



# NREL HPC

## FY22 Allocation Webinar

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Webinar

May 14, 2021

# FY22 Changes

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

- Dates have been changed, with requests due earlier.
- Tweaks to the form:
  - Additional information on keywords and categories.
  - Confusing wording cleared up in several parts of the application.
  - Optional request for explanation of large storage amounts.
- Threshold for pilot allocations increased from 20,000 to 50,000 AUs.
- 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.*

# FY22 Allocation Process Intro

## What's Available?

The allocation process covers approximately 65 million “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.
- 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.*

# FY22 Allocation Process Intro

## What projects are eligible?

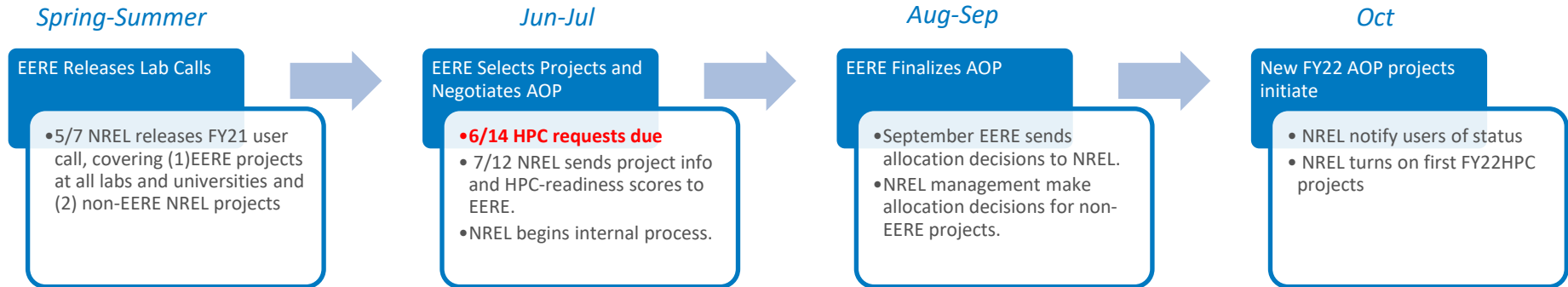
- All EERE-funded projects at all national laboratories and universities. (HPC4EI projects should consult with program management, because some are Office of Fossil Energy-funded.)
- All NREL projects, regardless of funding source.
- Projects should apply for allocations if: (1) funded, (2) a proposal is under consideration, or (3) if a proposal will be submitted during summer 2021.
- 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 Eagle 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.**

# FY 22 Allocation Process Intro

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.

# 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 May 7, 2021.

### Submit Allocation Request

- Before midnight **June 7, 2021**.

## 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, 2021**.

## 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, 2021**

### Communication

- HPC Operations prepares memos in response to each allocation request.
- Memos are planned to be sent by **late September, 2021**.

## 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, 2021.

### Provisional Allocations

- Provisional allocations will be set to start when authorized.

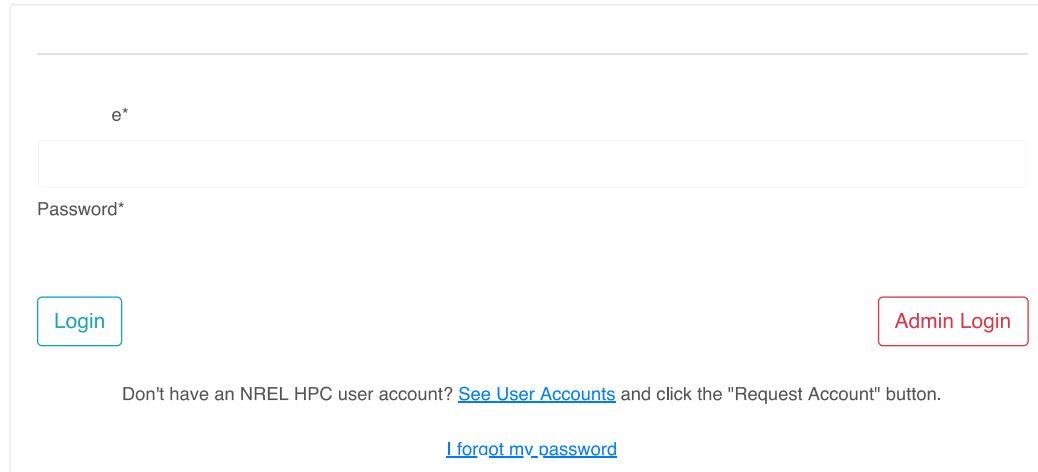
# Online Submission: Login

Go to [hpcprojects.nrel.gov](https://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\*" to its left.
- 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 FY22 allocation request.

- Use the FY21 button if you need a pilot allocation to test code, otherwise use FY22.
- If you are updating a FY21 allocation *where you are the lead* there is an option to copy the information over as a starting point.

## Allocation Requests

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

Allocation Requests for the FY21 cycle (October 1, 2020 to September 30, 2021) were open from **June 3, 2020** to **July 1, 2020**.

Pilot Project and Out-of-Cycle requests may be submitted any time. Pilot allocations are limited to 50,000 allocation units.

[Create New FY22 HPC Allocation Request](#)

[Create New FY21 HPC Allocation Request](#)

# Online Submission: Project Information

- Be simple, descriptive, and accurate.

Replace default. This will be used repeatedly. Avoid using the year and "HPC."

EERE focus areas for categorizing HPC use:

1. Materials Science
2. Integrated Energy Systems
3. Computational Fluid Dynamics
4. Forecasting
5. Manufacturing
6. Other

Handle short&clear!

Fiscal Year FY21

Title Should match the funded project, or a subtask of the funded project. Word count: 12

Short Abstract A top level summary to explain the project. This will appear on a summary slide to DOE and NREL decision makers. Word count: 21

Abstract This is a longer explanation if EERE wants to look at the project in more depth. Word count: 16

Primary Project Focus -----




Keywords Just like if you were writing up a journal paper...

Use info buttons for more information.


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

# 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.



May be contacted by EERE for program reasons.



# Funding Information and Project Goals

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.

**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	This helps us make sure the project goes to the right decision maker.	EERE	AOP
Funding Status ●	Funding End Date ●	AOP WBS or Contract # ●	
Requested			
AOP or Project Title ●		DOE/Federal Contact ●	
Program or Project Tasks ●			
Describe in as much detail as possible how you will use Eagle for specific project tasks.			
Character count: 89			
Program or Project Milestones ●			
Describe which project milestones are explicitly linked to Eagle use.			
Character count: 69			
Most Critical Milestone ●			
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# Online Submission: Funding Information and Project Goals

Awards are for FY22 but EERE wants long-term plan.

## 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 AUs 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.

FY	AUs	/projects	MSS	Use Pattern
FY22	100000	5	5	Development in Q1, production in Q2 or later
FY23	200000	20	20	Distribute equally across 4 quarters
FY24	100000	20	40	Use in first half of FY

Minimum AUs

80000

Implication of Minimum AUs

What is the absolute minimum you need to meet your milestones with little margin for error?

Character count: 91

Maximum AUs

150000

Implication of Maximum AUs

If you had a larger allocation, what would you get done? More accurate results? A larger ensemble?

Character count: 104

AU Estimator

Use as needed.

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

# Why Use Patterns?

**Eagle is a resource that must be scheduled: If nothing runs, the AUs aren't kept in a bank, they "expire."**

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

- Distribute equally across 4 quarters: 25% each quarter, *for ongoing projects.*
- Development in Q1, production in Q2 or later: 10% in Q1, 30% each in Q2-Q4, *designed for projects that are starting off and need time to develop their code.*
- Start in 2<sup>nd</sup> Quarter: 33% each in Q2-Q4, *designed for projects with late starts.*
- Use in first half of FY: 45% each in Q1 and Q2, 5% each in Q3 and Q4, *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, *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)

Allows 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 <a href="#">delete</a>	50% ▾	Yes ▾	Proj ▾	Yes ▾	Yes ▾	N/A ▾	1-2 ▾	not ▾
Python <a href="#">delete</a>	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 (Pt 2)

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.

## AU Request Explanation

Ideally this should be built from the "bottom up."

We will need to run 500 cases of our simulation. Each case takes 10 hours on 8 nodes.

$500 \text{ cases} \times 10 \text{ hours} \times 8 \text{ nodes} \times 3 \text{ AUs/node hour} = 120,000 \text{ AUs}$ .

Character count: 206

## I/O Requirements

This will be important if you expect to move large amounts of data in and out of Eagle in a short time.

Character count: 103

## Storage Request Explanation (only required if over 10 TB)

If you need large amounts of storage, especially for machine learning, explain the size of your request.

Character count: 104

## Other Computational Resources

List other HPC or cloud resources you have access to. There is no need to list desktop computing.



# 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:

- Your project will undergo an initial review to make sure it is complete and a *Technical Readiness Review* to ensure it is appropriate for Eagle. 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](mailto:hpc-requests@nrel.gov) and we will do our best to update request. If appropriate, we will notify EERE that the request has changed.

# After the Allocation Decision

## 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, justifying the size of the allocation request now more important than ever:

- 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.)

# After the Allocation Decision

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

- The machine 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.

Changes in storage and input and output to existing projects can usually be accommodated through requests to HPC Operations.

# Closing Comment

Eagle is overbooked and will almost certainly remain so for the rest of its operational life.

Providing the best possible data, including how use of Eagle 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 Eagle's successor*, which hopefully will reduce overbooking.

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

# Thank you

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[www.nrel.gov](http://www.nrel.gov)

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