

Rapid-Response Simulation of Forward and Inverse Problems in Atmospheric Transport and Dispersion

Inanc Senocak

Department of Mechanical and Biomedical Engineering
Boise State University

Environmental sensors have been deployed in various cities for early detection of contaminant releases into the atmosphere. Rapid-response contaminant dispersion and event reconstruction capabilities are needed to backtrack the dispersion source and then project the contamination extent with quantified uncertainty. To enable rapid-response simulations on small-footprint desktop supercomputers, we have taken a major computational effort to develop a computational fluid dynamics code for contaminant dispersion in urban environments using the GPU computing paradigm. GPUs that are traditionally designed for graphics rendering have emerged as massively-parallel "co-processors" to the Central Processing Unit (CPU). Small-footprint desktop supercomputers with hundreds of stream processors that can deliver several teraflops peak performance at the price of conventional workstations have been realized. In this talk, we describe the development of a novel Cartesian grid CFD code for urban environments using the NVIDIA CUDA programming model on desktop supercomputers with up to four GPUs. Harnessing the full compute-potential of GPUs from NVIDIA requires a clear understanding of the fundamentally new CUDA programming models, device architectures and memory-access patterns. Our results have confirmed the tremendous compute-potential of the GPU computing paradigm with two orders of magnitude speedup over a serial CFD code executed on a conventional CPU.

The second part of the seminar focuses on the inverse modeling problem and presents a stochastic event reconstruction capability that can process information from an environmental sensor network. The inference is based on the Bayesian paradigm with Markov chain Monte Carlo (MCMC) sampling. Given the observations, simple approximate dispersion models are substantially enhanced by introducing stochastic variables in turbulent diffusion parameterization schemes and estimating them within the Bayesian inference framework. Additionally, parameters in the event reconstruction model are estimated in a principled way using data and prior probabilities to avoid tuning in the overall method. The event reconstruction method is successfully validated for both real and synthetic dispersion problems, and posterior distributions of the model parameters are used to generate probabilistic plume envelopes with specified confidence levels to aid emergency decisions.