High Performance Computing and Computational Science

MPCS51087

Spring, 2022

Counting Problem

- What is chance that two people in this room have same birthday?

- How do we carry out an experiment to find the answer?

Numerical Experiment

```
for each experiment m
  for each student n
     select random number 1…365

  if match
    counter++

probability = counter/m
```

Implementation (*Code*)

```
function [ p ] = birthday( n, m )
count = 0;

for i=1:m
    r = randi(365,n,1);
    if (numel(unique(r)) ~= numel(r))
        count = count + 1;
    end
end

p = count/m;
end
```

Some Questions

- Under what conditions will the experimental result converge to the true expected value?
- What is the rate of convergence?
- How can a computer generate *random numbers*?
- How can this be efficiently implemented on a digital computer?
- What hardware and programming model abstractions are appropriate?
- Can I use the tool to solve my problem <u>well enough</u>?

The Monty Hall Problem

- Choose one of the three doors
- The grand prize is behind one of the doors
- The other doors have consolation gifts (pig)

- You choose door 1, for example

- Monte reveals a pig behind one of other doors (3)

- Monte gives option of switching to 2 or staying with 1

Do you switch?

Numerical Experiment

For each experiment ***m***

-select prize door ***x***: URN 1..3

-select audience choice ***y***: URN 1..3

-select Monte Hall reveal ***z***: Randomly not ***x*** or ***y***

-update audience choice to not **y** or ***z***

-if choice == ***x***

increment ***wins***

end

probability = ***win***/***m***

Matlab Code

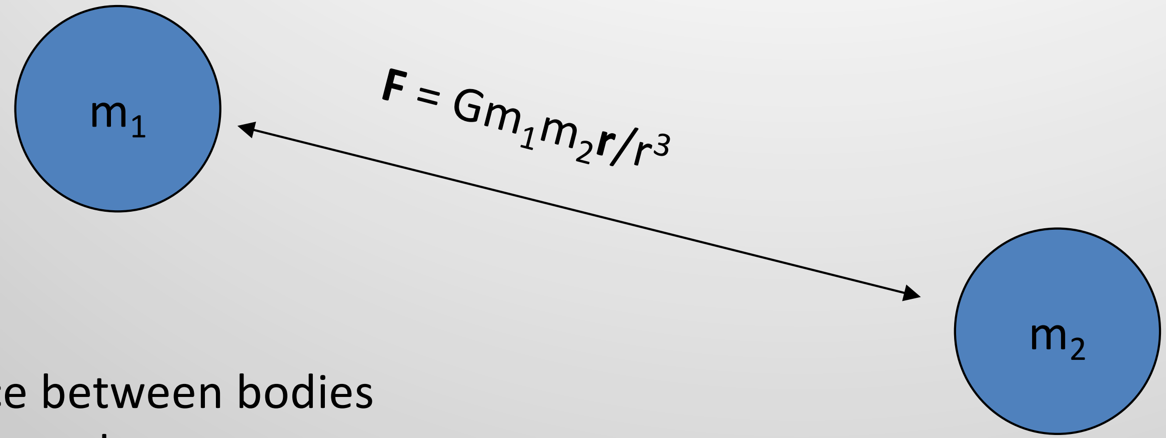
```
function win = MonteHall(method)
% method = 1: stay with original guess
% method = 2: switch after Hall reveal

x = randi([1 3]);                  %prize door
y = randi([1 3]);                  %audience choice
z = setdiff([1 2 3],[x y]); %monte hall reveal
z = z(randi([1 numel(z)]));
if (method ~= 1)
    y = setdiff([1 2 3],[y z]);
end
if (y == x)
    win = true;
end
```

Numerical experiments and Big Computers – n-body problem

Two-body Gravitational Attraction

This is a completely integrable, non-chaotic system.

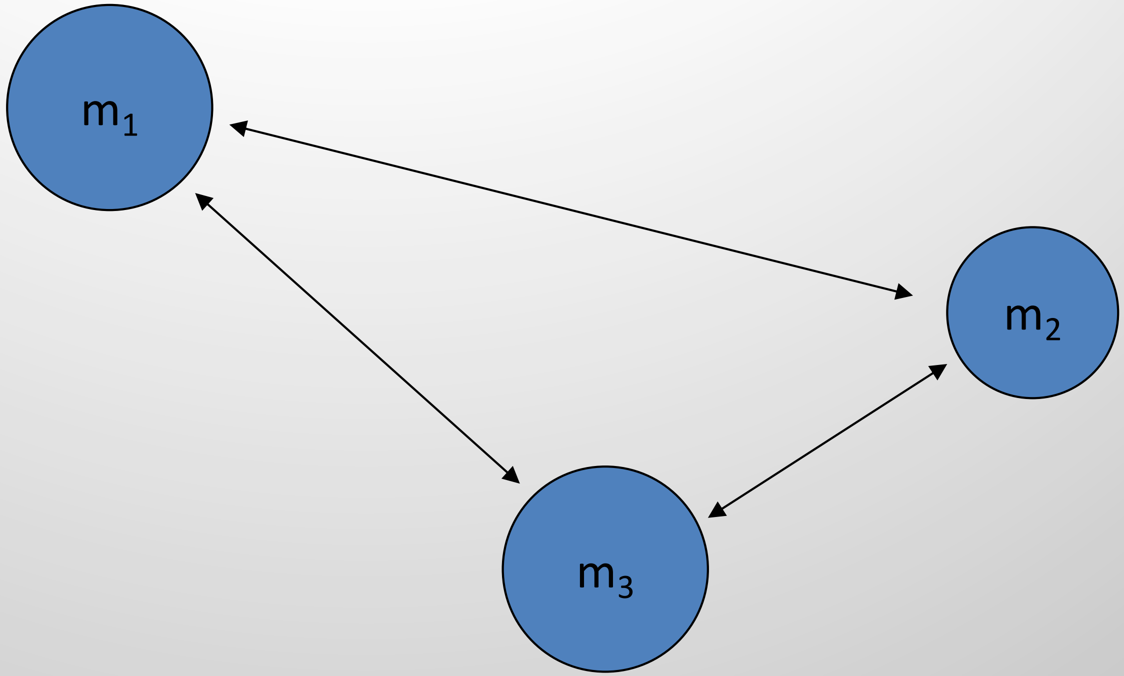


F: Force between bodies
G: universal constant
m_1: mass of first body
m_2: mass of second body
r: position vector = (x,y)
r: scalar distance

$\Longrightarrow$

$\mathbf{a} = \mathbf{F}/m$	**a**:acceleration
$\delta\mathbf{v} = \mathbf{a}\,\delta\mathbf{t} + \mathbf{v_o}$	**v:** velocity
$\delta\mathbf{x} = \mathbf{v}\,\delta t + \mathbf{x}_0$	**x**: position

Three-body problem



Case for three-bodies

$$\mathbf{F}_1 = Gm_1m_2\mathbf{r}_{1,2}/r^2 + Gm_1m_3\mathbf{r}_{1,3}/r^2$$

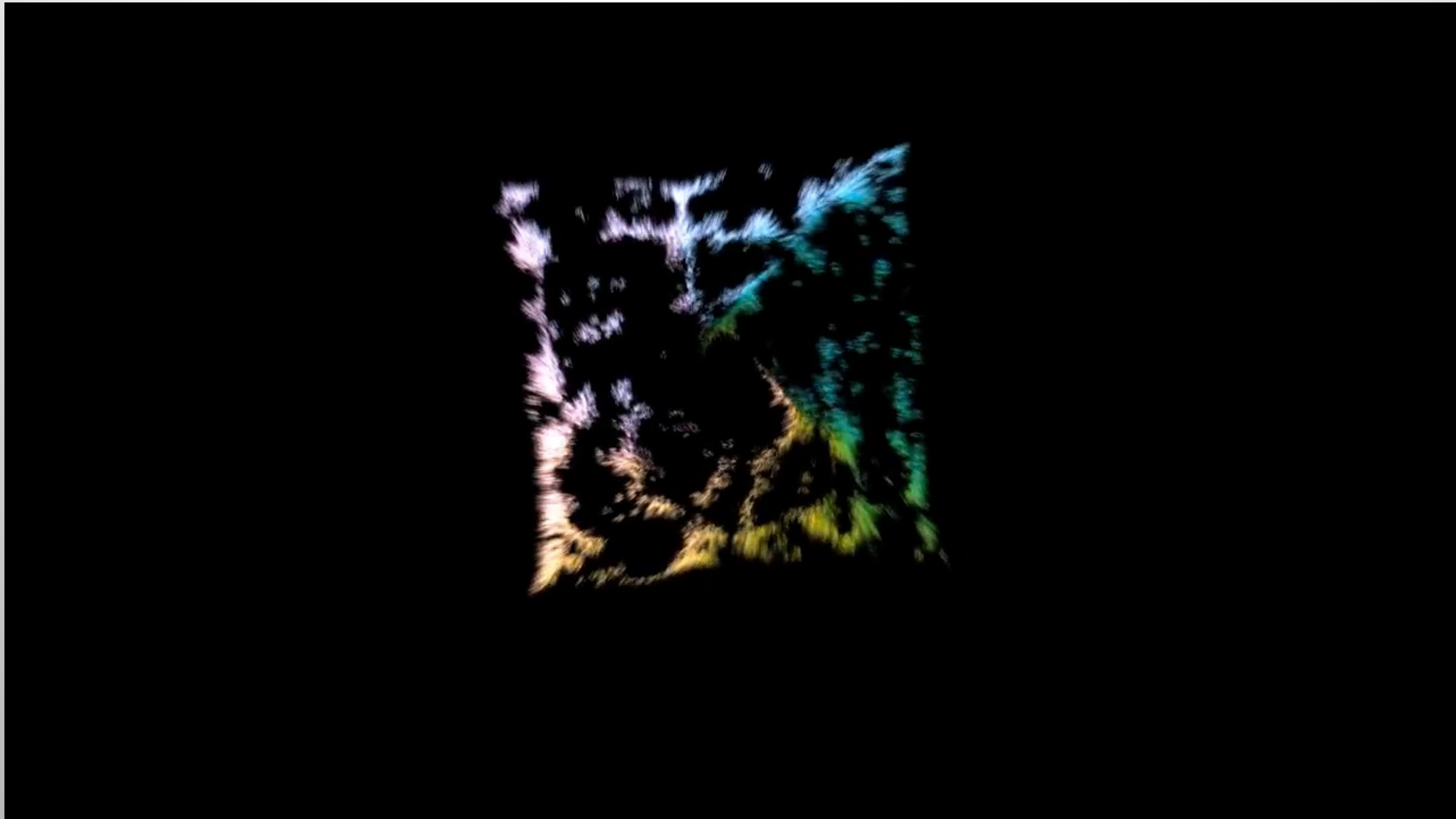
$$\mathbf{F}_2 = Gm_2m_1\mathbf{r}_{2,1}/r^2 + Gm_2m_3\mathbf{r}_{2,3}/r^2$$

$$\mathbf{F}_3 = Gm_3m_1\mathbf{r}_{3,1}/r^2 + Gm_3m_2\mathbf{r}_{3,2}/r^2$$

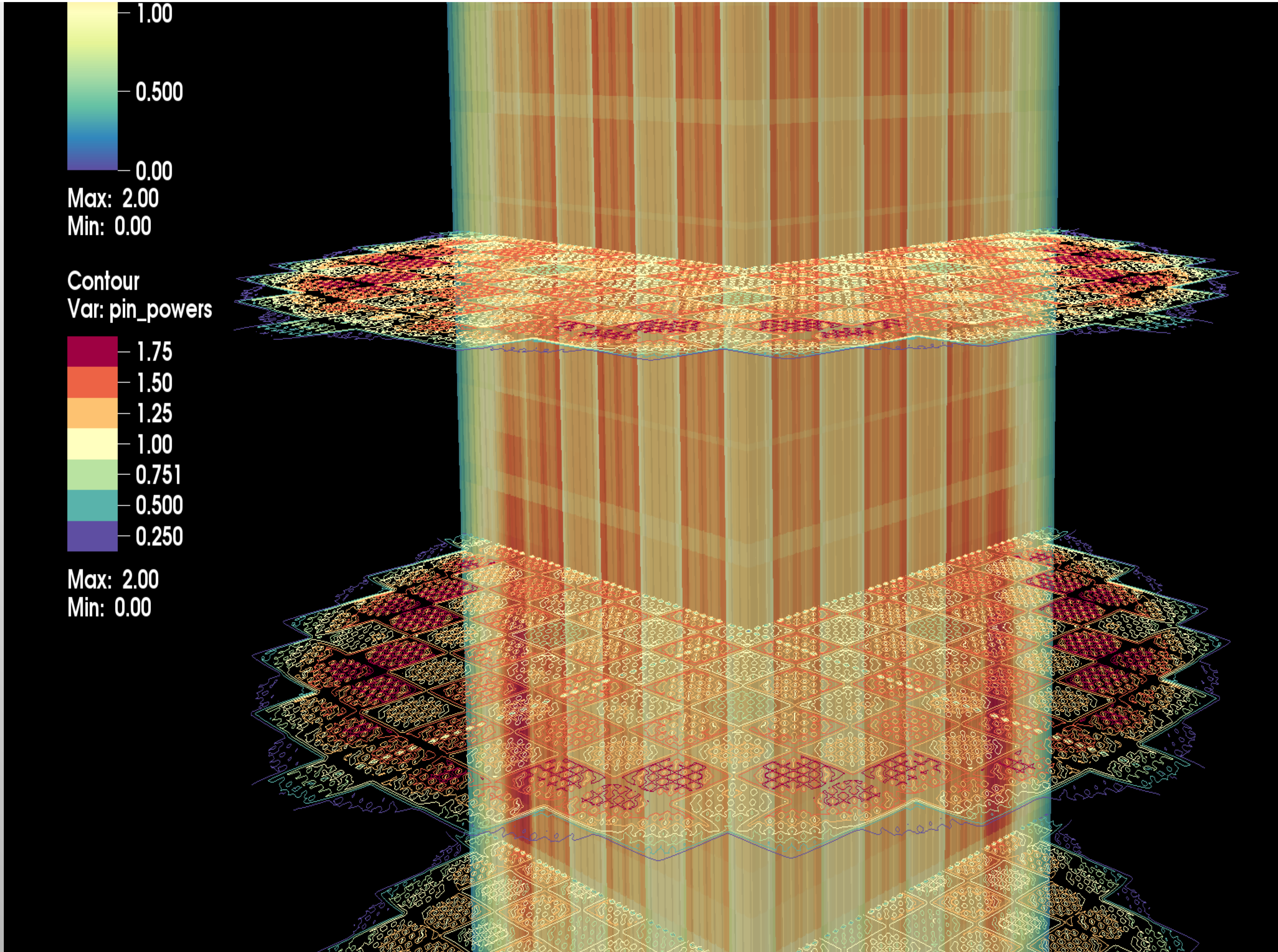
General case for n-bodies

$$\mathbf{F}_n = \Sigma_k Gm_nm_k\mathbf{r}_{n,k}/r^2$$

Gravitational Collapse



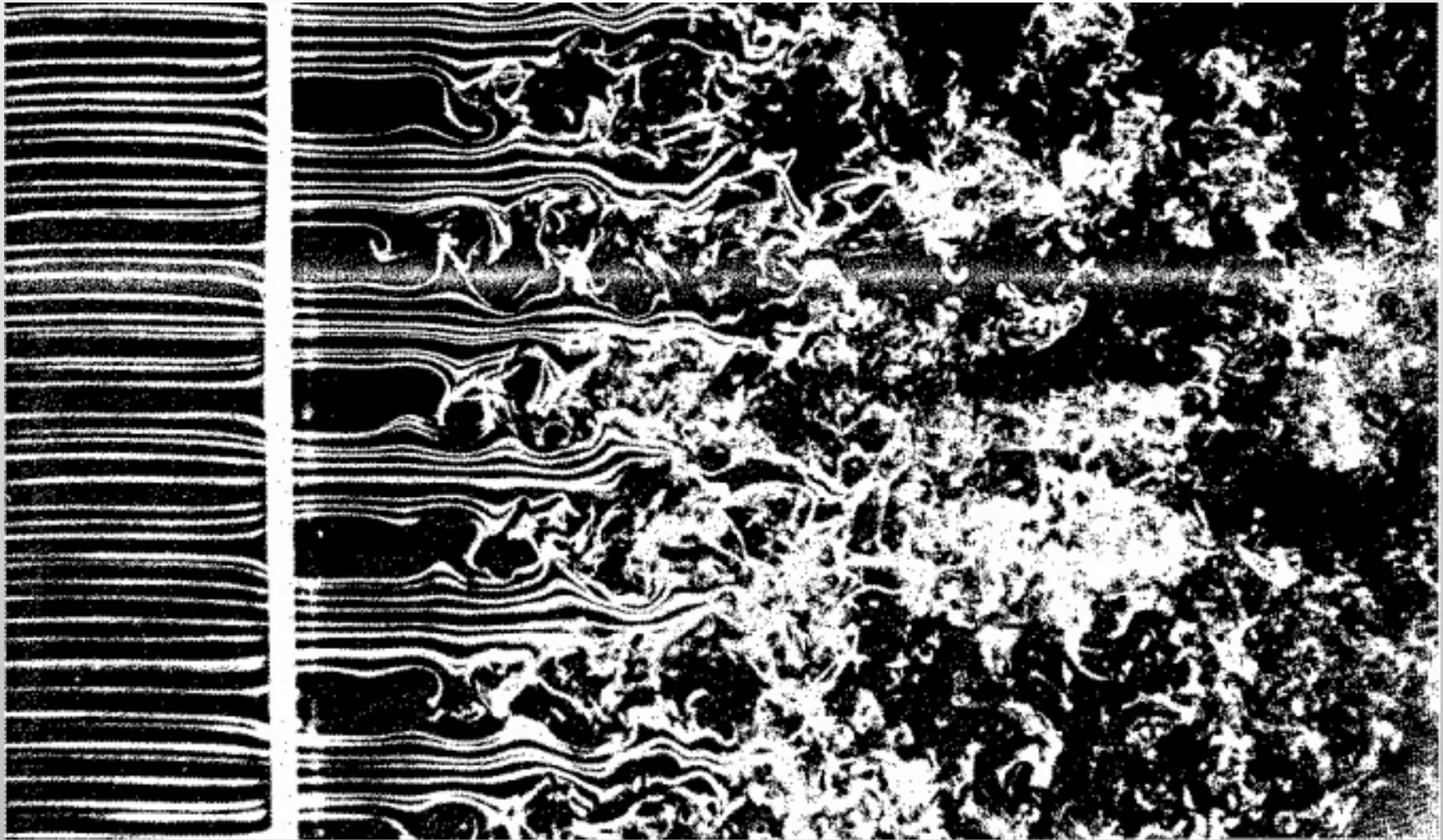
Numerical experiments and Big Computers – neutron population in a power reactor



1.00
0.500
0.00
Max: 2.00
Min: 0.00
Contour
Var: pin_powers
1.75
1.50
1.25
1.00
0.751
0.500
0.250
Max: 2.00
Min: 0.00

Numerical experiments and Big Computers – fluid flow

Turbulent Flow



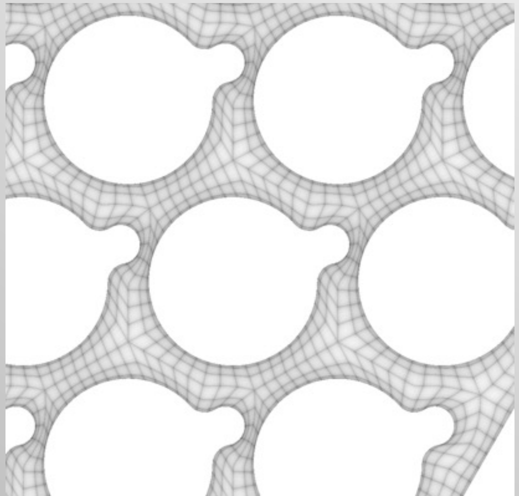
Van Dyke, “An Album of Fluid Motion”

PDE Example: Fluid flow

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}$$

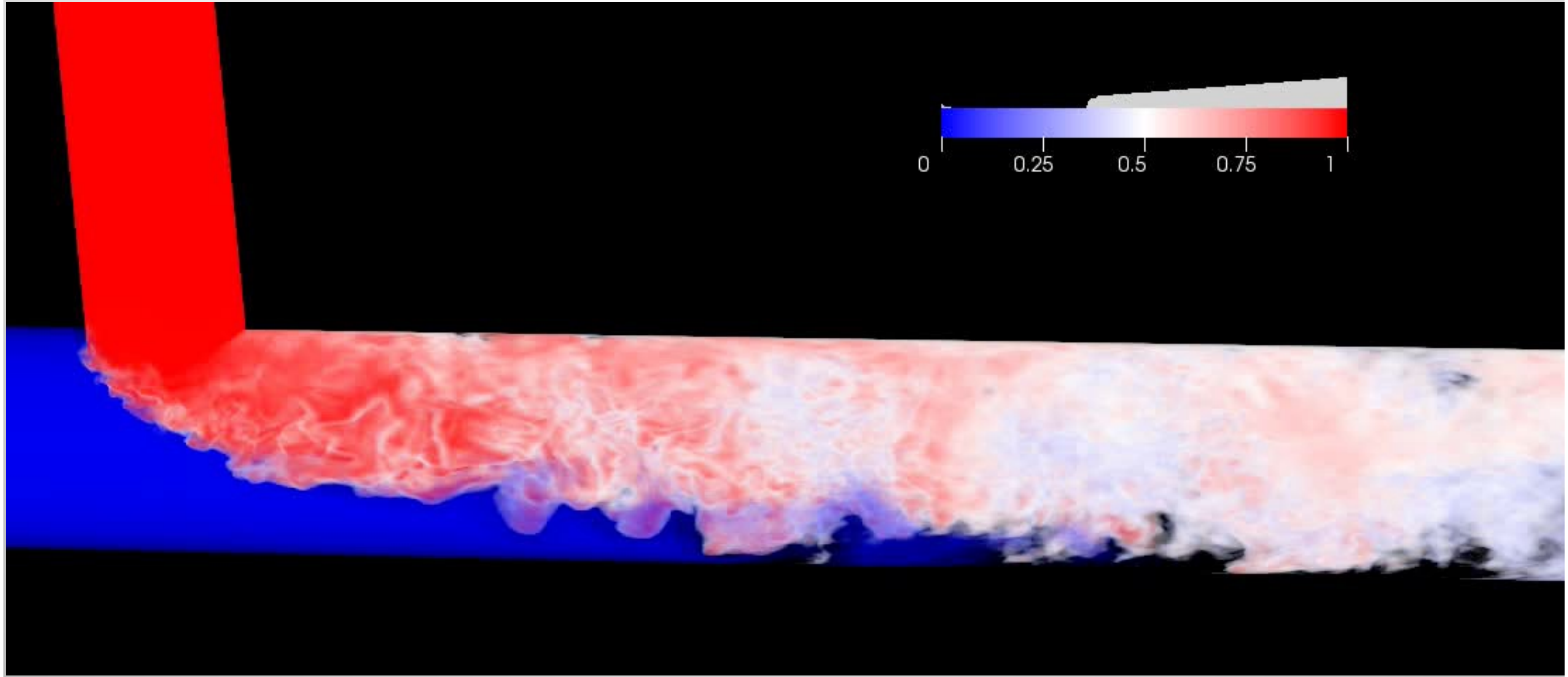
$$\nabla \cdot \mathbf{u} = 0$$

- *u(x,y,z,t): Fluid Velocity*
- *P(x,y,z,t): Fluid pressure*

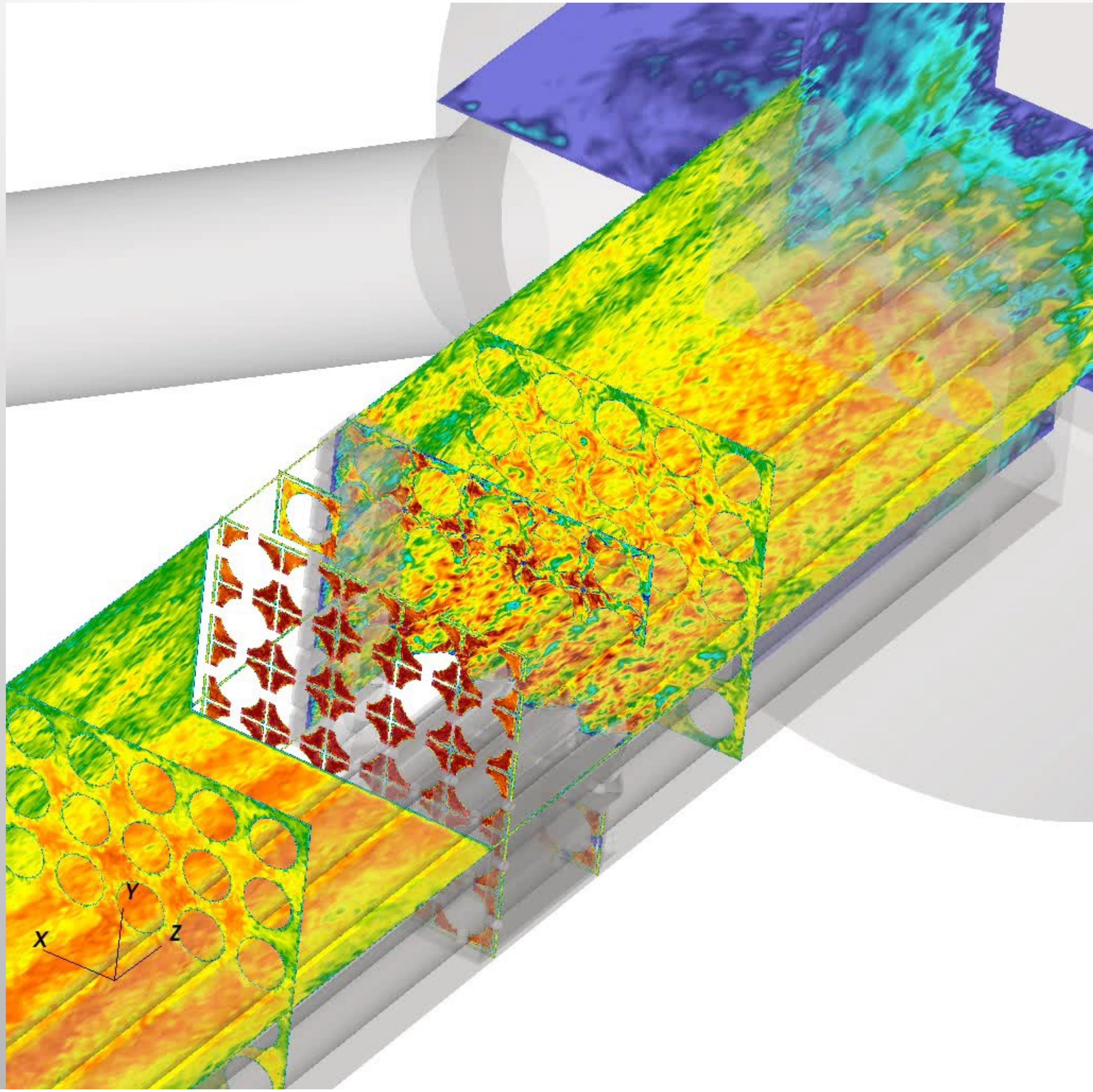


Big whirls have little whirls which feed upon their velocity
and little whirls have lesser whirls and so on to viscosity
-L.F. Richardson

T-Junction Benchmark

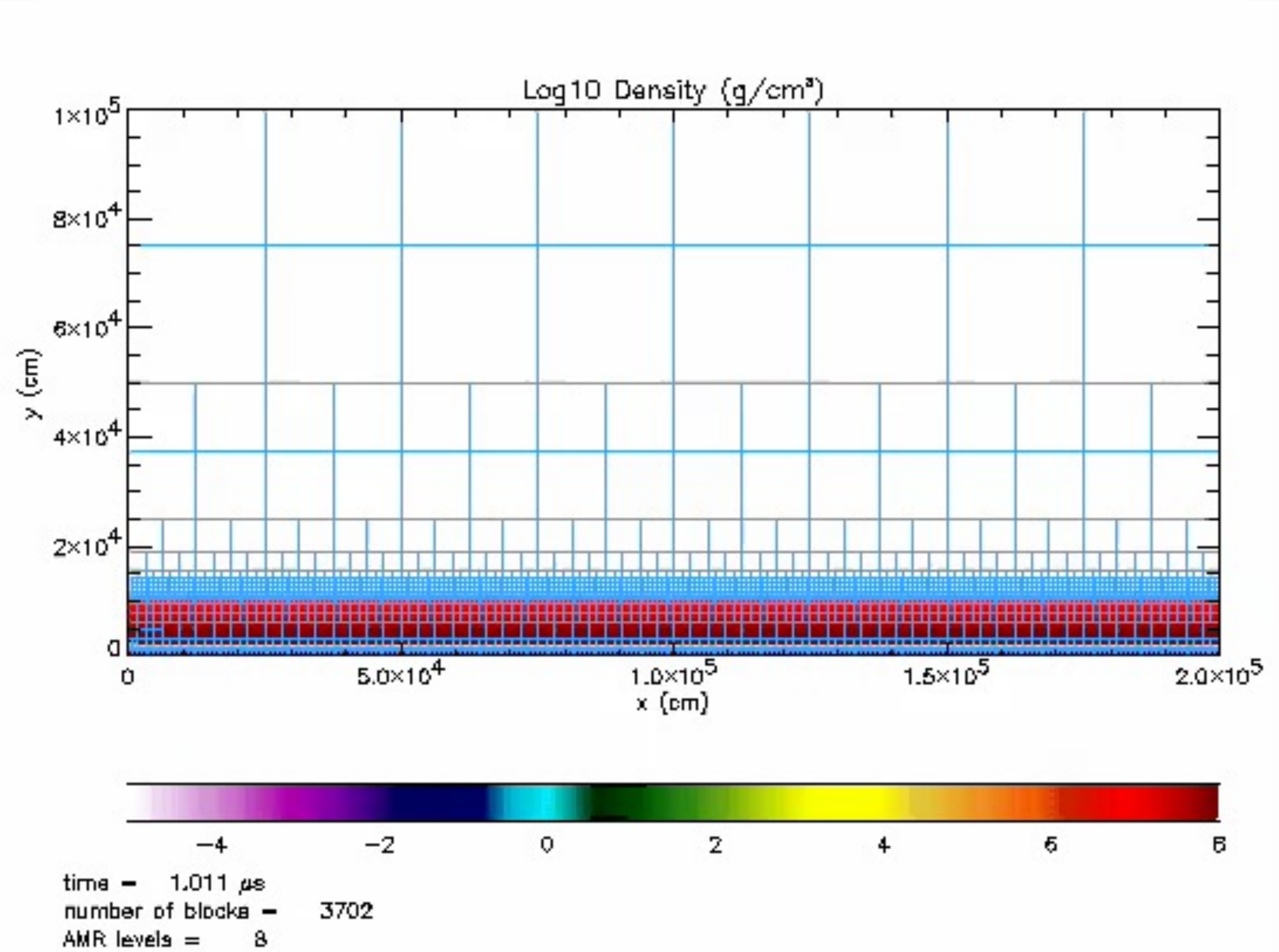


Coolant flow in Modular Reactor Core



Numerical experiments and Big Computers – exploding stars

X-ray burst on surface of neutron star



"An important development in sciences is occurring at the intersection of computer science and the sciences that has the potential to have a profound impact on science. It is a leap from the application of computing … to the *integration of computer science concepts, tools, and theorems* into the very fabric of science." -*Science* 2020 Report, March 2006

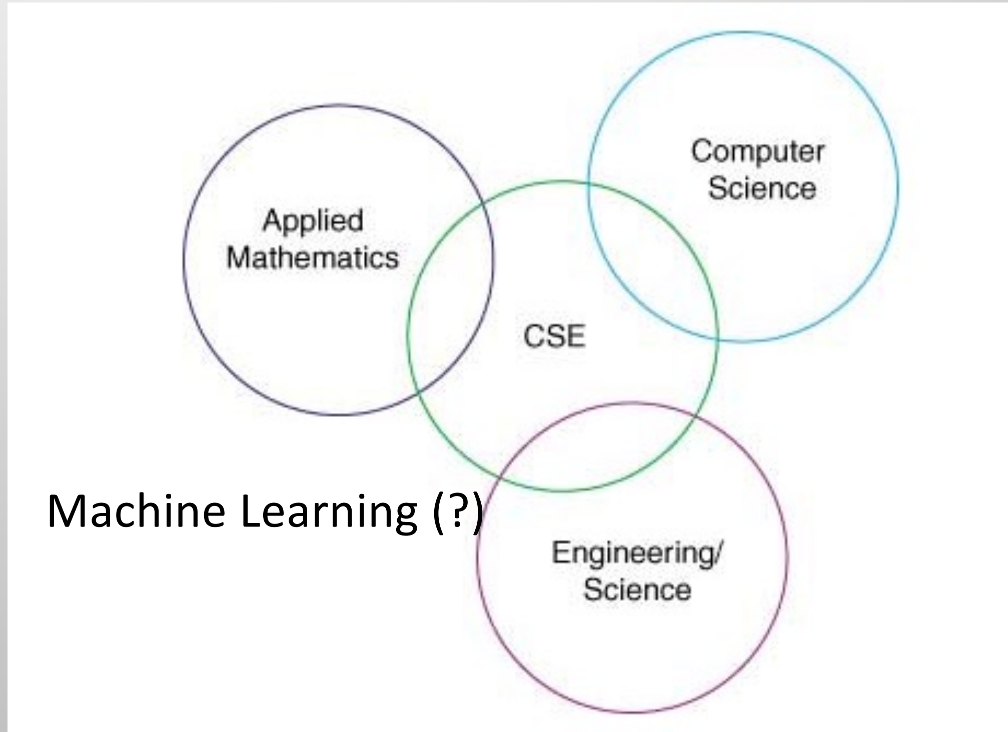
Nature, March 23, 2006

2020
SCIENCE

SIAM Report on Computational Science

"CSE is a broad multidisciplinary area that encompasses applications in science and engineering, applied mathematics, numerical analysis, and computer science. Computer models and computer simulations have become an important part of the research repertoire, supplementing (and in some cases replacing) experimentation. Going from application area to computational results requires domain expertise, mathematical modeling, numerical analysis, algorithm development, software implementation, program execution, analysis, validation and visualization of results. CSE involves all of this."

"Numerical simulation enables the study of complex systems and natural phenomena that would be too expensive or dangerous, or even impossible, to study by direct experimentation. The quest for ever higher levels of detail and realism in such simulations requires enormous computational capacity, and has provided the impetus for dramatic breakthroughs in computer algorithms and architectures."



Supercomputers

Expert Predictions

- "I think there is a world market for maybe five computers."
  - Thomas Watson, chairman of IBM, 1943.
- "There is no reason for any individual to have a computer in their home"
  - Ken Olson, president and founder of Digital Equipment Corporation, 1977.
- "640K [of memory] ought to be enough for anybody."
  - Bill Gates, chairman of Microsoft,1981.
- "On several recent occasions, I have been asked whether parallel computing will soon be relegated to the trash heap reserved for promising technologies that never quite make it."
  - Ken Kennedy, CRPC Director, 1994

Slide source: Warfield et al.

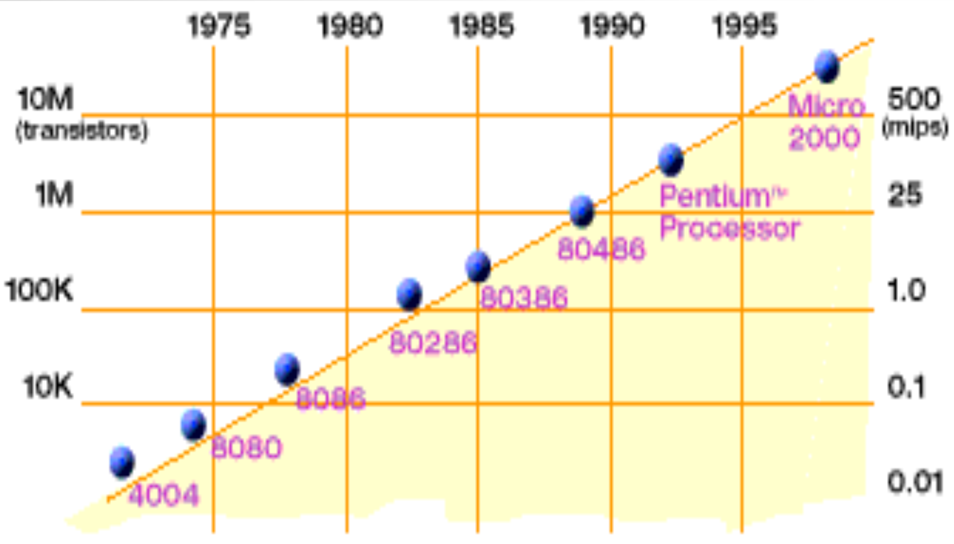
Units of Measure

- High Performance Computing (HPC) units are:
  - Flop: floating point operation, usually double precision unless noted
  - Flop/s: floating point operations per second
  - Bytes: size of data
  - Typical sizes are millions, billions, trillions…

Mega	**Mflop/s = 10^6 flop/sec**	**Mbyte = 2^{20} ~ 10^6 bytes**
Giga	**Gflop/s = 10^9 flop/sec**	**Gbyte = 2^{30} ~ 10^9 bytes**
Tera	**Tflop/s = 10^{12} flop/sec**	**Tbyte = 2^{40} ~ 10^{12} bytes**
Peta	**Pflop/s = 10^{15} flop/sec**	**Pbyte = 2^{50} ~ 10^{15} bytes**
Exa	**Eflop/s = 10^{18} flop/sec**	**Ebyte = 2^{60} ~ 10^{18} bytes**
Zetta	**Zflop/s = 10^{21} flop/sec**	**Zbyte = 2^{70} ~ 10^{21} bytes**
Yotta	**Yflop/s = 10^{24} flop/sec**	**Ybyte = 2^{80} ~ 10^{24} bytes**

- Current fastest machine
  - 442 PFlop/s (“petaflops” measured on HPL)
  - Fugaku at RIKEN Center, Japan
  - Up-to-date lists of fastest machines at www.top500.org

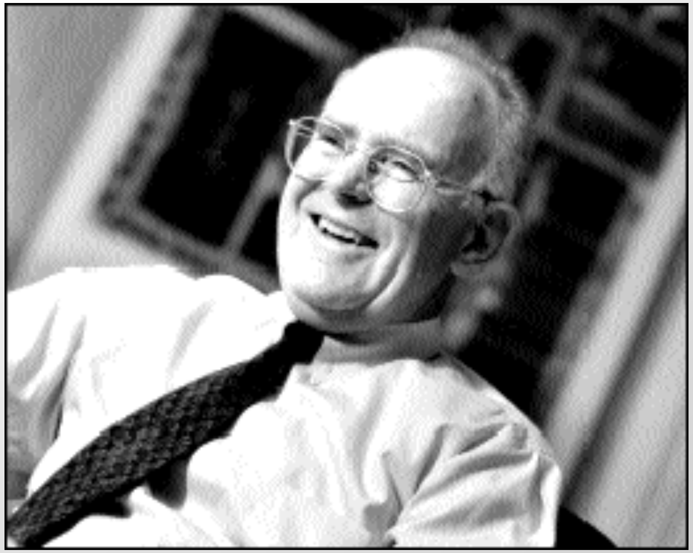
Technology Trends: Microprocessor Capacity



2X transistors/Chip Every 2 years

Called "Moore's Law"

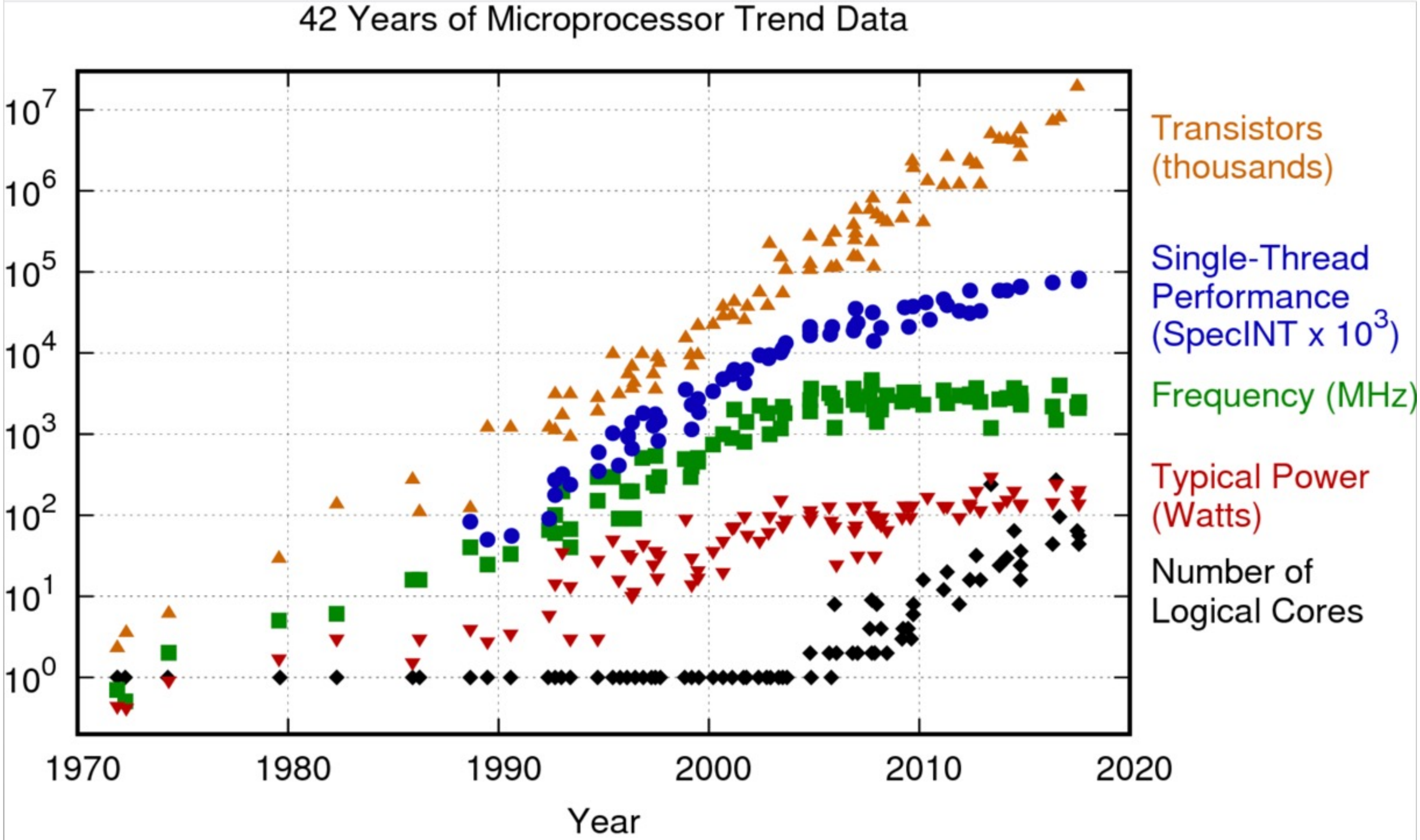
Microprocessors have become smaller, denser, and more powerful.



Gordon Moore (co-founder of Intel) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 2 years.

Slide source: Jack Dongarra

Microprocessor Transistors / Clock (1970-2020)



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2017 by K. Rupp

Top 10 Fastest Computers

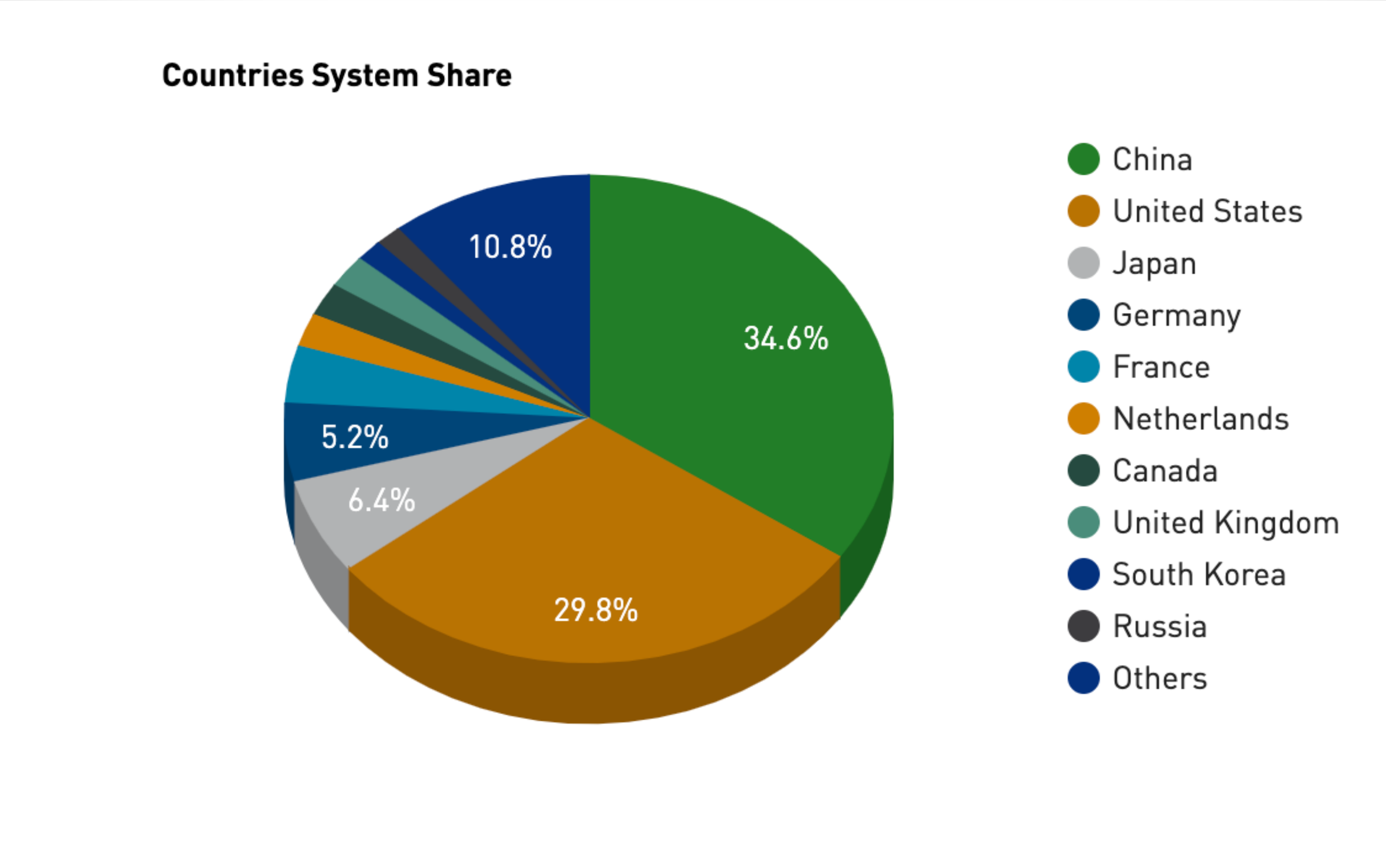
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
5	**Perlmutter** - HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE DOE/SC/LBNL/NERSC United States	761,856	70,870.0	93,750.0	2,589

6	**Selene** - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	555,520	63,460.0	79,215.0	2,646
7	**Tianhe-2A** - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000, NUDT National Super Computer Center in Guangzhou China	4,981,760	61,444.5	100,678.7	18,482
8	**JUWELS Booster Module** - Bull Sequana XH2000 , AMD EPYC 7402 24C 2.8GHz, NVIDIA A100, Mellanox HDR InfiniBand/ParTec ParaStation ClusterSuite, Atos Forschungszentrum Juelich (FZJ) Germany	449,280	44,120.0	70,980.0	1,764
9	**HPC5** - PowerEdge C4140, Xeon Gold 6252 24C 2.1GHz, NVIDIA Tesla V100, Mellanox HDR Infiniband, DELL EMC Eni S.p.A. Italy	669,760	35,450.0	51,720.8	2,252
10	**Voyager-EUS2** - ND96amsr_A100_v4, AMD EPYC 7V12 48C 2.45GHz, NVIDIA A100 80GB, Mellanox HDR Infiniband, Microsoft Azure Azure East US 2 United States	253,440	30,050.0	39,531.2	

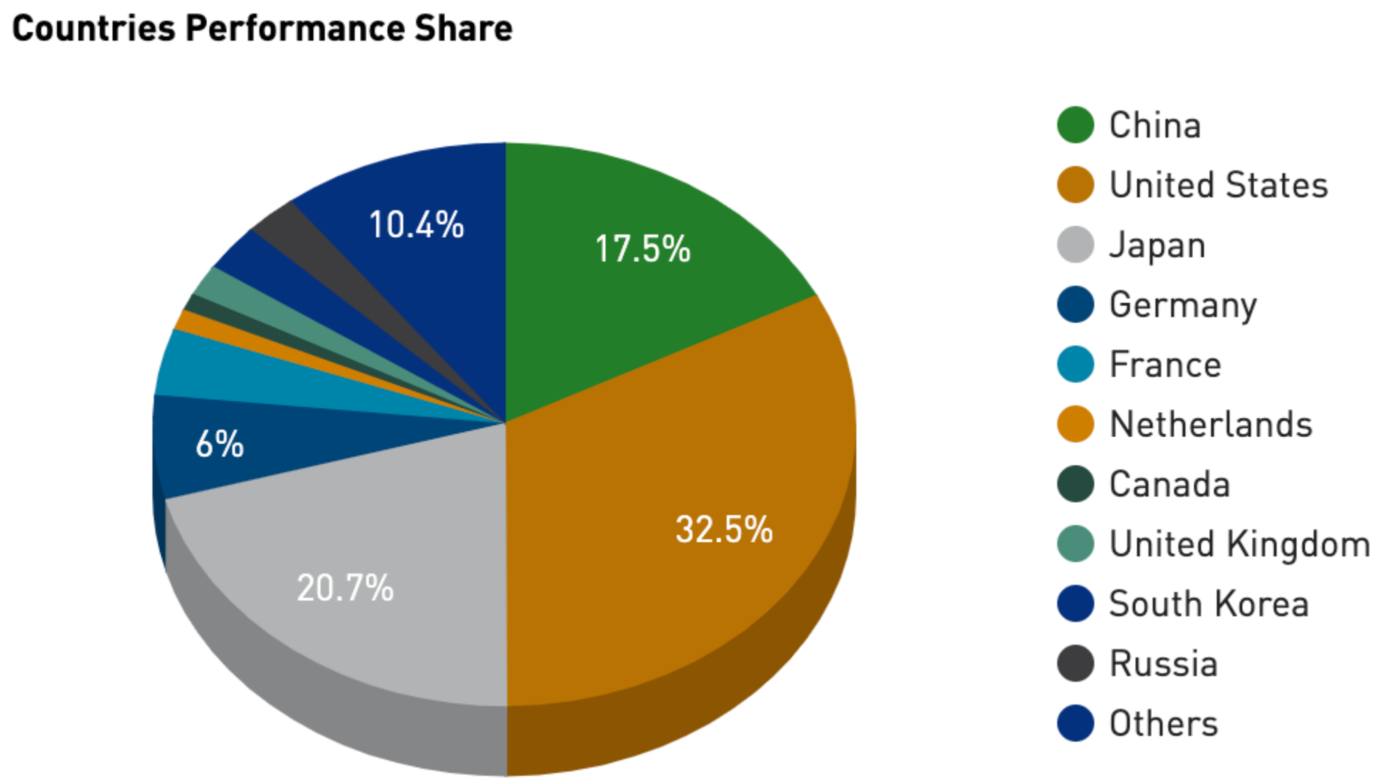
Going Beyond Linpack -- HPCG

Rank	TOP500 Rank	System	Cores	Rmax (TFlop/s)	HPCG (TFlop/s)
1	1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	16004.50
2	2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	2925.75
3	5	**Perlmutter** - HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE DOE/SC/LBNL/NERSC United States	706,304	64,590.0	1905.44
4	3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	1795.67
5	6	**Selene** - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	555,520	63,460.0	1622.51

Number of computers on top 500 list by country

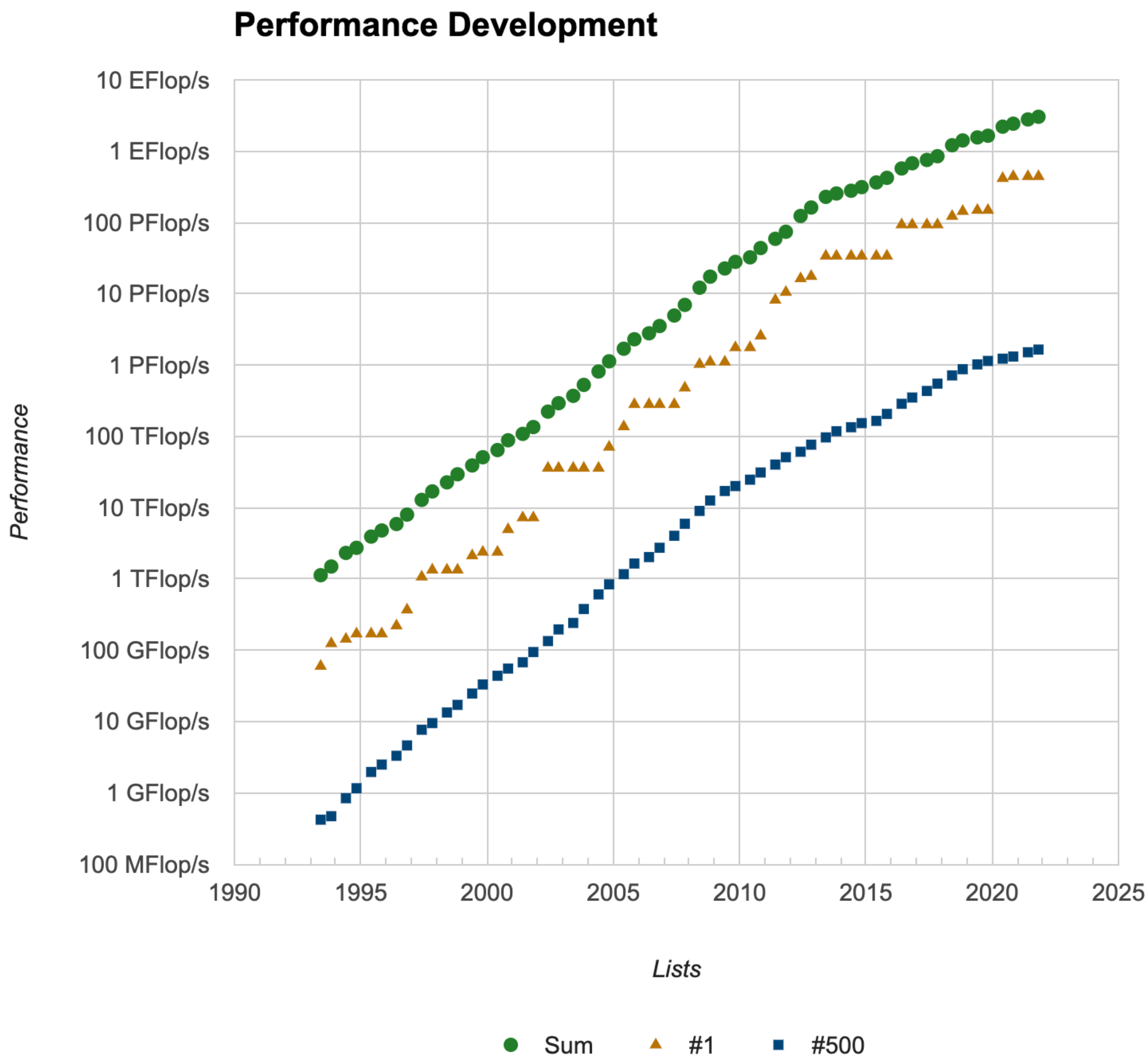


Aggregate performance of top 500



Historical Performance

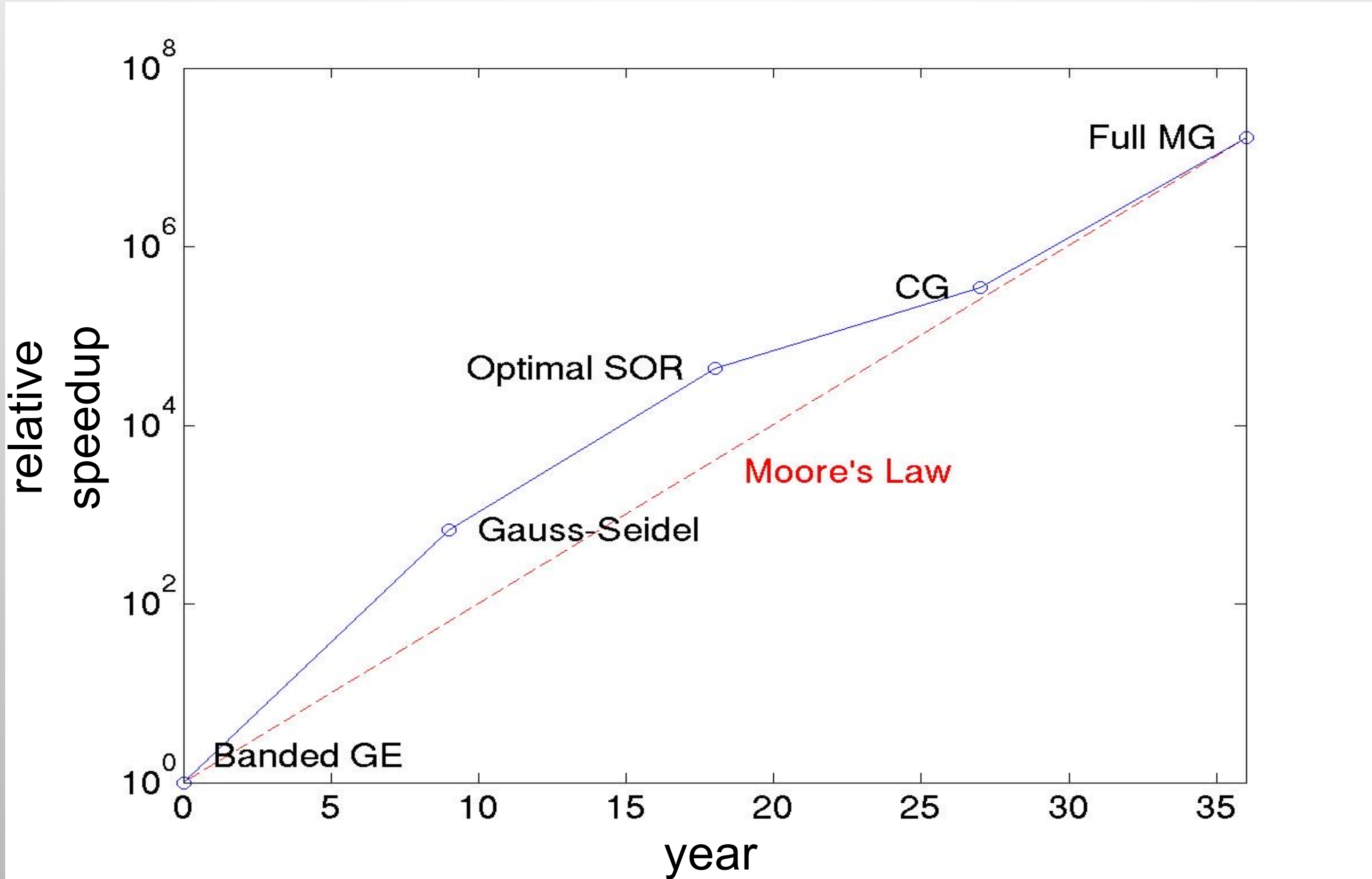
Question: what year was the fastest computer equal to a present-day commodity desktop system?



Performance Development
10 EFlop/s
1 EFlop/s
100 PFlop/s
10 PFlop/s
1 PFlop/s
100 TFlop/s
10 TFlop/s
1 TFlop/s
100 GFlop/s
10 GFlop/s
1 GFlop/s
100 MFlop/s
Performance
1990
1995
2000
2005
2010
2015
2020
2025
Lists
Sum
#1
#500

It's not all about architectures

- This advance took place over a span of about 36 years, or 24 doubling times for Moore's Law
- $2^{24} \approx 16$ million $\Rightarrow$ the same as the factor from algorithms alone!



Final Words

*“**Computational science** and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics and computer science. CSE focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems. We believe that CSE will play an important if not dominating role for the future of the scientific discovery process and engineering design.*” –SIAM report