Large Scale Simulation of Chem/Bio Dispersion in Urban Areas for Homeland Security

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ABSTRACT

The dispersion of biological and chemical aerosols is a significant security concern. The biological or chemical agents released from a suitcase, truck, or other mobile containers can quickly spread to a broader geographic area and put many people's lives at risk. High performance computing (HPC) technologies can be used to assess potential threats and to calculate the dispersion rates and the level of concentrations of these agents at various times and locations and support emergency response efforts.

The stabilized finite element formulations are developed and applied to solve buoyancy-driven incompressible flows with heat and mass transfer. The stabilizations are based on the SUPG (Streamline-Upwind/Petrov-Galerkin) and PSPG (Pressure-Stabilization/Petrov-Galerkin) methods. The SUPG stabilization term allows us to solve flow problems at high speeds (advection dominant flows) and the PSPG term eliminates instabilities associated with the use of equal order interpolation functions for both pressure and velocity. The finite element formulations are implemented in parallel using MPI. In parallel computations, the finite element mesh is partitioned into contiguous subdomains using METIS, which are then assigned to individual processors. To ensure a balanced load, the number of elements assigned to each processor is approximately equal. To solve nonlinear systems in large-scale applications, we developed a matrix-free GMRES iterative solver. Here we totally eliminate a need to form any matrices, even at element levels. Detailed geometric models of urban areas are built using a variety of methods including morphology data, GIS databases, and other sources. The application includes the simulation of dispersion of contaminant in city of Atlanta. Three different unstructured meshes are made with 6.9, 55, and 440 tetrahedral million elements. The solutions are obtained on the Cray T3E.

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