ADAPTIVE URBAN DISPERSION INTEGRATED MODEL

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## 1. INTRODUCTION

Numerical simulations represent a unique predictive tool for understanding the three-dimensional flow fields and associated concentration distributions from contaminant releases in complex urban settings (Britter and Hanna 2003). Utilization of the most accurate urban models, based on fully three-dimensional computational fluid dynamics (CFD) that solve the Navier-Stokes equations with incorporated turbulence models, presents many challenges. We address two in this work; first, a fast but accurate way to incorporate the complex urban terrain, buildings, and other structures to enforce proper boundary conditions in the flow solution; second, ways to achieve a level of computational efficiency that allows the models to be run in an automated fashion such that they may be used for emergency response and event reconstruction applications.

We have developed a new integrated urban dispersion modeling capability based on FEM3MP (Gresho and Chan 1998, Chan and Stevens 2000), a CFD model from Lawrence Livermore National Lab. The integrated capability incorporates fast embedded boundary mesh generation for geometrically complex problems and full three-dimensional Cartesian adaptive mesh refinement (AMR). Parallel AMR and embedded boundary gridding support are

provided through the SAMRAI library (Wissink et al. 2001, Hornung and Kohn 2002). Embedded boundary mesh generation has been demonstrated to be an automatic, fast, and efficient approach for problem setup. It has been used for a variety of geometrically complex applications, including urban applications (Pullen et al. 2005). The key technology we introduce in this work is the application of AMR, which allows the application of high-resolution modeling to certain important features, such as individual buildings and high-resolution terrain (including important vegetative and land-use features). It also allows the urban scale model to be readily interfaced with coarser resolution meso or regional scale models.

This talk will discuss details of the approach and present results for some example calculations performed in Manhattan in support of the DHS Urban Dispersion Program (UDP) using some of the tools developed as part of this new capability.

## 2. BACKGROUND

The current CFD urban dispersion modeling capability used at LLNL is FEM3MP (Gresho and Chan 1998, Chan and Stevens 2000, Stevens et al. 2002), a stand-alone CFD code based on a finite element fluid flow solver. It includes chemistry and simplified aerosol physics as well as advanced subgrid scale turbulence models and runs on large-scale parallel computer systems. The data structures supported by the code are compatible with structured, logically rectangular, grids.

The model solves the incompressible Navier-Stokes equations through the pressure projection scheme of Gresho and Chan (1998). It has been validated with experimental data

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from wind tunnel tests, and from flow measurements around complex buildings and urban environments, such as Urban 2000 (Salt Lake City, 2000 October) and Joint URBAN 2003 (Oklahoma City, 2003 July). Examples of such studies are discussed in Chan et al. (2001), Chan and Leach (2004), Calhoun et al. (2005), Chan (2005), Chan and Lundquist (2005).

Traditionally, FEM3MP has modeled buildings on grids that utilize contour mapping, an approach widely used for other atmospheric calculations with complex terrain. Gridlines are wrapped around the buildings and points that reside inside the buildings are "blanked out". Although this approach yields accurate results in the flow calculation, problem setup steps of generating the grid are difficult and time consuming for large-scale cityscapes and geometrically complex buildings. The approach is generally not automated and thus requires efforts by a trained analyst to construct the grid. The contour-mapped approach is thus only applicable for longer-term studies and is not generally usable for quick-turnaround needs of operational applications; that is, unless grids for every possible scenario (i.e. regions of any city of interest) are pre-generated, which would be a very time consuming effort.

## 3. METHODOLOGY

In an effort to reduce the problem setup costs and enhance computational efficiency, we adopt an embedded boundary gridding approach with Cartesian AMR meshes (Fig. 1). Cartesian meshes offer the advantage of having faster numerics because, unlike contour mapped grids, there are no metric terms applied. Also, they more easily facilitate the use of adaptive mesh refinement to enhance fidelity in certain important regions and allow a more accurate solution with fewer gridpoints. Embedded boundary meshes are simple and automatic to construct and almost completely eliminate the complex and costly problem setup steps required for the contour-mapped approach.

In our approach, we continue to use the FEM3MP finite element algorithm for the flow solve. The adaptive Cartesian meshing and embedded boundary representations are provided the SAMRAI software framework (Hornung and Kohn 2002, Wissink et al. 2001).
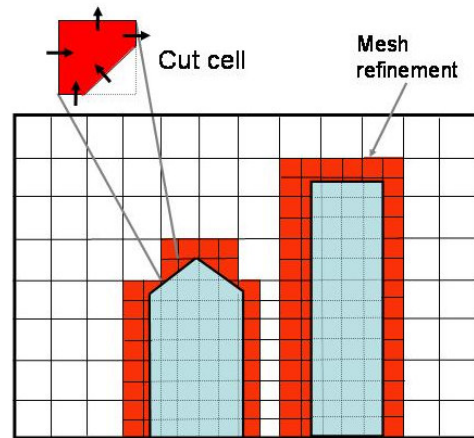


Fig. 1. Cartesian adaptive embedded boundary grid representation for buildings. Cells cut by building boundaries store their volume fraction, normal vector, etc.

The following subsections discuss details of the embedded boundary grid generation approach, the use of AMR, and software integration of FEM3MP and SAMRAI, respectively.

### 3.1 Mesh generation

Embedded or immersed boundary gridding has become a popular approach for geometrically complex problems (Berger and Aftosmis 1998). Unlike traditional mapped grids, the embedded boundary is constructed by simply overlaying the complex geometry over a standard Cartesian grid (Fig. 1). Cells that intersect the boundary are identified and certain information is stored, such as the volume fraction, surface normal, etc. The governing flow equations are then modified using these quantities to impose the appropriate boundary condition. The primary advantage of this approach is that it enables a high level of automation of the grid generation process, even for very complex geometries. The embedded or immersed boundary approach has been used by Tseng and Ferziger for geophysical flow applications involving complex terrain (2003) and by Landsberg and Boris for atmospheric flow around complex urban cityscapes (2001).

A key issue in developing an embedded boundary capability is the construction of the boundary and management of the data structures that hold the information. Each cut

cell must compute and store the volume fraction, normal direction, distance of nodes to the boundary, etc. The SAMRAI software from LLNL has links to packages that can construct the embedded boundary and maintains internal data structures that can hold this information and communicate it efficiently on a parallel computer system.
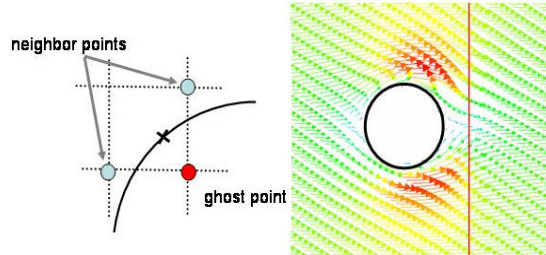


Fig. 2. "Ghost point" method to impose the presence of solid boundaries.

To enforce conditions at the embedded boundary we use the Immersed Boundary Method (IBM) as proposed by Tseng and Ferziger (2003). In this approach, "ghost points" are identified as the first node inside the boundary (Fig. 2). The distance and normal to the boundary are computed, as well as the distance from their nearest neighbor nodes outside of the boundary ("neighbor points"). From this information, the value of the primitive variables at the ghost point can be appropriately modified to enforce the boundary conditions, which are no slip (i.e. velocity = 0 in all directions) and a zero pressure gradient normal to the boundary.

### 3.2 Adaptive Mesh Refinement

The FEM3MP code operates on structured logically rectangular meshes. For this reason, it is most amenable to a patch-based block structured AMR approach. In patch-based AMR, a grid consists of a hierarchy of levels of logically rectangular variably-sized regions called patches (Fig. 3). FEM3MP numerical kernels are applied on the patches of the adaptive mesh hierarchy. Support for applying the numerics to interpolate between levels and communicating between different patches is supplied by the SAMRAI framework.

The SAMRAI framework provides parallel AMR support. Implementing AMR into an

existing application code is non-trivial. Algorithms to dynamically construct the adaptive mesh hierarchy, communication to manage data exchanges between irregularly spaced patches on different levels, and parallel load balancing must all be considered. Also, the solution technique becomes more complicated because solvers must properly operate on the adaptive grid hierarchy. The SAMRAI framework provides support for all of these operations – constructing and adapting the mesh hierarchy, communicating between levels and patches, and ensuring scalability on parallel computer systems. In our implementation, SAMRAI manages construction of the adaptive mesh hierarchy and provides parallel support, and FEM3MP numerical kernels are applied on each of the individual patches.
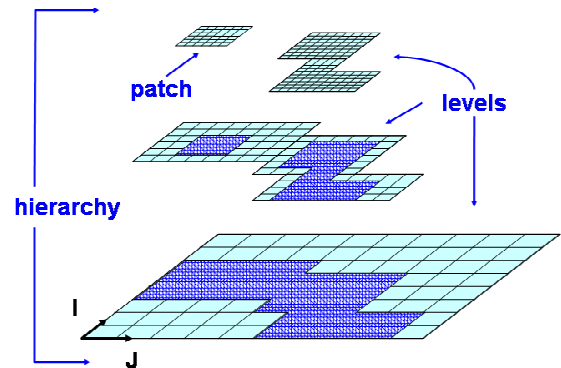


Fig. 3. Structured adaptive mesh grid consists of a hierarchy of nested patch levels.

In addition to parallel AMR support, SAMRAI also contains linear solvers specialized for AMR grids and contains links to a variety of solver packages. We utilize a specialized Fast Adaptive Composite (FAC) multigrid solver (Pernice and Hornung, 2004) for the pressure projection solves in our adaptive implementation.

We are currently investigating algorithmic issues in the AMR implementation of FEM3MP. Accuracy of the adaptive scheme is being assessed with simple flows around blocks and cylinders for which experimental results are available (Fig. 4).

The AMR code may be run with either static or dynamic refinement. That is, with static
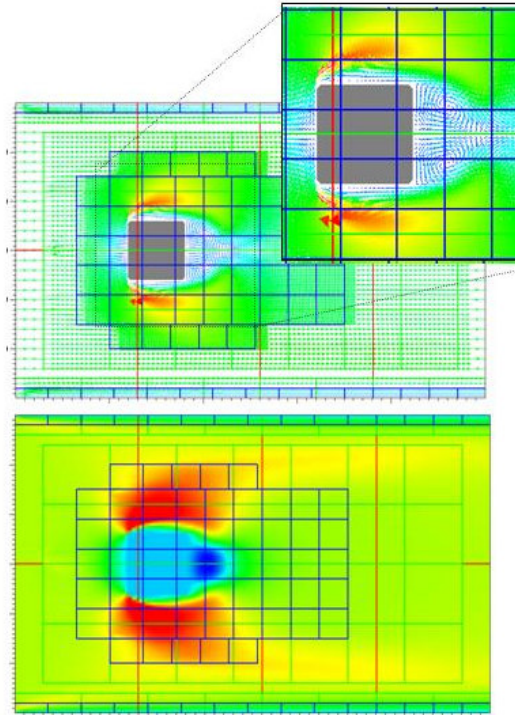
Fig. 4. Three level AMR implementation of FEM3MP for flow around square cylinder. Boxes represent patch boundaries on each level.

refinement a refined mesh hierarchy is constructed at the initial time but does not change during the simulation. An example case would be to generate a refined mesh around building boundaries with coarser meshes in the far field. This mesh would be used unchanged throughout the simulation. With dynamic refinement, the mesh is modified throughout the simulation to refine and/or coarsen around certain features. This could be used, for example, to track important features as the simulation evolves such as plume concentration, regions of high wind currents, etc. To date, we have not done a full analysis of which approach is best under certain conditions so this is a topic for future work.

### 3.3 Software Integration

The previous sections discussed the integration of FEM3MP with SAMRAI in order to provide parallel AMR and embedded boundary meshing capabilities. This section focuses on
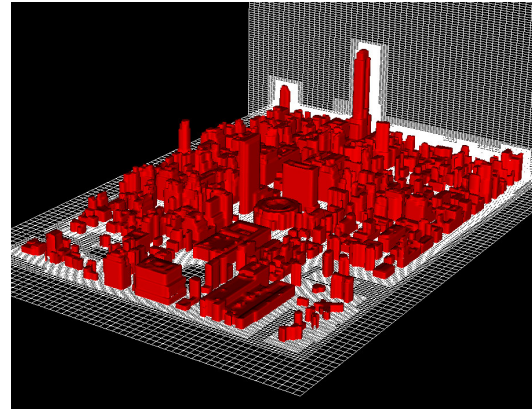


Fig. 5. Three-level adaptive Cartesian grid generated around Madison Sq. Garden area of Manhattan from ESRI shapefile description.

software developed to facilitate the grid generation steps, to automatically construct embedded boundary meshes from different building representations.

We have built software that is part of the Overture suite (Petersson 2003) which reads ESRI shapefile representations of buildings. From this information, it constructs a database of shapes which may then be used to build the Cartesian embedded boundary. The embedded boundary information is accessed by SAMRAI through library calls. Figure 5 shows a three-level adaptive embedded boundary mesh constructed from shapefiles of the Madison Square Garden area in Manhattan. Construction of this mesh was done automatically from shapefile input in about 10 minutes on a single processor workstation.

There are circumstances where urban topographies cannot be readily represented through shapefiles alone. Examples include geometrically complex buildings or those that lie in complex hilly terrain. For these cases, we have developed the capability to construct embedded boundary meshes directly from a triangulated surface description. Patch-based interfaces were built between SAMRAI and the fast embedded boundary grid generation tools in the Cart3D package from NASA Ames (Berger and Aftosmis 1998). This package, which was developed to model geometrically complex aerospace vehicles, is capable of meshing around very complex building geometries. Figure 6 shows the cross section of a five-level
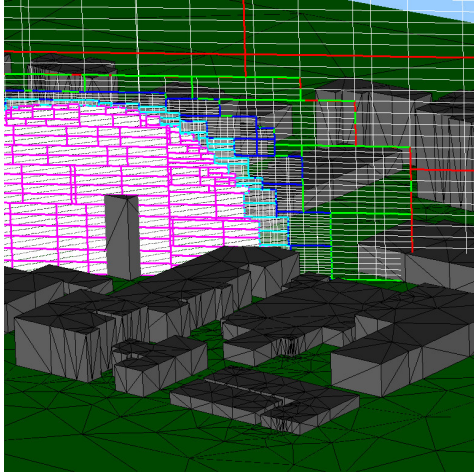
Fig. 6. Patch boundaries for a five-level adaptive Cartesian grid over a triangulated surface of buildings in Salt Lake City. The coarsest mesh resolution is 27m horizontal by 7m vertical, while on the finest resolution is 1m x 0.2m.

adaptive grid constructed around a triangulated surface of buildings in Salt Lake City.

## 4. APPLICATIONS

The rapid gridding tools described above are extremely useful in generating computational grids for use by a CFD model like FEM3MP (Gresho and Chan, 1998; Chan and Stevens, 2000; Chan and Lundquist, 2005) for simulating airflow and dispersion in the urban environment. Using such grids, FEM3MP has been used effectively and efficiently to perform simulations that aid the planning of field trials and in model evaluation studies, for instance, for the New York City Urban Dispersion Program (NYC UDP).

The NYC UDP research project was launched by the Department of Homeland Security in 2004, with the goal to improve the permanent network of wind stations in and around New York City and to enhance the city's emergency response capabilities. Encompassing both field studies and computer modeling, one of the program's objectives is to improve and validate urban dispersion models using the data collected from field studies and to transfer the improved capabilities to NYC emergency agencies. The first two field studies

were conducted in 2005 and an additional study is planned for the summer of 2006.

As an example, FEM3MP was used to simulate one of the field experiments around Madison Square Garden (MSG) conducted in March 2005. Details of the simulation and results can be found in Leach, et al. (2005). In the numerical simulation, a domain size of 1,750 m x 1,200 m x 800 m was discretized with 351 x 241 x 151 (~12.7 million) grid points. The embedded boundary grid, with a 5-m grid resolution in the horizontal directions and variable resolution in the vertical direction, was generated in about 10 minutes on a single processor workstation.
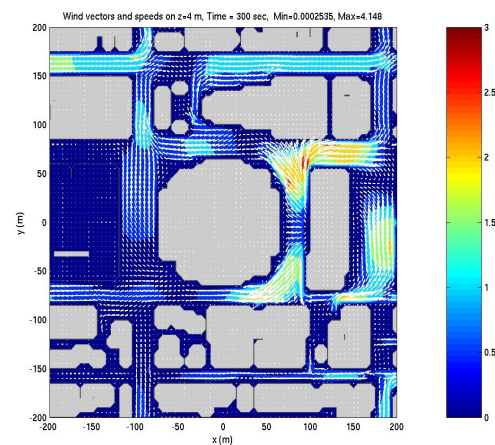


Fig. 7. Predicted wind vectors and wind speeds (color contours) near Madison Square Garden on z =4 m plane. MSG is in the middle of the picture.

Figure 7 shows a close-up view of the predicted wind vectors near MSG on the z=4m horizontal plane. Shown in the figure are the complexity of airflow around the buildings, in particular, the diverging flow towards the upwind and crosswind directions on the windward side of MSG and of Two Penn Plaza (to the east of MSG in the figure). In addition, there exists noticeable reverse flow along a couple of east-west running streets to the southwest corner of MSG. These results suggest that transport of a street level release in the area could extend for a few blocks in both upwind and crosswind directions relative to the prevailing wind direction above rooftops.

In Figure 8, predicted wind vectors and wind speeds (color contours) on the east-west vertical
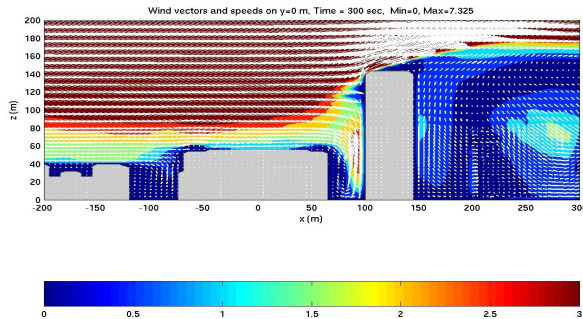
Fig. 8. Predicted wind vectors and wind speeds on the east-west vertical plane (y=0) passing through MSG.

plane (y=0) passing through MSG are shown. The variations and intensity of downdrafts and updrafts around Two Penn Plaza can be clearly seen. Also shown in the figure are two (clockwise) rotating vortices adjacent to MSG.

The existence of downdrafts and updrafts around Two Penn Plaza and the rotating vortices adjacent to MSG could have significant implications for the transport of contaminants. Such materials could be brought down or up around tall buildings, depending on the local wind direction. Once trapped in the vortices of the street canyons near MSG, the contaminants could linger much longer than they would in open areas.

### 4.1 Coupling with Large Scale Models

Urban scale models are able to resolve small-scale flows (e.g. flows around buildings) which must be parameterized in larger-scale models. However, flow and dispersion in urban boundary layers are driven by larger-scale motions that must be resolved using mesoscale and regional-scale models. Coupling numerical models to resolve different scales of motion is essential for high fidelity numerical simulations. Current work by our group has shown that the desired accuracy of urban-scale simulations can be attained only by faithfully integrating the natural fluctuations in larger-scale forcing in both time and space.

The grid nesting and refinement provided by the SAMRAI results in nearly seamless coupling of the CFD code with mesoscale models by aligning the coarse low-level grid with the mesoscale model grid. For example, Figure 6 shows a five-level mesh around Salt Lake City where the coarse resolution approaches that used in a mesoscale model while the fine resolution, in the regions immediately around the buildings, is on the order of 1m. In addition, adaptive meshing enables us to effectively address more complex scenarios such as those involving moving sources.

### 4.2 Turbulence Modeling

Two computational techniques used for turbulent flow simulations in urban boundary layers are Reynolds Averaged Navier-Stokes (RANS) and large-eddy simulations (LES). RANS is applicable to steady-state or slowly-evolving flows where quasi-equilibrium has been established. It is therefore valid for simulations involving longer time scales, and is more appropriate for continuous atmospheric releases. Due to the characteristics of real urban morphologies, associated release events and fast evolving flows, the LES approach, which resolves the most energetic eddies, is needed for highly accurate simulations. We are implementing improved turbulence (subgrid) models for LES, applicable to a full range of atmospheric stability conditions.

### 4.3 Performance

Our integrated CFD code incorporates MPI parallelization through the use of SAMRAI. This makes it suitable for use on distributed memory systems such as Linux clusters that are becoming a dominant computational platform for large-scale computations. Scalable adaptive calculations have been performed with SAMRAI on over 2000 processors so we are confident that our integrated model will be efficient on parallel computer systems.

### 5. SUMMARY

We have developed a prototype of a new integrated urban dispersion capability that utilizes adaptive grids and embedded boundary meshing. Our goal in developing this capability is to address the critical need for a fast, efficient and accurate tool for urban dispersion modeling to support a wide range of homeland and national security needs, vulnerability and risk

assessment studies, operational emergency response, critical infrastructure and facility protection, as well as forensic analysis applications.

While the adaptive CFD capability is still in the prototyping phase, the mesh generation tools have been successfully applied for studies in the Urban Dispersion Program. They have shown significant speedups that demonstrate their potential for operational use. For instance, meshes were generated over regions in Manhattan with over 1000 buildings in under 10 minutes on a standard workstation. Once we are able to effectively utilize dynamic adaptive meshes in the flow solver we anticipate a further order of magnitude reduction in computational cost, compared to a uniform mesh calculation.

We envision this new integrated urban dispersion CFD modeling framework to be a key core capability for integration into the Interagency Modeling and Atmospheric Assessment Center (IMAAC) emergency response system. It will also be an important component for atmospheric release event reconstruction in the urban environment.

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