ENG-270 Project

“Develop and use a computational model (e.g., simulation) of a real or hypothetical system to study its behavior.”

“All models are wrong, but some are useful.”
- George E. P. Box*

*British statistician 1919 – 2013

Today’s lecture

- Project deliverables
- What is a model
- The value of approximations and simple models
- Additional details

Deliverables

Project proposal

- for your stakeholder to highlight any major concerns

Final report for technical but non-coding stakeholders

- what problem did you solve
- what model / modeling approach did you use
- what were your findings

Accompanying code repository for technical, coding stakeholders

- code is well-documented
- automated
- reproduces your results

What is a model

Physical model

- physical replicas that capture main attributes

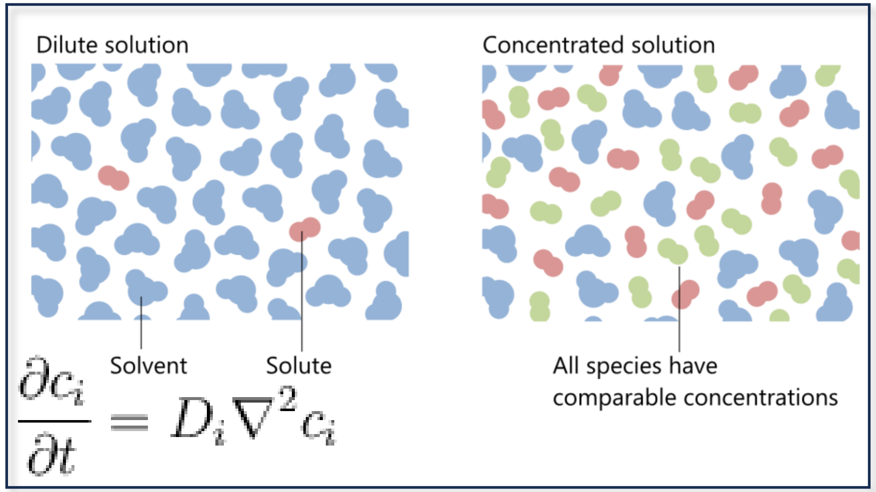
Mathematical model

- abstract description of a system using mathematical concepts

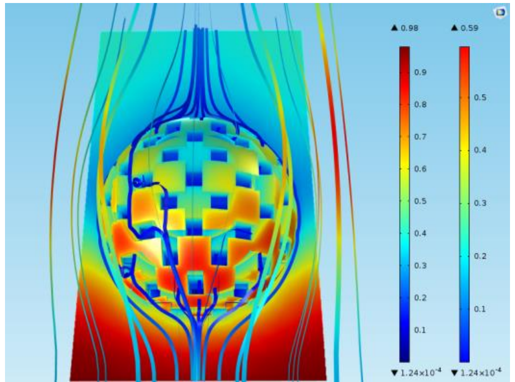
Numerical model

- Mathematical model implemented using numerical / computational methods

EPFL-LCH



COMSOL



COMSOL

Models

Classifications

- Mechanistic / Statistical
- Deterministic / Stochastic
- Analytical / Computational

Reasons for modeling

- Prediction / Forecasting
- Understanding or inference / hypothesis testing

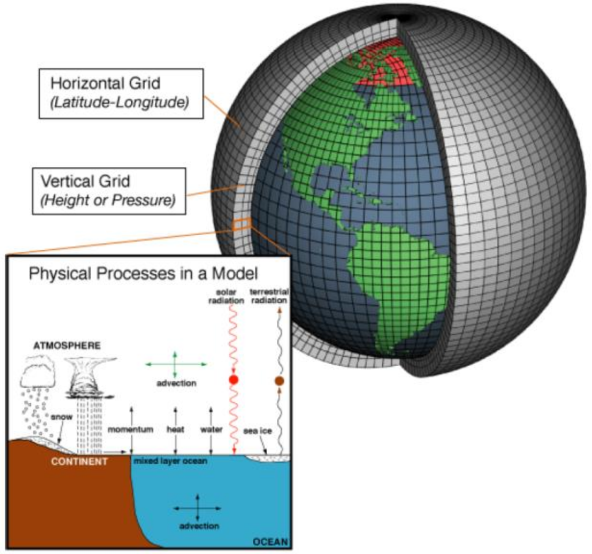
Application of computer methods (*iterative calculations*)

- Numerical integration (forward modeling)
- Parameter estimation (inverse modeling)
- Data analysis

Examples

- Simulation → generate data
- Data analysis → reduce amount of data

Mechanistic models
continuum models



source: NOAA

TABLE 1. Fundamental equations.

Conservation of momentum: (Newton's second law of motion)	$\frac{d\mathbf{V}}{dt} = -2\boldsymbol{\Omega} \times \mathbf{V} - \rho^{-1}\nabla p + \mathbf{g} + \mathbf{F}$	(T1)
Conservation of mass: (continuity equation)	$\frac{d\rho}{dt} = -\rho\nabla \cdot \mathbf{V} + C - D$	(T2)
Conservation of energy: (first law of thermodynamics)	$\frac{dI}{dt} = -p\frac{d\rho^{-1}}{dt} + Q$	(T3)
Ideal gas law: (approximate equation of state)	$p = \rho R T$	(T4)

Notation

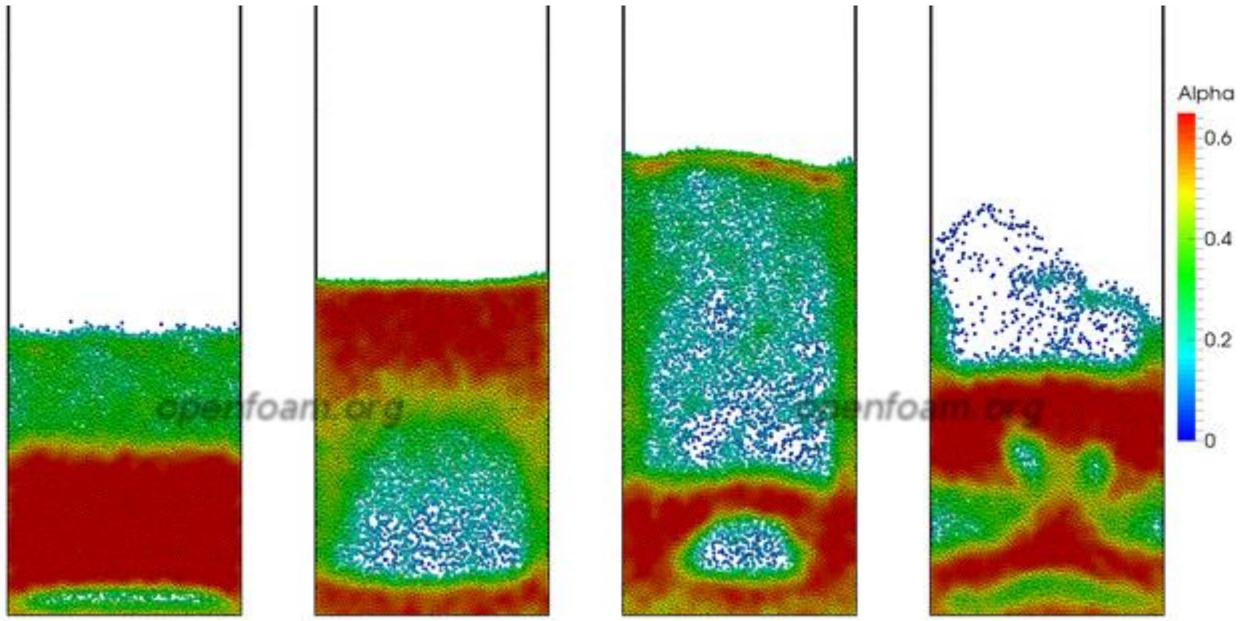
$\mathbf{V}$	velocity relative to rotating earth
t	time
$\frac{d}{dt}$	total time derivative $\left[= \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla\right]$
$\boldsymbol{\Omega}$	planet's angular rotation vector
ρ	atmospheric density
$\mathbf{g}$	apparent gravity [=true gravity $- \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \mathbf{r})$]
$\mathbf{r}$	position relative to planet's center
$\mathbf{F}$	force per unit mass
C	rate of creation of (gaseous) atmosphere
D	rate of destruction of atmosphere
I	internal energy per unit mass [$=c_v T$]
Q	heating rate per unit mass
R	gas content
c_v	specific heat at constant volume.

Hansen et al., 1983

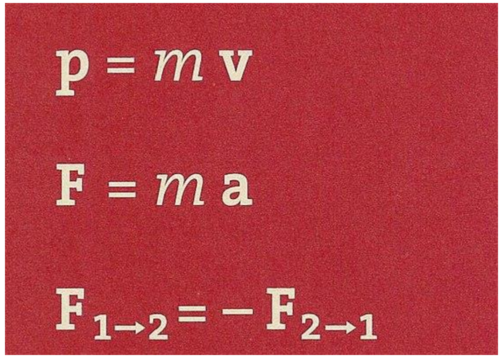
Numerically integrate over time/space

- Integration scheme
- Initial values
- Boundary values

Mechanistic models
discrete models



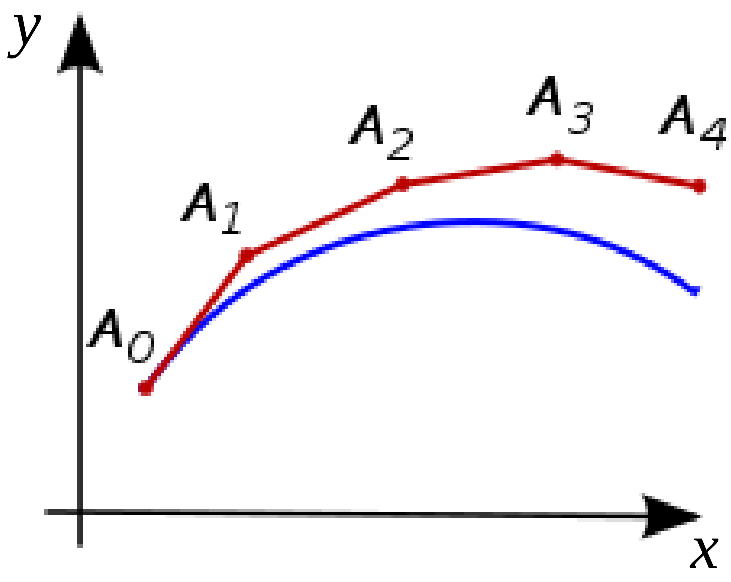
https://openfoam.org/



source: Wikipedia

Numerical integration

$$y_{n+1} = y_n + hf(t_n, y_n).$$

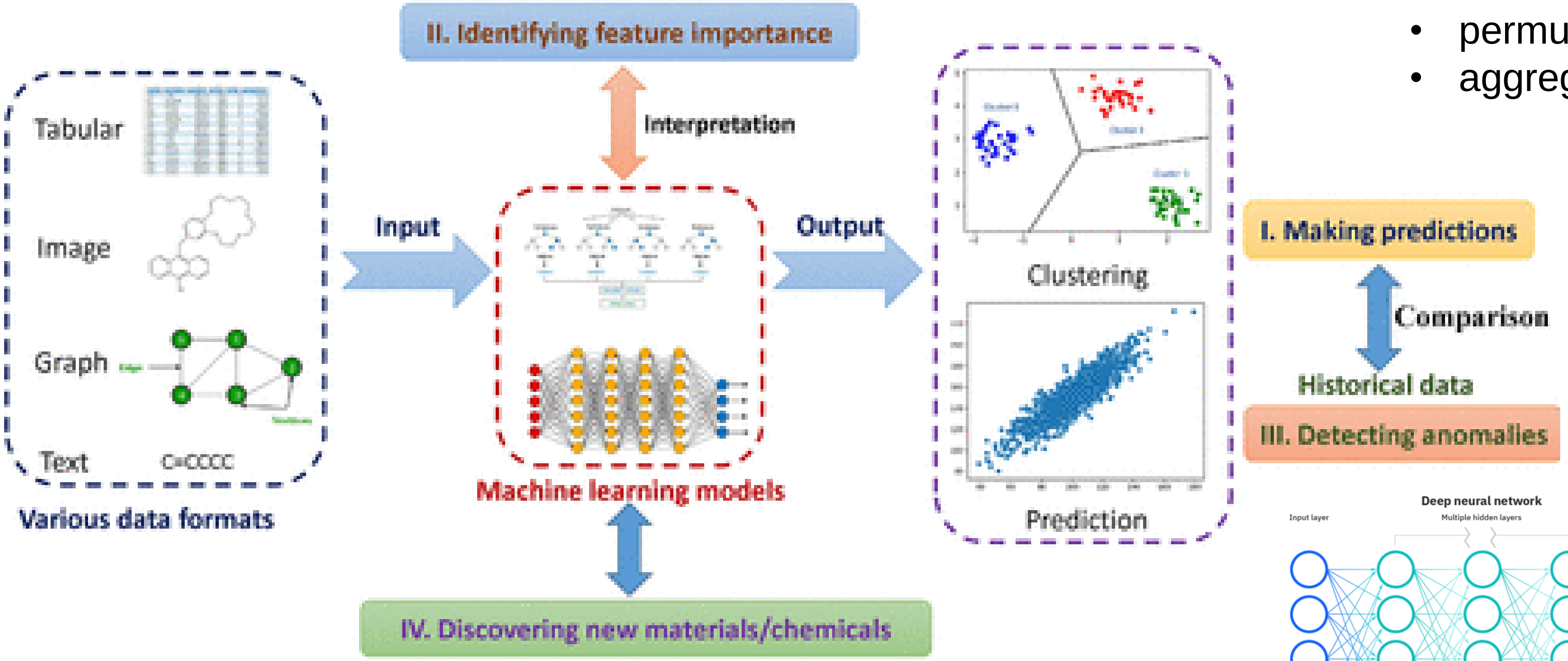


https://en.wikipedia.org/wiki/Euler_method

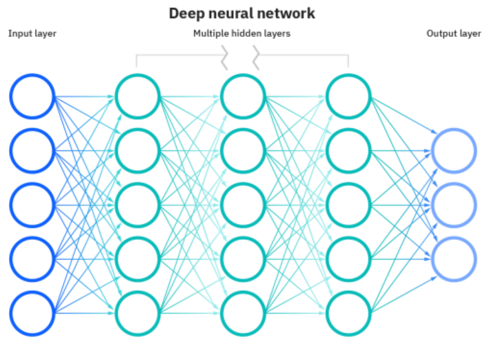
Statistical models

Data preparation:

- cleaning
- curation
- permutation
- aggregation



Zhong et al., *ES&T*, 2021



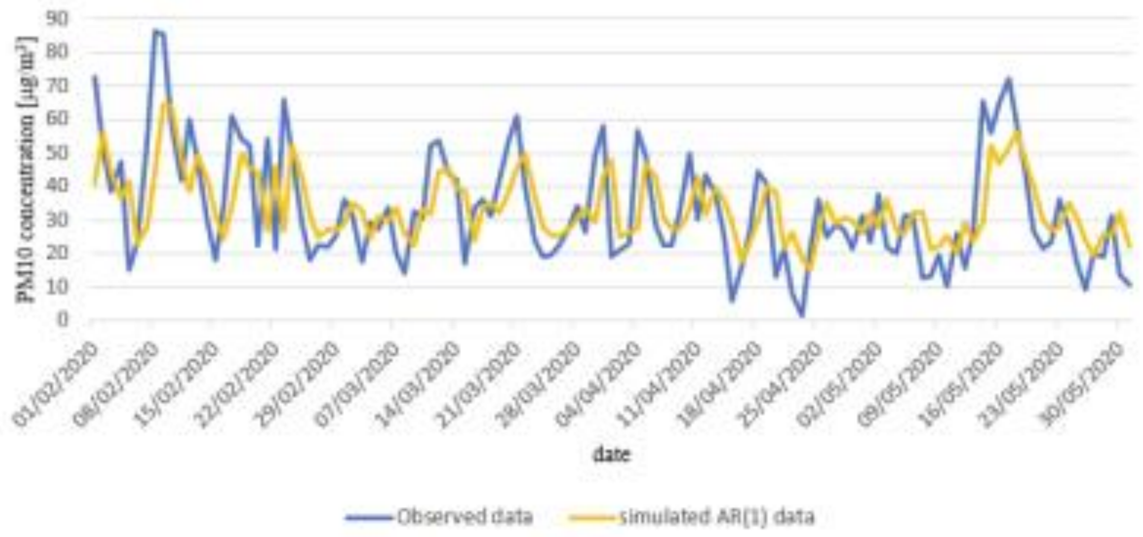
$$\sum_{i=1}^{m} w_i x_i + bias = w_1 x_1 + w_2 x_2 + w_3 x_3 + bias$$

$$\text{output} = f(x) = \begin{cases} 1 \text{ if } \sum w_1 x_1 + b \geq 0 \\ 0 \text{ if } \sum w_1 x_1 + b < 0 \end{cases}$$

https://www.ibm.com/cloud/learn/neural-networks

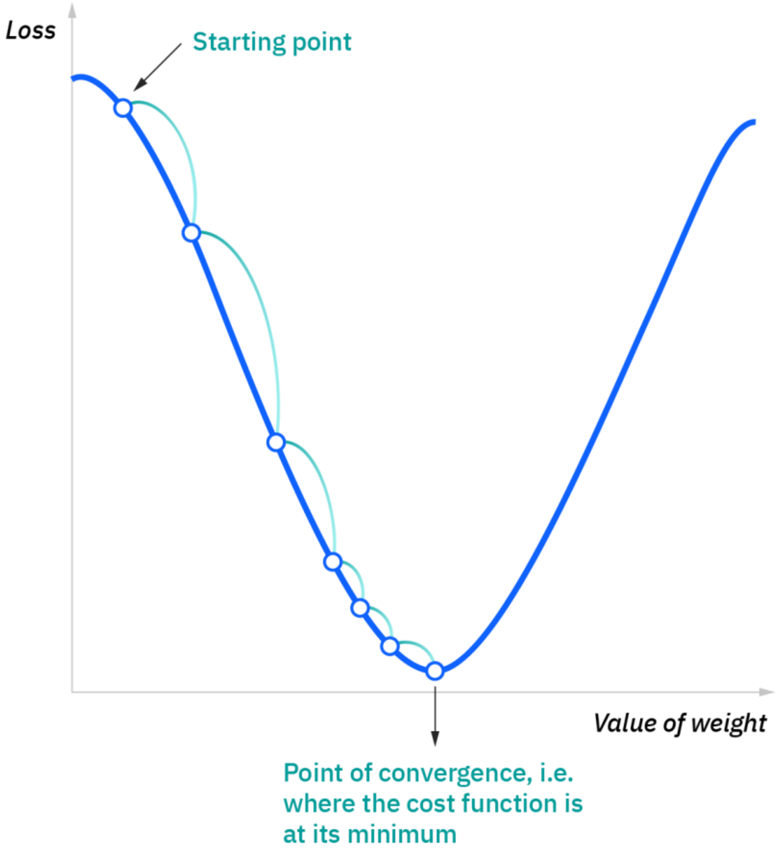
Statistical time series forecasting

$$X_t = \varphi_0 + \varphi_1 X_{t-1} + \ldots + \varphi_p X_{t-p} + \varepsilon_t - \theta_1 \varepsilon_{t-1} - \ldots - \theta_q \varepsilon_{t-q}$$



Mancini et al., *J. Phys.: Conf. Ser.,* 2022

Parameter estimation

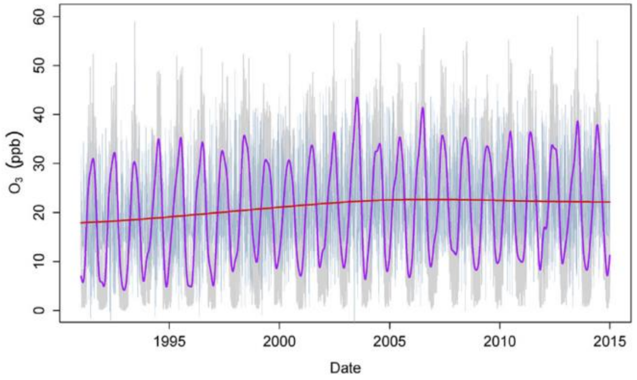


https://www.ibm.com/cloud/learn/gradient-descent

Atmos. Chem. Phys., 20, 9051–9066, 2020
https://doi.org/10.5194/acp-20-9051-2020

Atmospheric Chemistry and Physics

$$y(t) = LT(t) + S(t) + W(t) + E(t)$$



Temporal and spatial analysis of ozone concentrations in Europe based on timescale decomposition and a multi-clustering approach

Eirini Boleti[1,2], Christoph Hueglin[1], Stuart K. Grange[1,4], André S. H. Prévôt[3], and Satoshi Takahama[2]

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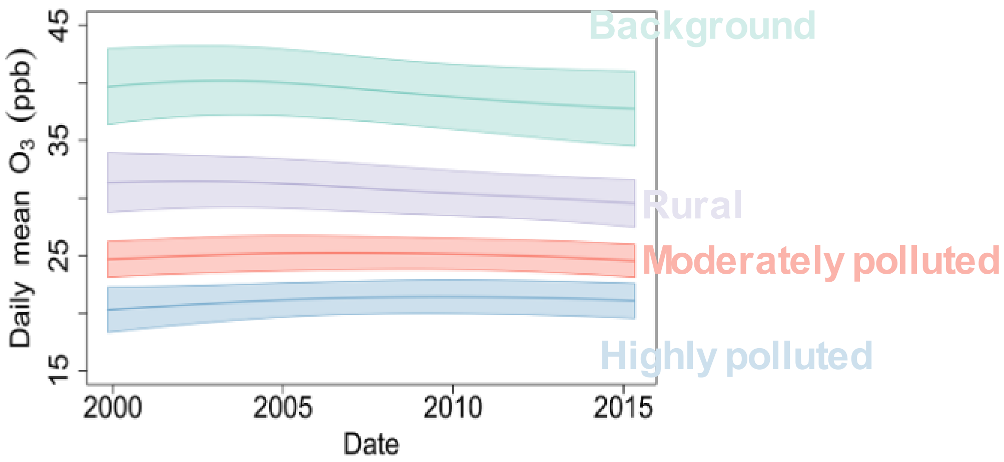
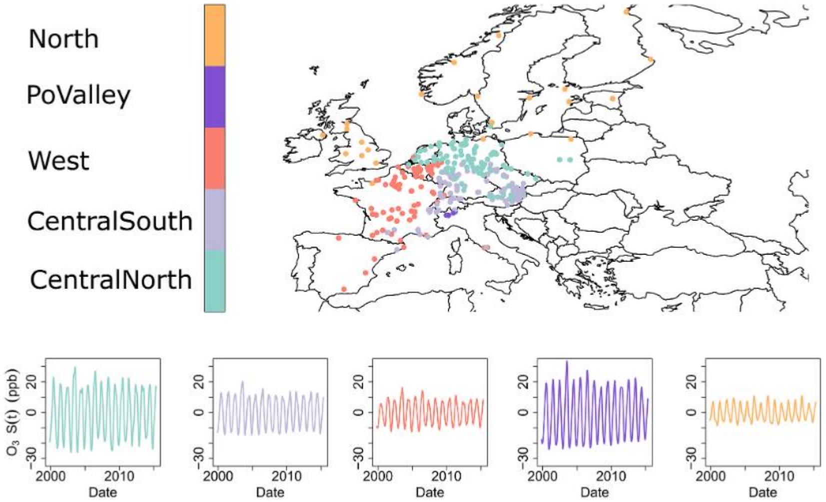




nature COMMUNICATIONS

ARTICLE

Check for updates

https://doi.org/10.1038/s41467-021-27484-1 OPEN

Secondary organic aerosol association with cardiorespiratory disease mortality in the United States

Havala O. T. Pye [1✉], Cavin K. Ward-Caviness [2], Ben N. Murphy [1], K. Wyat Appel[1] & Karl M. Seltzer [3]

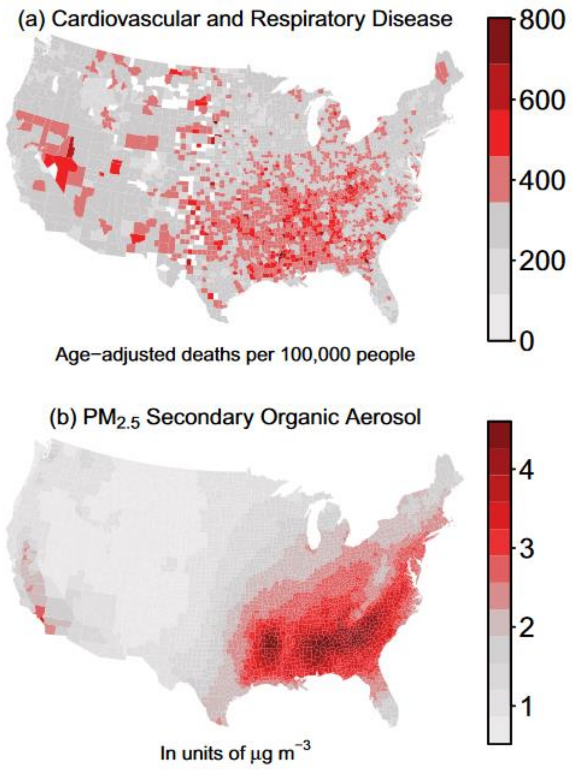
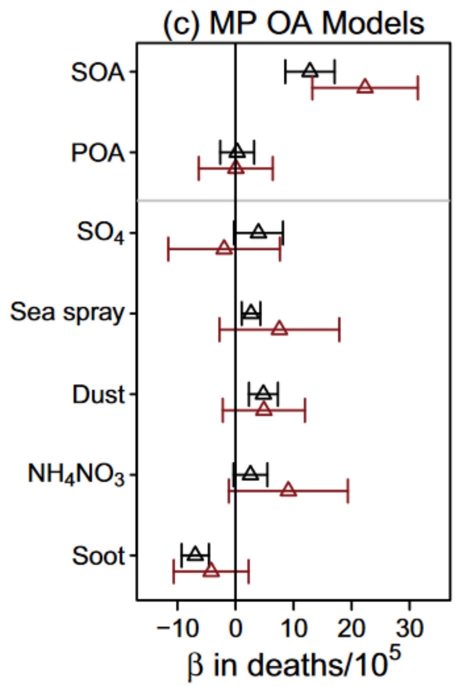
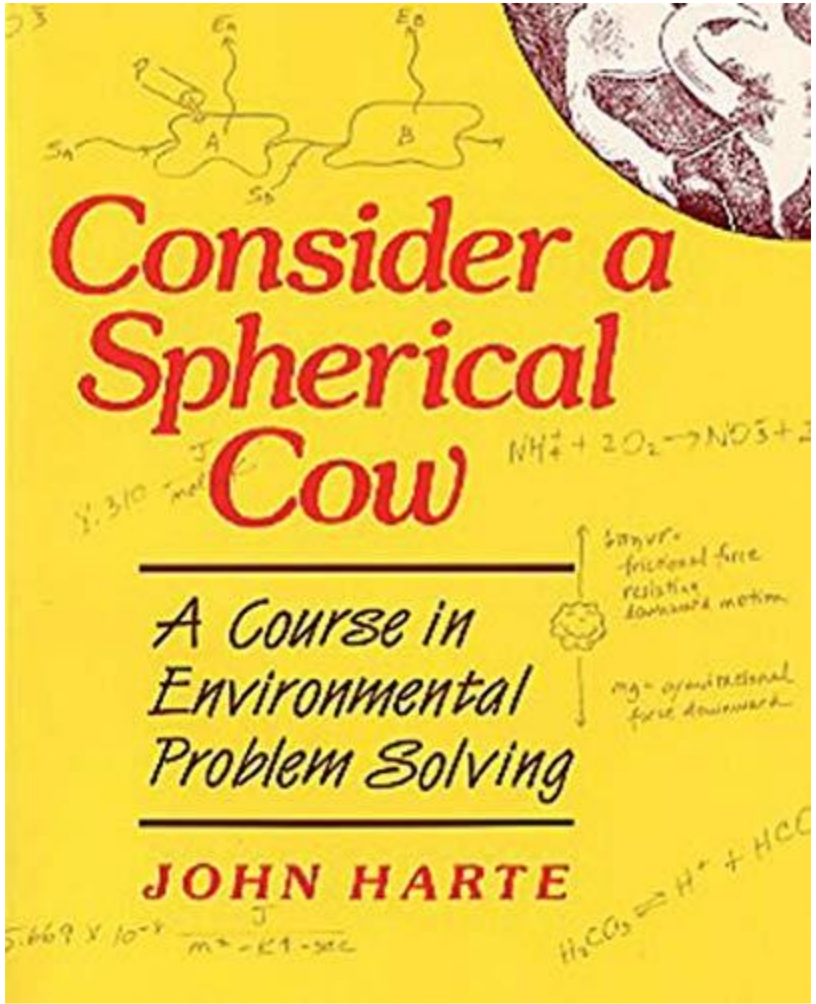


Fig. 1 Cardiorespiratory disease mortality rates and secondary organic aerosol concentrations. County-level, year 2016 (**a**) cardiovascular and respiratory disease age-adjusted death rates (per 100,000 in population) are from CDC and (**b**) $PM_{2.5}$ secondary organic aerosol concentrations are predicted by CMAQ. White in (**a**) indicates no death rate data while light gray indicates low reported rates.

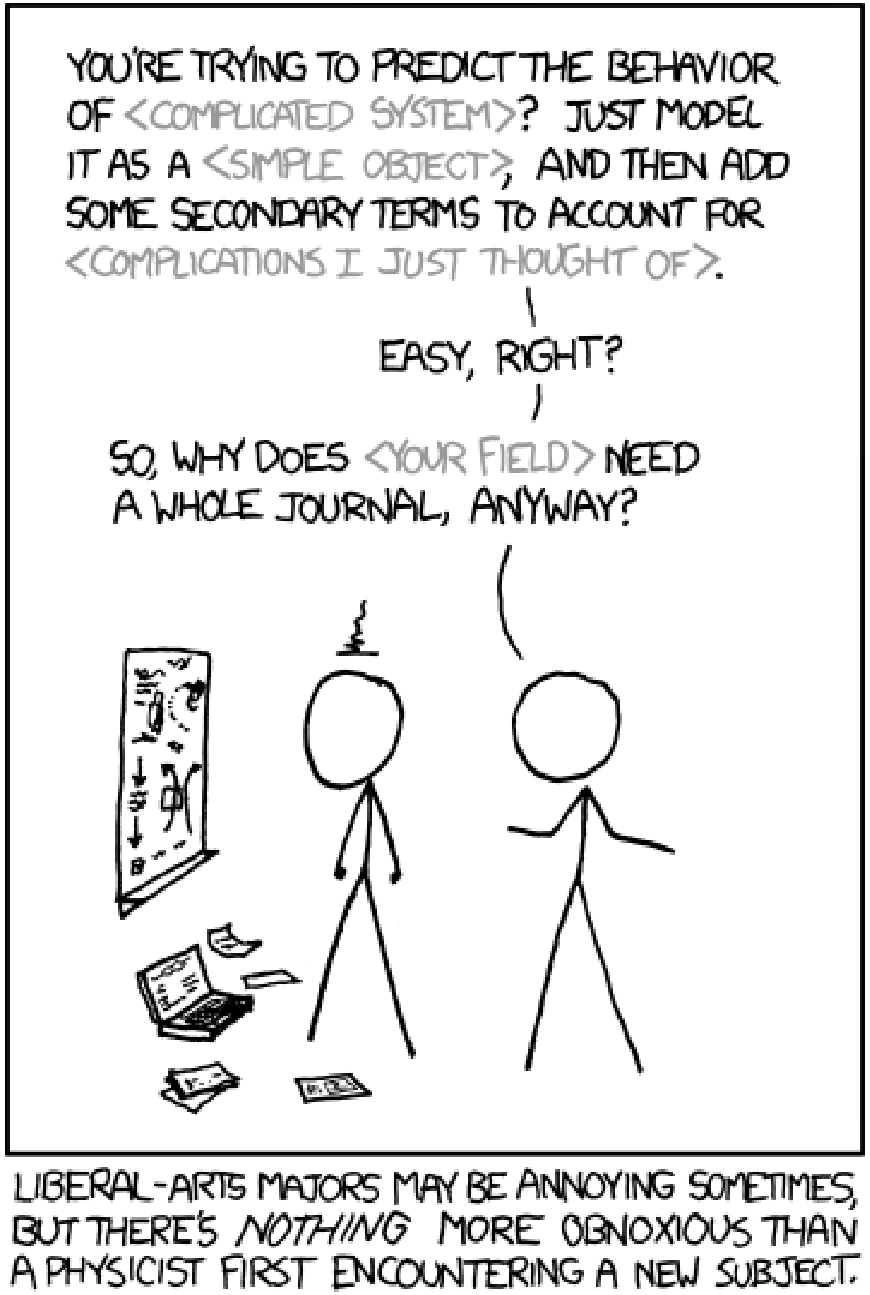
$$D = \beta_0 + \{\beta_1 PM_{SOA_{BVOC}} + \beta_2 PM_{SOA_{AVOC}} + \beta_3 PM_{POA}\} + \beta_4 PM_{Seaspray} + \beta_5 PM_{Soot} + \beta_6 PM_{NH_4NO_3} + \beta_7 PM_{SO_4} + \beta_8 PM_{Dust} + \sum_{j=1}^{N} \beta_j' C_j$$



The value of engineering approximations (and simple models)



https://en.wikipedia.org/wiki/Spherical_cow


YOU'RE TRYING TO PREDICT THE BEHAVIOR OF <COMPLICATED SYSTEM>? JUST MODEL IT AS A <SIMPLE OBJECT>, AND THEN ADD SOME SECONDARY TERMS TO ACCOUNT FOR <COMPLICATIONS I JUST THOUGHT OF>.
EASY, RIGHT?
SO, WHY DOES <YOUR FIELD> NEED A WHOLE JOURNAL, ANYWAY?
LIBERAL-ARTS MAJORS MAY BE ANNOYING SOMETIMES, BUT THERE'S *NOTHING* MORE OBNOXIOUS THAN A PHYSICIST FIRST ENCOUNTERING A NEW SUBJECT.

Source: XKCD

Project ideas

You can propose a project based on your own interests

Past project ideas: https://sieprog.ch/#projet

Some ideas (should be approx. 1/2 semester – make simplifications if necessary)
https://ch.mathworks.com/academia/students/project-ideas.html

Preparing the project proposal

- Is my topic okay? ***Yes***
- You can change everything about your project once you start; only need to document reasons for change in the beginning of your report.
- The question/problem does not need to be novel, but the code should not already be readily available.
- How much data do I need?
  - depends on your project
  - for data-driven modeling, you need data
  - for a simulation-based study, it is not necessary to validate against real data sets but justify that the range of input and output values are physically plausible

User interfaces to models

- Graphical user interfaces and command-line interfaces will not be part of the project assessment.

- The model you build will not be used by your stakeholder – you must be the user of the model to demonstrate its value in answering a question you propose.

- If you build a “general model”, demonstrate its use for several case studies that you choose and report the significance of your findings.

Preparing the final report and code repository

Report

- Include deviations from project proposal
- Motivate the problem (don’t refer to project proposal) and results

Approach

- *Report*: describe the model (some notion of model classification) and solution (numerical) approach but not the coding implementation
- *Code repository*: describe the coding implementation

Reproducibility

- Code should be documented + automated, and reproduce the figures / tables / calculations in your report

Citations

- Include proper attribution of others’ work, including any images, ideas