FY23 Changes

In case you are just here for the updates...

We will bring on a new computer, Kestrel, with 5 x the computing power of Eagle.

Kestrel is designed with a much larger GPU capacity than Eagle: approximately 50% of the computing power comes from GPU nodes.

Due to supply change issues, delivery has shifted....CPU nodes are expected to be available to users mid-FY23, while GPU nodes will be available later in the year (or potentially FY24).

All of this leads to large changes in the allocations process for FY23!
## Eagle vs Kestrel Technical Details

<table>
<thead>
<tr>
<th></th>
<th>Eagle</th>
<th>Kestrel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak Performance</td>
<td>8 Pflops peak</td>
<td>44 Pflops peak</td>
</tr>
<tr>
<td>Processors</td>
<td>Intel Xeon-Gold Skylake 18 cores</td>
<td>Intel Sapphire Rapids 52 cores</td>
</tr>
<tr>
<td>Nodes</td>
<td>2,114 nodes, 2 processors/node</td>
<td>2,304 nodes, 2 processors/node</td>
</tr>
<tr>
<td>Data Storage</td>
<td>14 PetaBytes Lustre</td>
<td>75 PetaBytes Lustre</td>
</tr>
<tr>
<td>Standard Nodes</td>
<td>1728@96GB, 288@192GB</td>
<td>2304@256GB memory</td>
</tr>
<tr>
<td>Accelerated Nodes</td>
<td>50 w/2x NVIDIA Tesla V100</td>
<td>132 w/4x NVIDIA H100 Dual socket AMD Genoa</td>
</tr>
<tr>
<td>Large Data Nodes</td>
<td>48@768GB memory</td>
<td>10@2TB memory</td>
</tr>
<tr>
<td>DAV Nodes</td>
<td>6 w/1x NVIDIA Quadro GV100</td>
<td>8 w/2x NVIDIA A40</td>
</tr>
<tr>
<td>Interconnect</td>
<td>InfiniBand EDR 8-Dimensional Enhanced Hypercube</td>
<td>HPE Slingshot Dragonfly</td>
</tr>
<tr>
<td>Efficient Computing</td>
<td>4.7 gflops/watt</td>
<td>10.4 gflops/watt</td>
</tr>
</tbody>
</table>
What really changes?

Because **GPUs are 50% of the computational power**, we are going to ask (1) is your code GPU ready, and (2) what would it take to make the code GPU-ready? (Note that not all code is expected to make the shift to GPUs.)

We are going to ask for an explicit transition plan, since Eagle is currently scheduled to shut down at the end of FY23. If a project will not continue past then, it does not need to plan a transition.

As many as 100M AUs may be available on Kestrel for the 2nd half of the year. This compares to the 65M AUs available for the entire year on Eagle. NREL and EERE are going to look closely at the “Maximum AUs” request to see which projects may be in a position to use Kestrel.
What’s Available?

The allocation process covers approximately 65 million “Allocation Units,” or AUs on Eagle, and potentially as many as 100 million AUs on Kestrel.

- Each AU is 1/3 of a node hour on Eagle. Note that even if a project uses just one core on a node, it will be charged for the entire node.

- ~85% of this is for EERE-funded projects, ~15% is for NREL non-EERE projects: LDRD, SPP, non-EERE DOE (ARPA-E, Office of Science), DoD, etc.

- A second cluster for VTO projects, “Swift,” will be available. VTO projects requesting time on Eagle will also be considered for time on Swift.

- A cluster for internal NREL projects, “Vermillion,” will be available. LDRD projects requesting time on Eagle will also be considered for time on Vermillion.
What projects are eligible?

– All EERE-funded projects at all national laboratories and universities. (HPC4EI projects should consult with program management, because some are Office of Fossil Energy-funded.)

– All NREL projects, regardless of funding source.

– Projects should apply for allocations if: (1) funded, (2) a proposal is under consideration, or (3) if a proposal will be submitted during summer 2022.

– One allocation per funded project. *Do not split projects up into multiple allocations, even if the project is scattered across several labs. Avoid using large “umbrella allocations” to cover multiple projects.*

Due to the large demand for resources, the allocation process is not able to support projects that do not have a link to either EERE or NREL, even if they support the clean energy mission.
NREL is not the decision maker for EERE projects: our role is to provide EERE with the information needed to make decisions.

- A separate NREL decision-making process is in place for non-EERE NREL projects.
- Allocation process is designed to be parallel to funding process.

Updates and off-cycle requests are possible but in-cycle requests are easier to accommodate: request compute time now if you think you will need it!
Technical Readiness Review: Part of how NREL makes sure EERE has the best possible information for decision-making.

- Is this an HPC task? “Ideal” uses large-scale parallelization capabilities, “Suitable” can run effectively, and “Unsuited” is just not ready. “Suitable” is an acceptable outcome to pass TRR.
- Is the project ready (if appropriate) to use GPUs?
- Is the size of the request justified?
- Is the storage request appropriate? Eagle is not for long-term storage of large data sets...
- Which software? Is the software available?
- NREL staff will follow up with submitter if there are issues.
Process

Request

HPC User Account
• Visit https://www.nrel.gov/hpc/user-accounts.html to request account if you don’t already have one.

Draft Allocation Request
Online
• Starting May 11, 2022.

Submit Allocation Request
• Before midnight June 8, 2022.

Review

Triage
• HPC Operations reviews requests for completeness and assigns Technical Readiness reviewer.

Technical Readiness
• CSC Center staff review requests for mission alignment (broadly), method and software compatibility with, and readiness to run on NREL HPC.

Packaging
• HPC Operations prepares a package, one for each EERE Office or DOE crosscutting activity. Package includes overview (hours requested), scorecard (for assignment of hours by project), and each request. Packages are transmitted no later than July 14, 2022.

Allocation

Apportion
• Allocation authorities meet to determine high-level distribution of hours to each EERE Office or DOE crosscutting activity.

Allocation
• Hours are assigned to each request within each office or DOE crosscutting activity. Allocation decisions are planned to be complete by early September, 2022.

Communication
• HPC Operations prepares memos in response to each allocation request. Memos are planned to be sent by late September, 2022.

Implementation

User Accounts
• HPC Operations will contact each PI to associate users with allocations and set up user accounts if necessary.

Full Allocations
• Full-year allocations will be set to start October 1, 2022.

Provisional Allocations
• Provisional allocations will be set to start when authorized.
Online Submission: Login

Go to hpcprojects.nrel.gov to prepare your submission.

Get an account ASAP if you plan to submit to avoid last-minute delays!
Online Submission: Landing Page

Once logged in, you can submit a FY23 allocation request.

– Use the FY22 button if you need a pilot allocation to test code, otherwise use FY23.

– If you are updating a FY23 allocation *where you are the lead* there is an option to copy the information over as a starting point.

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**Allocation Requests**

Allocation Requests for the FY22 cycle (October 1, 2021 to September 30, 2022) were open from **May 7, 2021 to June 7, 2021**.

Allocation Requests for the FY23 cycle (October 1, 2022 to September 30, 2023) are open from **May 11, 2022 to June 8, 2022**.

Create New FY22 HPC Allocation Request  
Create New FY23 HPC Allocation Request

*Pilot Project and Out-of-Cycle requests may be submitted any time. Pilot allocations are limited to 50,000 allocation units.*
Replace default. Avoid using the year and “HPC.”

Without this title, EERE will not be able to match your request to a funded project.

These are EERE focus areas for categorizing HPC use.

Use info buttons for more information.

Do you have this code and workflow up and running on Eagle?

Use similar keywords to what you would use for a journal.
Online Submission: Contact Information

- Need HPC point person and PI.

This is the person we will contact.

May be contacted by EERE for program reasons.
Even if a project is not linked to a specific EERE office, if it is in the technology area, it should be listed. Example: An ARPA-E project in wind energy should have WETO listed.

If the funding proposal has not yet been submitted, list “Requested.”

Tell us where HPC fits into the overall program.
# Online Submission: Computational Resources Requested

Requestors should take all possible care to provide an accurate estimate of the size and timing of their resource request. The size of the allocation request should be justified based on the number and length of runs given in the AU Request Explanation section of the Computational Readiness section below. Requests for more than 1 million AU's in particular will need both a strong AU Request Explanation, and a strong explanation of the value of the work in the Funding Information and HPC Goals sections. Requestors should also provide the best possible estimate of the timing of their use of resources, since, shifting unused resources between quarters may not be possible.

<table>
<thead>
<tr>
<th>FY</th>
<th>AUs</th>
<th>/projects</th>
<th>MSS</th>
<th>Use Pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY23</td>
<td>100000</td>
<td>5</td>
<td>5</td>
<td>Development in Q1, production in Q2 or lat</td>
</tr>
<tr>
<td>FY24</td>
<td>200000</td>
<td>10</td>
<td>10</td>
<td>Distribute equally across 4 quarters</td>
</tr>
<tr>
<td>FY25</td>
<td>200000</td>
<td>20</td>
<td>20</td>
<td>Distribute equally across 4 quarters</td>
</tr>
</tbody>
</table>

**Minimum AUs**

<table>
<thead>
<tr>
<th>Minimum AUs</th>
<th>Implication of Minimum AUs</th>
<th>Character count: 129</th>
</tr>
</thead>
<tbody>
<tr>
<td>50000</td>
<td>This should be the bare minimum number of AUs the project needs to accomplish its milestones, etc., with little margin for error.</td>
<td></td>
</tr>
</tbody>
</table>

**Maximum AUs**

<table>
<thead>
<tr>
<th>Maximum AUs</th>
<th>Implication of Maximum AUs</th>
<th>Character count: 244</th>
</tr>
</thead>
<tbody>
<tr>
<td>200000</td>
<td>This should be the amount of AUs that will enable the project to do the best possible science, through larger simulation data sets or higher fidelity results. For FY23, it is important to think big because of the large increase in available AUs.</td>
<td></td>
</tr>
</tbody>
</table>

Awards are for FY23 but EERE wants long-term plan. AUs are consistent across machines and from year to year.

If you don’t fit any of these patterns, comment in "Approach."

Use as needed.

We will look at this when allocating Kestrel.
Why Use Patterns?

Eagle is a resource that must be scheduled: If nothing runs and the computer is unused, the AUs aren’t kept in a bank. They “expire” & can’t be made up (like an empty seat on an airplane or table at a restaurant.)

We need to have some idea of how you plan to use your AUs!

– Distribute equally across 4 quarters: 25% each quarter, \textit{for ongoing projects}.
– Development in Q1, production in Q2 or later: 10% in Q1, 30% each in Q2-Q4, \textit{designed for projects that are starting off and need time to develop their code}.
– Start in 2\textsuperscript{nd} Quarter: 33% each in Q2-Q4, \textit{designed for projects with late starts}.
– Use in first half of FY: 45% each in Q1 and Q2, 5% each in Q3 and Q4, \textit{designed for projects with mid-year end dates or early milestones}.
– Use in second half of FY: 5% each in Q1 and Q2, 45% each in Q3 and Q4, \textit{designed for projects with mid-year start dates or late milestones}.

The closer your use matches your pattern, the better priority you will have and the less likely you are to lose Aus.
**Computational Readiness (Part 1)**

<table>
<thead>
<tr>
<th>Software Requested</th>
<th>Code Source</th>
<th>Estimated Use</th>
<th>Essential?</th>
<th>Platform/Environment</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANSYS Fluent</td>
<td>Proprietary/commercial code</td>
<td>50%</td>
<td>Yes</td>
<td>CPU</td>
</tr>
<tr>
<td>MPI</td>
<td>OpenMP</td>
<td>Partially</td>
<td>Impossible</td>
<td>6</td>
</tr>
<tr>
<td>Yes</td>
<td>Unknown</td>
<td></td>
<td>4x</td>
<td></td>
</tr>
</tbody>
</table>

- **Helps show EERE how Eagle is used.**
- **Should add up to 100%.**
- **Allows NREL check to make sure code is ready.**
- **Need to help understand Eagle vs. Kestrel.**
Computational Readiness (Part 2)

<table>
<thead>
<tr>
<th>Name</th>
<th>Code Source</th>
<th>Estimated Use</th>
<th>Essential?</th>
<th>Platform/Environment</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANSYS Fluent</td>
<td>Proprietary/commercial code</td>
<td>50%</td>
<td>Yes</td>
<td>CPU</td>
</tr>
</tbody>
</table>

**What are all of these?**

**Platform/Environment:** Does the code run mostly on the conventional CPU nodes, does it use GPU nodes, or does it use the highly specialized DAV (Data Analysis and Visualization) nodes? If you don’t know, the answer is almost certainly CPU nodes (the default.)

**GPU Readiness:** Can the code currently run on GPUs?

**GPU Effort:** If the user has some control over the code, how hard is it to move it over to GPUs? If it is commercial code, you have no control and should say “impossible.”

**GPU Quantity:** How many GPUs does it use?
Computational Readiness (Pt 3)

Will this project use DAV nodes?
Yes

DAV Node Use Explanation
If you expect to use the specialized DAV (Data Analysis and Visualization) nodes please explain why and what for.

Computational Approach
Give an overall explanation of what you are trying to do:

Example:

In this project, we will perform a large number of simulations of various battery chemistries using the LAMPPS molecular dynamics code to build a training set. We will then use Tensorflow-based machine learning to model the data and attempt to predict additional chemistries that may improve durability. We will re-run promising chemistries using molecular dynamics.
Tell us your plan for moving from one machine to another (and “It’s all ok” is acceptable!)

Kestrel Transition Plan

Delay moving to Kestrel (explanation required).

Kestrel Transition Plan Explanation

Explain to us why you want to do what you wish to do when it comes to moving from Eagle to Kestrel.

Percentage of Allocation Required to Run on Eagle

20%
Absolutely critical to showing that your request is realistic.

Only required if you are doing something unusual.

Do you have large data sets or output files that you need to keep?

Are you applying for, or do you have access to other resources? EERE prefers allocations over 1 million AUs also apply for other computing.
Submitting Your Request

Before submission:
– You can save as many times as you want, but submit only once, so please check and recheck.
– Keep in mind that the number of AUs available will increase mid-year when Kestrel comes on-line & set your “high end” request accordingly.

After submission:
– Your project will undergo an initial review to make sure it is complete and a Technical Readiness Review to ensure it is appropriate for NREL HPC. If you are asked questions, please respond as quickly as possible so NREL can submit to EERE on time.
– VTO users will be asked for follow up to determine if the project can run on Swift cluster.
– If project changes, email hpc-requests@nrel.gov and we will do our best to update request. If appropriate, we will notify EERE that the request has changed.
Decisions:
– Your decision may occur very close to the start of FY22, so be patient!
– Projects that do not receive an allocation will receive a pilot allocation of up to 50,000 AUs.
– There is very little room for adding AUs to projects. If you do not believe you can complete project milestones, etc., within your allocation, talk to your project sponsor immediately. If the scope of your project changes, you should ensure you have the AUs to accommodate the changes.
Dealing With Resource Restrictions

Because of limited resources in Q1 and Q2, justifying the size of the allocation request remains:

– Realistically justify number of AUs required per case and number of cases. You can request a pilot allocation request if you need to figure out how many AUs will use on Eagle.

– Large allocations (greater than 1 million AUs) should show that they are seeking additional resources.

– If you were low (or high) in your AU usage in FY21 allocations, be responsive when NREL operations asks for updates at the end of Q3.

– Pay attention to when you will use allocation and pick appropriate schedule. ("Distribute evenly across 4 quarters," "Development in Q1, production in Q2 or later," etc.)

– Balance this with thinking big once Kestrel is available...
After the Allocation Decision

What if I find out after allocations are done that I need HPC?

– Eagle will be completely booked, but there are opportunities to get time on the machine.

– Projects requesting time after the allocation process has concluded will be given pilot allocations of 50,000 AUs.

– Larger requests will be considered for additional AUs on a “space available” basis on the quarter boundaries.
Eagle is overbooked and will almost certainly remain so for Q1 and Q2 - but Kestrel is coming!

Providing the best possible data, including how use of HPC fits into milestones, and showing your estimate of use, helps NREL and EERE plan the most effective use of the machine, and makes it more likely your request will be filled.

This information also feeds the planning process for buying Kestrel's successor, which hopefully will reduce overbooking.

Please take the time to give the most accurate answers possible!
Thank you

www.nrel.gov

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