Express Risk Analysis of Aerosol Transport in Urban Environments

Research Proposal

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1 Background

In the event of the release of airborne harmful substances in an urban environment, it is important to have the ability to quickly predict the spread of the contaminants. Considering the complexity of urban landscapes, as well as the great variety of factors affecting the aerosol transport, accurate predictions can only be made on high performance computing facilities. Combined with the need for a quick response in an emergency situation, the solution becomes not feasible should the conventional physically-based models be used for making predictions. The important criteria for an efficient risk analysis system would be its speed and availability. Thus preferred implementations of the system are either web-based or workstation or even laptop-based.

Keeping this in mind, the problem of express risk analysis of aerosol dispersion in a complex city landscape was addressed in a preliminary study, financed by West Virginia University Research Corporation. The study resulted in a solution method for aerosol transport modeling which enables a reduction in the amount of data needed to analyze various aerosol dispersion scenarios, as well as in a drastic reduction of time to analyze the scenarios (from several day to several minutes). The method is implemented in a prototype software for distributed simulation and express risk analysis of aerosol transport, as well as a web-based data retrieval and visualization system. The results of the study will be reported at the forthcoming conferences [1, 2], and the corresponding papers are attached to this document. A demo-version web-based simulator has also been developed to illustrate the concepts of the method¹. The method will form the basis of a complete express risk analysis system for aerosol transport, RASAT, the development of which is the subject of the proposed work. The following sections provide a brief description of the method, outline the directions for future research and justify the need for further funding.

2 Project description

2.1 Methodology

The main idea behind this method is to conduct physical modeling of an aerosol transport process ahead of time and store the results in a database of different aerosol spreading scenarios. In the even of an emergency, this database can be queried and the needed scenarios retrieved in a timely manner. According to this, the risk analysis system consists of two stages: a slow preparation stage, including physically-based simulations, and a fast analysis stage, involving data retrieval and visualization. This idea is not new and has already been suggested in the past [3]. However, because of the variety of factors affecting the aerosol transport, such as the local weather situation, the nature of aerosols, etc., combined with all possible release locations, the number of possible aerosol dispersion scenarios becomes prohibitively large.

To make the problem manageable, it has been suggested in this study to modify the scheme by replacing the database of aerosol dispersion scenarios with a database of so-called *domain transfer probabilities* (DTP). These probabilities will be computed as before in the stage of physically based modeling. At the same time a separate simulation procedure is introduced into the analysis stage which will use the computed DTPs to simulate various aerosol dispersion scenarios. This procedure will be of a probabilistic nature and will not involve any complex physical models. Thus the analysis can still be done in a timely manner. The authors have shown in preliminary studies (attached) that by using DTPs instead of the set of all aerosol dispersion scenarios the total amount of simulated data can be significantly reduced.

¹http://mulphys.mae.wvu.edu/sim/demo

Another advantage of the approach is that it enables a very efficient implementation on distributed computer platforms, such as workstation clusters or grid computing environments. More details of the method can be found in the attached paper [4], which will be reported at the forthcoming International Aerosol Conference 2006.

2.2 Proposed Work

Preliminary studies have shown the feasibility of the proposed method of analyzing aerosol dispersion scenarios in urban environments; however, there are still several steps to be done to fully validate the method and implement it in a functional express risk analysis system.

Testing and Validation. The method has been tested on a limited case of an urban landscape prototyped after the Pittsburgh downtown area [5]. The landscape representation was done on a 92x92x32 grid and a simplified particle transport model was employed. Also the number of processors engaged in the simulations was limited to 16. In the opinion of the authors, this study was enough to prove the viability of the proposed approach; however, a larger scale study will be needed to fully assess the efficiency of the proposed method in realistic situations. These validation studies should involve the high resolution representation of urban environments, massive parallel computations, improved physical models, and more efficient data representation and post-processing techniques.

Improved Physical Models. The currently used aerosol transport model was based on the assumption of simplified atmospheric conditions defined by a uniform wind velocity with varying direction. The OpenFOAM open source CFD solver (openfoam.org) and the RFG subgrid turbulence model [6] developed earlier by the one of the authors was used to account for turbulent diffusion. These simplified assumptions used in a preliminary study enabled the authors to emphasize the essential features of the method while conducting the study in a relatively short time-frame and with limited computer resources.

More relevant and sophisticated physical models should be considered in the future. In addition, a thorough investigation of different aspects of aerosol transport should be conducted to fully validate the model. The discrete set of aerosol release locations and wind directions should be replaced by a more comprehensive set of release scenarios. A potentially promising scheme would involve a continuous generation of new release scenarios by a stochastic selection procedure using Monte-Carlo method. This on-going simulation process will constantly update the database of DTPs and provide a set of data with ever increasing accuracy.

Advanced Data Representation. The sets of DTP data generated during the physical high-performance simulations are well structured and can be significantly reduced in size using a variety of compression and data reduction techniques. In preliminary studies, a simple data reduction technique based on exclusion of zero counts enabled to reduce the data size by a factor of 3 on the average. A more flexible reduction technique can be applied which will retain most significant probabilities based on a predefined cutoff level. Then the risk analysis problem can be formulated as a trade-off between the accuracy of predictions and the required speed of execution. The appropriate optimum will be selected based on the available hardware, e.g. workstation vs. laptop.

The standard LZ77 compression (gzip) applied to DTP data has led to an average reduction of the data sets by four times of their original size. Other compression schemes can be considered, which can lead to higher compression ratios.

Finally, the proposed method can be combined with other acceleration approaches, such as neural networks and general high dimensional model representations schemes [7]. It should be noted that the proposed method is not a replacement for these approaches. In fact, these techniques can introduce high uncertainties and unexpected errors in predictions. This is because they depend on a control set of sparse data points to make heuristic predictions about different scenarios outside of the control set. This makes these techniques less reliable in risk analysis applications. In contrast the current method has the advantage of retaining the high accuracy of the physically based solutions. It does not depend on a control set of scenarios, but uses all the available information from physically based models as it is without modifications or extrapolations.

Data Retrieval and Visualization. A preliminary demo version of the web-interface for data remote retrieval and processing [5] will have to be

replaced with a more complete query and visualization system. The express simulator developed within the preliminary study, and based on the original probabilistic implicit particle tracking technique [4] (attached), should be integrated into the interface as well.

In practice the DTP database should be available on local media (CD/DVD) and remotely via the Internet. The issues of generation and distribution of DTP database on local media should also be considered.

References

- Andrei Smirnov, Steven Rowan, Gouxiang Liu, and James McCormick. Probabilistic implicit tracking approach in parallel simulations of particle transport. In *International Conference on Parallel Computational Fluid Dynamics*, Busan, Korea, 2006.
- [2] Andrei Smirnov and Steven Rowan. A fast response system for aerosol dispersion forecasting. In 7th IASTED International Conference on Modeling and Simulation, number 530-050 in MS, 2006.
- [3] J. Thilmen. Harm's way. Mechanical Engineering, 127:22–24, 2005. bioterror CFD.
- [4] Andrei Smirnov, Steven Rowan, and James McCormick. Aerosol dispersion modeling with probabilistic implicit particle tracking algorithm. In 2006 International Aerosol Conference, St. Paul, Minnesota, 2006. American Association for Aerosol Research (AAAR).
- [5] Andrei Smirnov. Aerosol dispersion in a city: a java demo. http://mulphys.com/sim/demo, 2005.
- [6] A. Smirnov, S. Shi, and I. Celik. Random flow generation technique for large eddy simulations and particle-dynamics modeling. *Trans. ASME. Journal of Fluids Engineering*, 123:359–371, 2001.
- [7] G. Li and H. Rabitz. High dimensional model representation. Journal of Physical Chemistry, 105(33):7765–7777, 2001.