



New Capabilities for Urban Dispersion Modeling

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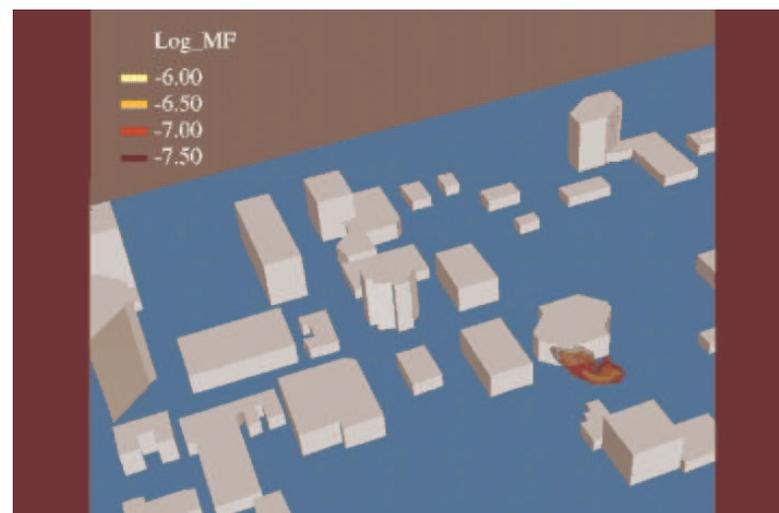
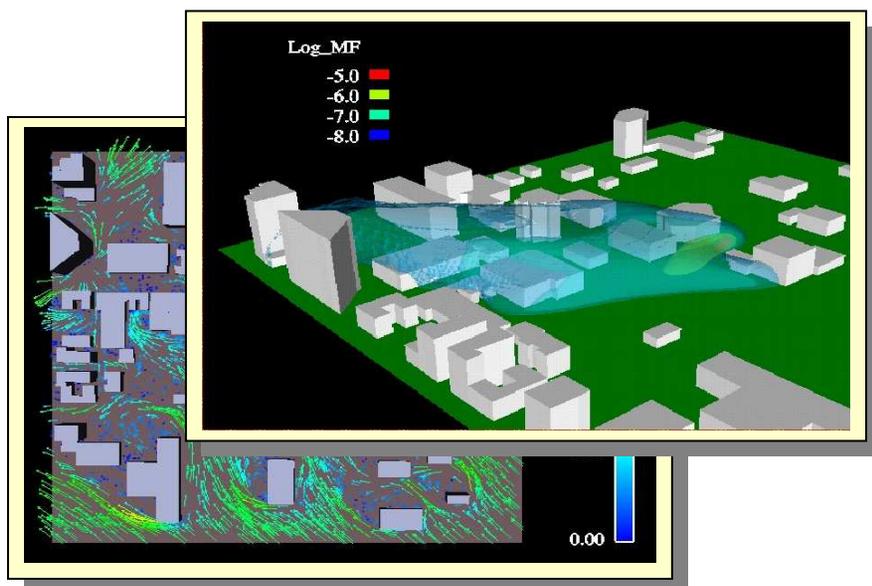




Prediction of aerosol dispersion is a critical homeland security need



- High fidelity models that predict the spread of airborne hazardous materials are important
 - Assist in emergency planning and response scenarios
 - Guide effective sensor placement
 - Event reconstruction (with measurements)





NARAC: An operational release advisory center at LLNL



- **National Atmospheric Release Advisory Center**
 - Supports the DHS Emergency Preparedness and Response (EPR) directorate
 - Provides detailed predictions of atmospheric releases for real-time emergency response, pre-planning, and post-incident assessments
 - Incorporates hierarchy of models for different types of release events, distance scales, and response times

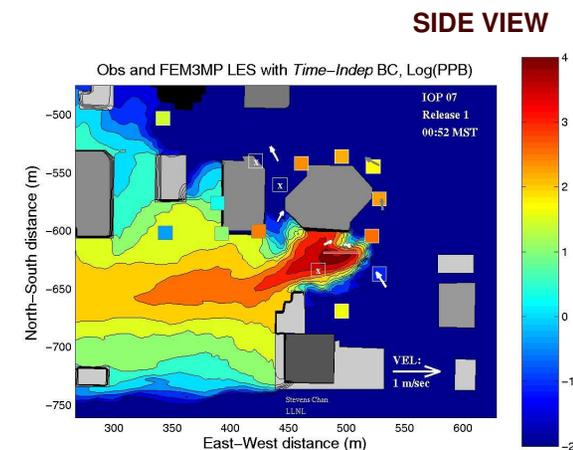
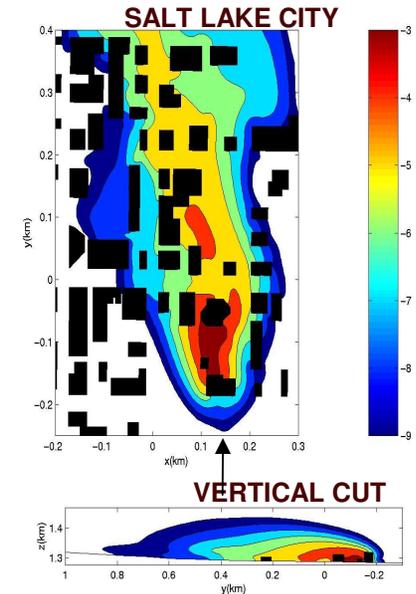




Computational Fluid Dynamics (CFD) necessary for urban dispersion



- **Fast parameterized plume models**
 - Parameters devised for specific conditions
 - Often not general enough to handle disparate urban environments
 - Require CFD model to validate, parameterize
- **FEM3MP is the primary CFD-based urban dispersion modeling code used in NARAC**
 - Finite element incompressible CFD
 - Structured mesh
 - LES & RANS turbulence models
 - Atmospheric chemistry

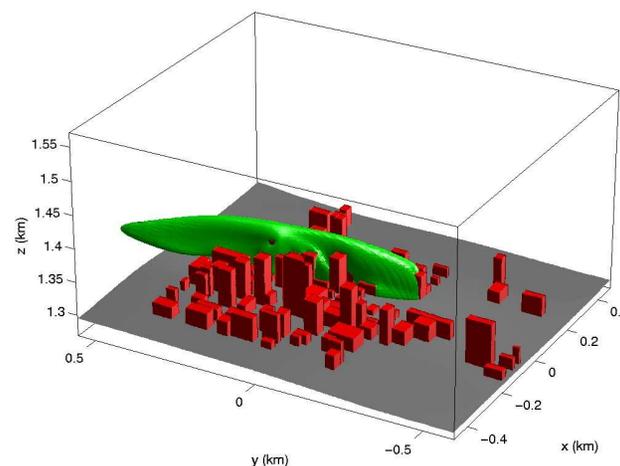
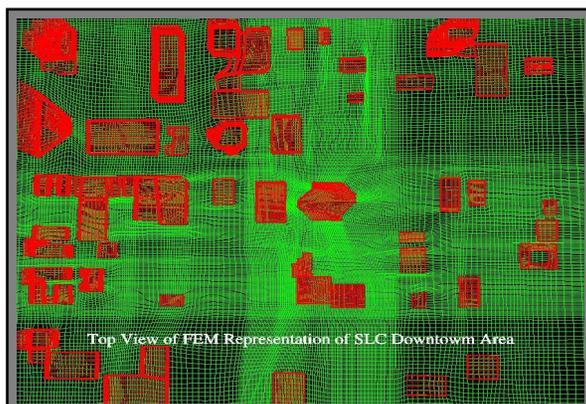




New technologies will significantly enhance operational capability



- Add capability to model complex building geometries
- Provide automatic grid generation capabilities that significantly reduce problem setup time
- Greatly improved computational efficiency



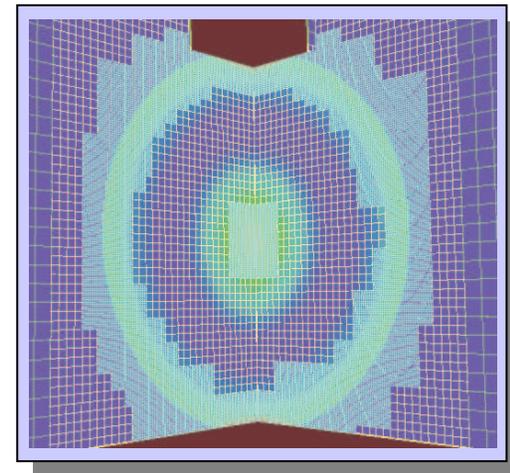
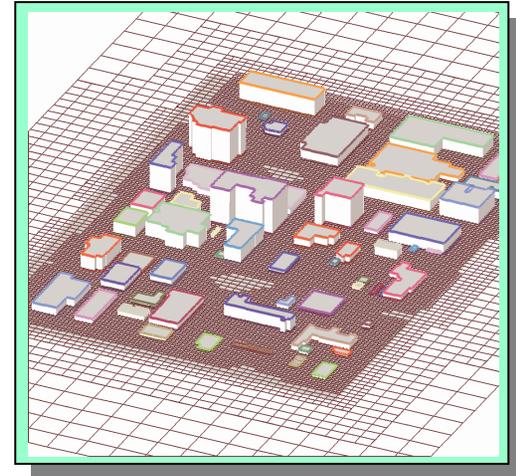
We will apply advanced meshing tools to deliver improvements in NARAC's operational capability



Utilize advanced meshing tools developed at LLNL

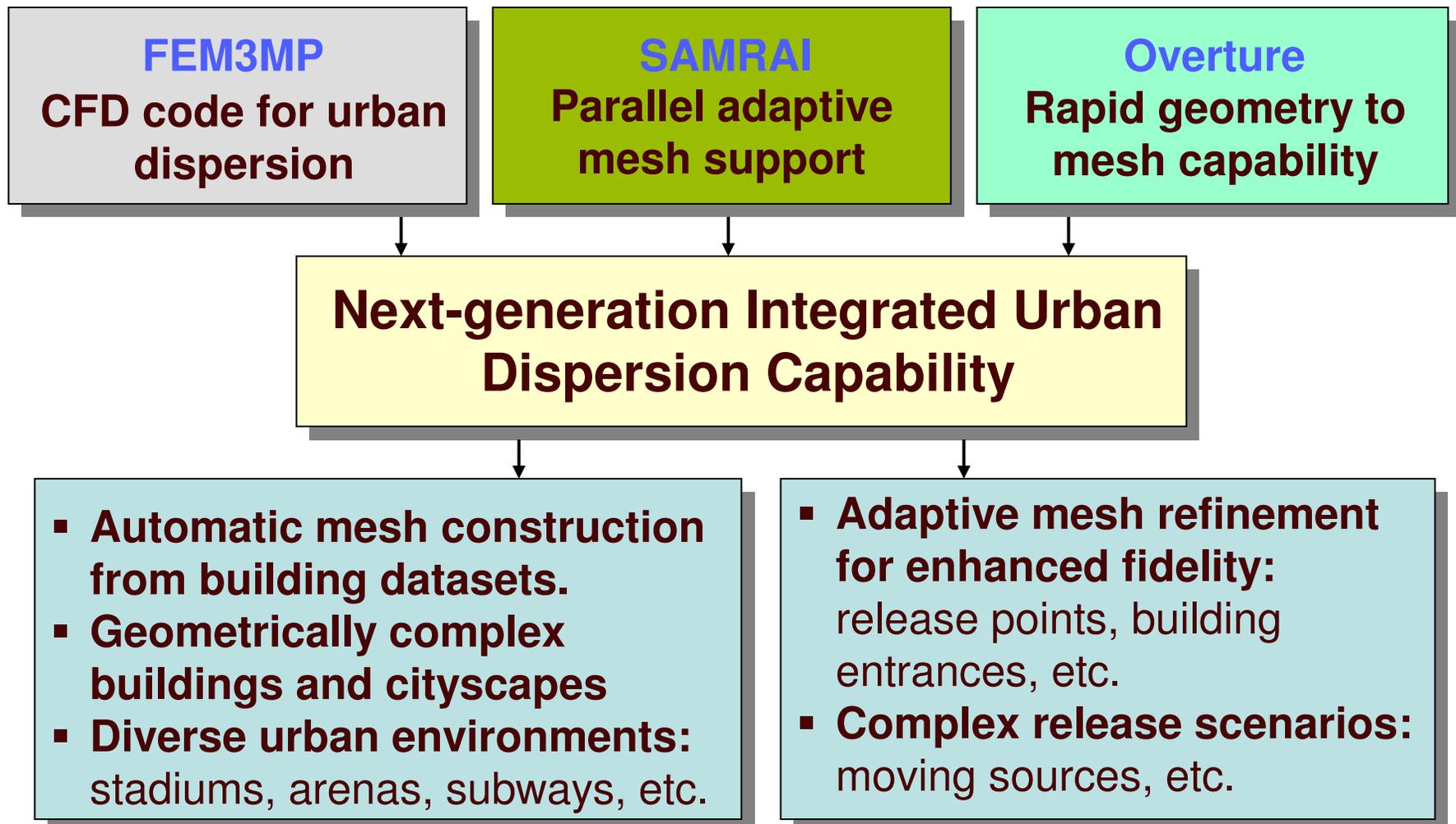


- **Overture** project has tools for rapid geometry-to-mesh (Rapsodi)
 - Rapid construction of surface grids from CAD data
 - Developed to handle complex geometries
- **SAMRAI** library supports parallel AMR applications
 - Adaptive mesh refinement (AMR) automatically enhances simulation resolution where needed.
 - Runs on large parallel computer systems



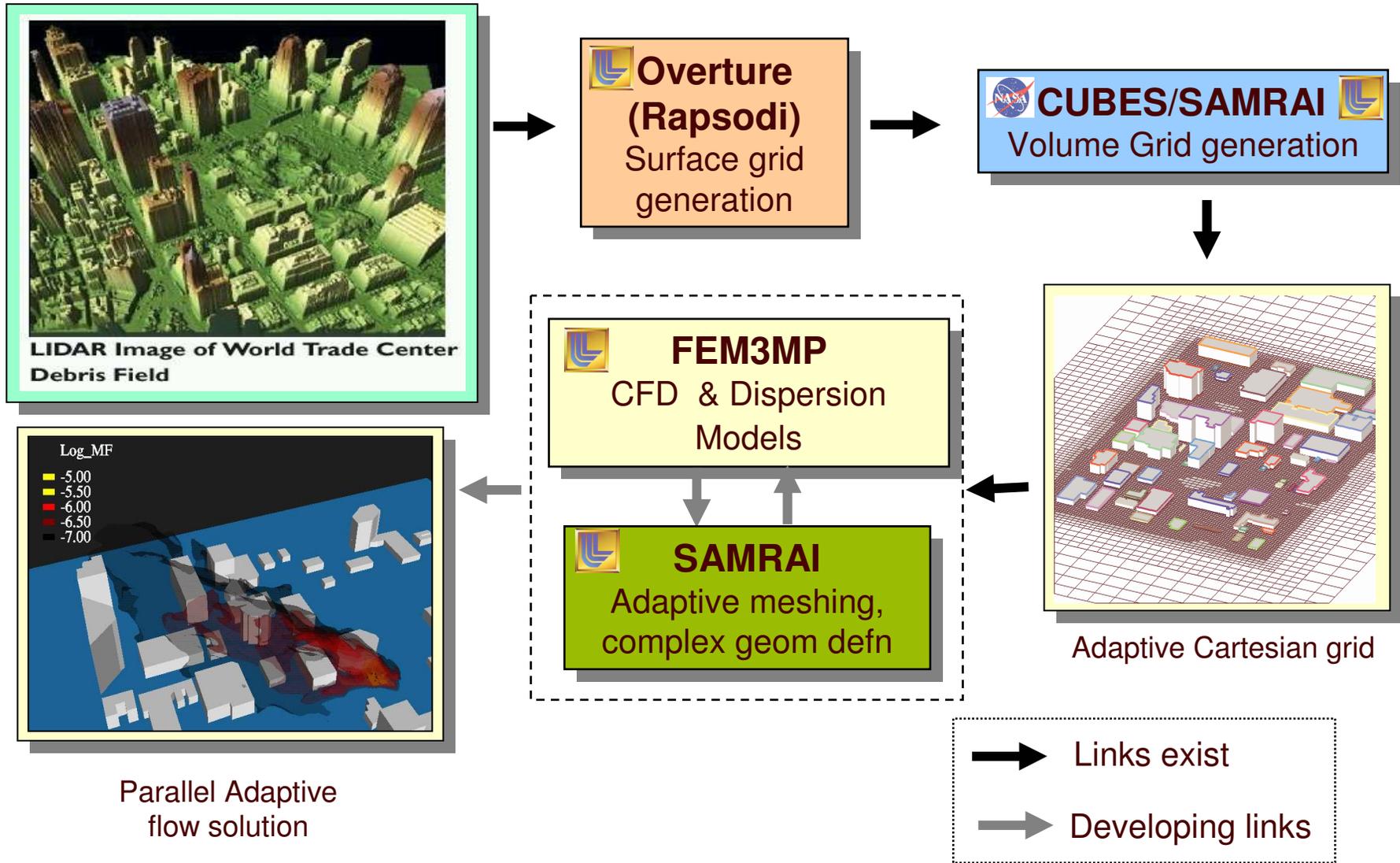


Couple advanced technologies to develop enhanced operational tool





Integrated approach will enable automated geometry to CFD analysis

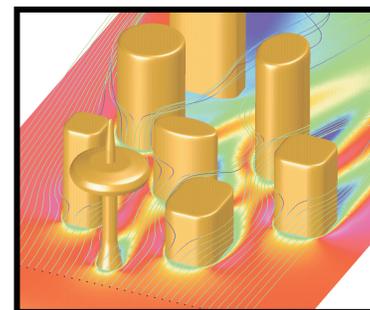
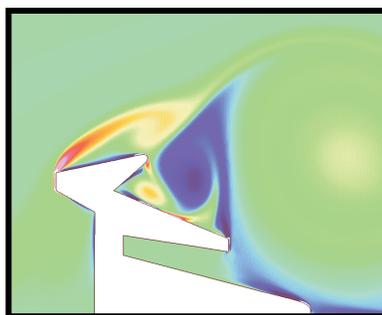
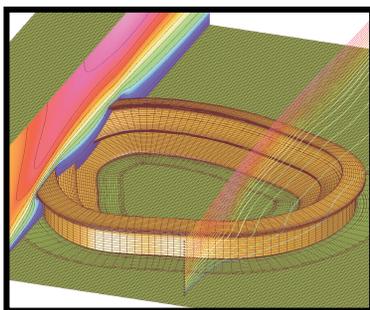




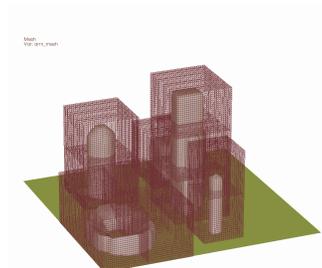
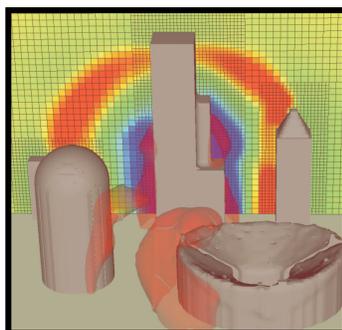
Some demonstration calculations around complex building geometries



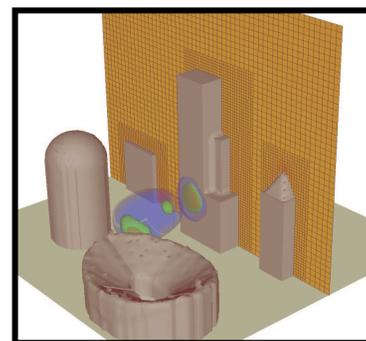
- Flow around stadium and sample cityscape



- Adaptive flow simulation over prototype cityscape



Refined region
around buildings



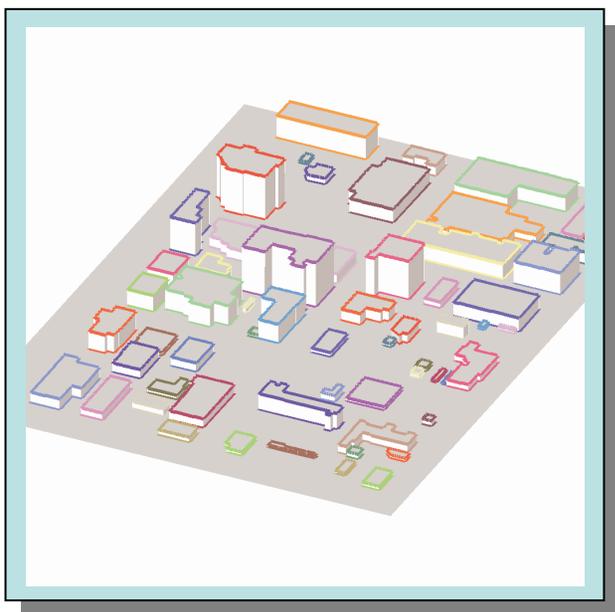
“Proof of concept” calculations – Q4 2003



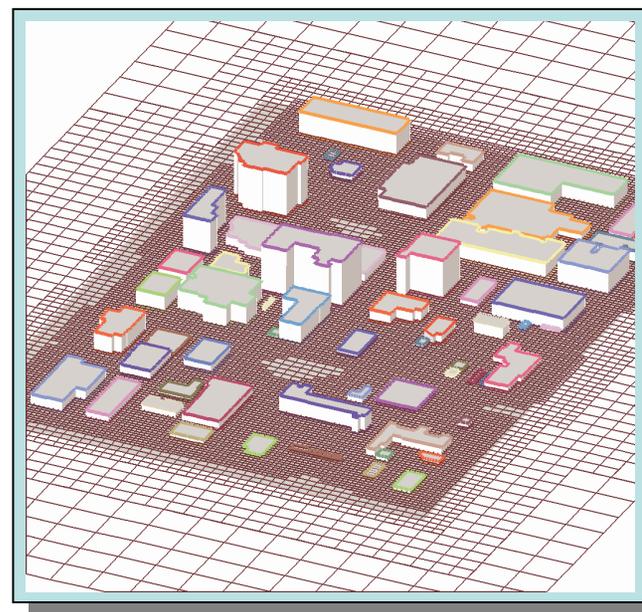
Automatic construction of grids from building datasets



- Tool developed to read polygonal geometry data from NARAC and generate Cartesian adaptive grids.



**Polygonal
geometry data
(Salt Lake City)**



**Adaptive volume mesh
by **metro/CUBES****

Q2 2004

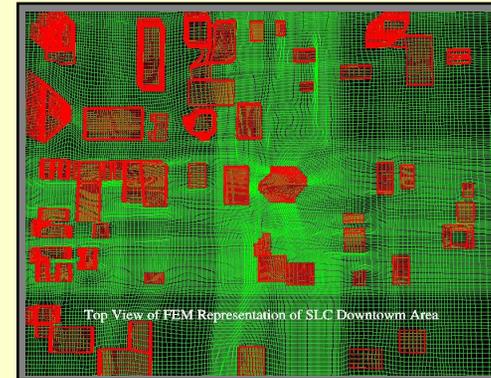


Grid generation time reduced from weeks to minutes



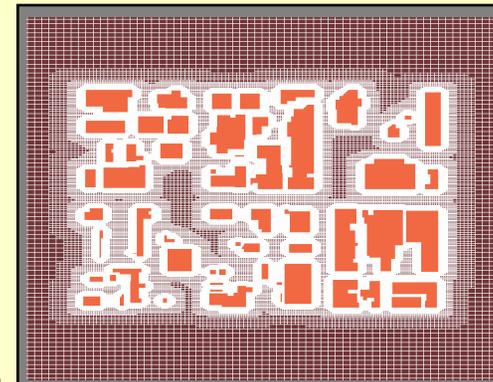
Downtown Salt Lake City gridding example

- Structured grid constructed with existing tools required about 1 week



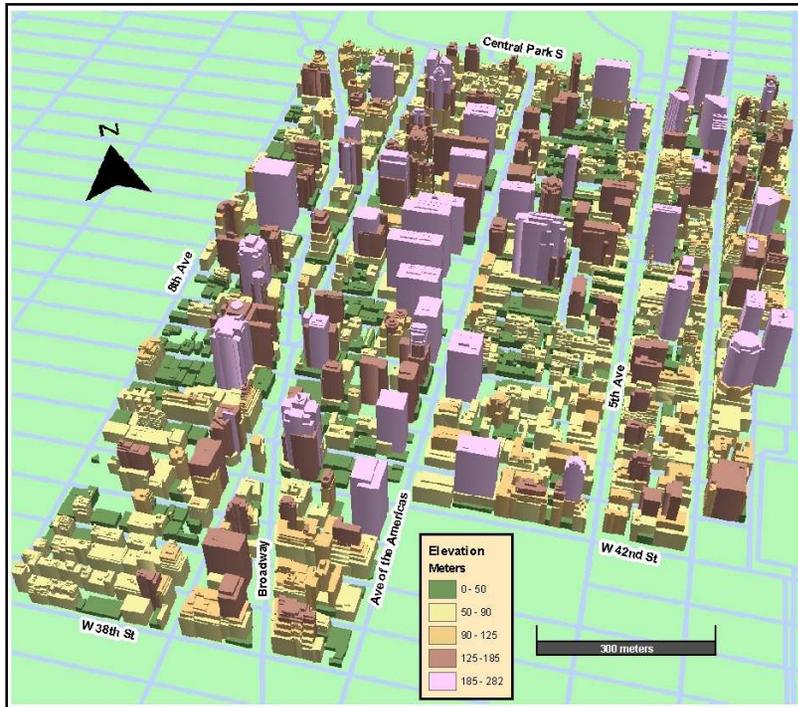
- Adaptive cut-cell grid generated with **metro/CUBES** required about 2 minutes

1.7M gridpoints, 6 levels refinement
Surface grid – 30 sec with “metro”
Volume grid – 45 sec with “CUBES”



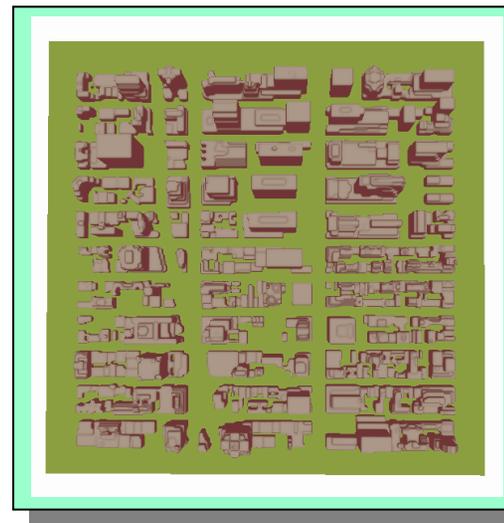


Tools utilized to mesh complex cityscapes



Midtown Manhattan

Times Square

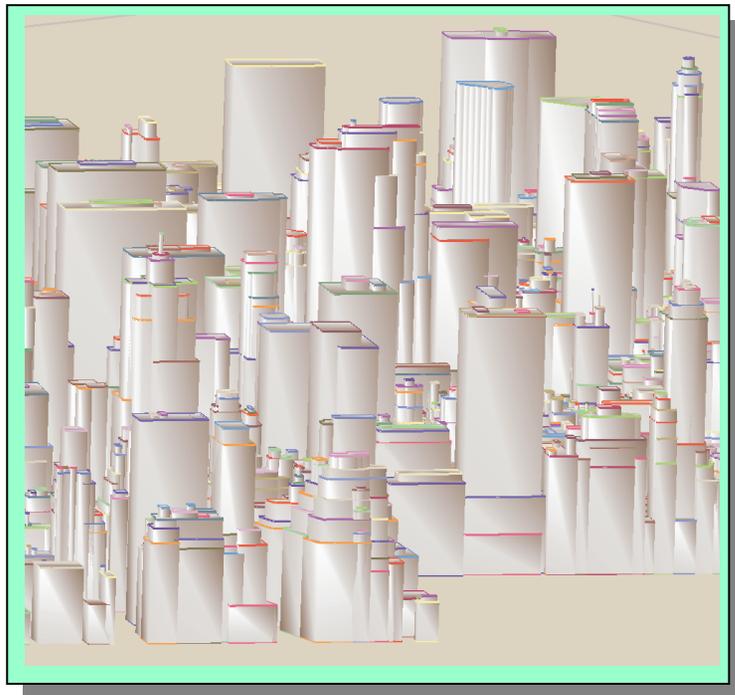


Polygonal geometry representation by **metro** (3600+ polygons)

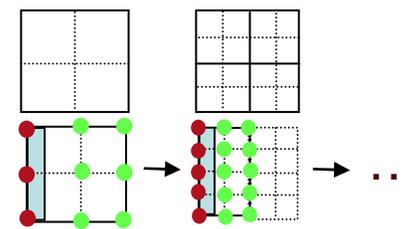
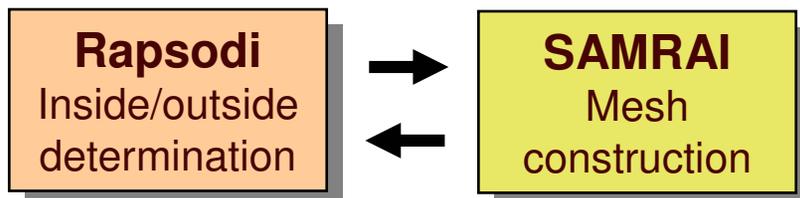
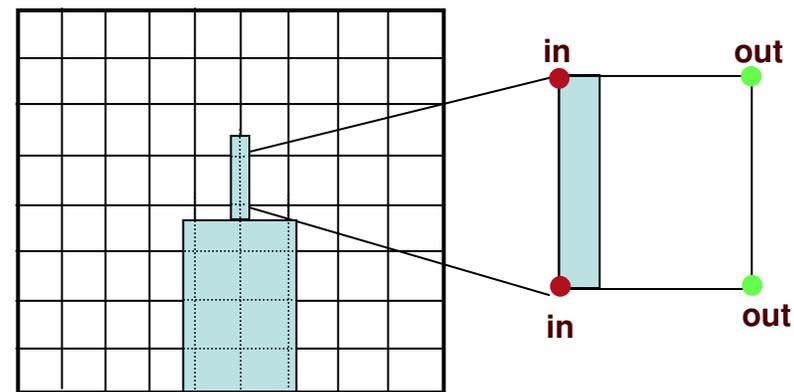
Q3 2004



New efficient grid construction strategies for complex cityscape data



- Generating triangulated surface difficult or impossible
- Inside/outside determination using Polygons



Enhanced accuracy through refinement

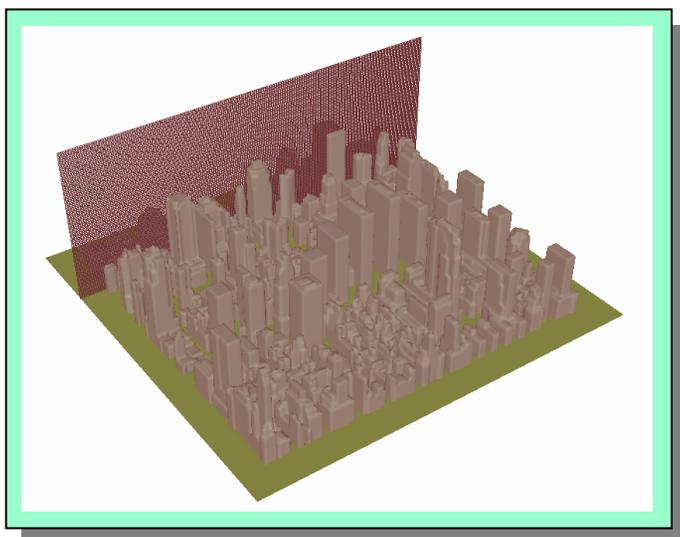


First set of delivered tools will be used for Manhattan in Fall 2004



Manhattan simulations

- DHS-funded study of urban dispersion in Manhattan
- Meshing tools used for CFD simulations
- Very computationally intensive calculations (using non-adaptive solver)
- When fully developed, our adaptive solver will enable higher resolution at lower computational cost



Manhattan meshes
Rapsodi/SAMRAI

Navier-Stokes Flow Solver

Adaptive
SAMRAI+FEM3MP

Expected availability mid 2005

Non-adaptive
FEM3MP standalone

Currently available

Q4 2004



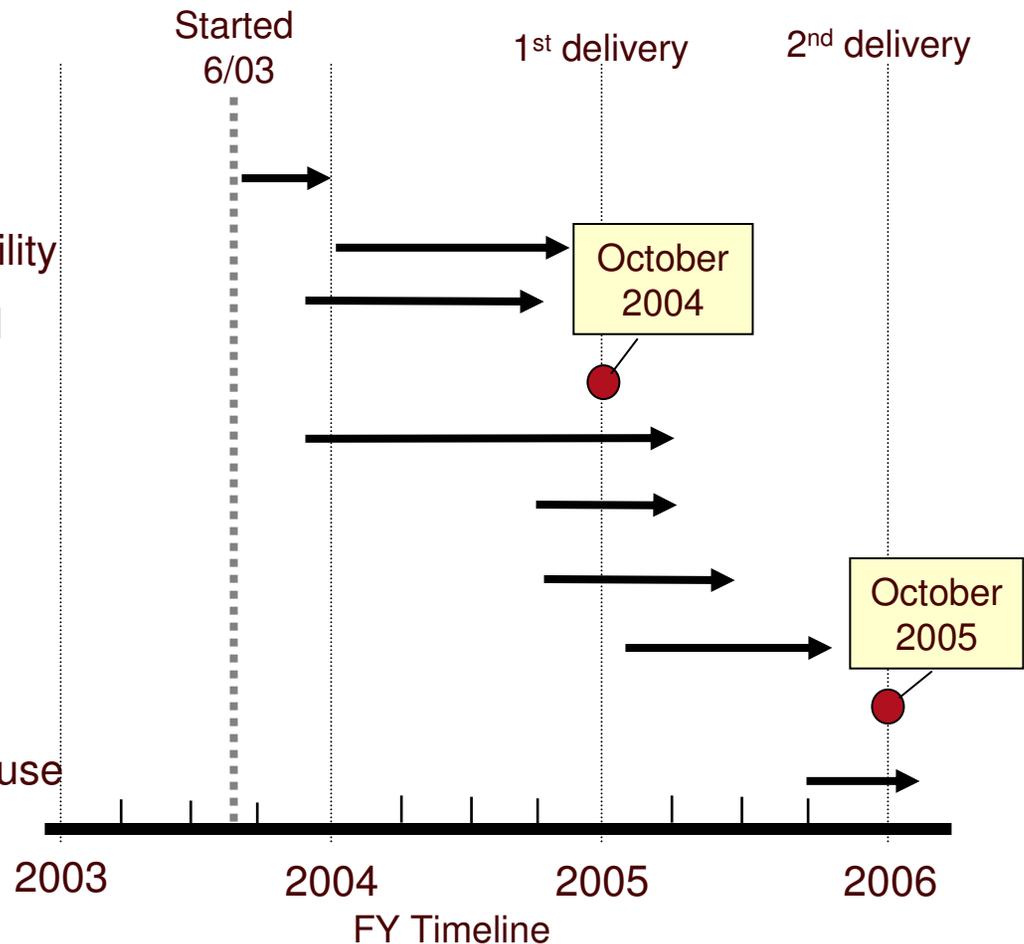
netcdf
files



Project tasks and timeline



- Demonstration calc with prototypes
- Demonstrate geometry-to-mesh capability
- Develop complex geometry in SAMRAI
- **Deliver gridding tools for NYC**
- SAMRAI-FEM3MP integration
- Develop cut cell FE algs
- Develop AMR capability
- **Deliver adaptive flow solver**
- Fine-tune performance for operational use

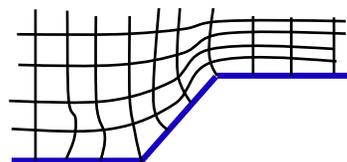




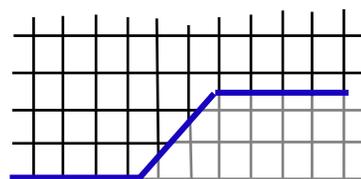
Algorithmic research issues to be addressed in 2005



- Finite element boundary representation on cut-cell grids using “fictitious domain” algorithm



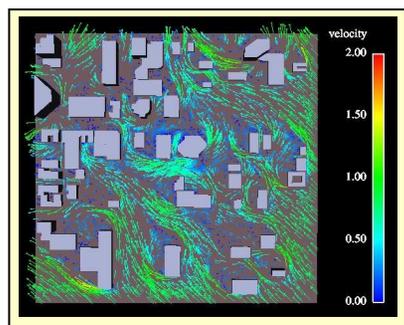
“conforming” mesh (old)



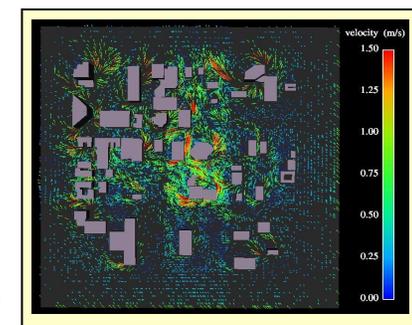
“cut-cell” mesh (new)

- Adaptive algorithms for finite element CFD solver
- Turbulence models

RANS



LES



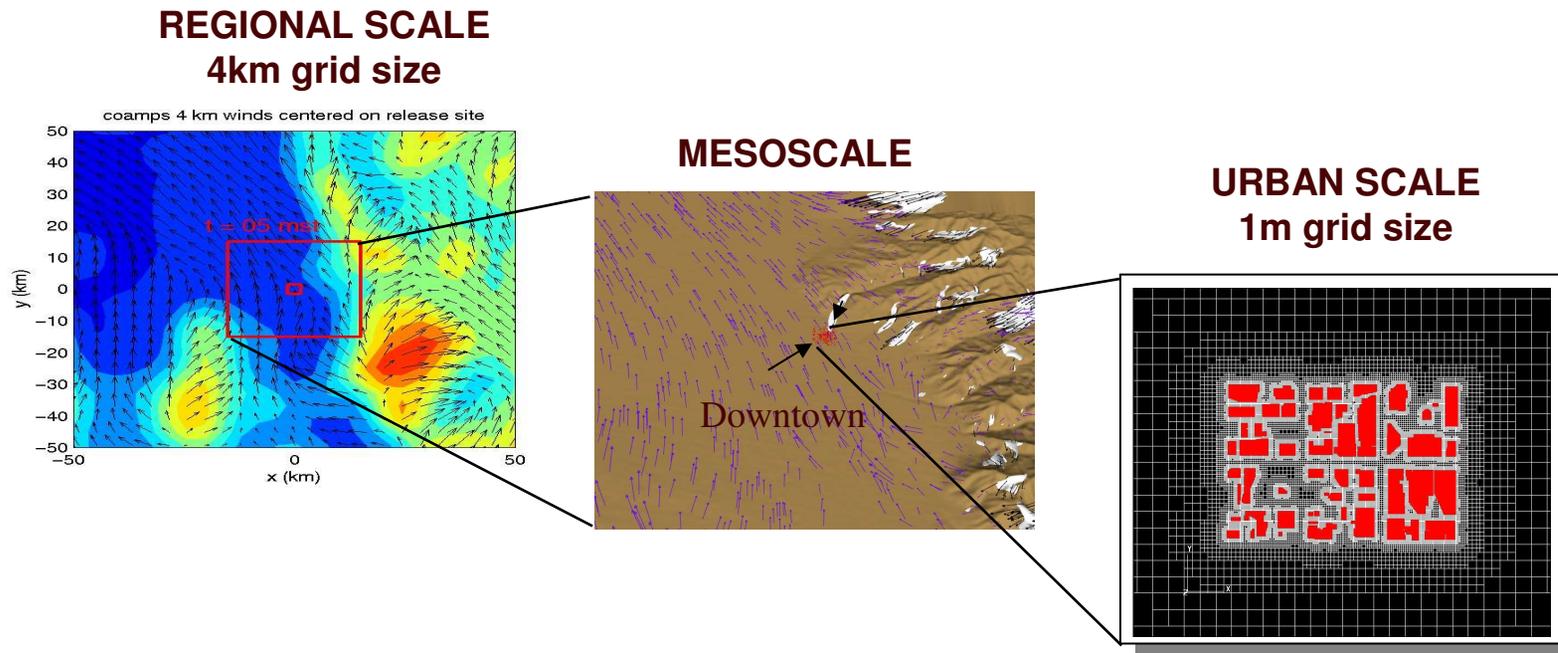
- Building geometry information that incorporates new features (e.g. terrain)



Longer term research issues



- Coupling models with different scales
- Integrate our external model with internal flow models (subways, arenas, etc.) – J. Shadid, SNL
- Performance on diverse parallel architectures

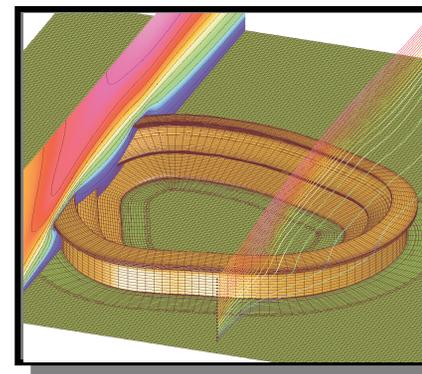
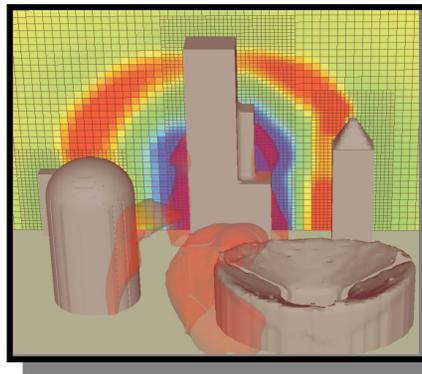
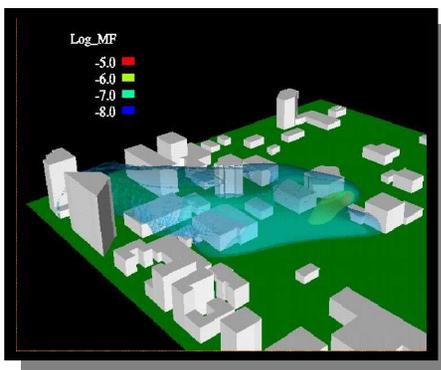




Summary



- We are developing new capabilities by combining tools by two groups at LLNL – COMP and NARAC
- Automatic geometry-to-mesh and adaptive gridding tools will significantly enhance NARAC's operational urban capability
- Preliminary tools delivered Fall 2004, fully developed adaptive solver to be delivered Fall 2005



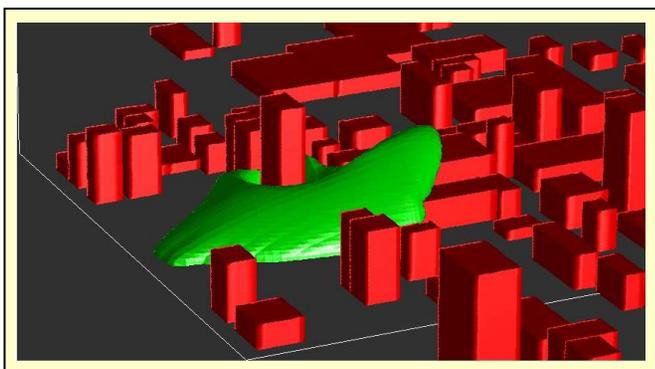
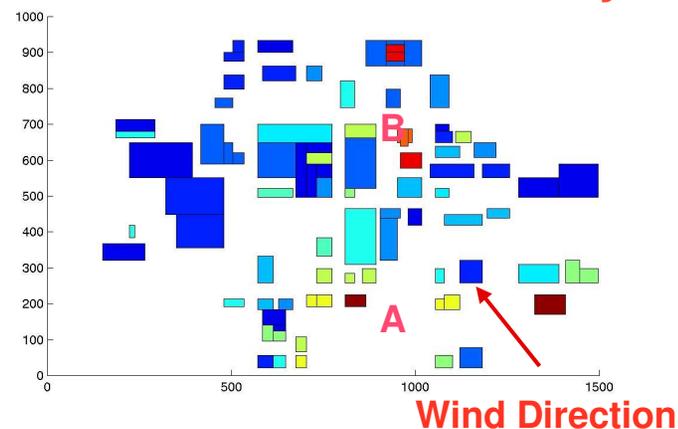


We will use experimental data to verify and validate model accuracy

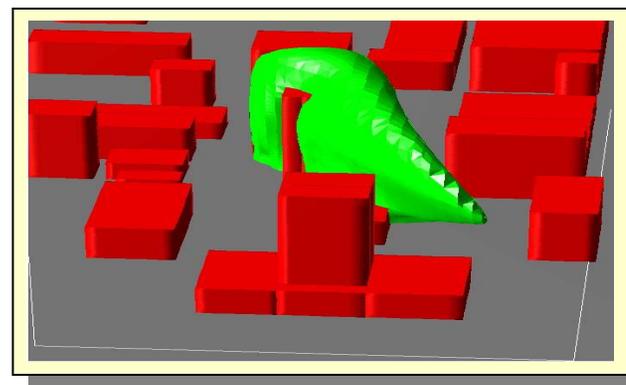


- Joint-Urban 2003 in Oklahoma City
- Urban 2000 in Salt Lake City
- Wind tunnel experiments

Downtown Oklahoma City



Release south of downtown (A)



Release in downtown area (B)



Acknowledgments



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