

# Training the Next Generation of Seismologists: Delivering Research-Grade Software Education for Cloud and HPC Computing through Diverse Training Modalities

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## Abstract

With the rise of data volume and computing power, seismological research requires more advanced skills in data processing, numerical methods, and parallel computing. We present the experience of conducting training workshops over various forms of delivery to support the adoption of large-scale High-Performance Computing and Cloud computing to advance seismological research. The seismological foci were on earthquake source parameter estimation in catalogs, forward and adjoint wavefield simulations in 2 and 3 dimensions at local, regional, and global scales, earthquake dynamics, ambient noise seismology, and machine learning. This contribution describes the series of workshops, the learning outcomes of the participants, and lessons learned by the instructors. Our curriculum was grounded on open and reproducible science, large-scale scientific computing and data mining, and computing infrastructure (access and usage) for HPC and the cloud. We also describe the types of teaching materials that have proven beneficial to the instruction and the sustainability of the program. We propose guidelines to deliver future workshops on these topics.

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## Supplemental Material

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## Introduction

Seismological research is advancing rapidly with the rise of computational power and big data, similar to other branches of geosciences (Morra et al., 2021). Seismological research encompasses a vast range of scientific inquiries and methodological practices. Driven by often sparse but fundamental observations of earthquake phenomena at all spatial and temporal scales, seismological research has historically relied mostly on first-principle theories that supported observations. Higher education in earthquake sciences builds on this rich legacy. Most undergraduate and graduate curricula are centered around foundational textbooks, such as “Introduction to Seismology” by Shearer (2019), “Introduction to Seismology, Earthquakes, and Earth Structure” by Stein and Wysession (2009), or advanced seismological theory, such as “Quantitative Seismology” by Aki and Richards (2002). These theoretical foundations for seismological research are typically taught in class lecture settings.

Numerical methods and the rise of high-performance computing have fueled the development of computational seismology, notably to solve the wave equation in complex media (e.g., Komatitsch and Vilotte, 1998; Komatitsch et al., 2002) and coupled to complex source models for purposes of physics-based ground-motion simulations (e.g., Graves et al., 2011) and for seismic imaging (e.g., Liu and Gu, 2012; Tromp, 2020). As examples, the SPECFEM package (Komatitsch and Tromp, 2002a; Komatitsch et al., 2004) have supported a new era of passive-source (earthquake, ambient noise) full-waveform-inversion (FWI) (e.g., Tape et al., 2009; Peter et al., 2011; Bozdağ et al., 2016; Chow et al., 2020) and the SeisSol software enables realistic simulations of 3D earthquake rupture dynamics (e.g., Käser et al., 2010; Pelties et al., 2012, 2014; Krenz et al., 2021; Gabriel et al., 2023; Uphoff et al., 2024).

Big data seismology is also vastly expanding, as continuous seismic data is recorded by hundreds or thousands of seismic stations worldwide. New methods emerged to include array processing (e.g., Rost and Thomas, 2009), ambient field (noise) seismology (e.g., Nakata et al., 2019), and machine learning (e.g., Kong et al., 2019; Mousavi and Beroza, 2022). Discoveries of new tectonic and environmental phenomena invigorate the collection of large seismic data sets, leading to an exponential growth in data volumes and bringing our community to an era of petabyte-scale archives (Arrowsmith et al., 2022). Novel computing infrastructures such as cloud computing are particularly well suited for big data seismological research (MacCarthy et al., 2020; Krauss et al., 2023; Ni et al., 2023).

The broad adoption of open-source software based on Python (e.g., Beyreuther et al., 2010) or Julia (e.g., Jones et al., 2020), as well as version control hosted on GitHub, Bitbucket, and GitLab is transforming research practice and standards (Chue Hong et al., 2022; Barker et al., 2022). Scientific journals require publicly hosted repositories or software availability, and Jupyter notebooks have become a popular avenue for sharing simple workflows (Pérez and Granger, 2007; Pimentel et al., 2019).

Educational approaches responding to the rise of computational and big data seismology have mostly leveraged advanced theoretical seismology and well-established numerical methods at the graduate student level. Computational Infrastructure for Geodynamics (CIG) has established best practices for both software development and training workshops (CIG, 2016a,b). “Computational Seismology” by Heiner Igel (Igel, 2017) and the associated Coursera course on “Computers, Waves, Simulations: A Practical Introduction to Numerical Methods using Python” (last accessed August 12, 2024) has effectively equipped STEM graduate students with the skills needed to solve the wave equation with a syllabus that blends numerical methods with seismological research problems. The textbook provides Jupyter notebooks, is entirely open source in Python, and can be run for simple problems from the associated Binder hub (Krischer et al., 2018). Despite this, we see a growing gap between higher education curricula and research practice. Open science and novel cyberinfrastructure present opportunities to train students and researchers in current research practices.

The COVID-19 pandemic has transformed education: students and teachers had to transition from in-person to remote, online learning. Several efforts have contributed to improving remote access to seismology education, such as the ROSES program (Brudzinski et al., 2021). These contributions have democratized education through pedagogical approaches analyzing small datasets, using approximate solutions, or performing modest simulations using single nodes and Python notebooks. However, a gap remains in the adoption of advanced computing platforms, such as high-performance computing (HPC) infrastructure and cloud computing. This article presents recent developments by the project SCOPED (Seismological COmputational Platform to Empower Discovery Tape et al. (2022); Wang et al. (2023); Denolle et al. (2024)) and col-

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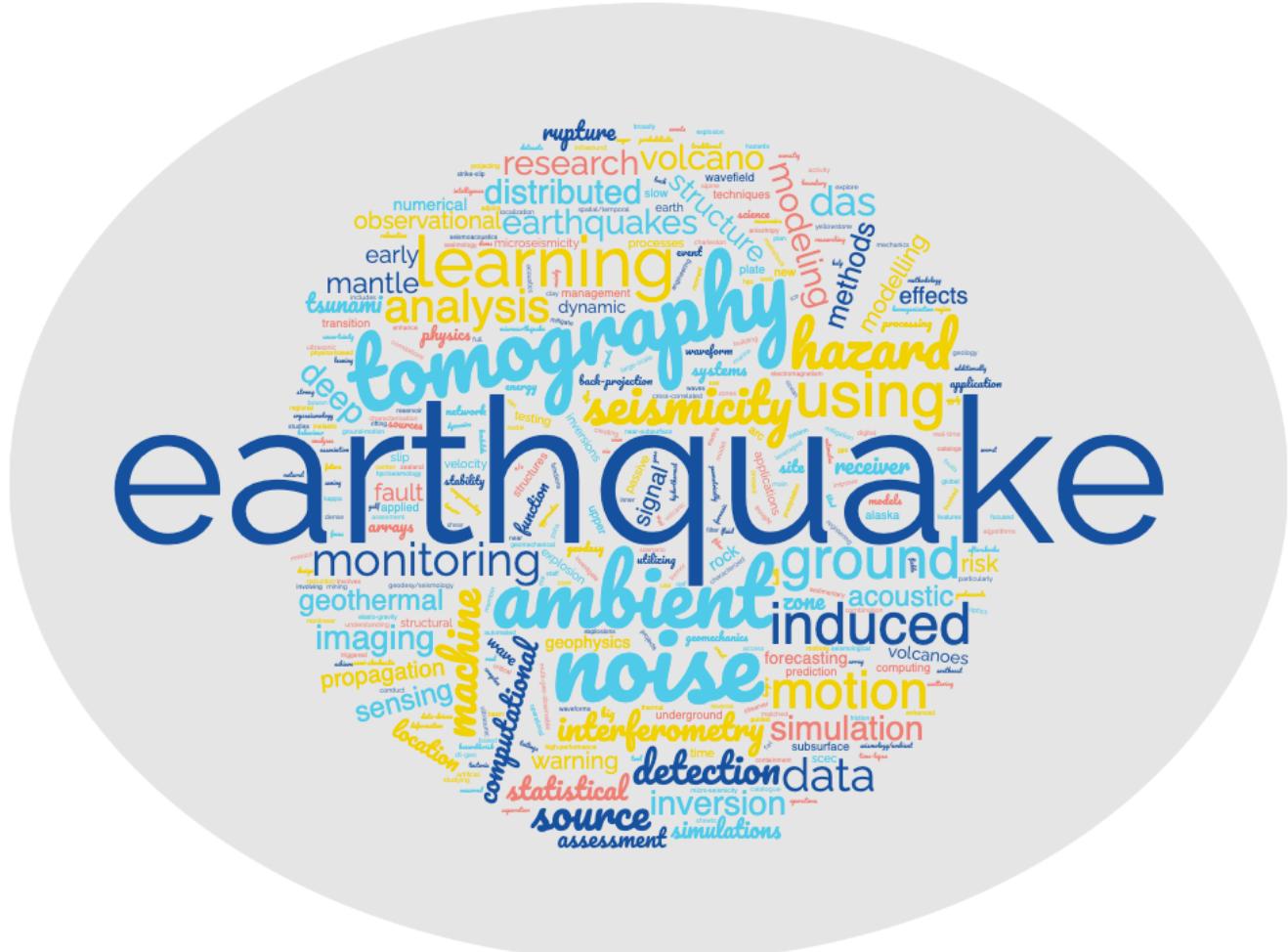


Figure 1: Word cloud illustrating the participant-reported research areas of the 2023 CyberTraining workshop.

laborations with other projects (e.g., the Statewide California Earthquake Center (SCEC), EarthScope, and the European projects Geo-Inquire, DT-GEO and ChEESE-2P (Folch et al., 2023)) to help close that gap for students and researchers with multi-modal educational efforts.

The goal of the **SCOPED** project is to develop a cyber-infrastructure that enables hybrid model–data research in seismology by utilizing cloud and HPC infrastructures, open-source software, and containerization. Research enabled by **SCOPED** includes 1) AI-enhanced earthquake source characterization and catalog building, 2) full-waveform inversion for source mechanisms, 3) full-waveform inversion for Earth imaging across scales, and 4) time-lapse imaging of the subsurface. The **SCOPED** community expressed their research interest, which we illustrate with Fig. 1. This article discusses the workshops held as part of the **SCOPED** project (Table 1), and in particular by its use of containers.

Name	Date (mo/yr)	Attendance mode	Range of participants
MTUQ	04/2022	Virtual	77
SPECFEM Users	10/2022	Virtual	50-183
SPECFEM Developers	10/2022	Hybrid	~ 30
HPS	04/2023	Virtual	30-80
CyberTraining			
SSA	04/2024	In-person	80
SCOPED	05/2024	Hybrid	100
MsPASS	06/2024	Virtual	54

TABLE 1. : Dates and Attendance modes of the workshops. MTUQ stands for Moment Tensor estimates and Uncertainty Quantification from broadband seismic data. SPECFEM stands for SPECtral Finite Element Method. High-Performance Seismology (HPS) cybertraining. SSA stands for the Seismological Society of America. MsPASS stands for Massive Parallel Analysis System for Seismology.

## A Broad Survey of the Seismology Community

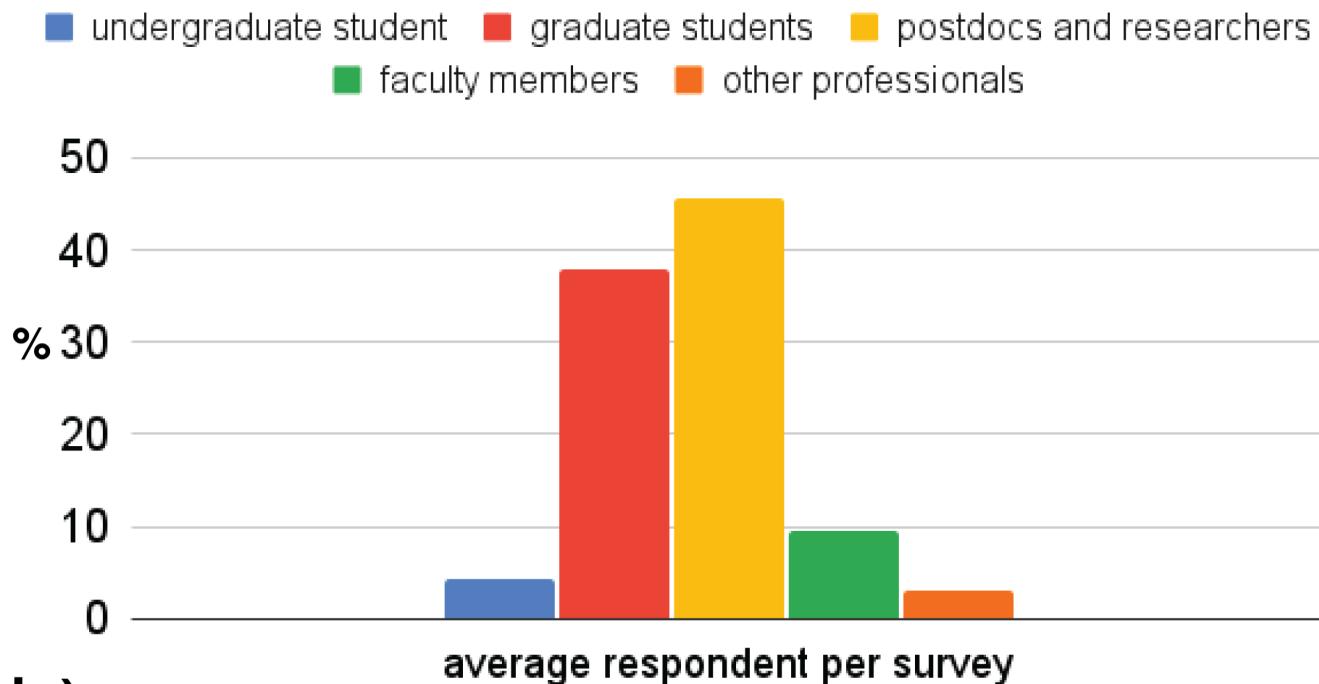
We ran multiple surveys to gauge the community interest in using widely employed seismological software in advanced computing environments such as HPC and the Cloud in anticipation of workshops between spring 2022 and spring 2024. The workshops were delivered in virtual, hybrid, and in-person formats. Surveys and workshops were announced in domain-specific mailing lists, such as the EarthScope Consortium and SCEC, and social media platforms (X formerly Twitter and LinkedIn). The surveys were tailored to each workshop, and the data collected mainly focused on familiarity with the required technical skills. Overall, we received 976 responses, although some may come from the same individuals. Our workshops had a total of 574 participants, with over 130 joining in-person. Some of the surveys presented here has a broad community reach, and our post-event surveys only had the workshop participants. We found that the timing and frequency of surveys had an effect on the response rate. Post-event surveys were successful only if participants completed them during the event. Due to differences in response rates for pre- and post-event surveys, our analysis combines common questions and categories from both types. The response rate was above 96% for requests during the workshop, whether the meeting was in person or virtual, while it was 13% in the case of the 2024 SSA workshop.

Survey questions were designed to minimize the imposter syndrome as suggested by [Huppenkothen et al. \(2018\)](#). For instance, we asked participants about their familiarity with shell scripting in various forms: “How familiar are you with computing programming from a command line (i.e., within a terminal window)?” with the response fields of “No experience, Some Experience, Extensive Experience.” We also asked their familiarity with version control was assessed with questions such as “All of my active research projects over the past year are on GitHub with many check-ins”. Another example to assess their proficiency in Python was “I use Python in my life” with the multiple-choice answer “several hours a week and mostly in the classroom”, “several hours a day in my research”, “all and every day!”, and “Never-ever”. We also gathered preliminary knowledge about the technical skill levels of the survey respondents. We emphasize that our surveys were a “self-assessment,” which likely provided a biased response. To limit these effects, we employed strategies similar to [Huppenkothen et al. \(2018\)](#). For example, we assessed version control (e.g., GitHub) familiarity by asking how many research project participants were hosted on the platform. Another example is assessing Python familiarity by asking how many hours a week a participant uses Python.

Our surveys canvassed career levels of interested workshop participants, which is illustrated in Figure 2a. The surveys included multiple choice questions with various career levels and sometimes received multiple answers. For instance, participants responded to both “graduate student” and “research scientist” or added an additional category of “PhD candidate”. While some surveys distinguished between “postdoctoral researcher” and “research scientist”, we have grouped these two categories as they both represent researchers with advanced technical skills and dedicated project-based research. Out of the 976 survey responses, the demographic of the surveyed community exhibited a great majority of graduate students and researchers, with a significant participation (15%) of faculty members. Undergraduate students have a distinctly lower participation level, likely due to our choice of communication channels and the required technical skills advertised in the announcements.

a)

### Career levels of survey respondents



b)

### Self-assessment of proficiency

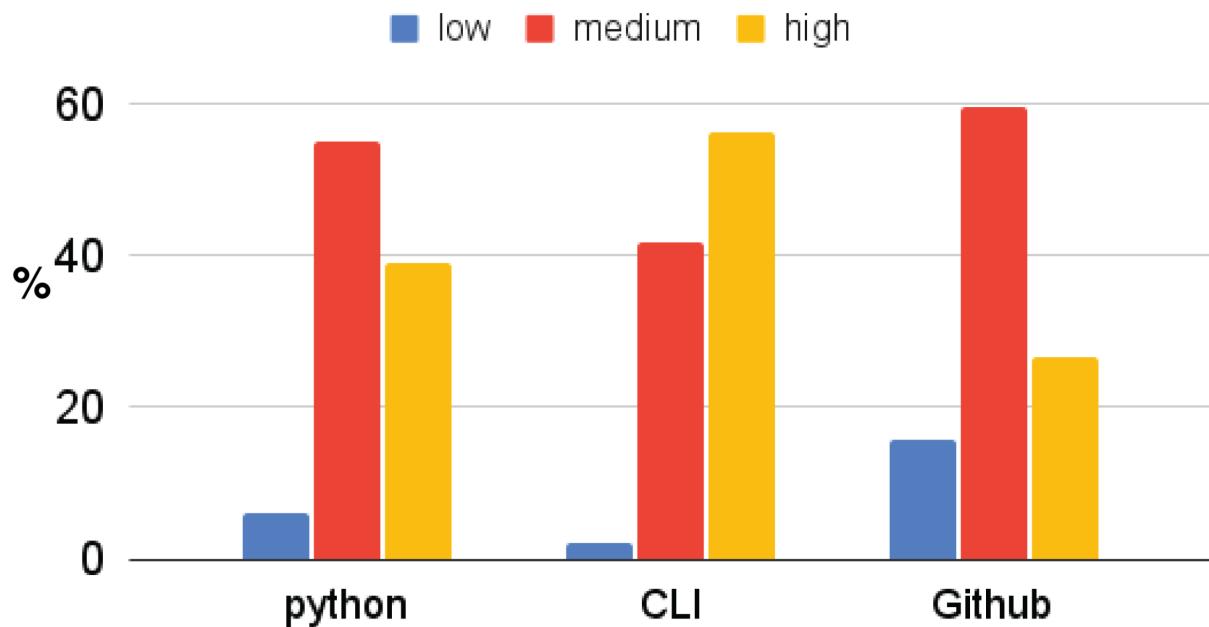


Figure 2: Proportion of participants as a summary over 7 workshop surveys for a) career levels and b) self-assessed proficiency in computing tools (CLI=command line interface).

We use three skill-based proficiency levels as a relative metric for the seismological community in Figure 2b. Overall, most participants felt comfortable with CLI tools. 90% of the participants reported having a sufficient level of familiarity with Jupyter notebooks and Docker. 40% of the participants declared being sufficiently experts in Python for their research, though a majority declared having a medium level of familiarity. Interestingly, version control using Git ranks last in our assessment, as most participants report having a medium level of comfort, and 16% declare having no experience with GitHub.

## Novel CyberInfrastructure (CI)

### CI on HPC

The main computing environment benefiting seismology today is HPC, which is enabled by clusters of thousands of tightly connected nodes managed by large computing centers, such as the [Texas Advanced Computing Center \(TACC\)](#), the [San Diego Supercomputing Center \(SDSC\)](#). Clusters are designed for parallelized workflows that require large shared memory and up to thousands of nodes. They require optimized software with demonstrated efficient performance scaling and proficiency in job scheduler-memory management and storage architecture. HPC centers often provide training.

Over the course of the workshops, we have trained participants in various aspects of HPC. The lectures entailed training on the fundamentals of HPC, how to write allocation proposals for HPC resources, and the parallelization of workflows leveraging shared or distributed memory architectures. We also trained a few selected groups of participants to access and run forward and adjoint simulations to compute 3D synthetic seismograms and data sensitivity kernels with SPECFEM3D\_GLOBE ([Komatitsch and Tromp, 2002a,b](#)) for FWI and dynamic rupture simulations with SeiSol ([Käser et al., 2010](#)) on the Frontera system ([Stanzione et al., 2020](#)) at the Texas Advanced Computing Center (TACC).

### CI on Cloud Computing

Cloud computing is a new paradigm for computing, where users rent hardware from commercial computing centers such as [Amazon Web Services \(AWS\)](#), or [Microsoft Azure](#), which provide on-demand and a-la-carte hardware choices. Computing is done on “virtual machines” (VM), an abstraction of hardware that contains up to a few hundred CPU cores, up to a few GPUs, and a tunable amount of memory. Maximum-size instances can have up to about 200 cores, 10 GPUs, and 1TB of memory and are designed mostly for big-data processing, for example, when training complex machine-learning models. VMs have a pre-loaded operating system on which users install dependencies from scratch, from Docker images, or from previously saved virtual images.

We trained participants in cloud computing concepts, such as its design to interact with storage and perform large-scale deployments, which is still in its infancy in seismology, and user access remains a challenge ([Krauss et al., 2023](#)). We presented diverse strategies for using cloud resources. They accessed Google Colab notebooks provided by Google Cloud Platform, which are pre-configured Python-based jupyterhubs, and learned how to customize them by manually installing additional dependencies. Accessibility is a major benefit of the Colab approach, as VM specifications can easily be modified on the Google Colab web interface. The free version is limited in size.

The SCOPED project chose AWS as the cloud provider due to the availability of large seismic datasets already hosted on AWS Simple Storage Service (S3). The workshop covered 1) various ways to access AWS cloud resources, 2) how to launch an AWS computing resource on the Elastic-Computing (EC2) referred to as an *instance* from scratch via the web console, 3) how to install basic research software into their instances, and 4) how to run research-grade problems on the Cloud. We used the typical AWS web console to deploy compute resources during one of our workshops and illustrated it in Figure 3. We taught popular tools for software environments and versioning, such as `git`, `Docker`, and `conda`. It should be noted that significant effort was required to simplify and prepare instructions for streamlined access and use of AWS instances. In particular, it is not trivial to open and access a jupyter lab, and we curated the training materials to achieve this ([HPS](#)).

Additionally, we taught various ways to conduct research workflows on the cloud: cloud-native workflows that incorporate cloud services as part of the design (e.g., `NoisePy`, [Jiang and Denolle \(2020\)](#), [HPS](#)), and, alternatively, workflows that are lifted to the cloud, e.g the Lamont-Doherty Earth Observatory earthquake catalog production workflow ([Wang et al., 2024](#)) that includes algorithms for event detection and phase arrival time measurements (QuakeFlow , [Zhu et al. \(2023\)](#)), discrimination (SpecUFEx, [Holtzman et al. \(2018\)](#); [Sawi et al. \(2022\)](#) ), and relocation (HypoDD , [Waldhauser and Ellsworth \(2000\)](#)).

### Open-Source and Containerized Software

The SCOPED platform gathers open-source software that tackles big data and large-scale simulation research. When writing this paper, SCOPED includes full waveform modeling and inversion, AI-aided earthquake catalog building and source characterization, ambient field seismology, and earthquake dynamic rupture simulations.

Name	Instance ID	Instance state	Instance type	Status check	Alarm status	Availability Zone
HC22222	i-01cc78bcf846cf45d	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
claudio	i-0cd3001ef7305051b	Running	t2.xlarge	2/2 checks passed	View alarms	us-west-2b
	i-030d5fad8a4766c4c	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
aaaaaaa	i-01b5f777657b555f2	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
nthapa_event	i-0551f45b26de0780f	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
Stevens_Event_Classific...	i-0f563d76c6c5bad96	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
KIM	i-0d9ede39d65e913b3	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
jyotis	i-0a39d5fb3b60913f5	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
ahutko_Fri_PM	i-0771f324131c1b310	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
utpal-ml	i-09ebfd2c2848dac1c	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
kyungmin	i-075e7aa4e6d94cd3	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
akash_kharita_scoped	i-05a7331a4a3649315	Running	c5.12xlarge	2/2 checks passed	View alarms	us-west-2b
rodrigo-test-friday-aft...	i-01876e0adf800fbfc	Running	t2.2xlarge	2/2 checks passed	View alarms	us-west-2b

Figure 3: Web browser screenshot showing AWS instances created by workshop participants during the 2024 SCOPED workshop, illustrating multiple instances running simultaneously on the same allocation. Instance participants chose names.

The underpinning strategy for deploying our software is containerization, which enhances portability and exploits negligible computing overhead (Wang et al., 2019) once successfully containerized. Containers are isolated images of software and its dependencies that can be deployed on various operating systems and hardware (Docker, Singularity). To grow our user and developer community, SCOPED flagship software is containerized with tutorials provided in the form of Jupyter notebooks. We developed a [SeisSCOPED container registry](#) in which the container base holds minimum dependencies. Additional dependencies can be added to the container base: for instance, an HPC-specific container loads modules for Message-Processing Interface - MPI, and a cloud-specific container has cloud-provider Command-Line-Interface CLI-specific packages. One major advantage of the containerized software approach is long-term stability; workshop users and future students alike are able to leverage the same workshop container and its pinned software dependencies, training materials, and test data. Another powerful use of notebooks is integrating shell scripting within notebook cells using system commands. As an example, one can deploy parallelized Python scripts on Azure Pool (Krauss et al., 2023), AWS Batch resources in a single notebook, or run parallelized SPECFEM simulations through JupyterLab (HPS).

While high-performance computing favors the use of scripting, compiled executables, and minimal container sizes, training materials benefit from attaching small test data and notebooks for documentation and visualization of results. Containers may add `IPython` and `ipykernel` dependencies to support Jupyter notebooks and small test data to a given container. Opening Jupyter notebooks from remote servers can pose a challenge in group settings, especially on cloud instances. Throughout workshops, our team scripted the following command line to easily allow access to Jupyter notebooks from a container by fixing the token and IP address:

```

1 sudo docker run -p 80:8888 --rm -it ghcr.io/seisscoped/noisepy:centos7_jupyterlab\
2     nohup jupyter lab --no-browser --ip=0.0.0.0 --allow-root --IdentityProvider.token=scoped &
```

where `IdentityProvider.token=scoped` gives a specific token (this avoids users tracking it in the long logs printed on the terminal), `allow-root` grants root access for users inside the container volume, `ip=0.0.0.0` tells the server to listen on all available network interfaces, and `nohup jupyter lab --no-browser &` opens JupyterLab without launching the browser, which is not possible on remote virtual machines protected by a private IP address. This small code snippet was designed to accelerate research rather than being hung up on infrastructure.

## Open Education

Open Education, a set of practices and principles aimed at making learning opportunities more accessible and equitable for everyone, is a promising future direction for higher education as research becomes increasingly specialized and training

materials require extensive, globally distributed expertise. JupyterBook is an appropriate platform for collaborative research education, as many instructors can contribute, and students receive up-to-date materials. Such an example is shown in Figure 4. The challenge remains in curating training materials, as many come from complex research literature and free, non-peer-reviewed online materials.

We are compiling a dynamic textbook titled “High-Performance Seismology” that the workshop participants have contributed to [HPS](#).

## SCOPED-related events

### Virtual Events

We have conducted several virtual events, which offer great potential for democratizing access to advanced computing globally. To maximize participation, we structured events into short sessions ( $\sim 45$  min) with adequate breaks and scheduled them at times that accommodate participants across various time zones. Pre-event surveys of user locations helped in selecting optimal event times, ensuring broad participation. Additionally, we recorded the training events and made them asynchronously available on our [SCOPED Youtube channel](#) to address time zone conflicts.

In April 2022, we organized a two-day workshop on moment tensor estimation using the open-source MTUQ software. The first day featured a 2-hour session introducing key concepts and tutorials. The second day consisted of a 4-hour session that demonstrated how to calculate a library of Green's functions for a specified 1D layered model using a frequency-wavenumber code ([Zhu and Rivera, 2002](#)) and obtain a seismic moment tensor solution. Attendance was strong, with 78 on day 1 and 68 on day 2, indicating sustained interest in the more detailed content. In preparation, software containers for four systems (Windows/PC, Linux, Mac OS Intel and Mac OS Apple Silicon processors) were developed and tested, resulting in high success rates for participants running the examples.

Building on the success of the previous workshop, we held a three-day SPECFEM users' workshop in October 2022. Each of the three daily, 4-hour sessions had a specific focus: the forward wavefield (day 1), sensitivity kernels (day 2), and seismic imaging (day 3). Each session included short (20-minute) science lectures, 45-minute tutorials that participants could run locally using pre-downloaded software containers, and wrap-up discussion sessions. Participation ranged from 187 attendees in the day 1 opening seminar to 63 in the day 3 discussion (Figure 5). This was the first SPECFEM workshop featuring seismic imaging, providing a natural progression from synthetic seismograms (day 1) to sensitivity kernels (day 2) to iterative tomographic inversion using SeisFlows and Pyatoa (day 3) ([Modrak et al., 2018](#); [Chow et al., 2020](#)). Crafting a pedagogical but research-grade notebook took dedicated efforts.

In 2023, we held a four-day virtual training workshop in collaboration with the SCEC and several European and NSF-funded projects. Each day focused on a specific theme, starting with an opening day of lectures on open science, reproducibility, software best practices, and an introduction to HPC and Cloud Computing. Subsequent days were divided into subdisciplines and platforms. The workshop attracted over 200 interested participants, with 80 joining on Zoom at the workshop's start, though attendance varied due to time zone challenges. Designed for tool adoptions and relatively fast-paced, participants were exposed to diverse topics in seismology, including earthquake simulations focusing on dynamic rupture (with SeisSol, [Käser et al. \(2010\)](#); [Uphoff et al. \(2024\)](#)) and wave propagation (SPECFEM, [Komatsitsch et al. \(2002\)](#)), machine learning phase picking (ELEP, [Yuan et al. \(2023\)](#)), earthquake probabilistic forecasting (pyCSEP, [Savran et al. \(2022\)](#)), and user access to Community Earth Models maintained by SCEC, (e.g., [Plesch et al., 2007](#); [Small et al., 2017](#)).

The 2024 MsPASS training short course was hosted in collaboration with EarthScope during the week of July 8, 2024, as part of their 2024 Technical Short Course series. The event featured two hours of lectures and hands-on sessions over three days. Participants could attend the course in real time or access recordings on YouTube afterward. Daily homework assignments were given, and an optional final project. The application-based enrollment process received 99 valid applications, from which 53 participants were accepted to attend. The cohort was notably diverse, with 38% self-identifying as underrepresented in the geoscience community and 26% identifying as female. This short course was the first event on EarthScope's [GeoLab](#) platform, a new experimental cloud-based JupyterLab platform hosted by EarthScope. MsPASS ([Wang et al., 2022](#)) was the first application to run parallel processing workflows on the GeoLab platform. Participants were exposed to topics such as using MsPASS to process waveform data in the cloud, managing datasets with a document database, and executing data processing workflows in parallel.

### In-person Events

We held a one-day workshop at the SSA meeting in Anchorage in 2024 that was in-person only, a fast-paced event with an introduction to cloud computing and research workflow. We successfully had 80 participants launch their own cloud instances on AWS, where they detected earthquakes in cloud-hosted SCEDC data and output data products to a shared MongoDB database. Participants also ran machine learning workflows for earthquake catalog building, including supervised and unsupervised learning approaches for event-type classification. The SSA participants enrolled as a first-come, first-serve approach, and communication with the participants was not as well-established as in the other SCOPED events. This slowed down the initial steps of setups, and advanced participants had to follow the pace of beginners.

Our last SCOPED workshop was a five-day hybrid meeting at the University of Washington in Seattle in May 2024 (<https://seisscoped.org/workshop-2024/>, last accessed 09/10/2024). About 50 participants, including instructors, attended the workshop in person (example of room layout in Fig. 6), along with a varying number of online participants (on average



High Performance Seismology

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## SSA Workshop Data Mining and Cloud 101 (2024)

This workshop will introduce participants to cloud computing, from concept and best practices to practice, for two main approaches of data mining in seismology: correlation seismology and machine learning. Participants will learn how to port their Python scripts from their laptops to the cloud, analyze their intermediate data products, and download the final data product. Participants will learn ambient noise seismology software noise and run it on cloud-hosted data sets of broadband seismometers and distributed acoustic sensing data. Participants will learn machine learning in seismology (earthquake catalog building and data discovery of various geohazards). The workshop curriculum is supported by the NSF project SCOPED.



## Schedule

Time	Topics	Instructors	Link to notebook or slides
9:00-9:30m	Welcome	Marine Denolle and Felix Waldhauser	
10:00-11:15am	Cloud 101	Yiyu Ni, Zoe Krauss, Marine Denolle	<a href="https://github.com/SeisSCOPED/seis_cloud_book">https://github.com/SeisSCOPED/seis_cloud_book</a>
11:15-12:30	Ambient Noise	Yiyu Ni, Kuan-Fu Feng, Marine Denolle	<a href="https://github.com/SeisSCOPED/noisepy_book">https://github.com/SeisSCOPED/noisepy_book</a>

Figure 4: A page of the HPS JupyterBook for the SSA 2024 workshop, which embeds a Google slide presentation for the introduction presentation, the schedule of the specific workshop, and links to relevant book pages

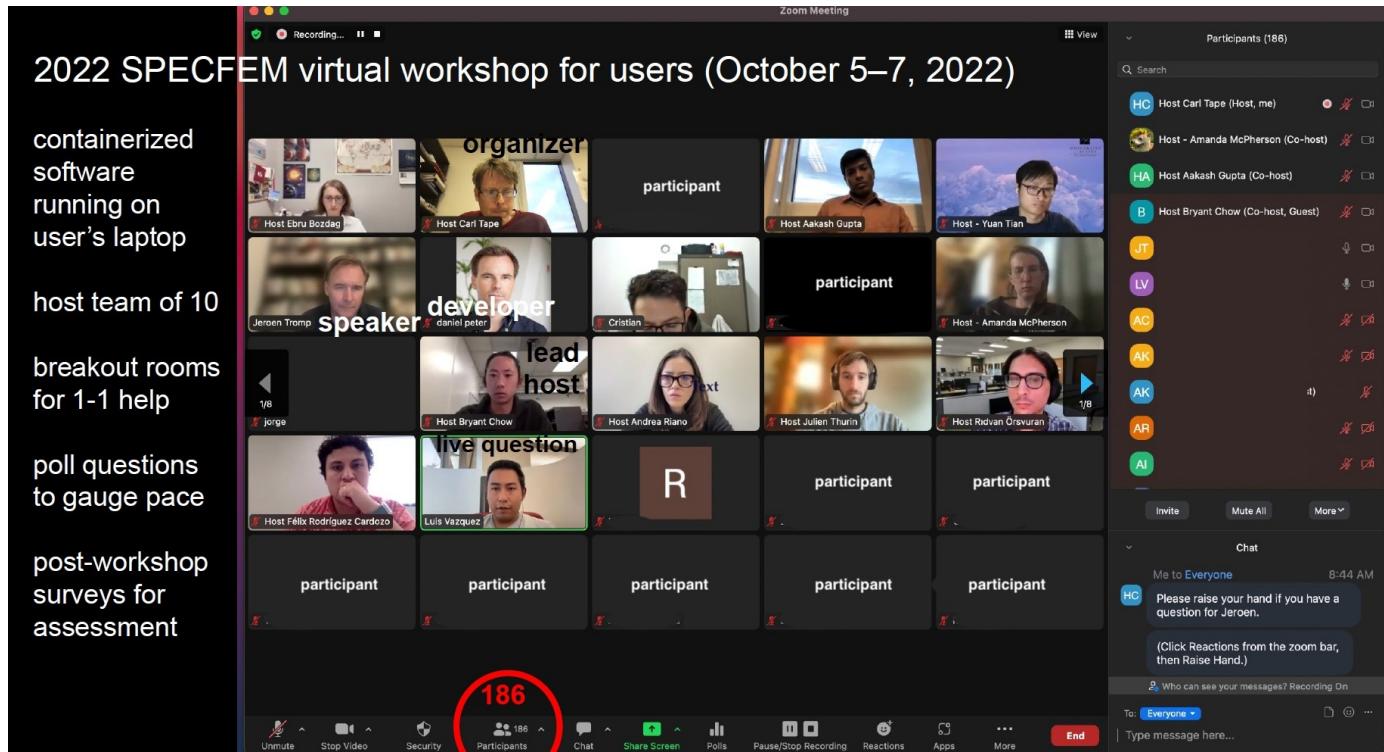


Figure 5: Annotated zoom screenshot from the SPECFEM virtual workshop for users (October 5, 2022). At this stage in the workshop, there were 186 participants (red circle). The annotations and windows show the hosts, the speaker, the lead software developer, the lead host/instructor, the organizer, and a participant asking a question.



Figure 6: In-person component of the 2024 SCOPED workshop. Participants engaged in live exercises. The OWL camera and directional microphone (bottom center), together with Zoom (speaker's laptop at lower left), enabled hybrid participation. Participants' posters can be seen on the walls.

about 50 per day). The training program was led by the research groups of the SCOPED PIs and Dr. Alice-Agnes Gabriel from the University of California San Diego, supported by several NSF- and European-funded projects. Day 1 covered subjects and practicals with an introduction to HPC and Cloud computing and best practices for developing and maintaining open-source software. Day 2 was dedicated to 2D and 3D wave simulations with SPECFEM packages and a tutorial on introduction to full-waveform inversion by SeisFlows and moment tensor inversions with the MTUQ software. Day 3 focused on 3D dynamic rupture and finite source earthquake simulations with SeisSol and 3D wave simulations and computation of 3D adjoint data sensitivity kernels (Tromp et al., 2005; Bozdağ et al., 2011) for full-waveform inversion on a one-chunk mesh with SPECFEM3D\_GLOBE (Komatitsch and Tromp, 2002a,b). Day 4 focused on high-precision earthquake catalogs (Wang et al., 2024), where they combined machine learning algorithms (QuakeFlow; Zhu et al. (2023)) with large scale cross-correlation and double-difference methods (HypoDD; Waldhauser and Ellsworth (2000); Waldhauser and Schaff (2008)) and demonstrated the use of unsupervised machine learning (SpecUFEx; Holtzman et al. (2018); Sawi et al. (2022)). The participants also had a session on MsPASS (Wang et al., 2022) to learn how to manage big data on HPC and the Cloud. Day 5 addressed ambient noise seismology on the cloud (NoisePy; Jiang and Denolle (2020)), and the trainees were given tutorials on machine learning workflows for seismology on the cloud. All the workshop tutorials were prepared in Jupyter notebooks hosted on GitHub, containerized versions of the open-source SCOPED software were used, and lectures were recorded and uploaded to the [SCOPED YouTube channel](#). All 3D simulations on Day 3 were performed by the trainees on the Frontera system, and the observational seismology tutorials were on AWS.

### Learning Outcomes

Surveys following the SSA and HPS CyberTraining workshops enabled us to evaluate learning outcomes. In the SSA survey, we evaluated the learning outcomes of each module, which were about cloud computing and research-grade applications in ambient noise seismology and machine learning in earthquake catalog building. Eleven survey respondents out of eighty participants noted improved cloud computing skills and a more moderate improvement in disciplinary topics. Overall, the surveyed participants had a positive learning outcome, and improvements in workshop materials and delivery will enhance the impacts of the training.

In the HPS CyberTraining survey, 23 participants responded and expressed positive learning outcomes, with 70% ranking their satisfaction 5/5 and 62.5% indicating that the workshop was a valuable use of their time (rank 5/5). Positive learning outcomes were on Docker and reproducible & open science, frontier seismological topics, and HPC and cloud computing. Several participants expressed verbally or via the survey, that the pace was fast and that instructors should slow down when going through code blocks in notebooks, along with improving participant-led exercises in the notebooks with empty cells.

## A Guide to Advanced Computing Workshops

The development of teaching materials requires dedicated effort from both faculty and participants. In-person workshops need a participant-to-assistant ratio of about 15 to 1 for effective debugging. Creating a new email address for event management may add more load. Recruiting participants with similar technical skill levels ensures consistent progress, or additional instruction time can be provided for beginners..

### Surveys

Evaluation surveys can be useful for quantifying learning outcomes, and crafting them with consideration can benefit professional educators and evaluators. Employing a more standardized approach to the surveys may improve their usefulness. For example, metrics such as “None, Little, Moderate, Quite a bit, Complete” for levels 1 through 5 are similar to the Likert 6-point, “strongly disagree, disagree, somewhat disagree, somewhat agree, agree, strongly agree.” More standard metrics, such as the Likert 6-point, will be incorporated in future surveys to provide a more nuanced measure of fields (Huppenkothen et al., 2018). It is also important to allow only one response per question, as multiple answers can hinder post-event quantitative analysis.

### Content

Each of the SCOPED workshops had various designs and, overall, was packed with tutorials. We developed or used several forms of pedagogy for training workshops, which individual workshops may have combined:

- scientific lectures, especially those that motivate the use of advanced computing resources.
- lectures on cyberinfrastructure, research ethics, and software best practices.
- core package tutorials to train participants in using a specific software in its generic form.
- research-grade workflow tutorials with assisted walk-throughs.

- group or participant-led activity (hackathon-style).

Complete virtual meetings can be spread over multiple days and time zones to help attract foreign participants. Virtual meetings can be topical, even narrowly topical, with two sessions: one 2–3 hour session to motivate the science and present a problem for rapid execution of the software and a second 3-hour session for participant-led practice to run the software at scale. This worked well for the SPECFEM and MTUQ workshops.

## Before the event

### *Instructor Coordination*

Coordination of the workshop instructional team is extremely valuable for the instructors themselves and ultimately improves the flow and delivery of the workshop. We had various degrees of coordination, mostly strong within the PI's group but less so in the multi-PI workshops. Organizing a workshop, even virtual, requires additional administrative tasks prior to and after the workshop, which were not fully supported for these workshops. The team of instructors should meet frequently and perform at least one full-scale mock event prior to the actual event. We find that the most successful events had a ratio of preparation time over delivery time of 2 or 3, even for workshops that used the same platform and software throughout. It is important to meet frequently with all instructors to build a unified cohort and ensure smooth transitions and delivery during the workshop. Organizers are encouraged to ask non-participating students and colleagues to join mock events and try to follow instructions prior to the workshop in an effort to catch major issues that might otherwise cause undue delays.

### *Materials & Platforms*

We recommend using Jupyterbooks or Google Docs as shareable platforms to organize the workshop schedule and share training materials, with a clear first page with the schedule that links to the sources (e.g., YouTube recording, Zoom links, GitHub repositories, etc.). Communication platforms like Slack or Teams, or other forms of group communication and direct messaging, allow for rapid, practical communication among instructors and between participants and organizers. Pre-workshop materials are particularly valued and desired by participants. Examples of such materials may be background knowledge, resources, and recorded videos of previous workshops, such as the fundamentals necessary to have acquired by the start of the workshop. Instructors may pre-download data, e.g., pre-processed data and static visualization, to ensure the workshop runs smoothly even with network connectivity of unforeseen technical issues.

### *Accounts*

The participants' accounts on the computing resources should be set up days in advance. We provide guidance to automatically create user accounts for AWS on the [HPS book](#). It is important to remind participants that workshop computing resources are *temporary*. Educational allocations at HPC centers are typically provided when supercomputer center research scientists are involved in the workshop. We recommend assigning the username as the prefix of the participant's email address, as well as a single generic password, to avoid manual and complicated intervention. Cloud accounts can be created at any time and managed during the workshop. For instance, a cloud manager can re-assign policies, roles, and temporary passwords during the event if needed. Through surveys and emails and possibly "Day 0" virtual help sessions, instructors should ensure that computing setups (accounts, software containers) are working in advance for all virtual participants.

## First Day

This is the day to onboard participants, ensure that the accounts to HPC and the Cloud are set up and accessible, install ancillary software, and download and test workshop containers to ensure they perform as expected on the participants' platforms. These tasks can also be done prior to the workshop to free up actual workshop time. Hybrid workshops can be challenging to deliver. They require multiple cameras and microphones for large rooms, attention to remote attendance, and interaction with remote participants. For hybrid events, organizers should ensure that there are sufficient staff/instructors online who can help manage remote participants. Engagement can be improved with frequent polling.

## During the Event

The feedback on workshops has been positive, especially for focused, single-tool, and single-platform sessions. We found that spending 3 hours per module was reasonable, but 2 hours was too dense and didn't allow for independent exploration. For virtual workshops, a helpful strategy is to ask "Are you ready to move on?" with the options "Yes, Almost, and No." This helps pace the session and provides instant feedback on participant experience, showing engagement levels and areas needing assistance. Research-grade software often includes advanced workflows tailored to specific use cases, making it challenging to strike a balance between teaching fundamental concepts and realistic scenarios. Some tutorials include additional cells in

the notebooks so that participants can test various parameters independently, which was implemented in SPECFEM, MTUQ, and SeisSol. Teaching cloud and HPC computing strategies can be challenging for participants if the content is not relevant to their work. Coordination among instructors with diverse research backgrounds is crucial for effective delivery. One example is to adapt a homegrown software stack based on a specific platform to provision a cloud instance.

### Post Event

Surveying the participants is a good way to measure learning outcomes. We found that participants will mostly not fill out post-event surveys unless asked **at the time of the events**, both for virtual and in-person meetings. To improve on evaluation, the exit survey should have similar questions to the incoming survey. Leaving an empty box at the end permits participants to speak freely of things that worked and things to improve.

Assessments need to be more quantitative, with more structured responses than were provided in many of the surveys we ran. Some respondents provided several answers to the same question, posing additional problems in the analysis of the survey in post-processing. Further automation of the survey, such as more rigorous Python-based post-processing, will improve the reproducibility of the survey analysis.

## Conclusions

The diversity of workshops is important to reach multiple pedagogical goals. Large attendance in virtual meetings allows for a global reach and democratization of training and access to computing resources. The size of these virtual meetings was not optimal for spontaneous communication and career network — although future workshops could take this into account. We found that at that scale (200+ participants), it was easier to have participants run containers and software locally, whereas for smaller, virtual meetings, it is possible to provision remote participants with temporary cloud accounts.

In-person meetings are well suited for career development, building collaborations, and provisioning participants with more advanced computing resources, which may be limited to certain countries. These in-person meetings can run longer than virtual events, with the caveat that organizers should pace the delivery of the materials more slowly than they anticipate and even include participant-led hackathons for better learning outcomes and stronger cohort building.

Advanced computing with projects such as JupyterHubs (e.g., Infrastructure-as-a-Service such as [Coiled](#) or [2i2c](#)) and science gateways (e.g., [Marru et al., 2011](#); [McLennan and Kennell, 2010](#); [Stubbs et al., 2021](#)) promote access to resources, potentially benefiting the user community. Nevertheless, training the community in the concepts of cloud computing and HPC for new *developers* remains important so that they can continue innovating solutions for large-scale computing for seismological research.

Our efforts in conducting these workshops reflect a positive outlook for seismologic research in the 21st century. As big seismic data become more widely accessible, seismologists at all career levels desire to pursue training in HPC and Cloud computing. We highlight the benefits of our workshop model by uniting cyberinfrastructure and research professionals skilled in HPC and Cloud computing. They leverage large-scale computing to solve seismologic problems. Through these workshops and their associated teaching materials, we are able to disseminate that collective knowledge in an open, sustainable, and reproducible manner, all to accelerate the pace of seismologic discovery.

## Data and Resources

The survey data came from Google Forms responses. Because of the lack of anonymity in the responses, the authors decided not to share the original data. All SCOPED educational materials are open-source (e.g., [HPS](#)). Video recordings of our workshops are available on [SCOPED YouTube channel](#).

## Declaration of Competing Interests

The authors acknowledge that no conflicts of interest have been recorded.

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## Figure legends

Figure 7: Word cloud illustrating the participant-reported research areas of the 2023 CyberTraining workshop.

Figure 8: Proportion of participants as a summary over 7 workshop surveys for a) career levels and b) self-assessed proficiency in computing tools (CLI=command line interface).

Figure 9: Web browser screenshot showing AWS instances created by workshop participants during the 2024 SCOPED workshop, illustrating multiple instances running simultaneously on the same allocation. Instance participants chose names.

Figure 10: A page of the HPS JupyterBook for the SSA 2024 workshop, which embeds a Google slide presentation for the introduction presentation, the schedule of the specific workshop, and links to relevant book pages

Figure 11: Annotated zoom screenshot from the SPECFEM virtual workshop for users (October 5, 2022). At this stage in the workshop, there were 186 participants (red circle). The annotations and windows show the hosts, the speaker, the lead software developer, the lead host/instructor, the organizer, and a participant asking a question.

Figure 12: In-person component of the 2024 SCOPED workshop. Participants engaged in live exercises. The OWL camera and directional microphone (bottom center), together with Zoom (speaker's laptop at lower left), enabled hybrid participation. Participants' posters can be seen on the walls.