January 23, 2026

Center for Accelerated Application Readiness for Discovery

Call for Proposals Informational Webinar

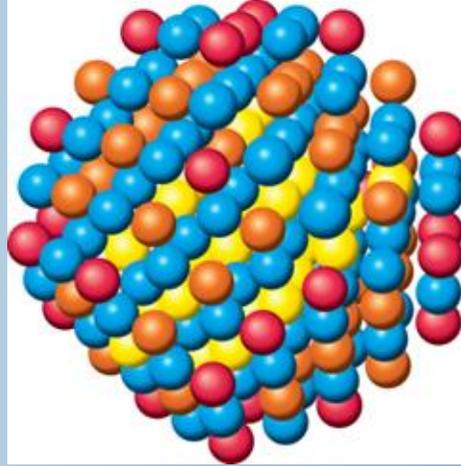Bronson Messer

OLCF

CAAR Goals and Anticipated Outcomes

- Scalable, accelerated scientific applications at the start of Discovery operations
  - <u>Demonstrate a number of applications achieving >= 5x FOM speedups vs. baseline run Frontier</u>
  - **Early Science** accomplishments on the Discovery system
- Experience translated to robust training program and Best Practices documentation
- Close collaboration with OLCF staff and HPE/AMD Center of Excellence
  - Improving the environment for users and application developers
  - Engaging with standards committees and (system) software vendors
- Further hardening of the Discovery system at scale with a broader set of applications beyond OLCF's own testing
- Communications
  - Best Practices in conference papers
  - Reports to ASCR
- Build OLCF staff expertise to enable a smooth transition and effective support of user programs on Discovery

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CAAR projects on Titan

WL-LSMS
Illuminating the role of material disorder, statistics, and fluctuations in nanoscale materials and systems.

3.8 performance ratio XK7/XE6

LAMMPS
A molecular description of membrane fusion, one of the most common ways for molecules to enter or exit living cells.
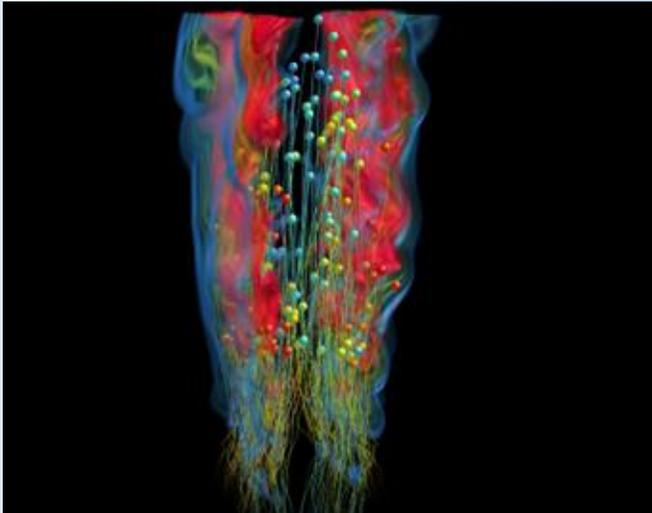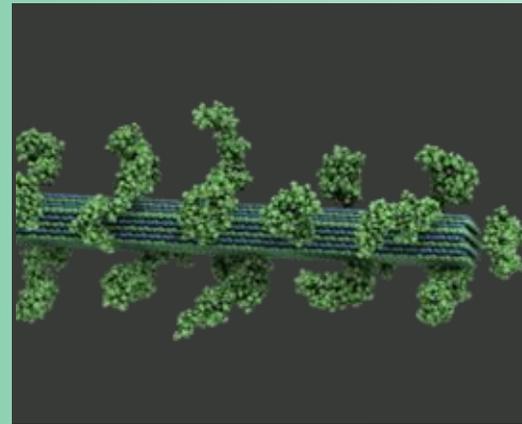
7.4 performance ratio XK7/XE6

S3D
Understanding turbulent combustion through direct numerical simulation with complex chemistry.
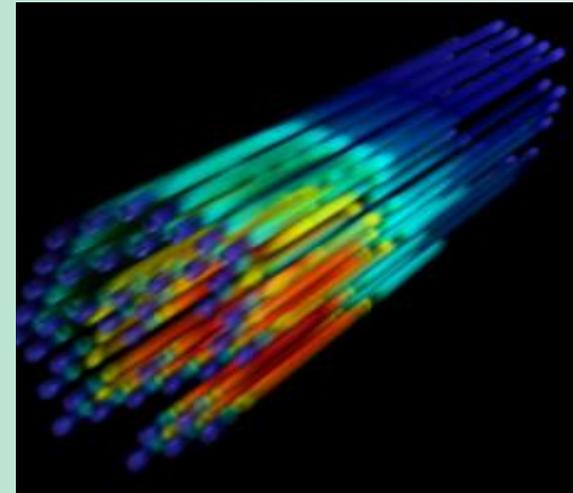
2.2 performance ratio XK7/XE6

Denovo
Discrete ordinates radiation transport calculations that can be used in a variety of nuclear energy and technology applications.

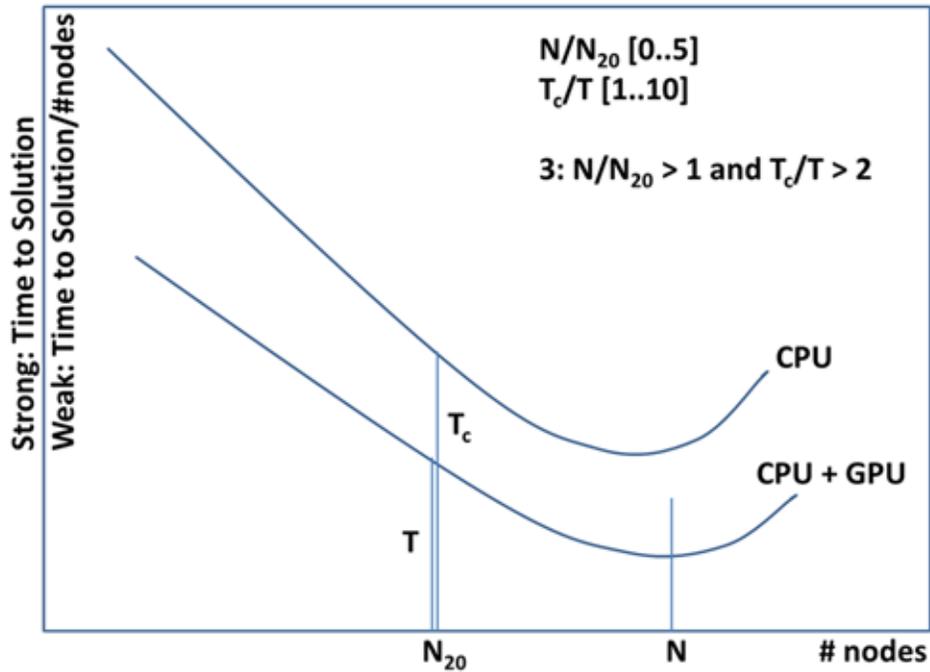3.8 performance ratio XK7/XE6

Titan: Cray XK7 (Kepler GPU plus AMD 16-core Opteron CPU)
Cray XE6: (2x AMD 16-core Opteron CPUs)

CAAR Projects on Summit

Preliminary status of the 8 CAAR projects in meeting the stated goals:

1. Scalability to 20% of the number of Summit nodes

1. Performance improvement with factor 2 or better from utilizing the GPUs at N_{20}

N/N_{20} [0..5]
T_c/T [1..10]

3: $N/N_{20} > 1$ and $T_c/T > 2$

E3SM	✔	1024	8.1
FLASH	✔	4592	3.1
XGC	✔	2048	13.2
NUCCOR	✔	1024	4.1
QMCPACK	✔	4096	24.7
RAPTOR	✔	3888	4
SPECFEM	✔	960	4.9
DIRAC	✔	1024	>9
HACC	✔	1024	30
NAMD	✔	1024	5.7
NWChem	✔	928	~5
LS-DALTON	✔	1024	2.1
GTC	✔	928	20

+5 community efforts (lower level of support)

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CAAR for Frontier

- Used application-specific FOMs to measure improvement versus Summit (target – 4x)

Application	Measured FOM Ratio	Notes
Cholla	22.3	Significant algorithmic improvements. 8000 Frontier nodes.
CoMet	5.2	9074 Frontier nodes
GESTS	5.9	8192 Frontier nodes (code requires 2^n nodes)
LBPM	4.6	Mixed single/double precision on Frontier. 4096 Frontier nodes.
LSMS	9.4	8192 Frontier nodes
NAMD	10.0 (single-node only)	GPU-resident code has markedly increased the single-node performance. However, lack of CHARM++ on Frontier rendered multi-node performance lower compared to Summit at beginning of Frontier's operation
NUCCOR	6.0	4096 Frontier nodes
PIConGPU	4.1	8704 Frontier nodes

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CAAR Project Selection Criteria

Category	Description
Science	• Compelling scientific vision alignment with Nation's science needs • Broad coverage of science domains
Implementation	• Broad coverage of relevant programming models, environment, languages, implementations • Broad coverage of relevant algorithms and data structures • Take advantage of Discovery system characteristics to enable new applications
Development Plan	• Feasibility: Measure of success is "Figure of Merit" compared to Frontier > 5x • Clear challenge problem for execution on Discovery
Development Team	• Commitment from development team • Plan for integration with other active development directions • OLCF liaison domain-specific skills and expertise with the application

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CAAR Proposal Format

Principal Investigators will be asked to include the following in their proposals:

1. Primary Funding Source(s)

2. Name and description of the software application, that includes a summary description of the employed methods and algorithms as well as the language(s) and programming model used.

3. Formulation of Figure of Merit (FOM).

4. Current Parallelization and Acceleration. Current degree of parallelization and the programming model (e.g. MPI, MPI + X, PGAS, etc.), and description of use of GPU in the code.

5. Description of the challenge problem you wish to attack first on Discovery. How will solving this problem and subsequent work on Discovery advance your science?

6. Description of acceleration plan and anticipated challenges on Discovery. How will you achieve 5X FOM speedups on Discovery?

7. What resources can you commit over the lifetime of the project? Describe the composition of the proposing team.

8. Information for export control, etc.

Key questions

- Can your CAAR plan achieve a 5x ratio Discovery/Frontier?

  - Discovery will have

    - 5x the memory bandwidth on the node

    - 5x the per GPU performance for FP32 and FP 64

    - A network with more bandwidth than Frontier's (but, "fatter" endpoints)

- Is your FOM a rate, allowing it to grow via both strong and weak scaling?

CAAR Proposal Reviews

- Impact of scientific result -- Is the Discovery Challenge Problem scientifically important, ambitious, and attainable?

- Team Commitment -- Does the team commit enough resources to the project to be successful? Are they the main developers? If not, are they known contributors?

- Figure of Merit -- Does the proposal provide a reasonable notion for the formulation of a measurable, rate-like figure of merit?

- Acceleration Plan -- Does the proposal present a reasonable path to achieve accelerated performance on Discovery?

- Will incorporation in CAAR expand the pool of applications able to effectively use Discovery?

- **OLCF Scientific Computing Liaisons**

- **Other ORNL Computational Experts**

- **Science Experts**

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CAAR Selection Criteria

Scientific Impact
- Assessment of anticipated scientific impact of ported application
- Compelling vision of an Early Science project
- Application user base

Team Expertise
- Composition, experience, and commitment of application development team
- Technical domain expertise of OLCF liaison
- Technical expertise of HPE/AMD Center of Excellence

Quality of Figure of Merit and Acceleration Plan
- FOM – requires a measurable rate of work
- Acceleration plan that can be enabled by the HPE/AMD SW stack

Program diversity
- Coverage of science domains in CAAR portfolio and support for DOE and US mission
- Coverage of algorithms, programming approaches, languages, data models

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Questions?

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