Parallel Computing & Accelerators

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# **Purpose of this talk**

This is the 50,000 ft. view of the parallel computing landscape. We want to orient you a bit before parachuting you down into the trenches to deal with OpenACC. The plan is that you walk away with a knowledge of not just OpenACC, but also where it fits into the world of High Performance Computing.

## **FLOPS we need: Climate change analysis**



#### Simulations

- Cloud resolution, quantifying uncertainty, understanding tipping points, etc., will drive climate to exascale platforms
- New math, models, and systems support will be needed

#### **Extreme data**

- "Reanalysis" projects need 100× more computing to analyze observations
- Machine learning and other analytics are needed today for petabyte data sets
- Combined simulation/observation will empower policy makers and scientists

## **Exascale combustion simulations**

- Goal: 50% improvement in engine efficiency
- Center for Exascale Simulation of Combustion in Turbulence (ExaCT)
  - Combines M&S and experimentation
  - Uses new algorithms, programming models, and computer science





Courtesy Horst Simon, LBNL

## The list is long, and growing.

- Molecular-scale Processes: atmospheric aerosol simulations
- AI-Enhanced Science: predicting disruptions in tokomak fusion reactors
- Hypersonic Flight
- Modeling Thermonuclear X-ray Bursts: 3D simulations of a neutron star surface or supernovae
- Quantum Materials Engineering: electrical conductivity photovoltaic and plasmonic devices
- Physics of Fundamental Particles: mass estimates of the bottom quark
- Digital Cells











#### And many of you doubtless brought your own immediate research concerns. Great!



### Welcome to The Exascale Era!

exa = 10<sup>18</sup> = 1,000,000,000,000,000,000 = quintillion

64-bit precision floating point operations per second



There may also be a Chinese machine, OceanLight, or 3letter-agency machines on the scene. Copyrighted Material

### COMPUTATIONAL PHYSICS

Revised and expanded

in very little time. Performing a billion operations, on the other hand, could take minutes or hours, though it's still possible provided you are patient. Performing a trillion operations, however, will basically take forever. So a fair rule of thumb is that the calculations we can perform on a computer are ones that can be done with *about a billion operations or less*.

Mark Newman

# Where are those 10 or 12 orders of magnitude?

### How do we get there from here?

BTW, that's a bigger gap than



VS.



IBM 709 12 kiloflops

### Moore's Law abandoned serial programming around 2004



#### Courtesy Liberty Computer Architecture Research Group

### But Moore's Law is only beginning to stumble now.

### Intel process technology capabilities



0nm	65nm	15nm					
		451111	32nm	22nm	14nm	10nm	7nm
2	4	8	16	32	64	128	256
	2	2 4	2 4 8	2 4 8 16	2 4 8 16 32	2 4 8 16 32 64	2 4 8 16 32 64 128



#### Transistor for 90nm Process

Source: Intel



Influenza Virus Source: CDC

#### And at end of day we keep using getting more transistors.



### That Power and Clock Inflection Point in 2004... didn't get better.



Fun fact: At 100+ Watts and <1V, currents are beginning to exceed 100A at the point of toact.

#### Courtesy Horst Simon, LBNL

# Not a new problem, just a new scale...



Cray-2 with cooling tower in foreground, circa 1985

# And how to get more performance from more transistors with the same power.





# **Parallel Computing**

One woman can make a baby in 9 months.

Can 9 women make a baby in 1 month?

But 9 women can make 9 babies in 9 months.

First two bullets are Brook's Law. From *The Mythical Man-Month*.

A must-read for serious project programmers that includes many other classics such as: "What one programmer can do in one month, two programmers can do in two months."

# Prototypical Application: Serial Weather Model



# First Parallel Weather Modeling Algorithm: Richardson in 1917



Courtesy John Burkhardt, Virginia Tech

## Weather Model: Shared Memory (OpenMP)



#### Weather Model: Distributed Memory (MPI)



call MPI\_Send( numbertosend, 1, MPI\_INTEGER, index, 10, MPI\_COMM\_WORLD, errcode)

call MPI\_Recv( numbertoreceive, 1, MPI\_INTEGER, 0, 10, MPI\_COMM\_WORLD, status, errcode)

call MPI\_Barrier(MPI\_COMM\_WORLD, errcode)

50 meteorologists using a telegraph.

## Weather Model: Accelerator (OpenACC)



1 meteorologists coordinating 1000 math savants using tin cans and a string.

## The pieces fit like this...



#### Top 10 Systems as of June 2024

#	Computer	Site	Manufacturer	CPU Interconnect [ <i>Accelerator</i> ]	Cores	Rmax (Pflops)	Rpeak (Pflops)	Power (MW)
1	Frontier	Oak Ridge National Laboratory <b>United States</b>	HPE	AMD EPYC 64C 2GHz Slingshot-11 AMD Instinct MI250X	8,699,904	1194	1692	22.7
2	Aurora	Argonne National Laboratory <b>United States</b>	НРЕ	Intel Xeon Max 9470 52C 2.4GHz Slingshot-11 Intel Data Center GPU Max	4,742,808	585	1059	24.6
3	Eagle	Microsoft United States	Microsoft	Intel Xeon 8480C 48C 2GHz Infiniband NDR NVIDIA H100	1,123,200	561	846	
4	Fugaku	RIKEN Center for Computational Science Japan	Fujitsu	ARM 8.2A+ 48C 2.2GHz Torus Fusion Interconnect	7,630,072	442	537	29.9
5	LUMI	EuroHPC Finland	HPE	AMD EPYC 64C 2GHz Slingshot-11 AMD Instinct MI250X	2,752,704	379	531	7.1
6	Leonardo	EuroHPC Italy	Atos	Intel Xeon 8358 32C 2.6GHz Infiniband HDR NVIDIA A100	1,824,768	238	304	7.4
7	Summit	Oak Ridge National Laboratory <b>United States</b>	IBM	Power9 22C 3.0 GHz Dual-rail Infiniband EDR <i>NVIDIA V100</i>	2,414,592	148	200	10.1
8	MareNostrum 5	EuroHPC/BSC <b>Spain</b>	EVIDEN	Intel Xeon 8460Y+ 40C 2.3GHz, Infiniband NDR200 NVIDIA H100 64GB	680,960	138	256	2.5
9	Eos NVIDIA DGX SuperPOD	500 <b>TX-Green2</b> - 2.4GHz, 25G	PowerEdge C6420 Ethernet, ACTION	, Xeon Platinum 8260 24C	43,200 2	.02 53.08	188	
10	Sierra	MIT Lincoln l United States	_aboratory Superco s	omputing Center			125	7.4

## The word is *Heterogeneous*

And it's not just supercomputers. It's on your desk, and in your phone.



How much of this can you program?

## We can do better. We have a role model.

- We hope to "simulate" a human brain in real time on one of these Exascale platforms with about 1 - 10 Exaflop/s and 4 PB of memory
- These newest Exascale computers use 20+ MW
- The human brain runs at 20W
- Our brain is a million times more power efficient!



# Why you should be (extra) motivated.

- This parallel computing thing is no fad.
- The laws of physics are drawing this roadmap.
- If you get on board (the right bus), you can ride this trend for a long, exciting trip.

Let's learn how to use these things!