Argonne Training Program on Extreme-Scale Computing

Introduction to ATPESC

Ray Loy
ATPESC Program Director

Outline

- Motivation
- Overview
- Curriculum
- Public training materials
- Applying for ATPESC 2023

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Motivation for ATPESC

- Today's most **powerful supercomputers** have **complex hardware architectures** and **software environments**
  - and even greater complexity is on the horizon on next-generation and exascale systems
- The **scientific and engineering applications** developed for these systems are themselves **complex**
- There is a **critical need for specialized, in-depth training for the computational scientists** poised to facilitate breakthrough science and engineering using these systems

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ATPESC Overview

- Founded by Paul Messina in 2013
- Conceived as a 2-week retreat
- Renowned computer scientists and HPC experts from US national laboratories, universities, and industry serve as lecturers and guide hands-on sessions.
- Target audience: advanced doctoral students, postdocs, and early career computational scientists
- No fee to participate. Domestic travel, meals, and lodging provided.
- Competitive application process reviewed by committee
  - Must have experience in MPI and/or OpenMP and/or Data Science frameworks
  - Experience with at least one HPC system
  - Concrete plans to conduct CSE research on large-scale computers

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ATPESC Website

extremecomputingtraining.anl.gov

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Argonne – a part of DOE National Laboratory System

Office of Science Laboratories

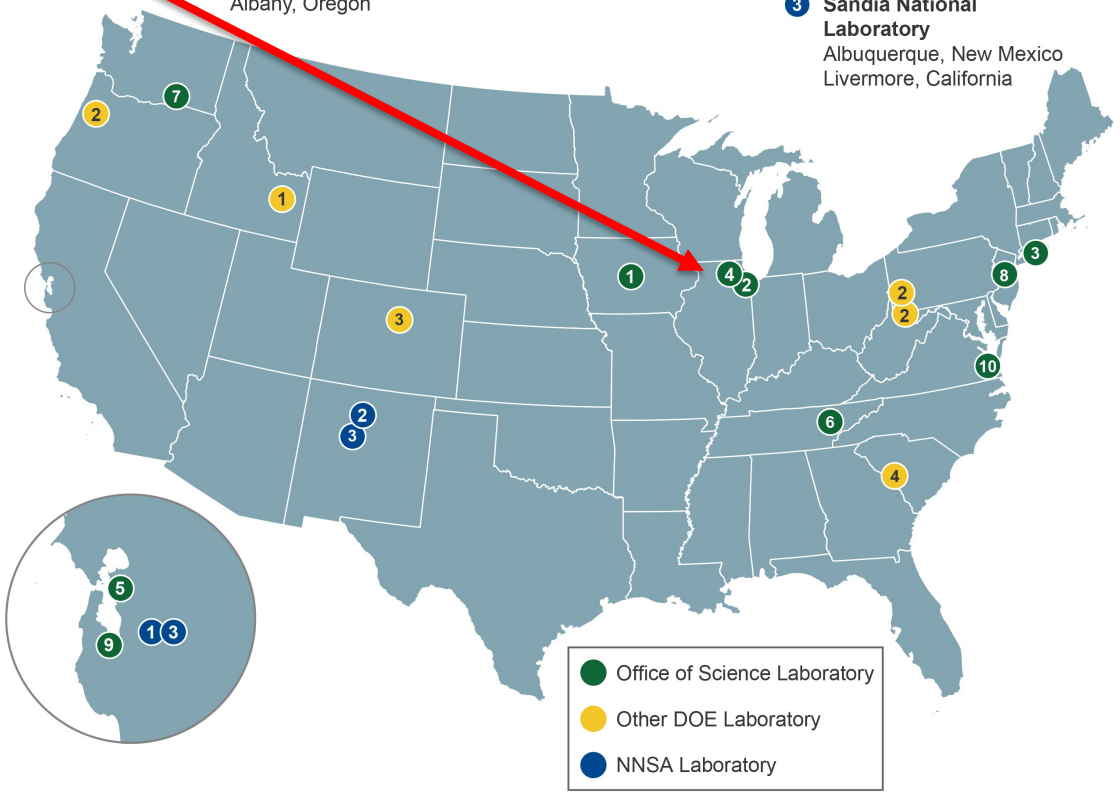
1. **Ames Laboratory**
   Ames, Iowa
2. **Argonne National Laboratory**
   Argonne, Illinois
3. **Brookhaven National Laboratory**
   Upton, New York
4. **Fermi National Accelerator Laboratory**
   Batavia, Illinois
5. **Lawrence Berkeley National Laboratory**
   Berkeley, California
6. **Oak Ridge National Laboratory**
   Oak Ridge, Tennessee
7. **Pacific Northwest National Laboratory**
   Richland, Washington
8. **Princeton Plasma Physics Laboratory**
   Princeton, New Jersey
9. **SLAC National Accelerator Laboratory**
   Menlo Park, California
10. **Thomas Jefferson National Accelerator Facility**
    Newport News, Virginia

Other DOE Laboratories

1. **Idaho National Laboratory**
   Idaho Falls, Idaho
2. **National Energy Technology Laboratory**
   Morgantown, West Virginia
   Pittsburgh, Pennsylvania
   Albany, Oregon
3. **National Renewable Energy Laboratory**
   Golden, Colorado
4. **Savannah River National Laboratory**
   Aiken, South Carolina

NNSA Laboratories

1. **Lawrence Livermore National Laboratory**
   Livermore, California
2. **Los Alamos National Laboratory**
   Los Alamos, New Mexico
3. **Sandia National Laboratory**
   Albuquerque, New Mexico
   Livermore, California



Source: https://science.energy.gov/~/media/_/images/laboratories/DOE_Laboratories_Map_2014_Hi-res.jpg

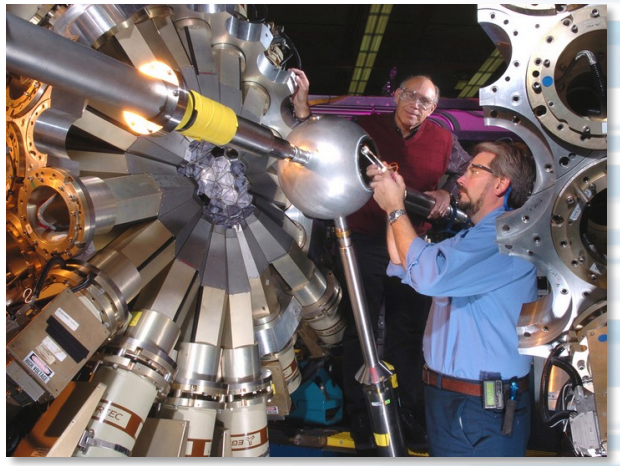
Together, the **17 DOE laboratories** comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities. The laboratories:

- Execute long-term government scientific and technological missions, often with complex security, safety, project management, or other operational challenges;
- Develop unique, often multidisciplinary, scientific capabilities beyond the scope of academic and industrial institutions, to benefit the Nation's researchers and national strategic priorities; and
- Develop and sustain critical scientific and technical capabilities to which the government requires assured access.

Major Scientific User Facilities at Argonne

Advanced Photon Source

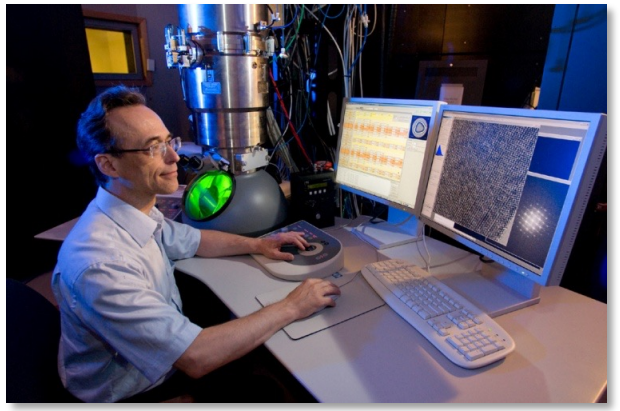
Argonne Tandem Linear Accelerator System



Center for Nanoscale Materials

Argonne Leadership Computing Facility Aurora

Electron Microscopy Center



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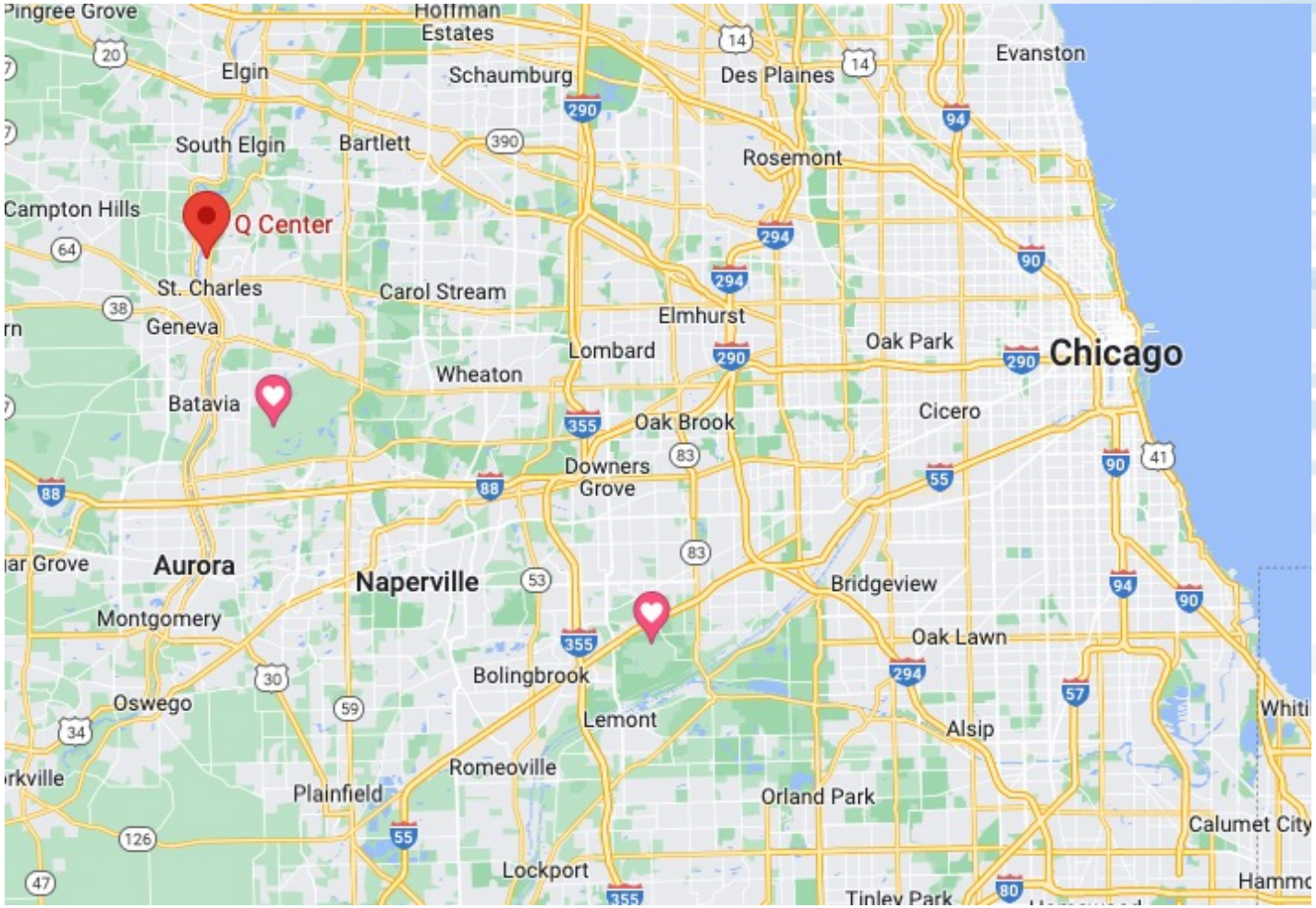
ATPESC 2023 Venue



Source: Google Maps, shutterstock, NASA

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ATPESC 2022

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Curriculum Tracks *(over 100 hours of content)*

- **Track 1:** Hardware Architectures
- **Track 2:** Programming Models and Languages
- **Track 3:** Data-intensive Computing and I/O
- **Track 4:** Visualization and Data Analysis
- **Track 5:** Numerical Algorithms and Software for Extreme-Scale Science
- **Track 6:** Performance Tools and Debuggers
- **Track 7:** Software Sustainability
- **Track 8:** Machine Learning and Deep Learning for Science

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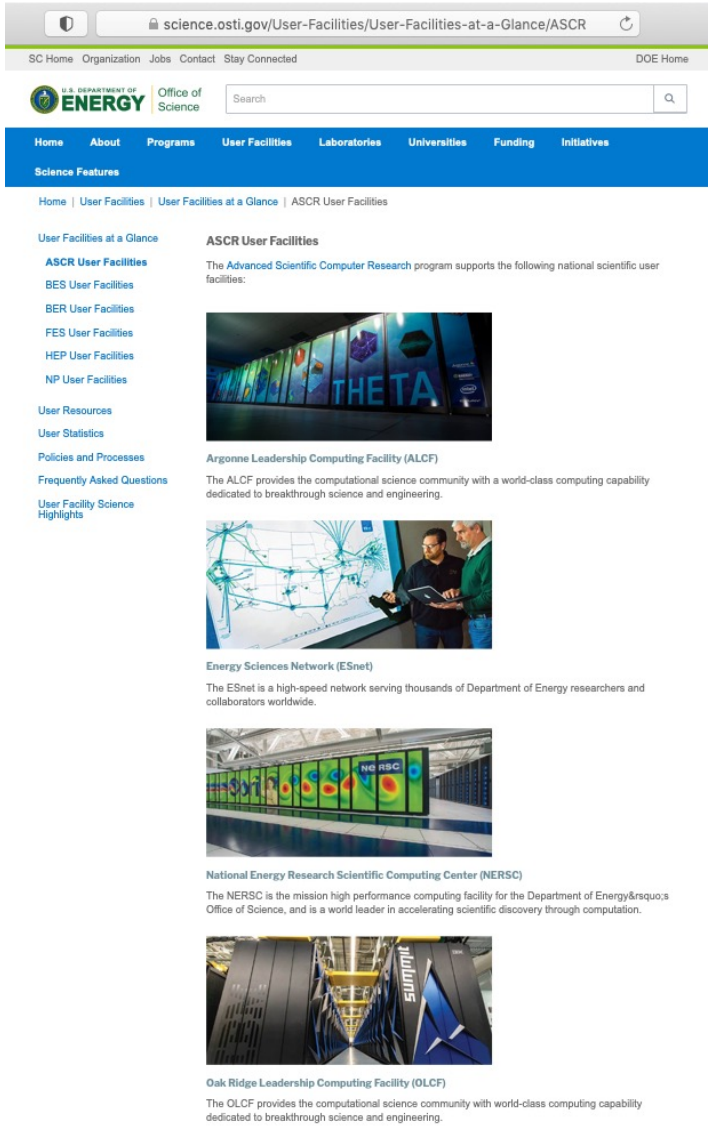
ATPESC Computing Resources



- **ALCF** – Polaris and Theta/ThetaGPU
- **OLCF** - Ascent
- **NERSC** – Cori et al.
- **Intel Devcloud**

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Goals for Attendees

Exposure to New ideas

Take advantage of ATPESC Resources

Talk F2F with Lecturers, other Participants, Support

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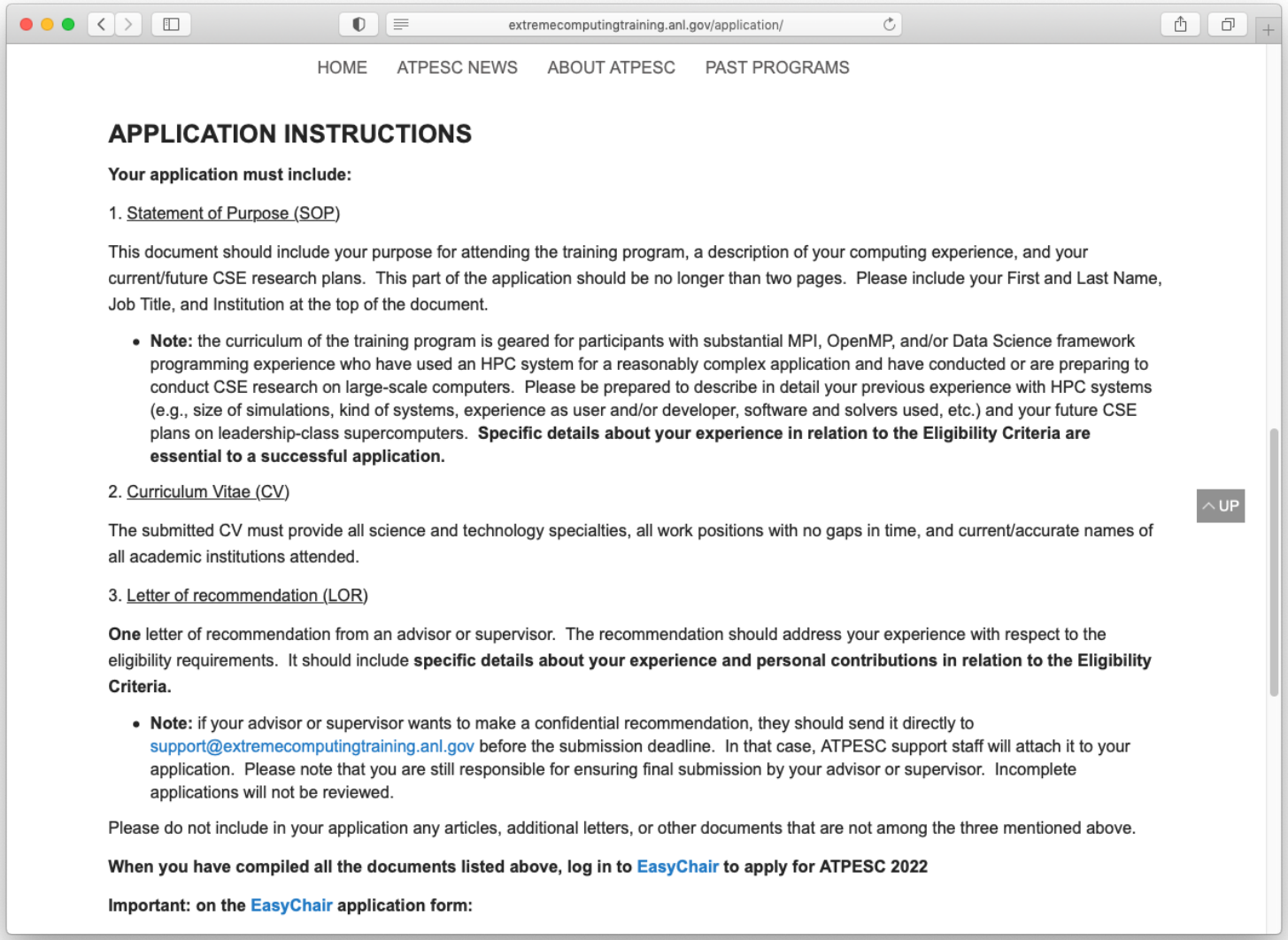
Application Instructions



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Eligibility

"Doctoral students, postdocs, and computational scientists interested in attending ATPESC can review eligibility and application details on the application instructions web page."

- These are the most common applicants but in general, **anyone who is qualified and who would benefit from the program may apply**.
- *If your situation is unusual, just address that in your Statement of Purpose.*

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Eligibility

- Substantial experience in MPI and/or OpenMP programming. Equivalent experience with Data Science frameworks will also be considered.
- Experience using at least one HPC system for a reasonably complex application.
- Plans to conduct computational science and engineering (CSE) research on large-scale computers.

Application Components

- Statement of Purpose
- Curriculum Vitae (CV)
- Letter of Recommendation (LOR)

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The Key to success

Provide details

The #1 problem a reviewer faces is trying to guess your qualifications when the materials are not clear.

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1. Substantial experience in MPI and/or OpenMP programming. Equivalent experience with Data Science frameworks will also be considered.

- Weak statements
  - "I took a class on MPI"
  - "I ran a code that uses MPI"
- Stronger statements
  - "I work on the NNN code. I implemented, tested, and benchmarked the message-passing routines for the boundary exchange of the MMM solver which has a communication pattern that communicates between…"

- If you are part of a group-developed code or working on a community code, be specific about your individual contribution.

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Experience using at least one HPC system for a reasonably complex application.

- We do not expect that you have access to a world-class system
  - University/corporate clusters are relevant
- Be clear if you are developing code and running it vs. running an existing code
- What types of runs have you accomplished?
  - Core/node counts are informative
  - Did you perform scaling studies or other performance inquiries?
- What type of queuing system(s) were involved?
  - Did you construct job scripts?
  - Did you run a large campaign and employ any workflow techniques to manage jobs?

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Plans to conduct computational science and engineering (CSE) research on large-scale computers.

- The training should be put to good use
- What is your current situation?
  - Are you currently part of a research effort?
- Where are you headed in your career?
  - If you are a student, what positions are you applying to?
  - How do you expect your current work to carry over?

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ATPESC 2023 Updates

- Subscribe to "info" mailing list linked from the homepage
  - https://extremecomputingtraining.anl.gov (bottom of page)
- Direct inquiries to
  - support@extremecomputingtraining.anl.gov

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Acknowledgments

Exascale Computing Project

Website: https://exascaleproject.org

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Questions/Discussion

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