ECP Application Development

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HPC User Forum

Argonne National Laboratory

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Exascale Computing Project: Application Development

**Goal:** Ensure that exascale hardware impacts DOE science/engineering mission

**Approach:** Significant investment in scientific applications well in advance of exascale machines

- Code Porting
- Algorithmic Restructuring
- New Numerical Approaches
- Alternate choice of Physical Models

Hardware has significant impact on all aspects of simulation strategy
## Portfolio of ECP Applications

<table>
<thead>
<tr>
<th>Application Categories</th>
<th>Number of Projects</th>
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<tbody>
<tr>
<td>Chemistry and Materials</td>
<td>6</td>
</tr>
<tr>
<td>Energy (generation)</td>
<td>5</td>
</tr>
<tr>
<td>Earth and Space Sciences</td>
<td>5</td>
</tr>
<tr>
<td>Data Analytics and Optimization</td>
<td>4</td>
</tr>
<tr>
<td>National Security</td>
<td>4</td>
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</table>

- **24 Domain Science/Engineering Simulation Projects**
- **50+ separate codes**
- **2/3 C ; 1/3 Fortran**
- **Most pure MPI, or MPI+OpenMP at outset**
- **Well defined, evolving dependencies on ECP software technology projects**
What defines an application project?

1. Scientific or Engineering exascale challenge problem.

2. Detailed completion criteria for (1) on exascale platform

3. A Figure of Merit (FOM) > 50 for project success

New physics capabilities – Not just faster/bigger version of existing codes
Quick Flyover of all 21 non-NNSA AD Application Projects
## Energy Applications

### ExaWind: Turbine Wind Plant Efficiency

Harden wind plant design and layout against energy loss susceptibility; higher penetration of wind energy

Lead: NREL DOE EERE

### ExaSMR: Design and Commercialization of Small Modular Reactors

Virtual test reactor for advanced designs via experimental-quality simulations of reactor behavior

Lead: ORNL DOE NE

### WarpX: Plasma Wakefield Accelerator Design

Virtual design of 100-stage 1 TeV collider; dramatically cut accelerator size and design cost

Lead: LBNL DOE HEP

### MFIX-Exa: Scale-up of Clean Fossil Fuel Combustion

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

Lead: NETL DOE EERE

### Combustion-PELE: High-Efficiency, Low-Emission Combustion Engine Design

Reduction or elimination of current cut-and-try approaches for combustion system design

Lead: SNL DOE BES, EERE

### WDMApp: High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas

Prepare for ITER experiments and increase ROI of validation data and understanding; prepare for beyond-ITER devices

Lead: PPPL DOE FES
## Chemistry and Materials Applications

<table>
<thead>
<tr>
<th>Project</th>
<th>Description</th>
<th>Lead</th>
<th>Agencies</th>
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<tbody>
<tr>
<td><strong>QMCPACK</strong>: Find, Predict, Control Materials &amp; Properties at Quantum Level</td>
<td>Design and optimize next-generation materials from first principles with predictive accuracy</td>
<td>Lead: ORNL</td>
<td>DOE BES</td>
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<tr>
<td><strong>ExaAM</strong>: Additive Manufacturing of Qualifiable Metal Parts</td>
<td>Accelerate the widespread adoption of AM by enabling routine fabrication of qualifiable metal parts</td>
<td>Lead: ORNL</td>
<td>DOE NNSA / EERE</td>
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<tr>
<td><strong>LatticeQCD</strong>: Validate Fundamental Laws of Nature</td>
<td>Correct light quark masses; properties of light nuclei from first principles; &lt;1% uncertainty in simple quantities</td>
<td>Lead: FNAL</td>
<td>DOE NP, HEP</td>
</tr>
<tr>
<td><strong>NWChemEx</strong>: Catalytic Conversion of Biomass-Derived Alcohols</td>
<td>Develop new optimal catalysts while changing the current design processes that remain costly, time consuming, and dominated by trial-and-error</td>
<td>Lead: PNNL</td>
<td>DOE BER, BES</td>
</tr>
<tr>
<td><strong>GAMESS</strong>: Biofuel Catalyst Design</td>
<td>Design more robust and selective catalysts orders of magnitude more efficient at temperatures hundreds of degrees lower</td>
<td>Lead: Ames</td>
<td>DOE BES</td>
</tr>
<tr>
<td><strong>EXAALT</strong>: Materials for Extreme Environments</td>
<td>Simultaneously address time, length, and accuracy requirements for predictive microstructural evolution of materials</td>
<td>Lead: LANL</td>
<td>DOE BES, FES, NE</td>
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## Earth and Space Science Applications

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<th>E3SM-MMF: Accurate Regional Impact Assessment in Earth Systems</th>
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<tbody>
<tr>
<td>Forecast water resources and severe weather with increased confidence; address food supply changes</td>
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<tr>
<td>Lead: SNL DOE BER</td>
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<th>Subsurface: Carbon Capture, Fossil Fuel Extraction, Waste Disposal</th>
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<td>Reliably guide safe long-term consequential decisions about storage, sequestration, and exploration</td>
</tr>
<tr>
<td>Lead: LBNL DOE BES, EERE, FE, NE</td>
</tr>
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<th>ExaSky: Cosmological Probe of the Standard Model of Particle Physics</th>
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<td>Unravel key unknowns in the dynamics of the Universe: dark energy, dark matter, and inflation</td>
</tr>
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<td>Lead: ANL DOE HEP</td>
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<th>EQSIM: Earthquake Hazard Risk Assessment</th>
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<td>Replace conservative and costly earthquake retrofits with safe purpose-fit retrofits and designs</td>
</tr>
<tr>
<td>Lead: LBNL DOE NNSA / NE, EERE</td>
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<th>ExaStar: Demystify Origin of Chemical Elements</th>
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<td>What is the origin of the elements? Behavior of matter at extreme densities? Sources of gravity waves?</td>
</tr>
<tr>
<td>Lead: LBNL DOE NP</td>
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Data Analytics and Optimization Applications

**ExaSGD: Reliable and Efficient Planning of the Power Grid**

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

Lead: PNNL
DOE EDER, CESER, EERE

**ExaFEL: Light Source-Enabled Analysis of Protein and Molecular Structure and Design**

Process data without beam time loss; determine nanoparticle size & shape changes; engineer functional properties in biology and material science

Lead: SLAC
DOE BES

**ExaBiome: Metagenomics for Analysis of Biogeochemical Cycles**

Discover knowledge useful for environmental remediation and the manufacture of novel chemicals and medicines

Lead: LBNL
DOE BER

**CANDLE: Accelerate and Translate Cancer Research**

Develop predictive pre-clinical models & accelerate diagnostic and targeted therapy thru predicting mechanisms of RAS/RAF driven cancers

Lead: ANL
NIH
Application Development Milestones

**AD**: Mapping of applications to target exascale architecture with machine-specific performance analysis including challenges and projections.

**CD-2/3 Approval**
- **AD**: Early results on pre-exascale architectures with analysis of performance challenges and projections.

**AD**: Results on early exascale hardware

**CD-4 Approve Project Completion**
- **AD, ST, HI**: Demonstration of Application Performance on Exascale Challenge Problems

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**FY18 Q1**
- **AD**: Assess application status relative to challenge problem

**FY19 Q1**
- **Q2**
- **Q4**

**FY20 Q1**
- **Q2**
- **Q4**

**FY21 Q1**
- **Q2**
- **Q4**

**FY22 Q1**
- **Q2**
- **Q4**

**FY23 Q1**
- **Q2**
- **Q4**
Current Figure of Merit Improvements on Summit/Sierra

AD KPP-1 FOM Status: Measured and Extrapolated FOM Increase

Measured KPP-1 values are the ratio of the highest reported FOM to the baseline FOM.
Extrapolated values assume perfect scaling to full machine size.
The Y-Axis default is limited to a maximum of 50 to ensure smaller FOM increases are shown.
Applications Face Common Challenges

1) Flat performance profiles
2) Strong Scaling
3) Understanding/analyzing accelerator performance
4) Choice of programming model
5) Selecting mathematical models that fit architecture
6) Software dependencies
Strong scaling on modern high throughput cores

• High throughput processors do not perform near their peak in starvation limit
  – High value of $n^{1/2}$
  – Require abundance of fine-grained tasks that are efficiently scheduled on available resources
  – Otten et al. e.g. demonstrate that, on Titan, certain problems can run faster by exploiting the additional granularity afforded through the all-CPU model rather than using the highly-tuned GPU code (albeit with a 2.5 increase in power)

• Important because work is linear in time, so 50x has major performance impact
Fast reductions is another key component of strong scaling

- **Conjugate Gradient**
  - If vector reductions performed in software
    - $\eta = 0.5 \frac{n}{P} \geq 8500\text{–}12000$ for $P = 10^6\text{–}10^9$
  - If vector reductions performed in hardware
    - $\eta = 0.5 \frac{n}{P} \geq 1200$ for $P = 10^6\text{–}10^9$!

- **Multigrid**
  - $\eta = 0.5 \frac{n}{P} \sim 10000\text{–}20000$ on machine like BG/Q
  - 2-4 times faster if hardware support for addition prefix ops
  - Bottom line: enables same simulation to run faster
Exemplar: Nuclear Engineering (ExaSMR)
Steve Hamilton (ORNL)
Approach: Monte Carlo Method

- Instead of solving equation, simulate individual neutrons directly
- Use known probability distributions for events (distance to collision, reaction, etc.)
- Count (or “tally”) the number of events that occur
- Simulating many (think millions+) particles gives average behavior

Why is this hard on accelerator architectures?
History-based Algorithm

for each particle do
  while particle is alive
    calculate next interaction
  endwhile
endfor

One particle at a time

Entire life of a particle
history

Thread divergence: not a natural fit for GPUs
Event-based Algorithm

Get vector of particles

\textbf{while} any particle alive \textbf{do}

\textbf{for} each event type \textbf{do}

\textbf{for} particle $\in$ event queue \textbf{do}

Process event

\textbf{end for}

\textbf{end for}

\textbf{end while}

- Do one step at a time
- Sort by event type
- Process as SIMD

Data-level parallelism?
Algorithmic mapping to hardware – neutron particle transport

- Reduce thread divergence – change from history- to event-based algorithm
- Flatten algorithms to reduce kernel size; smaller kernels = higher occupancy
- Partition events based on fuel and non-fuel regions
- Take advantage of other architectural improvements
Exemplar: SNAP Potential (Danny Perez, LANL)

- Machine-learned MD potential that seeks for quantum-chemistry accuracy
- Neighbors of each atom are mapped onto unit sphere in 4D
  \[
  (0, \ldots, 0) = (\max_0 \frac{r}{r_{\text{cut}}}, \cos^{-1}(z/r), \tan^{-1}(y/x))
  \]
- Density around each atom is expanded in a basis of 4D hyperspherical harmonics
- Bispectrum components of the 4D hyperspherical harmonic expansion are used as the geometric descriptors of the local environment
  - Preserves universal physical symmetries
  - Invariant to rotation, translation, permutation
  - Size-consistent
- SNAP uses linear regression to fit coefficients to DFT data
  \[
  u_{m,m'}^j = U_{m,m'}^j(0, 0, 0) + \sum_{r_{ii'}, R_{\text{cut}}} f_c(r_{ii'}) \omega_i U_{m,m'}^j(\theta, \theta, \phi)
  \]
  \[
  B_{j1,j2,j} = \sum_{m_1,m'_1=-j_1}^{j_1} \sum_{m_2,m'_2=-j_2}^{j_2} \sum_{m,m'=-j}^{j} (u_{m,m'}^j)^* H_{j1m1m'_1}^{j2m2m'_2} u_{m_1,m'_1}^j u_{m_2,m'_2}^j
  \]
SNAP GPU Performance Over Time

![Graph showing SNAP GPU performance over time from May to July 2019. The graph compares TestSNAP CUDA and LAMMPS Kokkos. The performance of TestSNAP CUDA improves significantly from May to June, while LAMMPS Kokkos shows a more stable performance. The OLCF GPU Hackathon is noted with an arrow pointing to the graph.](image-url)
SNAP Performance Improvements

- Aidan Thompson (Sandia) took the SNAP CPU code out of LAMMPS → TestSNAP stand-alone (realistic) force kernel, includes correctness check

- Idea from Nick Lubbers (LANL) → Aidan made algorithmic improvements that reduced FLOP count and eliminated some intermediate storage → ~2x speedup on CPUs

- Aidan reduced memory use by collapsing multidimensional arrays into compact lists

- Rahul Gayatri (NERSC):
  1. broke up the one monster kernel into many smaller kernels, reduces register pressure and allows tailoring launch parameters for each kernel, but blows up the memory
  2. inverted loops and changed data layouts to improve memory access

- Also had help from Sarah Anderson (Cray) and Evan Weinberg (NVIDIA)

- These improvements were ported to Kokkos SNAP in LAMMPS by Stan Moore
EXAALT FOM/KPP Projection for Summit

- Mira (IBM BG/Q) FOM baseline: 0.182 Katoms-steps/s/node * 49152 Mira nodes
- 2018 LAMMPS performance on Summit: 33.7 Katom-steps/s/node * 4608 Summit nodes: projected **17.4x faster than Mira baseline**
- New LAMMPS performance on Summit: 175.1 Katom-steps/s/node * 4608 Summit nodes: projected **90.2x faster than Mira baseline**
- Recently ported energy minimization in LAMMPS to Kokkos, which is needed by ParSplice
- Danny Perez (LANL) planning to validate these projections with large-scale Summit run soon
Overall …

• ECP is a very difficult project with many moving parts: specialized node architectures, system software, programming models, application level libraries, etc. enabling ambitious science and performance goals.

• Early adoption of intermediate (100PF) systems, test hardware, and hardware simulators critical to lowering risk by enabling progress tracking and early identification of issues.

• Surprisingly good progress to date, need to continue to push early adoption of exascale-type hardware, ensure proper balance of domain expertise and performance engineering. Facilities engagement programs are critical to achieving this.