Modeling and Simulation in Support of Chemical and Biological Defense Analysis

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Atmospheric Science and Engineering Solutions

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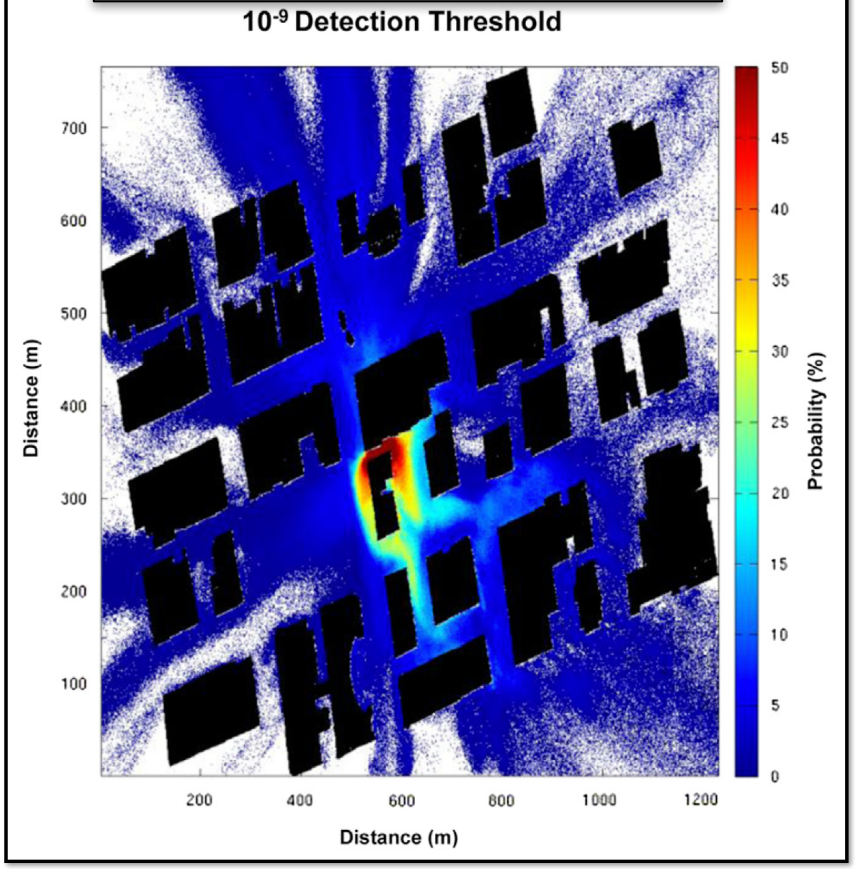
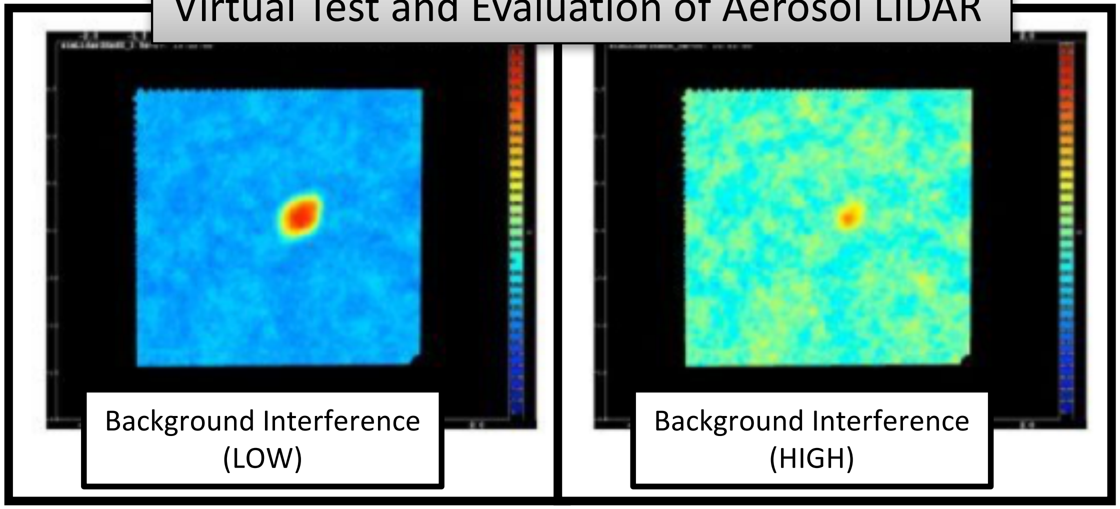
Modeling and Simulation (M&S) Applications

- **Chemical and Biological (CB) Asset Performance Analysis**
- **CB Asset Operational Optimization**
- **Critical Infrastructure Protection Design**
- **Strategic CB Scenario Risk Assessment**

Sensor Placement Optimization



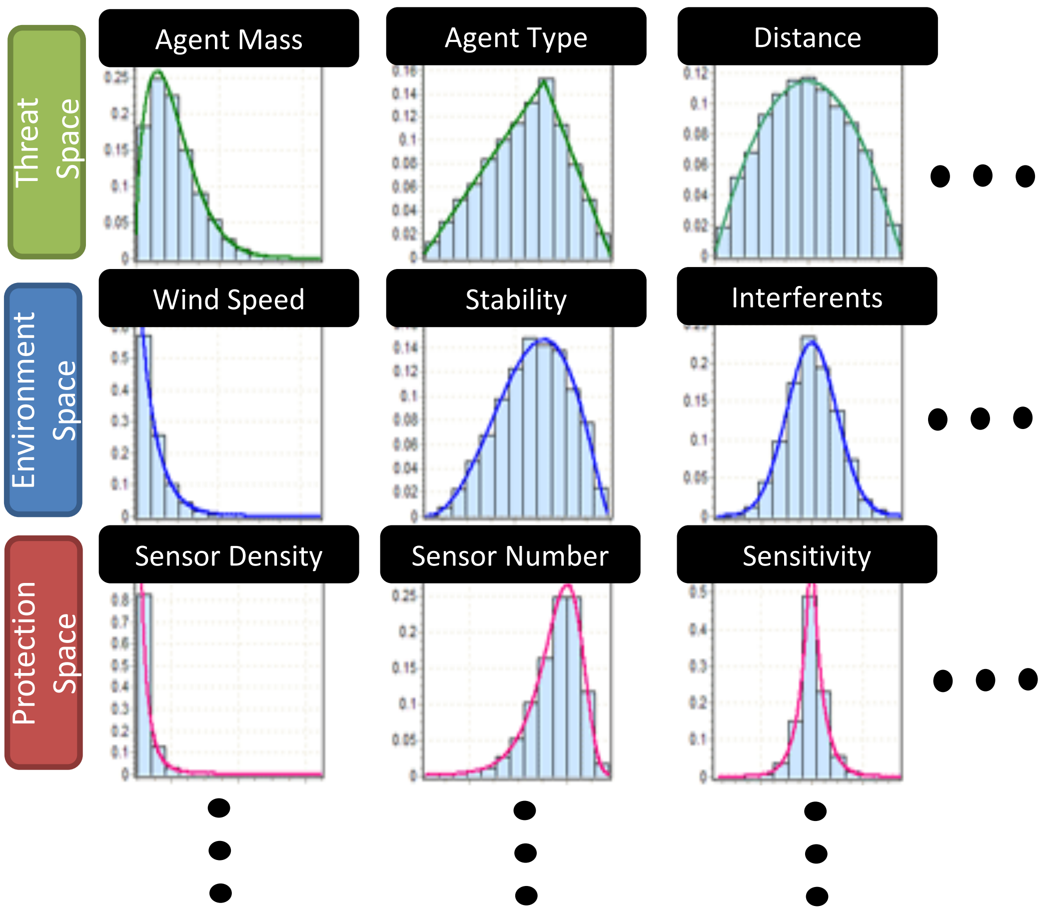
Virtual Test and Evaluation of Aerosol LIDAR



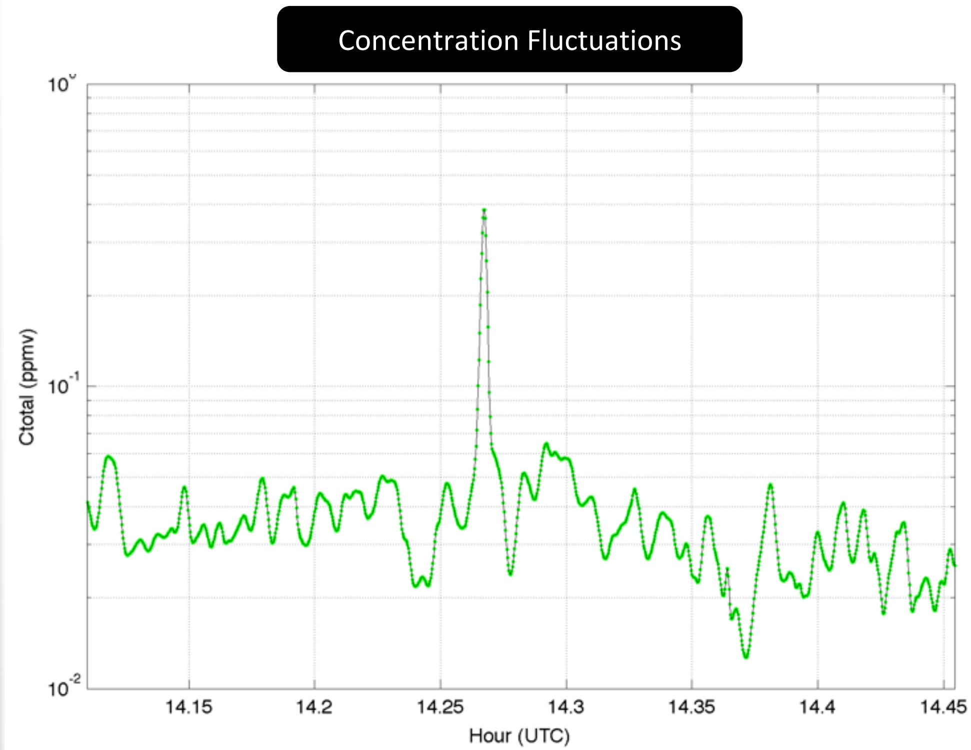
Material Source: Bieberbach (2005)
Bieringer et al (2013)

Elements of A Robust CB Defense M&S Analysis

Fully Represent CB Permutation Space



Adequately Resolve Critical Phenomena



Outline

- Elements of a robust CB Defense (CBD) analysis
  - Fully represent permutation space
  - Adequately resolve critical phenomena
- Enabling technologies and methods for improving CBD analysis robustness
  - Environmental data reduction via Self Organizing Maps (SOMs)
  - Graphics Processing Unit (GPU) accelerated High Performance Computing (HPC)
- Summary and conclusions

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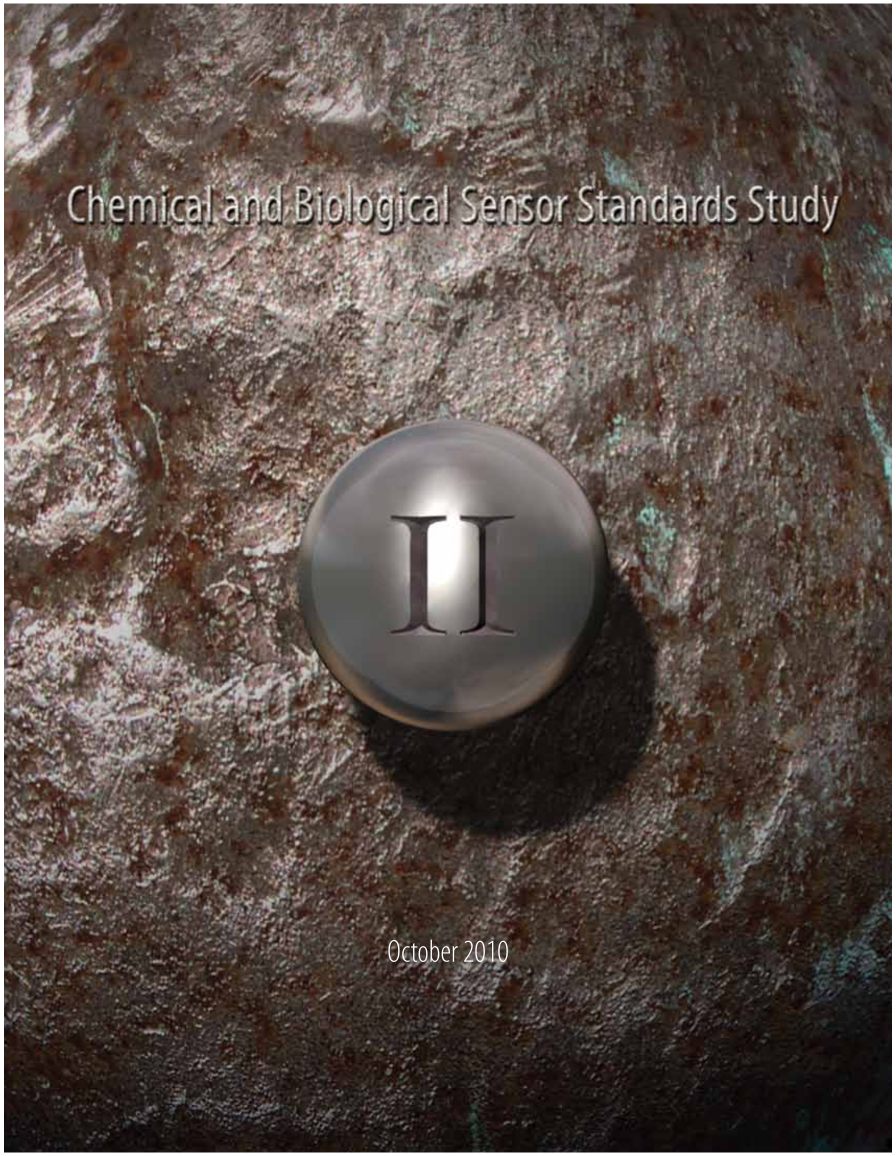
Representing Permutation Space
(CB Sensor Standards Study)

- **General CB sensor requirements study performed by Carrano and Jeys (2004, 2010)**
- **Attempted to identify key sensor performance requirements based on operationally relevant CB attack scenarios.**

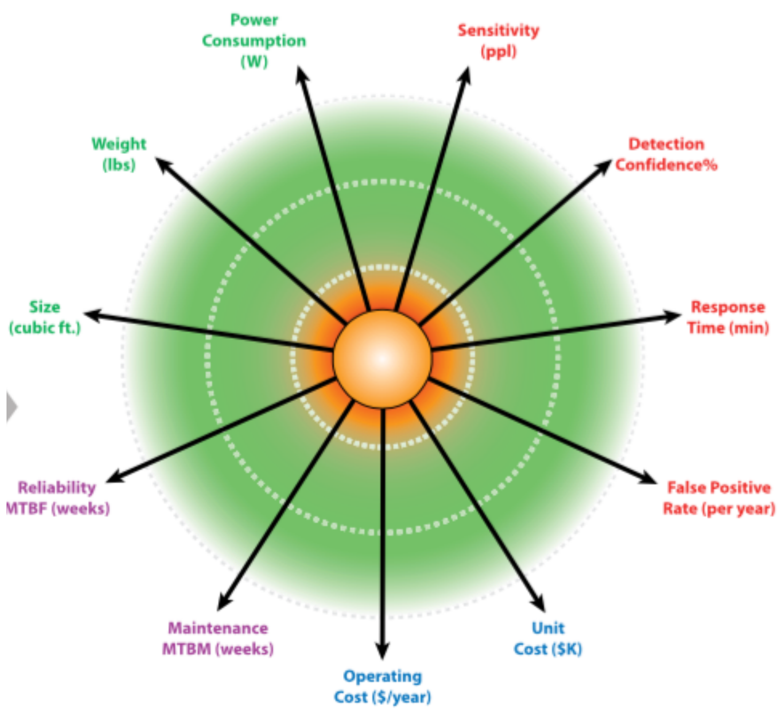


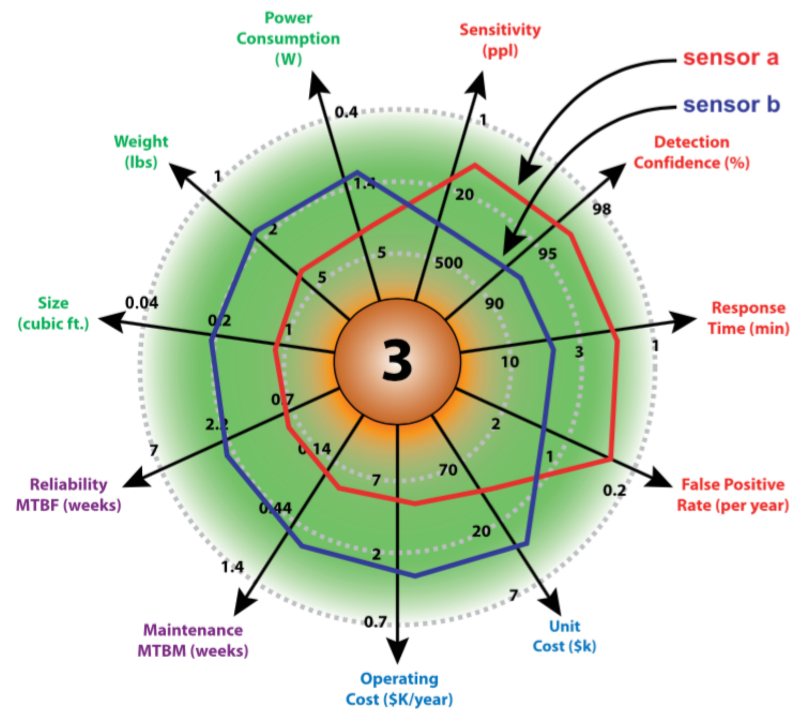
Representing Permutation Space

(Multi-parametric Methodology)

- **For each attack scenario, sensor requirements were derived based on a range of threat, environmental, and protection permutations.**
- **Results distilled into spider charts**

	Scenario	Agent	Sensor Sensitivity	Sensor Reaction Time (minutes)	Sensor Spacing (m)
1	Convoy Movement	Anthrax	1 – 500 ppl	1 – 10	50 – 500
2	Convoy Movement	Sarin	0.1 – 10 mg/m^3	1 – 10	50 – 100
3	Ground Forces Defense	Anthrax	1 – 500 ppl	1 – 10	50 – 100
4	Military Building (internal attack)	Smallpox	0.1 – 100 ppl	1 – 1	One per air duct
5	Military Building (external attack)	TIC	0.5 – 500 mg/m^3	0.1 – 1	One on roof
6	Amphibious Operation	Mustard	0.1 – 1 mg/m^3	1 – 30	500 - 100
7	OCONUS Forward Airbase	VX	0.01 – 2 mg/m^3	0 – 3	25 – 100
8	Terrain Denial	VX	0.1 - 10 mg/m^3	0 – 3	1 sensor per lead vehicle
9	CONUS Military Post	Anthrax	0.1 – 1 ppl	0 – 10	50 – 100
10	CONUS Military Post	Anthrax	0.1 – 25 ppl	1 – 7	500 – 1,000
11	Defensive Positions	Sarin	0.1 – 2 mg/m^3	1 – 6	500 – 1,000
12	Defensive Positions	Anthrax	0.1 – 10 ppl	0 – 2	500 – 1,000
13	Naval Port Facility	Anthrax	1 – 500 ppl	0 – 7	10 sensors on perimeter
14	Navy Ship in Littoral	Plague	1 – 500 ppl	0 – 0.25	10 sensors on deck





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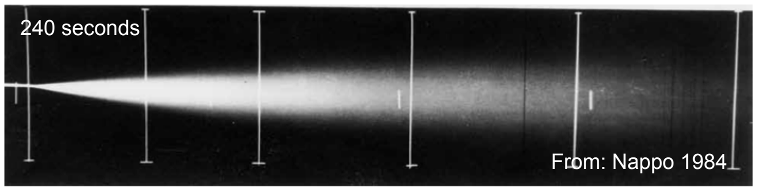
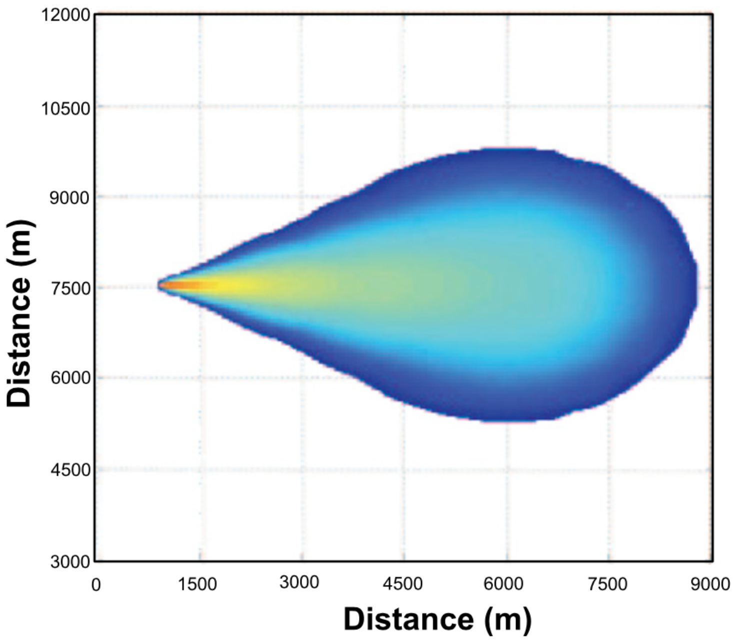
Material Source: Carrano and Jeys, (2004, 2010)

Representing Permutation Space
(CB Standard Study Limitations/Challenges)

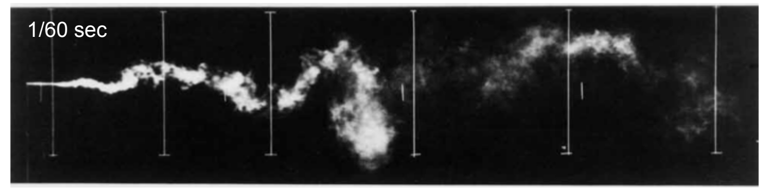
Ensemble-based gaussian puff model used to simulate the threat representation

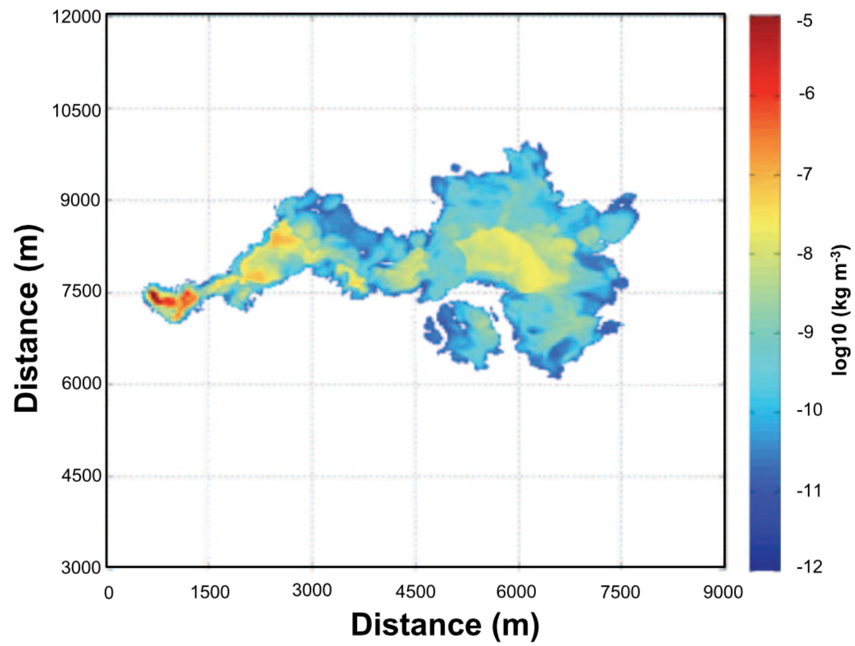
Ensemble-Based Simulation





Single-Realization Simulation





Continuous Release at 1450s After Initial Release

Representing Permutation Space

(CB Standard Study Limitations/Challenges)

CBD analysis examples where ensemble average models may not be appropriate

- **Sampling/response rates significantly exceed temporal fidelity of the simulation**
- **When the application relies on spatial/temporal correlations**
  - **Multi-sensor/location false alarm mitigation**
  - **Sensor network design**
  - **Standoff or remote detection**
- **When the application involves a non-linear transformation of CBRN concentration**

Contrasting the Use of Single-Realization versus Ensemble-Average Atmospheric Dispersion Solutions for Chemical and Biological Defense Analyses

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(Manuscript received 12 June 2013, in final form 2 January 2014)

ABSTRACT

Chemical and biological (CB) defense systems require significant testing and evaluation before they are deployed for real-time use. Because it is not feasible to evaluate these systems with open-air testing alone, researchers rely on numerical models to supplement the defense-system analysis process. These numerical models traditionally describe the statistical properties of CB-agent atmospheric transport and dispersion (AT&D). While the statistical representation of AT&D is appropriate to use in some CB defense analyses, it is not appropriate to use this class of dispersion model for all such analyses. Many of these defense-system analyses require AT&D models that are capable of simulating dispersion properties with very short time-averaging periods that more closely emulate a ''single realization'' of a contaminant or CB agent dispersing in a turbulent atmosphere. The latter class of AT&D models is superior to the former for performing CB-system analyses when one or more of the following factors are important in the analysis: high-frequency sampling of the contaminant, spatial and temporal correlations within the contaminant concentration field, and nonlinear operations performed on the contaminant concentration. This paper describes and contrasts these AT&D modeling tools and provides specific examples in which utilizing ensembles of single realizations of CB-agent AT&D is advantageous over using the statistical, ''ensemble-average'' representation of the agent AT&D. These examples demonstrate the importance of using an AT&D modeling tool that is appropriate for the analysis.

1. Introduction

In recent decades the materials of concern and delivery methods associated with the use of chemical and biological (CB) agents have continued to evolve. To combat these threats, the U.S. Department of Defense makes significant investments in technologies designed for CB-agent detection and defeat. CB defense-system analysis is a critical element in the defense-system acquisition process that includes identifying technology gaps, determining technology investment direction, and providing information that ultimately directs system acquisition and deployment decisions. While the use of live agents is the most advantageous approach for conducting CB defense-system analyses, their use is clearly difficult, and therefore agent simulants are frequently used in outdoor field-data-collection efforts (Przybylowicz et al. 2003). The use of agent simulants

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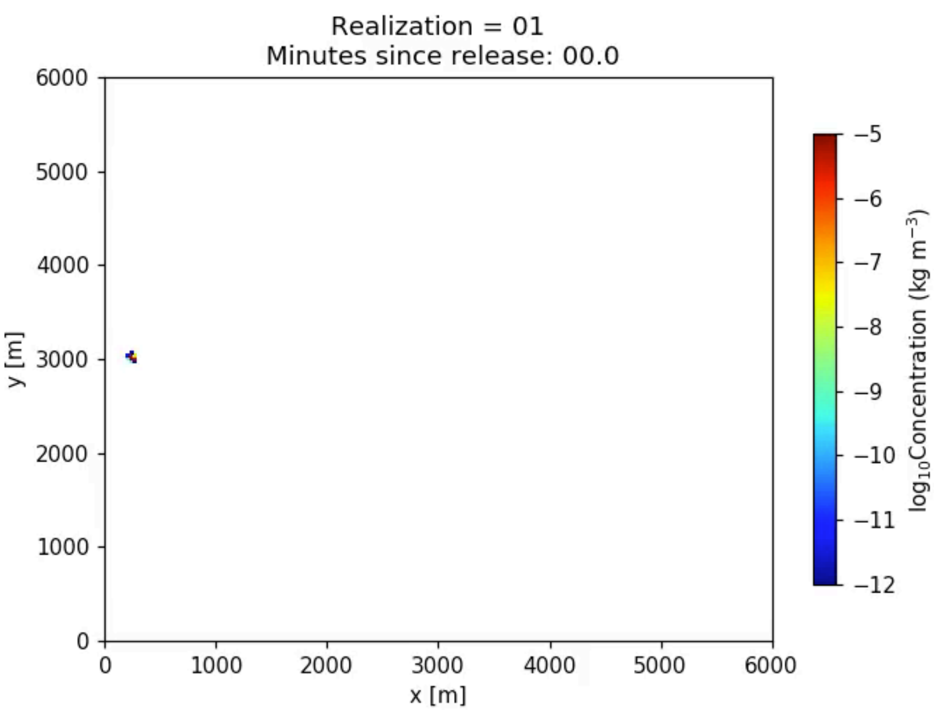
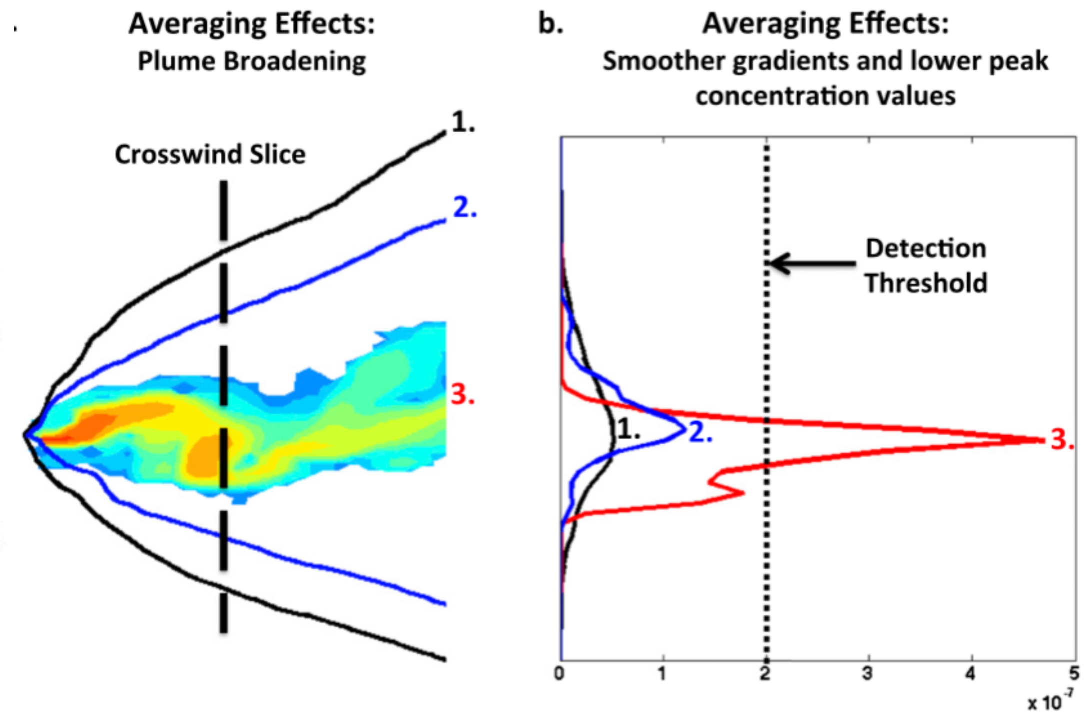
Material Source: Bieringer et al (2014)

Representing Permutation Space
(CB Standard Study Limitations/Challenges)

Not properly resolving the physics may lead to incorrect analysis conclusions





1. Time and Ensemble Average Concentration Values

2. Time Average Concentration Values

3. Instantaneous Concentration Values

Material Source: Bieringer et al (2014)

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Resolving Critical Phenomena

(Standoff CB Detector Analysis of Alternatives)

- **Standoff CB sensor analysis of alternatives study performed by Lawrence et al (2013)**
- **Attempted to examine value of different standoff sensor technologies and potential enhancements to those technologies for providing a detect-to-warn application.**

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Project Report
CB-3

Scientific Evaluation of Technology for Standoff Detection of Chemical and Biological Agents

W.G. Lawrence, E.C. Wack, D.C. Jamrog, J.C. Biddle, H.W. Lau, S.E. Holster, C.J. Smith, A.K. Goyal, F.D. D'Arcangelo, A.J. Annunzio, P.E. Bieringer, R. Cabell, G. Bieberbach

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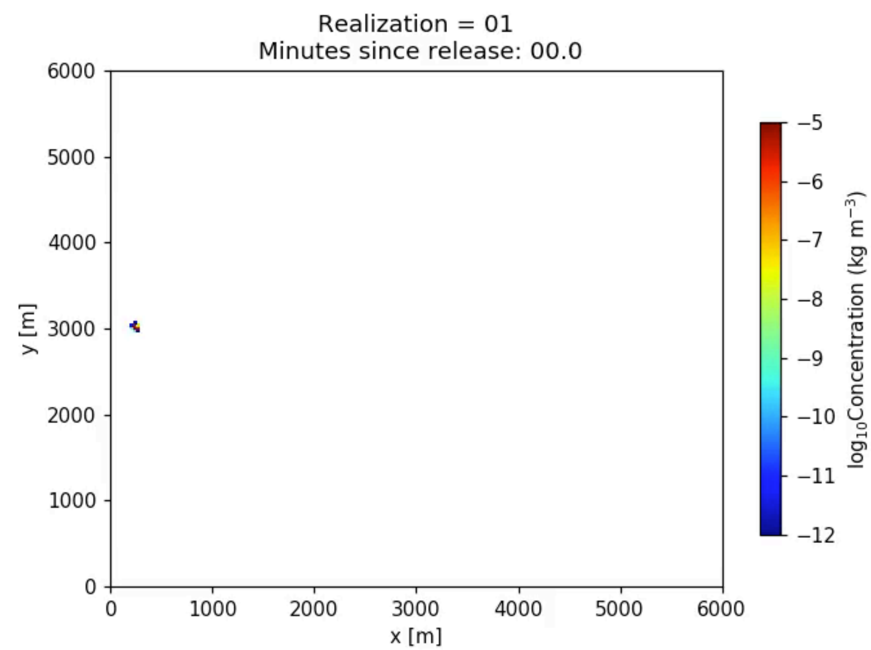
Resolving Critical Phenomena
(Large Eddy Simulation Dispersion Methodology)

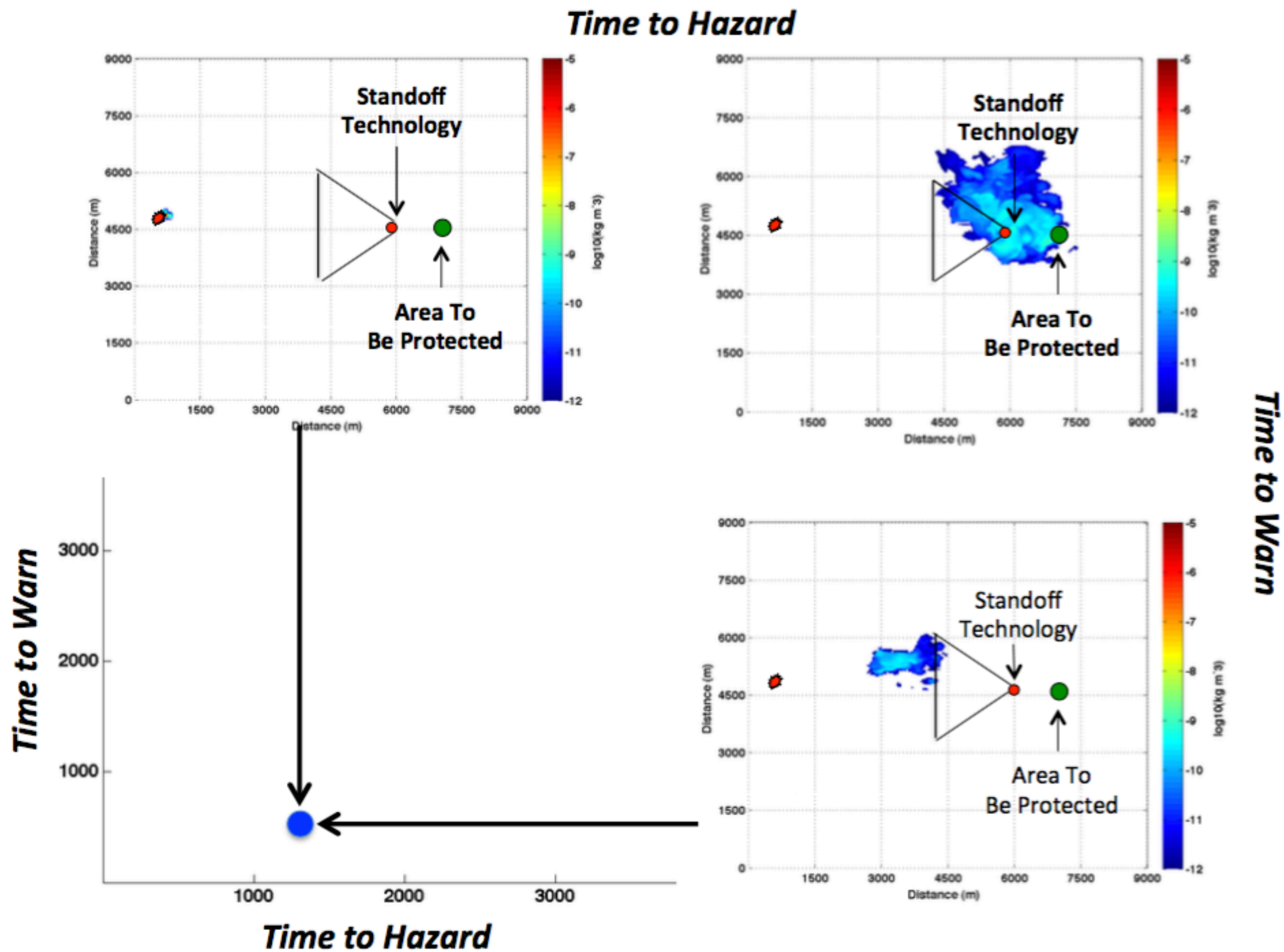
- **Leveraged metrics, scenarios, and lessons learned from CB Standards Study (Carrano and Jeys 2004, 2010).**
- **Utilized Large Eddy Simulation (LES) based dispersion model to simulate the CB threats**
  - **Generated multiple realizations of threat for each scenario and meteorological condition**
- **Utilized a variety of detailed standoff sensor models**

	Scenario	Attack Type	Agent	Release Type	Delivery Mechanism
Fixed Site	Ground Forces Defense (on move but stopped)	Chemical/ Biological	Sarin, VX, Anthrax	Single point	Stationary sprayer
	Defensive Positions (on move but stopped)	Chemical/ Biological	Anthrax, VX	Multiple Point	Artillery
	Military Post	Biological	Anthrax	Line	Truck with sprayer
Maneuver	Convoy Movement	Chemical/ Biological	Sarin, VX, Anthrax	Single Point	Stationary sprayer
	Convoy Movement	Chemical	Sarin, VX	Multiple Point	Artillery



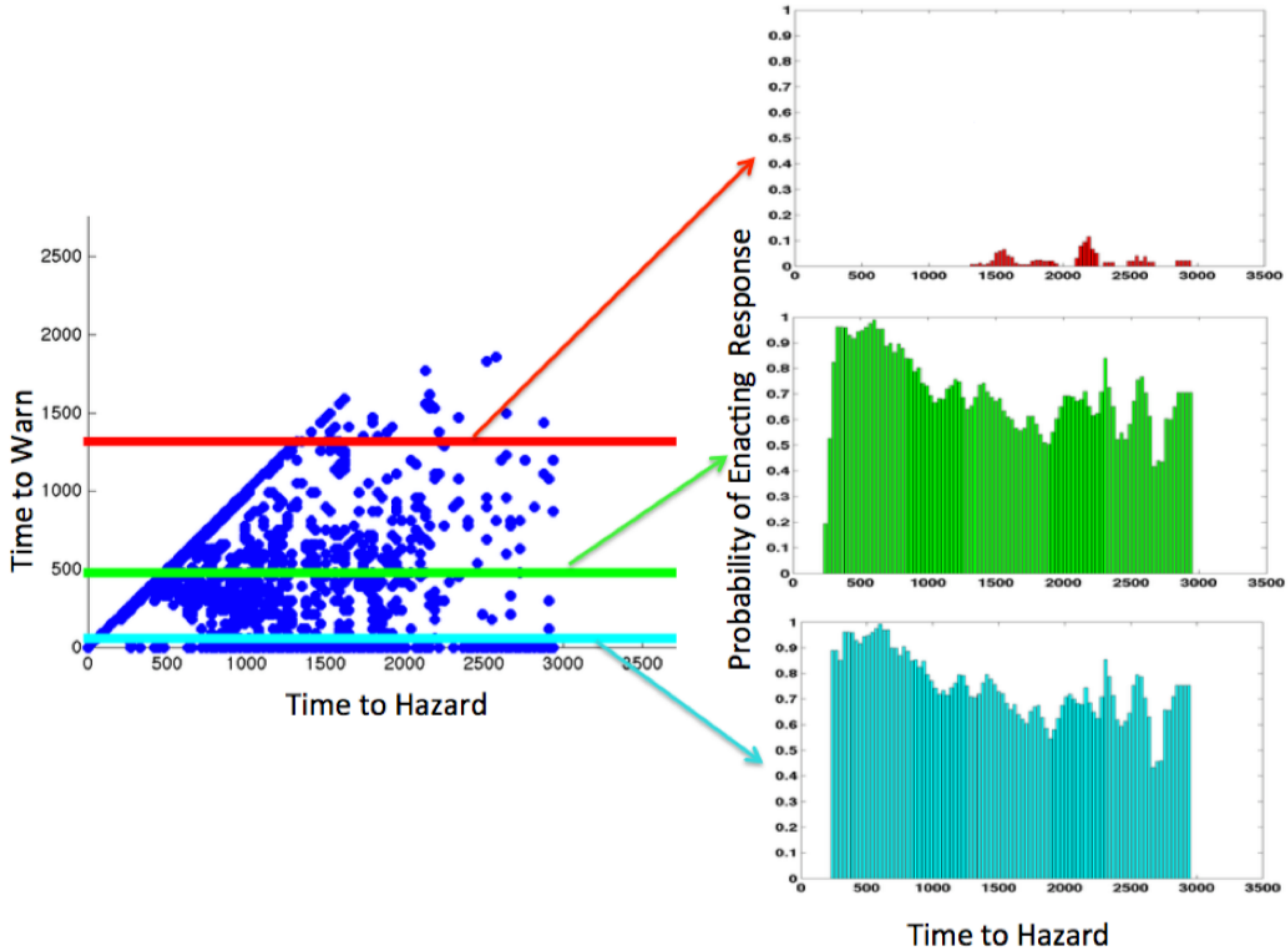
Resolving Critical Phenomena

(Allowed Correlations and Peak Concentrations To Be Properly Resolved)



Resolving Critical Phenomena

(Enabled Probabilistic Assessment of Operational Effectiveness)



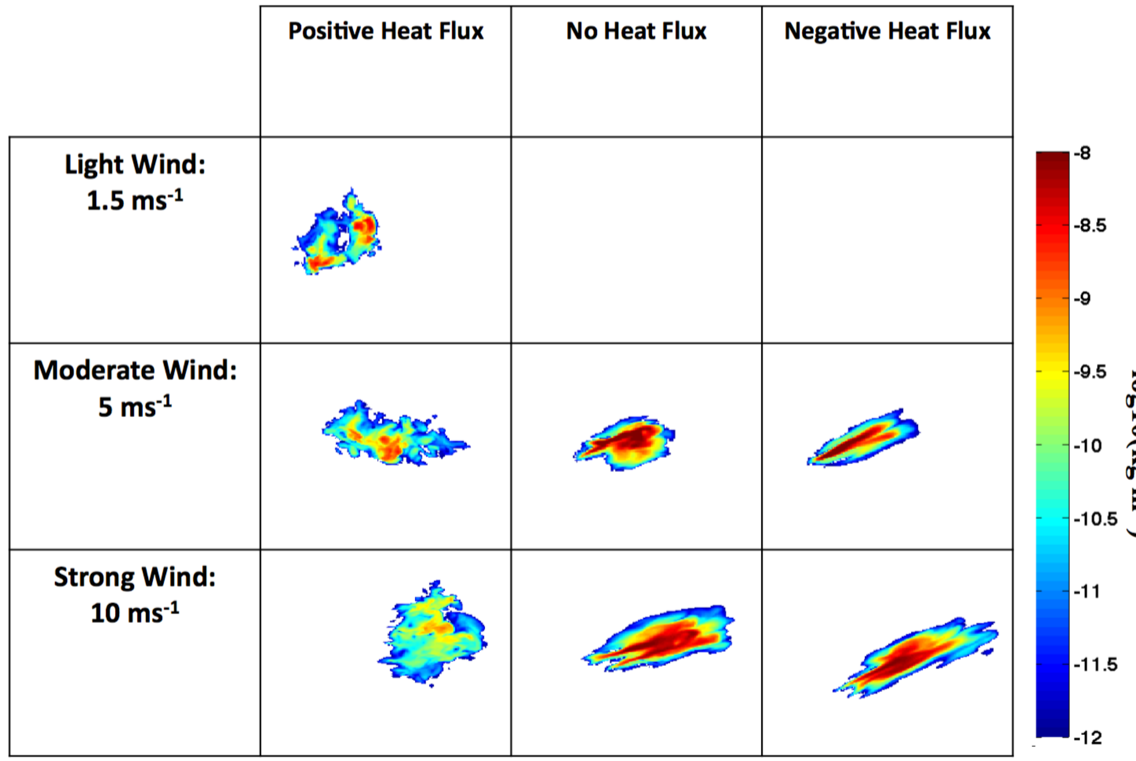
Material Source: Lawrence et al (2013)

Resolving Critical Phenomena

(CB Standoff Study Challenges/Limitations)

Study limited to a small set of environmental conditions

- **LES model simulations were very computationally expensive**
- **Required over 6 months of non-stop simulation time on large CPU based High Performance Computing (HPC) resources**
- **Generated 10s of TBs data, which was then analyzed/interrogated over an additional 6 month period**



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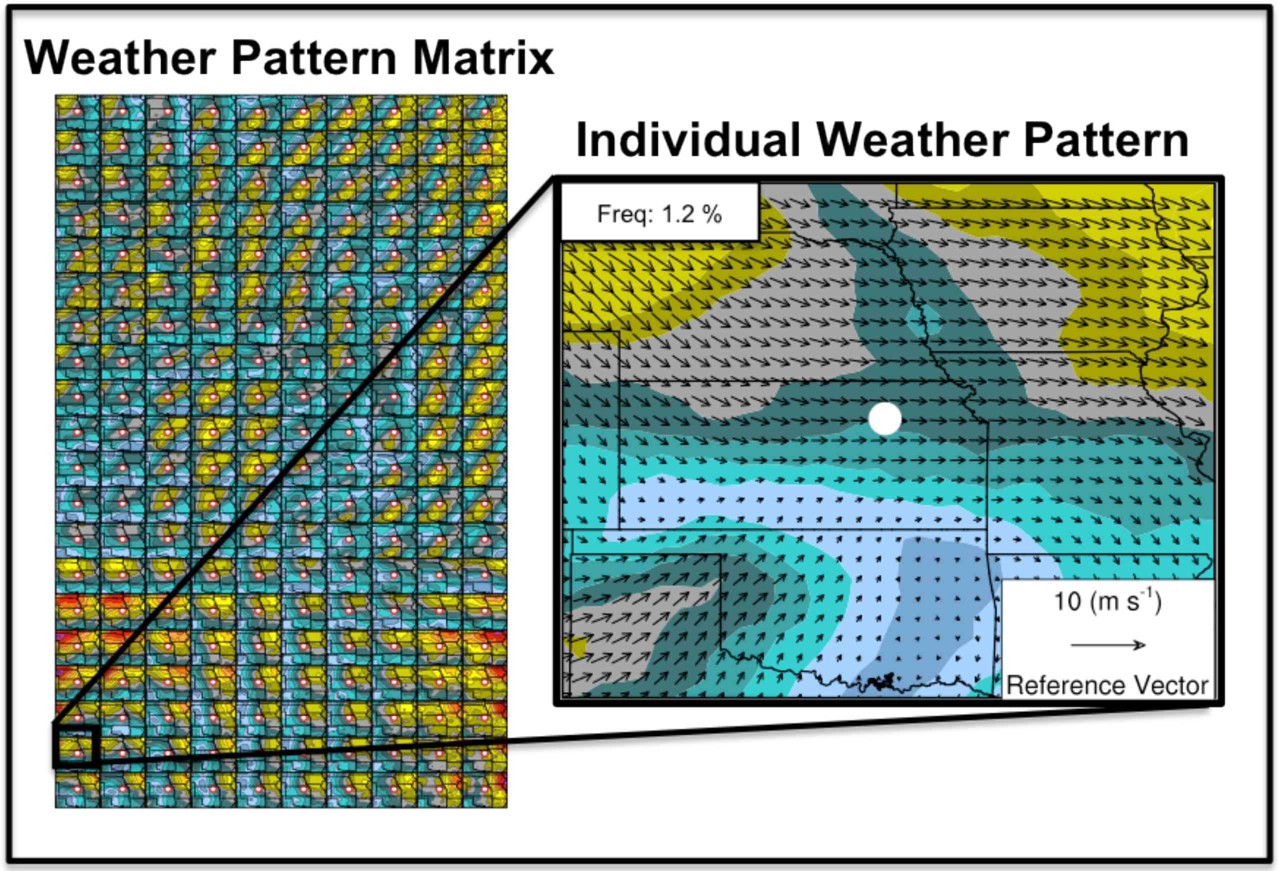
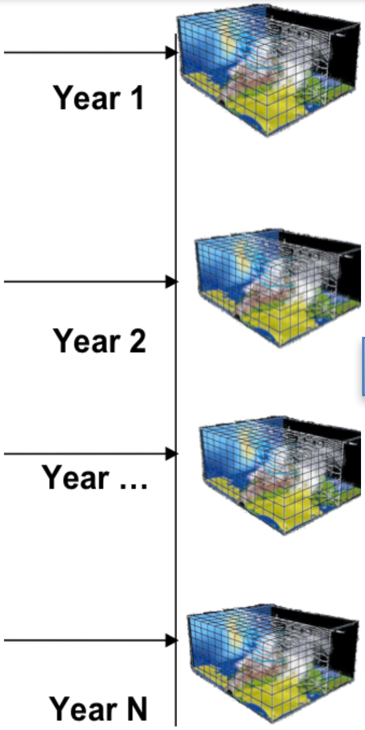
Enabling Technologies
(Environmental Data Reduction via Self Organizing Map)

- **The SOM is a neural network pattern recognition and classification algorithm (Kohonen 1990)**
- **Utilized by the atmospheric science community to distill large amounts of atmospheric data into a small set of characteristic patterns.**



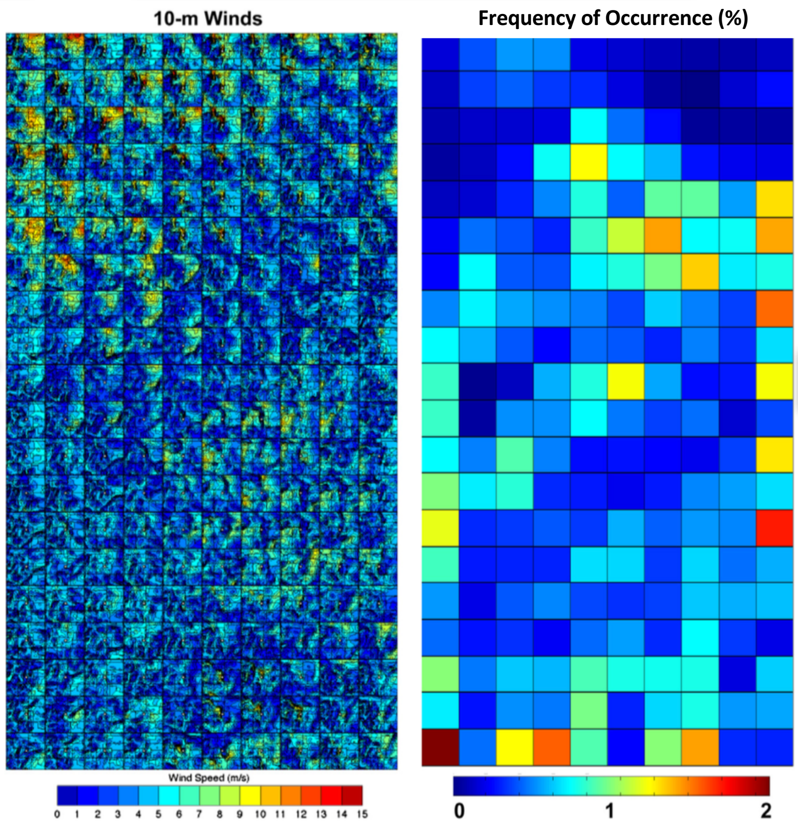
Enabling Technologies
(Environmental Data Reduction via Self Organizing Map)

21 Years of Climate Data (183,960 Meteorological Conditions)



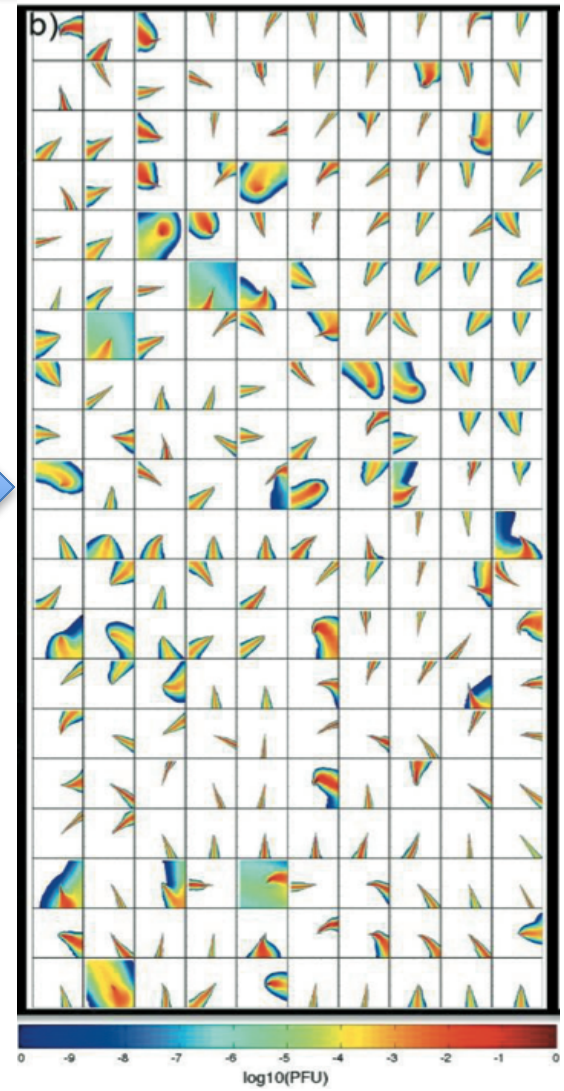
SOM

200 Representative Meteorological Patterns



AT&D

200 Representative Dispersion Patterns



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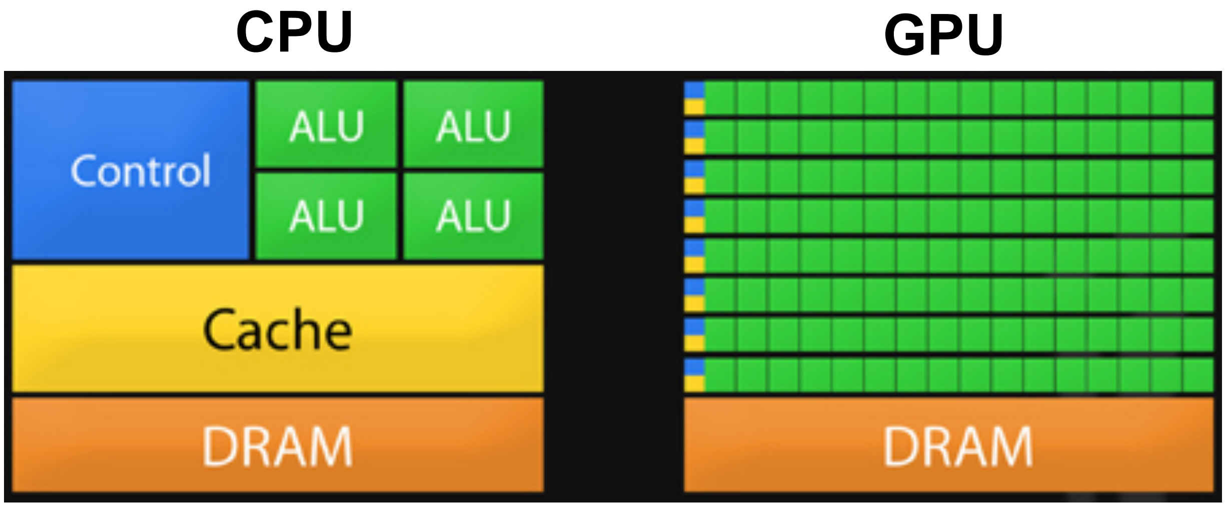
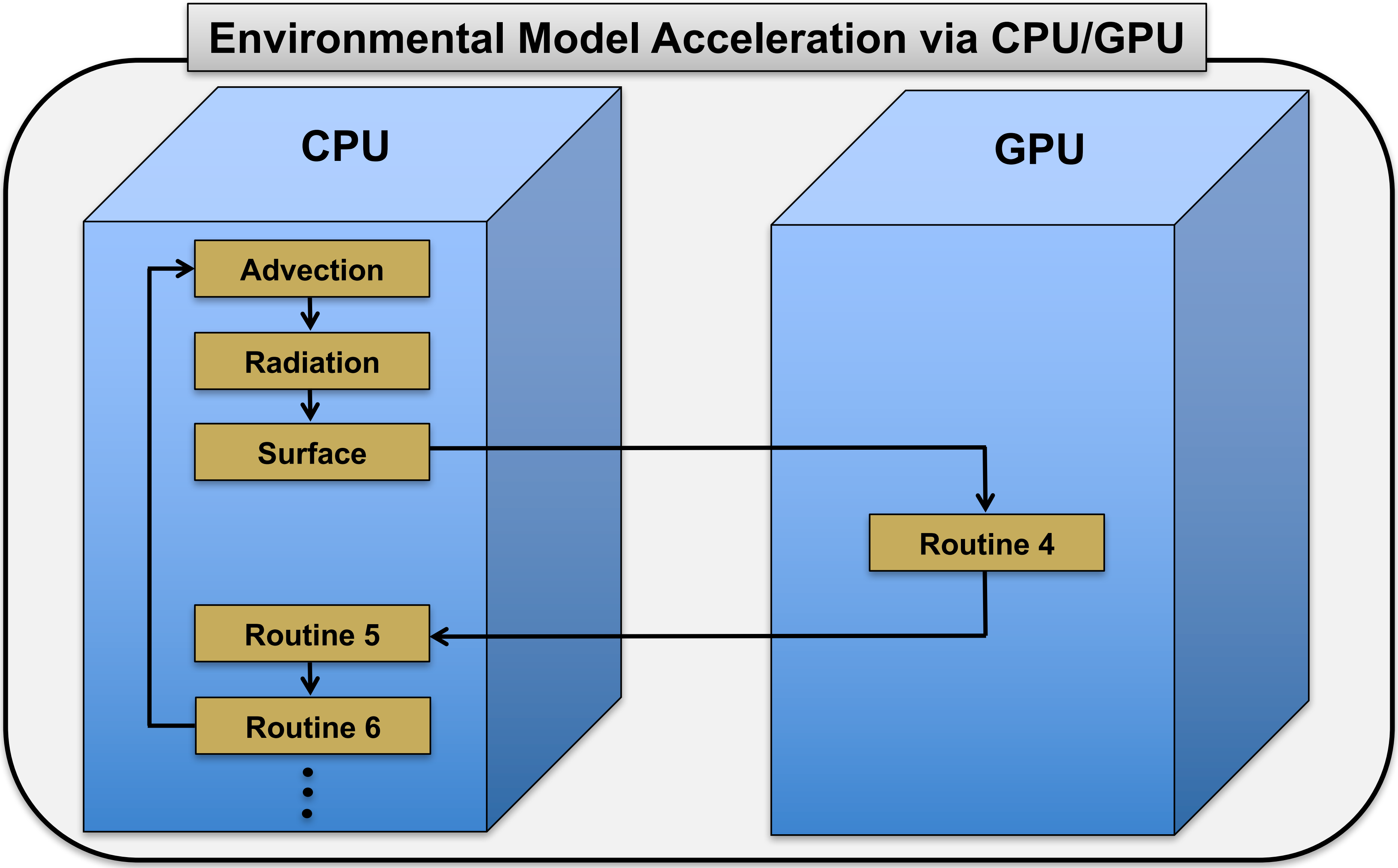
Enabling Technologies
(Graphics Processing Unit Accelerated HPC Computing)



ALU:	**Arithmetic and logic unit**
Control:	**Directs the operation of the processor**
Cache:	**Static memory (fast access)**
DRAM:	**Dynamic random access memory (slow access)**

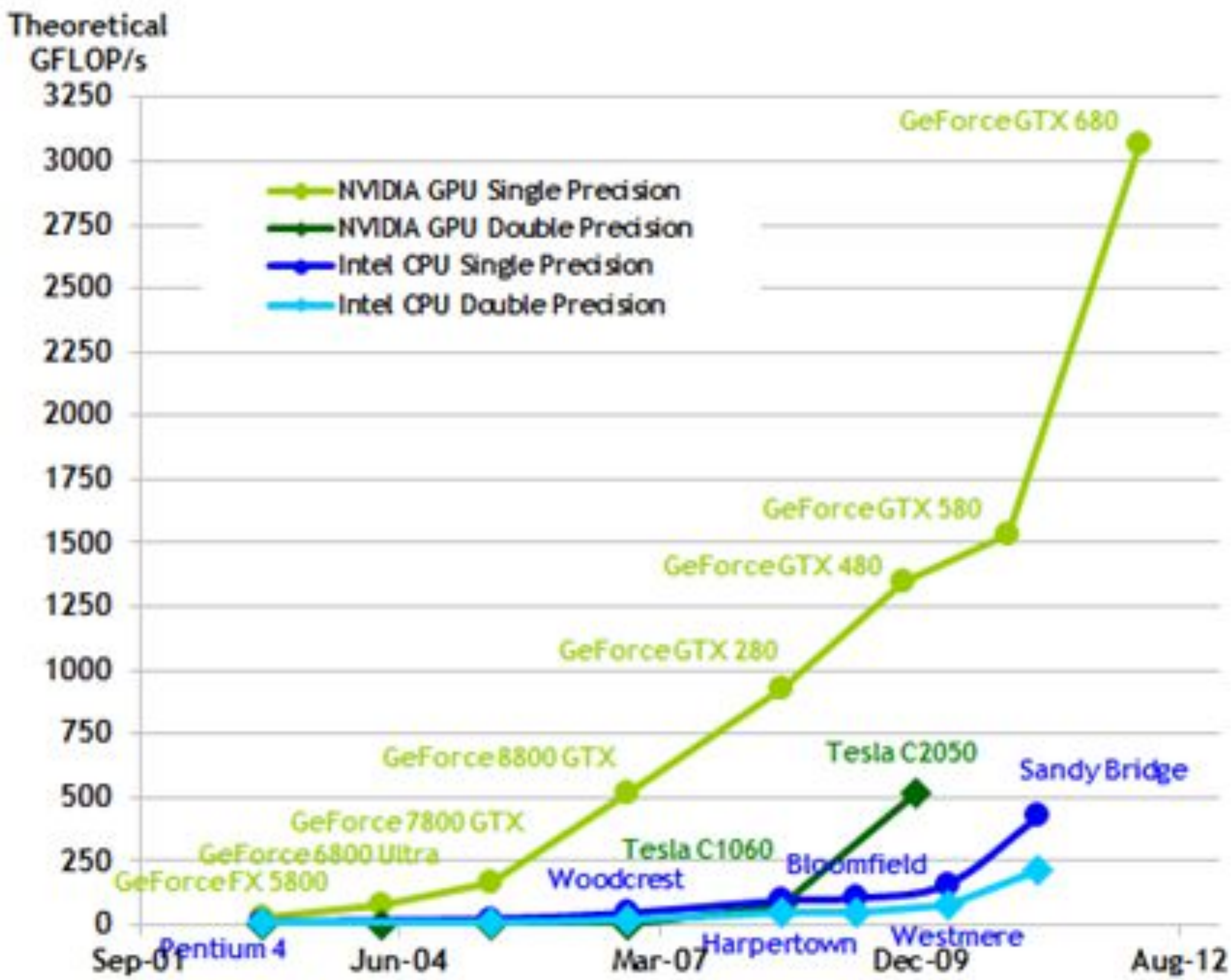
- **CPU is optimized to perform sequential operations**
  - **Multiple ALU's (cores) enable some parallel performance**
  - **Typically has a large cache memory availability compared to GPU**
- **GPU is optimized to perform highly parallel operations**
  - **Numerous ALU's (1000's on a single GPU card)**
  - **Faster and more advanced memory interfaces**
- **Primary challenge is refactoring of CPU based model codes to optimize utilization on GPU**

Enabling Technologies
(Graphics Processing Unit Accelerated HPC Computing)



Enabling Technologies
(Graphics Processing Unit Accelerated HPC Computing)

GPU Technology has continued to rapidly advance in terms of both Floating Point Operations per second (FLOP/s) and size/speed of the available fast access memory (Cache)



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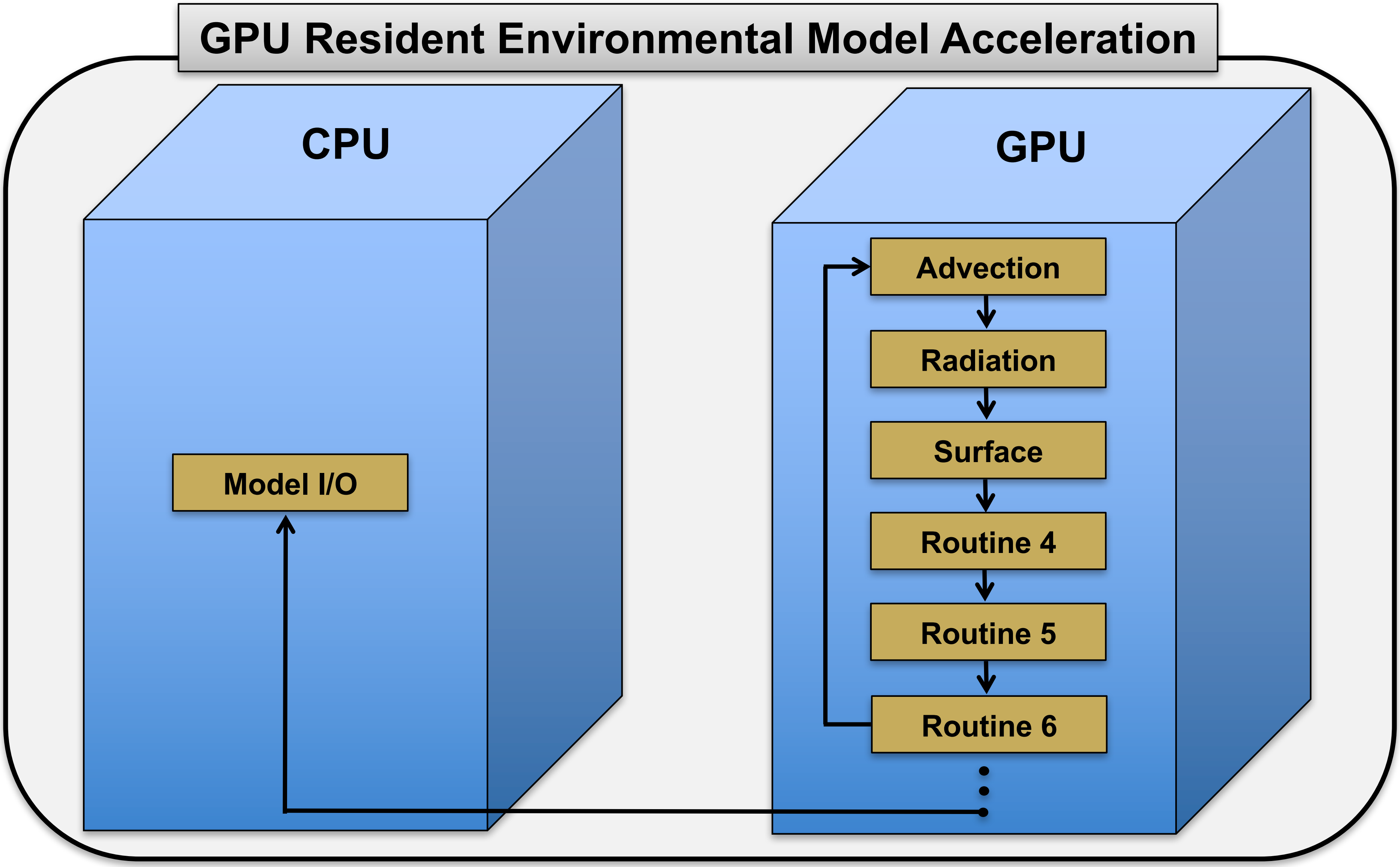
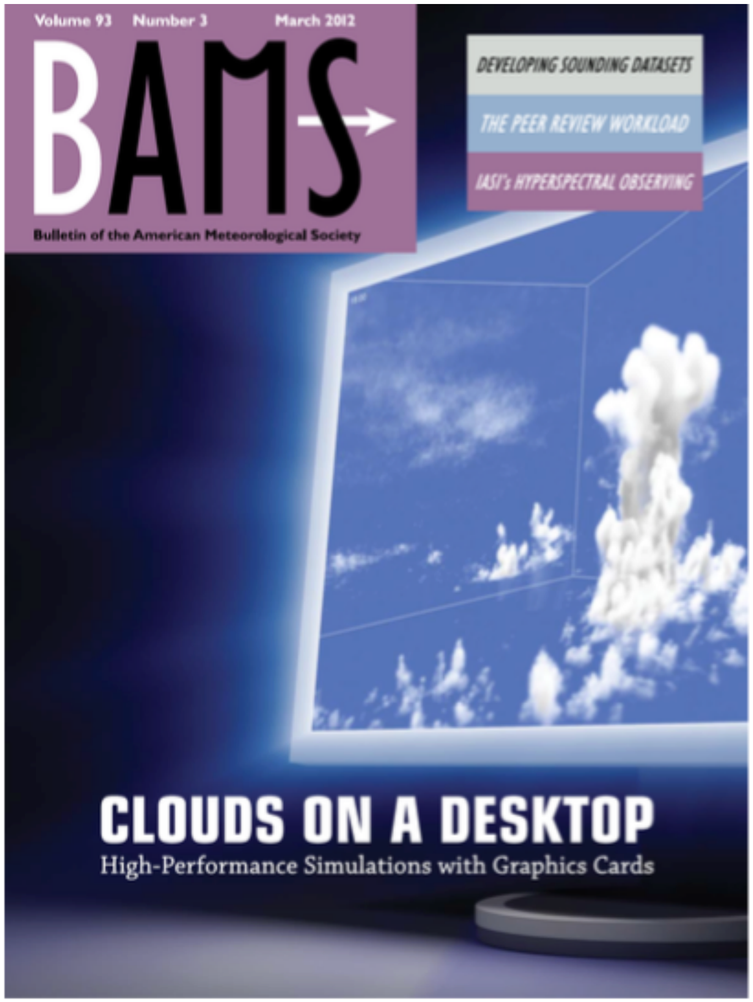
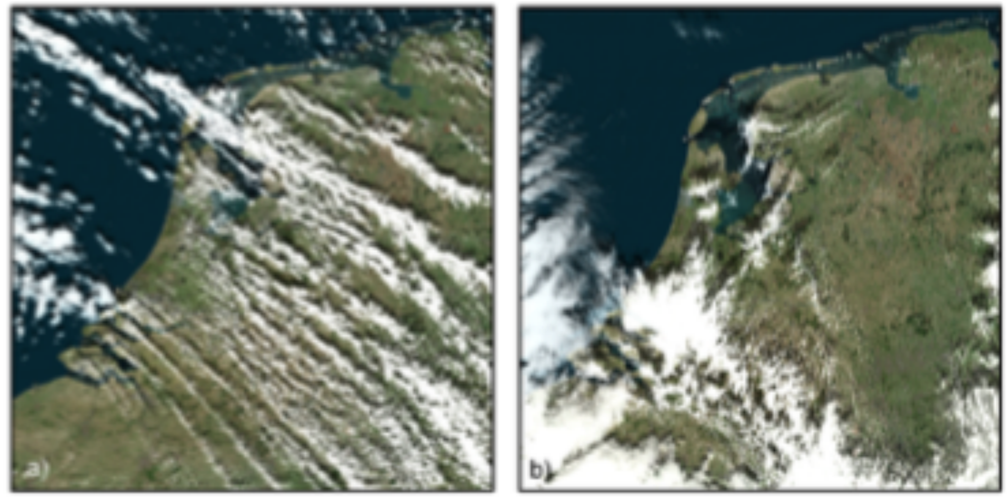
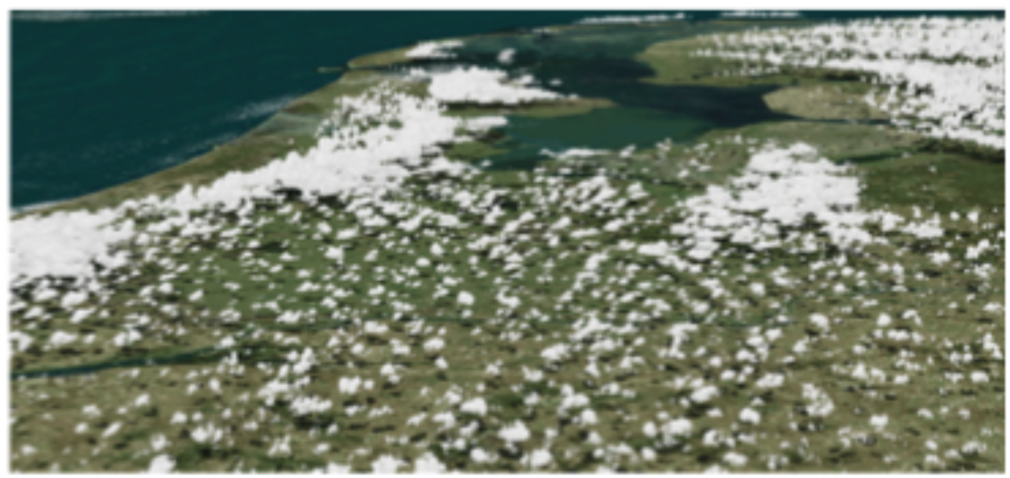
Enabling Technologies
(Graphics Processing Unit Accelerated HPC Computing)



Enabling Technologies
(GPU Resident Atmospheric Simulation Program (GRASP))



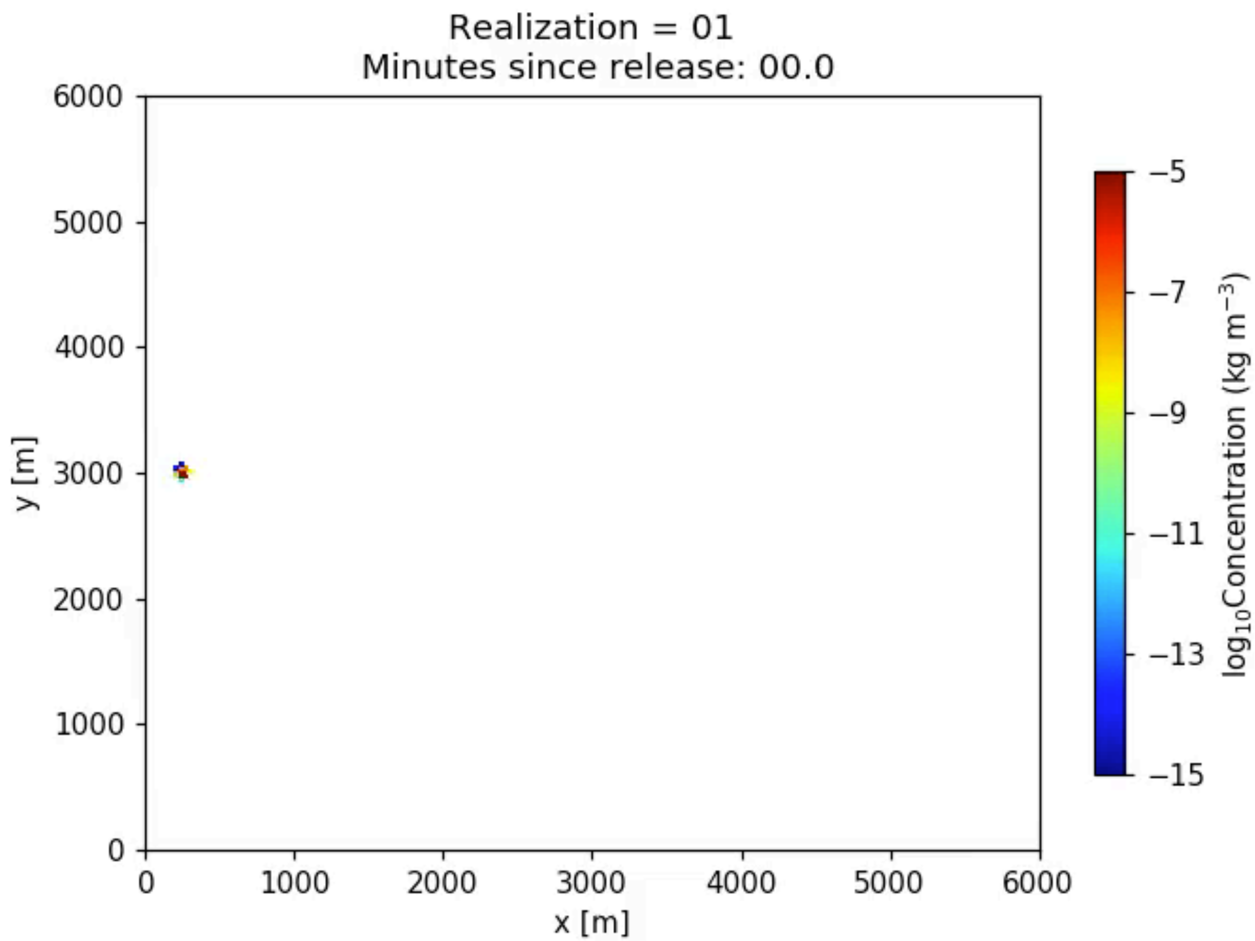




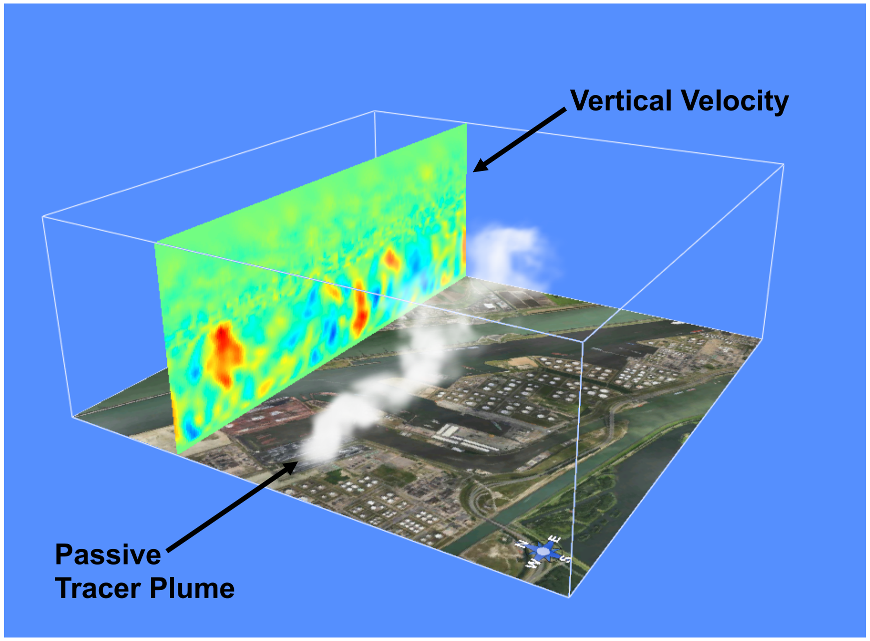
Material Source: Schalkwijk et al. BAMS 2012
Schalkwijk et al. BAMS 2015

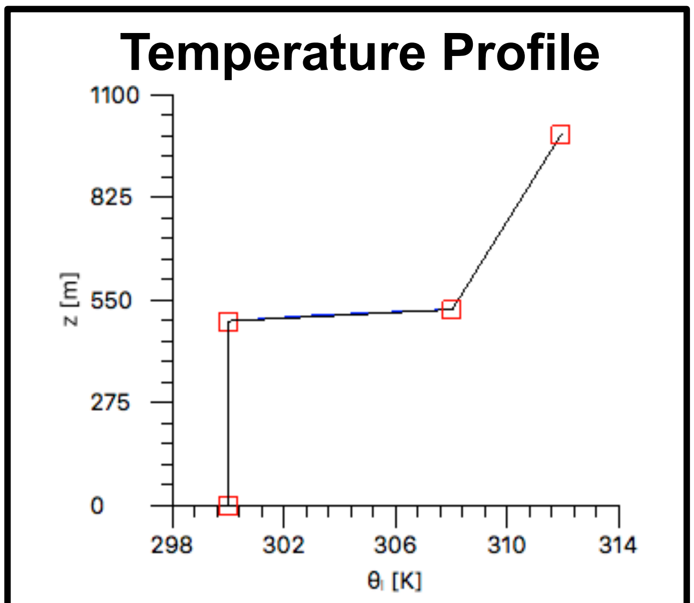
Enabling Technologies
(GPU Resident Atmospheric Simulation Program (GRASP))

AT&D capability recently added to allow generation of dispersion realizations in a fraction of the time, as compared to traditional CPU based LES solution



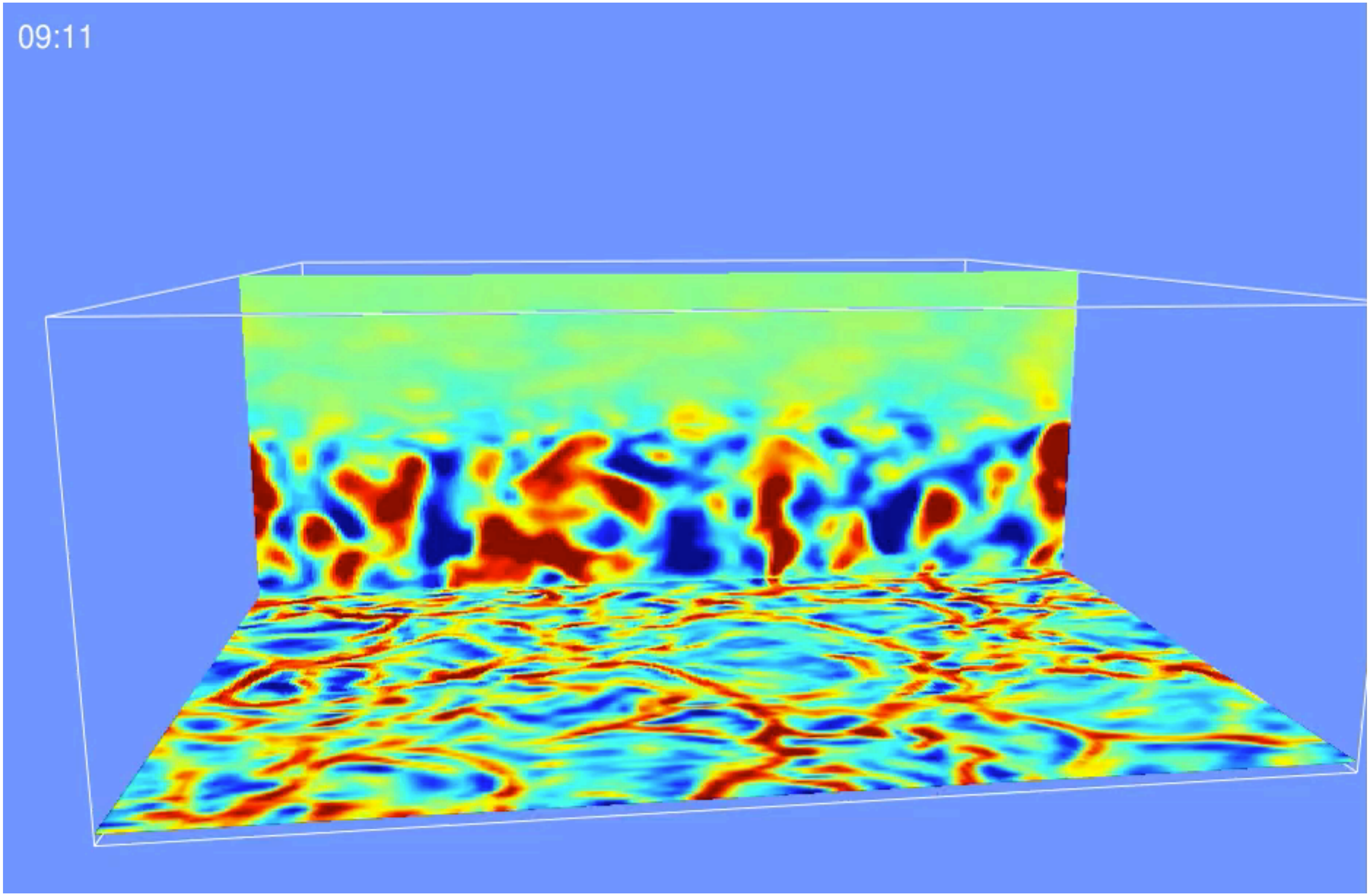
Enabling Technology
(GRASP AT&D Rural Simulation Demonstration)





- **Simulation specifications**
  - 128 x 128 x 64 grid
  - Horizontal resolution: 20 m
  - Vertical resolution ~17 m
  - 1-hr simulation
- **Performance on CPU based system (8-core Xenon): 5,520 seconds (~ 1.5 hours)**
- **Performance on NVIDIA K40 GPU Card: 36 seconds**

Enabling Technology
(GRASP AT&D Rural Simulation Demonstration)



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Summary and Conclusions

- **A robust M&S methodology should attempt to:**
  - Incorporate full distribution of possible cases/inputs, including associated probabilities/likelihoods.
  - Utilize models which adequately resolve critical phenomenon.
- **The ability to meet these requirements is historically limited by:**
  - Time and funds allocated to complete the analysis
  - Current state of methods, technologies, and computational resources available to perform the analysis
- **Various emerging technologies hold promise to better meet these analysis goals:**
  - Environmental data reduction methods such as the Self Organizing Map (SOM) are a useful tool for reducing the input dimensionality, while retaining the associated probability distributions.
  - GPU model optimization is becoming an effective means to accelerate more sophisticated computationally expensive M&S codes, making their utilization more feasible for CBD analysis studies.

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