P1.11 INTEGRATED URBAN DISPERSION MODELING CAPABILITY

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1. INTRODUCTION

Numerical simulations represent a unique predictive tool for developing a detailed understanding of three-dimensional flow fields and associated concentration distributions from releases in complex urban settings (Britter and Hanna 2003). The accurate and timely prediction of the atmospheric dispersion of hazardous materials in densely populated urban areas is a critical homeland and national security need for emergency preparedness, risk assessment, and vulnerability studies.

The main challenges in high-fidelity numerical modeling of urban dispersion are the accurate prediction of peak concentrations, spatial extent and temporal evolution of harmful levels of hazardous materials, and the incorporation of detailed structural geometries. Current computational tools do not include all the necessary elements to accurately represent hazardous release events in complex urban settings embedded in high-resolution terrain. Nor do they possess the computational efficiency required for many emergency response and event reconstruction applications.

We are developing a new integrated urban dispersion modeling capability, able to efficiently predict dispersion in diverse urban environments for a wide range of atmospheric conditions, temporal and spatial scales, and release event scenarios. This new computational fluid dynamics capability includes adaptive mesh refinement and it can simultaneously resolve individual buildings and high-resolution terrain (including important vegetative and land-use features), treat complex building and structural geometries (e.g., stadiums, arenas, subways, airplane interiors), and cope with the full range of atmospheric conditions (e.g. stability). We are developing approaches for seamless coupling with mesoscale numerical weather prediction models to provide realistic forcing of the urban-scale model, which is critical to its performance in real-world conditions.

2. BACKGROUND

Our current urban dispersion modeling capability, FEM3MP (Chan and Stevens 2000, Chan et al. 2001a, Stevens et al. 2002) is a stand-alone computational fluid dynamics (CFD) code based on a finite element fluid flow solver. The CFD code was parallelized using the Message Passing Interface (MPI) and includes chemistry and simplified aerosol physics. The data structures supported by the code are compatible with globally structured (logical) grids. To meet the challenges involved in accurate high-fidelity predictions of hazardous releases for a wide range of urban conditions the new integrated urban dispersion capability includes new flexible data structures that enable more efficient coupling with large-scale models and specification of more realistic boundary conditions. It also includes advanced subgrid turbulence models.

3. METHODOLOGY

Our approach to the development of the integrated urban dispersion capability consists of integration of the existing FEM3MP incompressible flow solver with the structured adaptive mesh refinement framework. We are also developing meshing tools for rapid embedded boundary grid generation around the complex configurations characteristic of the urban environment.

3.1 *Framework Integration*

We are currently integrating our flow solver (FEM3MP) with the Structured Adaptive Mesh Refinement Application Infrastructure (SAMRAI) framework. SAMRAI provides us with flexible and extensible tools for structured adaptive mesh refinement application development involving complex coupled physics models, sophisticated numerical solution methods, and high-performance parallel computing hardware (Hornung and Kohn 2002, Wissink et al. 2003). SAMRAI. We will introduce a virtual building concept that will allow us to represent building effects outside of the focus area via a drag force and an immersed boundary technique via distributed Labrangian multipliers (DLM) where the effect of impermeable boundaries is achieved through application of appropriate body forces. This will make it possible to focus high resolution on the areas of interest and eliminate the high computational penalty of our current globally structured grids. We will also take advantage of SAMRAI's parallel communication infrastructure for large-scale applications on massively parallel platforms.

3.2 *Mesh Generation*

Converting input geometries for urban environments to a mesh-appropriate representation is often difficult and time consuming. We are developing new tools that will enable a high level of automation of the grid generation process. Our mesh generation tools are based on Rapsodi algorithms for rapid computational generation of meshes for complex geometries in support of large-scale scientific simulations in three space dimensions (Petersson 2002). Rapsodi's grid generation technology automatically determines all the information needed to construct a reference triangularization of the surface. Integrating Rapsodi tools into our dispersion simulation process enables rapid geometry-to-mesh construction process that can be carried out on a standard workstation through an interactive graphic user interface.

By using these mesh generation tools we will be able to take full advantage of new detailed urban mapping databases currently under development (e.g. USGS/NIMA Metro Area Initiative, a component of the National Map program). Our integrated urban CFD capability will thus potentially be applicable in all major urban areas for emergency response and other consequence assessments.

3.3 *Coupling with Large Scale Models*

Urban scale models are able to resolve small-scale flows (e.g. flows around buildings) but they 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. In addition to that, adaptive meshing enables us to effectively address more complex scenarios such as those involving moving sources.

3.4 *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.

3.5 *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.

3.6 *Verification and Validation*.

The new, advanced features of all the components of our integrated CFD capability will be tested and their effectiveness demonstrated using a series of benchmark tests based on experimental data and previously validated numerical simulations (Chan et al. 2001b). Data will be derived from both wind tunnel experiments and recent urban field study campaigns, such as Urban 2000 (Salt Lake City, 2000 October) and Joint Urban 2003, (Oklahoma City, 2003 July).

4. SUMMARY

Our new integrated urban dispersion capability will 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.

This new urban dispersion CFD model will be a key core capability for integration into a next-generation National Atmospheric Release Advisory Center (NARAC) emergency response system. The CFD model will also be an important component for atmospheric release event reconstruction in the urban environment.

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