Large Scale Simulation on Clusters using COMSOL 4.2

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Outline

- Introduction and History
- What is a cluster?
- Simulation results
  1. Test problems
  2. Criteria
  3. Evaluations
- What's coming

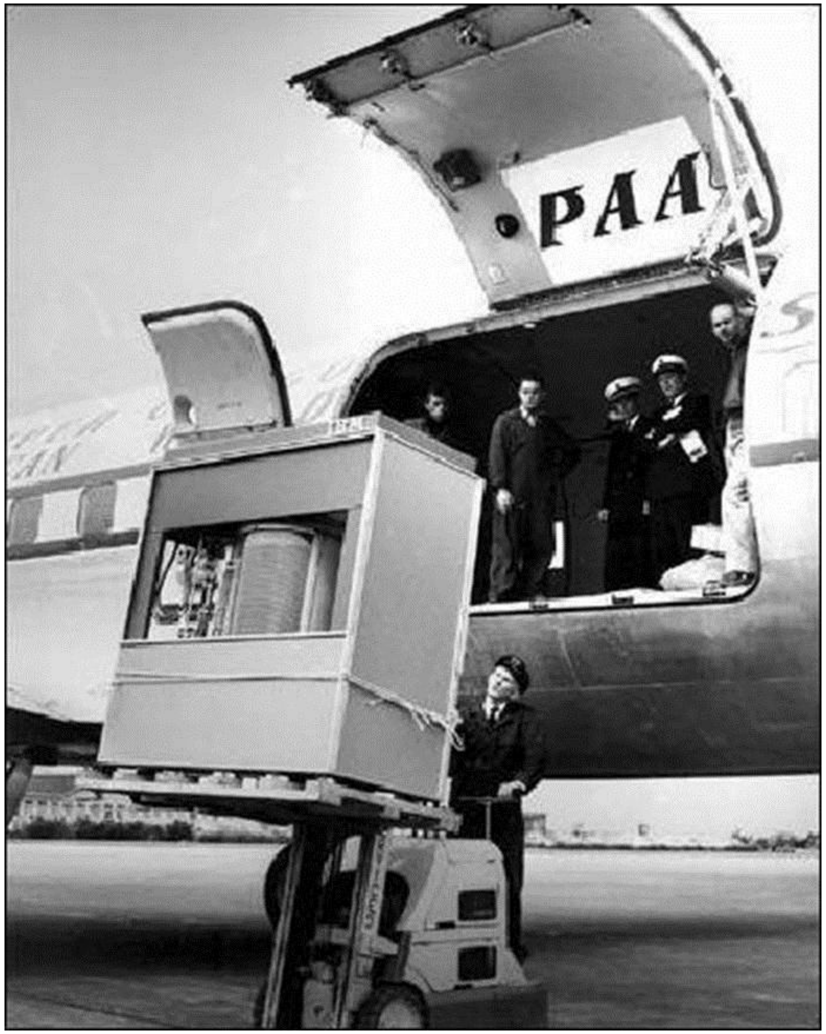
Introduction

- History of COMSOL Benchmarking
  - 2007 – 3.4
  - 2009 – 3.5a
  - 2012 - 4.2
- Need for HPC
  - Examine capabilities of COMSOL Multiphysics 4.2 running on a computer cluster

History of HPC

- 1954 – IBM introduced 704 – used FPA
- 1958 – IBM idea of parallel programming
- 1962 – Burroughs Corp – 4-processor computer; 16 memory
- 1967 – Amdahl's Law – define limit of speed-up
- 1969 – Honeywell introduces 8 processor parallel system
- 1964 – ILLIAC IV – a SIMD machine w/ 256 processors – LLNL
- 1976 – SRL clustered VAX and DEC systems
- 1976 – Cray-1; XMP, YMP
- 1996 – SGI-Cray merged
- 2002 – SGI-Cray created Origin 3800

What is this?



What is this?

- 5MB hard drive circa 1956 – IBM launched the 305 RAMAC first supercomputer HDD – weight > 1 ton

Computer platform – 4.2 vs 3.5

PC Hardware:

- Platform 1: Pentium(R) D CPU 2.80GHz, 4.0GB this configuration was used to test the first four benchmark problems.
- Platform 2: Intel ® Core ™ 2 Quad CPU Q9300 CPU 2.50GHz, 4.0GB RAM. This configuration was used for the four CFD-CHT benchmark problems.

Test Problems

- Benchmark criteria
  - Computational accuracy (comparison difference is less than or equal to 5%)
    - Contours of key variables
    - Extreme values
    - Experimental data
  - Mesh independent study
    - Comparisons are made for results obtained for different mesh densities for a selected test problem
    - Increase in the number of elements leads to negligible differences in the solutions.

Test Criteria

- Benchmark criteria
  - Memory
    - Provided by software package whenever possible
    - COMSOL “Mem Usage” shows the approximate memory consumption, the average memory during the entire solution procedure
  - CPU time
    - Execution times can be recorded from immediate access to the CPU time by the program or from measuring wall-clock time
    - To obtain accurate CPU time, all unnecessary processes were stopped

Comparison between 4.2 and 3.5

Benchmark case	Software Used	Number of elements	Memory cost (MB)	CPU time (s)	Compared values
Case 1: FSI	COMSOL 4.2	3,341	468	164	$\text{Tot}_{\text{dis-max}}$:27.62μm
	COMSOL 3.5	3,372	264	240	$\text{Tot}_{\text{dis-max}}$:21.97μm
Case 2: Actuator	COMSOL 4.2	5,051	299	4	$X_{\text{dis-max}}$=3.065μm
		9,635	434	5	$X_{\text{dis-max}}$=3.069μm
		20.101	489	8	$X_{\text{dis-max}}$=3.067μm
	COMSOL 3.5	5,032	170	3	$X_{\text{dis-max}}$=3.065μm
		10,779	360	8	$X_{\text{dis-max}}$=3.069μm
		16,893	480	22	$X_{\text{dis-max}}$=3.066μm
Case 3: Circulator	COMSOL 4.2	14,031	338	23	reflection, isolation and insertion loss
	COMSOL 3.5	14,089	280	103	
Case 4: Generator	COMSOL 4.2	32,850	441	13	$B_{\max}$=1.267T
	COMSOL 3.5	32,395	190	17	$B_{\max}$=1.257T

What is a cluster?

- A group of loosely coupled computers that work together closely – multiple standalone machines connected by a network
- *Beowulf* cluster – multiple identical commercial off-the-shelf computers connected with a TCP/IP Ethernet LAN

PC Clusters

- 1994 – first PC cluster at NASA Goddard – 16 PCs – 70 Mflops (Beowulf)
- 1996 – Cal Tech & LANL built Beowulf clusters > 1 Gflops
- 1996 – ORNL used old PCs and MPI and achieved 1.2 Gflops
- 2001 – ORNL was using 133 nodes

Beowulf

Massively Parallel Processor

- A single computer with many networked processors; each CPU contains its own memory and copy of the operating system, e.g., Blue Gene
- Grid computing – computers communicating over the Internet to work on a given problem (SETI@home)

SIMD vs MIMD

- Single-instruction-multiple-data (SIMD) – doing the same operation repeatedly over a large data set (vector processing – Cray; Thinking Machines – 64,000)
- Multiple-instruction-multiple-data (MIMD) – processors function asynchronously and independently; shared memory vs distributed memory (hypercube)

Test Measures

- Speedup
  - $S_p = T_1/T_p$ = $\text{time}_{\text{node-1}}/\text{time}_{\text{nodes-p}}$

  Parallel Efficiency

  $E_p = S_p/p$

  Scale-up

  Solution time where work/node is constant

  Memory

  Usage as a function of increasing p

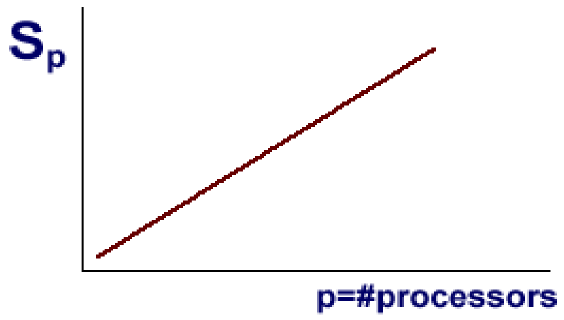
Speedup

- ***Speedup*** is the length of time it takes a program to run on a single processor, divided by the time it takes to run on multiple processors.
  - Speedup generally ranges between 0 and p, where p is the number of processors.
- ***Scalability***
  - When you compute with multiple processors in a parallel environment, you will also want to know how your code scales.
  - The scalability of a parallel code is defined as its ability to achieve performance proportional to the number of processors used.

Linear Speedup

If it takes one processor an amount of time t to do a task and if p processors can do the task in time t/p, then you have perfect or linear speedup (S_p= p).

- running with 4 processors improves the time by a factor of 4, running with 8 processors improves the time by a factor of 8, etc



Slowdown

- **When a parallel code runs slower than sequential code**
  - When S_p<1, it means that the parallel code runs slower than the sequential code.
  - This happens when there isn't enough computation to be done by each processor.
  - The overhead of creating and controlling the parallel threads outweighs the benefits of parallel computation, and it causes the code to run slower.
  - To eliminate this problem you can try to **increase the problem size or run with fewer processors**.

Efficiency

- Efficiency is a measure of parallel performance that is closely related to speedup and is often presented in a description of the performance of a parallel program.
  - Efficiency with p processors is defined as the ratio of speedup with p processors to p.
- Efficiency is a fraction that usually ranges between 0 and 1.
  - $E_p = 1$ corresponds to perfect speedup of $S_p = p$.
  - You can think of efficiency as describing the average speedup per processor.

$$E_p = \frac{S_p}{p}$$

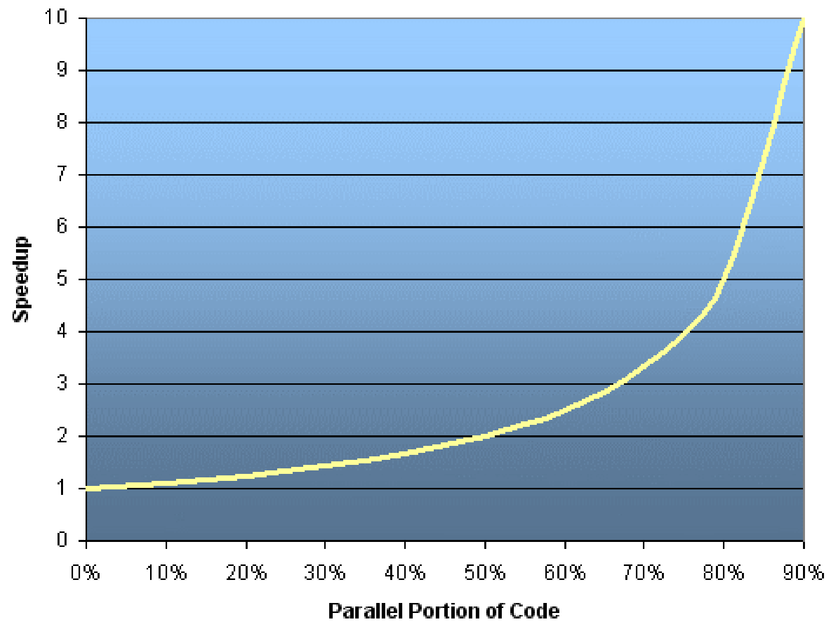
Amdahl's Law

- An alternative formula for speedup is Amdahl's Law - attributed to Gene Amdahl.
    - This formula, introduced in the 1980s, states that no matter how many processors are used in a parallel run, a program's speedup will be limited by its fraction of sequential code (a fraction of the code that doesn't lend itself to parallelism).
    - This is the fraction of code that will have to be run with just one processor, even in a parallel run.
- Amdahl's Law defines speedup with p processors as follows:

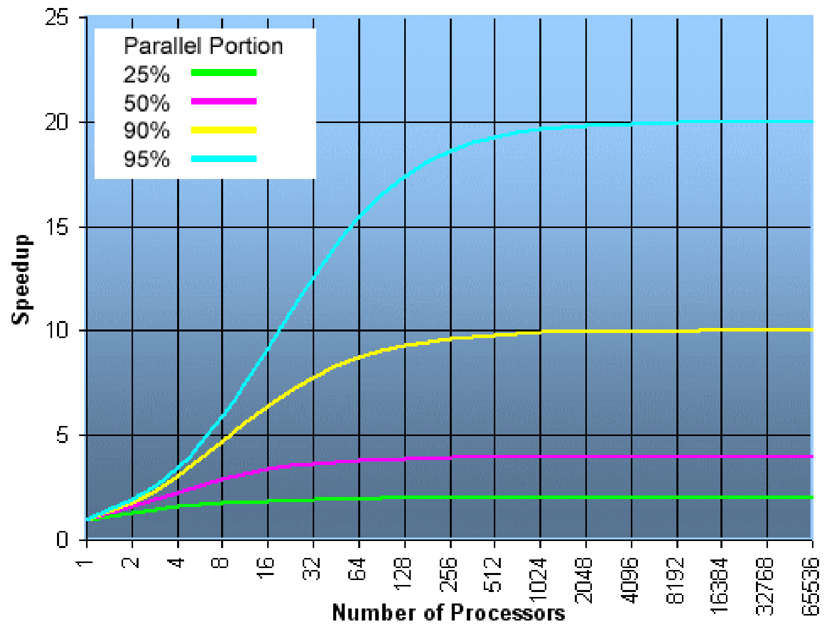
$$S_p = \frac{1}{f + (1 - f)/p}$$

- where *f* = fraction of operations done sequentially with just one processor, and *(1 - f)* stands = fraction of operations done in perfect parallelism with *p* processors.

Amdahl’s Law



Speedup
0
1
2
3
4
5
6
7
8
9
10
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
Parallel Portion of Code



Parallel Portion
25%
50%
90%
95%
Speedup
0
5
10
15
20
25
1
2
4
8
16
32
64
128
256
512
1024
2048
4096
8192
16384
32768
65536
Number of Processors

Amdahl's Law – con't

- Amdahl's Law shows that the sequential fraction of code has a strong effect on speedup

  - Need for large problem sizes using parallel computers

  - You cannot take a small application and expect it to show good performance on a parallel computer

  - For good performance, you need **large applications**, with large data array sizes, and lots of computation

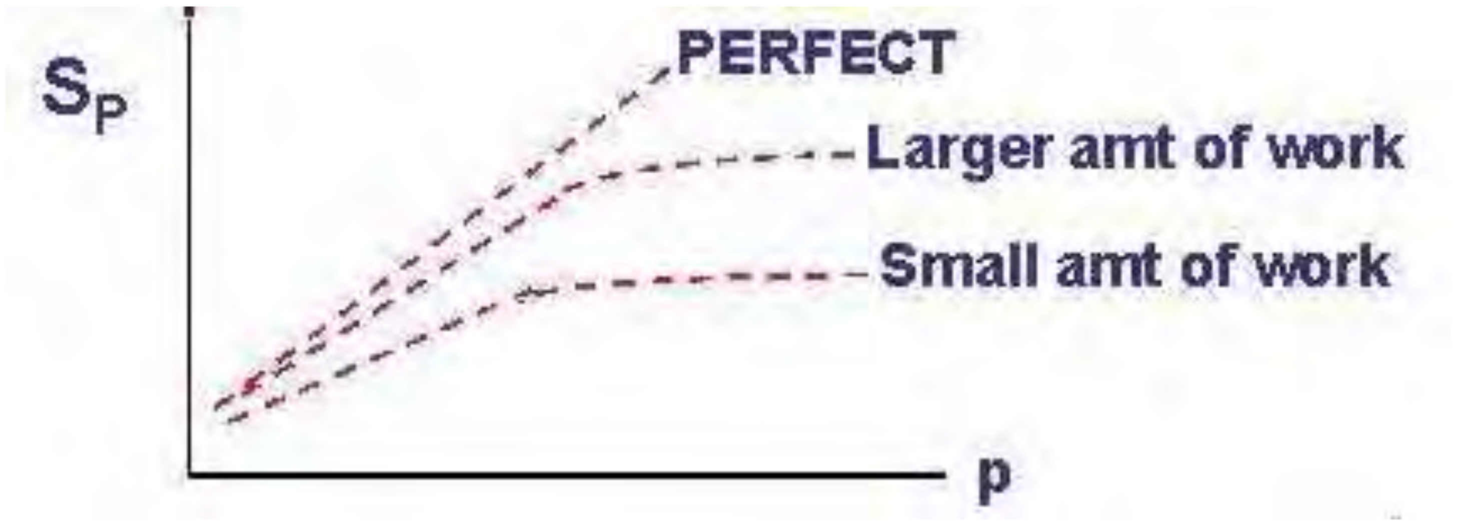
  - As problem size increases, the opportunity for parallelism grows, and the sequential fraction shrinks

Speedup Limitations

- *Too much I/O*
  - Speedup is limited when the code is I/O bound
- *Wrong algorithm*
  - **Numerical algorithm is not suitable** for a parallel computer
- *Too much memory contention*
  - You need to redesign the code with attention to data locality
- *Wrong Problem Size*
  - **Too small a problem**
- *Too much sequential code or too much parallel overhead*
  - Too much overhead compared to computation
- *Too many idle processors*
  - Load imbalance

Problem Size

- **Small Problem Size**
  - Speedup is almost always an increasing function of problem size.
  - If there's not enough work to be done by the available processors, the code will show limited speedup.

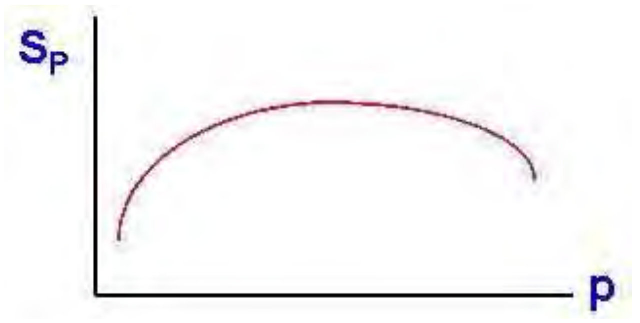


Problem Size Fixed

When the problem size is fixed, you can reach a point of negative returns when using additional processors

As you compute with more and more processors, each processor has less and less amount of computation to perform

The additional parallel overhead, compared to the amount of computation, causes the speedup curve to start turning downward as shown in the following figure.



HPC Computer platforms

SGI Altix 4700 - USAFA

- 18 nodes (512 processors/node)
- 9216 Processors (59 Peak TeraFLOPS)
- 2-4 GB Memory/Compute Processor
- 440 Terabyte Workspace

HPC Computer platforms – con’t

Cray XE6 - USAFA

- 2732 Compute Nodes (16 Cores/Node)
- 43,712 Cores (410 Peak TeraFLOPS)
- 2 GB Memory/Core
- 1.6 Petabyte Workspace

SGI - USAFA

COMSOL Tests

- The following codes were tested on the SGI Altix System at the USAFA

1. sar_in_human_head (RF)
2. Induction motor
3. Turbulence backstep
4. Free convection
5. Tuning fork

(plus other models now being run)

Preliminary Test Results

Model	DOF	node time (s)	p node time (s)	S_p	E_p
RF Module	780308	108	5.62	19.21	0.800
Induction Motor	95733	51	2.6	19.61	0.817
	86786	67	3.48	19.25	0.802
Turbulent Backstep	70405	99	5.15	19.22	0.800
	46557	56	2.91	19.24	0.801
Free Convection	10360	11	0.57	19.29	0.803
Tuning Fork	96822	204	10.62	19.20	0.800

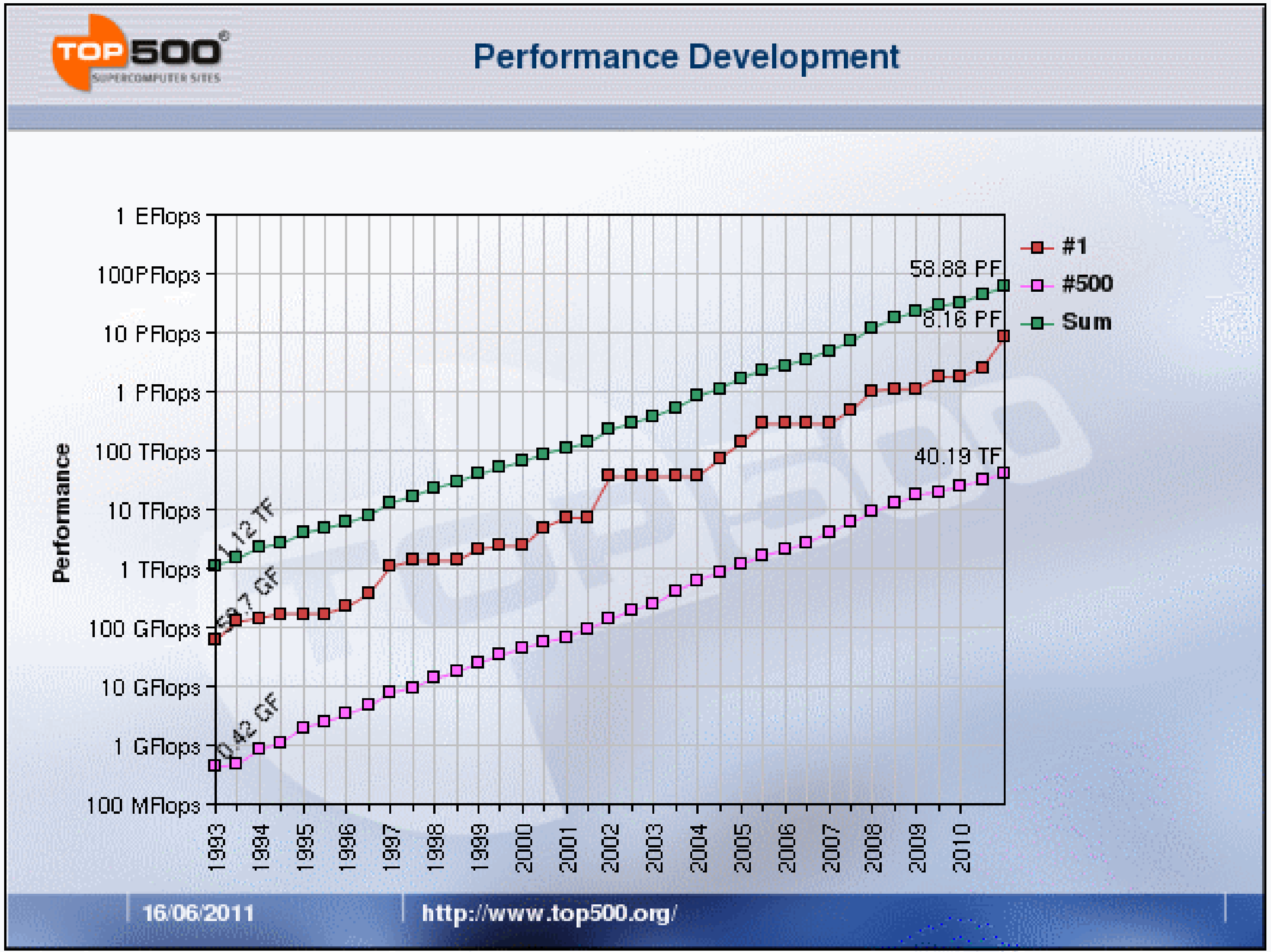
What’s coming?

- Refinement in adaptation (include p) – hp
  - BEM; Meshless Methods
- More robust modeling techniques
- More multiphysics – with multiscale
- Easier access to cluster/cloud computing
- Quantum Computing – Qubits (quantum bits; particle spin; entanglement; D::Wave – Canada)
- Ipad example –accessing COMSOL

Accessing COMSOL on iPad

- GoTo My PC – set up app on iPad and on host machine
- Bring up internet, click on COMSOL – you can now run remotely
- Beware of using two monitors on host system

Computer performance

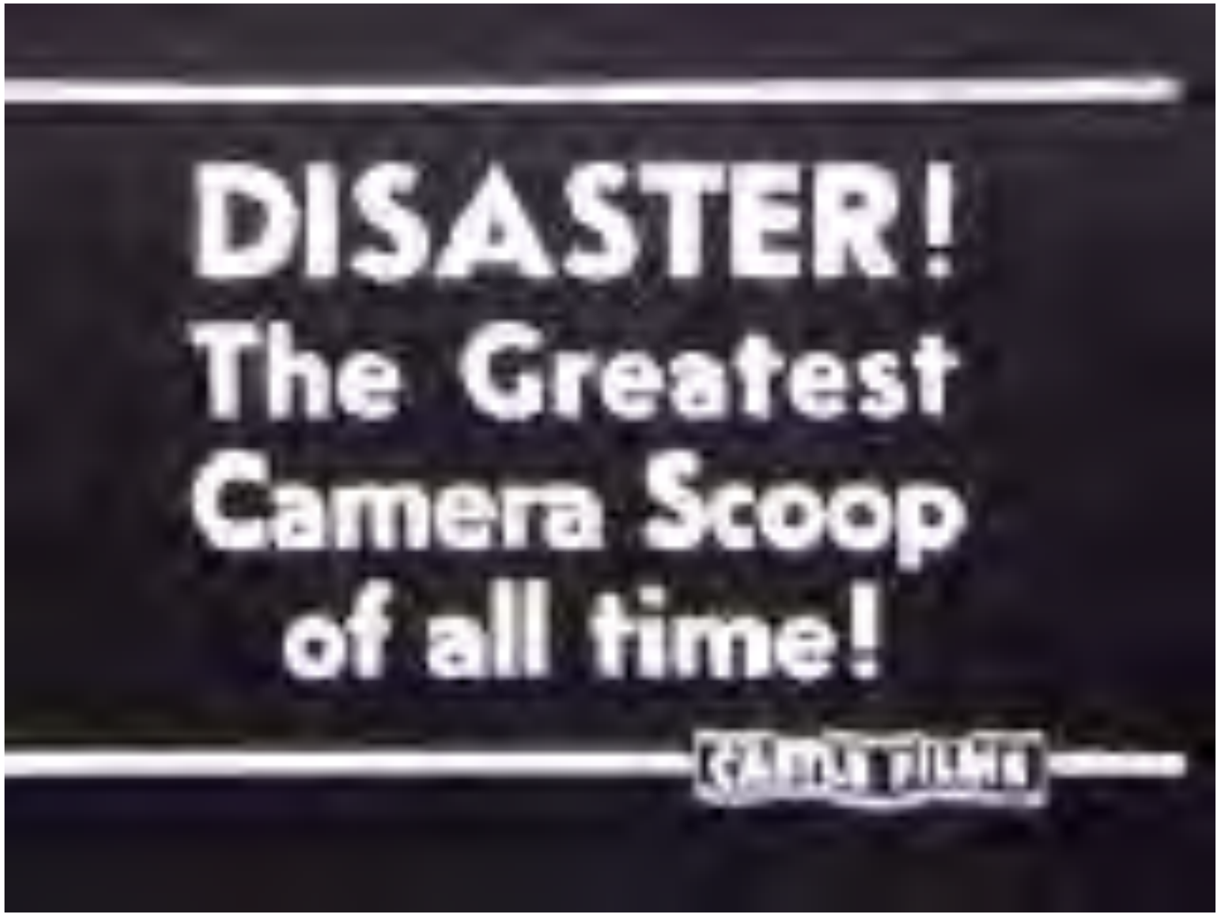


Name	FLOPS
yottaFLOPS	10^{24}
zettaFLOPS	10^{21}
exaFLOPS	10^{18}
petaFLOPS	10^{15}
teraFLOPS	10^{12}
gigaFLOPS	10^{9}
megaFLOPS	10^{6}
kiloFLOPS	10^{3}

Tacoma Narrows Bridge

- Vortex shedding frequency matching bridge resonance
- Structural shells coupled with turbulent flow
- Classic FSI problem

TNB



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