COMPUTATIONAL MATHEMATICS IN ENVIRONMENTAL SCIENCES

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THE ENVIROCOMP INSTITUTE

INVITED LECTURE

ARL/USMA TECHNICAL SYMPOSIUM (AUTS)

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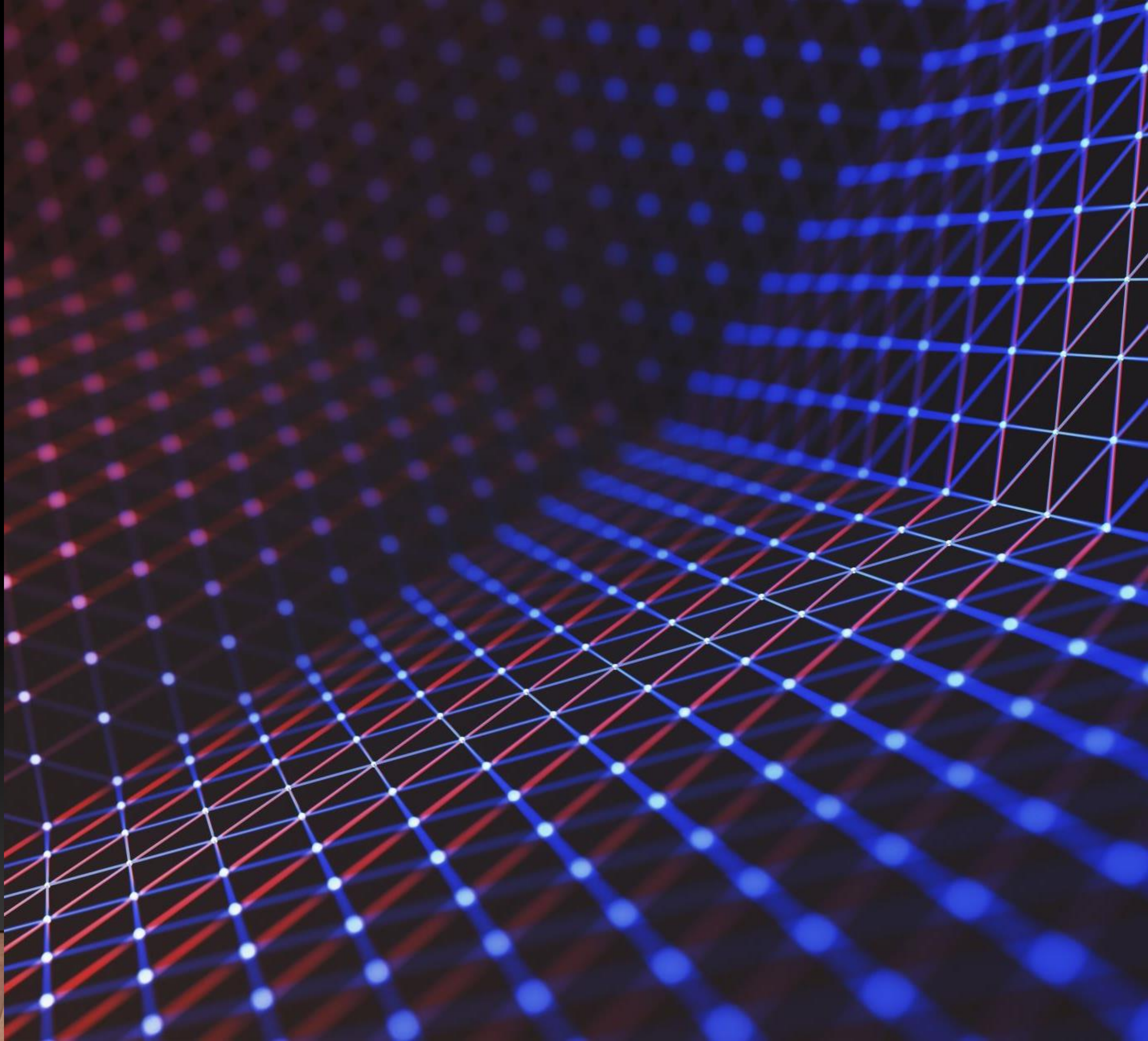


COMPUTATIONAL ENGINEERING MATHEMATICS

- It existed before computers
  - Use of numerical approximation instead of symbolic manipulation
  - Tables of pre-calculated logarithms, trigonometric functions, square roots, and commonly-used integrals
  - Use of slide ruler and nomograms
  - Analog computers
- Enormous improvements with digital electronic computers after WWII
  - Meteorology
  - Nuclear Physics

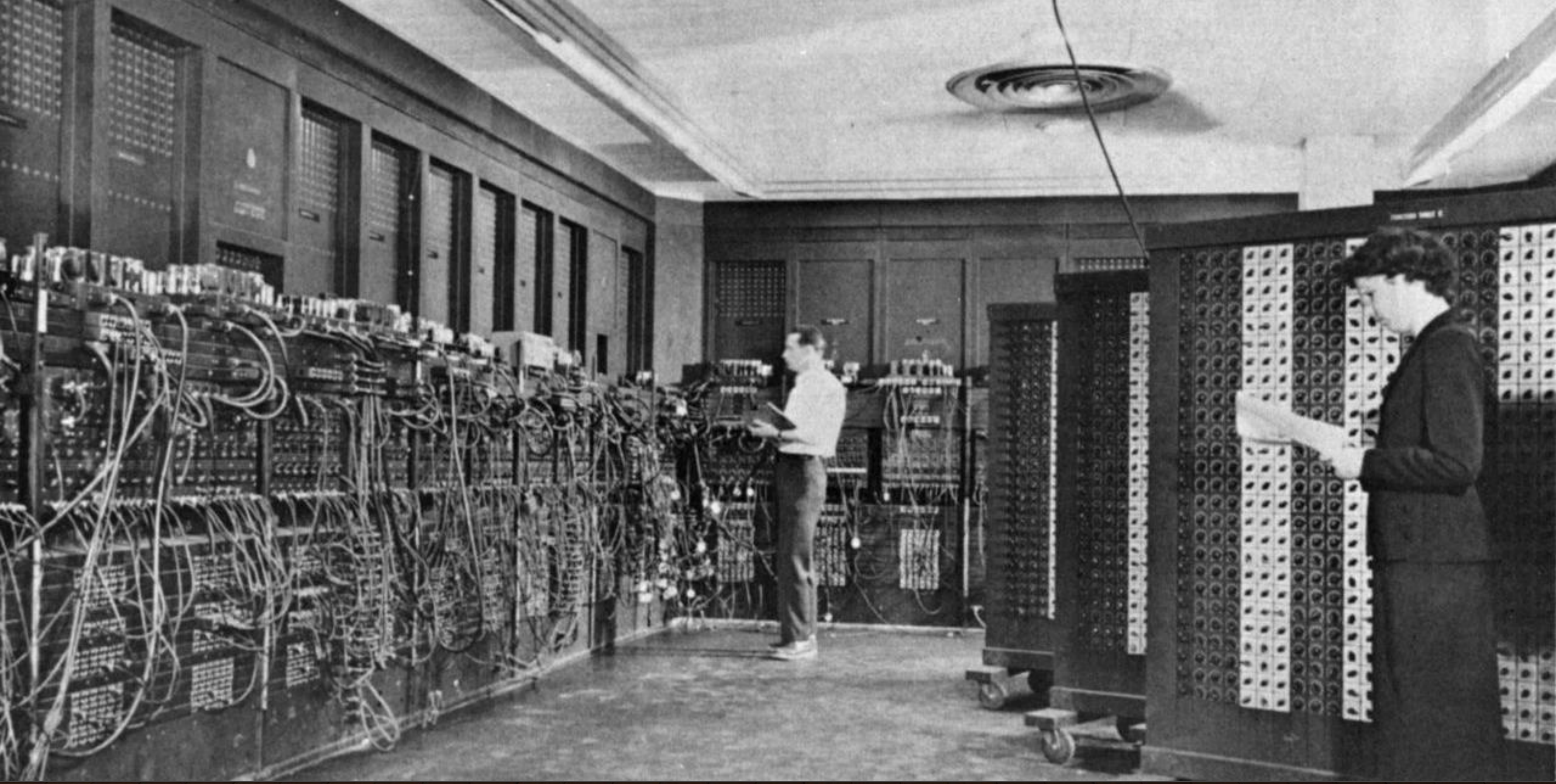
COMPUTER SIMULATIONS IN SCIENCE (HTTPS://PLATO.STANFORD.EDU/ENTRIES/SIMULATIONS-SCIENCE/)

- Start: meteorology and nuclear physics
- Later: astrophysics, particle physics, materials science, engineering, fluid mechanics, climate science, evolutionary biology, ecology, economics, decision theory, medicine, sociology, epidemiology, and many others
- Computer simulation today: a comprehensive method for studying systems; an entire process which includes: choosing a model; finding a way of implementing that model in a form that can be run on a computer; calculating the output of the algorithm; and visualizing and studying the resultant data
- Future: AI …

THE DAWN OF DIGITAL: ENIAC (FEB 1946)

(HTTPS://WWW.ATOMICHERITAGE.ORG/HISTORY/COMPUTING-AND-MANHATTAN-PROJECT)

- ENIAC was built for the purpose of calculating artillery-firing tables
- ENIAC was used to create the first weather predictions via computer in 1950
- ENIAC weighed more than 60,000 pounds, covered 1800 square feet of area, consumed 150 kilowatts of power, and cost $500,000 to build (about $6,000,000 in today's dollars)
- The processor could handle 50,000 instructions per second (an iPhone processor today, by contrast, can handle about five billion)



COMPUTER SIMULATIONS IN ENVIRONMENTAL SCIENCES

1. Simulation of environmental flows (winds, water currents, groundwater flows)
2. Simulation of materials (pollutants) carried by environmental flows
   - Dispersion
   - Chemistry, Deposition
   - Ultimate fate
     - SO_2, CO, O_3 (hours/days) vs. **Persistent, Bioaccumulative and Toxic Chemicals (PBTs), e.g., metals**

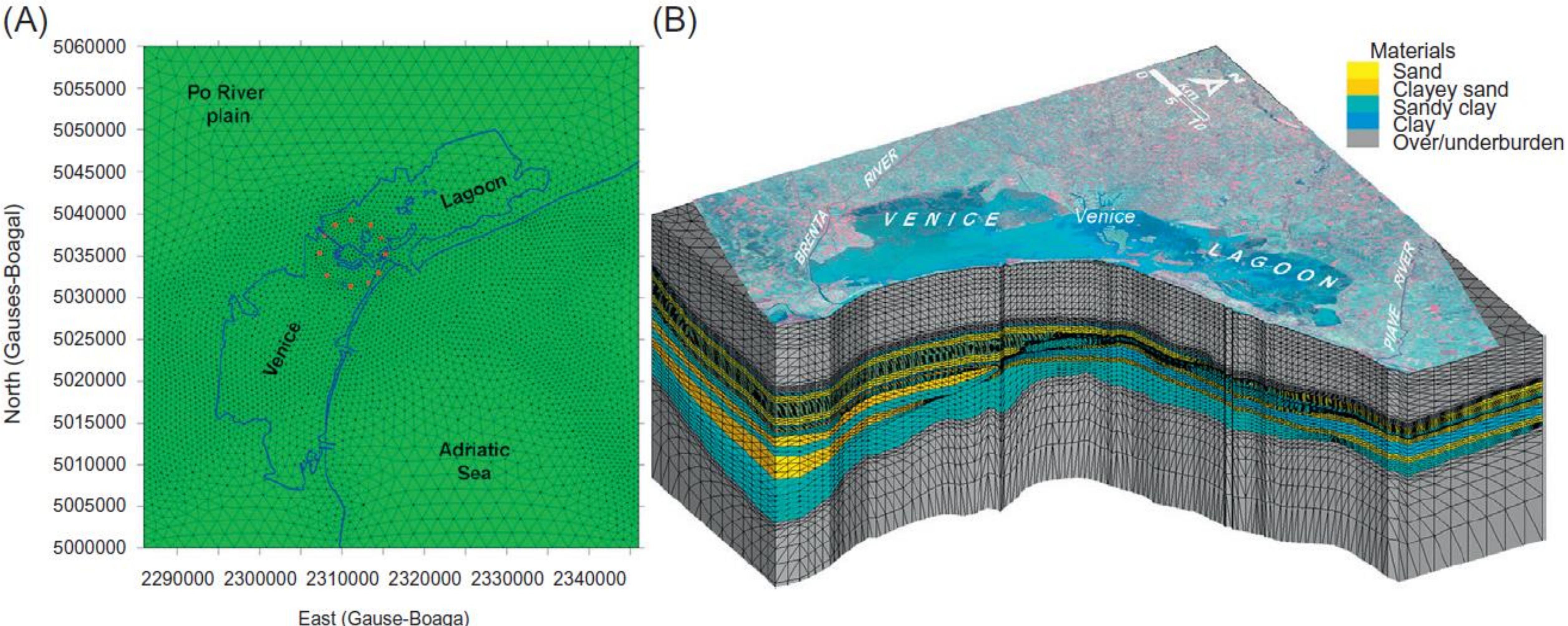
MAIN FIELDS OF APPLICATION

- Air
  - Meteorological modeling (different scales)
- Water
  - River/ocean modeling
- Soil and groundwater
  - Flow of subsurface water
- ALL: Transport and fate of pollutants in different media

MODELING OF LIFTING OF VENICE

8

THE PROJECT CONSISTS OF INJECTING SEAWATER INTO A NUMBER OF SANDY LAYERS INTERSPERSED WITHIN A BRACKISH WATER AQUIFER SYSTEM LYING BETWEEN 650 AND 1000 M BELOW THE SURFACE OF THE LAGOON (VENICE SHALL RISE AGAIN - ENGINEERED UPLIFT OF VENICE THROUGH SEAWATER INJECTION GIUSEPPE GAMBOLATI AND PIETRO TEATINI, ELSEVIER, 2014)



10-Y PREDICTION

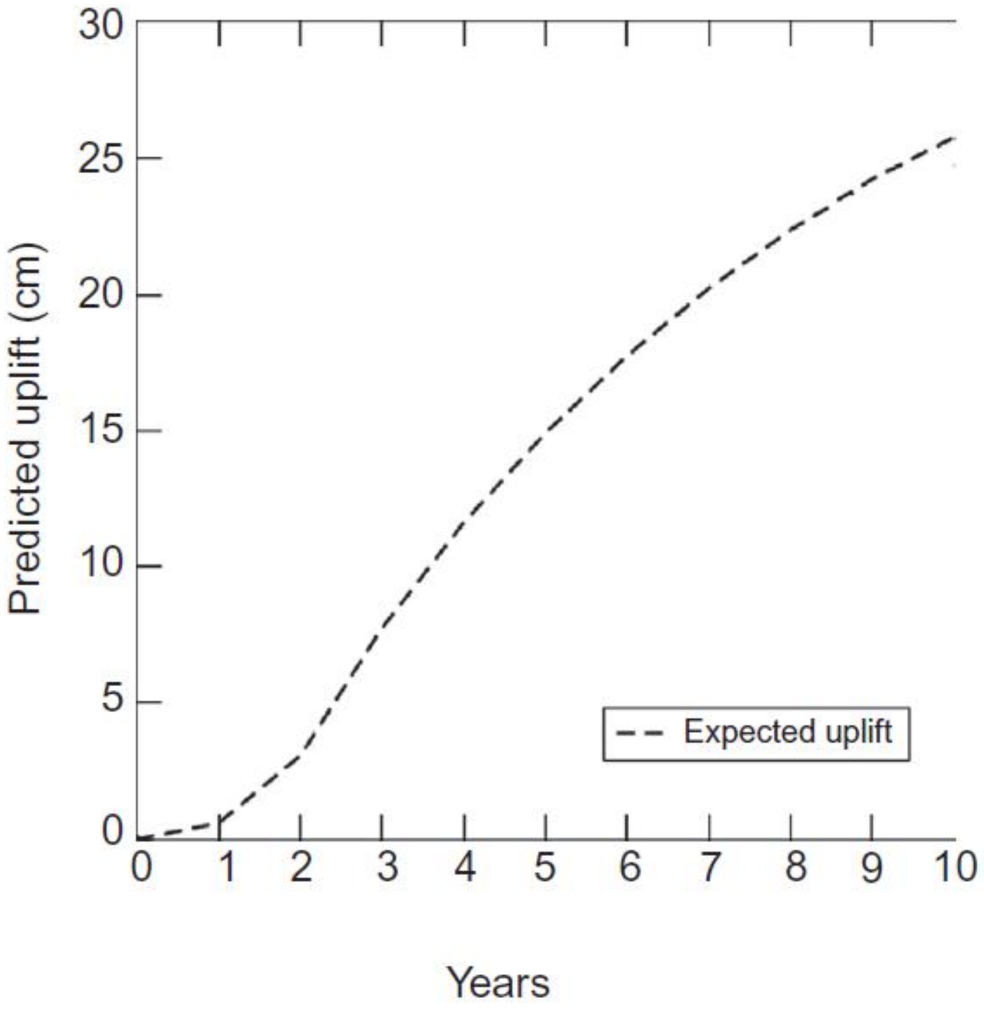
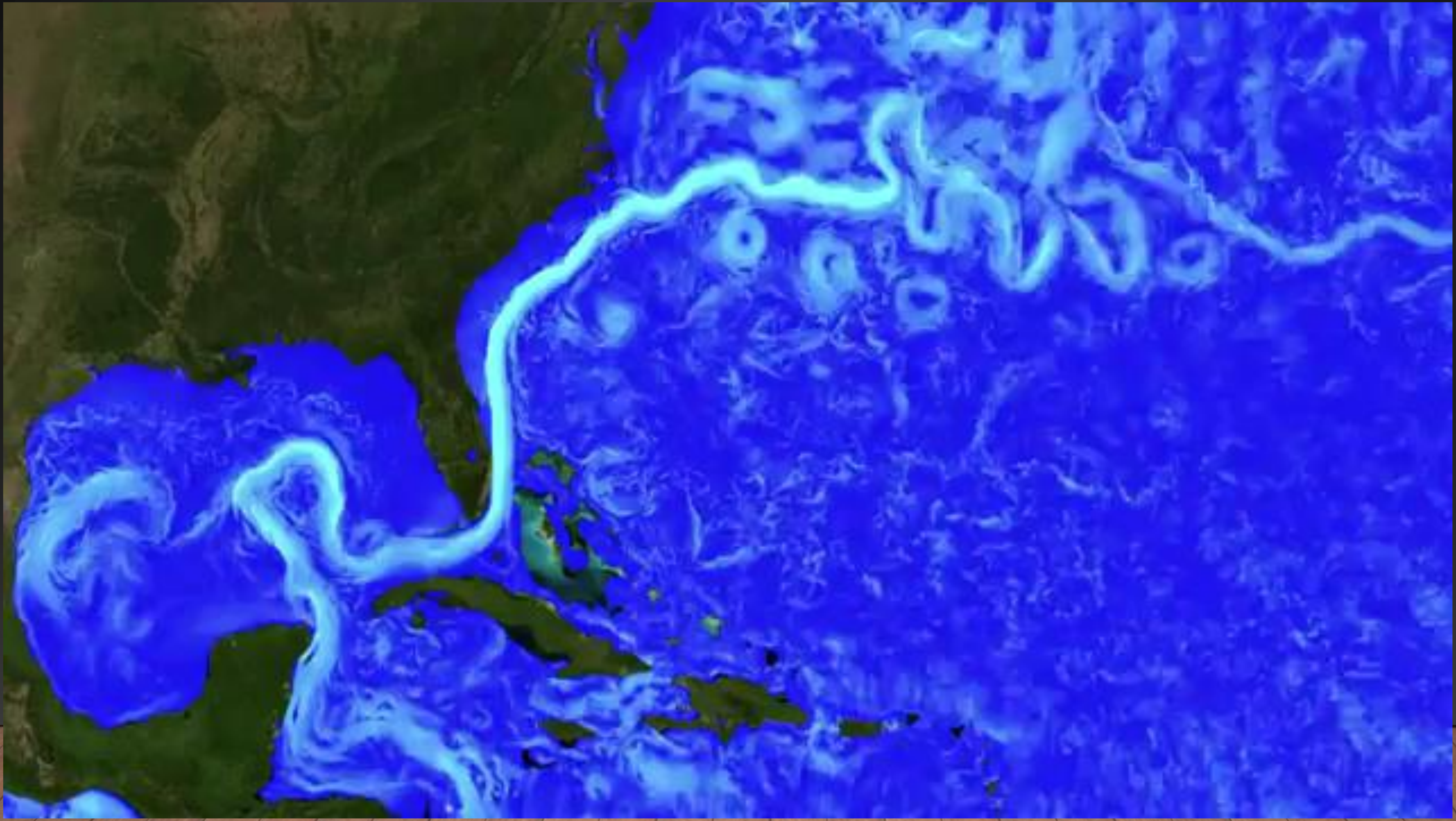


Figure 5.10 Predicted uplift versus time at Rialto Bridge.

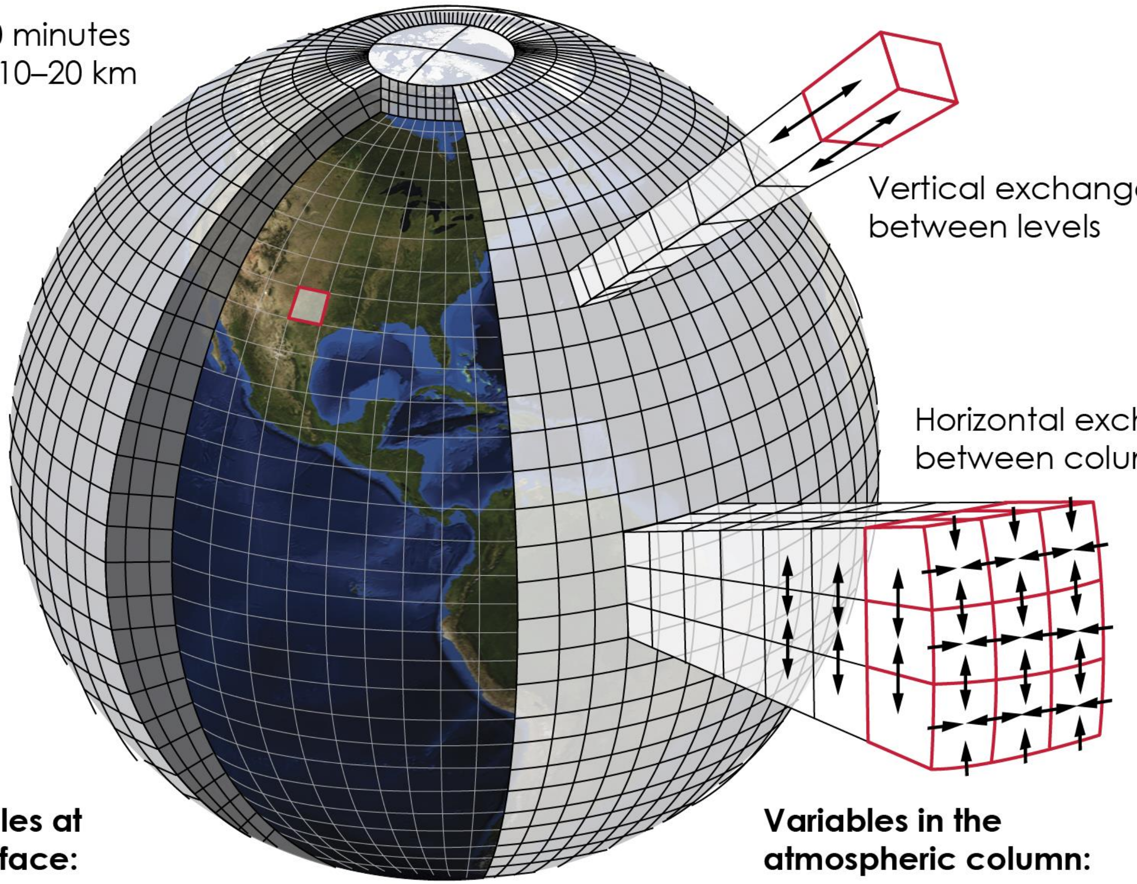
10 SUPERCOMPUTER SIMULATION OF OCEAN FLOWS



WEATHER FORECAST – GLOBAL SCALE

Weather forecast modeling

american geosciences institute
connecting earth, science, and people



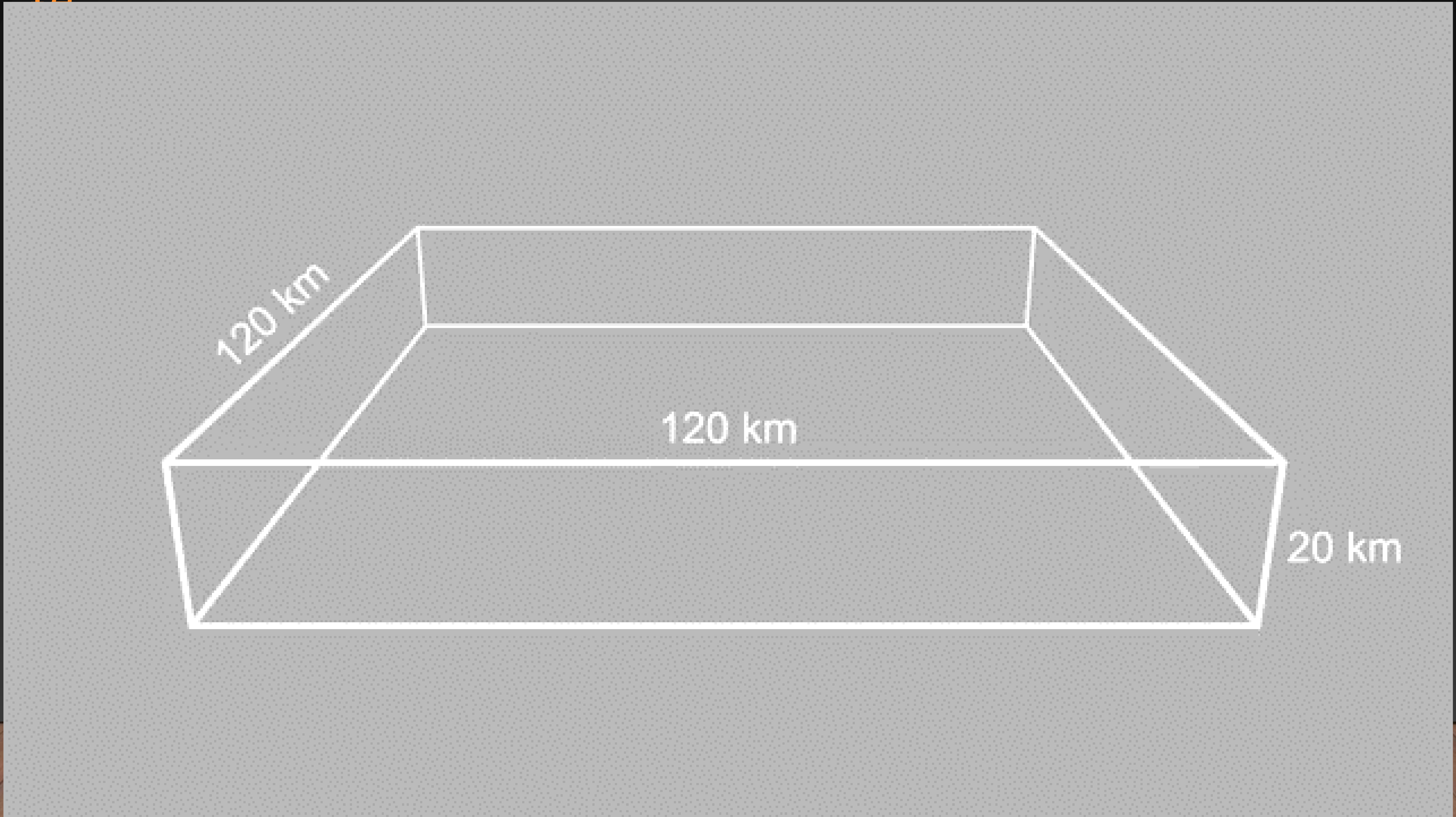
Variables at the surface:

Temperature
Humidity
Pressure
Moisture fluxes
Heat fluxes
Radiation fluxes

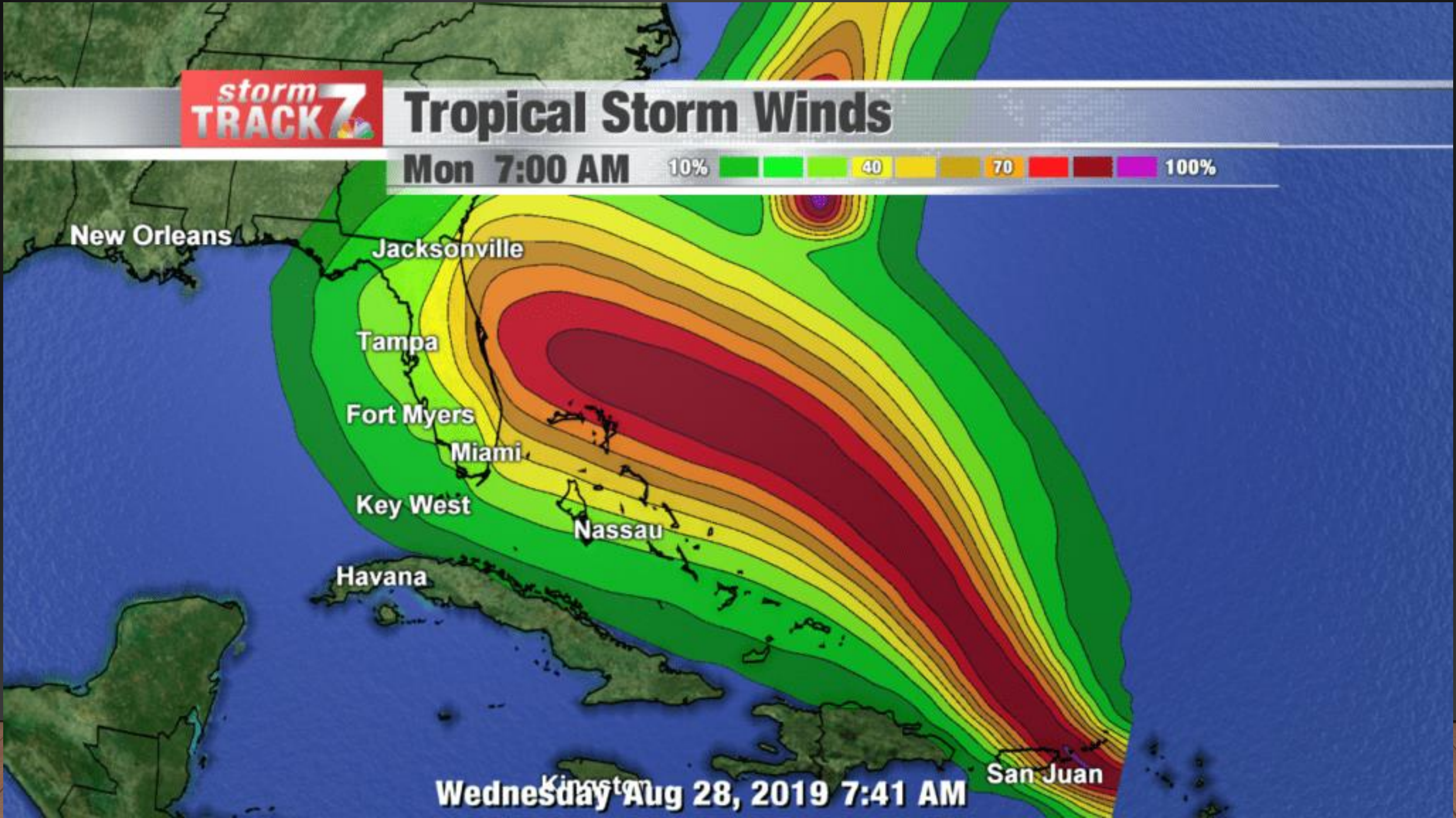
Variables in the atmospheric column:

Wind vectors
Humidity
Clouds
Temperature
Height
Precipitation
Aerosols

SUPERCOMPUTER SIMULATION OF A TORNADO



TRACKING HURRICAN DORIAN (2019)



MAJOR CHALLENGE: TURBULENCE

- Many systems evolve in a way that is dominated by initial and boundary conditions ➔ computer simulations are reliable (e.g., trajectories of objects in space)
- Other systems (especially in the atmosphere) evolve with chaotic components and soon “forget” initial conditions and are almost unaffected by boundary conditions
- Challenge: incorporate “chaos” in the calculations
  - ➔ MONTECARLO techniques ➔ air pollution

MONTECARLO MODELING OF AIR POLLIUTION

MONTECARLO AIR POLLUTION MODELING

- Conceptually simple: pollution is “traced” by particles and particles move according to the average wind + a semi random component
- The semi-random component is properly generated (intensity, auto-correlation, cross-correlation) from theoretical or semi-empirical meteorological parameterizations
- Very suitable for short-term accidental releases

LAPMOD

https://www.enviroware.com/lapmod/

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Formulation of the Lagrangian particle model LAPMOD and its evaluation against Kincaid SF_6 and SO_2 datasets

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H I G H L I G H T S

- The theory behind a new Lagrangian particle model (LAPMOD) is described.
- Directly coupled with CALMET, meteorological processor of the US-EPA CALPUFF model.
- Coupled to AERMET output files through its LAPMET processor.
- Detailed accounting of peak-to-mean concentration fluctuations, for odor modeling.
- Evaluated against Kincaid SO_2 and SF_6 field experiments with good results.

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Model evaluation
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A B S T R A C T

This paper presents the Lagrangian particle model LAPMOD for modeling time-variable emissions in atmosphere of inert and radioactive gases and aerosols. LAPMOD is fully interfaced with the meteorological model CALMET (Scire et al., 1999a), part of the US-EPA recommended CALPUFF modeling system (EPA, 2017), and can also use the meteorological input files produced with the AERMET meteorological processor of US-EPA recommended model AERMOD (EPA, 2004).

The paper outlines the theory on which LAPMOD is based and provides the results of the evaluation of LAPMOD against the Kincaid SF_6 and SO_2 classical field studies and tracer experiments. The performance of LAPMOD is successfully evaluated with the Model Evaluation Kit (Olesen, 2005) and compared with that of other air quality models.

1. Introduction

In the last decades, Lagrangian particle dispersion models (LPDMs) have become more appealing as modeling tools to simulate the atmospheric dispersion of pollutants thanks to their ability to reproduce the stochastic nature of turbulence (e.g. Thomson and Wilson, 2012). Lagrangian particle models simulate pollutant releases by following a number of independent computational particles – each one representing a fraction of the released mass - in a sequence of finite time intervals. The motion of each particle is driven by a time-varying velocity field, which can be divided into an average component, the average wind, plus a fluctuation velocity describing the effects of atmospheric turbulence and those wind variations not included in the mean component. The fluctuation velocity can be described by a non-linear form of the Langevin stochastic differential equation.

While particles in Lagrangian particle models are generally considered computational markers of the atmospheric fluid that allow the reconstruction of the concentration field of the pollutant at later times, the description of released matter in terms of particles allows easy incorporation of some physical processes the pollutant may undergo, including radioactive decay and deposition. Since particles can represent the pollutants as gas or aerosol, deposition and gravitational settling can also be taken into account.

The advantages of Lagrangian particle models with respect to Eulerian models and analytical models are described for example in Zannetti (1990).

LPDMs are widely used tools in the field of atmospheric pollution studies. For example, they are used to estimate the emission rates of specific sources starting from monitored concentrations (e.g. Park et al., 2016) and to simulate atmospheric dispersion over

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atmosphere

MDPI

Article

Incorporation of Numerical Plume Rise Algorithms in the Lagrangian Particle Model LAPMOD and Validation against the Indianapolis and Kincaid Datasets

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Abstract: This paper describes the methodology used to incorporate two numerical plume rise algorithms, one by Janicke and Janicke and another by Webster and Thomson, into the Lagrangian particle model LAPMOD. LAPMOD is fully interfaced with the diagnostic meteorological model CALMET, which is part of the widely used CALPUFF modeling system. LAPMOD can also use the meteorological input files produced with the AERMET meteorological processor of the US-EPA recommended model AERMOD. This paper outlines the theory behind the two plume rise algorithms and the details of their implementation in LAPMOD. The paper also provides the results of the evaluation of LAPMOD and its included plume rise algorithms against the well-known Indianapolis and Kincaid SF_6 and SO_2 field studies and tracer experiments. The performance of LAPMOD is successfully evaluated with the Model Evaluation Kit and compared with that of other air quality models.

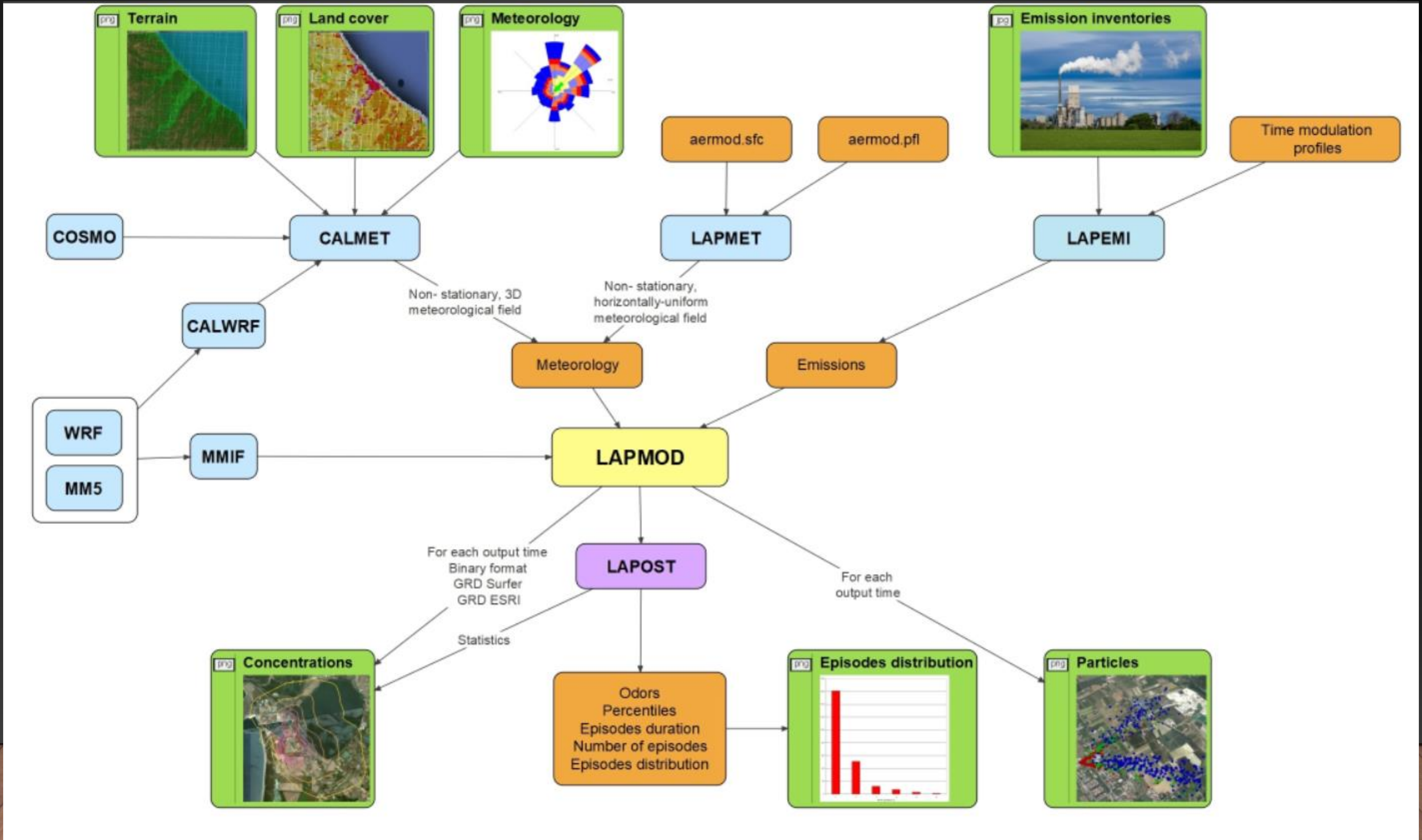
Keywords: Lagrangian particle model; plume rise; wet plume; model validation

1. Introduction

In most countries, Gaussian models are the reference tool recommended for atmospheric regulatory modeling applications. The most widely used of such Gaussian models is AERMOD, developed and distributed by the US-EPA [1]. The success of Gaussian models is due to several important factors, such as the simplicity of the algorithm, the direct physical interpretation of the parameters involved, and the limited number of input parameters required. Moreover, practical applications for regulatory purposes typically require the calculation of statistical parameters based on multi-year hourly values of concentration of pollutants emitted by several sources. Gaussian models are particularly fit for such simulations because of their fast execution, even on desktop computers.

However, Gaussian models show various limitations. For example, the stationarity of the solution over one hour implies constant meteorology and does not allow the simulation of accumulation and recirculation effects. In addition, the horizontal homogeneity of the meteorological conditions for any fixed height above terrain does not allow the treatment of variable land-use and orographic effects and limits the extent of the modeling domain where meteorological conditions are representative. The Gaussian solution to the dispersion equation is valid only for non-zero wind speed. For this reason, calm or very low wind conditions cannot be accounted for. Turbulence is assumed to be Gaussian via

HTTPS://WWW.ENVIROWARE.COM/LAPMOD/



THANK YOU!

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