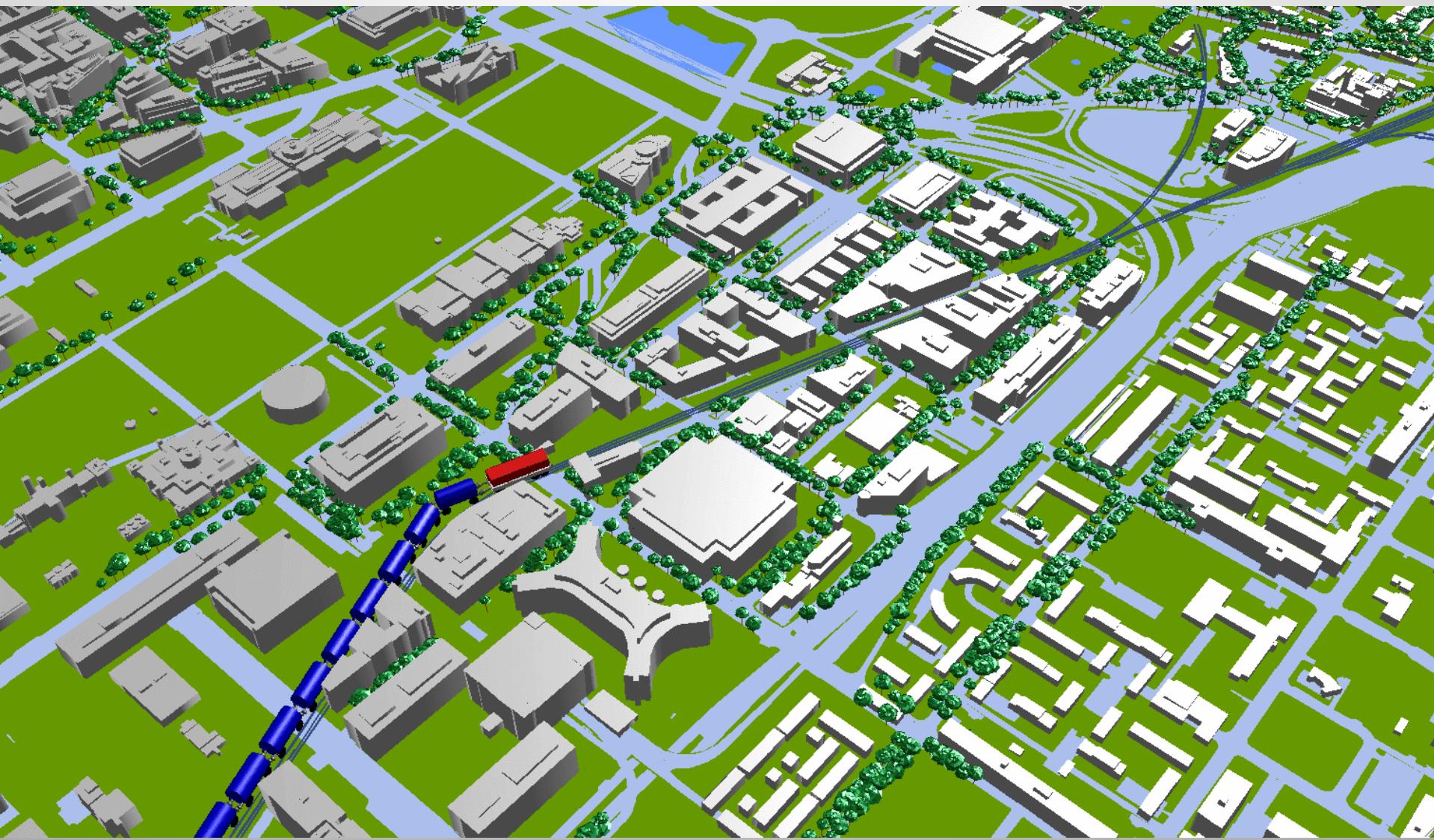
TIME = 1100 s



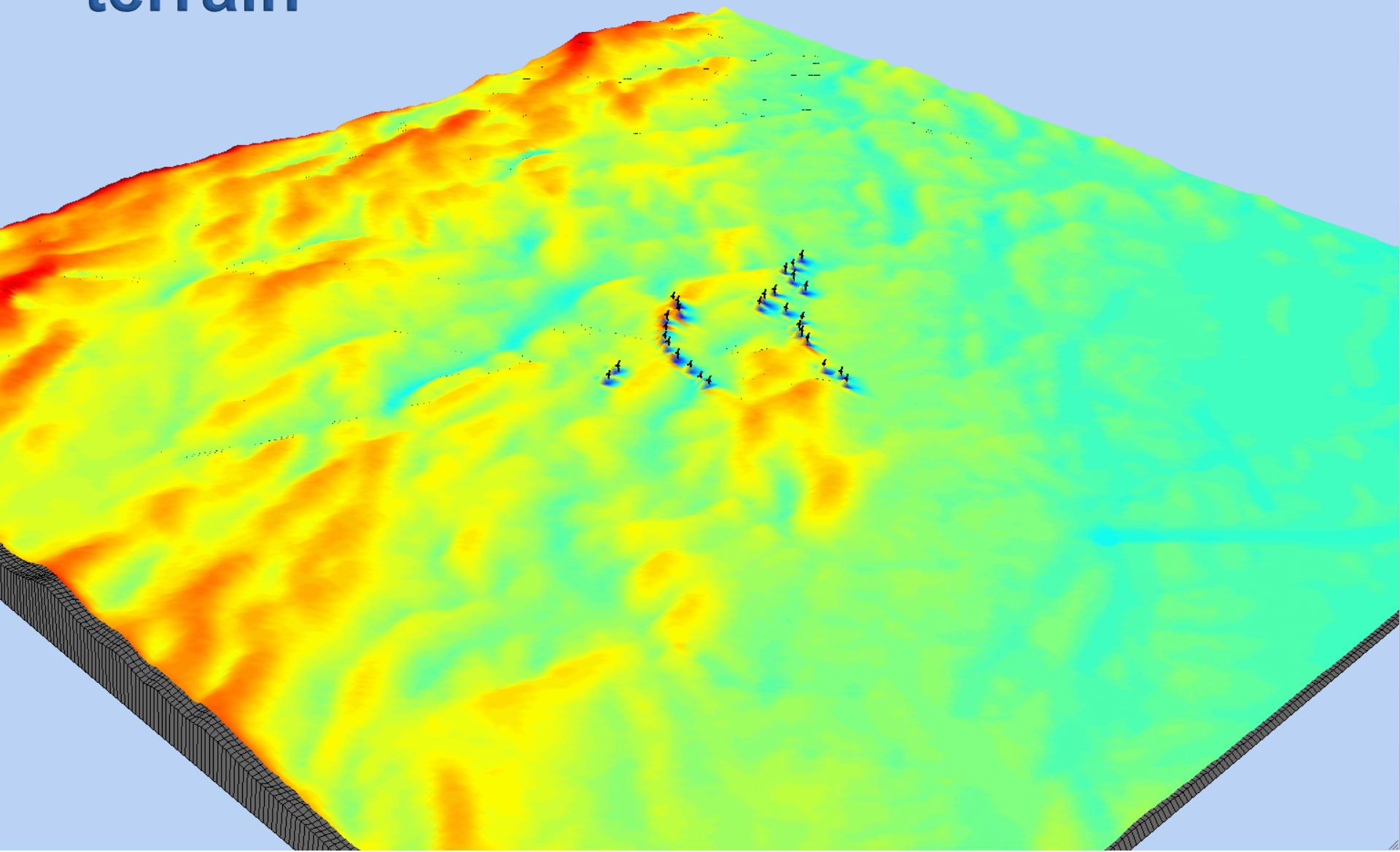
Deposition on Building Surfaces



Dense Gas Dispersion Simulation



Simulation of flow over complex terrain





**Lawrence Livermore
National Laboratory**