How to be skeptical of computer simulations

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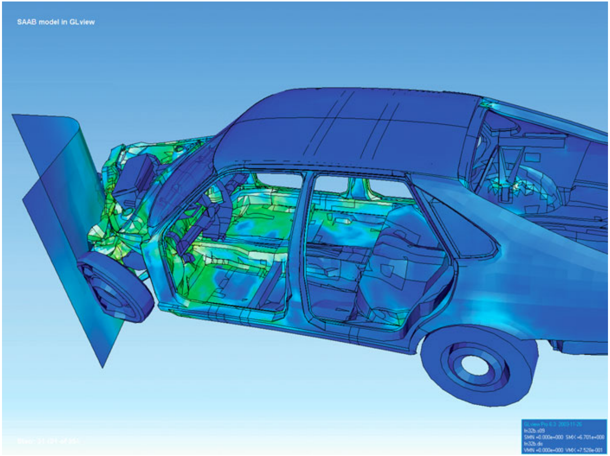
Skepticamp DC 2012

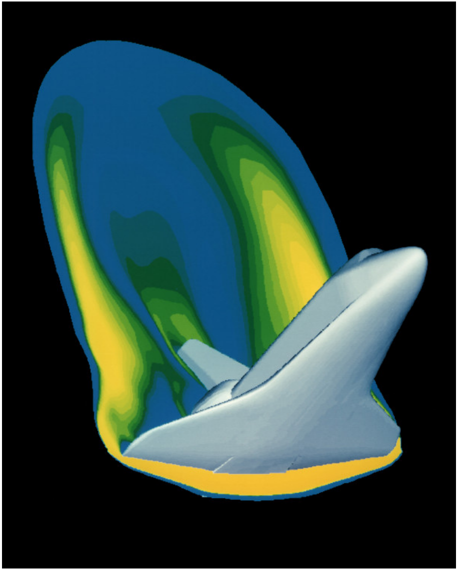
Categories of simulations

- physical systems
  - weather
  - climate
  - flow around planes, cars, etc.
  - combustion
  - material deformation
  - etc.
- economic
  - derivatives
- psychological
  - traffic
  - evacuation



https://en.wikipedia.org/wiki/File:FAE_visualization.jpg

Another example



http://www.nasa.gov/multimedia/imagegallery/image_feature_431.html

Why simulate anything?

If simulations are potentially untrustworthy, can't we avoid this problem by testing or checking everything? Not always.

- You can't test or check everything.
  - fire safety of building — too expensive to build tons of houses just to burn them down
  - aerodynamics — tweaking the model airplane to test different configurations often is too slow
  - future or past climate — no time machines
- The test only occurs when you need the knowledge.
  - weather
- It's illegal.
  - nukes

Sleipner A offshore platform

underprediction of stress by 47% in the concrete lead to

- the sinking of part of the base of the offshore platform and...
- a crash registering at 3.0 on the Richter scale and...
- $700 million in losses for the company.
- Thankfully no one was hurt or killed.

http://ta.twi.tudelft.nl/users/vuik/wi211/disasters.html

Commonly heard quote about simulations

> *Everyone believes the experiment except the person who did it. No one believes the simulation except the person who did it.*

a similar quote with "simulation" replaced by "theory" was attributed to Albert Einstein.

`http://www.aphids.com/cgi-bin/quotes.pl?act=ShowListingsForSub&Subject=S33`

Basic skepticism: no special knowledge needed

Basic skepticism: garbage in, garbage out[1]

- All input data must be sourced, preferably with known uncertainty (and units).
- This data should be checked:
  - Does the source have the same value?
  - Does the source cite another source? (You might have to go down the rabbit hole.)
  - Does the value make sense?

[1] Usually. You can get the right answer *by coincidence*. Getting a plausible result is no guarantee that the input data is good.

Basic skepticism: assumptions

- Sometimes certain physics are ignored or changed.
  - The phenomena is demonstrably unimportant.
  - "It's what I was taught." (e.g., linearization)
  - Laziness.
  - "Ignoring it is a model."

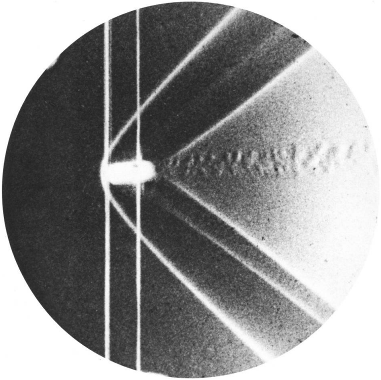
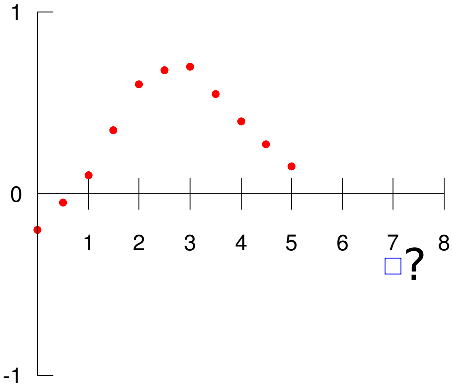


Photo by Ernst Mach.

Basic skepticism: extrapolation

- Imagine this plot shows temperature at different times. Can you estimate where the temperature is going next?



https://en.wikipedia.org/wiki/File:Extrapolation_example.svg

Basic skepticism is not enough

- Questioning assumptions, justifications, and input data in a physically based model is not enough!
- *Even if* a simulator has perfect assumptions a poorly designed or poorly implemented simulator *can produce garbage results*.
- Even technical people are not immune. Most of them are unaware of what I will discuss today.
- Simulations are not a "black box". They are not magic. They do have problems people should be aware of. If you don't understand the basics of what's going on inside then you are not qualified to analyze their results (in my opinion).

How computer simulations work
and how to question their results

Necessary approximations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

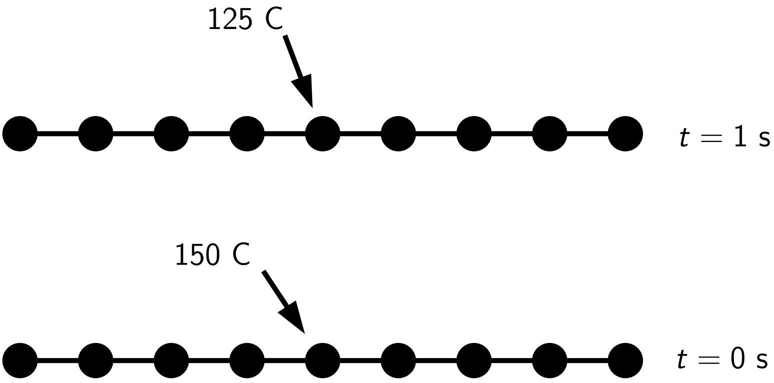
$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_i}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\mu\frac{\partial u_i}{\partial x_i}\right]$$

$$\frac{\partial \rho \phi_k}{\partial t} + \frac{\partial \rho u_i \phi_k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho\alpha_k\frac{\partial \phi_k}{\partial x_i}\right)$$

- Computers can't really do anything we can't, so if we can't solve these equations, computers probably can't either. But we can change this from an exact calculus to an *approximate* algebra problem that computers solve much faster than we do.
- The approximation introduces an error. The accuracy is usually specified with the "order" of the method, e.g., a *1st-order* error. Higher is (usually) better.

How many physical simulations work: grids

In most physical simulations, everything is on a grid in some way, whether through "time-stepping", space gridding, or both. Reality is *continuous*. The simulation is *discrete*.



The finer (smaller) the grid, *usually* (hopefully!) the more accurate the simulation.

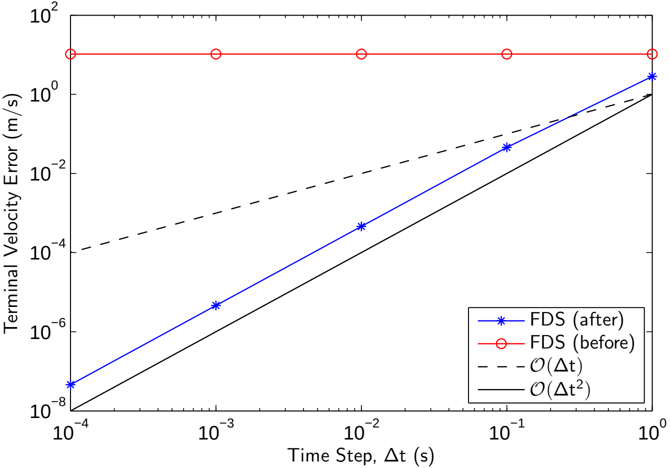
Bugs in the code

- Who writes bug-free code? (No one best I can tell.)
- In 2009, the Climatic Research Unit at the University of East Anglia was hacked. Many emails and documents in the back described bugs in the code, e.g.:
  - "Yup, my awful programming strikes again"
- Climate change "skeptics" railed about how CRU scientists were terrible programmers, but they didn't realize the full extent of the problem: *few scientific and engineering programmers follow best practices*.
- What can we do to eliminate bugs and otherwise test simulations?

`http://www.nature.com/news/2010/101013/full/467775a.html`

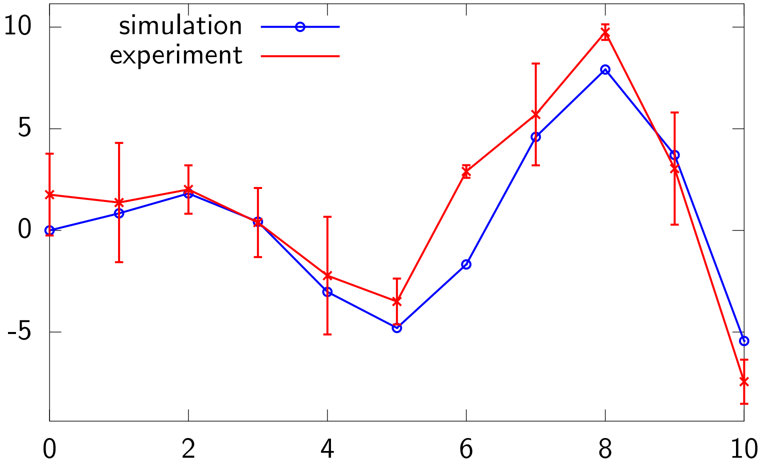
Verification

- verification — checking the math — comparing exactly known results against the simulation



Validation

- validation — checking the model — comparing experiments against the simulation



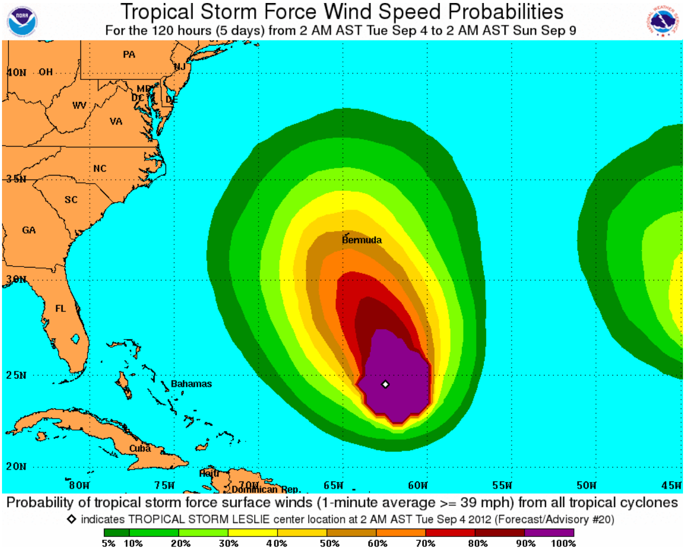
Unfortunately...

Passing verification and validation tests are necessary for a simulation to be correct, but *not sufficient*.

Testing every part of the simulation often is difficult if it's even possible.

Uncertainty quantification

- Can a simulation account for uncertainties in the inputs and the models and give you a range of possible results? **Yes**.



How could things go wrong?

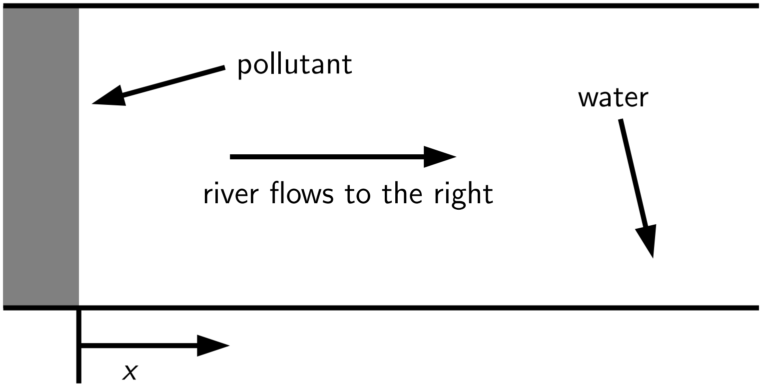
example: pollutants released in a river

https://commons.wikimedia.org/wiki/File:ColumbiarivergorgeJRH.jpg

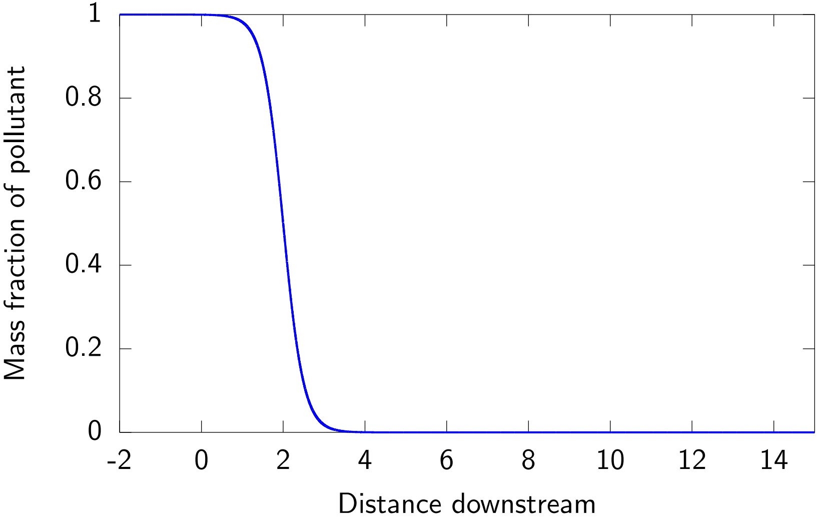
Modeling pollutants in a river

$$\frac{\partial Y}{\partial t} + v\frac{\partial Y}{\partial x} = 0$$

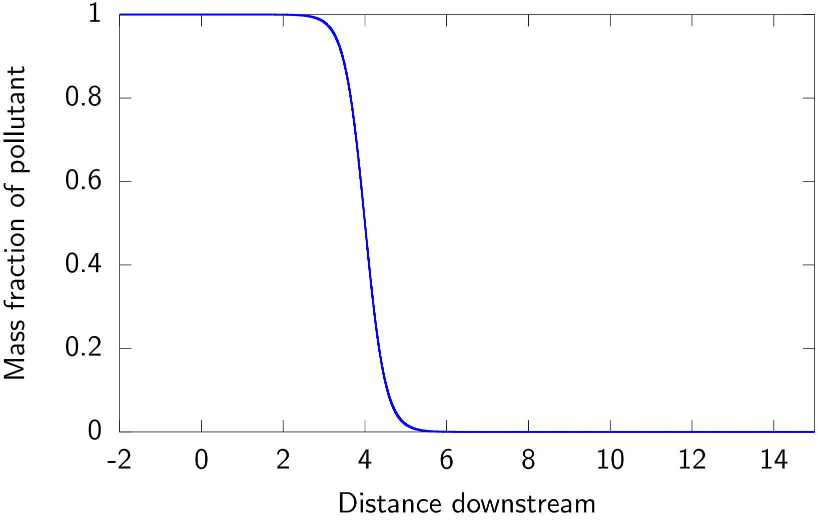
- Y — pollutant mass fraction
  - 1 if 100% pollutant, 0 if 0% pollutant (i.e., 100% water)



Exact solution



Exact solution



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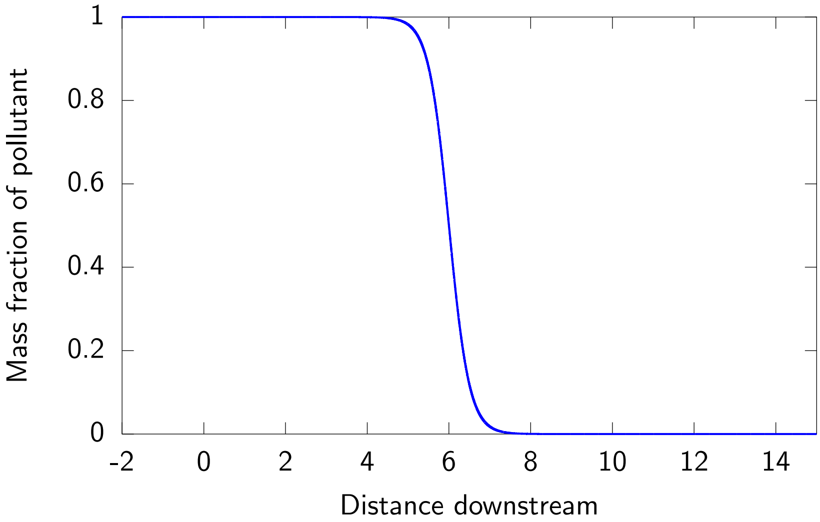

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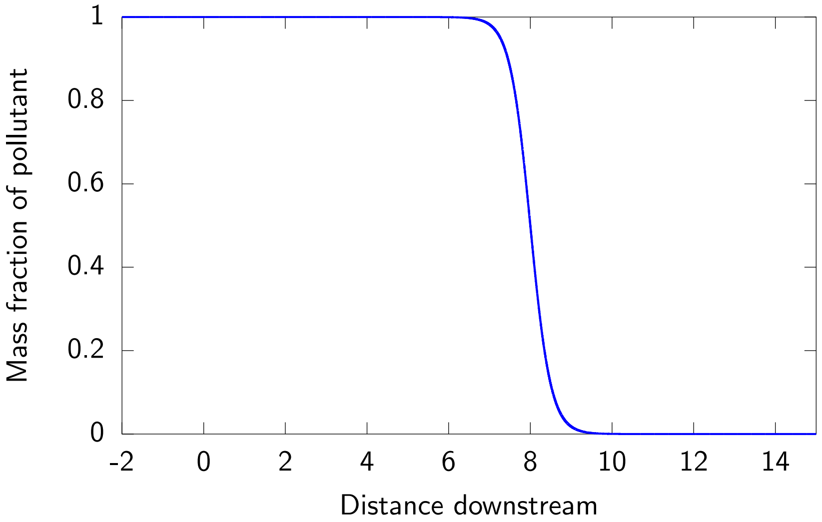
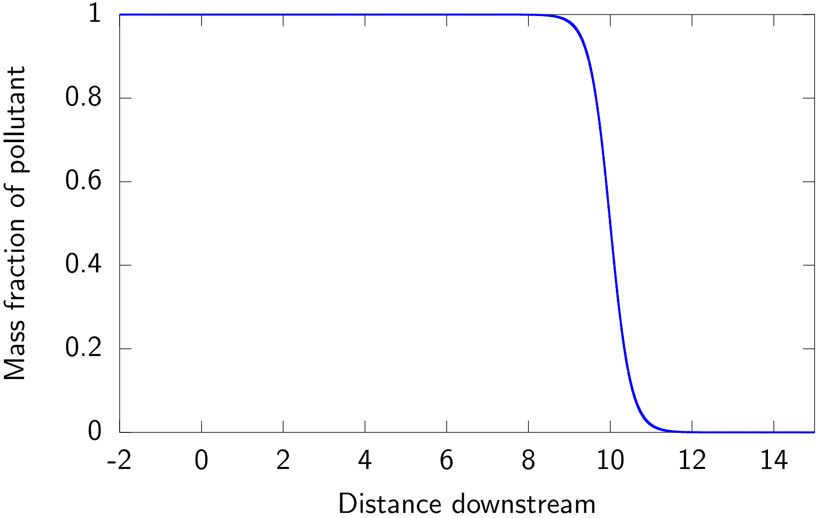
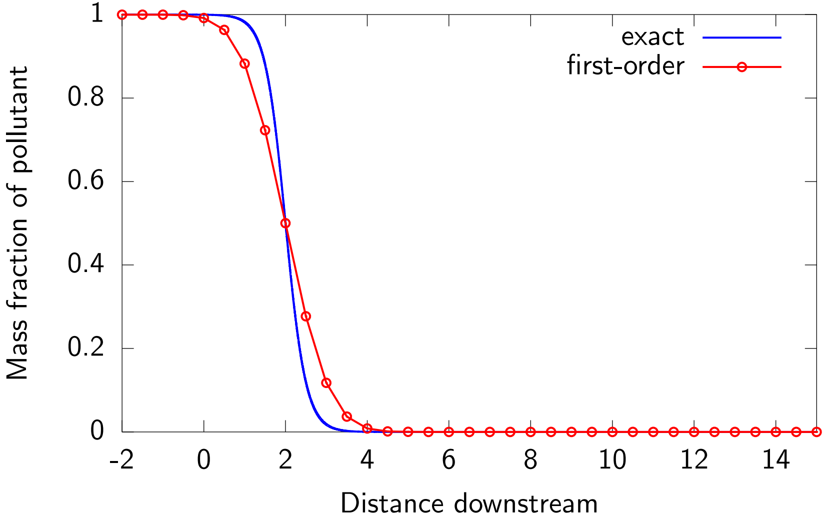


Exact solution

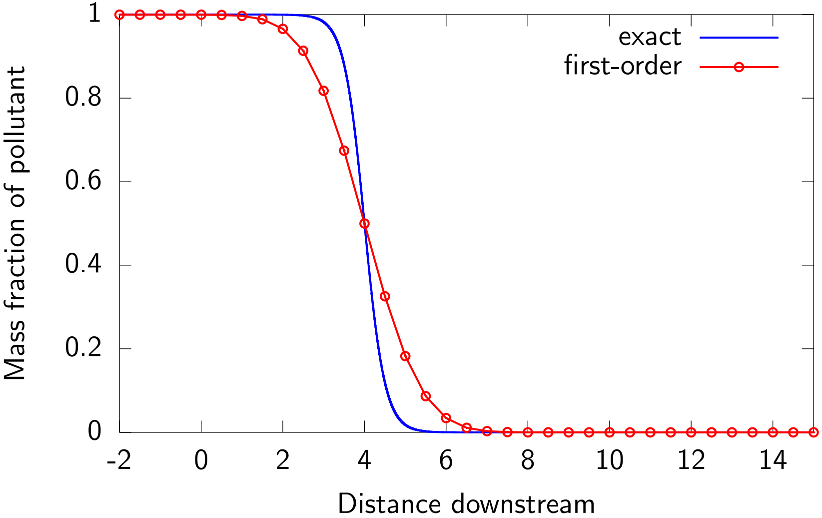


1^{st}-order numerical simulation

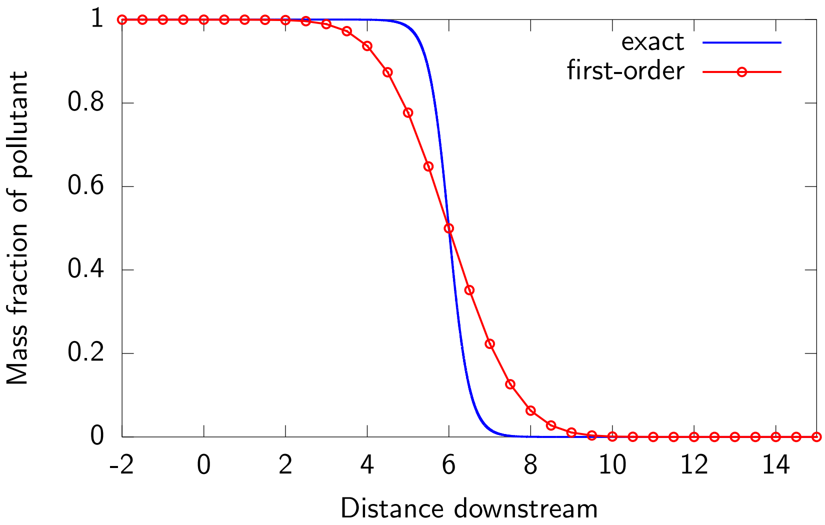
1^{st}-order solution



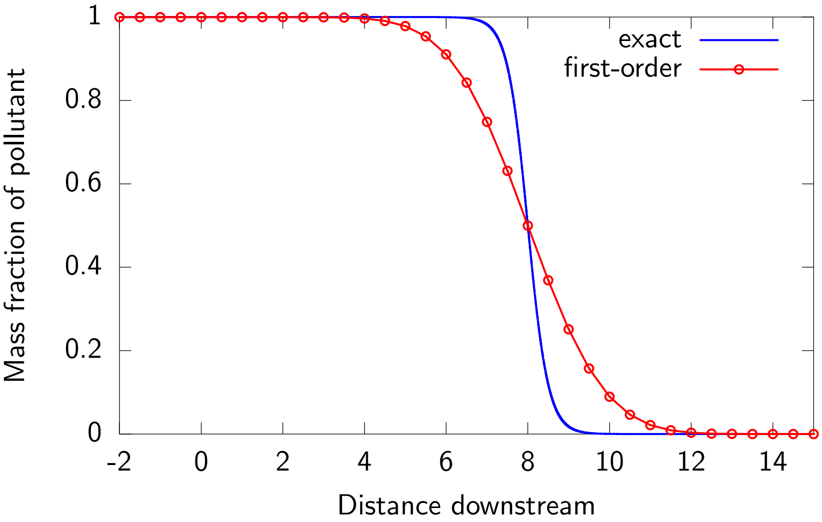
1^{st}-order solution



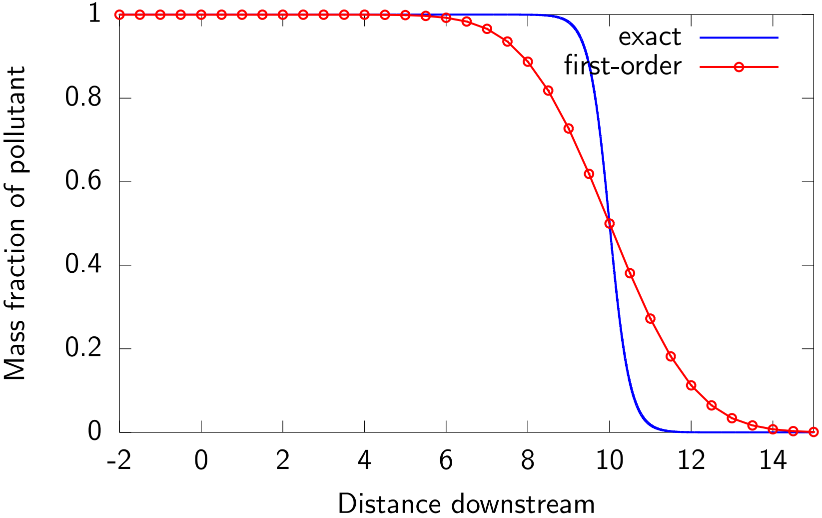
1^{st}-order solution



1^{st}-order solution



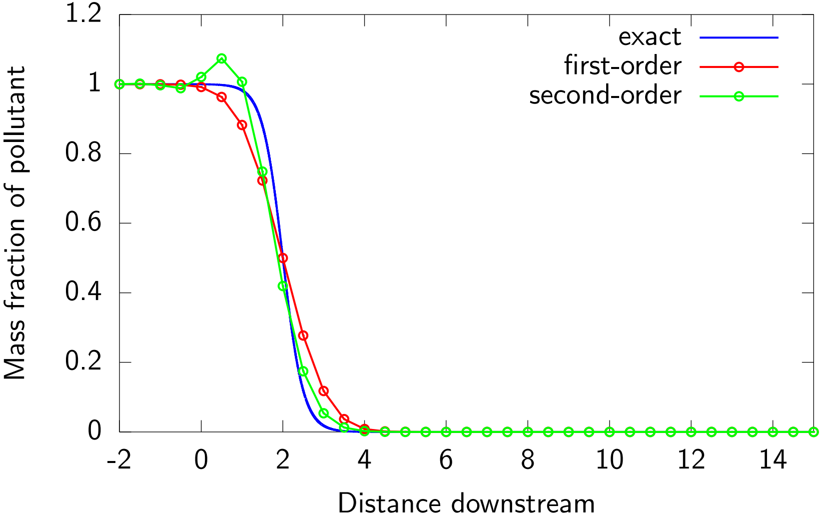
1^{st}-order solution



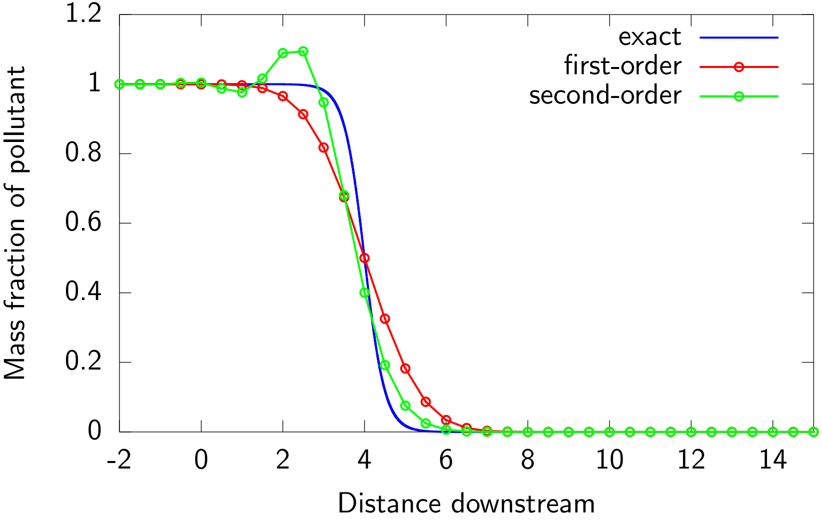
2^{nd}-order numerical simulation

Should be better?

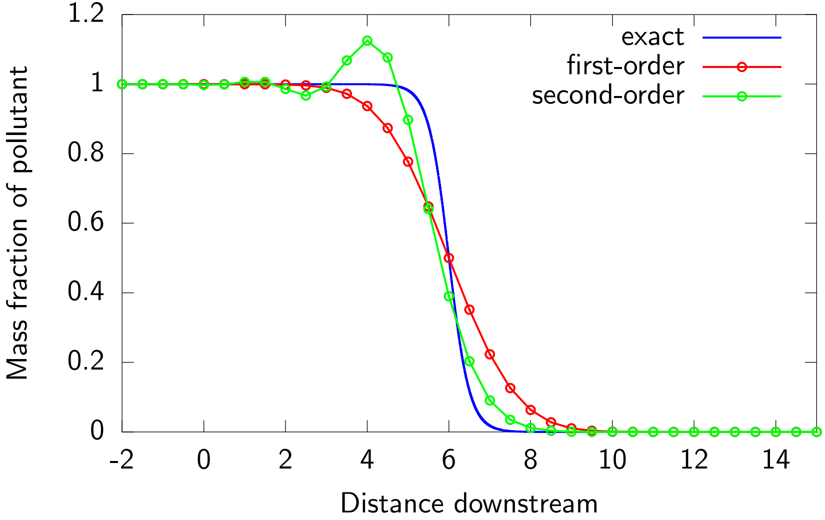
2^{nd}-order solution



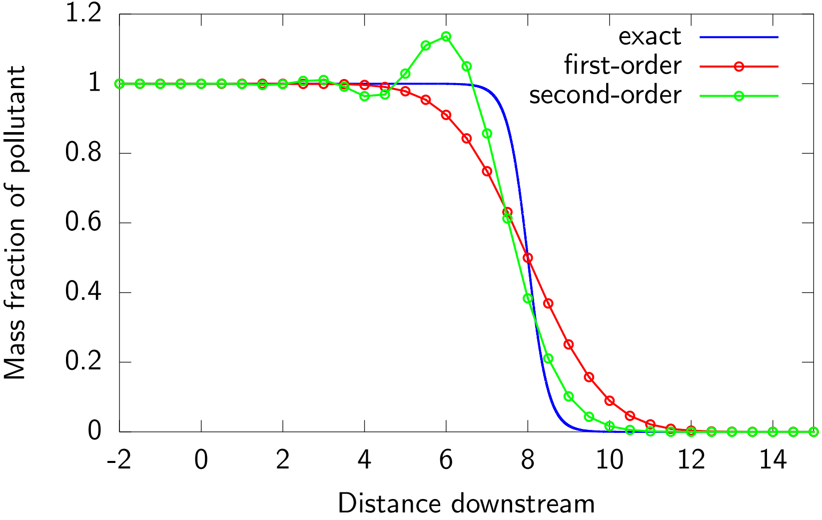
2nd-order solution



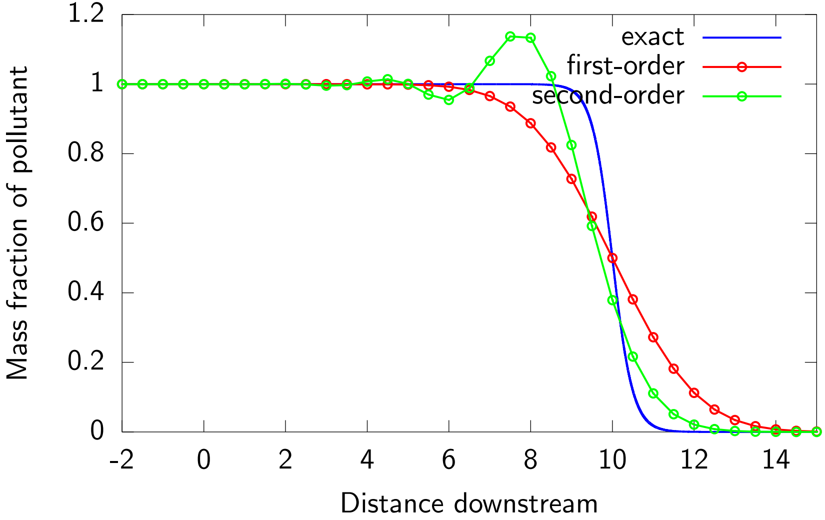
2nd-order solution



2^{nd}-order solution



1st-order solution



No silver bullet?

- Godunov's theorem — *linear* methods for PDEs that don't produce wiggles are at best 1^{st}-order accurate
- More advanced (non-linear) numerical methods have low dissipation and no (or less) wiggles, though they often require more computational cost and have other problems (e.g., create non-physical vorticity, a.k.a. fluid spinning).

Other potential problems with physically-based simulations

- Features of the physics are ignored:
  - energy conservation
  - shock wave propagation speed
  - physical bounds
- Unphysical (not real) oscillations
  - Non-monotone/TVD numerical schemes
  - "Stiff" equations
- Stability
- Grid convergence
- odd-even decoupling (a.k.a. "checkerboarding")
- tons more I forgot

Summary

To critically evaluate anything based on computer simulations (of physical phenomena):

- Question everything, especially data sources and assumptions. (Garbage in, garbage out.)
- Do some sanity checks. Can the simulation produce physically impossible results?
- Demand to see the results of verification and validation tests. Alternatively, do these tests yourself.
  - To any scientist or engineer who questions why you want to test "basic" things like this, ask in return what they are afraid of!
- Recognize that simulations are not magic. Even if the user of a simulation did everything right, the result still could be garbage. Simulations have tons of their own problems that the trained eye can recognize.
- Quantifying the uncertainty in a simulation result is intellectually honest and should be encouraged.

Thank you.

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