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LARGE EDDY SIMULATION (LES) BASED SYSTEM FOR PRODUCING COUPLED URBAN AND INDOOR AIRBORNE CONTAMINANT TRANSPORT AND DISPERSION SOLUTIONS

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Abstract: Recent advances in atmospheric modeling have demonstrated that it is now possible to resolve the detailed interactions between the atmosphere and the outdoor urban environment (Lundquist et al. 2012 and Tomas et al. 2017) that are necessary for producing short time averaged, "single-realization", dispersion solutions. These single-realization dispersion solutions have been shown to be critical for atmospheric dispersion applications associated with air sampling network designs, pollutant measurement systems performance, and characterizing the impact of hazardous airborne materials on human health (Bieringer et al. 2014). Here we describe a Large Eddy Simulation (LES) atmospheric and coupled outdoor urban dispersion model implemented on a Graphics Processing Unit (GPU) computer that has been linked to a building interior air exchange model. This system, referred to as the Joint Outdoor-indoor Urban LES (JOULES) system, is a physics-based quantitative modeling system that is being developed to provide high-fidelity simulations of urban and interior pollutant concentrations for use in the testing and evaluation of operational urban emergency response modeling tools and subsequent enhancements to these systems. JOULES provides physically realistic, time varying atmospheric conditions that interact with the urban landscape and influence the dispersion patterns at locations where air exchanges between the indoor and outdoor spaces occur. A key element of JOULES is the computationally efficient GPU-based LES that enables the development of solution ensembles that can then be used to resolve the distributions in material transport and scenario outcomes associated with the complex interactions between the indoor and outdoor spaces. This paper describes validations of the GPU-LES dispersion model solutions to field observations and provides example simulations that illustrate high temporal/spatial resolution urban contaminant transport and dispersion.

Key words: *Urban Dispersion Modeling, Indoor Dispersion Modeling, Large Eddy Simulation (LES), Graphics Processing Unit (GPU) Computing, Indoor-Outdoor Contaminant Transport and Dispersion*

INTRODUCTION

According to the 2010 United States (US) census, over 80% of the population resides in an urban area. Klepeis et al. (2001) suggest that as much as 86% of the day for an average person in the US is spent inside a structure or vehicle. These statistics highlight the need for airborne contaminant models to resolve both the complexities of the urban environment, and the air exchanges between outdoor and indoor spaces. To address this need, the Defense Threat Reduction Agency – Joint Science and Technology Office for Chemical and Biological Defense (DTRA-JSTO-CBD) is supporting the development of a coupled outdoor-indoor urban airborne contaminant modeling system. This system, called the Joint Outdoor-indoor Urban LES (JOULES), couples a building-aware Large Eddy Simulation (LES) atmospheric model with an integrated outdoor airborne material transport and dispersion model, and models that predict simulate the transport of contaminants across the building envelope.

The purpose of JOULES is to provide detailed, high-resolution, "single-realization", coupled outdoor-indoor contaminant dispersion solutions, which have been shown to be critical for applications associated with air sampling network designs, pollutant measurement systems performance, and characterizing the impact of hazardous airborne materials on human health (Bieringer et al. 2014). JOULES will be used to produce synthetic contaminant dispersion data sets for use in evaluating the performance of operational Chemical, Biological, and Radiological (CBR) emergency response modeling tools. This system will also support the scientific research necessary to better characterize the uncertainties present in these environments, and the impact that these uncertainties have on emergency response decisions. In this paper, we provide an overview of the models in JOULES, a description of work that has been done to validate its accuracy, and finally show some preliminary examples of JOULES simulations for open terrain and urban locations.

JOULES SYSTEM DESCRIPTION

GPU atmospheric and dispersion model

A key enabling technology within JOULES is a Graphics Processing Unit (GPU) LES atmospheric model called the GPU Resident Atmospheric Simulation Program (GRASP). GRASP is based on a central processing unit (CPU) version of an LES model originally developed at Delft University of Technology (TU Delft), and further adapted to run on GPU based architectures by scientists at TU Delft and Whiffle Ltd. GRASP provides computationally-efficient means to develop detailed simulations of the winds and turbulence in the planetary boundary layer (PBL), and has undergone extensive validation of its ability to accurately model the PBL (Schalkwijk et al. 2012, 2015, and 2016). Recently this model has been coupled with an atmospheric transport and dispersion (AT&D) modeling capability that solves for the advection and diffusion of a passive scalar (e.g. neutrally buoyant airborne tracer) directly in-line with other atmospheric variables within the LES model.

The implementation of an LES model on GPU hardware can provide a significant computational advantage over comparable LES simulations performed on a CPU based computing platform. To characterize these benefits, we conducted benchmark LES simulations using the Weather Research and Forecast (WRF) model with LES turbulence closure. The WRF and GRASP simulations used a grid of 128 X 128 X 64 points (X,Y,Z), with a spatial resolution of 20m X 20m X 17m. The simulation used a periodic lateral boundary condition to spin up convective eddies and turbulence over a 1 hour period. The simulation was performed on a Dell R640 running Red Hat v.7.6 Linux on an Intel Xenon E5 v4, 8 core, CPU. WRF was configured to use the distributed memory (i.e., Message Passing Interface (MPI)) option. On this hardware platform, a one-hour simulation required approximately 1 hour and 32 minutes of wall clock time to complete. A comparable 1 hour LES simulation with GRASP was performed on an NVIDIA Tesla K40 with 2880 cores operating at 745 MHz and 12 Gb of onboard fast access memory. The GRASP simulation completed in ~36 seconds of wall clock time, a ~150x speedup compared with the CPU based simulation. As will be discussed in the next section, this level of computational improvement enables us to efficiently produce tens to hundreds of dispersion solutions that can then be used to characterize dispersion variability. In addition, the GPU version has lower equipment costs, power consumption, cooling requirements, and physical space requirements. We estimate that a cluster of 19 Dell R640 Linux servers (comparable to the one used here) and an Infiniband high-speed network switch would be required to match the performance of a single NVIDIA Tesla K40.

JOULES performance evaluation

GRASP was initially developed to provide high-resolution simulations of wind, turbulence, and clouds. Throughout its development, GRASP has undergone a variety of evaluations to assess its accuracy and ability to provide high-resolution reconstructions of atmospheric variables and short-term weather predictions. Of particular relevance to this effort is a prior evaluation in which GRASP was coupled to a regional-scale atmospheric model and used to create a continuous, three-dimensional time series of turbulence and clouds for a year-long period. The results from this year-long set of LES model runs were then compared to detailed boundary layer observations collected at the Cabauw Experimental Site for Atmospheric Research (CESAR), located at Cabauw, Netherlands. This unique study included comparisons between the measured and simulated power spectrum of horizontal and vertical wind speed variance, and demonstrated the ability of GRASP to reproduce the wind and turbulence in this environment across a variety of temporal scales (Schalkwijk et al. 2015 and 2016). While this work provides an extensive evaluation of GRASP's ability to reproduce planetary boundary layer meteorological parameters and clouds, it did not include an assessment of the model's ability to accurately simulate the dispersion of airborne contaminants.

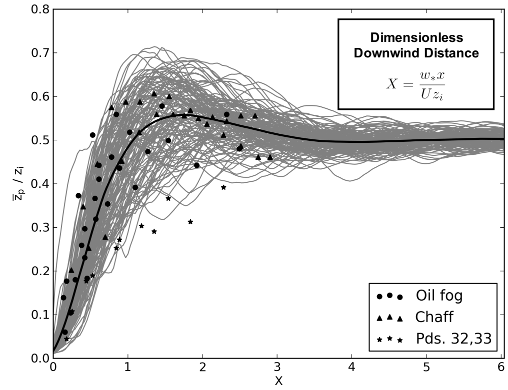

Figure 1. Plume height vs. downwind distance from the source.

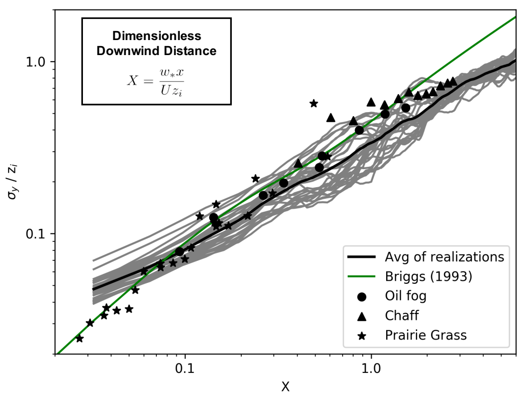

Figure 2. Plume crosswind dispersion vs. downwind distance.

In 2017, following the implementation of the passive airborne tracer capability in GRASP, we evaluated of the ability of this GPU-LES model to simulate the transport of airborne contaminants in an open terrain. Our assessment follows the methodologies used by Weil et al. (2004) and Weil et al. (2012), which evaluated the performance of a Lagrangian Particle Dispersion Model (LPDM) that utilized winds and turbulence information produced by an LES model developed at the National Center for Atmospheric Research (NCAR). The LES in our evaluations was configured to produce simulations within a 10 X 10 X 2 km domain at a spatial resolution of ~50 m in the horizontal and ~21 m in the vertical. We specified the initial meteorological conditions through a vertical profile of temperature, a random pattern of surface heat flux perturbations of 0.24 $ms^{-1}K$, a prescribed surface temperature of 300 K, and the use of periodic lateral boundary conditions. After allowing the turbulence to spin up for two hours, to a point where the average boundary layer winds and turbulence were stable, this configuration produced a convective boundary layer depth of 1 km with a mean horizontal wind of 3 ms^{-1}. We then created 130 uncorrelated dispersion realizations by varying the source location and the start of the continuous unit tracer release.

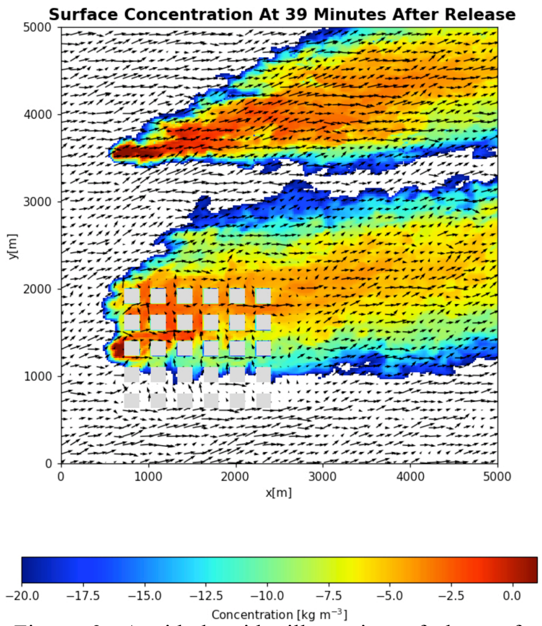

Figure 3. A side-by-side illustration of the surface concentrations and wind vectors for an open terrain area and within an array of thirty 20 m tall square surface obstacles.

Our analysis of the accuracy of the open terrain dispersion simulations in JOULES used a 10-minute averaging time and was patterned after the scaling methodologies employed by Willis and Deardorff (1976). We compared plume height normalized by PBL height, vertical profiles of crosswind integrated concentration (CWIC), surface CWIC, surface crosswind dispersion, and vertical dispersion to comparable dispersion metrics computed from observations. The observations used in this evaluation were derived from the Prairie Grass experiment (Barad 1956), Willis and Deardorff (1976), and the COnvective Diffusion Observed by Remote Sensor (CONDORS) experiments (Eberhard et al. 1988; Briggs 1993). The JOULES open terrain convective simulations showed close agreement with the observations for these parameters and closely matched the performance of the LPDM and NCAR LES model published in Weil et al. 2012 (Figure 1 and 2). Figure 1 depicts the average of the plume height normalized by the PBL height as a function of a dimensionless downwind distance. Figure 2 depicts the results from the surface crosswind dispersion as a function of a dimensionless downwind distance. In both figures, each grey line represents one of the 130 dispersion realizations, the black line denotes the average of all 130 realizations, and the markers represent observations from the CONDORS field program (Figure 1) and CONDORS and Prairie Grass (Figure 2) field programs. These figures are representative of the results for the other parameters that were examined.

JOULES SYNTHETIC DISPERSION ENVIRONMENT EXAMPLES

JOULES is currently being extended to incorporate surface obstacles, representing buildings, and to link these buildings to an envelope contaminant transport model. The outdoor building-aware LES implementation in JOULES uses an immersed boundary method (IBM) surface layer parameterization, analogous to that used in Lundquist et al (2012) and Tomas et al (2017). The indoor air contaminant model is based on work at Lawrence Berkeley National Laboratory (LBNL) (Chan et al. 2007). Figure 3 illustrates a simulation of wind flow and airborne contaminant dispersion through an array of 30 surface obstacles, representing 50 m tall buildings, side-by-side with an open-terrain region. This figure qualitatively illustrates the impact that the obstacles have on the near-surface wind flow patterns and the increased cross-wind dispersion that occurs when buildings are present. JOULES can also incorporate real-world buildings derived from lidar observations and/or building shapefiles. Figure 4 depicts preliminary simulation results of dispersion and a horizontal cross section of vertical velocity within the TU Delft campus. In this example the locations and heights of the buildings are based on an aerial LIDAR survey of the campus. A qualitative evaluation of these preliminary results found that the model is performing as expected, effectively resolving contaminant channeling between buildings. Furthermore, upward airflow on the windward side of buildings leads to the lofting of the neutrally-buoyant tracer above building tops, where downward airflow on the lee side leads to subsidence and, subsequently, pooling of elevated contaminant concentrations.

CONCLUSIONS

In this paper, we have described an effort to leverage the computational power of GPU hardware platforms to create simulations of the complex airflow and turbulence generated in urban areas, and the associated contaminant dispersion. The GPU platform on which these capabilities have been benchmarked shows ~150X speed improvement over a comparable CPU based simulation. We believe that the current generation of GPU hardware may lead to even larger performance gains, improvements on the order of 200 to 300X over comparable CPU-based simulations. The model is currently undergoing an extensive evaluation of its ability to accurately simulate atmospheric dispersion. Results from comparisons of JOULES simulations with open-terrain field trials during unstable atmospheric conditions show very good agreement with observations from the Prairie Grass, CONDORS field experiments and laboratory experiments conducted by Willis and Deardorff (1976). In the coming year, we plan to

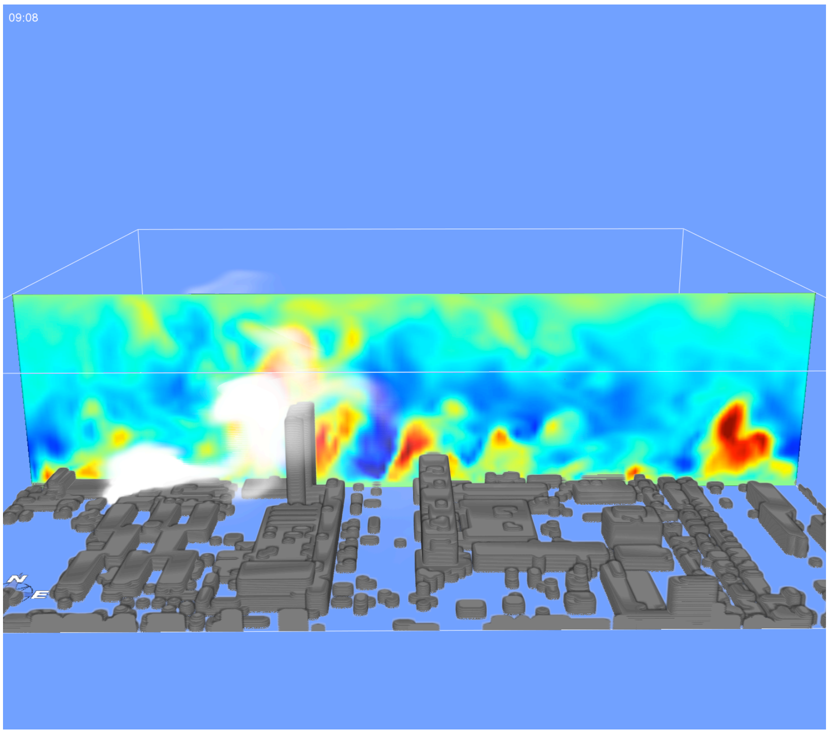

Figure 4. An illustration of a JOULES simulation of winds and dispersion over the TU Delft campus. The vertical cross-section illustrates vertical velocity.

extend our open-terrain validation following the methodologies of Venkatram et al. (2013) and others to cover both stable and neutrally buoyant open terrain PBL conditions. The evaluation of JOULES will also be extended to include field trials of outdoor urban environments like the Mock Urban Setting Test (MUST) (Biltoft, 2001) and Joint Urban 2003 (Allwine et al. 2004; Brown et al. 2004). Lastly, the interior modeling capabilities, developed by LBNL, will be fully integrated into JOULES, and evaluated for its ability to accurately simulate contaminant infiltration and exfiltration.

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