



NREL HPC

FY21 Allocation Webinar

Michael Martin

Webinar

June 11, 2020

Topics

 **Allocation Process Overview**

 **Online submission form**

 **Common questions**

FY 21 Allocation Process Intro

The allocation process covers approximately 53 M “Allocation Units,” or AUs.

- 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.

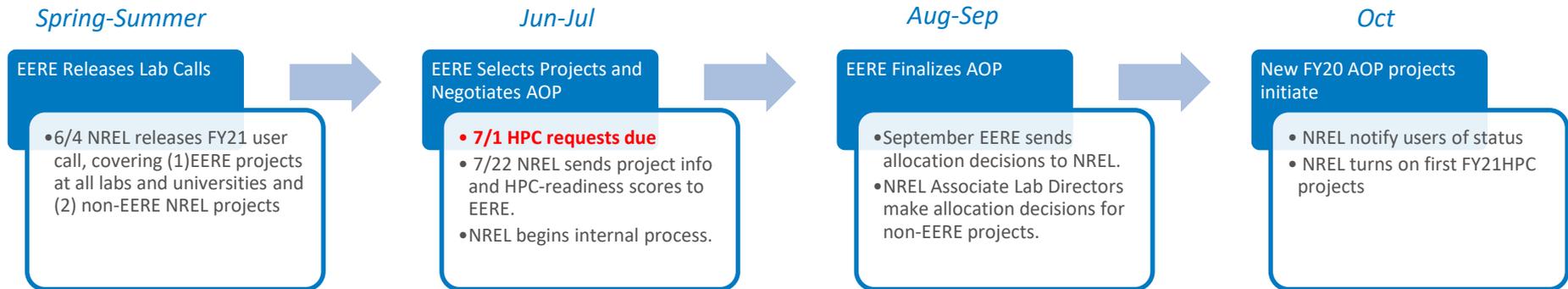
What projects are eligible?

- All EERE-funded projects at all national laboratories and universities. (HPC4EI projects should consult with program management.)
- 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 2020.

FY 21 Allocation Process Intro

NREL is not the decision maker: our role is to provide EERE with the information needed to make decisions.

Allocation process is designed to be parallel to funding process.



Updates and off-cycle requests are possible.

Dealing with resource restrictions

Because of limited resources, justifying the size of the allocation request now more important than ever:

- Realistically justify number of AUs required per case & 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 1M AUs) should show that they are seeking additional resources.
- If you were low (or high) in your AU usage in FY20 allocations, be responsive when NREL operations asks for updates in late June.
- 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.)

Technical Readiness Review

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 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 June 3, 2020,

Submit Allocation Request

- Before midnight **July 1, 2020**.

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 & 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 22, 2020**.

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 **September 9, 2020**.

Communication

- HPC Operations prepares memos in response to each allocation request
- Memos are planned to be sent by **September 16, 2020**.

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, 2020.

Provisional Allocations

- Provisional Allocations will be set to start when authorized

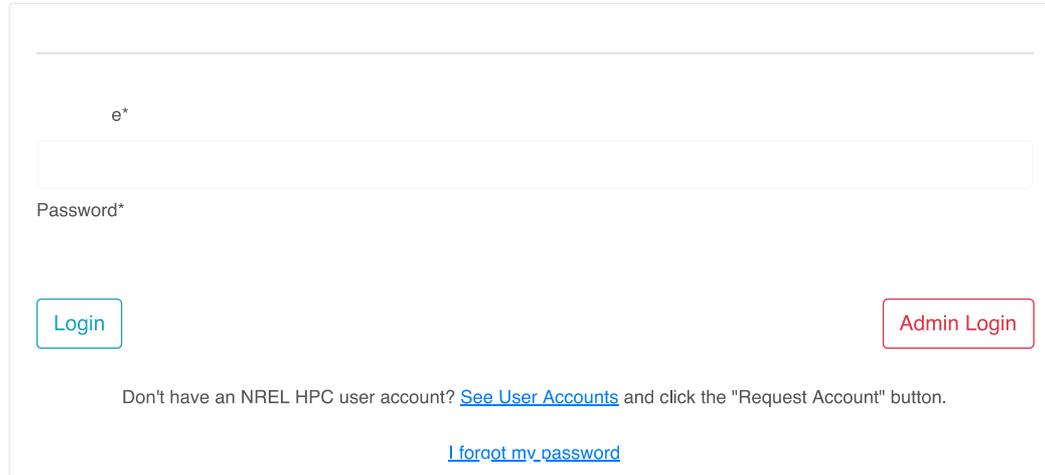
Online Submission: Login

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

Get an account ASAP if you plan to submit to avoid last minute delays!

6/10/2020

Lex



The screenshot shows a login form with the following elements:

- A horizontal line at the top of the form area.
- A text input field with the label "e*" above it.
- A password input field with the label "Password*" below it.
- A blue "Login" button.
- A red "Admin Login" button.
- A link: "Don't have an NREL HPC user account? [See User Accounts](#) and click the "Request Account" button."
- A link: "[I forgot my password](#)".

Online Submission: Landing Page

Once logged in, you can submit a FY21 allocation request.

- Use the FY20 button if you need a pilot allocation to test code, otherwise use FY21.
- If you are updating a FY20 allocation *where you are the lead* there is an option to copy the information over as a starting point.

Allocation Requests

The Fiscal Year (FY) 2021 NREL HPC Call for allocation requests starts **June 3, 2020**.

Requests for allocations for the FY21 cycle which runs October 1, 2020 to September 30 2021 are due **July 1, 2020**.

Pilot Project and Out-of-Cycle requests may be submitted any time. Pilot allocations are limited to 20,000 hours. Out-of-Cycle requests are considered quarterly.

Create New **FY20** Allocation Request

Create New **FY21** Allocation Request

Online Submission: Project Information

- Be simple and descriptive.

Replace default. This will be used repeatedly.

Handle ⓘ* Fiscal Year ⓘ*

Title ⓘ* Word count: 13

Short Abstract ⓘ Word count: 12

Abstract ⓘ Word count: 14

Use info buttons for more information.

Online Submission: Contact Information

- Need HPC point person and PI.

Contacts

HPC Lead Email 	HPC Lead First Name	HPC Lead Last Name	HPC Lead Institution
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
HPC Alternate Lead Email 	HPC Alternate Lead First Name	HPC Alternate Lead Last Name	HPC Alternate Lead Institution
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
PI Email 	PI First Name	PI Last Name	PI Institution
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

This is the person we will contact.

Online Submission: Funding Information and Project Goals

This is how you communicate to EERE how using Eagle fits into a funded or proposed project.

- Make VERY specific links to the goals of the project!
- Ensure EERE can match the request to a project or funding request.

Funding Information and HPC Goals

This section should provide the information needed to link the allocation to a project that is funded, under consideration, or expected to be submitted for funding. The descriptions given in "Program or Project Tasks" and "Program or Project Milestones" should provide a clear case for the use of HPC resources to complete this project.

Funding Area ●	Funding Source ●	Project Category ●	Project Type ●
VTO ▾	Helps make sure it gets to decision maker	EERE ▾	FOA ▾
Funding Status ●	Funding End Date ●	AOP WBS or Contract # ●	
Requested ▾			
AOP or Project Title ●	DOE/Federal Contact ●		
Self-explanatory			

Word count: 1

Program or Project Tasks ●

Describe in detail how you will use Eagle for specific project tasks.

Character count: 69

Program or Project Milestones ●

Indicate milestones are linked to Eagle usage

Character count: 45

Most Critical Milestone ●

Annual Milestone ▾

Online Submission: Funding Information and Project Goals

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 *Resource Justification* section of the *Computational Readiness* section below. Requests for more than 1 million AUs in particular will need both a strong resource justification, 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.

FY	AUs	/projects	MSS	Use Pattern
FY21	100000			Development in Q1, production in Q2 or later
FY22	100000			Distribute equally across 4 quarters
FY23	100000			Use in first half of FY

Minimum AUs: 80000
Implication of Minimum AUs: Show what you can do with a lower allocation. Typically meeting project milestones without much margin for things going wrong or doing good science...
Character count: 151

Maximum AUs: 120000
Implication of Maximum AUs: Show what you can do with a larger allocation.
Character count: 46

AU Estimator

Awards FY21 but EERE wants long-term plan.

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

Use as needed.

Computational Readiness (Part 1)

Lets NREL
check to
make sure
code is
ready

Computational Readiness

Software

Name	Usage	Essential?	Source	MPI	OpenMP	GPU Speedup	GPU Ready	GPU Qty
ANSYS-Fluent delete	50% ▾	Yes ▾	Proj ▾	Yes ▾	Yes ▾	N/A ▾	1-2 ▾	not ▾
Python delete	50% ▾	Yes ▾	Inte ▾	Yes ▾	No ▾	2x ▾	Nov ▾	2 ▾

[add](#)

Demographics

Size of runs ●
2-4 nodes ▾

Duration of runs ●
< 24 hours ▾

Is this project using/supporting ML/AI? (Check all that apply) ●

- Project uses Machine Learning/Artificial Intelligence
- Project generates data sets to be used for ML/AI

Computational Approach ●

Explain what codes you are using and how you are using them.

Character count: 60

Should add up to
100%.

Helps show EERE
how Eagle is
used.

Computational Readiness (Part 2)

I/O Requirements ●

Relevant when you are moving data in or out of Eagle.

Character count: 53

Resource Justification ●

Build your estimate from the ground up. If you need 500 cases of a code that takes 10 hours on 8 nodes, then

One case = 80 node hours = 240 AUs.

100 cases = 120,000 AUs.

Go through this for each code used if you have multiple steps.

Character count: 237

Other Computational Resources ●

Because of the limited resources, EERE urges PIs, especially ones with requests larger than 1M AUs, to pursue other resources in conjunction with Eagle requests.

Absolutely
critical to
showing that
your request
is realistic.



Submitting your request

Before submission:

- You can save as many times as you want, but submit only once, so please check and recheck.

After submission:

- If project changes, e-mail hpc-requests@nrel.gov and we will do our best to update request. If appropriate, we will notify EERE that the request has changed.

Questions? (2020)

Q: Does "NREL project" mean any project NREL is involved with?

A: For purposes of using the 15% of the machine allocated to non-EERE projects, this includes any project with NREL participation.

Q: How large can pilot allocations be? How long do they take to be approved?

A: Pilot allocations can be up to 20,000 AUs and generally take 10-14 days for approval. We will seek to expedite approval for pilot allocations that are requested to estimate AUs for FY21 requests.

Q: For NREL-run efforts that are a part of multi-lab projects should PI be the overall technical lead (potentially from other lab) or the NREL technical lead (still non-HPC lead)?

A: Please include the overall lead, even if they are not at NREL. You may wish to include the non-HPC technical lead as the alternate HPC contact.

Q: Is there a table describing the breakdown for the Use Patterns?

A: The list of options is in the dropdown menu of the online application.

Q: Can we submit a FY20 request for an extension in case we have used all node hours?

A: You may submit a request to hpc-requests@nrel.gov. However, because of current resource availability, it is unlikely that additional AUs will be provided for FY20.

Questions? (2020)

Q: Is there any way to share use of a node across multiple projects when running?

A: We do not have that capability at this time.

Q: Is the application form the same for pilot projects?

A: Yes, but because these are exploratory, there will be less scrutiny of the size of the request.

Q: Can we submit multiple requests per project (for example for different kinds of research/codes uses?)

A: No, each project should have one request.

Q: What happens if we realize our request was too small or too large after allocation? Is there there a reconciliation period?

A: Projects can always return a portion of their allocation if they realize their request was too large. Projects that have requested too few AUs can submit a request for more AUs through hpc-requests@nrel.gov.

Q: For pilot projects, what level of detail is required ? Does it need to reference a specific project as well?

A: The form is the same, but less detail is required, especially if the request is to support code validation. In general, these requests should reference a specific project. *However, if the request is to support code validation or scaling for a proposal or allocation request in progress, this requirement will be waived.*

Questions? (2020)

Q: Is there a maximum number of AUs a project can reasonably ask for?

A: There is no official cap. In practice, EERE will only support projects over 1M AUs with extraordinary justification.

Q: If the project is funded by EERE, is it required to have a NREL personnel in the request?

A: No, there is no requirement to include NREL staff, and many existing projects do not.

Q: If total AU's utilized for current allocation are under the allocated AU's, will under utilization have an impact on the current request. If so is there a limit on under utilization?

A: If a project is using 50 percent or less of its FY20 allocation, EERE may take that into account when deciding on FY21 allocations. PIs can reduce the risk of a reduced allocation by (1) seeking to return AUs they do not expect to use by July 1, and (2) explaining the reasons for the underutilization.

Questions? (Past years)

Q: Are separate allocation requests required if different software will be used?

A: A separate allocation request is required for each source of funding. Project activities including use of different software can be described in a single request under the “Computational Readiness” section of the request.

Q: The process described is for the EERE allocation pool. How is the process different for the NREL allocation pool to cover things like LDRD?

A: The process to determine within the NREL allocation pool is similar. NREL ALDs and LPMs participate in similar activities to EERE Office Directors.

Q: If the same team of people is working on multiple, inter-related projects with multiple funding streams, can jobs access an aggregated allocation to simplify management of resources used by the team?

A: We account for and report AUs use per allocation decision. So, a unique handle is needed for each project. However, storage can be shared by multiple allocations. HPC Operations will contact project leads in August to establish teams (list of members) and associate those teams with use of handles for job submission and project data storage.

Questions? (Past years)

Q: For a Multi-lab project, should one request per project or per lab be submitted?

A: If an AOP WBS spans multiple labs, a single allocation request will serve. Otherwise one is required for each AOP project ID.

Q: For large programs with future awards, how should those be handled?

A: A single allocation request to cover the program needs can be submitted. However, it is preferred that these be broke into individual requests as soon as possible.

Q: Will access to the large memory and accelerated nodes be handled with a “special” request?

A: We offer the large memory and GPGPU-accelerated nodes in normal queues. This may change during the system’s life as project needs evolve.

Q: How can I give critical jobs higher run priority?

A: Using the Slurm option “--qos=high” allows urgent jobs to jump to the top of the queue in exchange for a higher allocation burn rate. Note that routine use of this mechanism is not allowed.

Reservations are possible if situations require, see <https://www.nrel.gov/hpc/eagle-job-priorities.html>

Thank you

www.nrel.gov

NREL/PR-2C00-77068

This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

