OAK RIDGE National Laboratory

Frontier Tips and Tricks

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Frontier New User Training

Feb 28th, 2024

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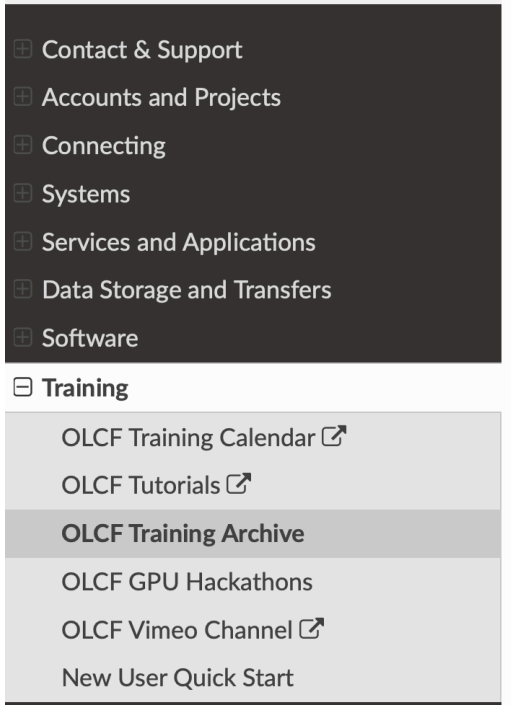
- Training Archive
- Programming Models
- AI on Frontier
- NVME
- Checkpointing
- Links to profiling talks and docs
- Link to debuggers and docs
- Link to Tips from Balint's February talk

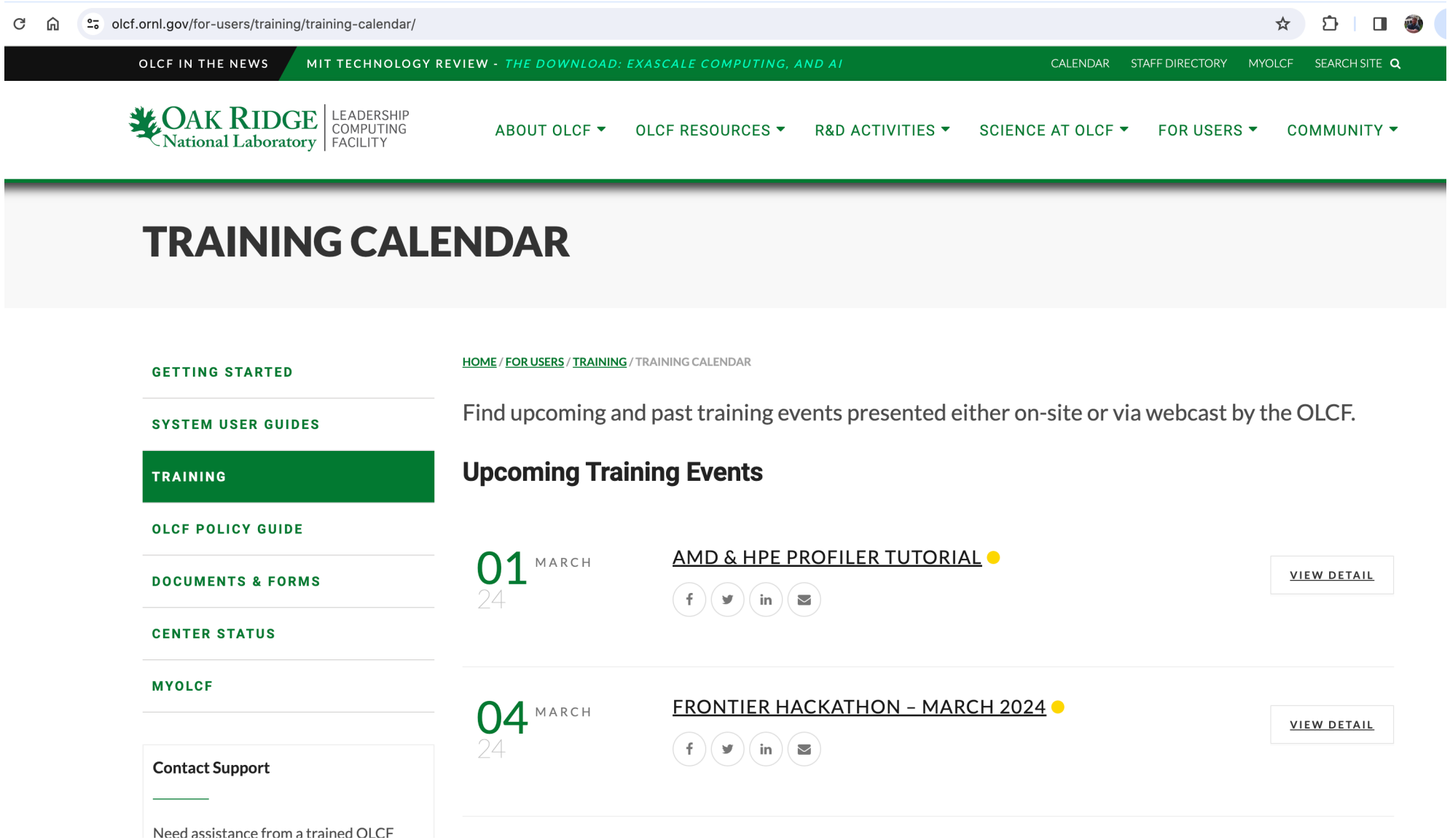
Training Calenar & Archive

- Training Calendar:
  - https://www.olcf.ornl.gov/for-users/training/training-calendar/
  - Includes past events back to Jan 2022

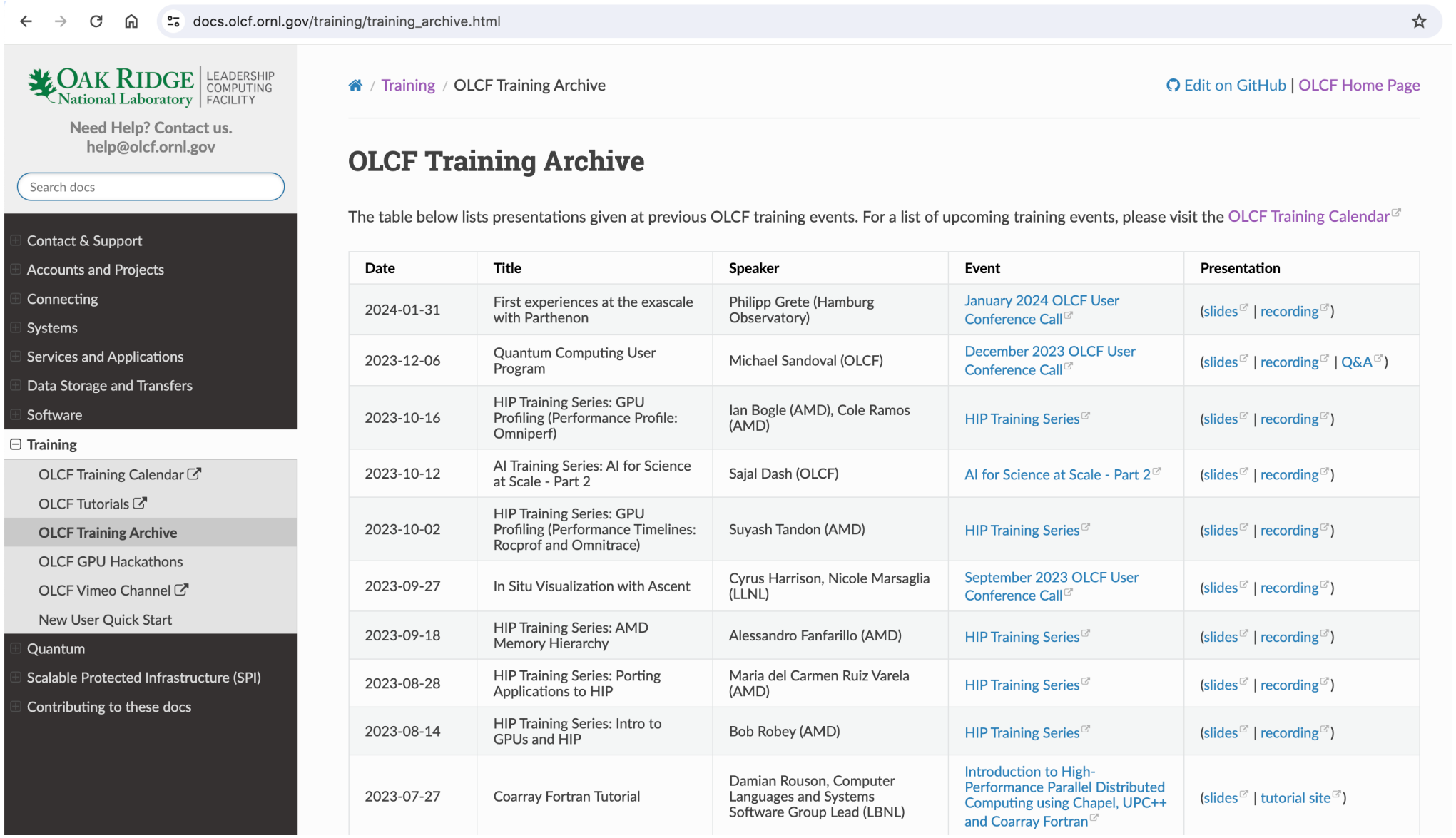
- Training Archive:
  - https://docs.olcf.ornl.gov/training/training_archive.html
  - Previous OLCF Training Events going back to 2017



Training Calendar



Training Archive



docs.olcf.ornl.gov/training/training_archive.html

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- Contributing to these docs

Training / OLCF Training Archive

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OLCF Training Archive

The table below lists presentations given at previous OLCF training events. For a list of upcoming training events, please visit the OLCF Training Calendar

Date	Title	Speaker	Event	Presentation
2024-01-31	First experiences at the exascale with Parthenon	Philipp Grete (Hamburg Observatory)	January 2024 OLCF User Conference Call	(slides | recording)
2023-12-06	Quantum Computing User Program	Michael Sandoval (OLCF)	December 2023 OLCF User Conference Call	(slides | recording | Q&A)
2023-10-16	HIP Training Series: GPU Profiling (Performance Profile: Omniperf)	Ian Bogle (AMD), Cole Ramos (AMD)	HIP Training Series	(slides | recording)
2023-10-12	AI Training Series: AI for Science at Scale - Part 2	Sajal Dash (OLCF)	AI for Science at Scale - Part 2	(slides | recording)
2023-10-02	HIP Training Series: GPU Profiling (Performance Timelines: Rocprof and Omnitrace)	Suyash Tandon (AMD)	HIP Training Series	(slides | recording)
2023-09-27	In Situ Visualization with Ascent	Cyrus Harrison, Nicole Marsaglia (LLNL)	September 2023 OLCF User Conference Call	(slides | recording)
2023-09-18	HIP Training Series: AMD Memory Hierarchy	Alessandro Fanfarillo (AMD)	HIP Training Series	(slides | recording)
2023-08-28	HIP Training Series: Porting Applications to HIP	Maria del Carmen Ruiz Varela (AMD)	HIP Training Series	(slides | recording)
2023-08-14	HIP Training Series: Intro to GPUs and HIP	Bob Robey (AMD)	HIP Training Series	(slides | recording)
2023-07-27	Coarray Fortran Tutorial	Damian Rouson, Computer Languages and Systems Software Group Lead (LBNL)	Introduction to High-Performance Parallel Distributed Computing using Chapel, UPC++ and Coarray Fortran	(slides | tutorial site)

Programming Models

- Frameworks/methodologies for software dev that can efficiently utilize HPC resources
  - MPI, OpenMP, and PGAS
  - optimizing performance for complex calculations and data-intensive tasks
- Training Calendar/Archive > Aug/Feb 2023 Frontier Workshops
  - GPU Programming Models (Subil Abraham)
  - HIP, Kokkos, OpenMP Offload
  - https://www.olcf.ornl.gov/wp-content/uploads/8-24-23-gpu_programming_models.pdf
  - https://vimeo.com/858462039?share=copy
- HIP Training series.
  - https://www.olcf.ornl.gov/hip-training-series/

AI on Frontier

- Enablement more efficient processing/analysis of vast datasets
- Optimizing HPC resource allocation
- Accuracy/speed improvement of simulations and predictive models
- Long-Term Goal: tackling complex analysis tasks that were previously unmanageable
- Pytorch on Frontier (Upcoming, April 24th 1-2pm, see training calendar)
- Aug 23/Feb 23 Frontier Workshops
  - AI on Frontier (Junqi Yin)
    - Recording: https://vimeo.com/858471449
    - Slides: https://www.olcf.ornl.gov/wp-content/uploads/8-24-23-AIonFrontier.pdf
- AI for Science at Scale
  - PART 1: https://www.olcf.ornl.gov/calendar/ai-for-science-at-scale-intro/
  - PART 2: https://www.olcf.ornl.gov/calendar/ai-training-series-ai-for-science-at-scale-part-2/
- SmartSim at OLCF
  - https://www.olcf.ornl.gov/calendar/smartsim-at-olcf/

NVMe's

- NVMe = Non-Volatile Memory express, "Burst Buffer"
  - Better I/O performance for high-I/O demand workloads

- Training Calendar > Aug 23/Feb 23 Frontier Workshops
  - NVMe Usage (Chris Zimmer)
    - Recording: https://vimeo.com/803630815
    - Slides: https://www.olcf.ornl.gov/wp-content/uploads/2-17-23_nvme.pdf

Checkpointing

- Practice of periodically saving the state of an ongoing job and data
- Allows computation to be restarted from the most recent checkpoint in case of a failure
- Minimizes the loss of computational work and effort
- Aug/Feb 2023 Frontier Workshops
  - Checkpointing Tips (Scott Atchley)
    - Recording: https://vimeo.com/803634715
    - Slides: https://www.olcf.ornl.gov/wp-content/uploads/Checkpointing-Tips-Frontier-Training-Workshop-20230217.pdf
- Mar 2023 User Call: Checkpointing Best Practices for Frontier
    - Recording: https://vimeo.com/814713985
    - Slides: https://www.olcf.ornl.gov/wp-content/uploads/Checkpointing-Tips-OLCF-User-Call-20230329.pdf

Profiling

- Analyzing performance bottlenecks within applications and systems
  - Measuring the execution time of application components
  - Mapping resource utilization
  - Finding where optimizations can boost efficiency and speed
- Goal: maximizing the performance of HPC applications
- MyOLCF Office HoursAug/Feb 23 Frontier Workshop
  - Application Profiling (Trey White, HPE)
    - Recording: https://vimeo.com/840552061
    - Slides: https://www.olcf.ornl.gov/wp-content/uploads/2-17-22_application_profiling.pdf
  - GPU Profiling (Asitav Mishra)
    - Recording: https://vimeo.com/858481088
    - Slides: https://www.olcf.ornl.gov/wp-content/uploads/8-25-23-Introduction-to-omniperf-with-roofline-AMishra-OLCF.pdf
- HIP Training series
  - https://www.olcf.ornl.gov/hip-training-series/

Debugging

- Identifying + resolving errors/bottlenecks
- Challenges: synchronization issues, memory access errors, I/O lag, etc.
- Specialized tools and techniques to ensure efficient and correct execution of applications at scale

- Aug/Feb 2023 Frontier Workshops
  - GPU Debugging (Mark Stock, HPE)
    - Recording: https://vimeo.com/840552596
    - Slides: https://www.olcf.ornl.gov/wp-content/uploads/2-17-23_GPU_Debugging_distribute-2.pdf

Balint Joo's Feb 2023 Workshop Tips & Tricks Talk

- Recording: https://vimeo.com/803633277
- Slides: https://www.olcf.ornl.gov/wp-content/uploads/Joo-FrontierTipsAndTricks.pdf
- Contents:
  - ROCm Building Tips
  - Interactive/Testing
  - SLURM Process binding and NIC Binding
  - Using the NVMEs
  - CMakeTips
  - Debugging
  - Profiling

Getting Help

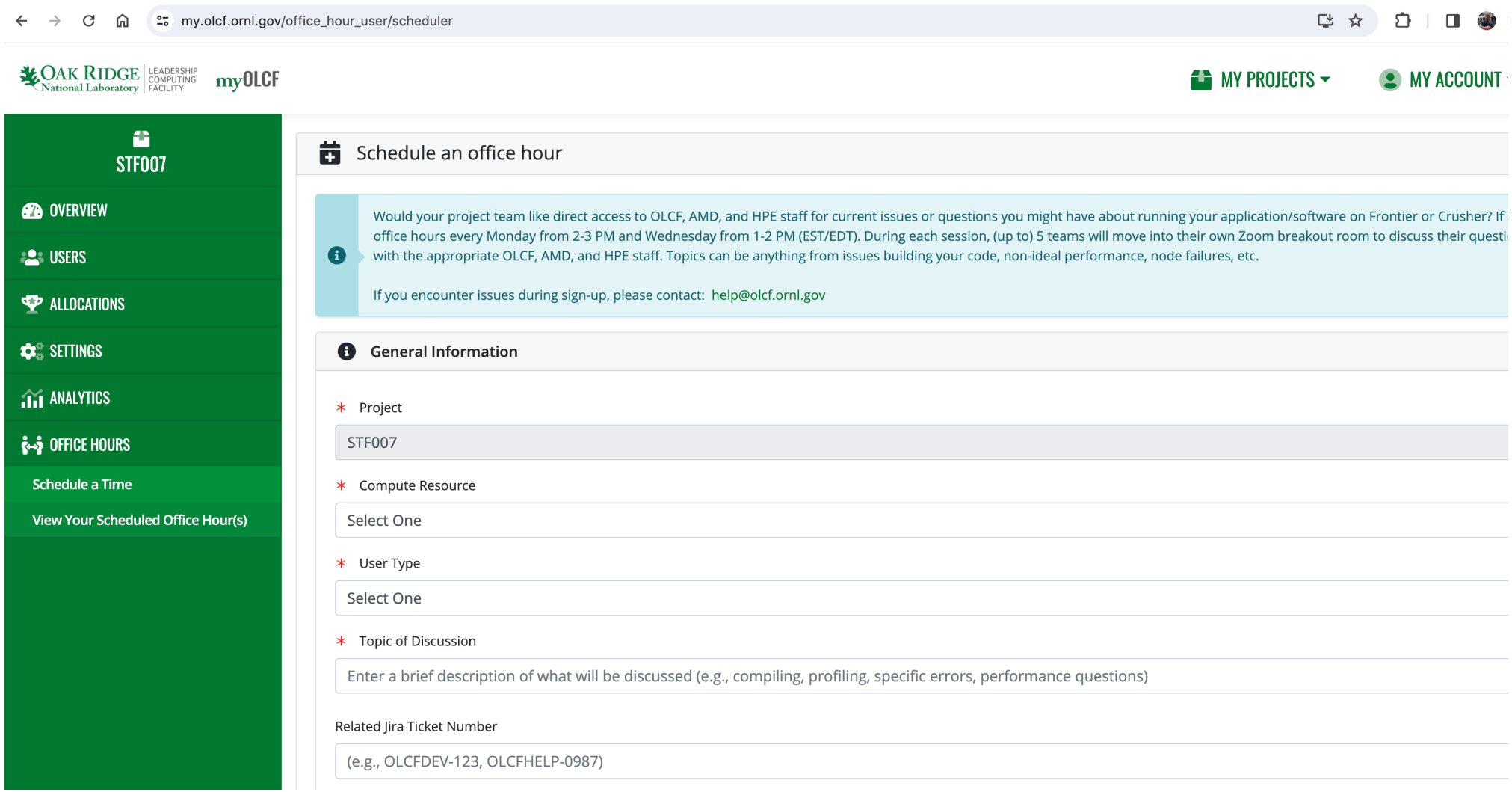
- Submit a ticket to help@olcf.ornl.gov

- Consult the documentation at:
  - https://docs.olcf.ornl.gov/systems/frontier_user_guide.html
  - https://docs.olcf.ornl.gov/systems/crusher_quick_start_guide.html

- Consider attending an "Office Hour"
  - Mondays 2-3pm ET & Wednesdays at 1-2pm ET
  - Sign up at https://www.my.olcf.ornl.gov/
    - Login to your Moderate account at myOLCF
    - Expand the OFFICE HOURS dropdown (on the sidebar navigation)
    - There are 2 options to select: **Schedule a Time** and **View Your Scheduled Office Hour(s)**

Getting Help

Office Hours



Ticket Tips

- The most helpful tickets
  - Clearly state the problem, the key modules/env vars
  - Have a small reproducer (either attached or identified in the text)
  - detail any other investigation you may have undertaken before you got stuck
- Less helpful tickets:
  - “Please help! My code stopped working.”
- The least helpful ticket:
  - “”

Thanks!

- Questions?