Simulation in hands-on science

Current trends and conjectures on the future

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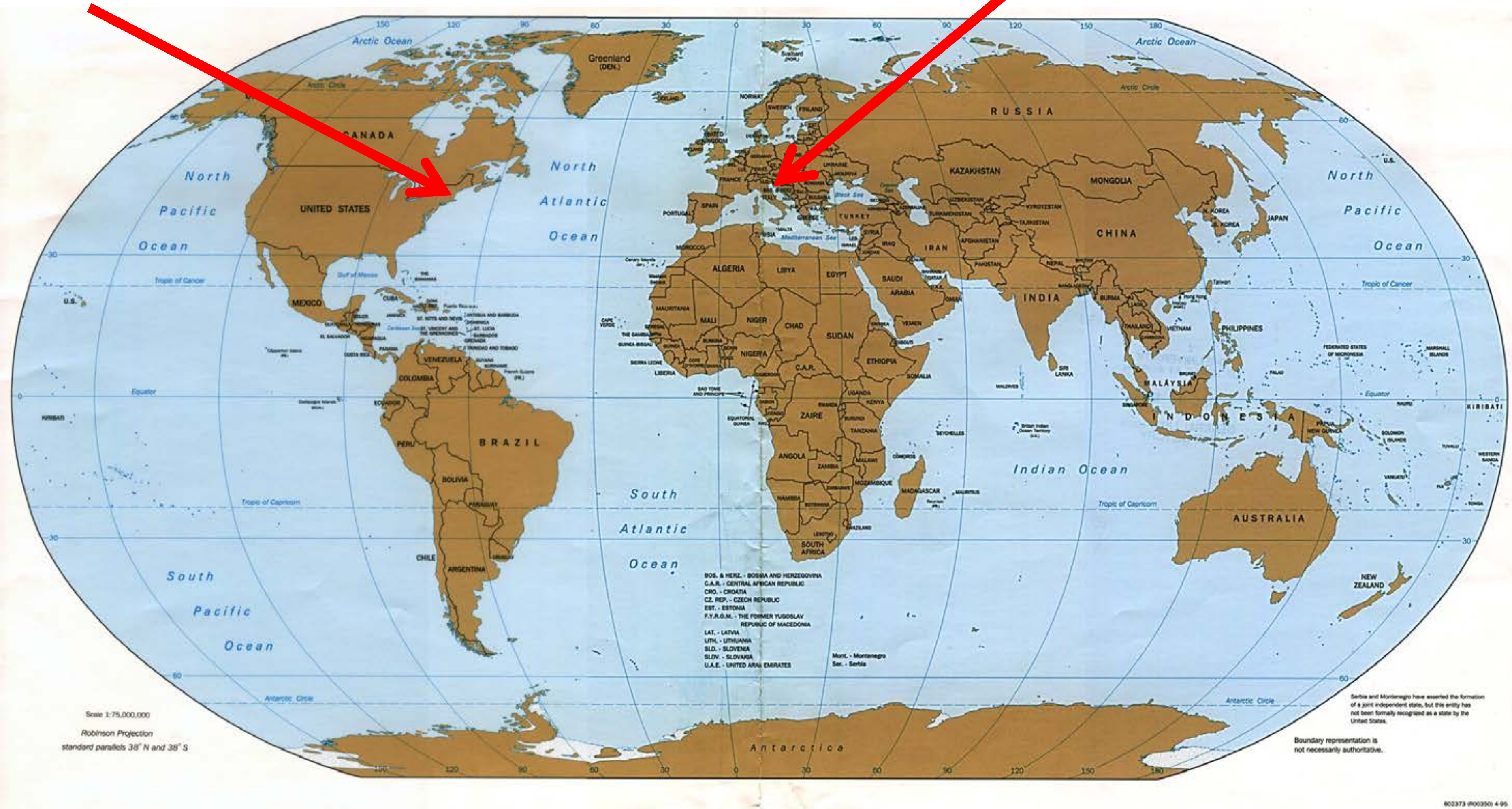
Olin College

Where am I from?

Suburban Boston (42.4°)

Trieste (45.6°)



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Fluid dynamics

Leonardo Da Vinci

Simulation

Big science

Tianhe - China
Power- 18 MW
Speed – 33 petaflops
Cores- 3 Million +
Many people to maintain
$ 4×10^8 USD

Hands-on science

Deterministic Nonperiodic Flow[1]

EDWARD N. LORENZ

Massachusetts Institute of Technology

(Manuscript received 18 November 1962, in revised form 7 January 1963)

ABSTRACT

Finite systems of deterministic ordinary nonlinear differential equations may be designed to represent forced dissipative hydrodynamic flow. Solutions of these equations can be identified with trajectories in phase space. For those systems with bounded solutions, it is found that nonperiodic solutions are ordinarily unstable with respect to small modifications, so that slightly differing initial states can evolve into considerably different states. Systems with bounded solutions are shown to possess bounded numerical solutions.

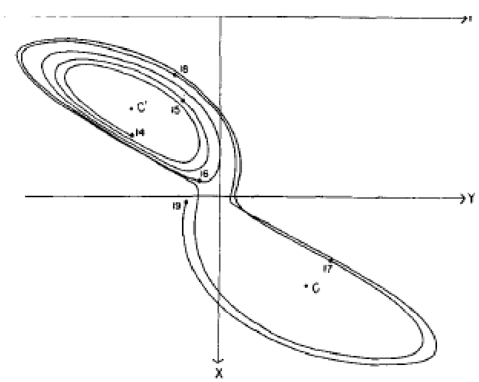
A simple system representing cellular convection is solved numerically. All of the solutions are found to be unstable, and almost all of them are nonperiodic.

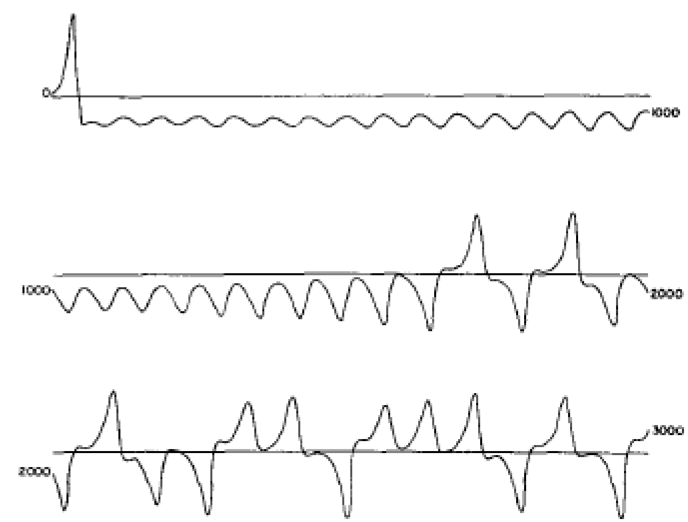
The feasibility of very-long-range weather prediction is examined in the light of these results.

$$\dot{X} = -\sigma X + \sigma Y,$$

$$\dot{Y} = -XZ + rX - Y,$$

$$\dot{Z} = XY - bZ.$$





Web of science: ~5000 citations

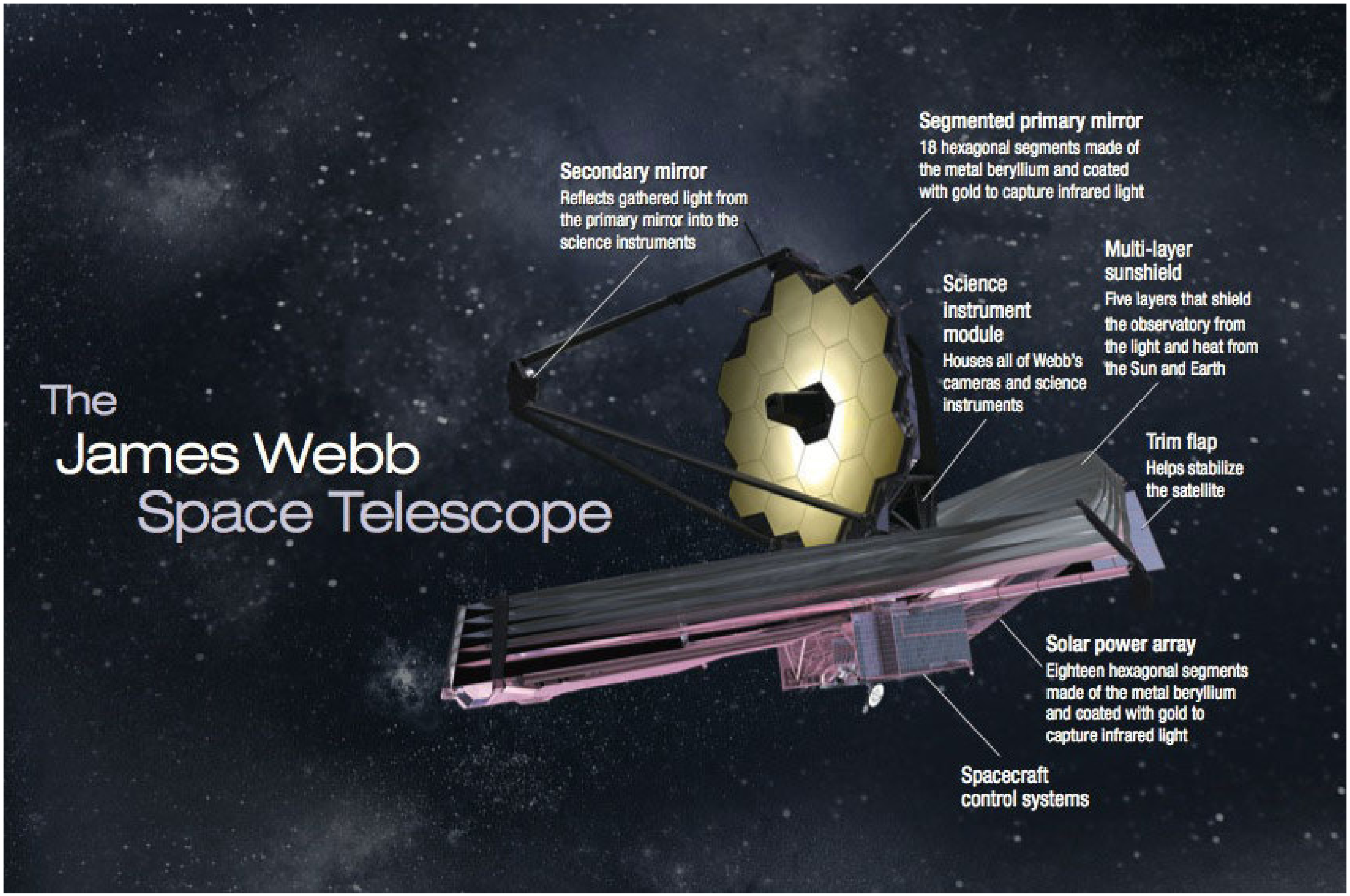
1963 – Royal McBee

Memory Size:	4096 word
Speed:	access times between two adjacent addresses 2.340 ms.
Clock Rate:	120 kHz
Power:	1500 watts
Technology:	113 vacuum tubes and 1350 diodes.
First Delivery:	September, 1956
Num. Produced;	~500
Price:	$47,000 (~$400,000 in today’s US dollars)
Weight:	740 pounds

Source: wikipedia

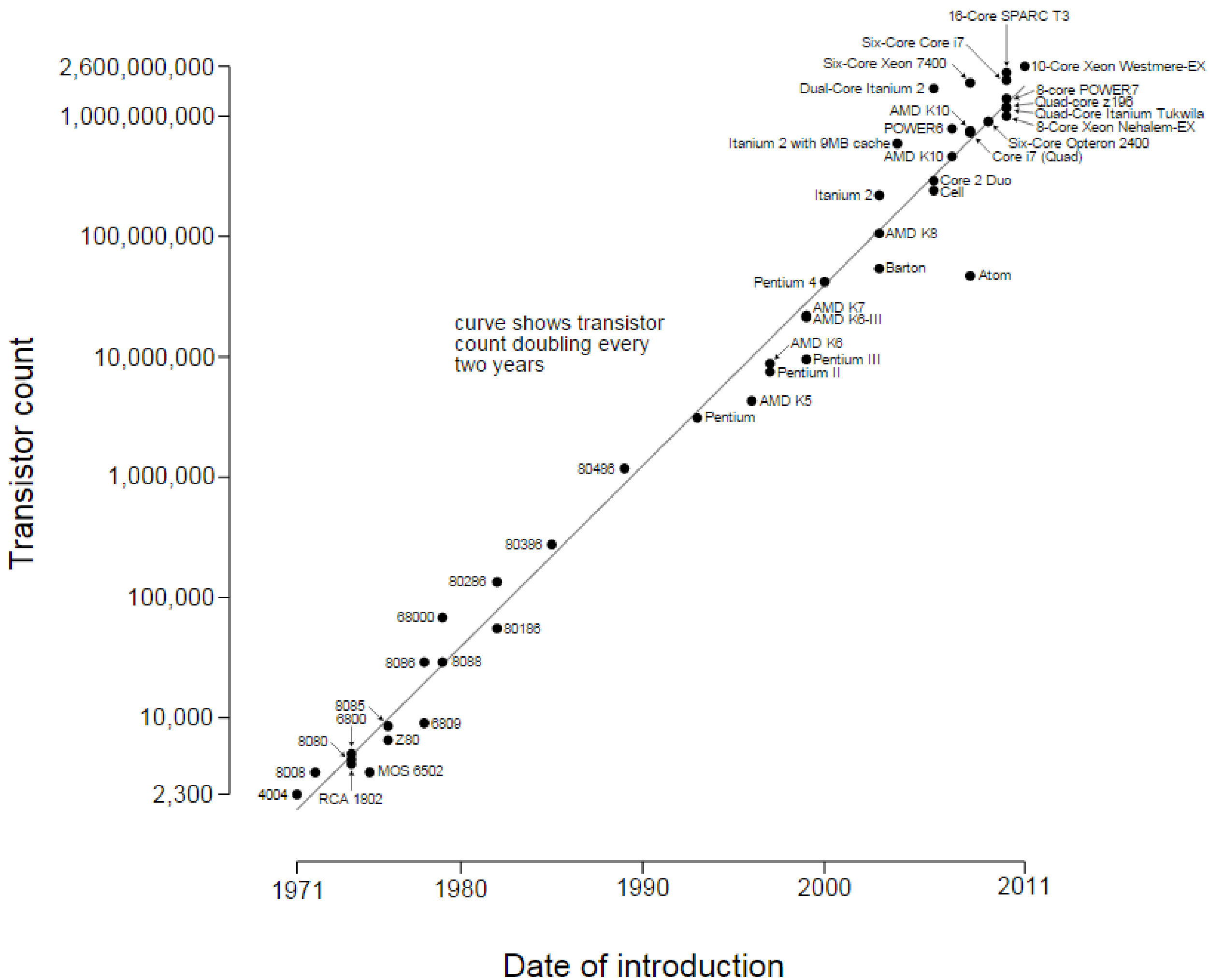
Scaling laws in simulation are different

Big physical things will always cost money

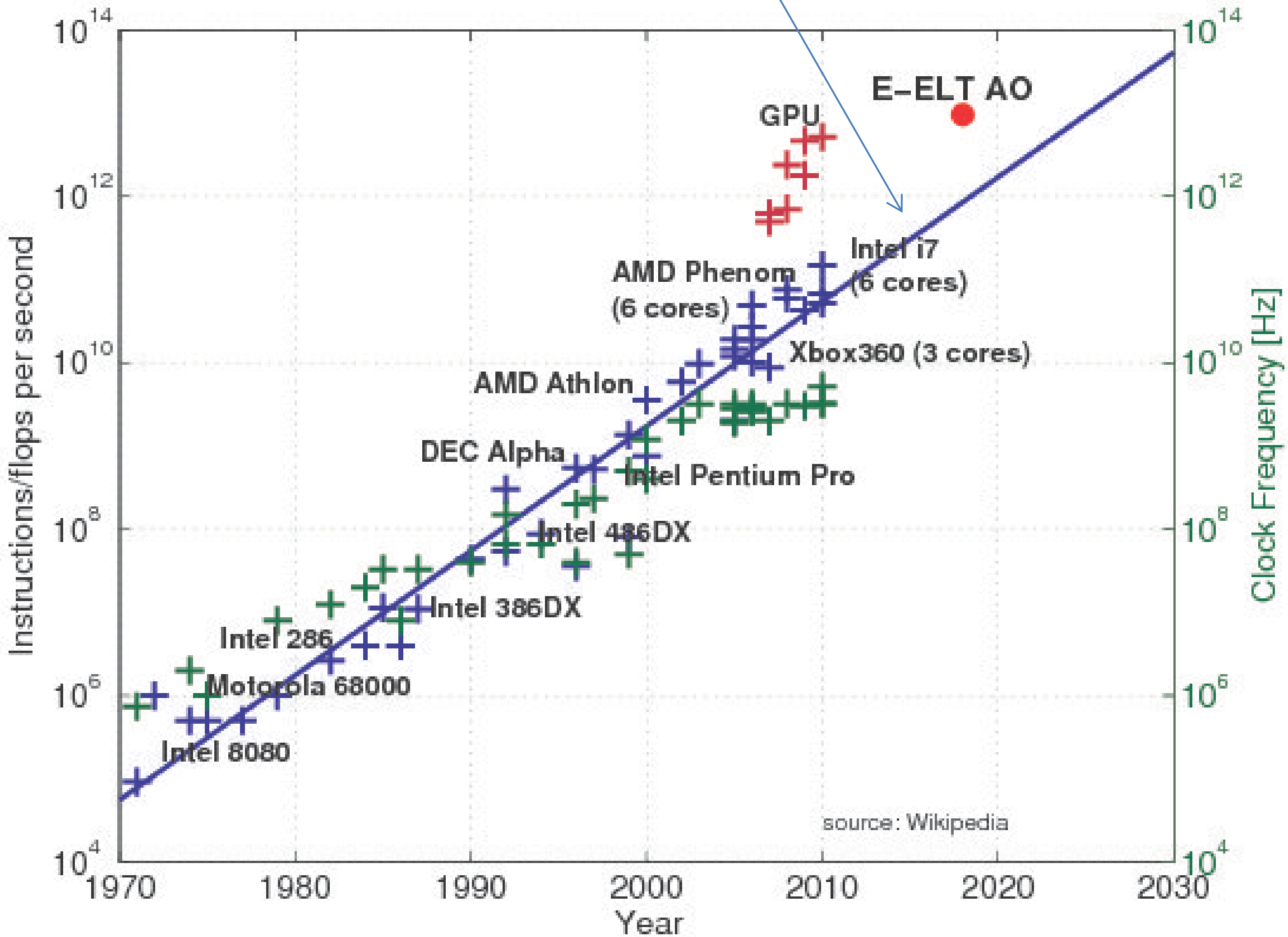


Moore's Law:

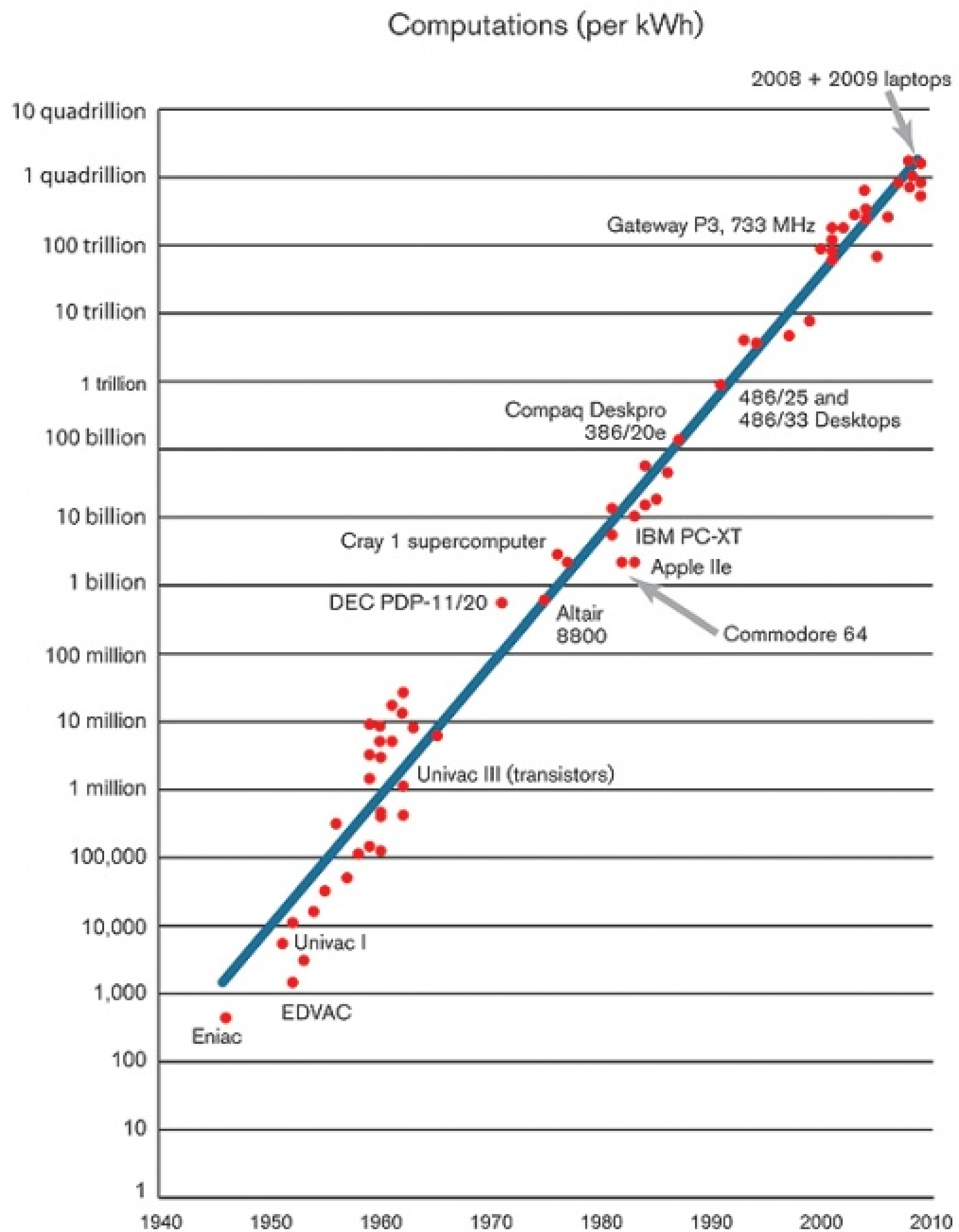
of transistors doubles every year (or two)



Today ~0.5 TFLOPS

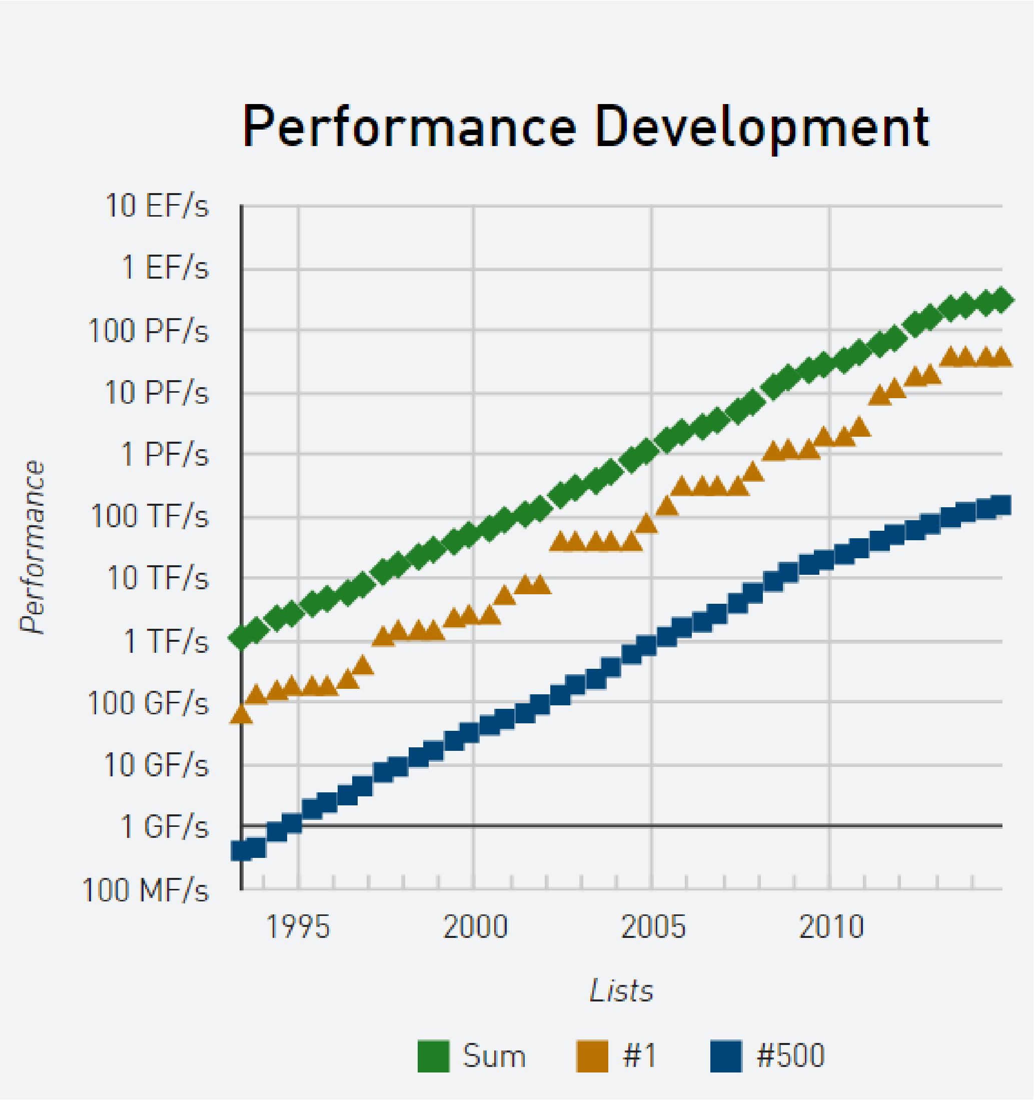


~100x in 10 years.



~100 x per decade

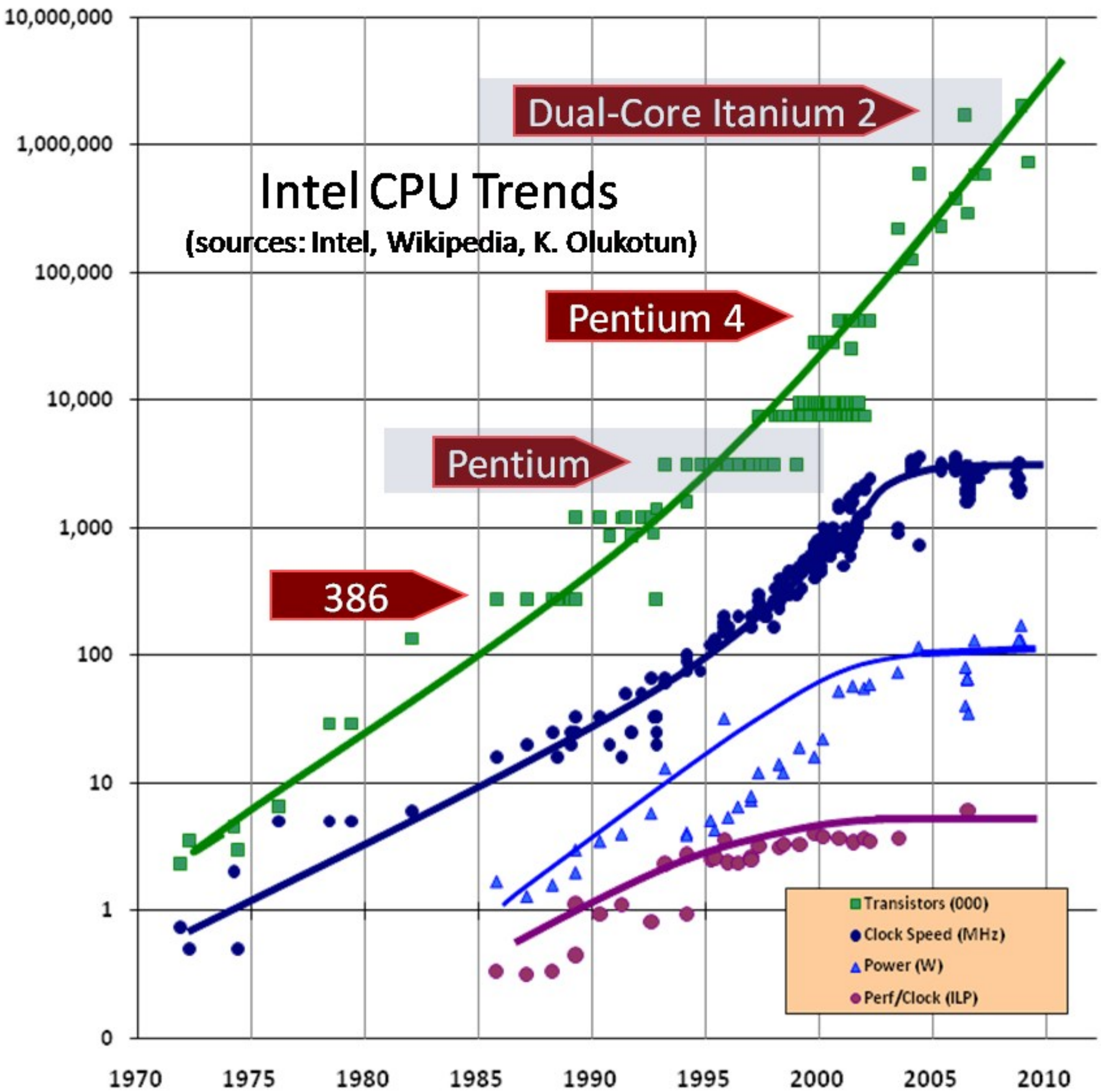
Supercomputer performance



~1000x in 10 years= doubles very year

Top500.org

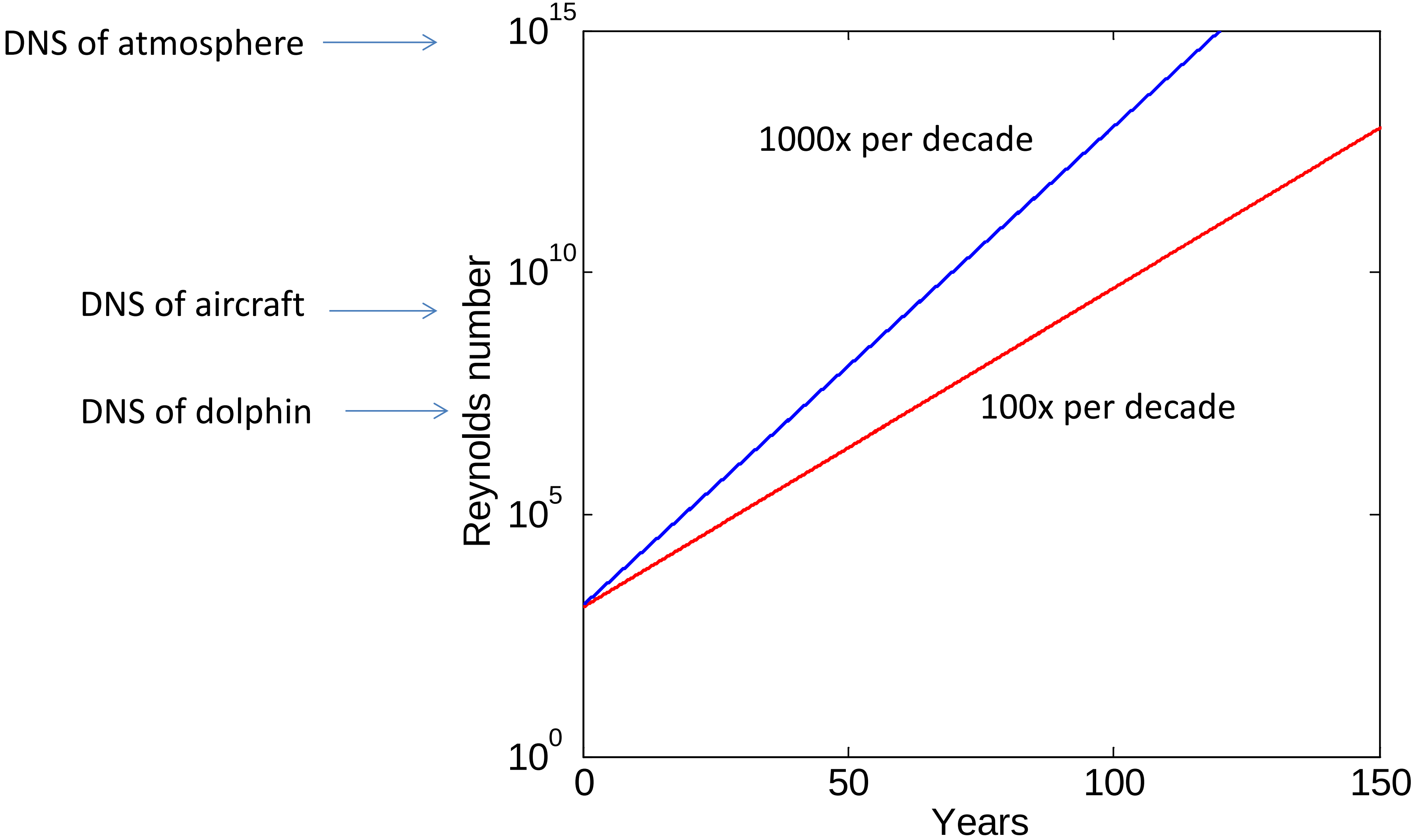
Will this continue?



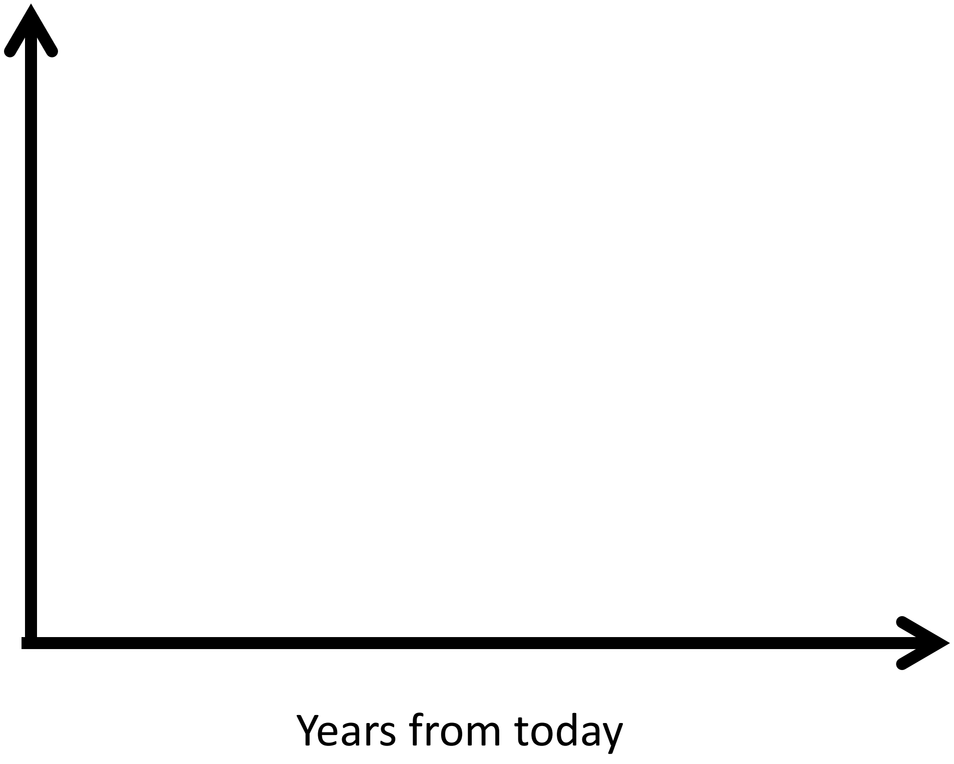
Current size is 14 nm

Estimates that it continue to 5-7 nm ~2020-2025

Future for fluid dynamics

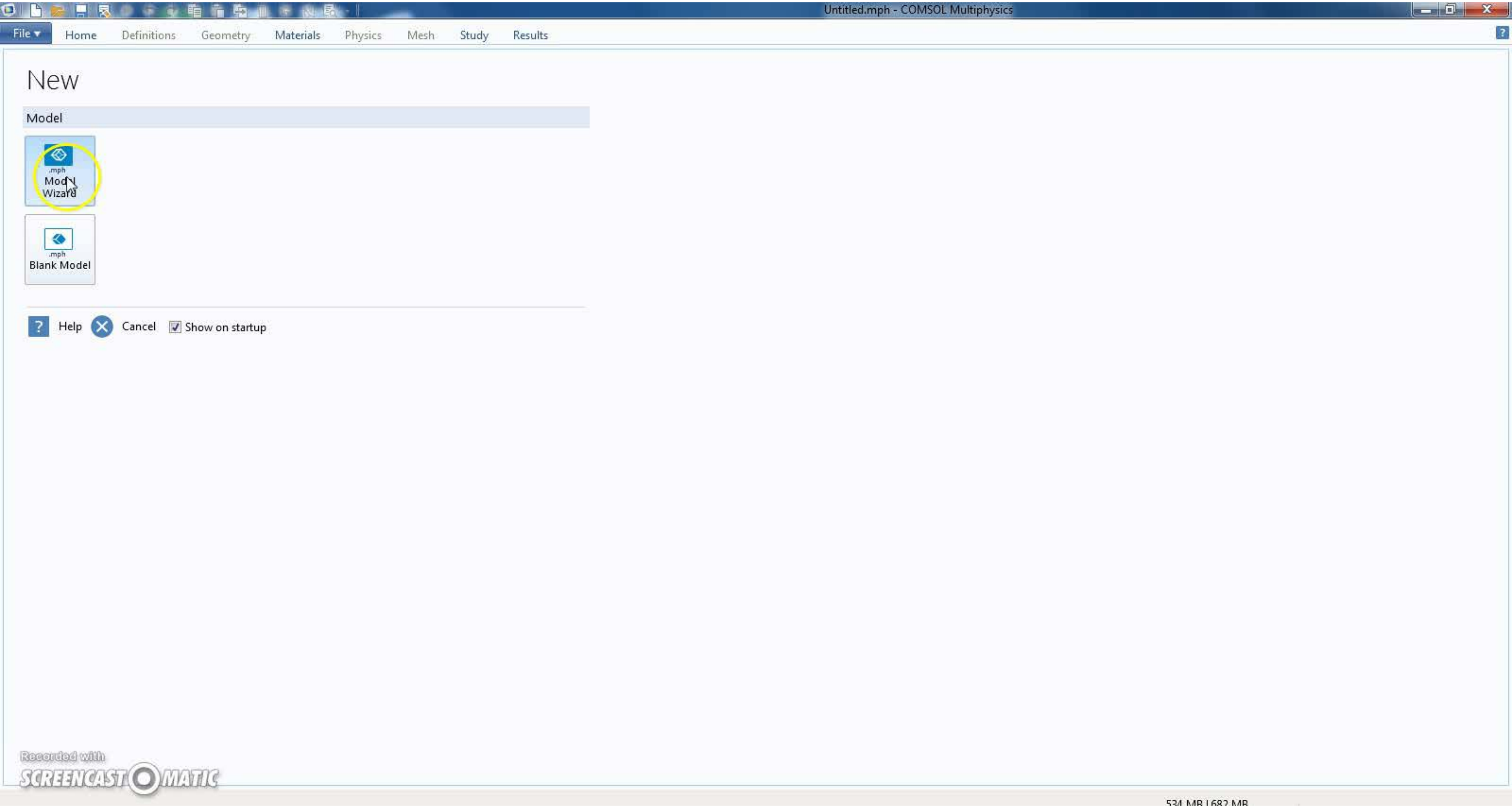


Your homework



For hands-on science

User training and time



Ten digit algorithm

Lloyd Trefethen – “Ten digits, 5 seconds, and just one page.”

WHY FIVE SECONDS?
“In computing with humans, response time is everything. If a program runs in less than five seconds, its author will effortlessly adjust, improve, and experiment. The process of scientific exploration becomes interactive and pleasurable. If the program runs for a minute or an hour, on the other hand, it is a very different situation from the human point of view “

WHY ONE PAGE?
“Again it’s a matter of linking to people. A code less than a page long can be read and studied.”

Survey

How long is it before an expert level computational problem becomes one that I can complete with one days work?

Take a minute to think, discuss with a neighbor, then get an answer in increments of 5 years.

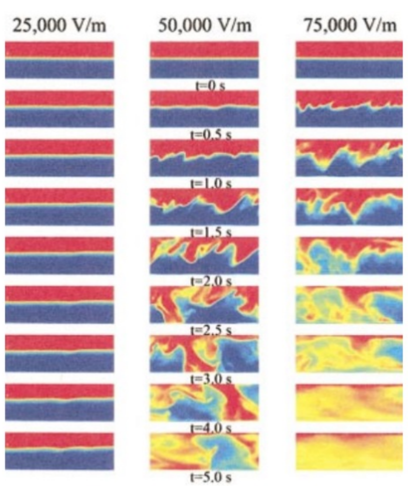
Case study (me)

2004 paper

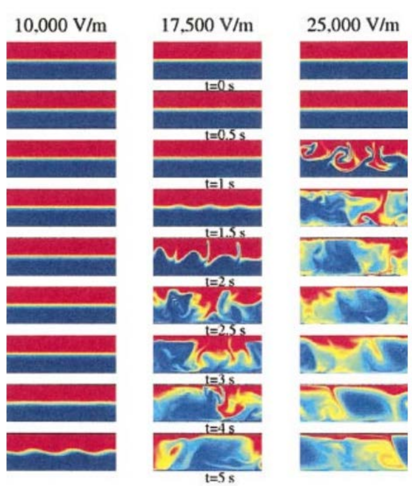
- Coupled flow and electrodynamics
- Experiments, analysis, & simulation
- Point of paper was the physics, so the paper still holds up pretty well
- Custom simulations, non-standard equations, months of code development

What changed?

- I replicated these results in ~30 min with Comsol.
- Now the graduate student who did the experiments would have done the sim.
- Can get instant results.

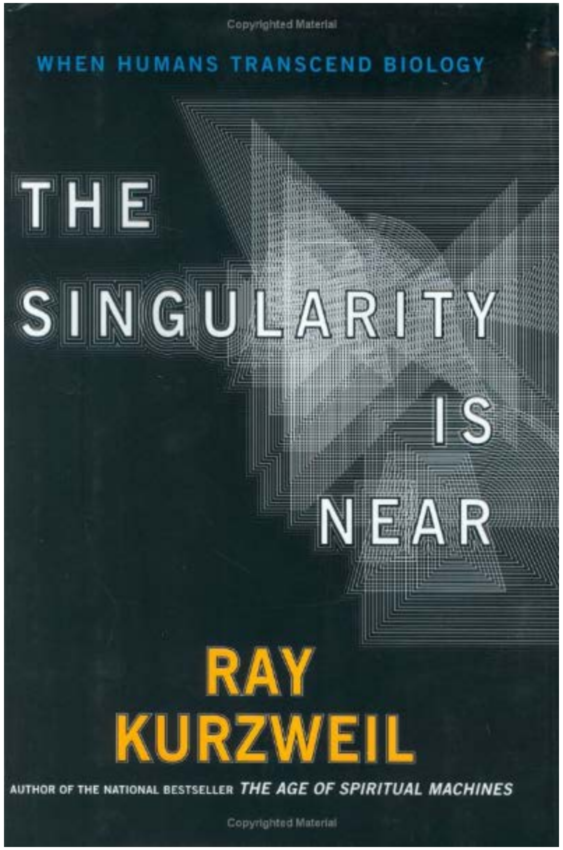


Experiment



Simulation

So what does the future look like?



Predictions- Computing power

- Moore’s law for # of transistors will pause in 5-10 years.
- Growth in computing power will continue. 100X per decade
- Computing power per watt will be driven by consumer demand. 100x per decade. Brain ~25 Watts.

Predictions – Big science

- Complex simulations become routine.
- Big science work will remain for my lifetime, but will become more and more specialized.
- Big simulations even more strongly focused in industry, national labs, and big research centers.

Predictions- CAE

- Industry needs will continue to grow
- The push to integrate analysis and design will allow non-specialists to run codes. Better results, less training.
- Industry has all new innovations.

Predictions – Hands-on science

- Interactive nature of simulation will change the way many people explore and learn science.
- Evolve away from traditional mode of simulation as bridge from theory to experiment.
- In hands-on work, the best papers will integrate analysis, simulation and experiment.
- All scientists and engineers will use simulation, but fewer people will understand the details.

Predictions - AI

- At some point, expect full cloud services for CAE. Fully integrated design, analysis, and manufacturing.
- Solvers will learn by experience from others.
- We will be able to click “simulate physics”

Predictions

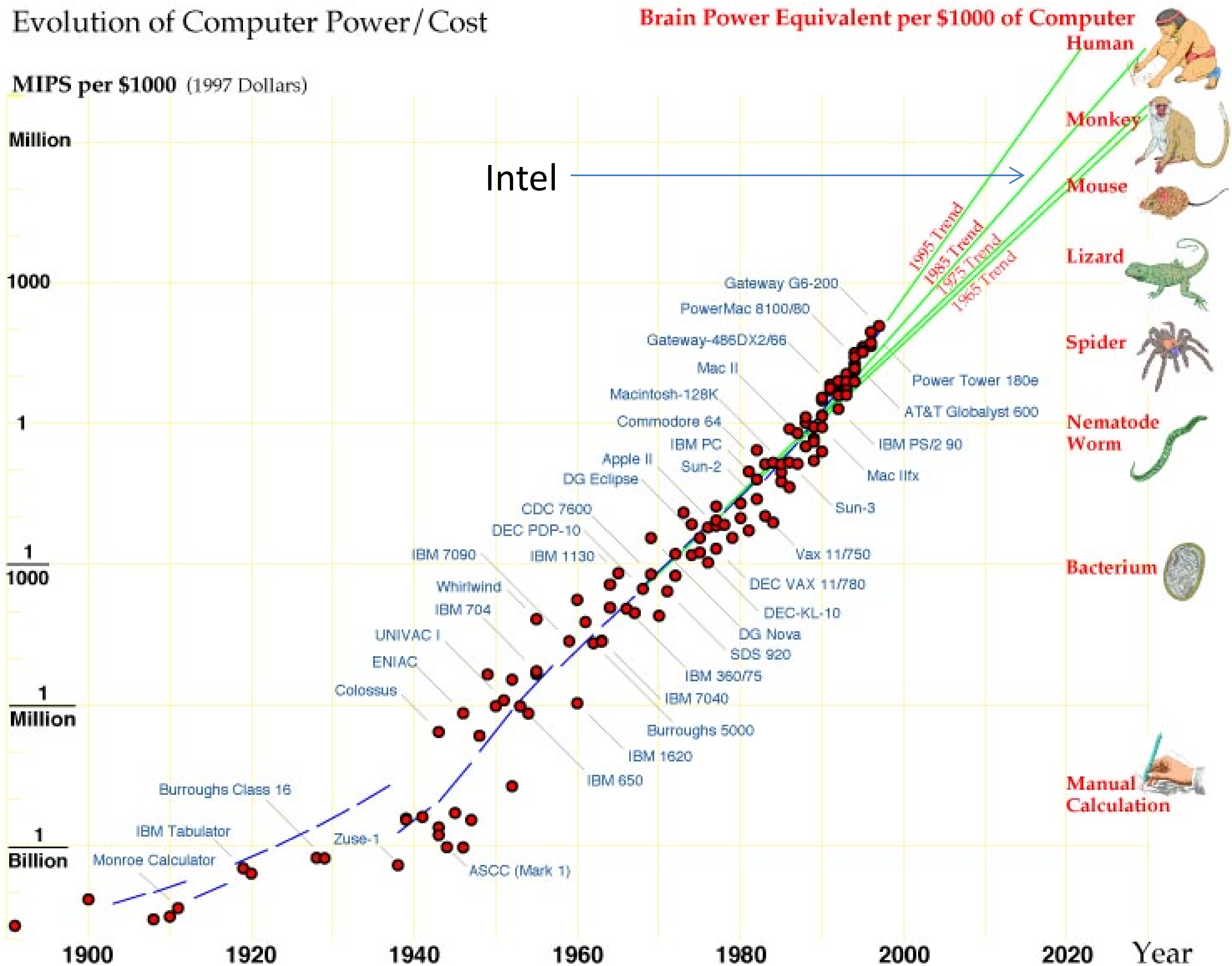
- Biology will remain an exception (for a while, anyway) – no universal equations to solve. Challenges are fundamental.

Opportunities in HOS

Increases in computing continue to rapidly change role of simulation

- More interactive (10 digit alg.)
- Used iteratively with experiments
- No specialization and little training required to get good results (skill is in interpreting the results)
- 10 years is the magic number
- As computing becomes easier for everyone, picking the right problems becomes even more important.
- <u>What</u> you compute is more important than <u>how</u>

What will happen to your field? What forces drive change? What are opportunities? How to you keep from being obsolete?



from [ROBOT](), *[Moravec]()*, [Oxford](), 1998, Chapter 3: *Power and Presence*, page 6

Software matters

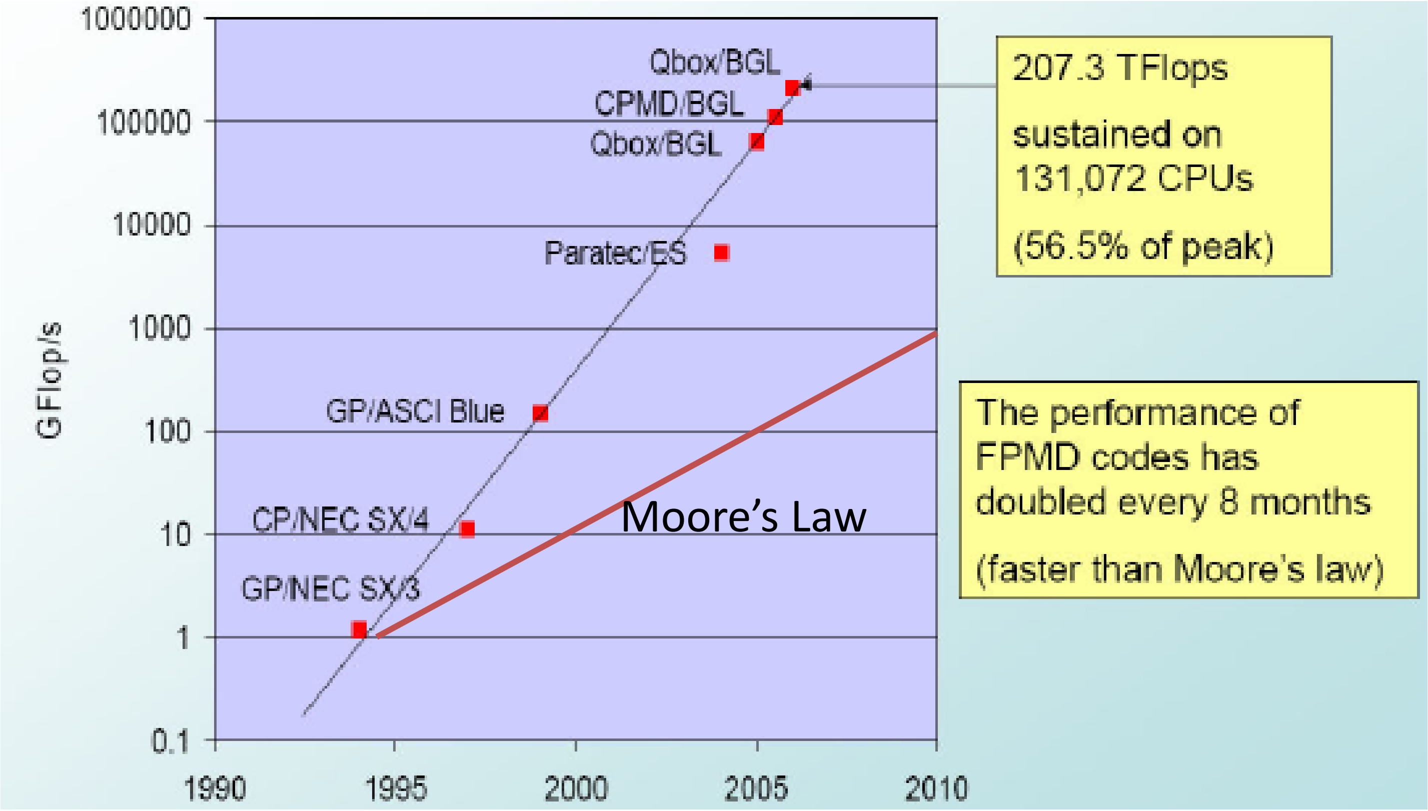


Figure 5.1. History of the performance of FPMD codes on different computer platforms (courtesy of Francois Gygi, University of California, Davis).