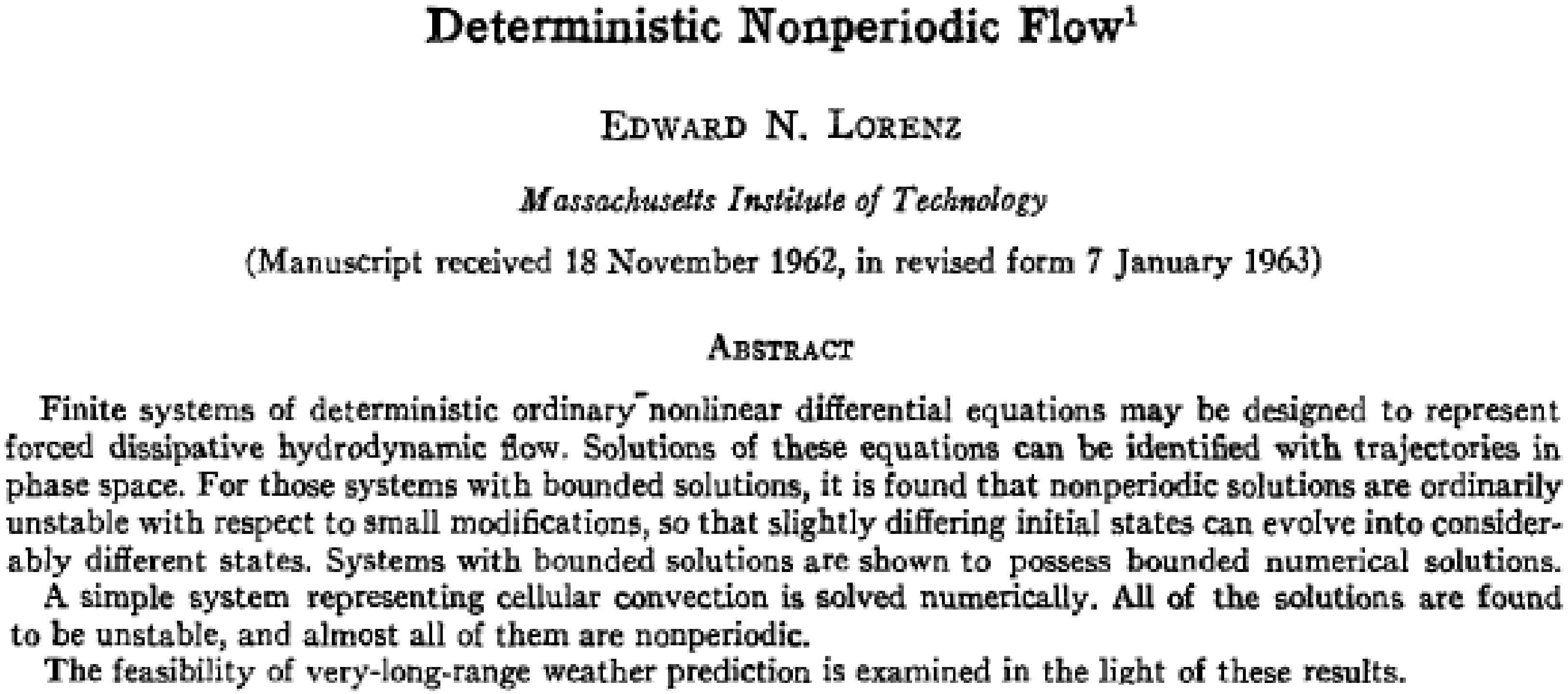
Computational science

from the supercomputer the personal computer

Brian D. Storey

Franklin W. Olin College of Engineering



Deterministic Nonperiodic Flow[1]

EDWARD N. LORENZ

Massachusetts Institute of Technology

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

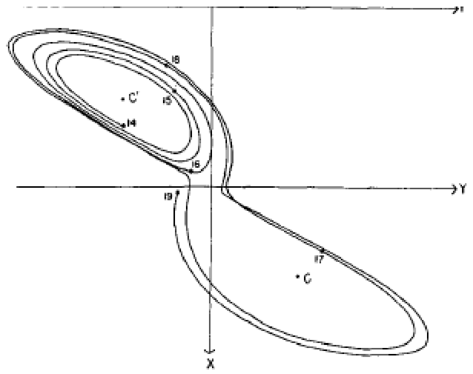
ABSTRACT

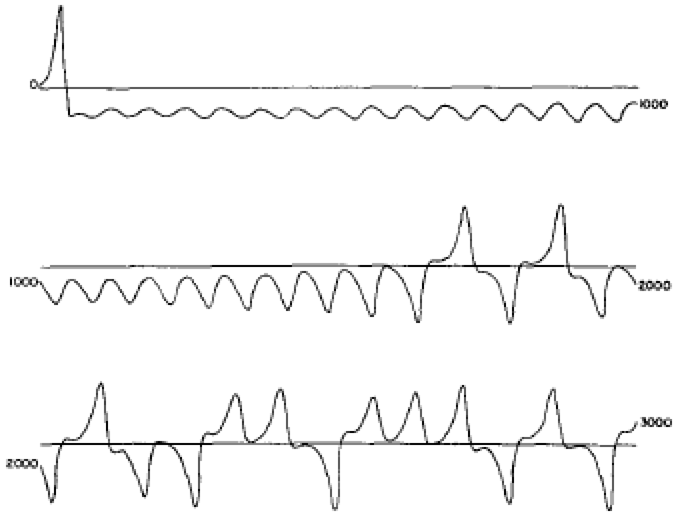
Finite systems of deterministic ordinary nonlinear differential equations may be designed to represent forced dissipative hydrodynamic flow. Solutions of these equations can be identified with trajectories in phase space. For those systems with bounded solutions, it is found that nonperiodic solutions 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.

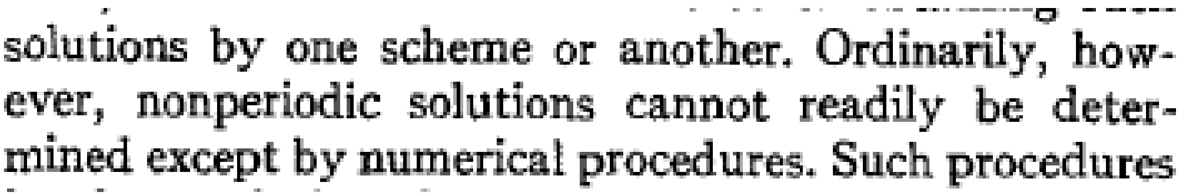
$$
\begin{aligned}
\dot{X} &= -\sigma X+\sigma Y,\\
\dot{Y} &= -XZ+rX-Y,\\
\dot{Z} &= XY -bZ.
\end{aligned}
$$

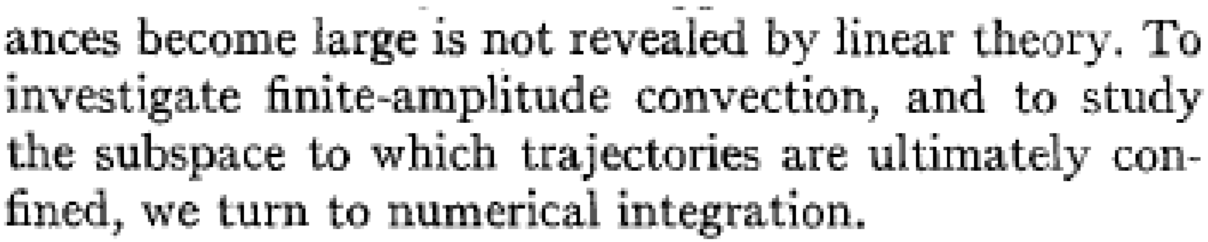


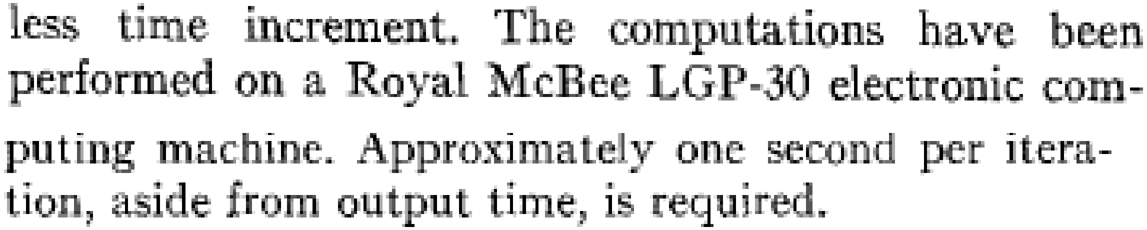


Web of science: ~5000 citations

1963


solutions by one scheme or another. Ordinarily, however, nonperiodic solutions cannot readily be determined except by numerical procedures. Such procedures


ances become large is not revealed by linear theory. To investigate finite-amplitude convection, and to study the subspace to which trajectories are ultimately confined, we turn to numerical integration.

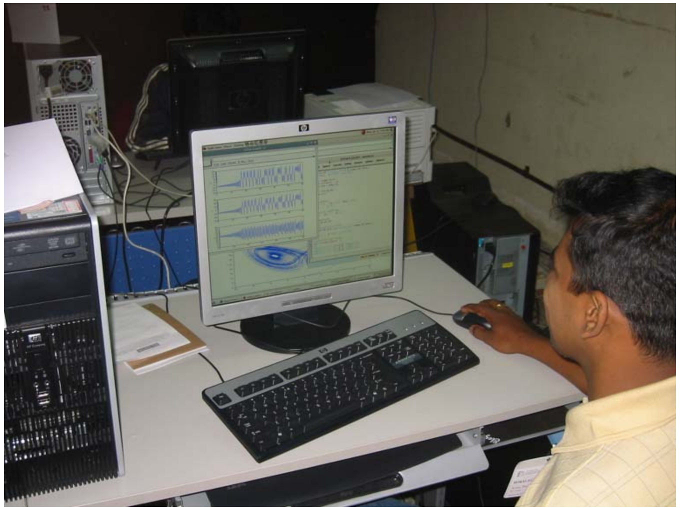

less time increment. The computations have been performed on a Royal McBee LGP-30 electronic computing machine. Approximately one second per iteration, aside from output time, is required.

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 dollars)
Weight:	740 pounds

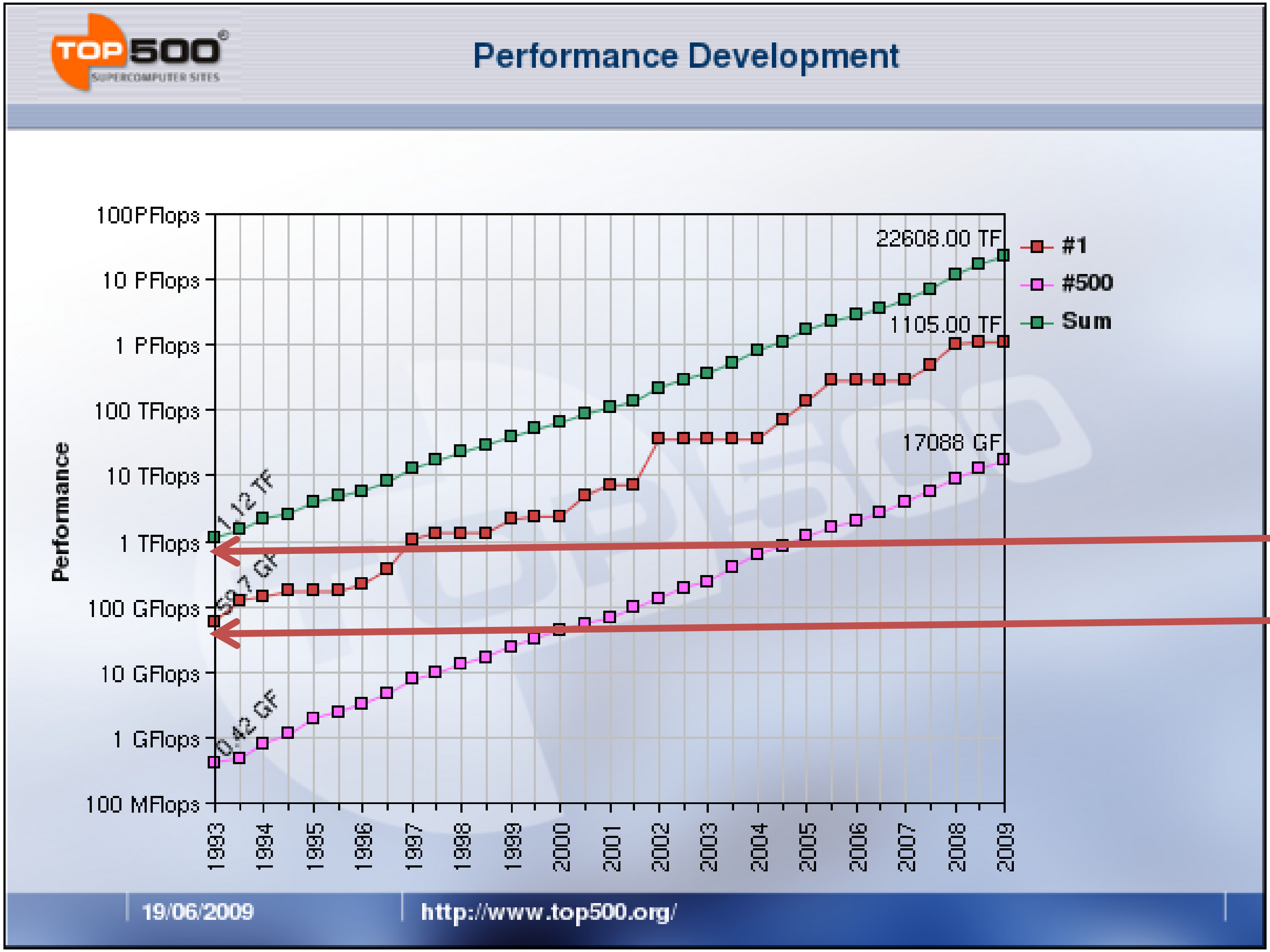
Source: wikipedia

2009



```
function lorenz

   sigma = 10;  rho = 28;  beta = 8/3;  tspan = 0:.01:60;

   x0 = 0;  y0 = 1;  z0 = 0;  Y0 = [x0;y0;z0];

   [T,Y] = ode45(@derivative,tspan,Y0,[],sigma,rho,beta);
   X = Y(:,1); Z = Y(:,3); Y = Y(:,2);

   plot(Y,X);


function dY = derivative(t,Y,sigma,rho,beta)
   x = Y(1);  y = Y(2);  z = Y(3);

   dx = sigma*(y-x);
   dy = x*(rho-z) - y;
   dz = x*y - beta*z;

   dY = [dx;dy;dz];
```

microseconds per iteration on my laptop
Fraction of a second instead of 1 ½ hours for 6000 iterations.



Performance Development

19/06/2009

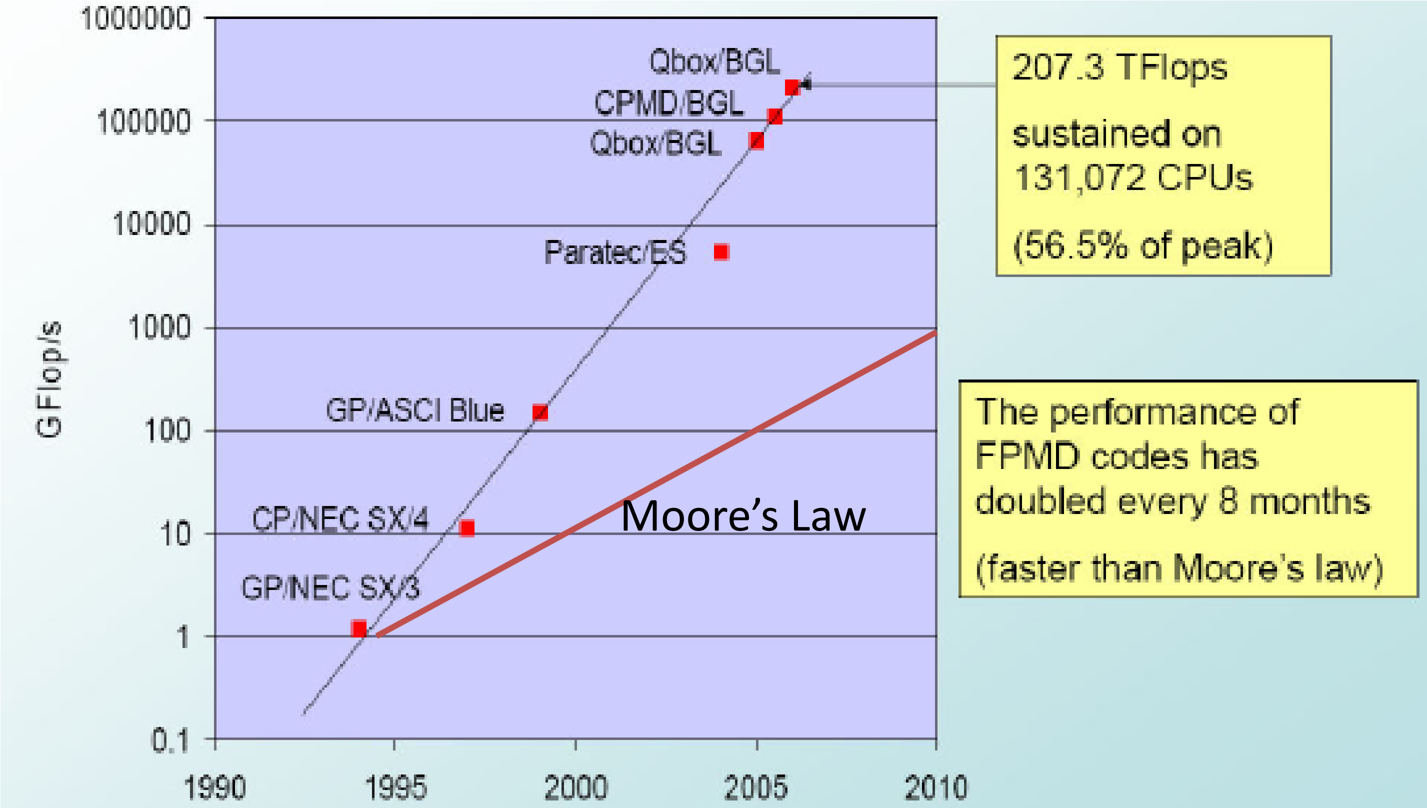
http://www.top500.org/

GPU (single)

PC (double)

www.top500.org

Software matters too



207.3 TFlops
sustained on
131,072 CPUs
(56.5% of peak)

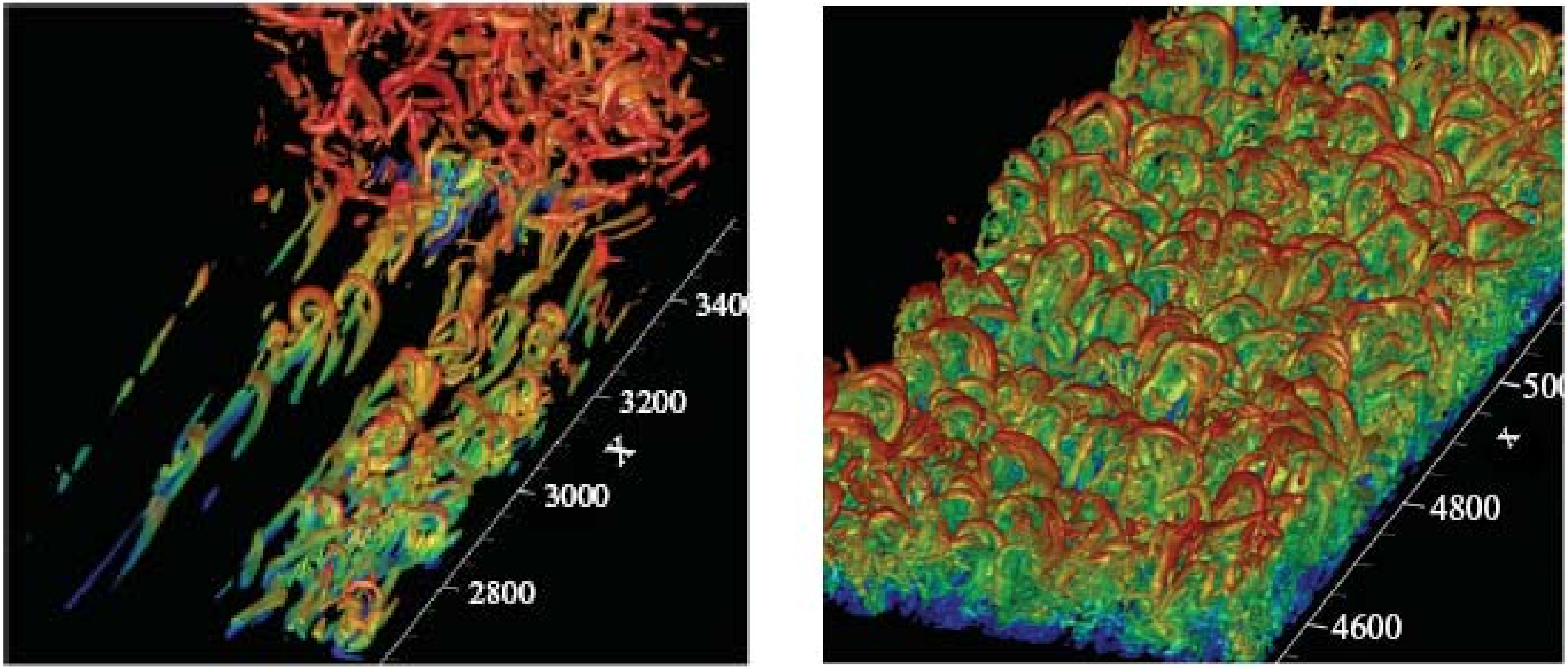
The performance of FPMD codes has doubled every 8 months
(faster than Moore's law)

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

INTERNATIONAL ASSESSMENT OF RESEARCH AND DEVELOPMENT IN SIMULATION-BASED ENGINEERING AND SCIENCE, NSF, 2009

So what’s possible with today’s supercomputers?

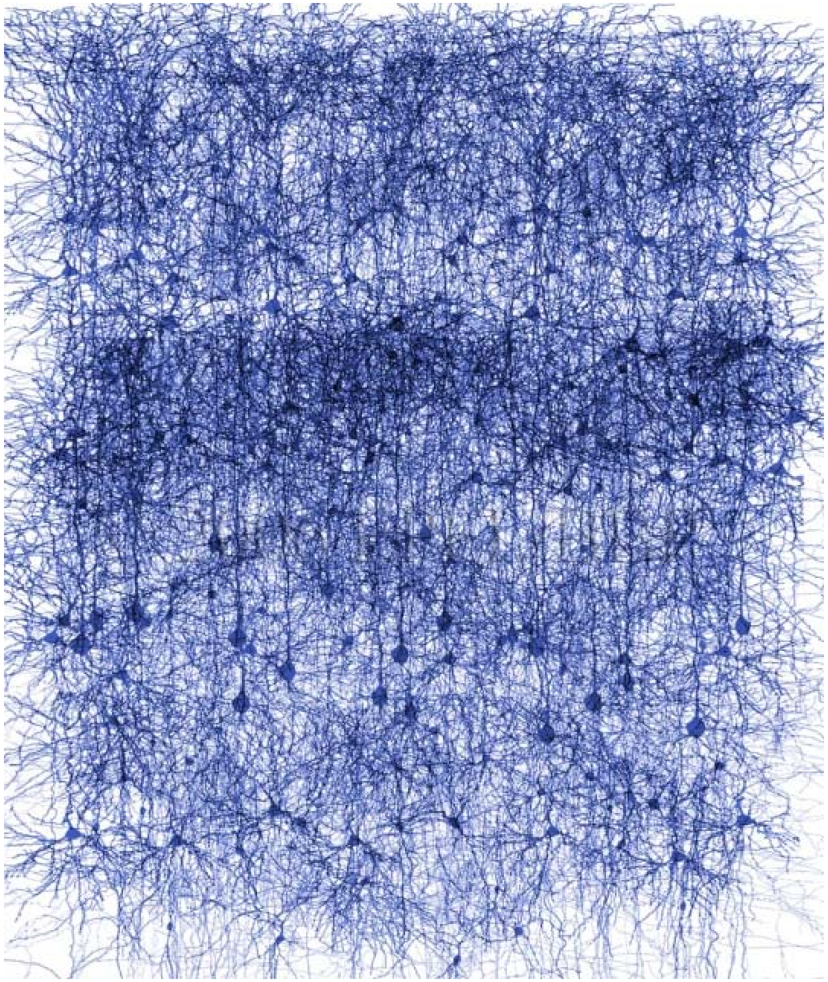
Fluid dynamics

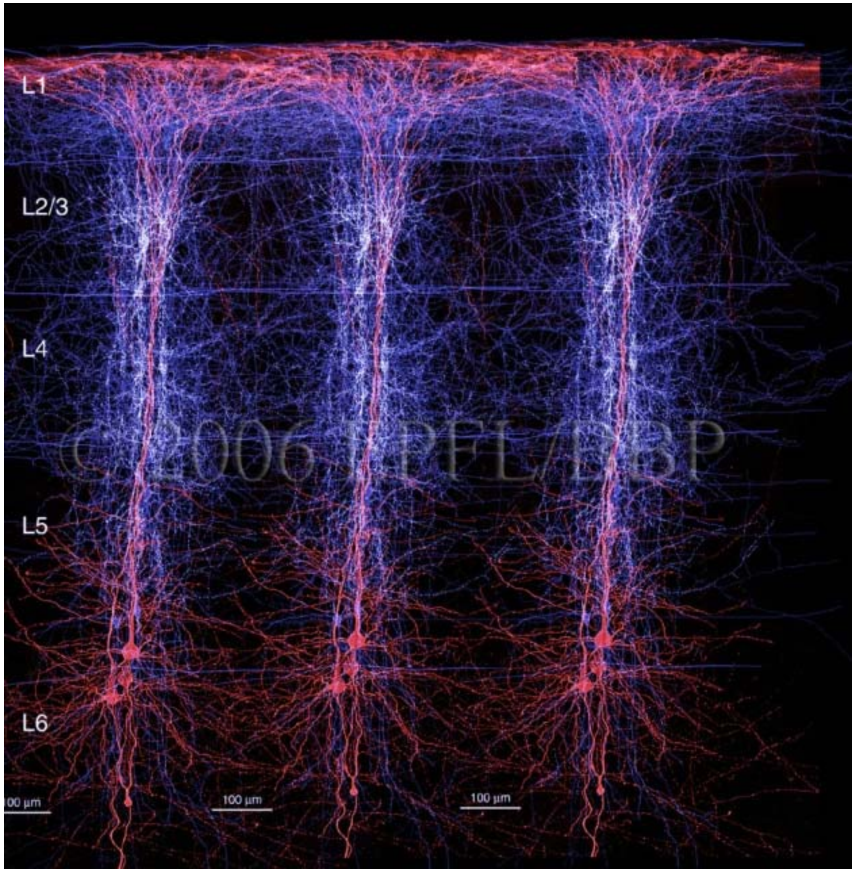


Wu and Moin, JFM 2009

Blue Brain

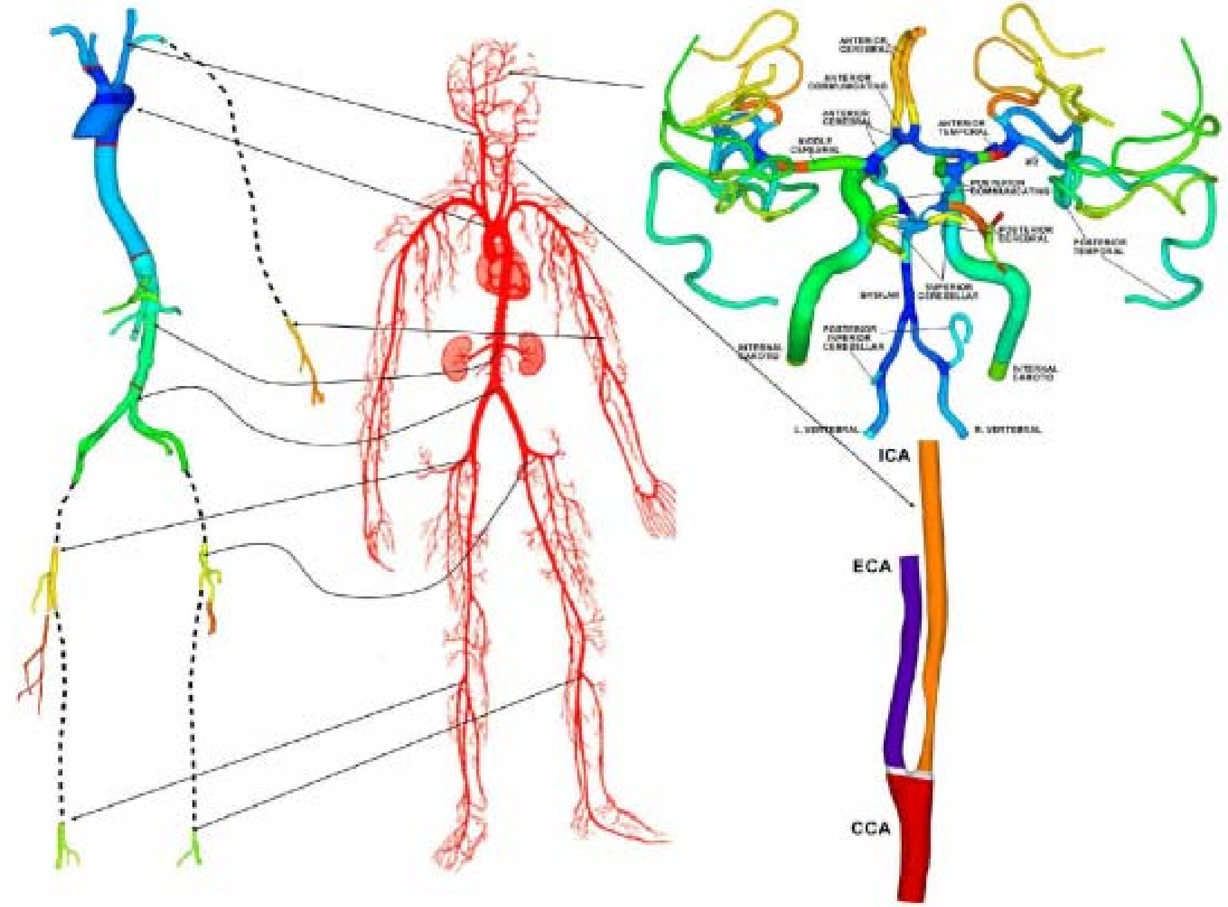
model of neocortical column





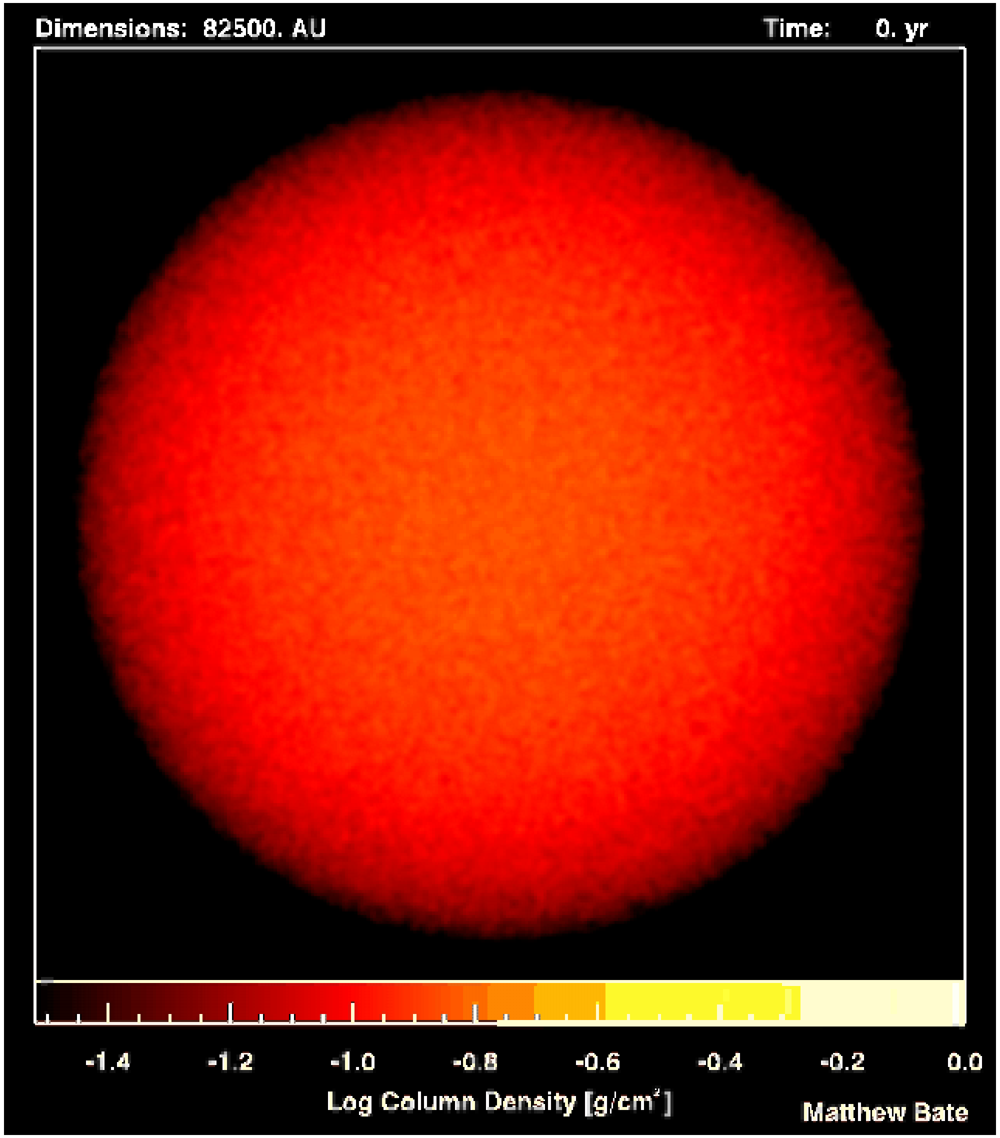
http://bluebrain.epfl.ch/

Virtual surgery



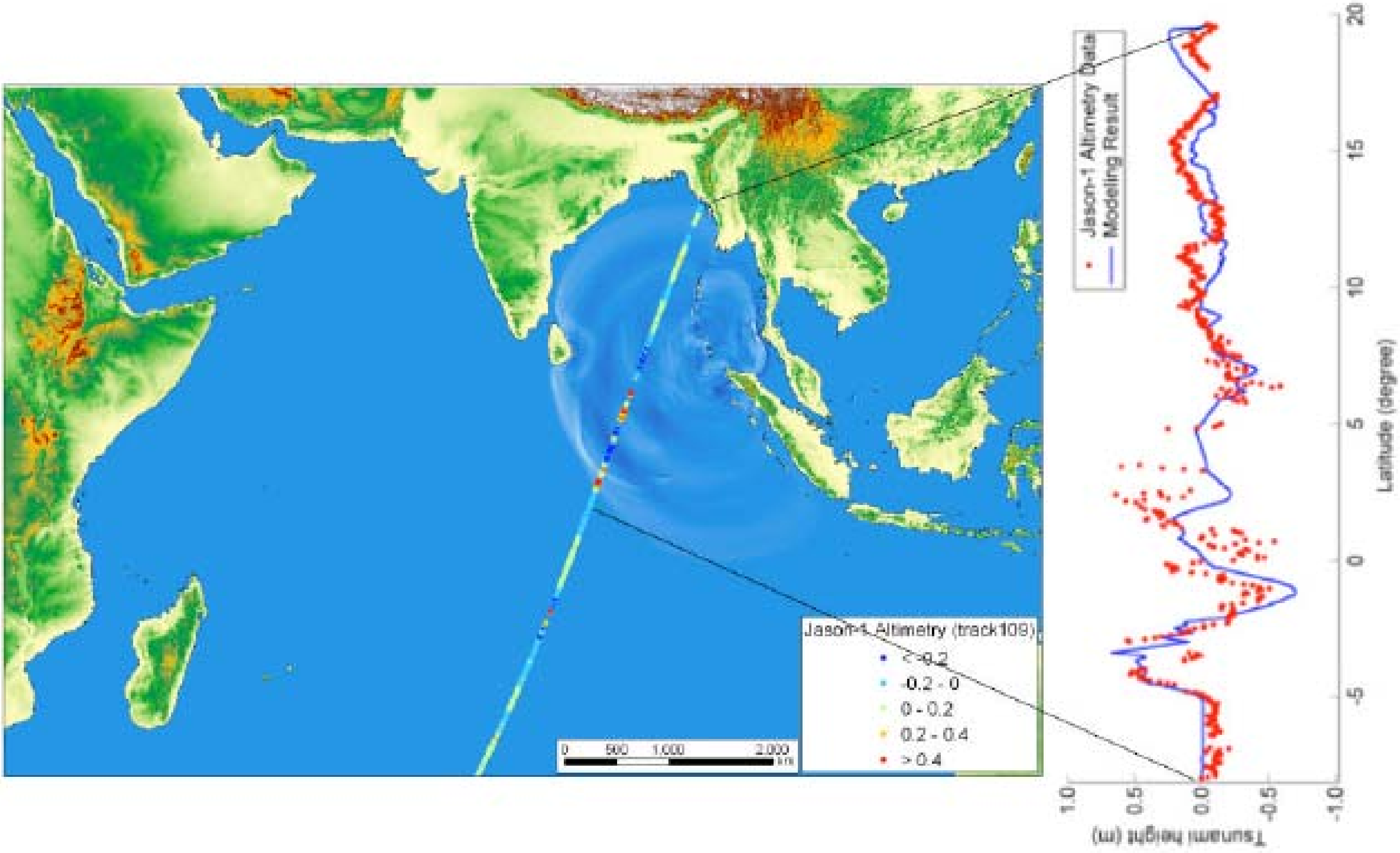
Grinberg etal, 2008

Star formation



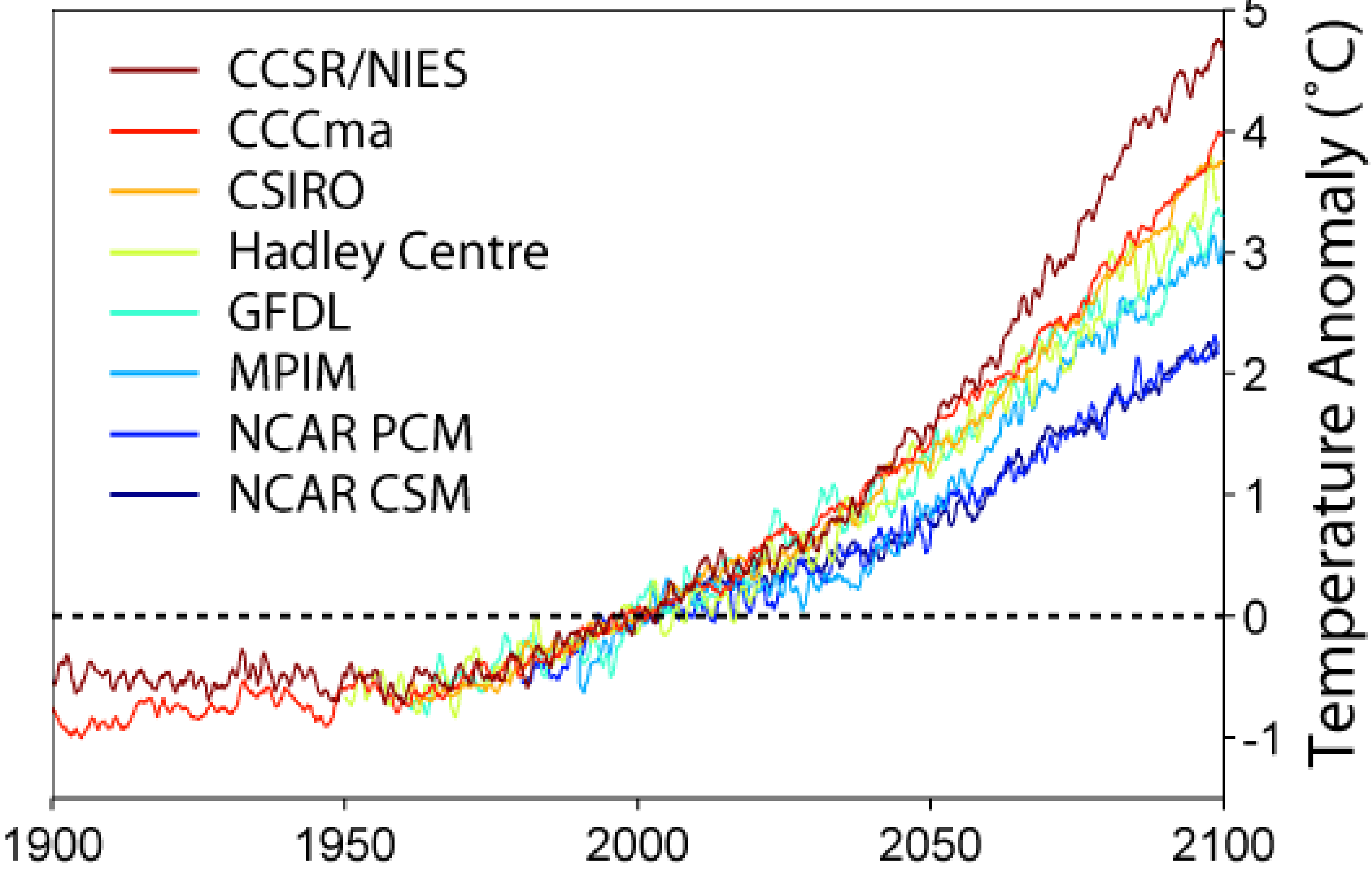
Matthew Bate
http://www.ukaff.ac.uk/starclus

Disaster planning



Koshimura & Yanagiswa, 2007

Global Warming Projections



But supercomputing can be expensive

Roadrunner

Power- 2.35 MW

Space - 296 racks, 560 m^2 (6,000 sq ft)

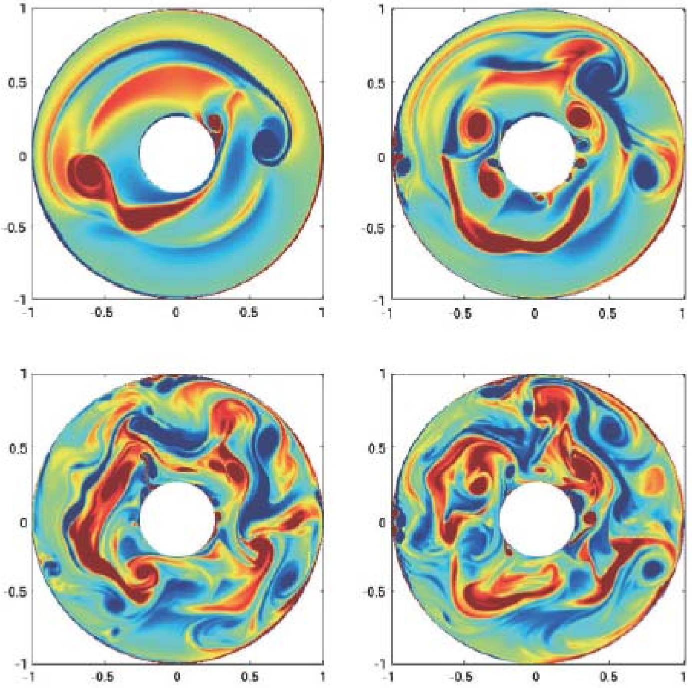
Memory - 103.6 TB

Speed - 1.71 petaflops

Cost - USD $133M

Processors - 12,960 IBM Power XCell 8i,
6,480 AMD Opteron

and supercomputing requires programming time, training, and access



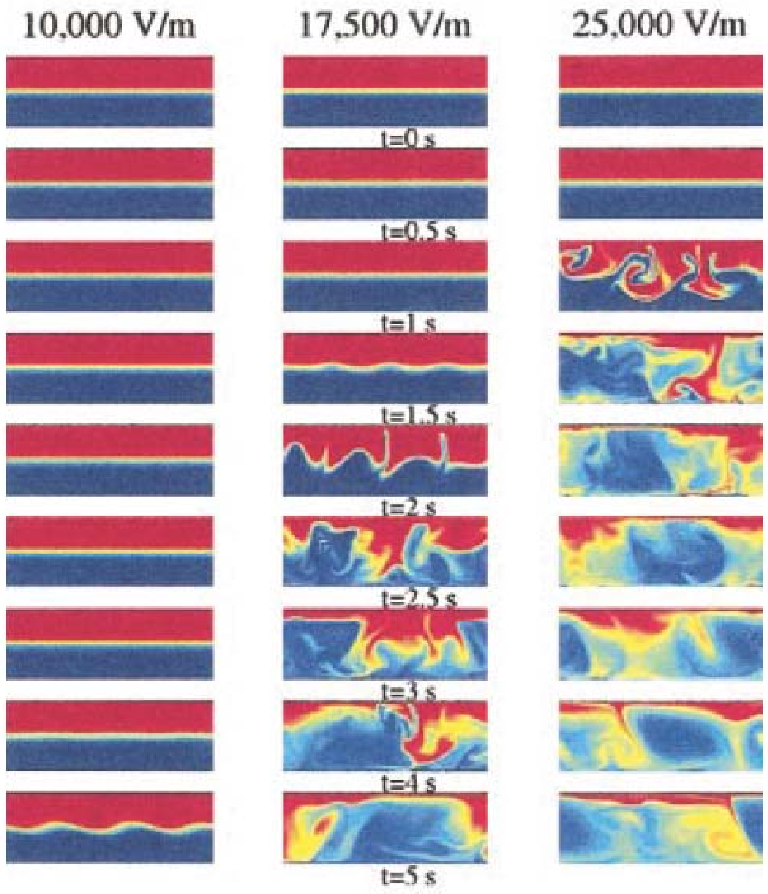
Storey, 2004. *Int J. Num. Meth. in Fluids*

- -2002 project run on 1998 SC
- -Needed to write a proposal to use SC.
- -Fortran 90 w/ MPI, 2285 lines of code, 41 pages printed
- -512 and 1024 resolution, long times.
- -A few hours per run (but there is a wait)
- -2 months to write, test, debug
- -Visualization and post-processing done separately

2D Equations for:

- **-streamfunction**
- **-vorticity**

PC based MATLAB simulation



Lin, Storey, Oddy, Chen, & Santiago 2004. *Phys. Fluids*

-2003 project, 2003 PC

-MATLAB, 704 lines of code, 12 pages printed

-256x128 resolution

-2 weeks to write, test, debug

-Overnight to run

-Visualization/processing can be done in code

2D Equations for:

-streamfunction

-vorticity

-electric field

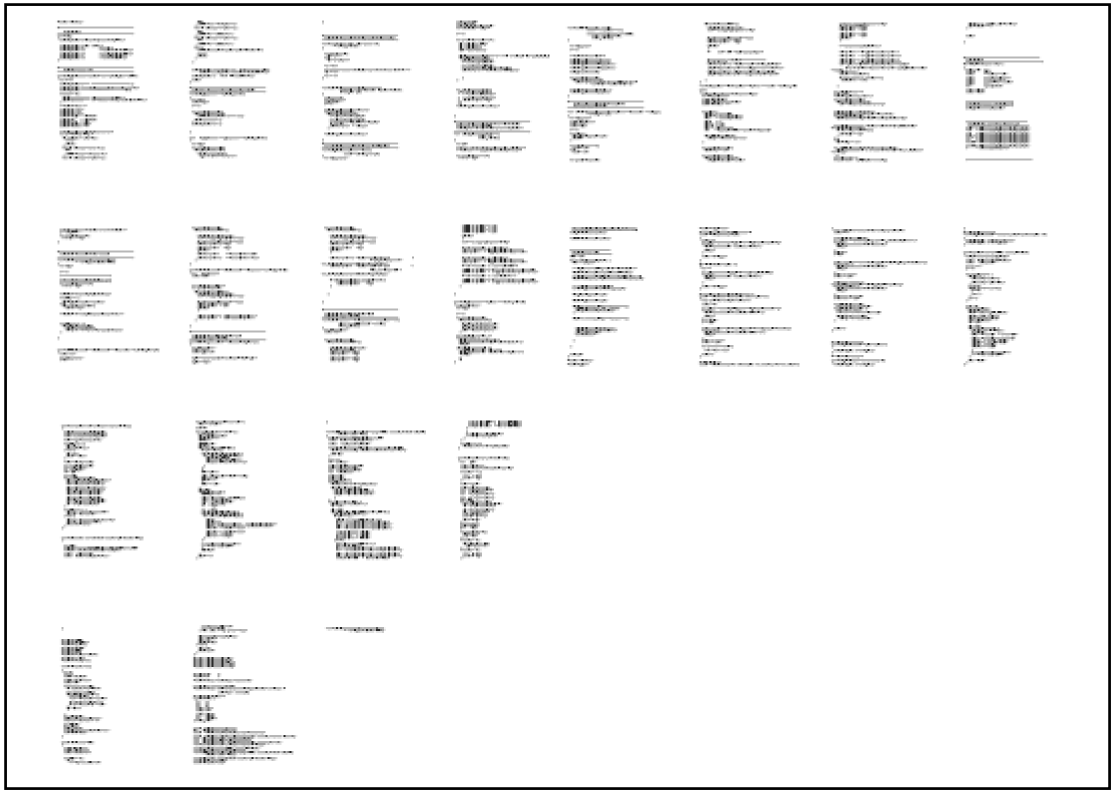
-electrical conductivity

-passive tracer

PC to PC comparison

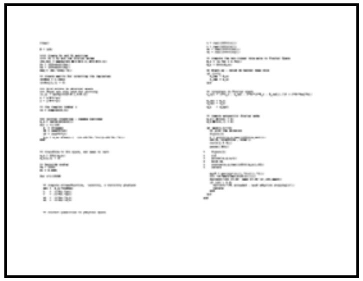
2D Turbulence simulation

C code, 1252 lines, 22 pages



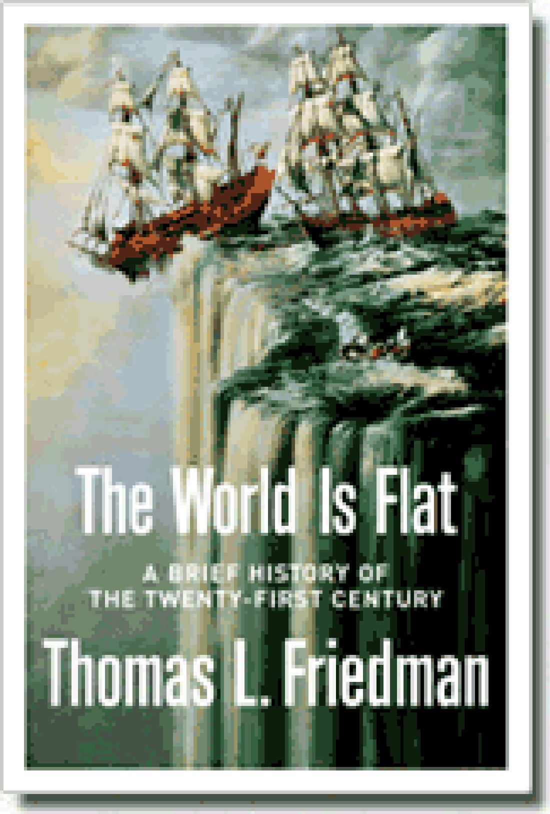
Too complicated!

MATLAB code,
110 lines, 2 pages



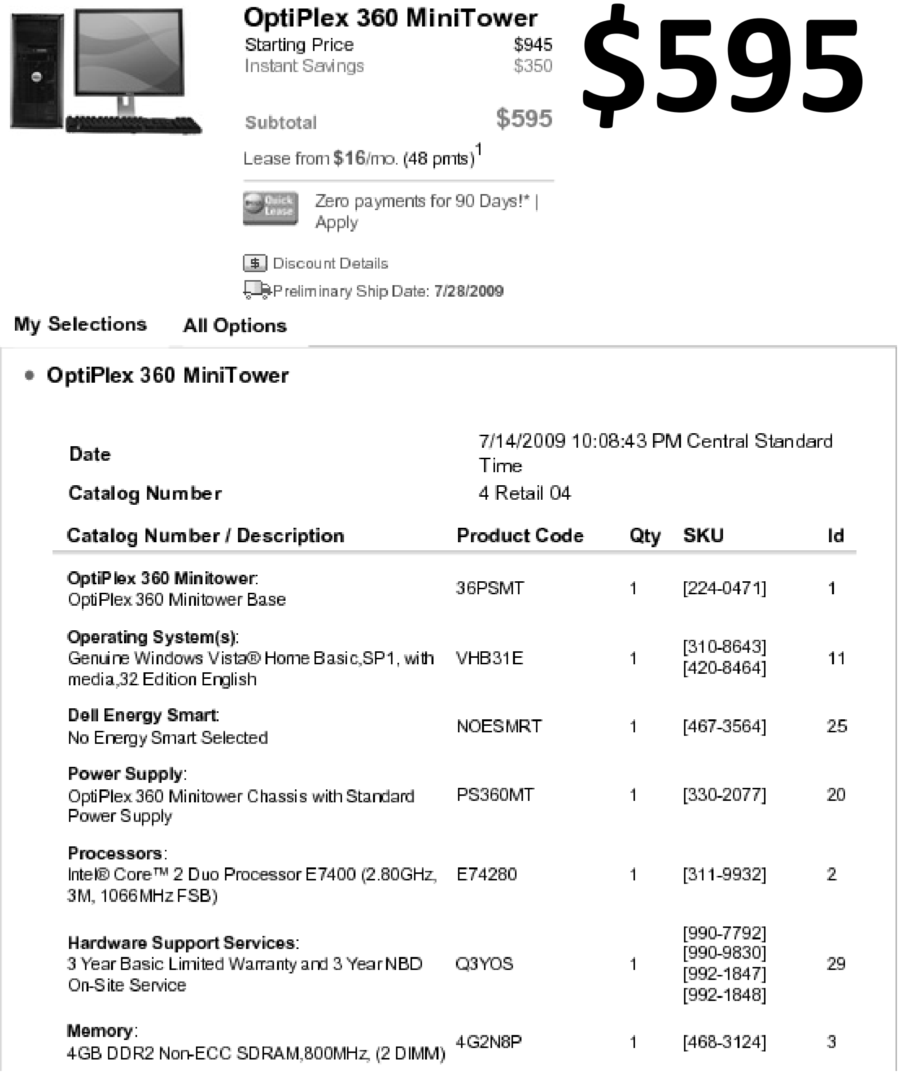
Student friendly

The world is flat



“the playing field is being leveled”

$595



OptiPlex 360 MiniTower

Starting Price	$945
Instant Savings	$350
Subtotal	$595

Lease from $16/mo. (48 pmts)[1]

Zero payments for 90 Days!* | Apply

Discount Details

Preliminary Ship Date: 7/28/2009

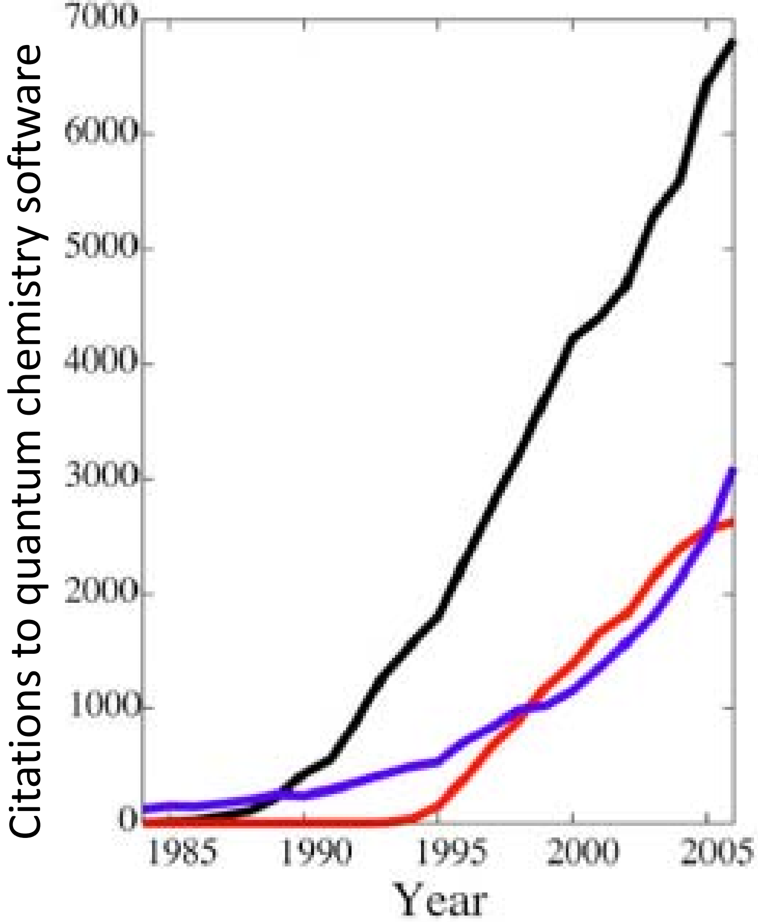
- **OptiPlex 360 MiniTower**

Date 7/14/2009 10:08:43 PM Central Standard Time

Catalog Number 4 Retail 04

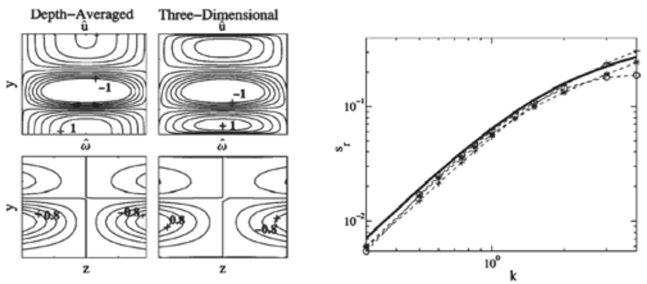
Catalog Number / Description	Product Code	Qty	SKU	Id
OptiPlex 360 Minitower: OptiPlex 360 Minitower Base	36PSMT	1	[224-0471]	1
Operating System(s): Genuine Windows Vista® Home Basic,SP1, with media,32 Edition English	VHB31E	1	[310-8643] [420-8464]	11
Dell Energy Smart: No Energy Smart Selected	NOESMRT	1	[467-3564]	25
Power Supply: OptiPlex 360 Minitower Chassis with Standard Power Supply	PS360MT	1	[330-2077]	20
Processors: Intel® Core™ 2 Duo Processor E7400 (2.80GHz, 3M, 1066MHz FSB)	E74280	1	[311-9932]	2
Hardware Support Services: 3 Year Basic Limited Warranty and 3 Year NBD On-Site Service	Q3YOS	1	[990-7792] [990-9830] [992-1847] [992-1848]	29
Memory: 4GB DDR2 Non-ECC SDRAM,800MHz, (2 DIMM)	4G2N8P	1	[468-3124]	3

Cost goes down, users go up

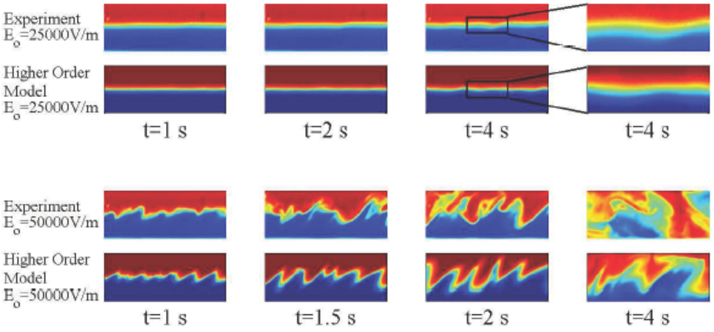


INTERNATIONAL ASSESSMENT OF RESEARCH AND DEVELOPMENT IN SIMULATION-BASED ENGINEERING AND SCIENCE, NSF, 2009

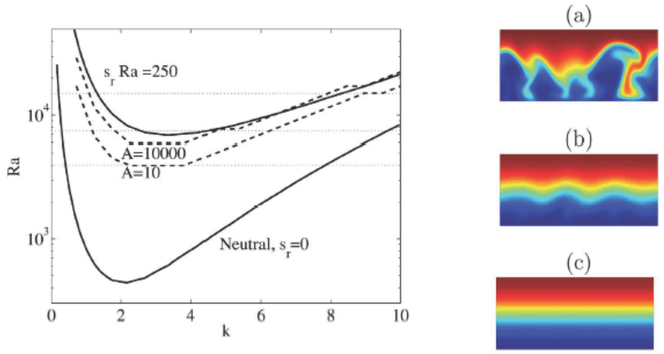
Can computational science be done with only a PC, a few students, and no money?



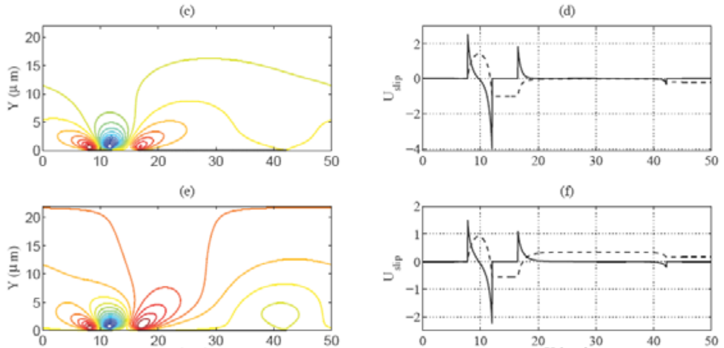
Storey, B.D., Tilley, B.S., Lin, H., & Santiago, J.G. 2005 *Physics of Fluids.*



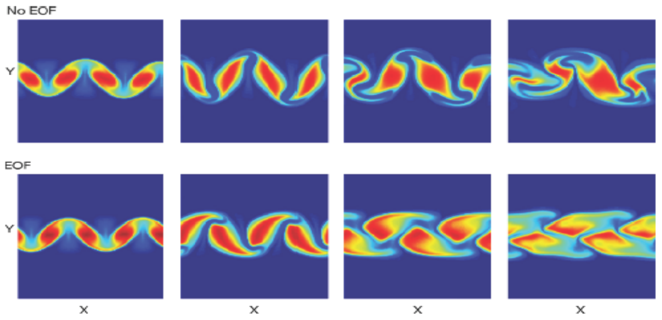
Lin, H., Storey, B.D., & Santiago, J.G. 2008 *Journal of Fluid Mechanics*,



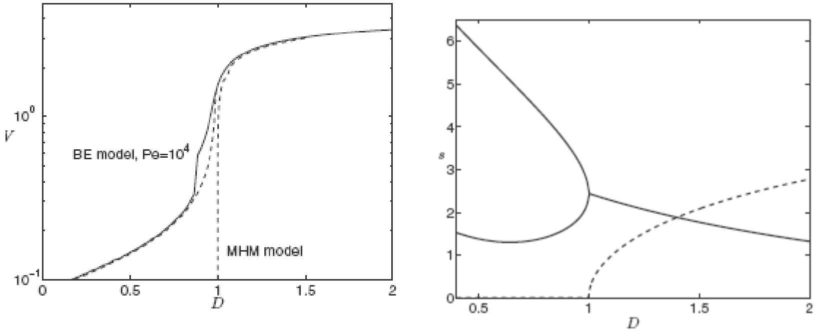
Boy, D.A. & Storey, B.D. 2007 *Physical Review E*



Storey, B.D., Edwards, L.R., Kilic, M.S., & Bazant, M.Z. 2007 *Physical Review E*



Storey, B.D. 2005 *Physica D*



Storey, B.D., Zaltzman, B., & Rubinstein, I. 2007 *Physical Review E*,.

Some tools I like

MATLAB

I like it for:
- Solving ODEs
- Custom but simple numerical codes for PDEs (especially NL ones)
- Integrating computation and visualization
- Integrating experiment and simulation

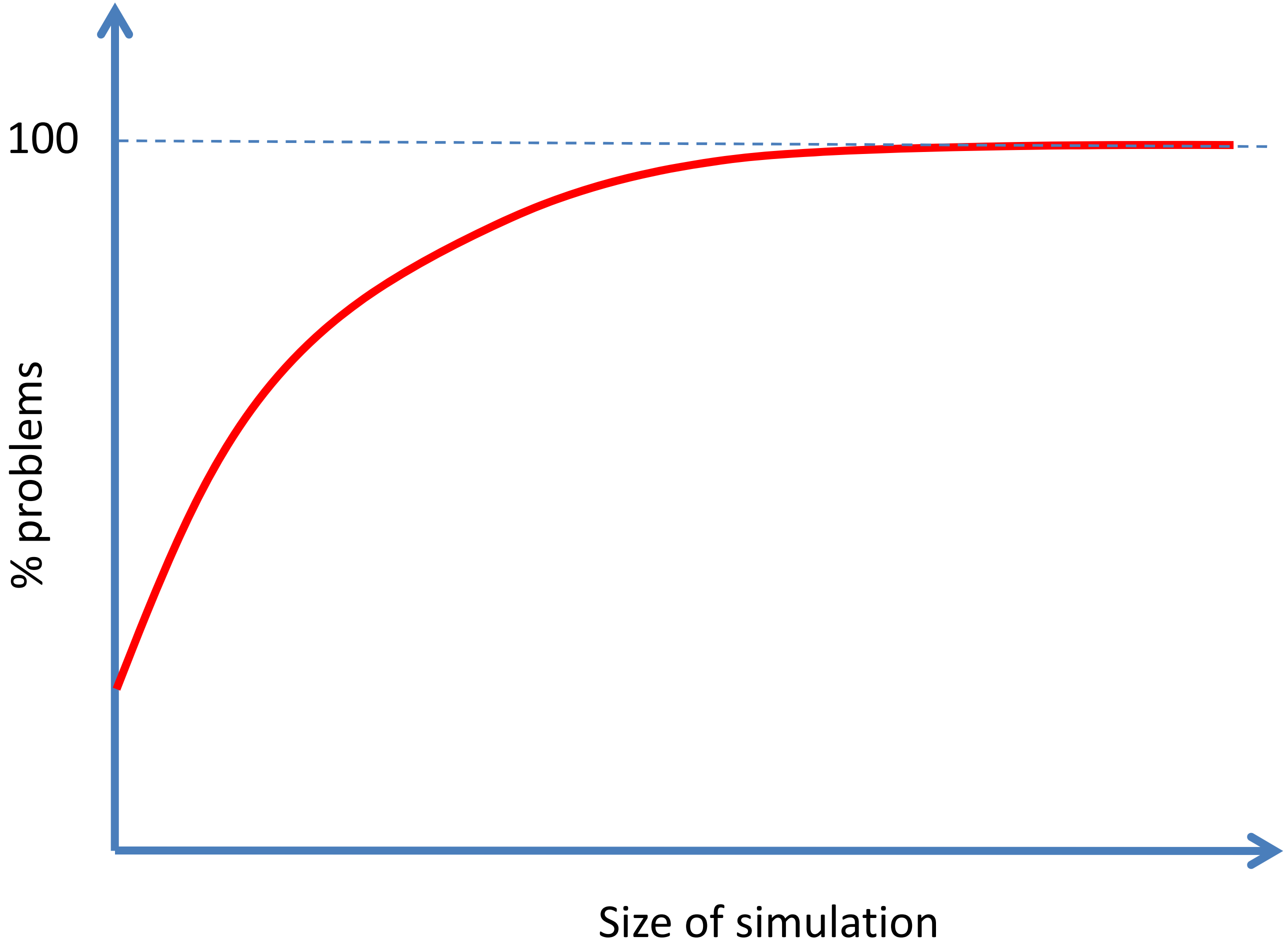
Maple 13

I like it for:
- Calculus calculator
- Algebra, keeping constants straight
- Linearization, matched asymptotics

COMSOL

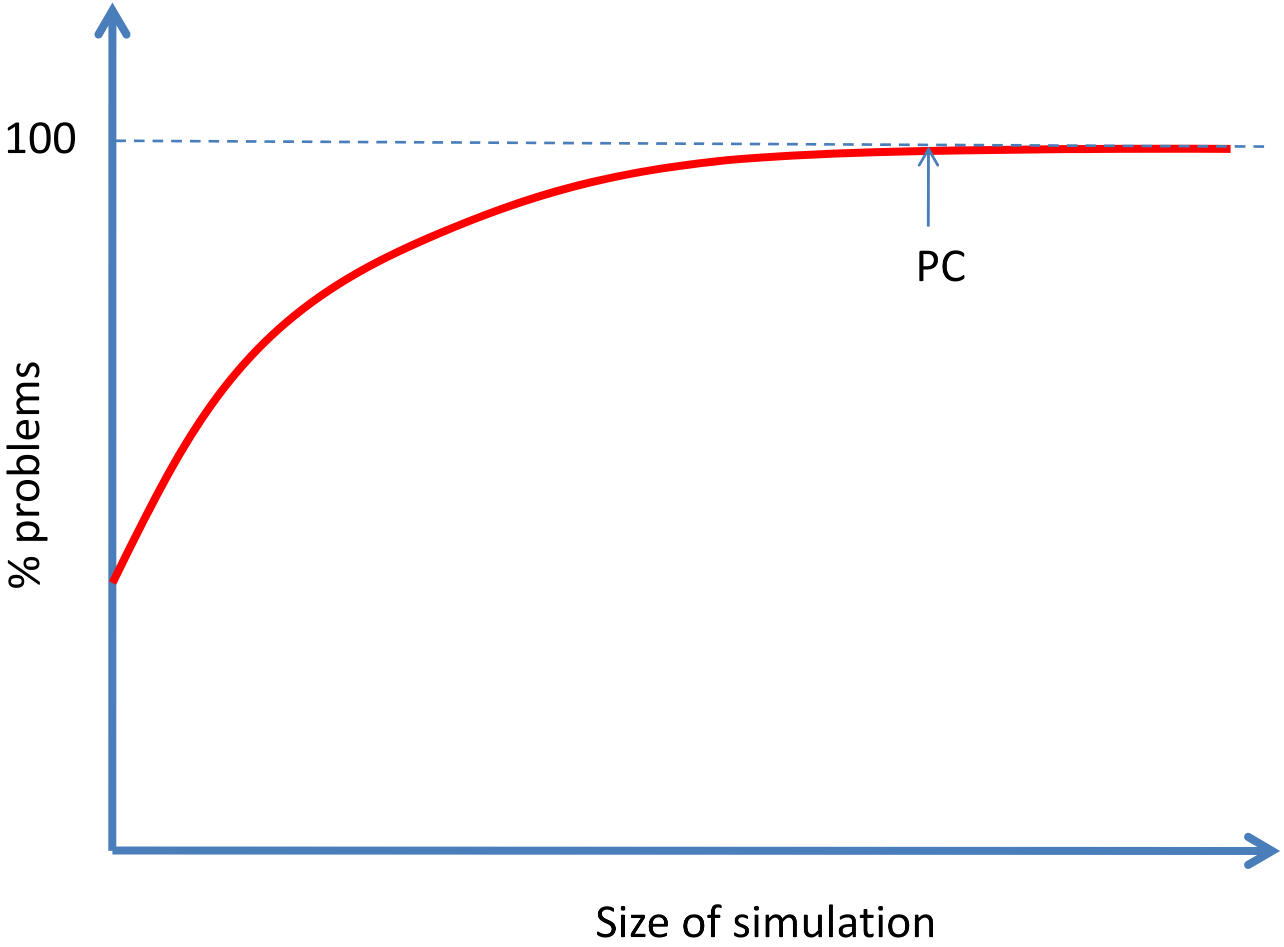
I like it for:
- Any PDEs problem (especially linear or weakly NL)
- Complex geometry
- Qualitative behavior
- Students to visual 3D phenomena

Where is your field?

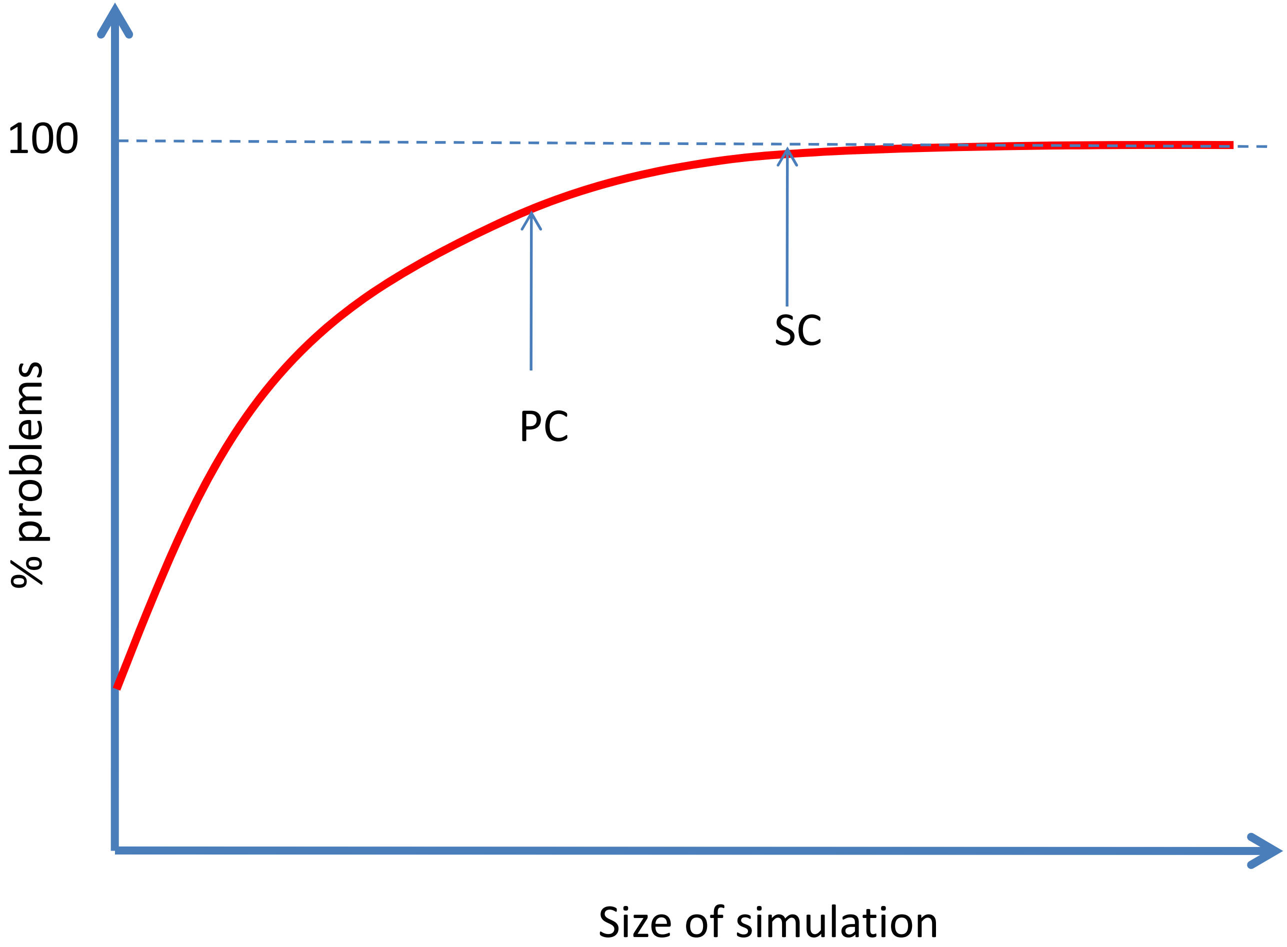


Dynamical systems (ODEs)

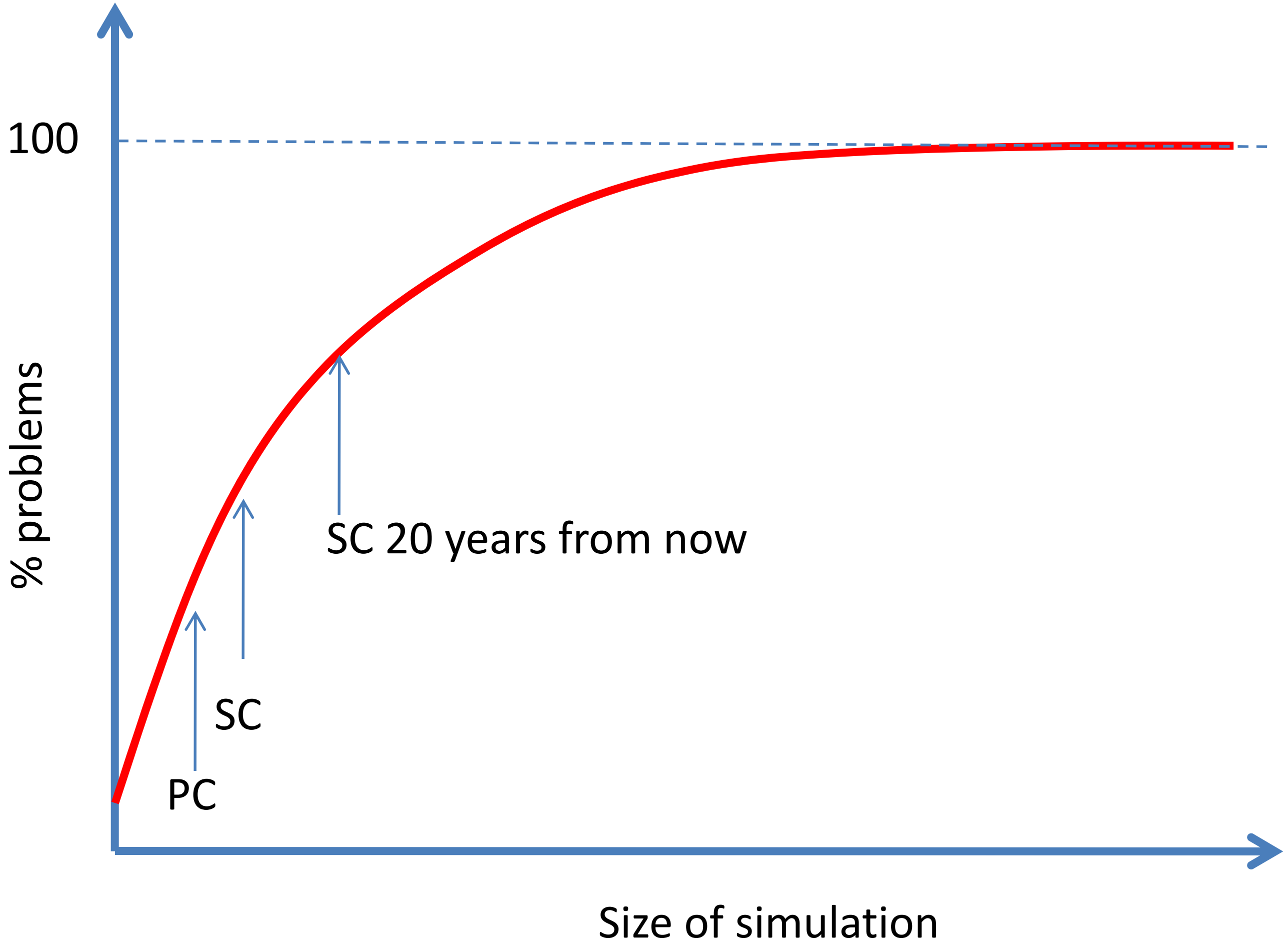
solving ODEs has become a commodity



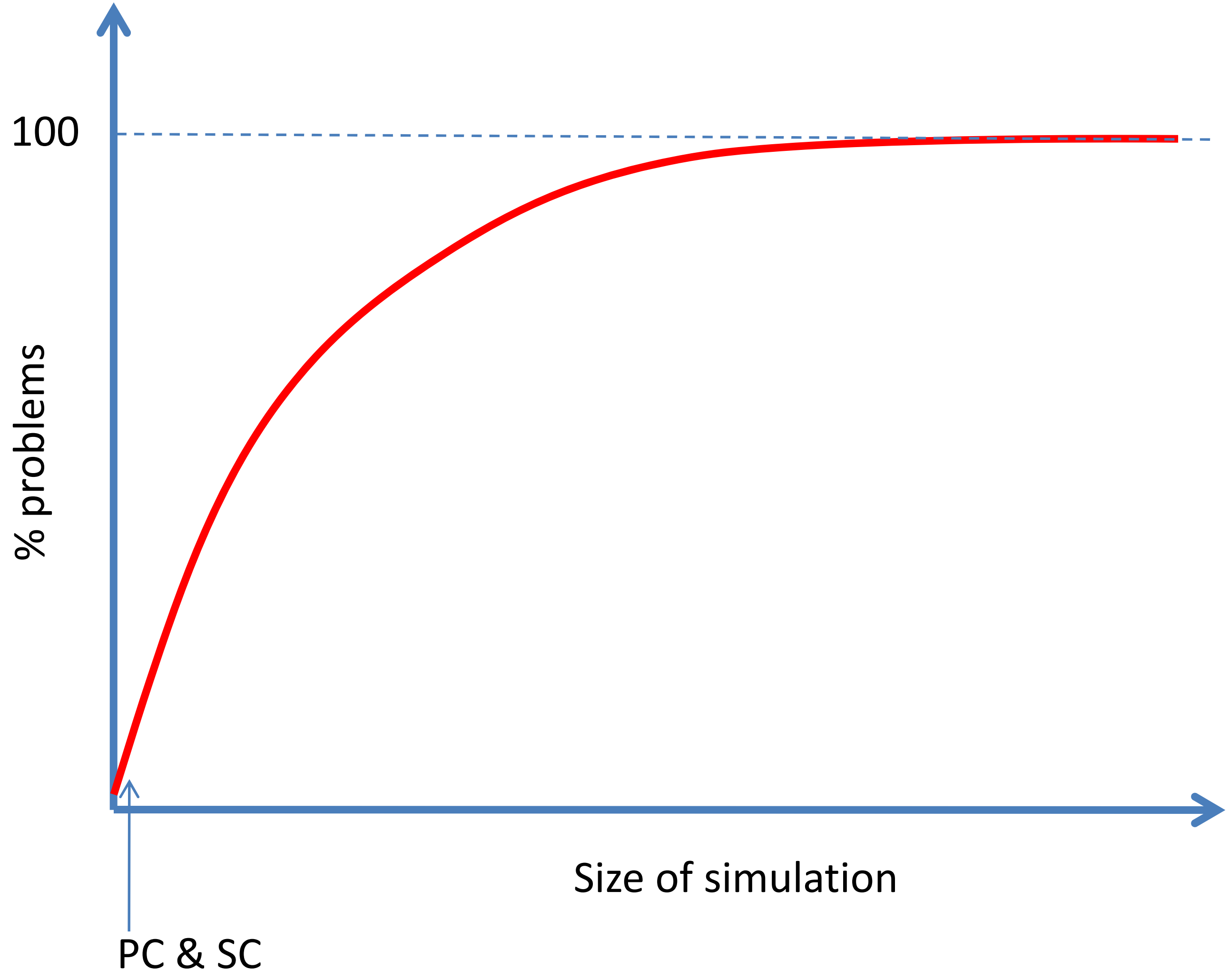
2D nonlinear, 3D linear PDEs



3D fluid mechanics or molecular dynamics



and some fields we don't even have equations to solve.



What does it mean?

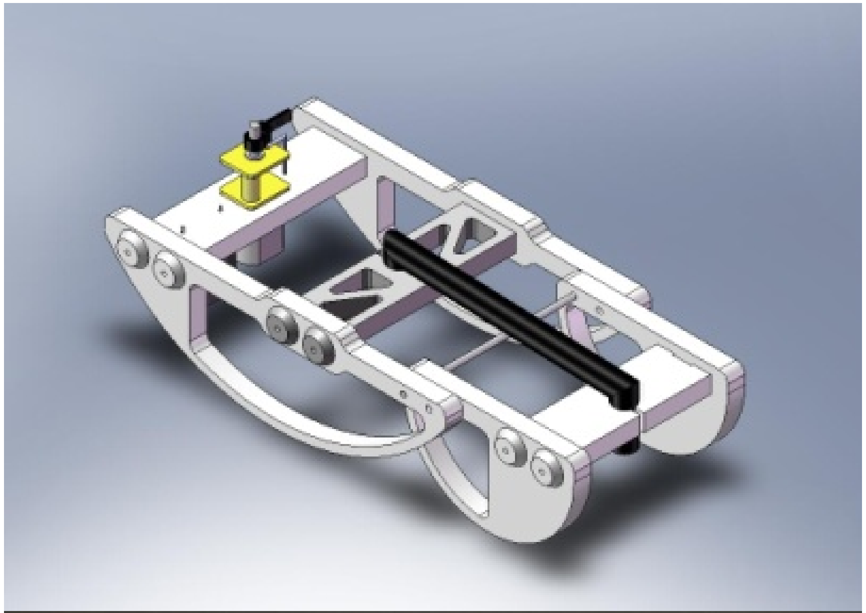
- Some fields, PC computing is a commodity (just like using a calculator for arithmetic).
- Just because most problems can be solved, doesn’t mean they have been. Lots of interesting math, physics, engineering problems. But make sure their interesting!
- Fields where PC computing is close to be a commodity have a lot of unsolved problems (research has not kept pace with advances in computing).
- If computation is a commodity (or close), strive for computational simplicity (and accuracy) over efficiency.
- Some problems just need large scale computing and infrastructure and will remain that way for decades.
- What will be possible in your field in 5 years, 10 years?

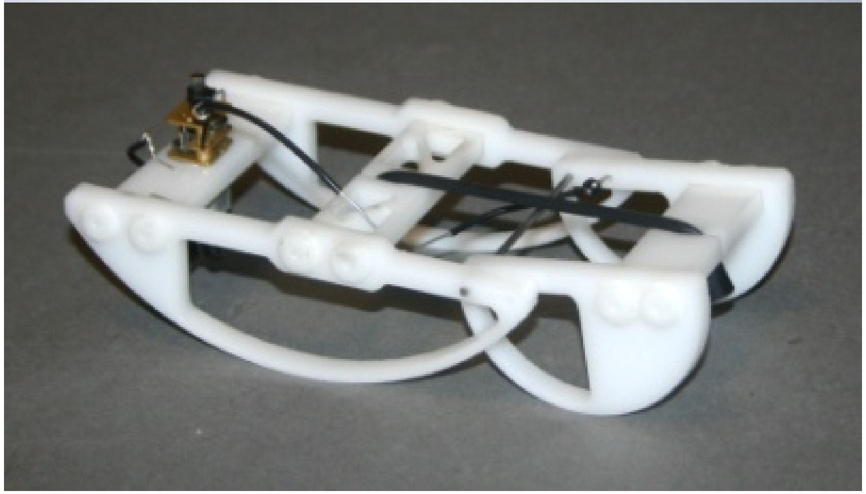
Computation and simulation in education

(both yours and the student)

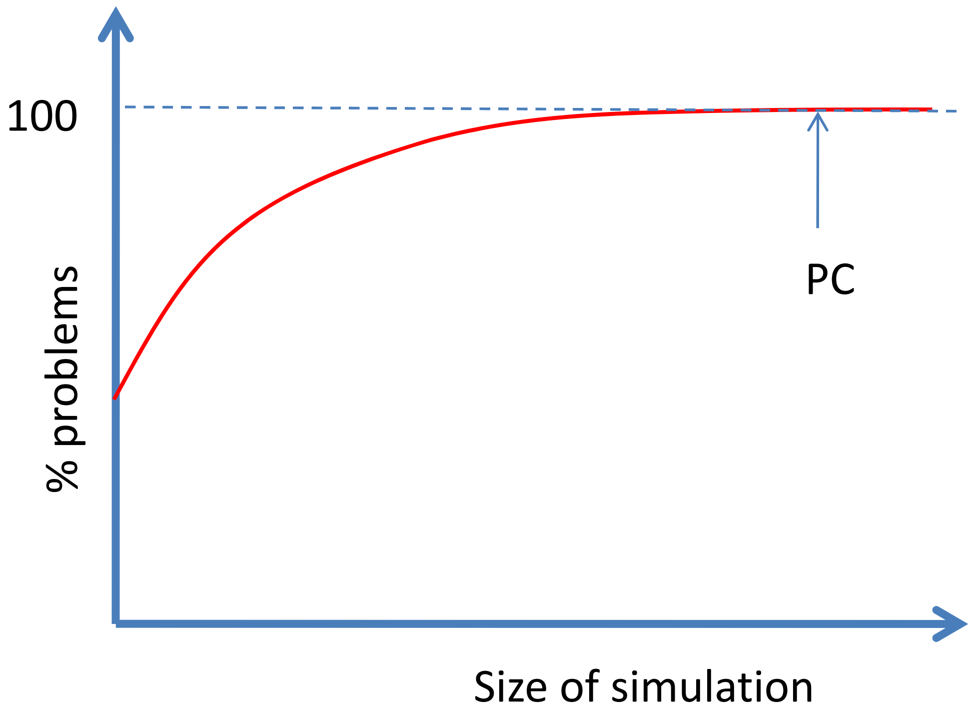
CAD/CAM

Migration from high-end platforms to the classroom





Courtesy Ben Linder, Olin



- If you can easily solve numerically, why learn the math?
- Teaching needs to recognize this reality.
- Don’t hold onto the past, but don’t abandon it.
- Simplicity should rule over efficiency.

“TEN DIGIT ALGORITHMS”

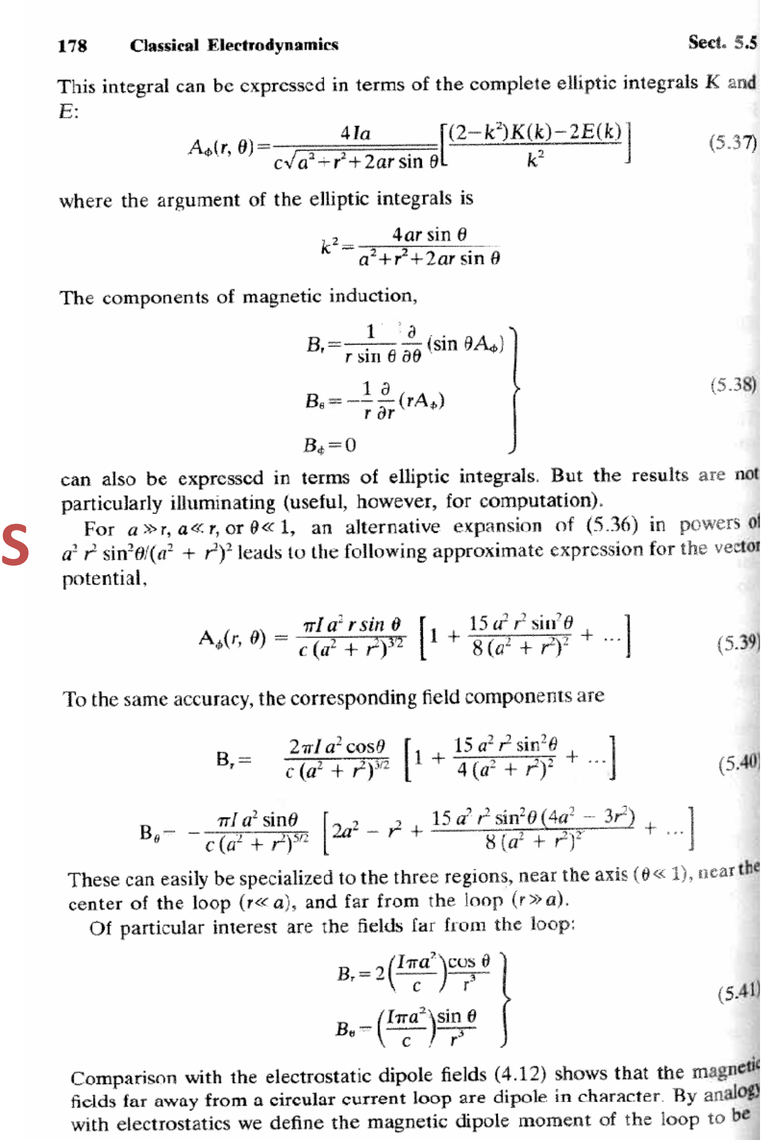
“Ten digits,
Five seconds,
And just one page. “

Lloyd Trefethen, Oxford University
http://web.comlab.ox.ac.uk/oucl/work/nick.trefethen/tda.html

Our visual bandwidth is extraordinary

http://web.mit.edu/8.02t/www/802TEAL3D/
TEAL project, MIT

VS



178 **Classical Electrodynamics** **Sect. 5.5**

This integral can be expressed in terms of the complete elliptic integrals K and E:

$$A_\phi(r,\theta)=\frac{4Ia}{c\sqrt{a^2+r^2+2ar\sin\theta}}\left[\frac{(2-k^2)K(k)-2E(k)}{k^2}\right] \tag{5.37}$$

where the argument of the elliptic integrals is

$$k^2=\frac{4ar\sin\theta}{a^2+r^2+2ar\sin\theta}$$

The components of magnetic induction,

$$\left.\begin{aligned} B_r&=\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\phi)\\ B_\theta&=-\frac{1}{r}\frac{\partial}{\partial r}(rA_\phi)\\ B_\phi&=0 \end{aligned}\right\} \tag{5.38}$$

can also be expressed in terms of elliptic integrals. But the results are not particularly illuminating (useful, however, for computation).

For $a \gg r$, $a \ll r$, or $\theta \ll 1$, an alternative expansion of (5.36) in powers of $a^2r^2\sin^2\theta/(a^2+r^2)^2$ leads to the following approximate expression for the vector potential,

$$A_\phi(r,\theta)=\frac{\pi I a^2 r\sin\theta}{c\,(a^2+r^2)^{3/2}}\left[1+\frac{15\,a^2r^2\sin^2\theta}{8\,(a^2+r^2)^2}+\dots\right] \tag{5.39}$$

To the same accuracy, the corresponding field components are

$$B_r=\frac{2\pi I a^2\cos\theta}{c\,(a^2+r^2)^{3/2}}\left[1+\frac{15\,a^2r^2\sin^2\theta}{4\,(a^2+r^2)^2}+\dots\right] \tag{5.40}$$

$$B_\theta=-\frac{\pi I a^2\sin\theta}{c\,(a^2+r^2)^{5/2}}\left[2a^2-r^2+\frac{15\,a^2r^2\sin^2\theta\,(4a^2-3r^2)}{8\,(a^2+r^2)^2}+\dots\right]$$

These can easily be specialized to the three regions, near the axis ($\theta \ll 1$), near the center of the loop ($r \ll a$), and far from the loop ($r \gg a$).

Of particular interest are the fields far from the loop:

$$\left.\begin{aligned} B_r&=2\left(\frac{I\pi a^2}{c}\right)\frac{\cos\theta}{r^3}\\ B_\theta&=\left(\frac{I\pi a^2}{c}\right)\frac{\sin\theta}{r^3} \end{aligned}\right\} \tag{5.41}$$

Comparison with the electrostatic dipole fields (4.12) shows that the magnetic fields far away from a circular current loop are dipole in character. By analogy with electrostatics we define the magnetic dipole moment of the loop to be

Jackson, Classical Electrodynamics

Cellular biology

Inner life of the cell

vs

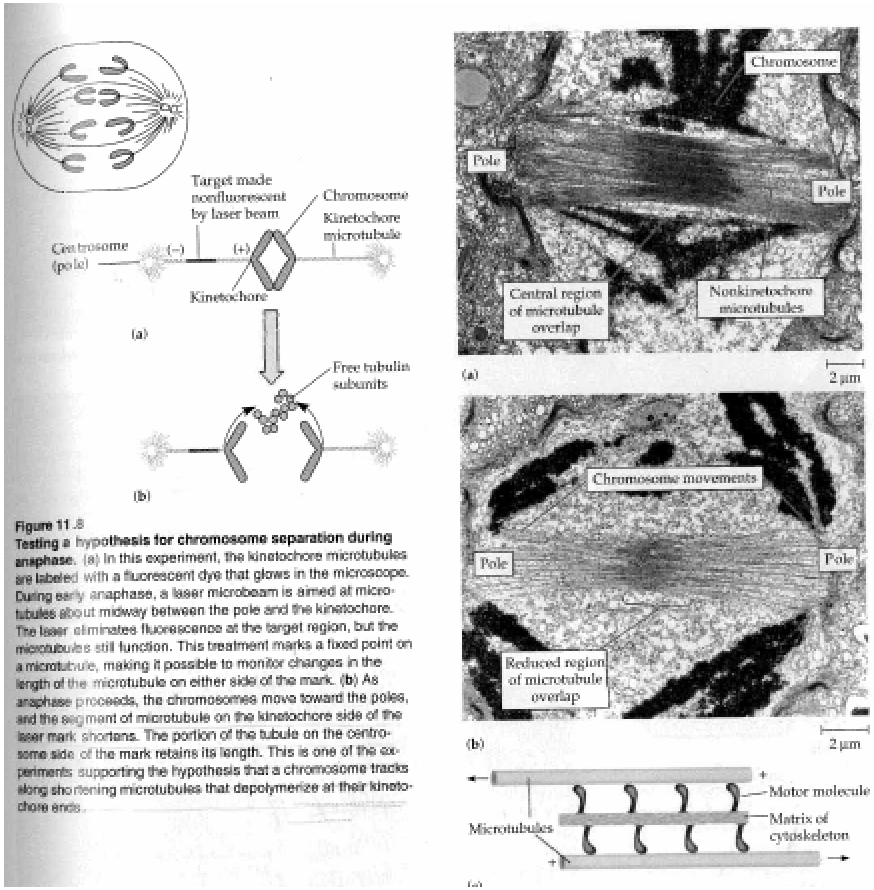


Figure 11.8

Testing a hypothesis for chromosome separation during anaphase. (a) In this experiment, the kinetochore microtubules are labeled with a fluorescent dye that glows in the microscope. During early anaphase, a laser microbeam is aimed at microtubules about midway between the pole and the kinetochore. The laser eliminates fluorescence at the target region, but the microtubules still function. This treatment marks a fixed point on a microtubule, making it possible to monitor changes in the length of the microtubule on either side of the mark. **(b)** As anaphase proceeds, the chromosomes move toward the poles, and the segment of microtubule on the kinetochore side of the laser mark shortens. The portion of the tubule on the centrosome side of the mark retains its length. This is one of the experiments supporting the hypothesis that a chromosome tracks along shortening microtubules that depolymerize at their kinetochore ends.

Conclusions

- Computation has fundamentally changed science and engineering.
- Computation has changed education, but today's technology is untapped.
- Let go of (but don't forget) the past.
- Extrapolate Moore's law 5 and 10 years. What will the future hold in your field?
- Don't build too much expertise that will soon be irrelevant.
- Don't solve problems, just because you can.