Future of HPC

John Urbanic
Parallel Computing Scientist
Pittsburgh Supercomputing Center
Moore's Law abandoned serial programming around 2004
But Moore’s Law is only beginning to stumble now.

Intel process technology capabilities

<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Feature Size</td>
<td>90nm</td>
<td>65nm</td>
<td>45nm</td>
<td>32nm</td>
<td>22nm</td>
<td>14nm</td>
<td>10nm</td>
<td>7nm</td>
</tr>
<tr>
<td>Integration Capacity</td>
<td>2</td>
<td>4</td>
<td>8</td>
<td>16</td>
<td>32</td>
<td>64</td>
<td>128</td>
<td>256</td>
</tr>
</tbody>
</table>

Transistor for 90nm Process  
Source: Intel

Influenza Virus  
Source: CDC
...but our metrics are less clear.

After a while, “there was no one design rule that people could point to and say, ‘That defines the node name’ … The minimum dimensions are getting smaller, but I’m the first to admit that I can’t point to the one dimension that’s 32 nm or 22 nm or 14 nm. Some dimensions are smaller than the stated node name, and others are larger.”

Mark Bohr, Senior fellow at Intel.
From The Status of Moore’s Law: It’s Complicated (IEEE Spectrum)
Now tradeoffs are stealing these gains.

The density and power levels on a state-of-the-art chip have forced designers to compensate by adding:

- error-correction circuitry
- redundancy
- read- and write-boosting circuitry for failing static RAM cells
- circuits to track and adapt to performance variations
- complicated memory hierarchies to handle multicore architectures.

All of those extra circuits add area. Some analysts have concluded that when you factor those circuits in, chips are no longer twice as dense from generation to generation. One such analysis suggests, the density improvement over the past three generations, from 2007 on, has been closer to 1.6 than 2.

And cost per transistor has gone up for the first time ever:

- 2012 20M 28nm transistors/dollar
- 2015 19M 16nm transistors/dollar
At end of day, we keep using all those new 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 load!

Source: Kogge and Shalf, IEEE CISE

Courtesy Horst Simon, LBNL
Not a new problem, just a new scale...

Cray-2 with cooling tower in foreground, circa 1985
How to get same number of transistors to give us more performance without cranking up power?

Key is that

\[ \text{Performance} \approx \sqrt{\text{area}} \]

Power = \( \frac{1}{4} \)

Performance = \( \frac{1}{2} \)
And how to get more performance from more transistors with the same power.

A 15% Reduction In Voltage Yields

RULE OF THUMB

<table>
<thead>
<tr>
<th>Frequency Reduction</th>
<th>Power Reduction</th>
<th>Performance Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>15%</td>
<td>45%</td>
<td>10%</td>
</tr>
</tbody>
</table>

A 15% Reduction In Voltage Yields

SINGLE CORE

- Area = 1
- Voltage = 1
- Freq = 1
- Power = 1
- Perf = 1

DUAL CORE

- Area = 2
- Voltage = 0.85
- Freq = 0.85
- Power = 1
- Perf = ~1.8
<table>
<thead>
<tr>
<th>Processor</th>
<th>Year</th>
<th>Vector</th>
<th>Bits</th>
<th>SP FLOPs / core / cycle</th>
<th>Cores</th>
<th>FLOPs/cycle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pentium III</td>
<td>1999</td>
<td>SSE</td>
<td>128</td>
<td>3</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Pentium IV</td>
<td>2001</td>
<td>SSE2</td>
<td>128</td>
<td>4</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>Core</td>
<td>2006</td>
<td>SSE3</td>
<td>128</td>
<td>8</td>
<td>2</td>
<td>16</td>
</tr>
<tr>
<td>Nehalem</td>
<td>2008</td>
<td>SSE4</td>
<td>128</td>
<td>8</td>
<td>10</td>
<td>80</td>
</tr>
<tr>
<td>Sandybridge</td>
<td>2011</td>
<td>AVX</td>
<td>256</td>
<td>16</td>
<td>12</td>
<td>192</td>
</tr>
<tr>
<td>Haswell</td>
<td>2013</td>
<td>AVX2</td>
<td>256</td>
<td>32</td>
<td>18</td>
<td>576</td>
</tr>
<tr>
<td>KNC</td>
<td>2012</td>
<td>AVX512</td>
<td>512</td>
<td>32</td>
<td>64</td>
<td>2048</td>
</tr>
<tr>
<td>KNL</td>
<td>2016</td>
<td>AVX512</td>
<td>512</td>
<td>64</td>
<td>72</td>
<td>4608</td>
</tr>
<tr>
<td>Skylake</td>
<td>2017</td>
<td>AVX512</td>
<td>512</td>
<td>96</td>
<td>28</td>
<td>2688</td>
</tr>
</tbody>
</table>
Putting It All Together

Transistors (thousands)

Single-Thread Performance (SpecINT x 10^3)

Frequency (MHz)

Typical Power (Watts)

Number of Logical Cores

Many Levels and Types of Parallelism

- Vector (SIMD)
- Instruction Level (ILP)
  - Instruction pipelining
  - Superscaler (multiple instruction units)
  - Out-of-order
  - Register renaming
  - Speculative execution
  - Branch prediction
- Multi-Core (Threads)
- SMP/Multi-socket
- Accelerators: GPU & MIC
- Clusters
- MPPs

Compiler (not your problem)

Also Important
- ASIC/FPGA/DSP
- RAID/IO
The pieces fit like this…
The Long-awaited Exascale - This year!

Courtesy Horst Simon, LBNL
Staying on track to Exascale

First boost: many-core/accelerator

Second Boost: 3D (2016 – 2020)
- We will be able to reach usable Exaflops for ~20 MW by 2021
- But at what cost?
- Will any of the other technologies give additional boosts after 2025?

Third Boost: SiPh (2020 – 2024)

• We will be able to reach usable Exaflops for ~20 MW by 2021
• But at what cost?
• Will any of the other technologies give additional boosts after 2025?

Courtesy Horst Simon, LBNL
## Top 10 Systems as of June 2020

<table>
<thead>
<tr>
<th>#</th>
<th>Site</th>
<th>Manufacturer</th>
<th>Computer</th>
<th>CPU Interconnect [Accelerator]</th>
<th>Cores</th>
<th>Rmax (Tflops)</th>
<th>Rpeak (Tflops)</th>
<th>Power (MW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>RIKEN Center for Computational Science Japan</td>
<td>Fujitsu</td>
<td>Fugaku</td>
<td>ARM 8.2A+ 48C 2.2GHz Torus Fusion Interconnect</td>
<td>7,299,072</td>
<td>415,530</td>
<td>513,854</td>
<td>28.3</td>
</tr>
<tr>
<td>2</td>
<td>DOE/SC/ORNL United States</td>
<td>IBM</td>
<td>Summit</td>
<td>Power9 22C 3.0 GHz Dual-rail Infiniband EDR NVIDIA V100</td>
<td>2,414,592</td>
<td>148,600</td>
<td>200,794</td>
<td>10.1</td>
</tr>
<tr>
<td>3</td>
<td>DOE/NNSA/LLNL United States</td>
<td>IBM</td>
<td>Sierra</td>
<td>Power9 3.1 GHz 22C Infiniband EDR NVIDIA V100</td>
<td>1,572,480</td>
<td>94,640</td>
<td>125,712</td>
<td>7.4</td>
</tr>
<tr>
<td>4</td>
<td>National Super Computer Center in Wuxi China</td>
<td>NRCPC</td>
<td>Sunway TaihuLight</td>
<td>Sunway SW26010 260C 1.45GHz</td>
<td>10,649,600</td>
<td>93,014</td>
<td>125,435</td>
<td>15.3</td>
</tr>
<tr>
<td>5</td>
<td>National Super Computer Center in Guangzhou China</td>
<td>NUDT</td>
<td>Tianhe-2 (MilkyWay-2)</td>
<td>Intel Xeon E5-2692 2.2 GHz TH Express-2 Intel Xeon Phi 31S1P</td>
<td>4,981,760</td>
<td>61,444</td>
<td>100,678</td>
<td>18.4</td>
</tr>
<tr>
<td>6</td>
<td>Eni S.p.A Italy</td>
<td>Dell</td>
<td>HPC5</td>
<td>Xeon 24C 2.1 GHz Infiniband HDR NVIDIA V100</td>
<td>669,760</td>
<td>35,450</td>
<td>51,720</td>
<td>2.2</td>
</tr>
<tr>
<td>7</td>
<td>Eni S.p.A Italy</td>
<td>NVIDIA</td>
<td>Selene</td>
<td>EPYC 64C 2.25GHz Infiniband HDR NVIDIA A100</td>
<td>272,800</td>
<td>27,580</td>
<td>34,568</td>
<td>1.3</td>
</tr>
<tr>
<td>8</td>
<td>Texas Advanced Computing Center/Univ. of Texas United States</td>
<td>Dell</td>
<td>Frontera</td>
<td>Intel Xeon 8280 28C 2.7 GHz InfiniBand HDR</td>
<td>448,448</td>
<td>23,516</td>
<td>38,745</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Cineca Italy</td>
<td>IBM</td>
<td>Marconi100</td>
<td>Power9 16C 3.0 GHz Infiniband EDR NVIDIA V100</td>
<td>347,776</td>
<td>21,640</td>
<td>29,354</td>
<td>1.5</td>
</tr>
<tr>
<td>10</td>
<td>Swiss National Supercomputing Centre (CSCS) Switzerland</td>
<td>Cray</td>
<td>Piz Daint Cray XC50</td>
<td>Xeon E5-2690 2.6 GHz Aries NVIDIA P100</td>
<td>387,872</td>
<td>21,230</td>
<td>27,154</td>
<td>2.4</td>
</tr>
</tbody>
</table>
Today

- Pflops computing fully established with more than 500 machines
- The field is thriving
- Interest in supercomputing is now worldwide, and growing in many new markets
- Exascale projects in many countries and regions
USA: ECP by the Numbers

A seven-year, $1.7 B R&D effort that launched in 2016

Six core DOE National Laboratories: Argonne, Lawrence Berkeley, Lawrence Livermore, Oak Ridge, Sandia, Los Alamos
  • Staff from most of the 17 DOE national laboratories take part in the project

Three technical focus areas: Hardware and Integration, Software Technology, Application Development supported by a Project Management Office

More than 100 top-notch R&D teams

Hundreds of consequential milestones delivered on schedule and within budget since project inception
The Plan

Pre-Exascale Systems

2012: TITAN (ORNL Cray/AMD/NVIDIA), MIRA (ANL IBM BG/Q)
2016: CORI (ORNL Cray/Intel), THETA (ANL Intel/Cray)
2018: SUMMIT (ORNL IBM/NVIDIA)
2020: PERLMUTTER (ORNL Cray/AMD/NVIDIA), FRONTIER (ORNL Cray/AMD)

Future Exascale Systems

2021–2023: Aurora (Intel/Cray), CROSSTROADS (LANL/SNL TBD), EL CAPITAN (LLNL Cray)
<table>
<thead>
<tr>
<th>System</th>
<th>Performance</th>
<th>Power</th>
<th>Interconnect</th>
<th>Node</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aurora (ANL)</td>
<td>&gt; 1 EF</td>
<td></td>
<td>100 GB/s Cray Slingshot Dragonfly</td>
<td>2 Intel Xeon CPU + 6 Intel Xe GPUs</td>
</tr>
<tr>
<td>El Capitan (LLNL)</td>
<td>&gt; 1.5 EF</td>
<td>30-40 MW</td>
<td>100 GB/s Cray Slingshot Dragonfly</td>
<td>AMD Epyc CPU + 4 Radeon GPUs</td>
</tr>
<tr>
<td>Frontier (ORNL)</td>
<td>&gt; 1.5 EF</td>
<td></td>
<td>100 GB/s Cray Slingshot Dragonfly</td>
<td>AMD Epyc CPU + 4 Radeon GPUs</td>
</tr>
<tr>
<td>Perlmutter (LBNL)</td>
<td></td>
<td></td>
<td>Cray Slingshot Dragonfly</td>
<td>2 AMD Epyc CPU + 4 Volta GPUs</td>
</tr>
</tbody>
</table>
One of the many groups established to enable this outcome (the Advanced Scientific Computing Advisory Committee) puts forward this list of 10 technical challenges:

- Energy efficient circuit, power and cooling technologies.
- High performance interconnect technologies.
- Advanced memory technologies to dramatically improve capacity and bandwidth.
- Scalable system software that is power and resilience aware.
- Data management software that can handle the volume, velocity and diversity of data.
- Programming environments to express massive parallelism, data locality, and resilience.
- Reformulating science problems and refactoring solution algorithms for exascale.
- Ensuring correctness in the face of faults, reproducibility, and algorithm verification.
- Mathematical optimization and uncertainty quantification for discovery, design, and decision.
- Software engineering and supporting structures to enable scientific productivity.
It is not just “exaflops” – we are changing the whole computational model. Current programming systems have WRONG optimization targets.

**Old Constraints**

- Peak clock frequency **as primary limiter for performance improvement**
- Cost: **FLOPs** are biggest cost for system: optimize for compute
- Concurrency: Modest growth of parallelism by adding nodes
- Memory scaling: **maintain byte per flop capacity and bandwidth**
- Locality: MPI+X model (uniform costs within node & between nodes)
- Uniformity: **Assume uniform system performance**
- Reliability: **It’s the hardware’s problem**

**New Constraints**

- **Power** is primary design constraint for future HPC system design
- **Cost:** Data movement dominates: optimize to minimize data movement
- **Concurrency:** Exponential growth of parallelism within chips
- **Memory Scaling:** Compute growing 2x faster than capacity or bandwidth
- **Locality:** must reason about data locality and possibly topology
- **Heterogeneity:** Architectural and performance non-uniformity increase
- **Reliability:** Cannot count on hardware protection alone

*Fundamentally breaks our current programming paradigm and computing ecosystem*

Adapted from John Shalf
End of Moore’s Law Will Lead to New Architectures

Non-von Neumann

NEUROMORPHIC ARCHITECTURE

Cerebras WSE
1.2 Trillion transistors
46,225 mm² silicon

Largest GPU
21.1 Billion transistors
815 mm² silicon

BEYOND CMOS

COMPUTING Progress and Prospects

TODAY

QUANTUM TECHNOLOGY
It would only be the 6th paradigm.
We can do better. We have a role model.

- Straight forward extrapolation results in a real-time human brain scale simulation at about 1 - 10 Exaflop/s with 4 PB of memory.
- Current predictions envision Exascale computers in 2021 with a power consumption of at best 20 - 30 MW.
- The human brain takes 20W.
- Even under best assumptions in 2020 our brain will still be a million times more power efficient.

Courtesy Horst Simon, LBNL
It has become a mantra of contemporary programming philosophy that developer hours are so much more valuable than hardware, that the best design compromise is to throw more hardware at slower code.

This might well be valid for some Java dashboard app used twice a week by the CEO. But this has spread and results in...

The common observation that a modern PC (or phone) seems to be more laggy than one from a few generations ago that had literally one thousandth the processing power.

Moore’s Law has been the biggest enabler (or more accurately rationalization) for this trend. If Moore’s Law does indeed end, then progress will require good programming.

No more garbage collecting, script languages. I am looking at you, Java, Python, Matlab.
Do you really care about software?

Of course you should. Here are a few reassuring words that software at exascale is not an afterthought, followed by more than a few application examples.
<table>
<thead>
<tr>
<th>National security</th>
<th>Energy security</th>
<th>Economic security</th>
<th>Scientific discovery</th>
<th>Earth system</th>
<th>Health care</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stockpile stewardship</td>
<td>Turbine wind plant efficiency</td>
<td>Additive manufacturing of qualifiable metal parts</td>
<td>Find, predict, and control materials and properties</td>
<td>Accurate regional impact assessments in Earth system models</td>
<td>Accelerate and translate cancer research</td>
</tr>
<tr>
<td>Next generation simulation tools for assessing nuclear weapons performance</td>
<td>High-efficiency, low-emission combustion engine and gas turbine design</td>
<td>Reliable and efficient planning of the power grid</td>
<td>Cosmological probe of the standard model of particle physics</td>
<td>Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols</td>
<td></td>
</tr>
<tr>
<td>Response to hostile threat environments and reentry conditions</td>
<td>Materials design for extreme environments of nuclear fission and fusion reactors</td>
<td>Seismic hazard risk assessment</td>
<td>Validate fundamental laws of nature</td>
<td>Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Design and commercialization of Small Modular Reactors</td>
<td></td>
<td>Demystify origin of chemical elements</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Subsurface use for carbon capture, petroleum extraction, waste disposal</td>
<td></td>
<td>Light source-enabled analysis of protein and molecular structure and design</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Scale-up of clean fossil fuel combustion</td>
<td></td>
<td>Whole-device model of magnetically confined fusion plasmas</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Biofuel catalyst design</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>
xSDK Version 0.4.0: December 2018 (even better today)

https://xsdk.info

Each xSDK member package uses or can be used with one or more xSDK packages, and the connecting interface is regularly tested for regressions.

xSDK functionality, Dec 2018
Tested on key machines at ALCF, NERSC, OLCF, also Linux, Mac OS X

Alquimia          SLEPc          hypre          SUNDIALS
PFLOTRAN          PETSc          Trilinos       MFEM
SuperLU           hypre          AMReX          Omega_h
More domain       PETSc          PUMI           deal.II
components        SUNDIALS       PHIST          More libraries
STRUMPACK

Domain components
- Reacting flow, etc.
- Reusable.

Libraries
- Solvers, etc.
- Interoperable.

Frameworks & tools
- Doc generators.
- Test, build framework.

SW engineering
- Productivity tools.
- Models, processes.

Impact: Improved code quality, usability, access, sustainability
Foundation for work on performance portability, deeper levels of package interoperability
The planned ECP ST SDKs will span all technology areas.
Appendix

Endless apps...
CEED is targeting several ECP applications:

- Compressible flow (MARBL)
- Climate (E3SM)
- Wind Energy (ExaWind)
- Modular Nuclear Reactors (ExaSMR)
- Urban systems (Urban)
- Additive Manufacturing (ExaAM)
- Subsurface (GEOS)
- Combustion (Nek5000)
- Magnetic Fusion (WDMApp)

PI: Tzanio Kolev (LLNL)
ECP’s Adaptive Mesh Refinement Co-Design Center: AMReX

- Develop and deploy software to support block-structured adaptive mesh refinement on exascale architectures
  - Core AMR functionality
  - Particles coupled to AMR meshes
  - Embedded boundary (EB) representation of complex geometry
  - Linear solvers
  - Supports two modalities of use
    - Library support for AMR
    - Framework for constructing AMR applications
- Provide direct support to ECP applications that need AMR for their application
- Evaluate software technologies and integrate with AMReX when appropriate
- Interact with hardware technologies / vendors

PI: John Bell (LBNL)
ECP’s Co-Design Center for Online Data Analysis and Reduction
CODAR

**Goal:** Replace the activities in HPC workflow that have been mediated through file I/O with in-situ methods / workflows. Data reduction, analysis, code coupling, aggregation (e.g. parameter studies).

**Cross-cutting tools:**
- Workflow setup, manager (Cheetah, Savanna); Data coupler (ADIOS-SST); Compression methods (MGARD, FTK, SZ), compression checker (Z-checker)
- Performance tools (TAU, Chimbuco, SOSFlow)

PI: Ian Foster (ANL)
ECP’s Co-Design Center for Particle Applications: CoPA

**Goal:** Develop algorithms and software for particle methods,

**Cross-cutting capabilities:**
- Specialized solvers for quantum molecular dynamics (Progress / BML).
- Performance-portable libraries for classical particle methods in MD, PDE (Cabana).
- FFT-based Poisson solvers for long-range forces.

**Technical approach:**
- High-level C++ APIs, plus a Fortran interface (Cabana).
- Leverage existing / planned FFT software.
- Extensive use of miniapps / proxy apps as part of the development process.

**PI:** Sue Mniszewski (LANL) recently replacing Tim Germann (LANL), who is taking on a larger role in ECP.
ECP’s Co-Design Center for Machine Learning: ExaLearn
Bringing together experts from 8 DOE Laboratories

- AI has the potential to accelerate scientific discovery or enable prediction in areas currently too complex for direct simulation (ML for HPC and HPC for ML)

- AI use cases of interest to ECP:
  - *Classification and regression*, including but not limited to image classification and analysis, e.g. scientific data output from DOE experimental facilities or from national security programs.
  - *Surrogate models* in high-fidelity and multiscale simulations, including uncertainty quantification and error estimation.
  - *Structure-to-function relationships*, including genome-to-phenome, the prediction of materials performance based on atomistic structures, or the prediction of performance margins based on manufacturing data.
  - *Control systems*, e.g., for wind plants, nuclear power plants, experimental steering and autonomous vehicles.
  - *Inverse problems* and optimization. This area would include, for example, inverse imaging and materials design.

- Areas in need of research
  - Data quality and statistics
  - Learning algorithms
  - Physics-Informed AI
  - Verification and Validation
  - Performance and scalability
  - Workflow and deployment

**Expected Work Product: A Toolset That . . .**
- Has a line-of-sight to exascale computing, e.g. through using exascale platforms directly, or providing essential components to an exascale workflow
- Does not replicate capabilities easily obtainable from existing, widely-available packages
- Builds in domain knowledge where possible “Physics”-based ML and AI
- Quantifies uncertainty in predictive capacity
- Is interpretable
- Is reproducible
- Tracks provenance

PI: Frank Alexander (BNL)
Machine Learning in the Light Source Workflow

**Beam Line Control and Data Acquisition (DAQ)**

- Data TB/s
- DAQ
- Data TB/s
- ML to design light source beam lines
- ML to control the beam line parameters
- ML at DAQ to control data as it is acquired

**Local Systems**

- Compressor Nodes
- Online Monitoring and Fast Feedback
- Data
- Model
- ML for data compression (e.g., hit finding). Use models learned remotely.
- ML for fast analysis at the experimental facility. Uses models learned remotely.
- 10 GB/s - 1Tb/s

**Network**

- Data
- Model
- ML networks for image classification, feature detection and solving inverse problems (how to change experiment params to get desired experiment result)

**Remote Exascale HPC**

- Exascale Supercomputer
- Data
- Model
- Model
- Model
- Simulate experiments, beam line control and diffraction images at scale to create data for training

PI: Frank Alexander (BNL)
Exascale apps can deliver transformative products and solutions

**ExaWind**

**Turbine Wind Plant Efficiency**  
(Mike Sprague, NREL)

- Harden wind plant design and layout against energy loss susceptibility
- Increase penetration of wind energy

*Challenges*: linear solver perf in strong scale limit; manipulation of large meshes; overset of structured & unstructured grids; communication-avoiding linear solvers

**ExaAM**

**Additive Manufacturing (AM) of Qualifiable Metal Parts**  
(John Turner, ORNL)

- Accelerate the widespread adoption of AM by enabling routine fabrication of qualifiable metal parts

*Challenges*: capturing unresolved physics; multi-grid linear solver performance; coupled physics

**EQSIM**

**Earthquake Hazard Risk Assessment**  
(David McCallen, LBNL)

- Replace conservative and costly earthquake retrofits with safe purpose-fit retrofits and designs

*Challenges*: full waveform inversion algorithms
EQSIM: Understanding and predicting earthquake phenomenon

- Vertical motion
- Horizontal motion
- Site ground motions
- Surface waves
- Body waves
- Site
- Source
- Ground motions tend to be very site specific

PI: David McCallen (LBNL)
EQSIM: The Exascale “Big Lift” – regional ground motion simulations at engineering frequencies

- Pipelines
- Long-span Bridges
- Tall Buildings
- Low-rise Buildings and Industrial Facilities
- Energy System Components
- Nuclear Power Equipment

PI: David McCallen (LBNL)

Doubling the frequency resolution = 16X computational effort!
Exascale apps can deliver transformative products and solutions

**MFIX-Exa**

**Scale-up of Clean Fossil Fuel Combustion**
(Madhava Syamlal, NETL)

- Commercial-scale demonstration of transformational energy technologies – curbing CO₂ emissions at fossil fuel power plants by 2030

*Challenges: load balancing; strong scaling thru transients*

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**GAMESS**

**Biofuel Catalyst Design**
(Mark Gordon, Ames)

- Design more robust and selective catalysts orders of magnitude more efficient at temperatures hundreds of degrees lower

*Challenges: weak scaling of overall problem; on-node performance of molecular fragments*

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**EXAALT**

**Materials for Extreme Environments**
(Danny Perez, LANL)

- Simultaneously address time, length, and accuracy requirements for predictive microstructural evolution of materials

*Challenges: SNAP kernel efficiency on accelerators; efficiency of DFTB application on accelerators*
# Exascale apps can deliver transformative products and solutions

<table>
<thead>
<tr>
<th>ExaSMR</th>
<th>Subsurface</th>
<th>QMCPACK</th>
</tr>
</thead>
</table>
| **Design and Commercialization of Small Modular Reactors**  
(Steve Hamilton, ORNL) | **Carbon Capture, Fossil Fuel Extraction, Waste Disposal**  
(Carl Steefel, LBNL) | **Materials for Extreme Environments**  
(Paul Kent, ORNL) |
| - Virtual test reactor for advanced designs via experimental-quality simulations of reactor behavior | - Reliably guide safe long-term consequential decisions about storage, sequestration, and exploration |  |
| *Challenges:* existing GPU-based MC algorithms require rework for hardware less performant for latency-bound algorithms with thread divergence; performance portability with OCCA & OpenACC not achievable; insufficient node memory for adequate CFD + MC coupling | *Challenges:* performance of Lagrangian geomechanics; adequacy of Lagrangian crack mechanics) + Eulerian (reaction, advection, diffusion) models; parallel HDF5 for coupling | *Challenges:* minimizing on-node memory usage; parallel on-node performance of Markov-chain Monte Carlo |

Exascale Computing Project
Exascale apps can deliver transformative products and solutions

**ExaSGD**

**Reliable and Efficient Planning of the Power Grid**
(Henry Huang, PNNL)

- Optimize power grid planning, operation, control and improve reliability and efficiency

*Challenges:* parallel performance of nonlinear optimization based on discrete algebraic equations and possible mixed-integer programming

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**Combustion-PELE**

**High-Efficiency, Low-Emission Combustion Engine Design**
(Jackie Chen, SNL)

- Reduce or eliminate current cut-and-try approaches for combustion system design

*Challenges:* performance of chemistry ODE integration on accelerated architectures; linear solver performance for low-Mach algorithm; explicit LES/DNS algorithm not stable
<table>
<thead>
<tr>
<th>E3SM-MMF</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Accurate Regional Impact Assessment in Earth Systems</strong> (Mark Taylor, SNL)</td>
</tr>
<tr>
<td>- Forecast water resources and severe weather with increased confidence; address food supply changes</td>
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</tbody>
</table>

*Challenges:* MMF approach for cloud-resolving model has large biases; adequacy of Fortran MPI+OpenMP for some architectures; Support for OpenMP and OpenACC

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<table>
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<th>NWChemEx</th>
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<tbody>
<tr>
<td><strong>Catalytic Conversion of Biomass-Derived Alcohols</strong> (Thom Dunning, PNNL)</td>
</tr>
<tr>
<td>- Develop new optimal catalysts while changing the current design processes that remain costly, time consuming, and dominated by trial-and-error</td>
</tr>
</tbody>
</table>

*Challenges:* computation of energy gradients for coupled-cluster implementation; on- and off-node performance

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<tr>
<td><strong>Metagenomics for Analysis of Biogeochemical Cycles</strong> (Kathy Yelick, LBNL)</td>
</tr>
<tr>
<td>- Discover knowledge useful for environmental remediation and the manufacture of novel chemicals and medicines</td>
</tr>
</tbody>
</table>

*Challenges:* Inability of message injection rates to keep up with core counts; efficient and performant implementation of UPC, UPC++, GASNet; GPU performance; I/O performance

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E3SM-Multiscale Modeling Framework (MMF)
Cloud Resolving Climate Model for E3SM

• Develop capability to assess regional impacts of climate change on the water cycle that directly affect the US economy such as agriculture and energy production.

• Cloud resolving climate model is needed to reduce major systematic errors in climate simulations due to structural uncertainty in numerical treatments of convection – such as convective storm systems

• Challenge: cloud resolving climate model using traditional approaches requires zettascale resources

• E3SM “conventional” approach:
  - Run the E3SM model with a global cloud resolving atmosphere and eddy resolving ocean.
    • 3 km atmosphere/land (7B grid points) and 15-5 km ocean/ice (1B grid points)
  - Achieve throughput rate of 5 SYPD to perform climate simulation campaigns including a 500 year control simulation
  - Detailed benchmarks on KNL and v100 GPUs show negligible speedups compared to conventional CPUs
    • Low arithmetic intensity of most of the code; throughput requirements lead to strong scaling and low work per node.

• E3SM-MMF: Use a multiscale approach ideal for new architectures to achieve cloud resolving convection on Exascale
  - Exascale will make “conventional” cloud resolving simulations routine for shorter simulations (process studies, weather prediction)
  - For cloud resolving climate simulations, we need fundamentally new approaches to take advantage of exascale resources

PI: Mark Taylor (SNL)
Exascale apps can deliver transformative products and solutions

**ExaSky**

Cosmological Probe of the Standard Model of Particle Physics (Salman Habib, ANL)
- Unravel key unknowns in the dynamics of the Universe: dark energy, dark matter, and inflation

*Challenges*: subgrid model accuracy; OpenMP performance on GPUs; file system stability and availability

**LatticeQCD**

Validate Fundamental Laws of Nature (Andreas Kronfeld, FNAL)
- Correct light quark masses; properties of light nuclei from first principles; <1% uncertainty in simple quantities

*Challenges*: performance of critical slowing down; reducing network traffic to reduce system interconnect contention; strong scaling performance to mitigate reliance on checkpointing

**WarpX**

Plasma Wakefield Accelerator Design (Jean-Luc Vay, LBNL)
- Virtual design of 100-stage 1 TeV collider; dramatically cut accelerator size and design cost

*Challenges*: scaling of Maxwell FFT-based solver; maintaining efficiency of large timestep algorithm; load balancing
## Exascale apps can deliver transformative products and solutions

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<tr>
<th>High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas (Amitava Bhattacharjee, PPPL)</th>
<th>Demystify Origin of Chemical Elements (Dan Kasen, LBNL)</th>
<th>Light Source-Enabled Analysis of Protein and Molecular Structure and Design (Amadeo Perazzo, SLAC)</th>
<th>Accelerate and Translate Cancer Research (Rick Stevens, ANL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Prepare for ITER exps and increase ROI of validation data and understanding</td>
<td>• What is the origin of the elements?</td>
<td>• Process data without beam time loss</td>
<td>• Develop predictive preclinical models and accelerate diagnostic and targeted therapy through predicting mechanisms of RAS/RAF driven cancers</td>
</tr>
<tr>
<td>• Prepare for beyond-ITER devices</td>
<td>• How does matter behave at extreme densities?</td>
<td>• Determine nanoparticle size and shape changes</td>
<td>Challenges: increasing accelerator utilization for model search; effectively exploiting HP16; preparing for any data management or communication bottlenecks</td>
</tr>
<tr>
<td><strong>Challenges:</strong> robust, accurate, and efficient code-coupling algorithm; reduction in memory and I/O usage</td>
<td>• What are the sources of gravity waves?</td>
<td>• Engineer functional properties in biology and materials science</td>
<td><strong>Challenges:</strong> improving the strong scaling (one event processed over many cores) of compute-intensive algorithms (ray tracing, M-TIP) on accelerators</td>
</tr>
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**WDMApp**

**ExaStar**

**ExaFEL**

**CANDLE**