The Application of Fine-Scale Computational Fluid Dynamics Simulations of Pollutant Concentrations in Support of Air Quality Studies and Potential Interfacing within the CMAQ System

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** 9/29/07: Retired from Federal Career*

Key Collaborators and Acknowledgments

- *Matt Freeman and Wei Tang,*
  Lockheed-Martin Operations Support
  US EPA Environmental Modeling and Visualization Laboratory, RTP, NC
  (Scientific Visualization, Model setup, and computing at US EPA.)

- *Walter Schwarz,*
  Ansys, Lebanon, NH
  (Consulting on development of best practices and specific applications of the FLUENT CFD Code.)

- *Michael Lazaro,*
  Argonne National Laboratory, Argonne, IL
  (Computing at Laboratory Computing Resources Center and consultation on potential multi-scale models interfacing)

- *Renaissance Computing Institute,*
  Topsail Computing Cluster, UNC, Chapel Hill, NC
  (Bulk of Recent Manhattan Simulations)

- *1st Career: National Exposure Research Laboratory,*
  NOAA in Collaboration with EPA

Why CFD?

- Growing needs in better (reality?) understand transport and dispersion of species in urban environments
  - Refined assessments for air quality studies
  - Homeland security concerns

- Results of CFD simulations can be used to
  - Directly simulate specific case studies

  - Support the development of more simplified algorithms that may be generally applied:

    Work from bottom detail up to larger scales

  - Substitute for single CMAQ Model Grid for Special Occasions where Source Characterization or Exposure Characterization is desired:

    Then Interface into a courser CMAQ model framework

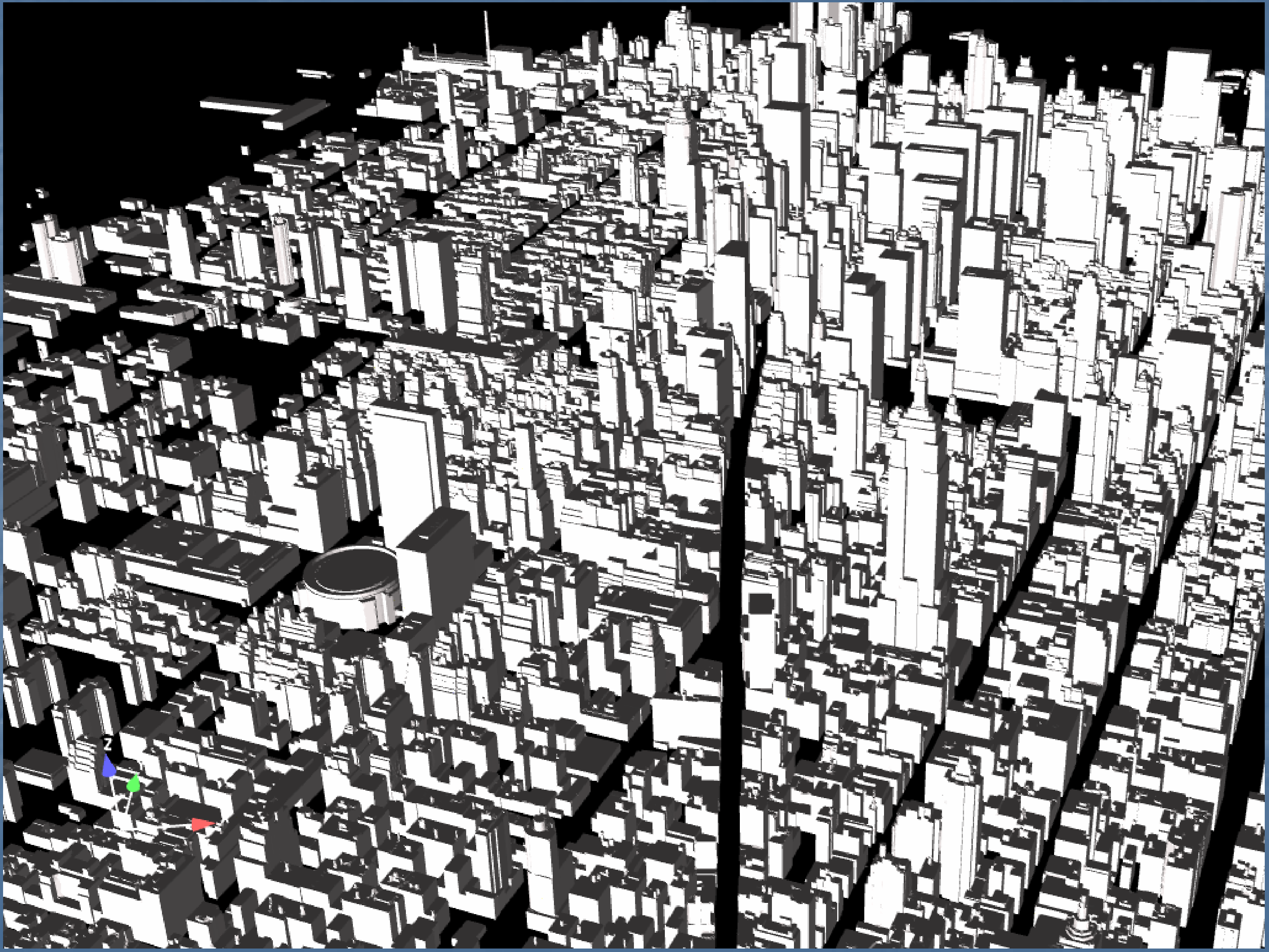
Total Exposure Concentration = Local Microenvironments (CFD Model) + Regional/Neighborhood (CMAQ Model)

Urban Exposures: Beyond the Lamppost

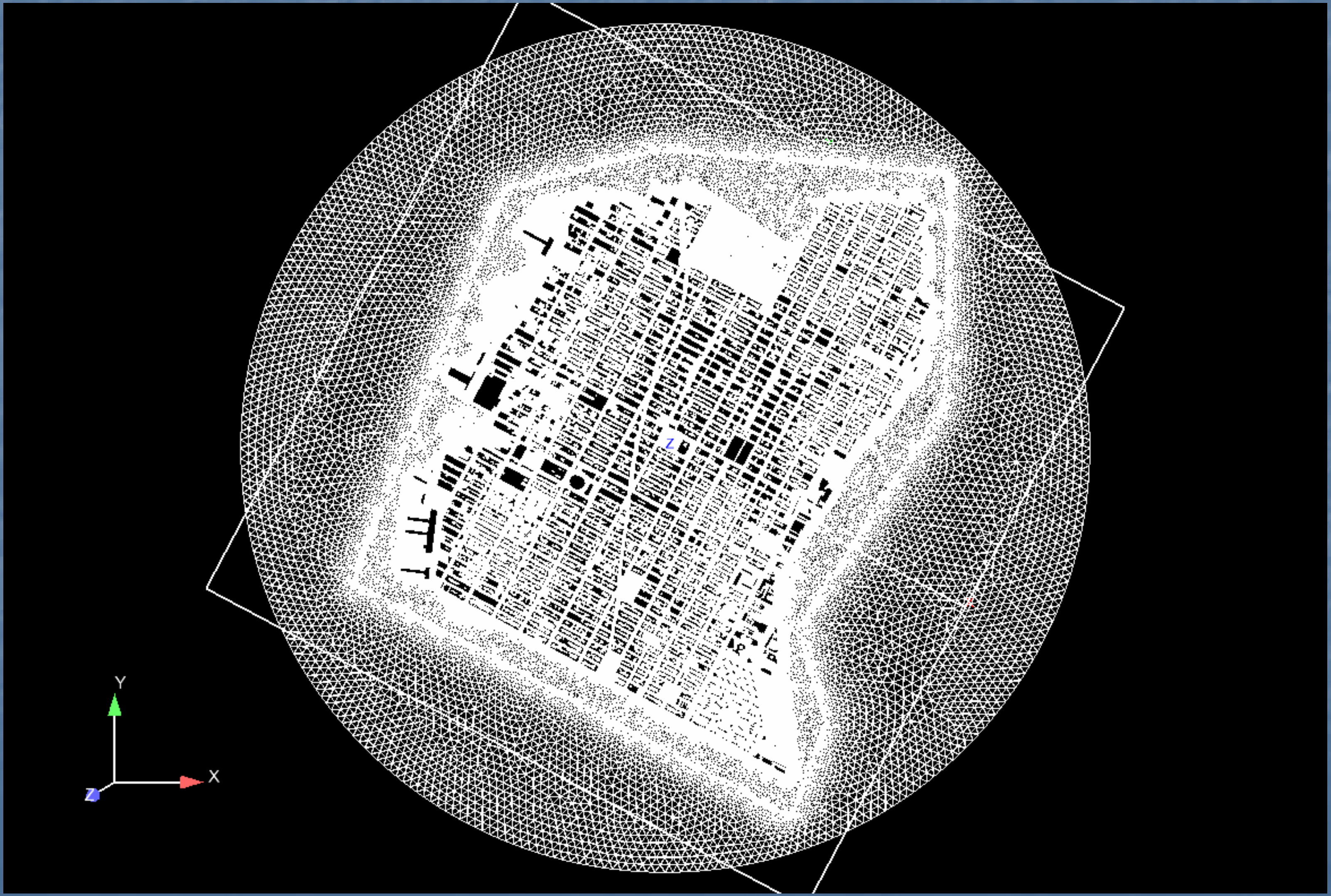
New York City CFD Modeling

- A model of Midtown Manhattan was developed to support the New York City Urban Dispersion Program.
(support from EPA and DHS)
- There were two major field studies during 2005.
(principally funded by DHS with field operation managed by PNNL – Jerry Allwine)
- Summer 2005 studies lead to support model comparison study including “blind tests.”
(now in waiting for review of draft report)
- The Spring 2005 studies in the vicinity of Madison Square Garden are now in the public domain.
(Present simulations are being run to examine model methods and performance)

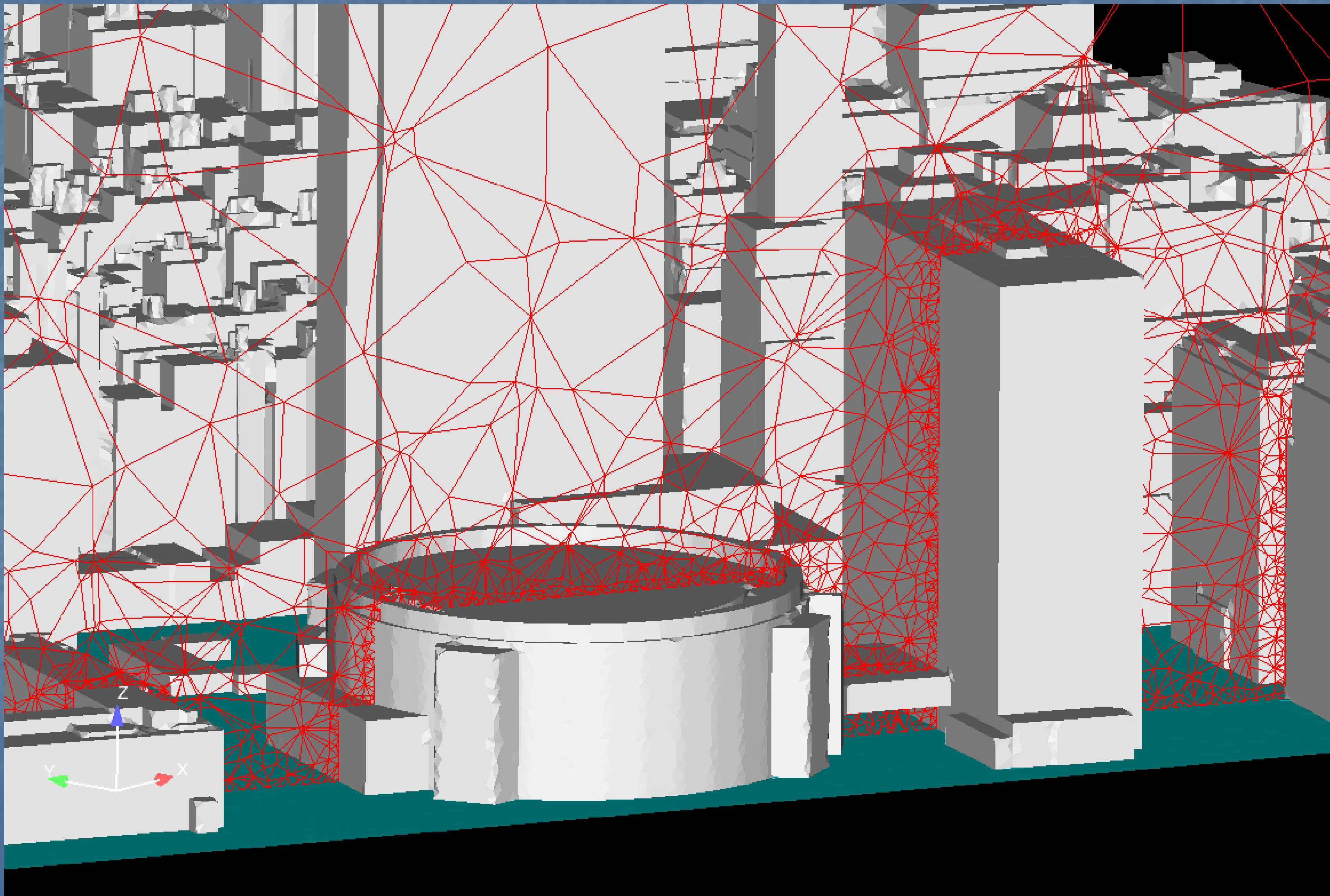
Midtown Manhattan Model



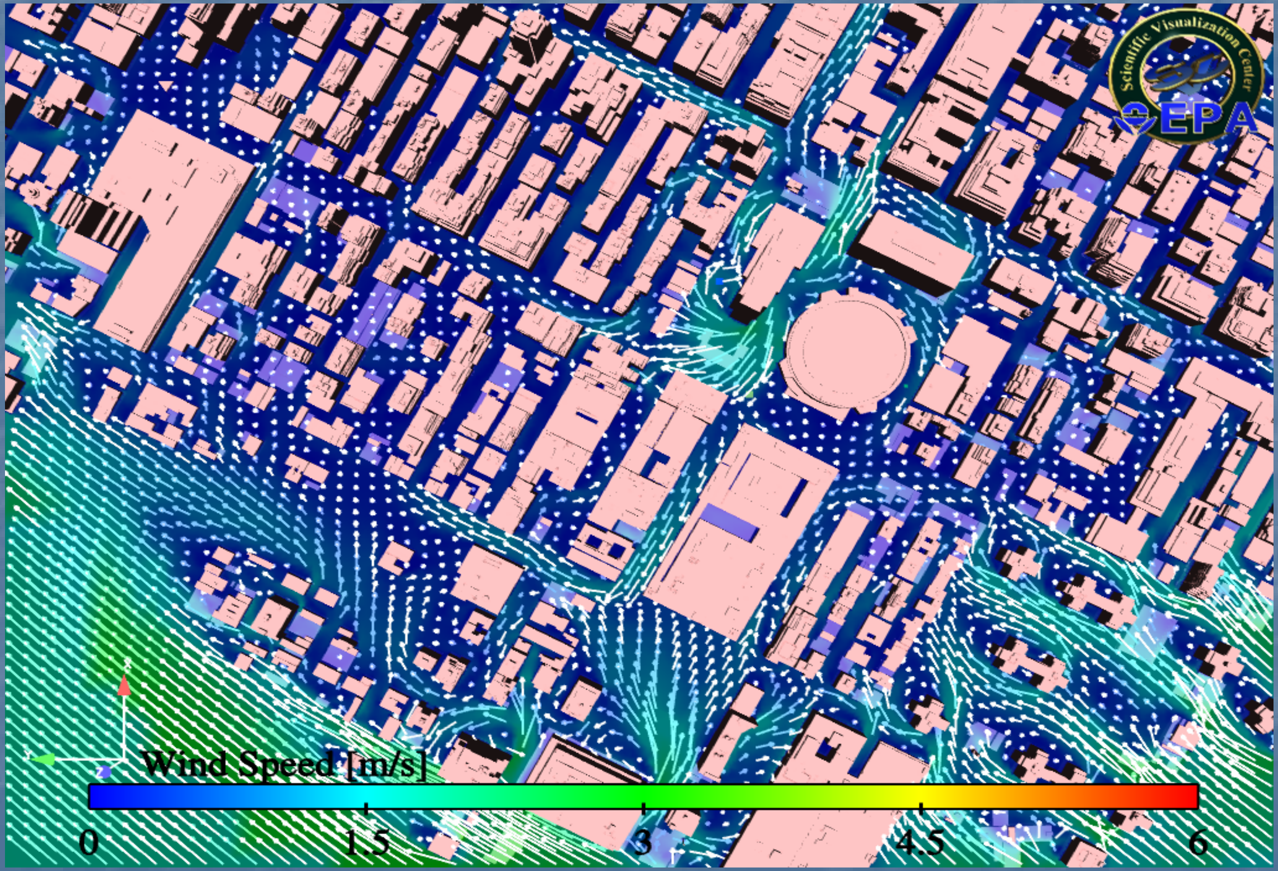
Overview of Full Domain with 54 Million Cells



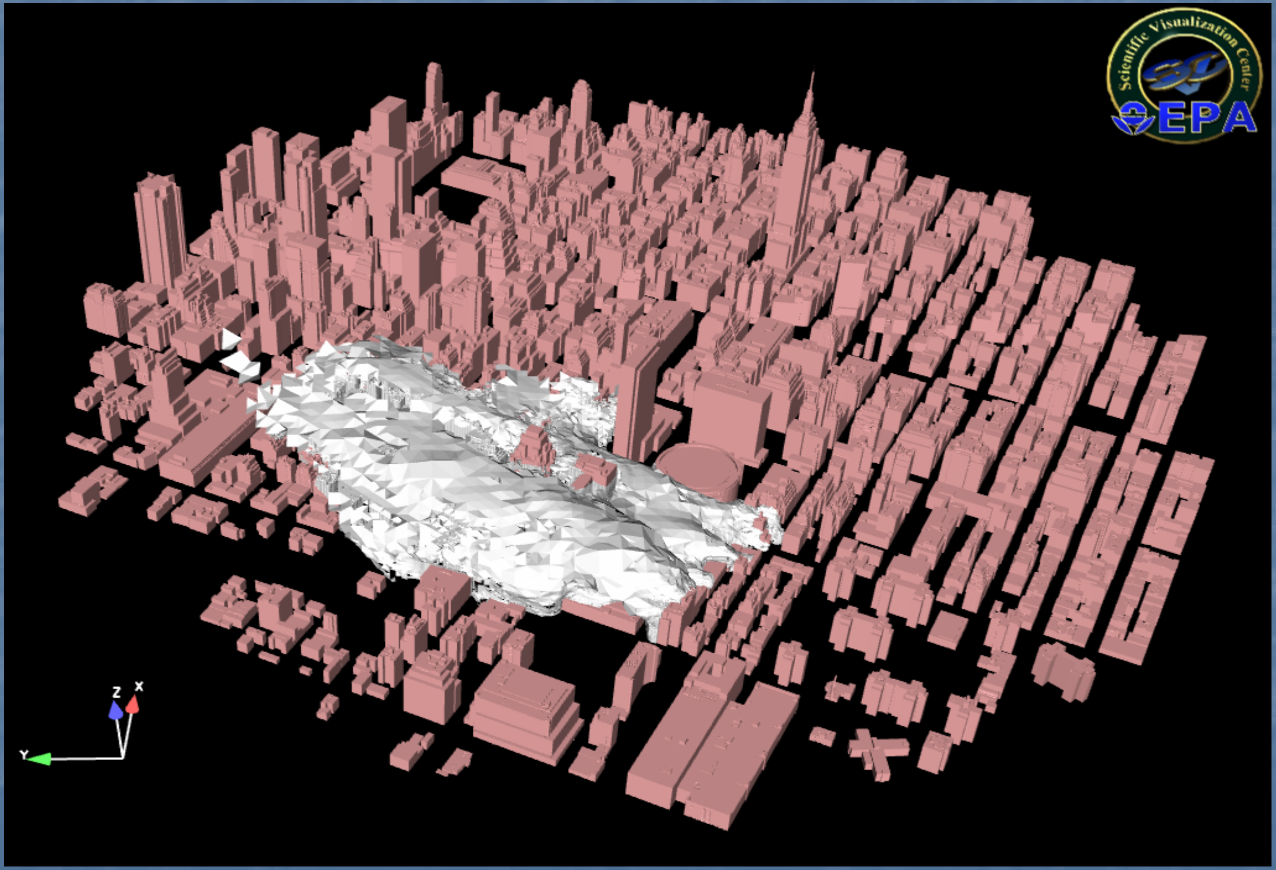
Example Vertical Profile of Mesh



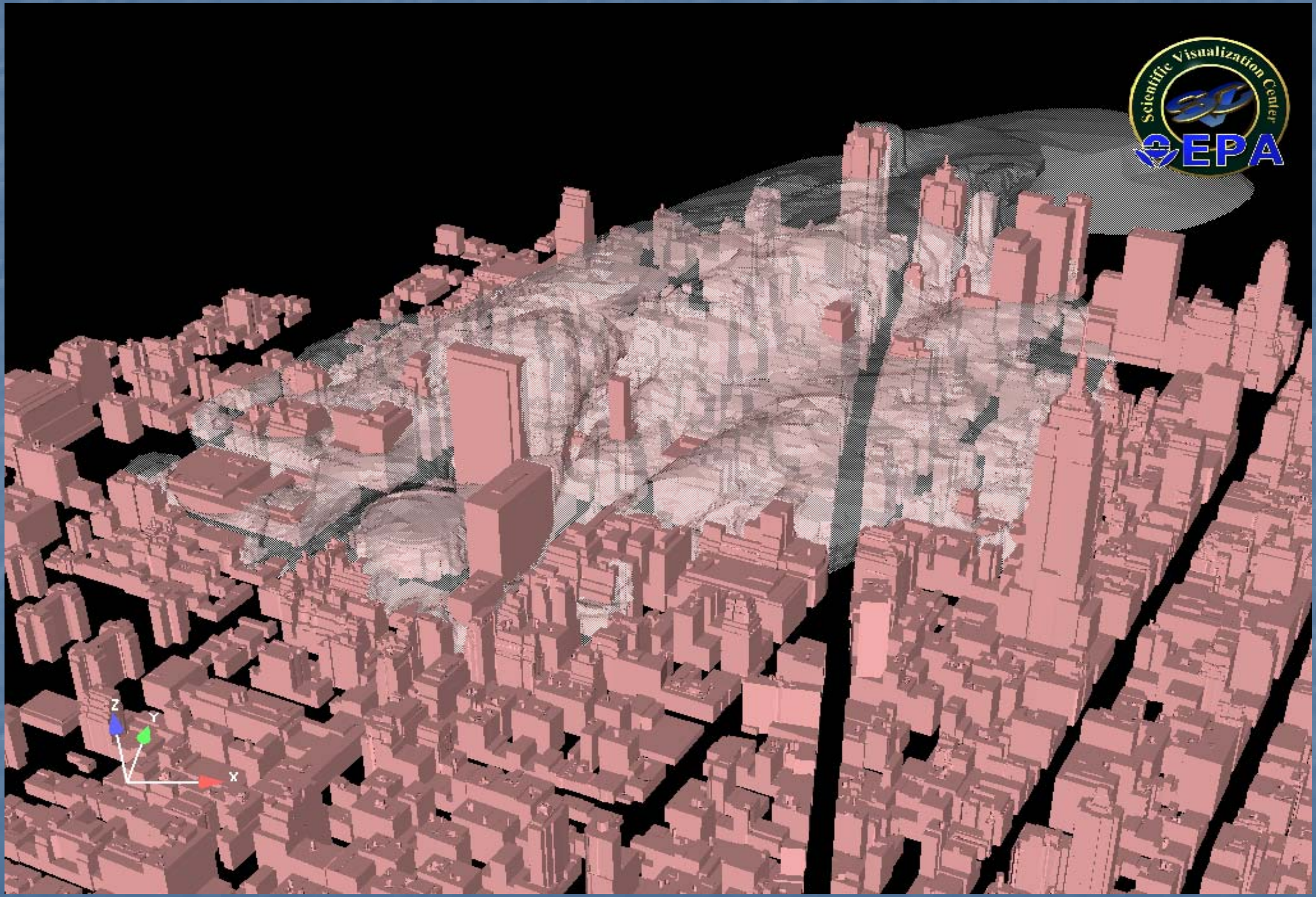
Preliminary Studies for Fixed Wind Directions



Example Plume 1



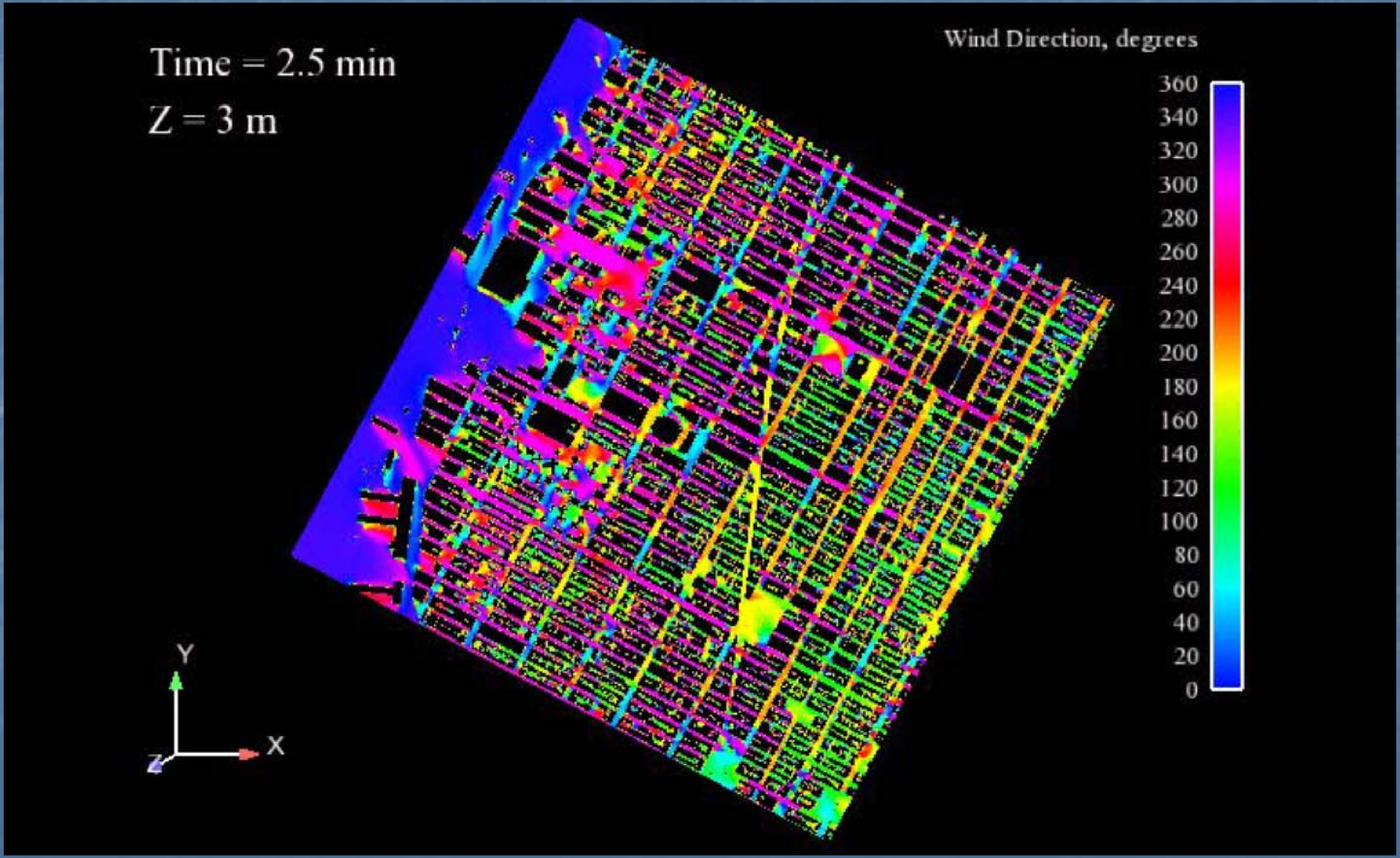
Example Plume 2



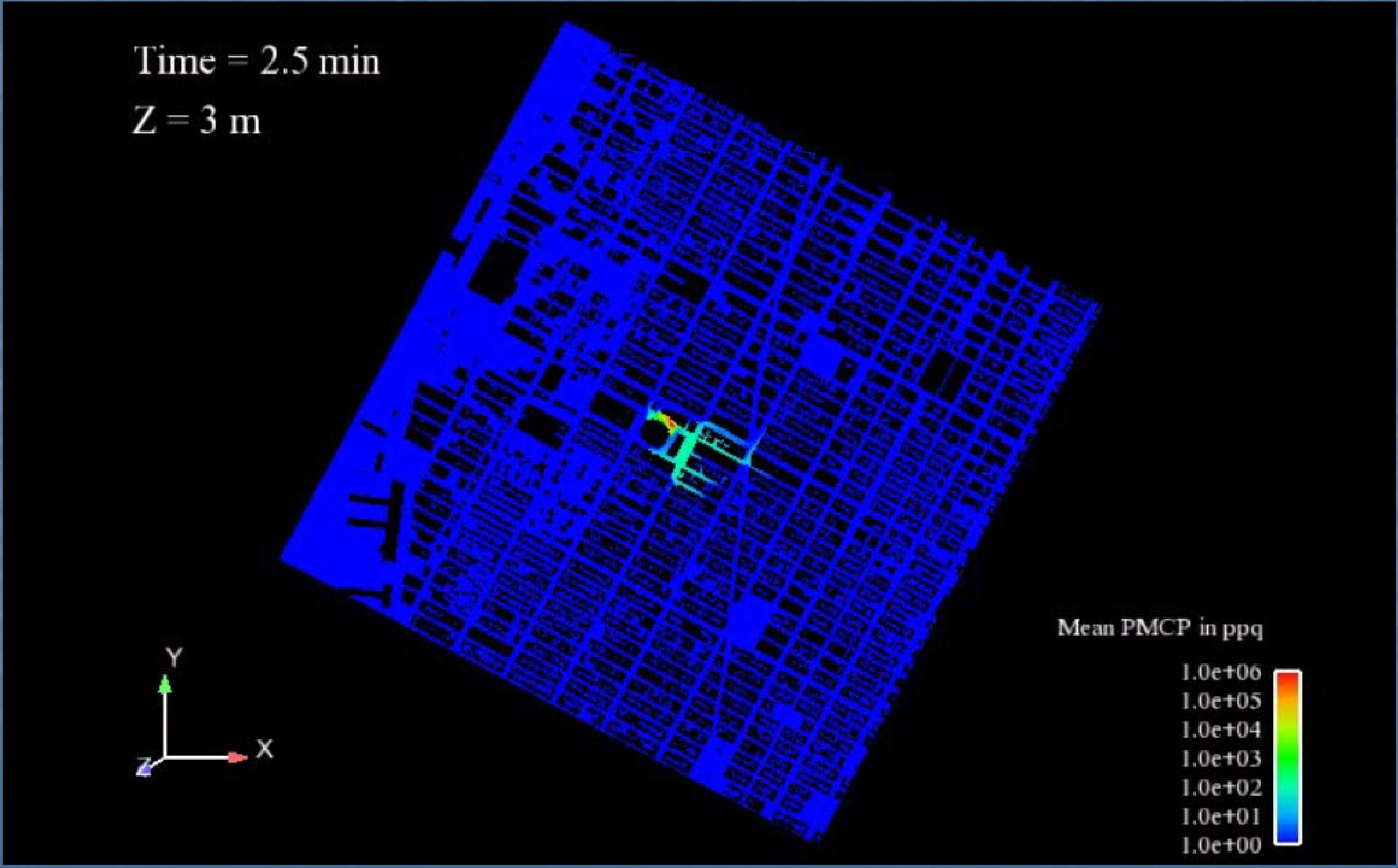
CFD Model Setup with Unsteady Winds:
Set to match real field conditions

- Single Inlet Boundary-layer Profile.
- Wind direction and wind speed changes every minute. Based on few measurements.
- 1-minute steady state solutions: usually output as 5-minute average.
- Uses Unsteady RANS, 2nd Order Numerics
- Realizable k-e Turbulence Model.

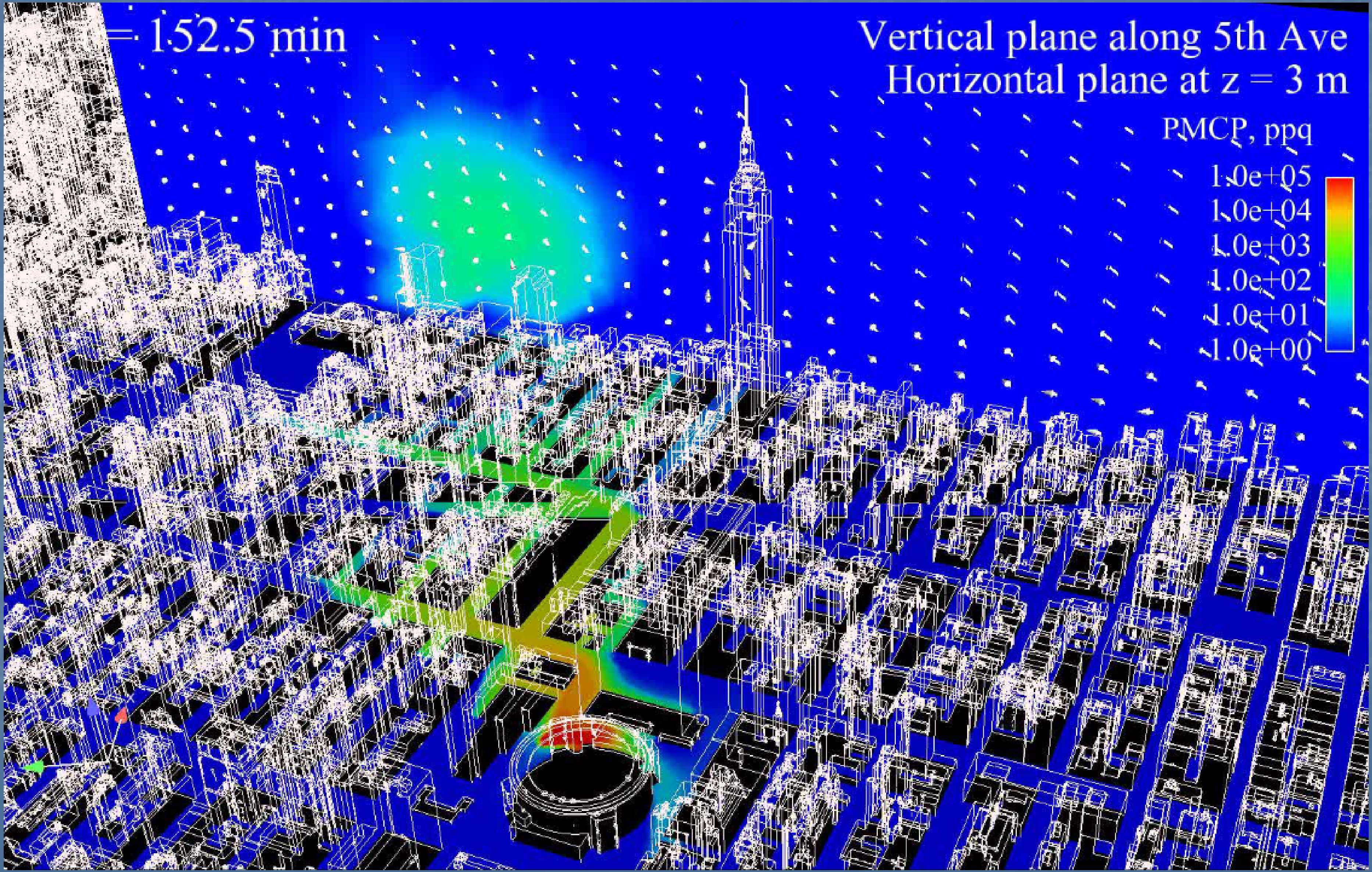
IOP2:
5 hours of 5-minute-averaged Wind Direction



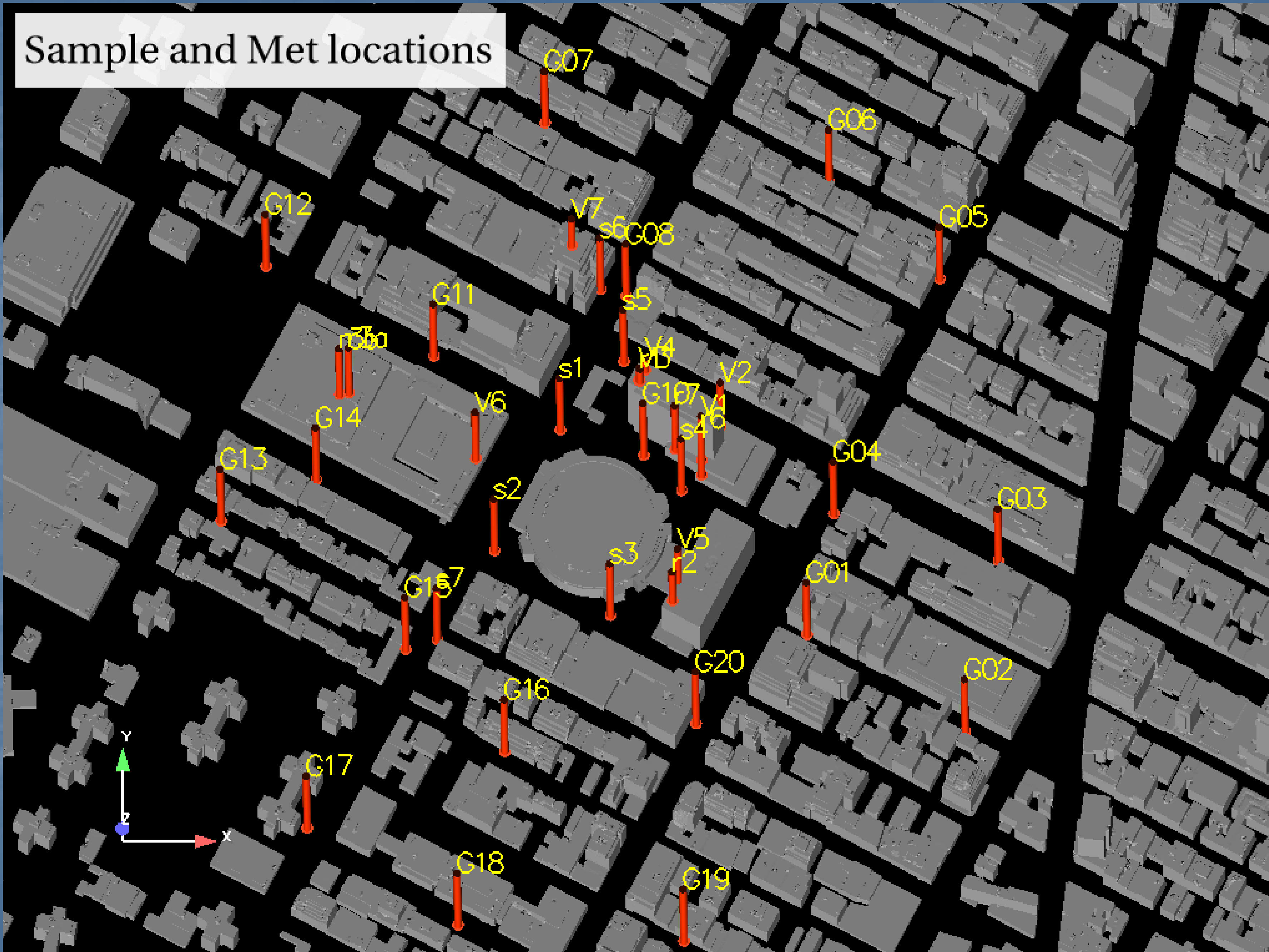
IOP2: Release 4:
5 hours of 5-minute-averaged Concentrations



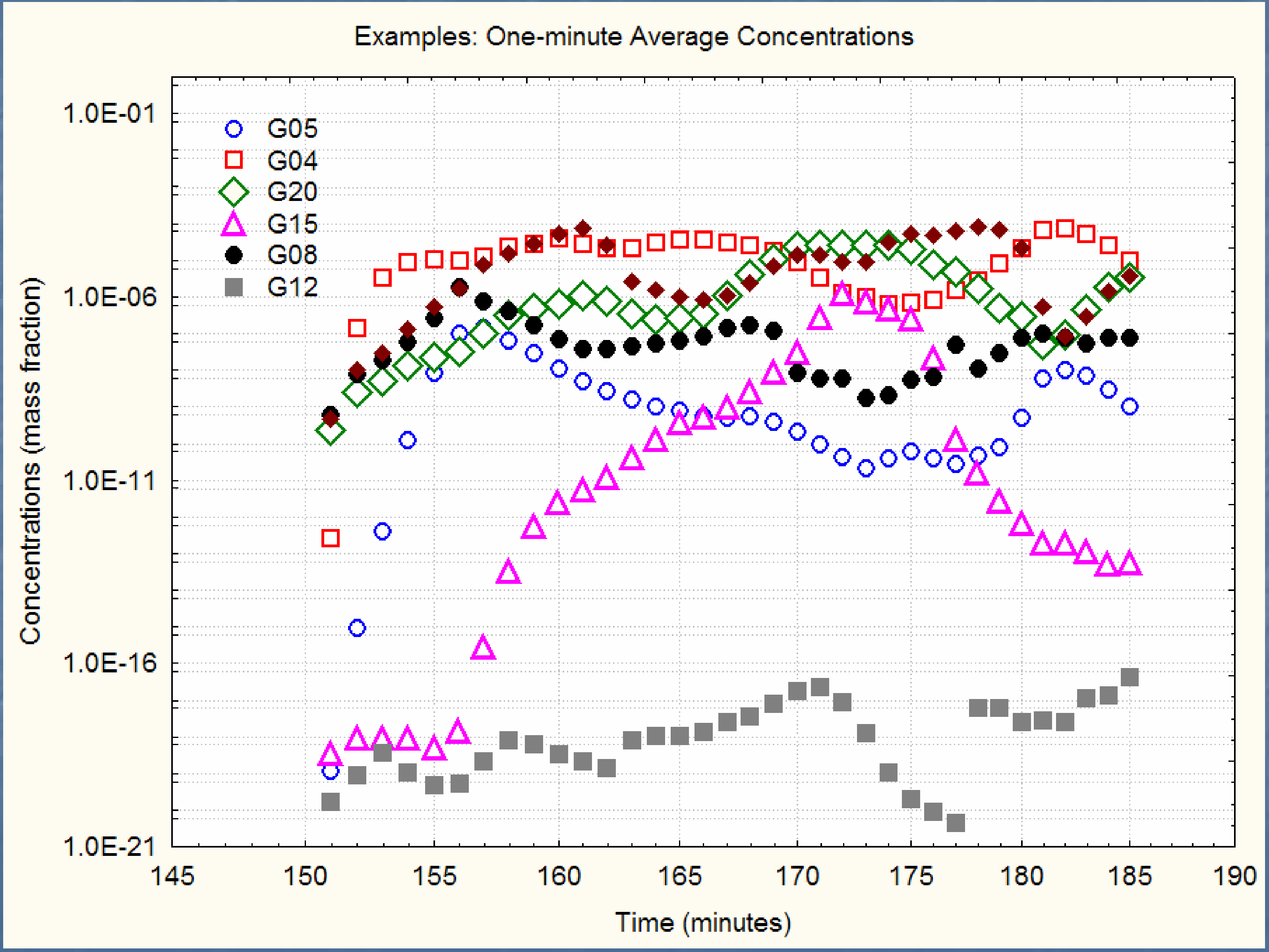
IOP2b: Release 4:
90 minutes of 5-minute-averaged Concentrations



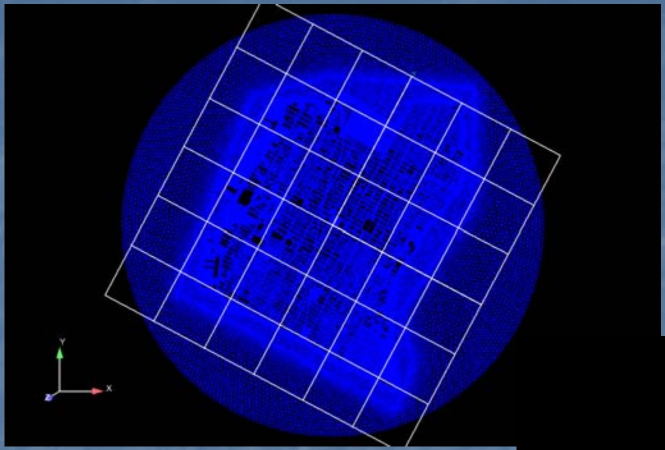
Sample and Met locations

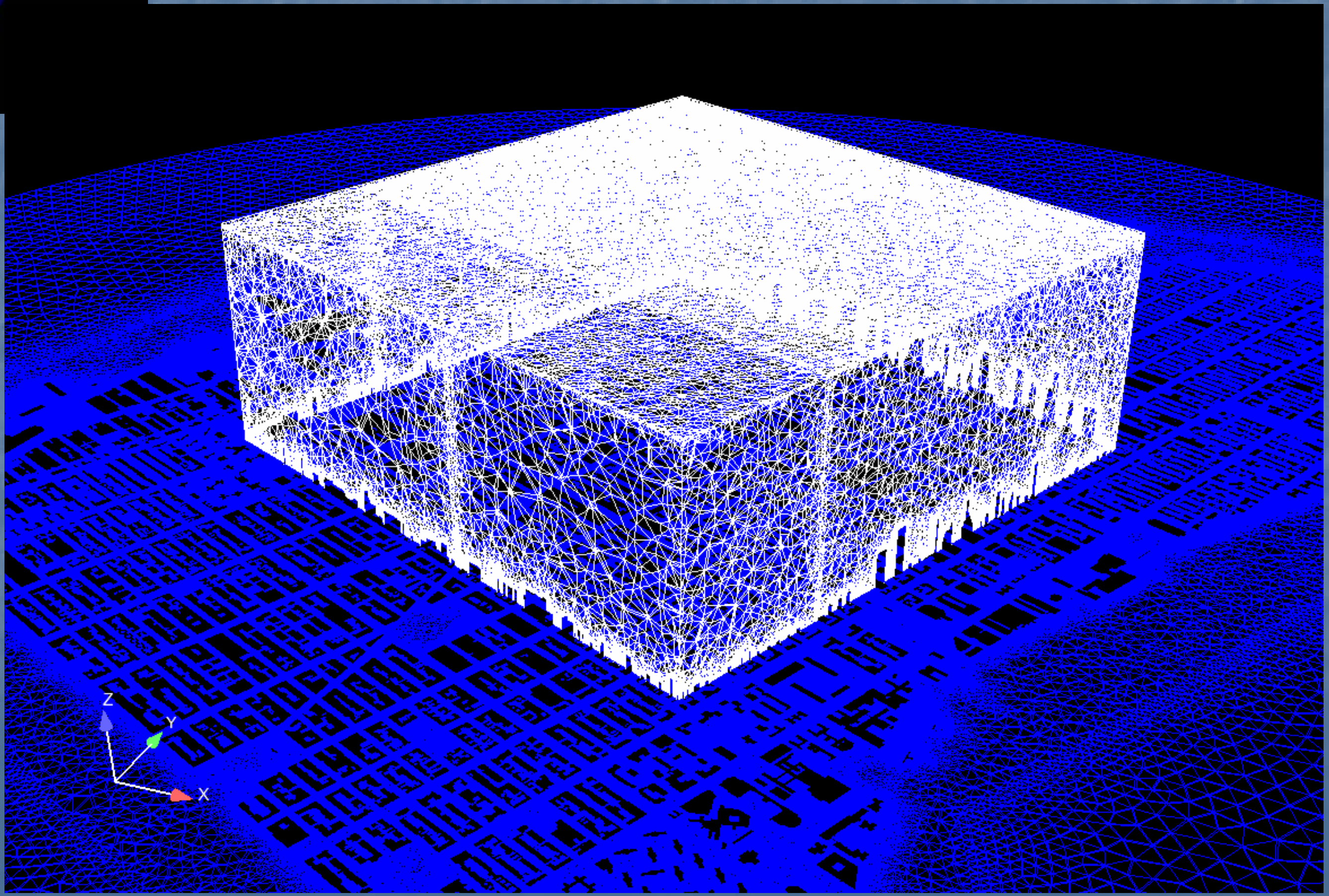


Sample 1-minute-average Concentrations

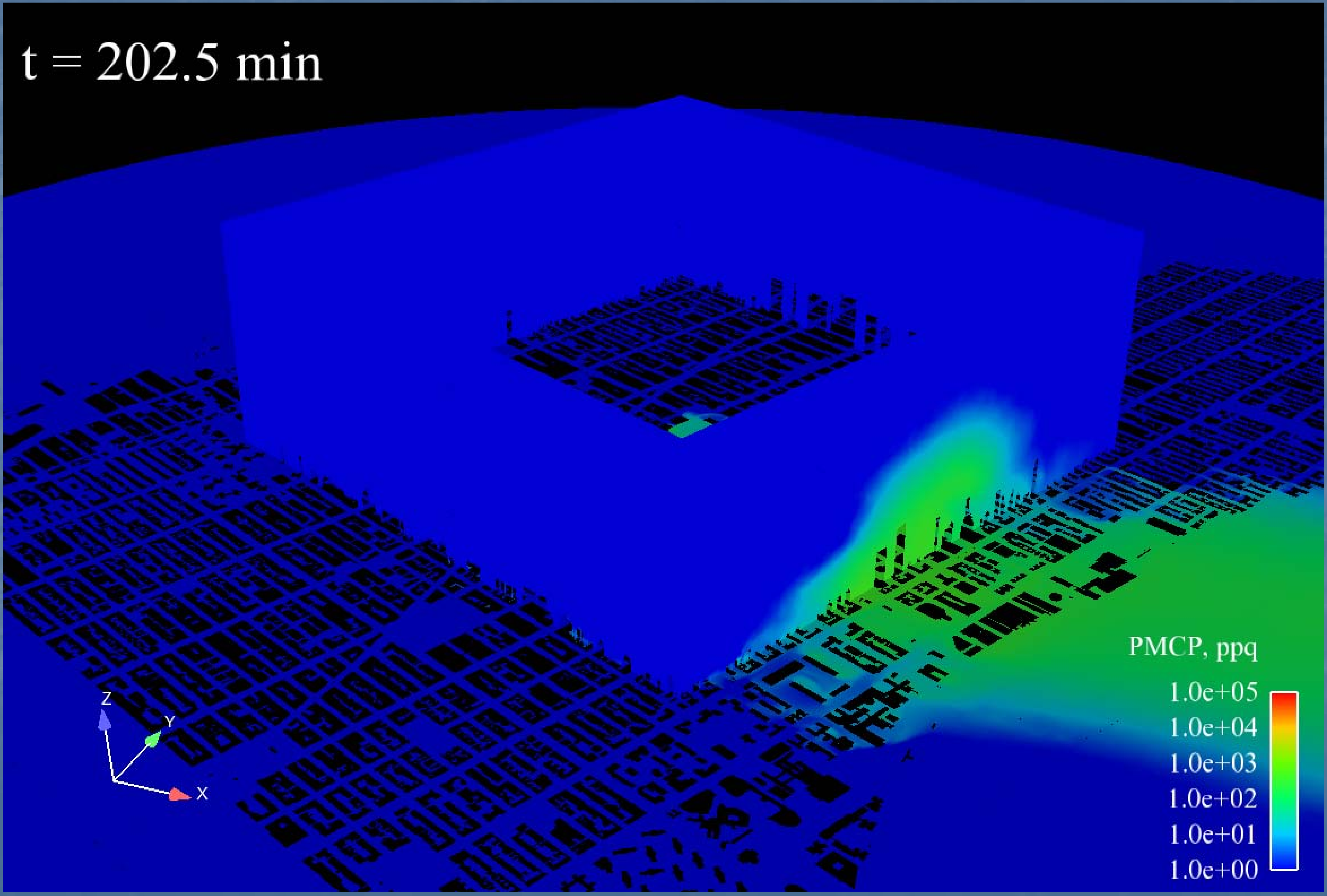


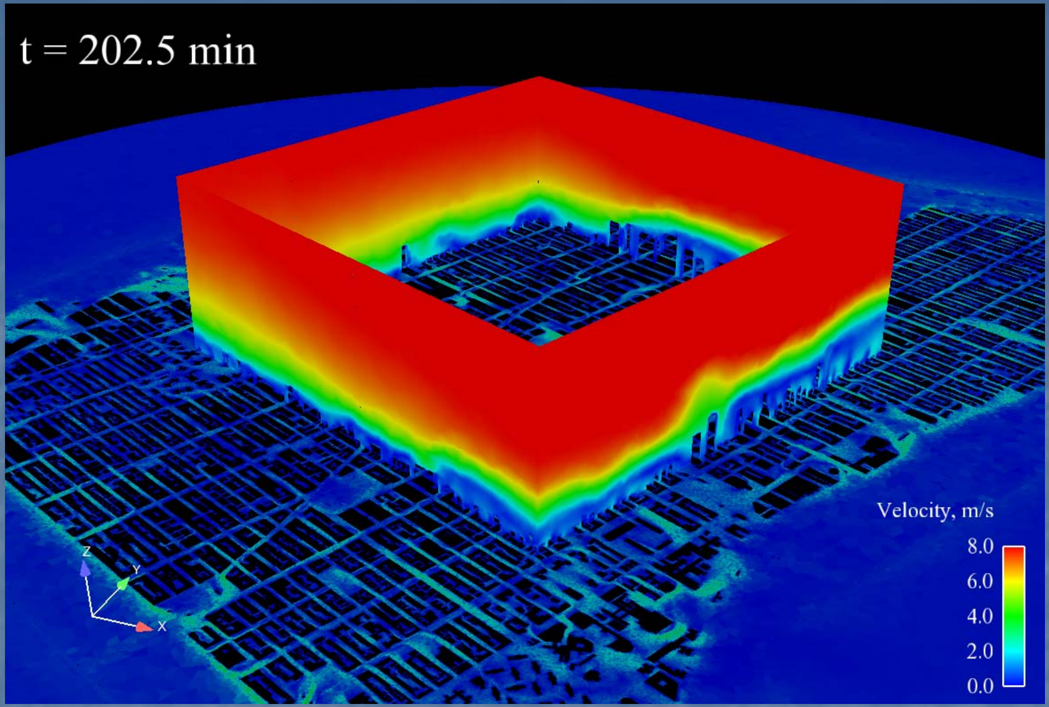
Overlay Course Model Framework to select CFD Resolved Volume

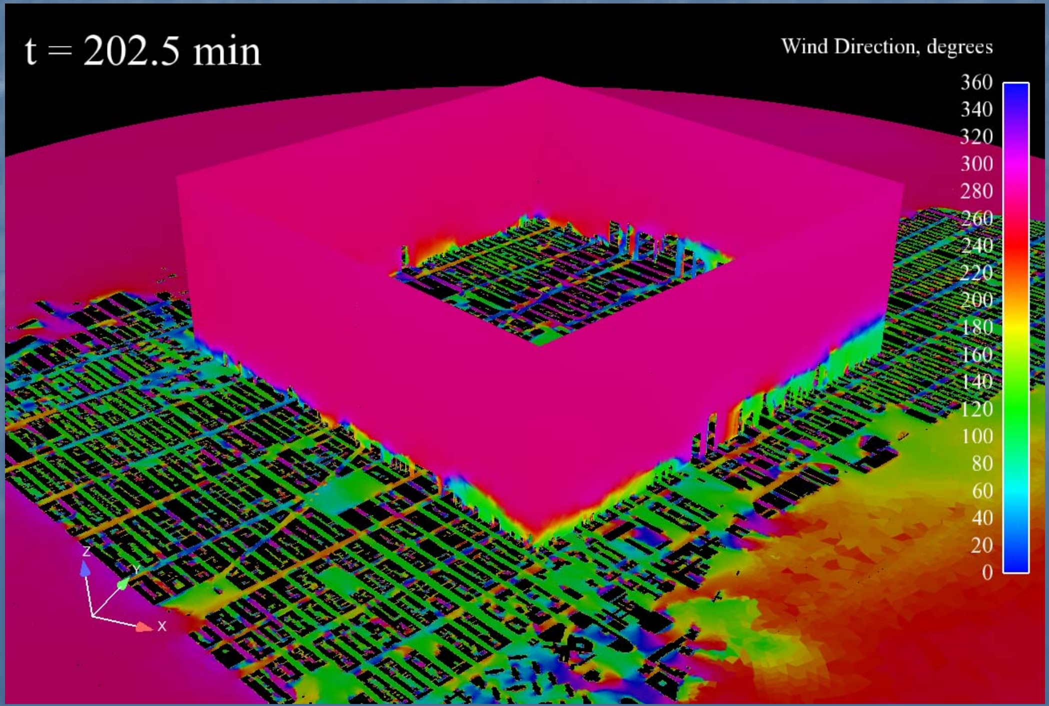




Examine and Interface the Plume



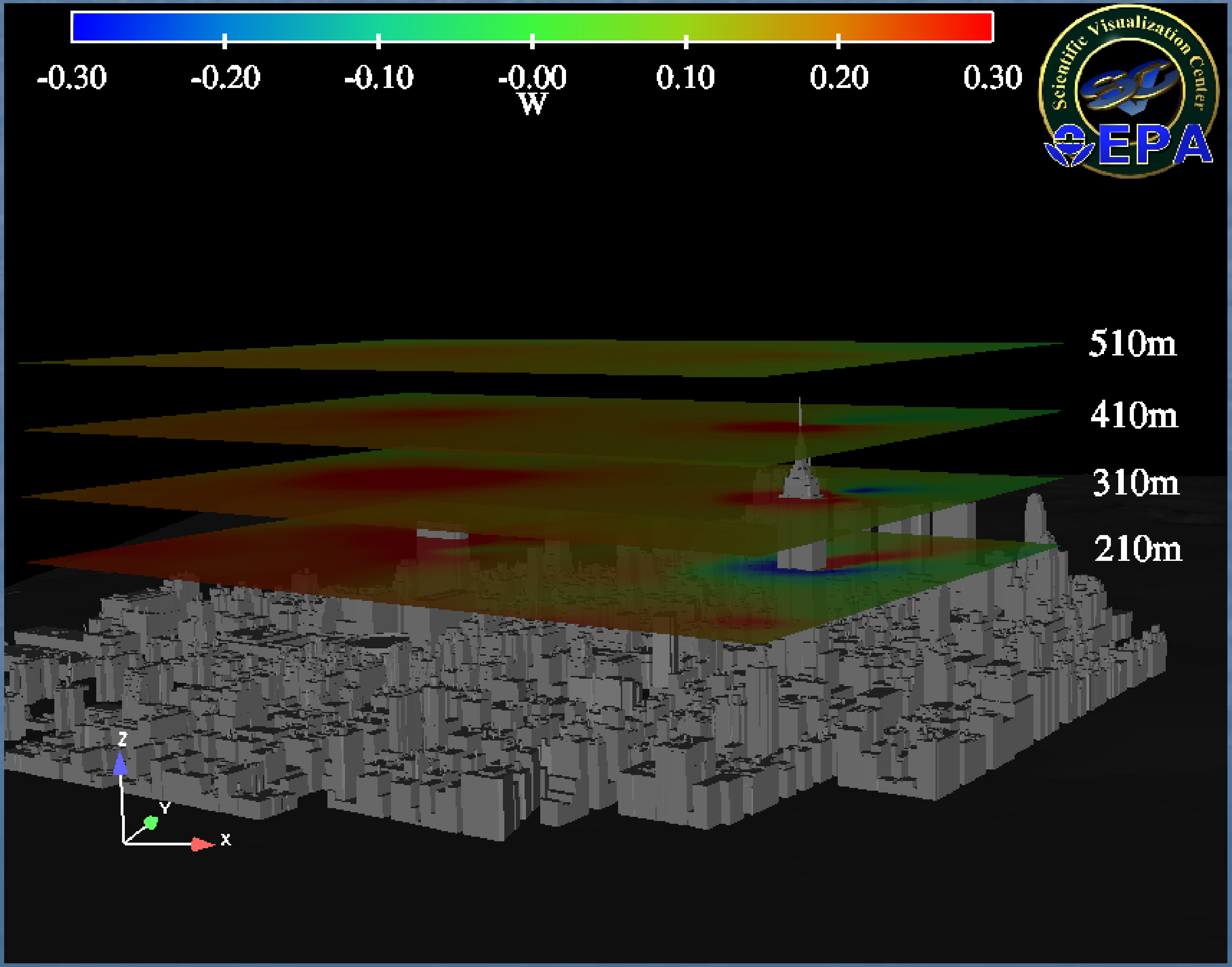




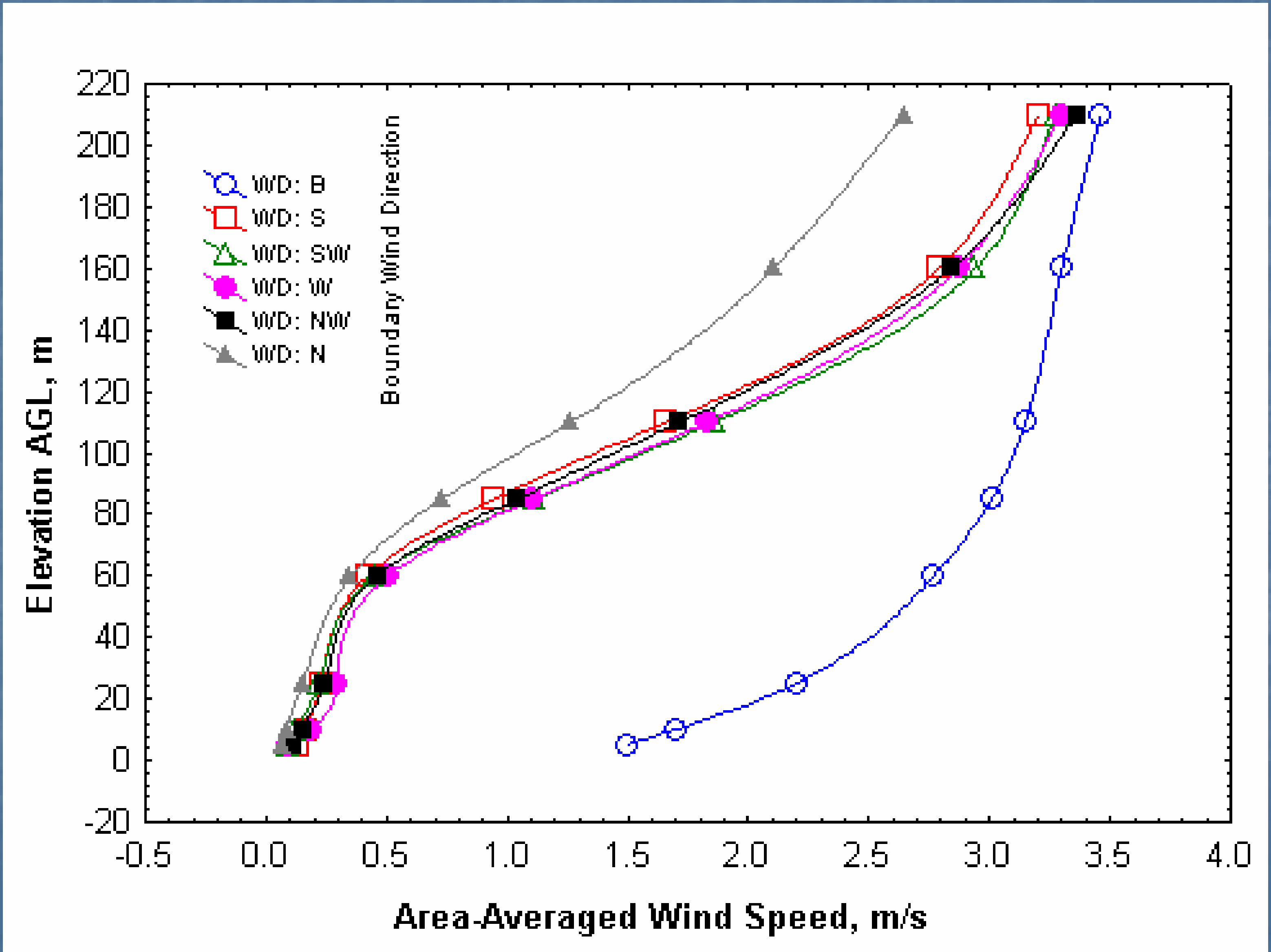
Examine and Interface Meteorology

City Specific CFD Can Provide Sub-grid Parameterizations

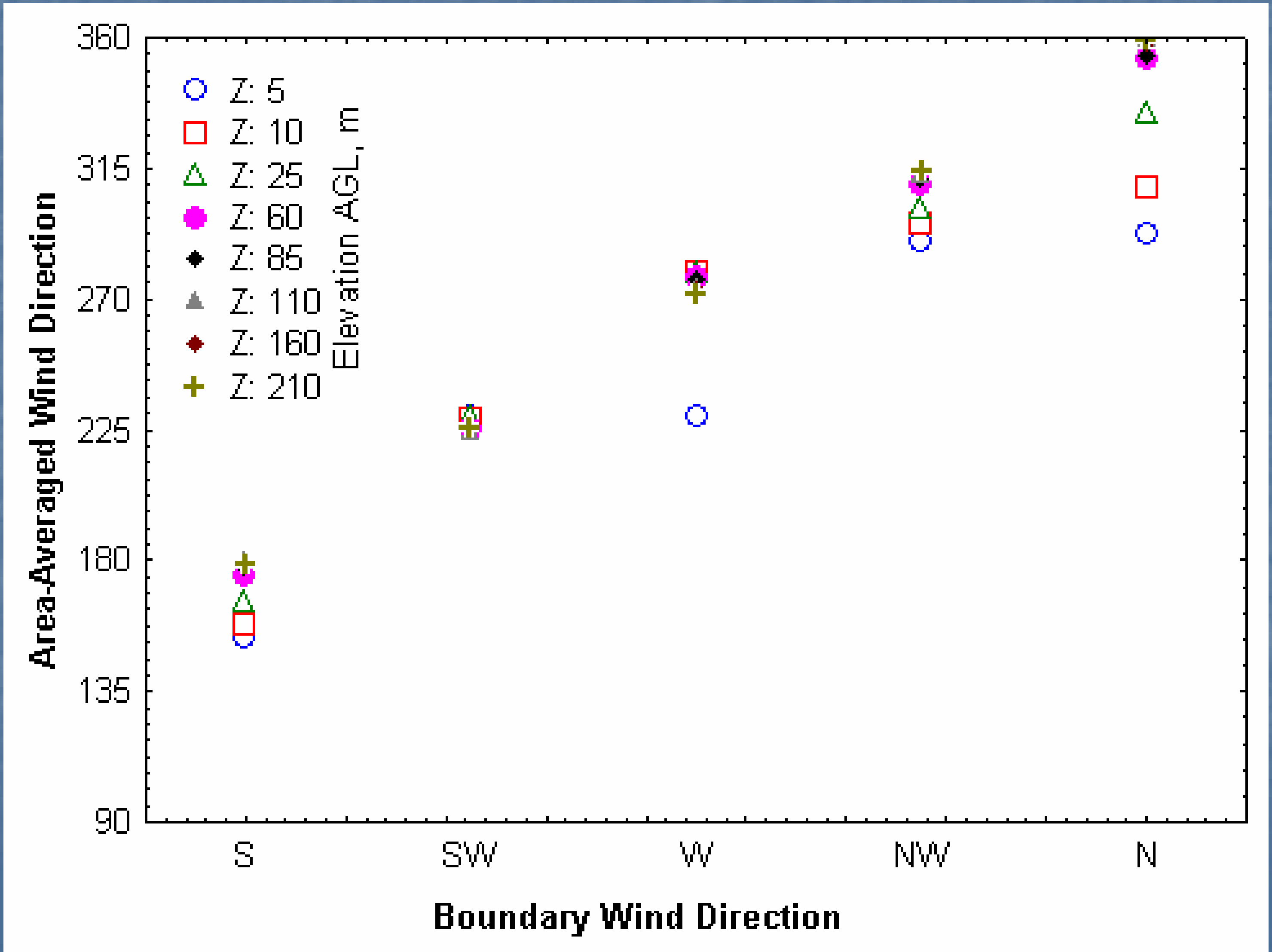
Example Horizontal Planes - Vertical Velocity



Example: Area-Averaged Wind Speed



Example: Area-Averaged Wind Direction



Chicago Urban Dispersion Modeling System

Proposal is being developed by Mike Lazaro with ANL Group.

Potential Cooperative/ Collaborative Partners

UIUC

UIC

Slide Provided by Mike Lazaro, ANL

Tiered Modeling System

- **Tier I** **(Scale: 1 – 25 km)**
  City Scale
  Simple/Fast Urban Codes
- **Tier II** **(Scale: 10 m – 1 km)**
  Neighborhood Scale
  Coupled Building
  Aware Urban Codes
- **Tier III** **(Scale: 1 m – 100 m)**
  Building Scale
  Coupled High-Fidelity
  Urban Codes

Rapid Response

- Real-Time/Near Real-Time

Preparedness

- **Support development and evaluation of Tier I & II is critical.**
- Next Generation Training with Unscripted Exercises

Refined/Post Response

- Bldg. Scale Flow/Evac. Zone
- **Contamination Mapping/Decon**
- Forensic Analysis
- Rapid Economic Recovery

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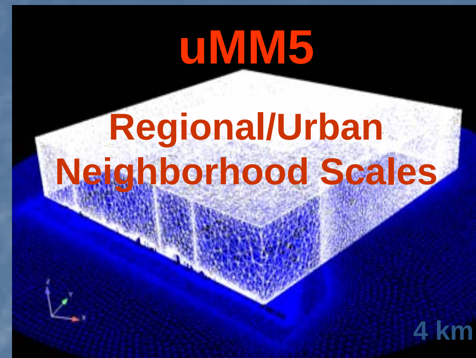
Chicago Urban Dispersion Modeling System

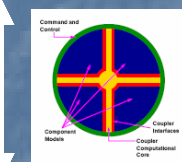


Tier II Coupled

Dispersion Models
Urban/Neighborhood Scale

Tier III Coupled

High Fidelity CFD Code
Building Scale

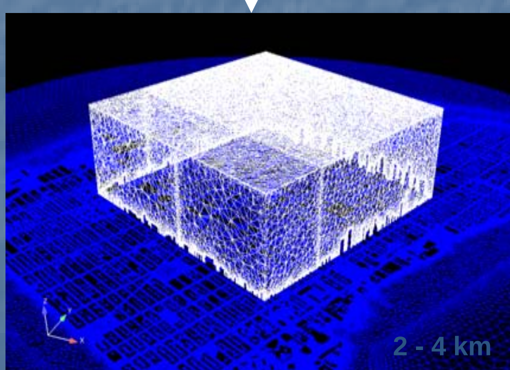


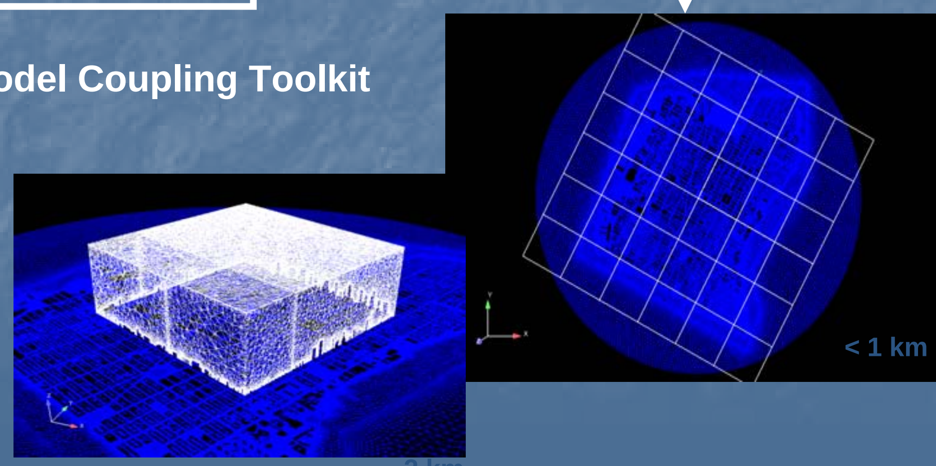
Interfacing/Downscaling
Grid Adaptation

Downscaling/ UPL
Parameter Exchanges

MCT*/MCEL
Coupler

* **Argonne Model Coupling Toolkit**





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Summary of CFD for Urban Modeling

- Atmospheric flows are complicated due to complex temporal-spatial wind fluctuations. They can reasonably be included.
- Bulk Transport and Dispersion through urban street canyons can be well simulated.
- Thermal effects should be added.
  (Bulk parameterizations should work well)
- Atmospheric Chemistry and Particle Physics should be added.
  (I hope progress can be reported at next years CMAS meetings)
- Work using present completed computed New York City simulations should be a priority for examining application of CFD and interfacing within a CMAQ framework.
- Work on other Cities should begin as opportunities arise.

CFD Simulations for Air Quality Modeling

- CFD simulations are applicable where other models should not go. They can NOW be used to support improved parameterization for CMAQ subgrid-scale modules as well as provide example direct simulations of exposures and of local emissions pathways.

- There is great potential for CFD development and their role in applications for air quality studies and it will grow with the rapidly advancing computational software and hardware. Interfacing of multiscale models WILL become seamless in not too many years.

  I expect to see it before I really retire.