

Performance Evaluation of GPU-accelerated HPC and AI applications using HPCToolkit, TAU, and ParaTools Pro for E4S™

Sameer Shende

Research Professor, University of Oregon

President and Director

ParaTools, Inc.

Presentation at EnergyHPC conference, Rice U., Houston

February 27, 2025



<https://tinyurl.com/e4stut>



U.S. DEPARTMENT OF
ENERGY

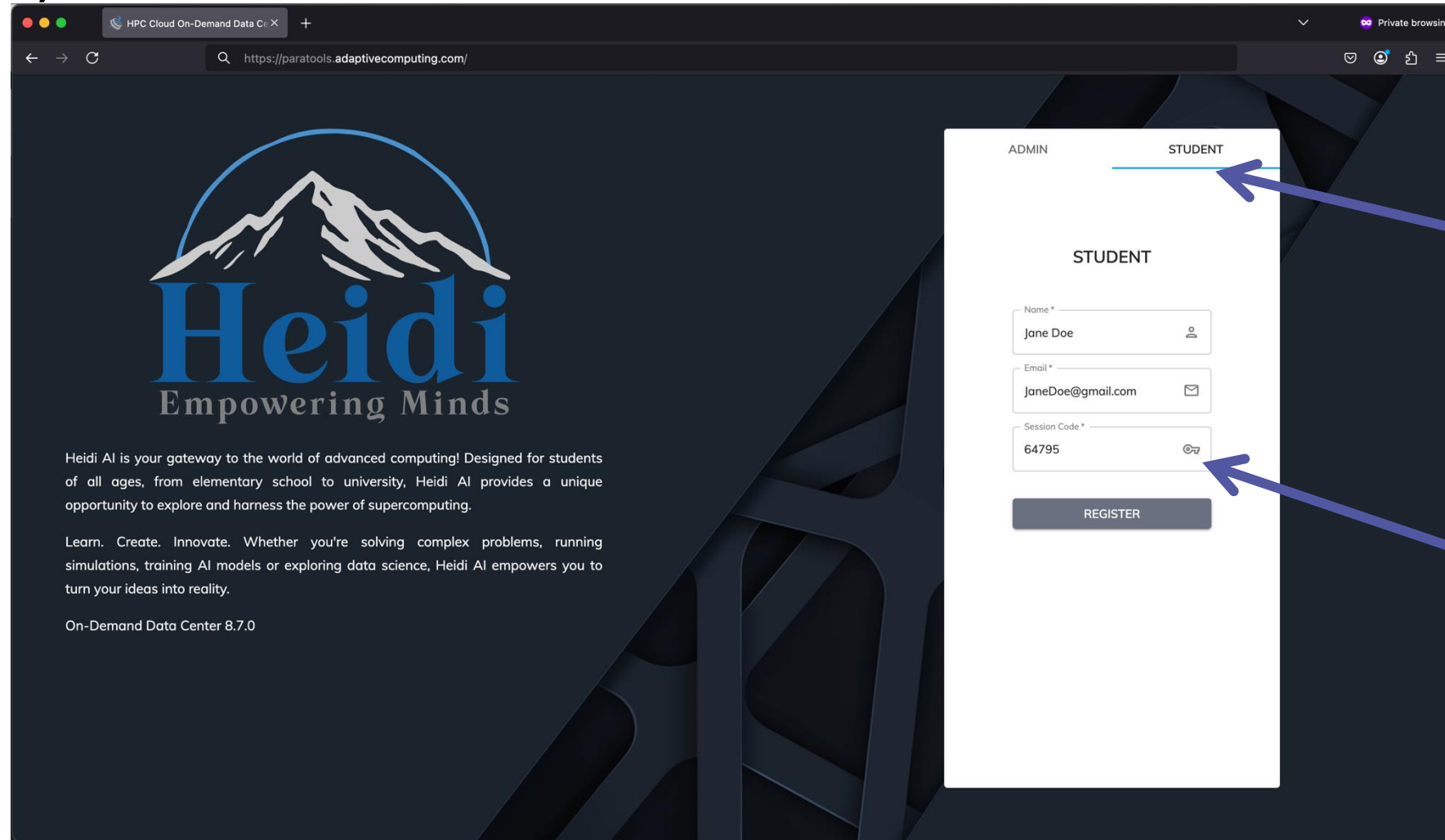
Office of
Science

Using Adaptive Computing's Heidi Workshops (aka ODDC)

Go to <https://tinyurl.com/e4stut> for slides

STEP 1: Click on Students tab at:
<https://paratools.adaptivecomputing.com>
Firefox recommended.

Adaptive Computing's Heidi: Go to STUDENT tab and enter Name, Email and enter the session code 64795



The screenshot shows a web browser window with the URL <https://paratools.adaptivecomputing.com/>. The page features the Heidi AI logo, which includes a mountain graphic and the text "Heidi Empowering Minds". Below the logo, there is a paragraph about Heidi AI being a gateway to advanced computing for students, followed by a list of activities: "Learn. Create. Innovate. Whether you're solving complex problems, running simulations, training AI models or exploring data science, Heidi AI empowers you to turn your ideas into reality." and the version "On-Demand Data Center 8.7.0". A white registration form is overlaid on the right side of the page. The form has two tabs: "ADMIN" and "STUDENT", with the "STUDENT" tab selected. The form fields are: "Name *" with the value "Jane Doe", "Email *" with the value "JaneDoe@gmail.com", and "Session Code *" with the value "64795". A "REGISTER" button is at the bottom of the form. Two blue arrows point from the text on the right to the "STUDENT" tab and the "Session Code" field.

ADMIN STUDENT

STUDENT

Name *
Jane Doe

Email *
JaneDoe@gmail.com

Session Code *
64795

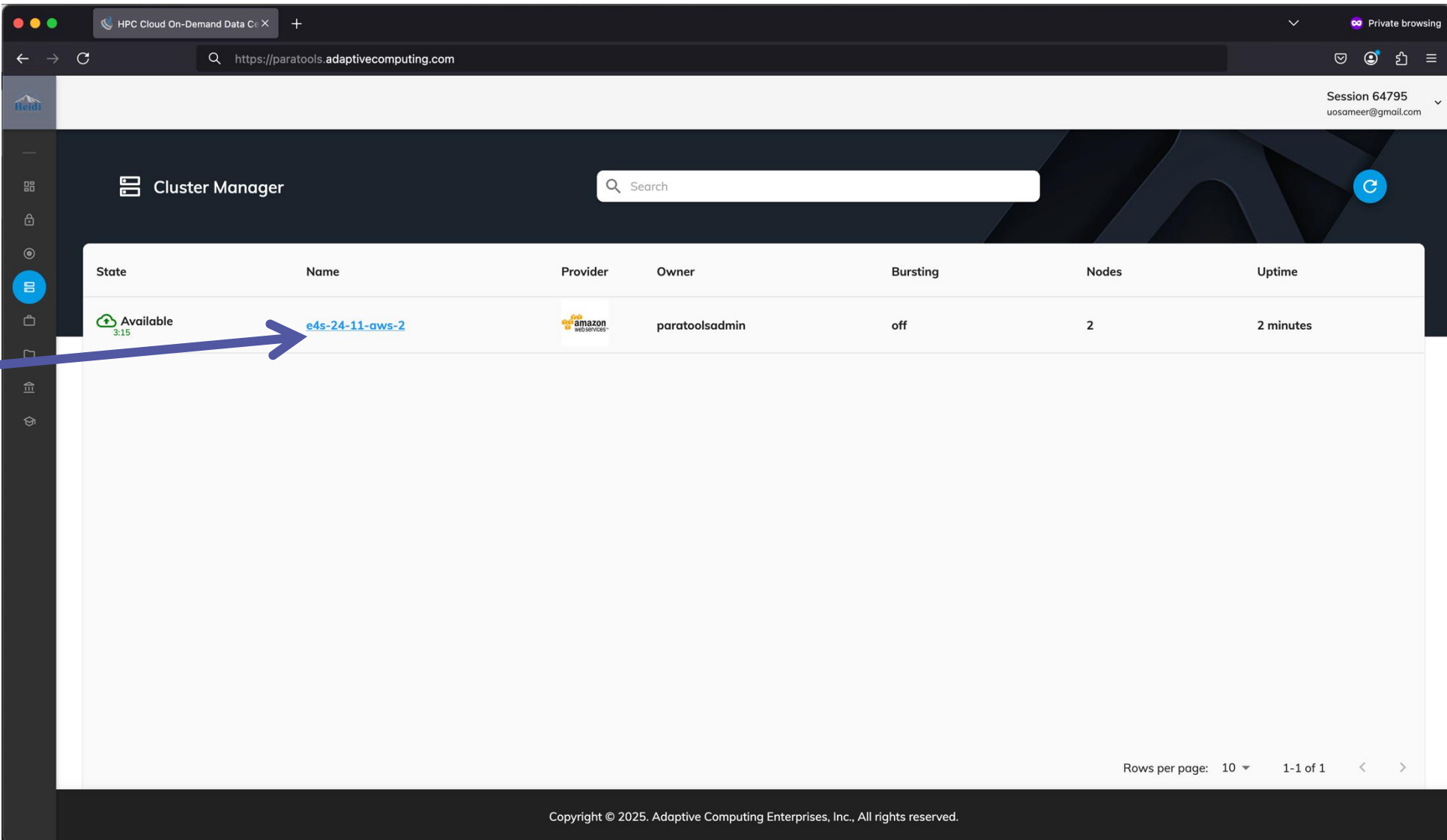
REGISTER

Click on Student tab

Enter name, email And **64795** session code

Launch VNC Viewer from Heidi's Configuration Tab

Click here



The screenshot shows the Heidi application interface. The top bar includes the Heidi logo, a search bar, and a session identifier 'Session 64795' with the email 'uosameer@gmail.com'. The main area is titled 'Cluster Manager' and contains a table with the following data:

State	Name	Provider	Owner	Bursting	Nodes	Uptime
Available 3:15	e4s-24-11-aws-2	amazon	paratoolsadmin	off	2	2 minutes

At the bottom of the interface, there is a footer with the text: 'Copyright © 2025. Adaptive Computing Enterprises, Inc., All rights reserved.'

Launch VNC Viewer from ODDC and allow popups

The screenshot shows a web browser window displaying the Adaptive Computing ODDC interface. A Firefox notification bar at the top indicates that pop-ups are blocked. A 'Preferences' dialog box is open, showing options to allow pop-ups for the current site. The main content area shows the 'Configuration' tab for a cluster named 'e4s-24-05-aws'. The 'Cluster Information' section includes details like Cluster ID, Head Node, Size, Mem, Head Node Disk Space, Image Name, Cluster IP, SSH Username, Created time, and Availability Zone. A blue 'OPEN VNC VIEWER' button is present, with a checkbox for 'Remote client' and a checkbox for 'Use popup'. The 'Participant Credentials' section shows Username, Password, and IP Address, along with a 'DOWNLOAD SSH KEY' button. A blue arrow points from the text 'Click here' to the 'OPEN VNC VIEWER' button. Another blue arrow points from the 'Use popup' checkbox to the 'Preferences' dialog box.

Click here

Cluster ID: 6626dd00a6069602bd755901
Head Node : g4dn.8xlarge - GPU: 1, vCPU: 32
Size Mem (GB): 128
Head Node Disk Space: 200 GB
Image Name: e4s-24-05-v18
Cluster IP: 44.233.148.21
SSH Username: ubuntu
Created: April 22, 2024 4:56 PM
Availability Zone: us-west-2a

OPEN VNC VIEWER

Remote client Use popup

Participant Credentials

Username: training1
Password: HPCLinux12!
IP Address: 44.233.148.21

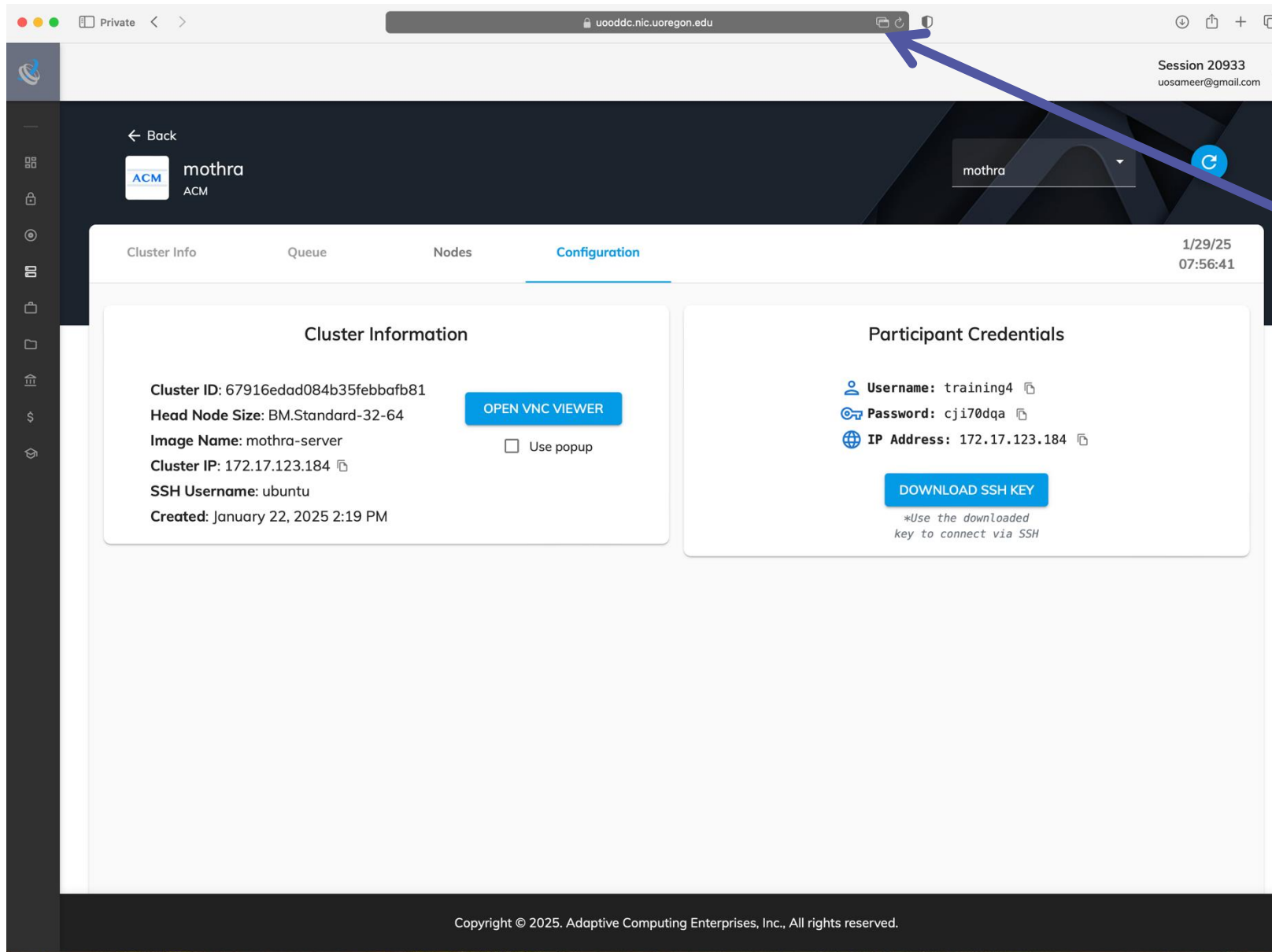
DOWNLOAD SSH KEY

*Use the downloaded key to connect via SSH

Cluster Compute Nodes

Copyright © 2024. Adaptive Computing Enterprises, Inc., All rights reserved.

Allow Popups by clicking on popup window in Safari

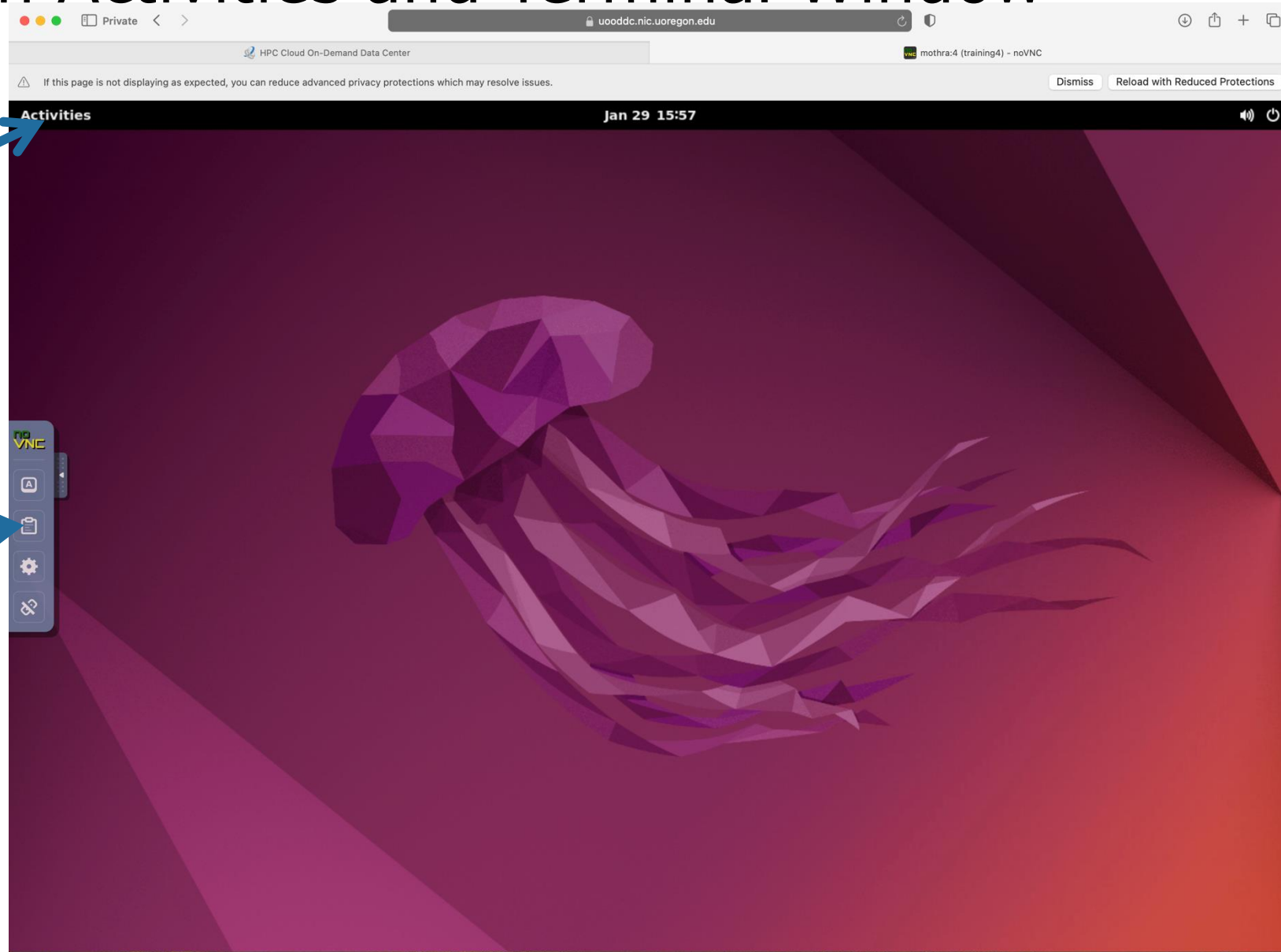


Click here
to open popup
window in
Safari

Launch Activities and Terminal Window

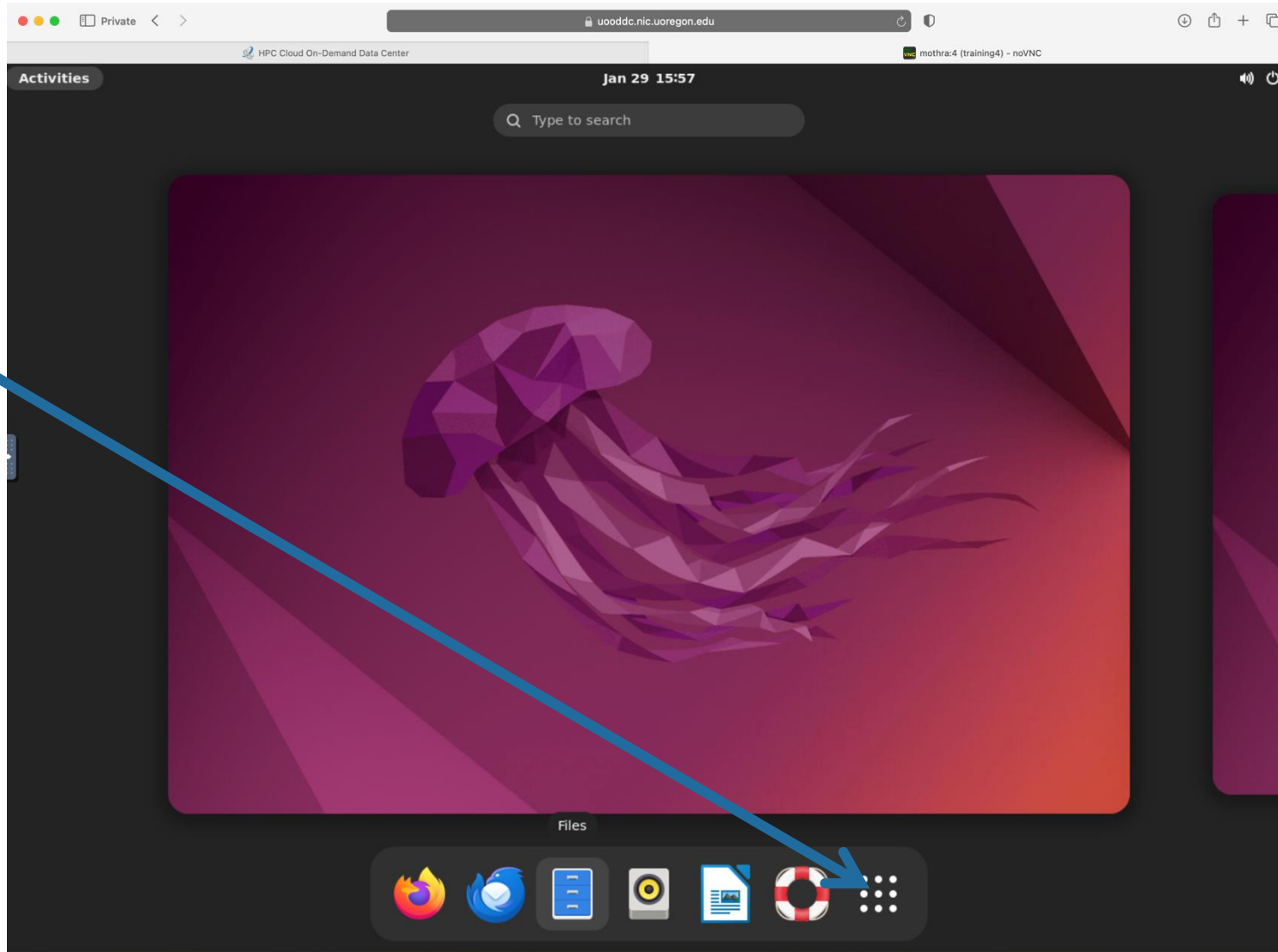
Click here

To cut and
paste to
windows
in Heidi



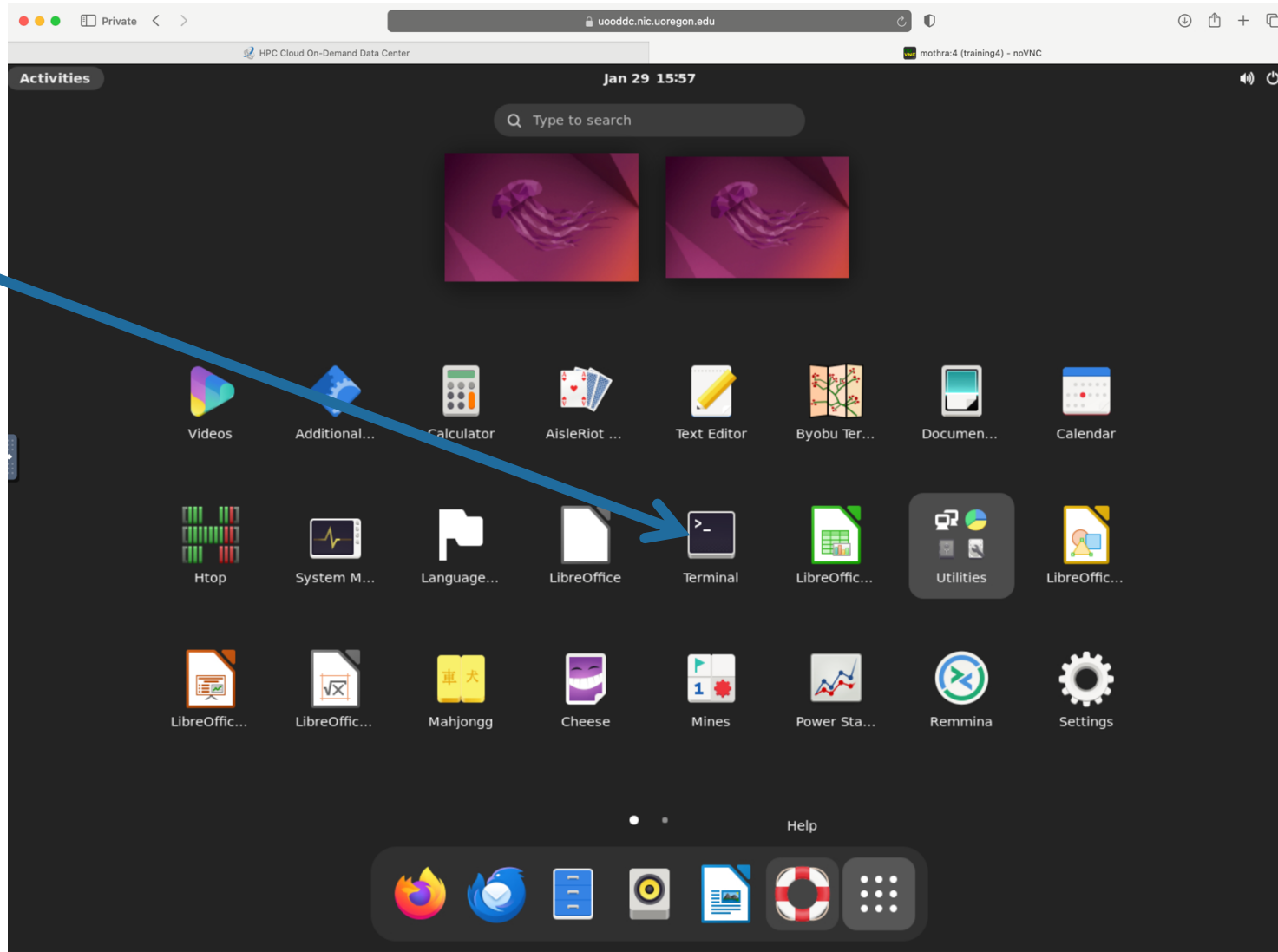
Launch Terminal Application from the desktop

Click here

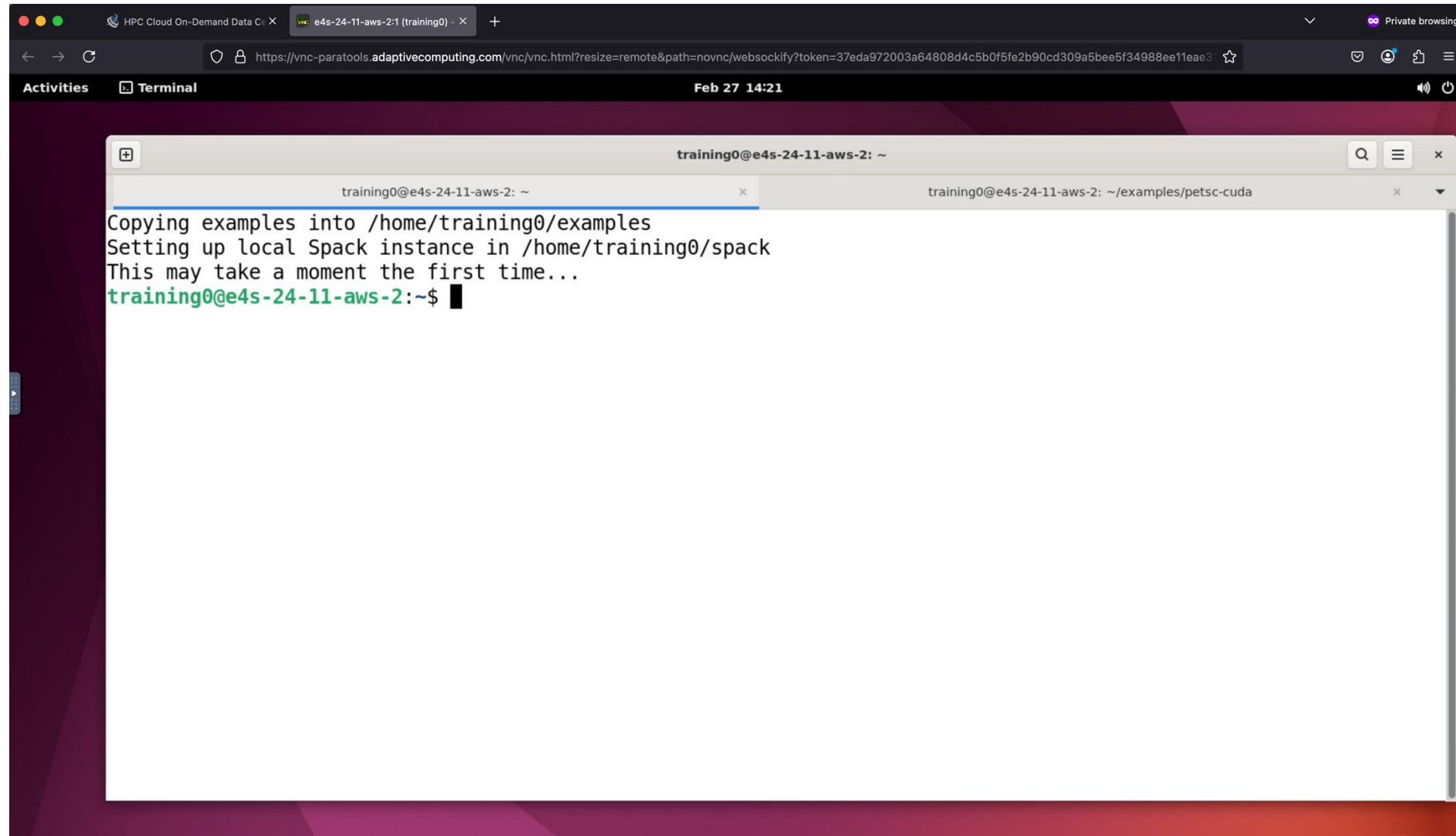


Launch Terminal from Applications

Click here



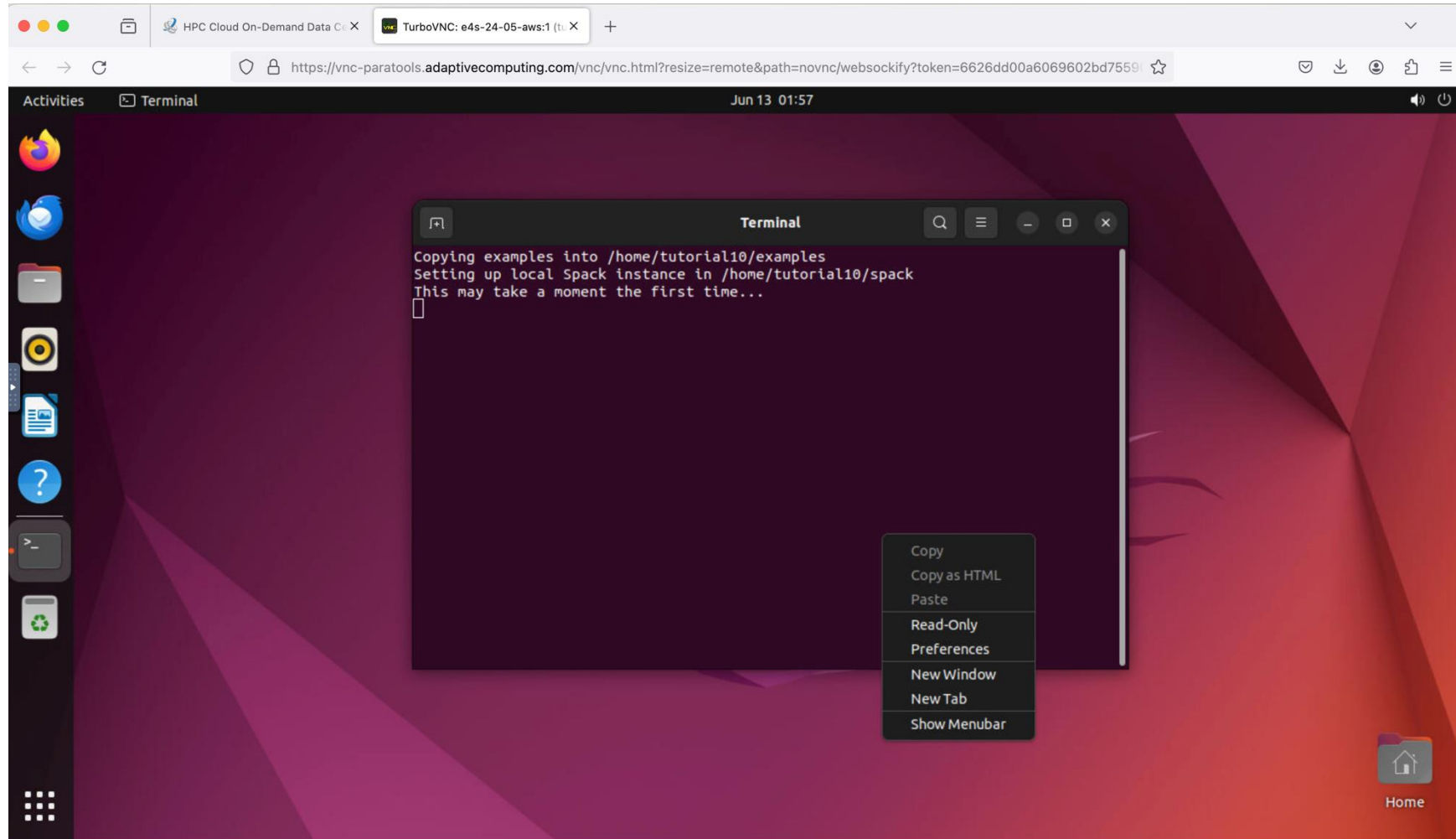
Launch Terminal from Applications



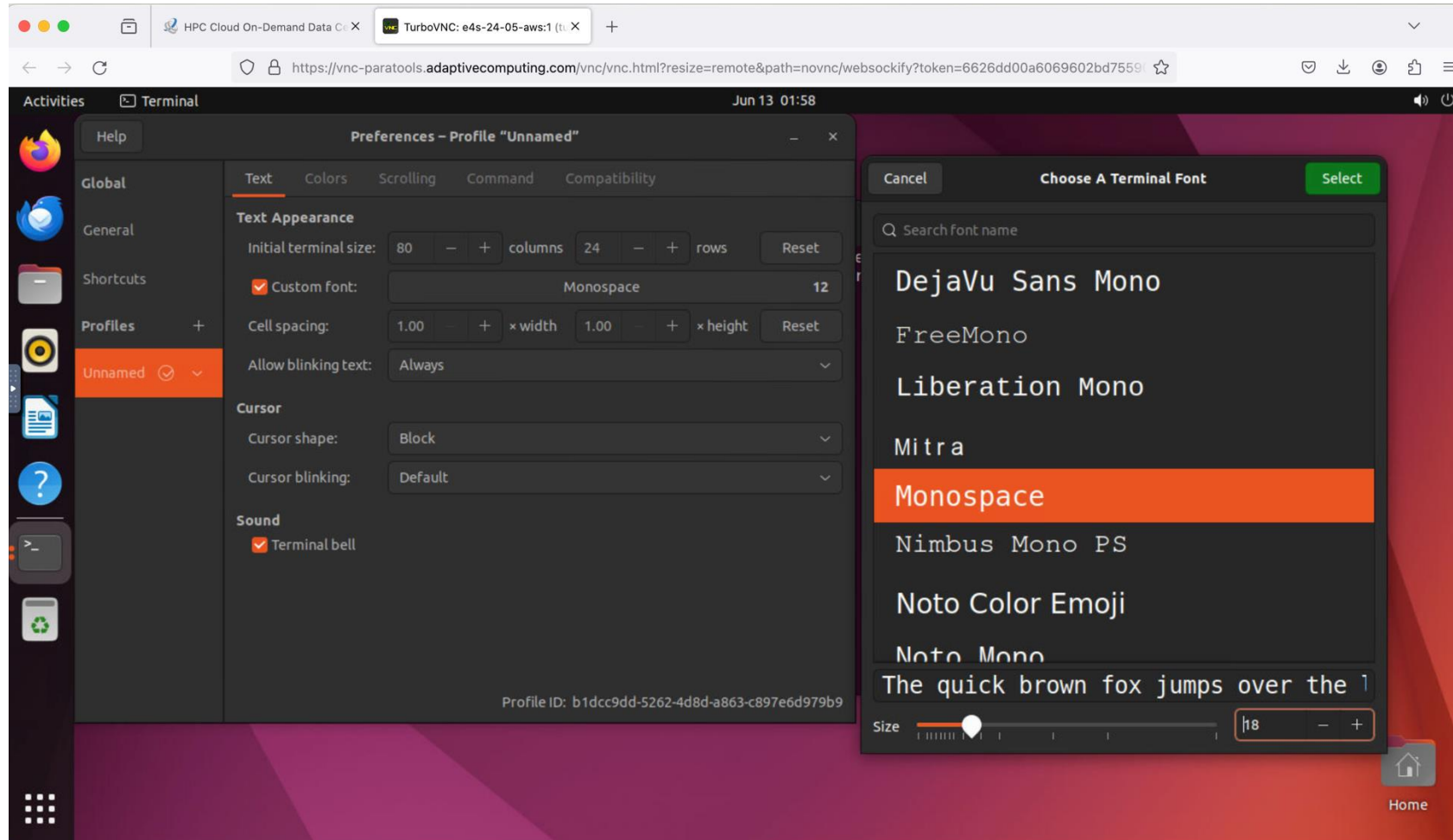
The screenshot shows a VNC viewer window titled "e4s-24-11-aws-2:1 (training0) - X". The address bar displays a URL from "https://vnc-paratools.adaptivecomputing.com". The desktop background is a dark purple gradient. A terminal window is open, titled "training0@e4s-24-11-aws-2: ~". It contains the following text:

```
training0@e4s-24-11-aws-2: ~  
Copying examples into /home/training0/examples  
Setting up local Spack instance in /home/training0/spack  
This may take a moment the first time...  
training0@e4s-24-11-aws-2:~$
```

To increase font size right click and choose preferences



Choose font size after clicking Custom Font for Terminal



Spack package manager

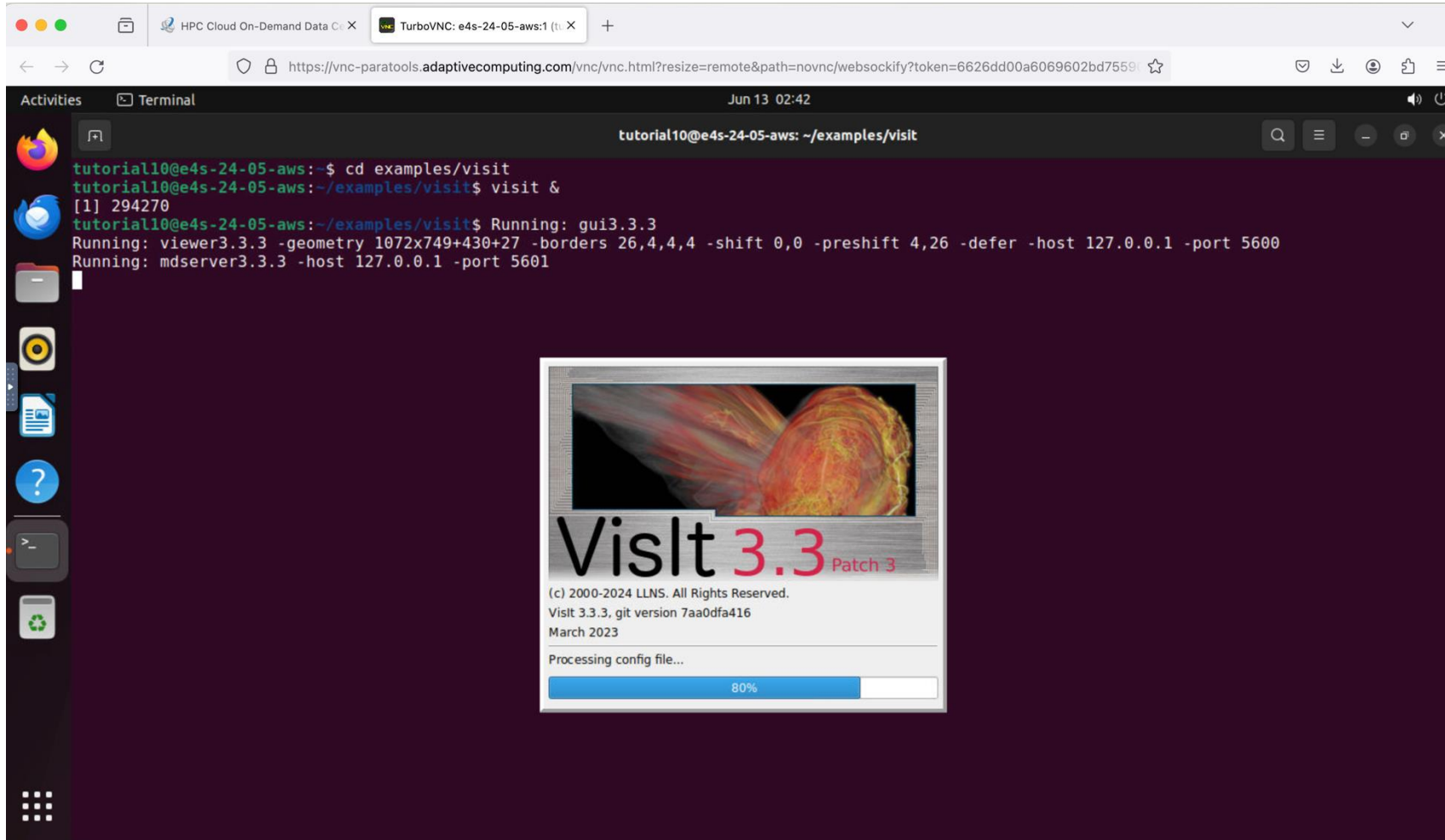
[<https://spack.io>]

```
tutorial10@e4s-24-05-aws: ~  
$ spack find -x  
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 -----  
adios@1.13.1 dealii@9.5.1 hdf5-vol-async@1.7 mercury@2.3.1 petsc@3.21.0 superlu-dist@8.2.1  
adios2@2.10.0 dealii@9.5.1 hdf5-vol-cache@v1.1 metall@0.25 phist@1.12.0 swig@4.0.2-fortran  
adios2@2.10.0 dyninst@13.0.0 hdf5-vol-log@1.4.0 mfem@4.6.0 plasma@23.8.2 sz@2.1.12.5  
alquimia@1.1.0 e4s-alc@1.0.2 heffte@2.4.0 mgard@2023-12-09 mpmc@2.9.0 sz3@3.1.7  
amL@0.2.1 e4s-cl@1.0.3 heffte@2.4.0 mgard@2023-12-09 mpmc@2.9.0 tasmanian@8.0  
amrex@24.04 ecp-data-vis-sdk@1.0 hpctoolkit@2024.01.1 mgard@2023-12-09 mpmc@2.9.0 tasmanian@8.0  
amrex@24.04 ecp-data-vis-sdk@1.0 hpctoolkit@2024.01.1 mgard@2023-12-09 mpmc@2.9.0 tau@2.33.2  
arborx@1.6 exago@1.6.0 hpx@1.9.1 mpi4py@3.1.1 py-cinemasci@1.7.0 trilinos@13.0.1  
arborx@1.6 flecsi@2.2.1 hpx@1.9.1 mpi4py@3.1.1 py-cinemasci@1.7.0 trilinos@15.1.1  
argobots@1.2 flecsi@2.2.1 hypre@2.31.0 mpi4py@3.1.1 py-deephyper@0.6.0 trilinos@15.1.1  
ascent@0.9.2 flit@2.1.0 hypre@2.31.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
axom@0.9.0 flux-core@0.61.2 kokkos@4.3.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
axom@0.9.0 flux-core@0.61.2 kokkos@4.3.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
boost@1.79.0 forttrilinos@2.3.0 kokkos-kernels@4.3.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
bricks@2023.08.25 fpm@0.10.0 kokkos-kernels@4.3.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
bricks@2023.08.25 gasnet@2023.9.0 laghos@3.1 lammps@20230802.3 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
butterflypack@2.4.0 ginkgo@1.7.0 lammps@20230802.3 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
cabana@0.6.0 ginkgo@1.7.0 lammps@20230802.3 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
cabana@0.6.0 globalarrays@5.8.2 legion@24.03.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
caliper@2.10.0 glvis@4.2 legion@24.03.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
caliper@2.10.0 gmp@06.2.1 legion@24.03.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
chai@2024.02.0 gotcha@1.0.6 libcatayst@2.0.0-rc4 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
chai@2024.02.0 gptune@4.0.0 libcatayst@2.0.0-rc4 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
chai@2024.02.0 gromacs@2024.1 libcatayst@2.0.0-rc4 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
charliecloud@0.37 gromacs@2024.1 libcatayst@2.0.0-rc4 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
conduit@0.9.1 h5bench@1.4 hdf5@1.12.2 loki@0.1.7 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
cp2k@2024.1 hdf5@1.12.3 loki@0.1.7 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
cusz@0.3.1 hdf5@1.14.3 magma@2.8.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
darshan-runtime@3.4.4 hdf5@1.14.3 magma@2.8.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
darshan-util@3.4.4 hdf5@1.14.3 magma@2.8.0 mpi4py@3.1.1 py-deephyper@0.6.0 umap@2.1.0  
==> 170 installed packages  
tutorial10@e4s-24-05-aws: ~$ which visit  
/usr/local/visit/bin/visit  
tutorial10@e4s-24-05-aws: ~$ which paraview  
/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/paraview-5.12.0-ytdziwgztxhb5jc6z2fn25bypuqqvq/bin/paraview  
tutorial10@e4s-24-05-aws: ~$
```

```
spack find -x
spack find

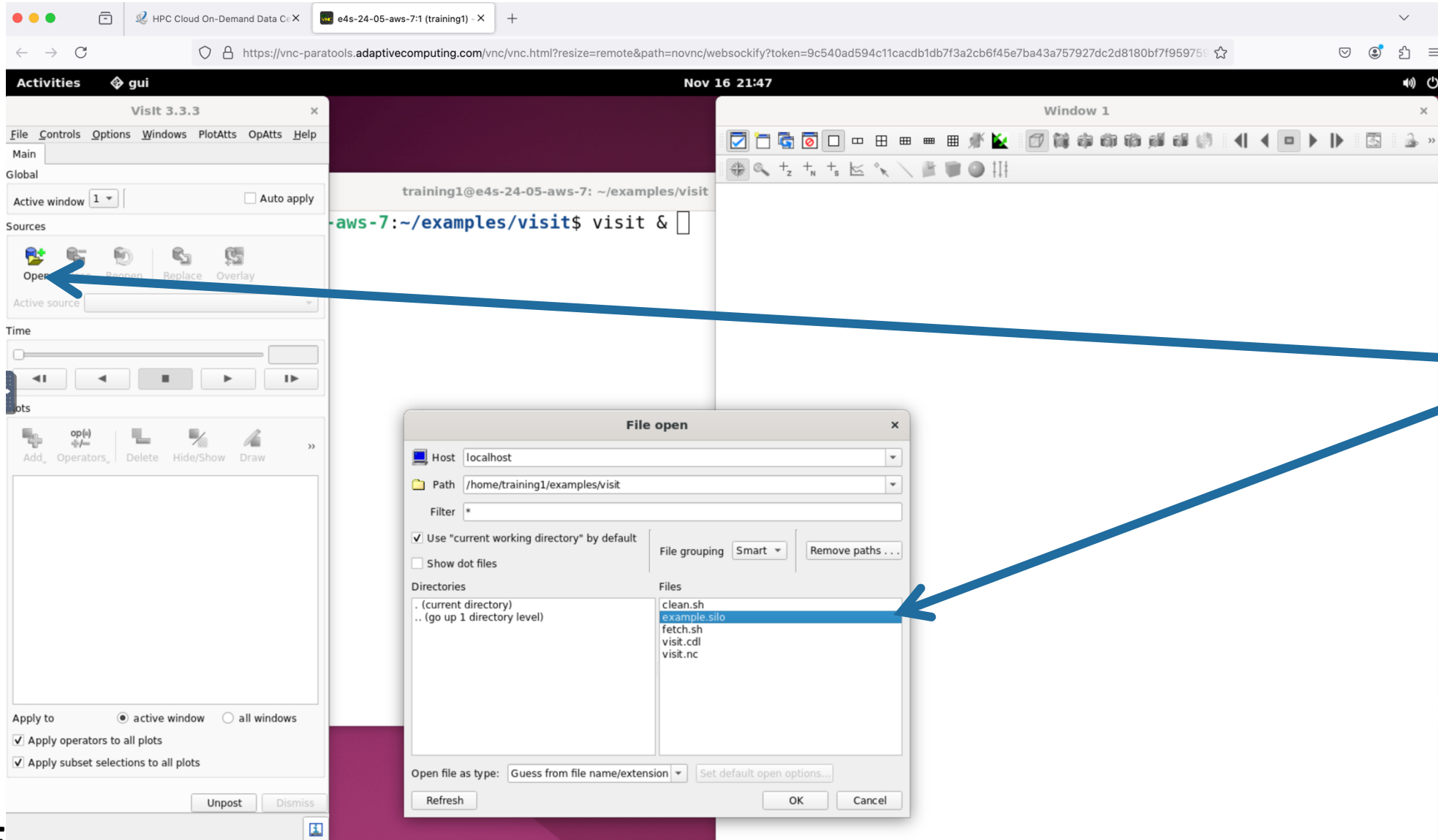
module avail
```


VisIt visualizer: 3D graphics on remote desktop



cd ~/examples/visit
visit &

VisIt visualizer: 3D graphics on remote desktop

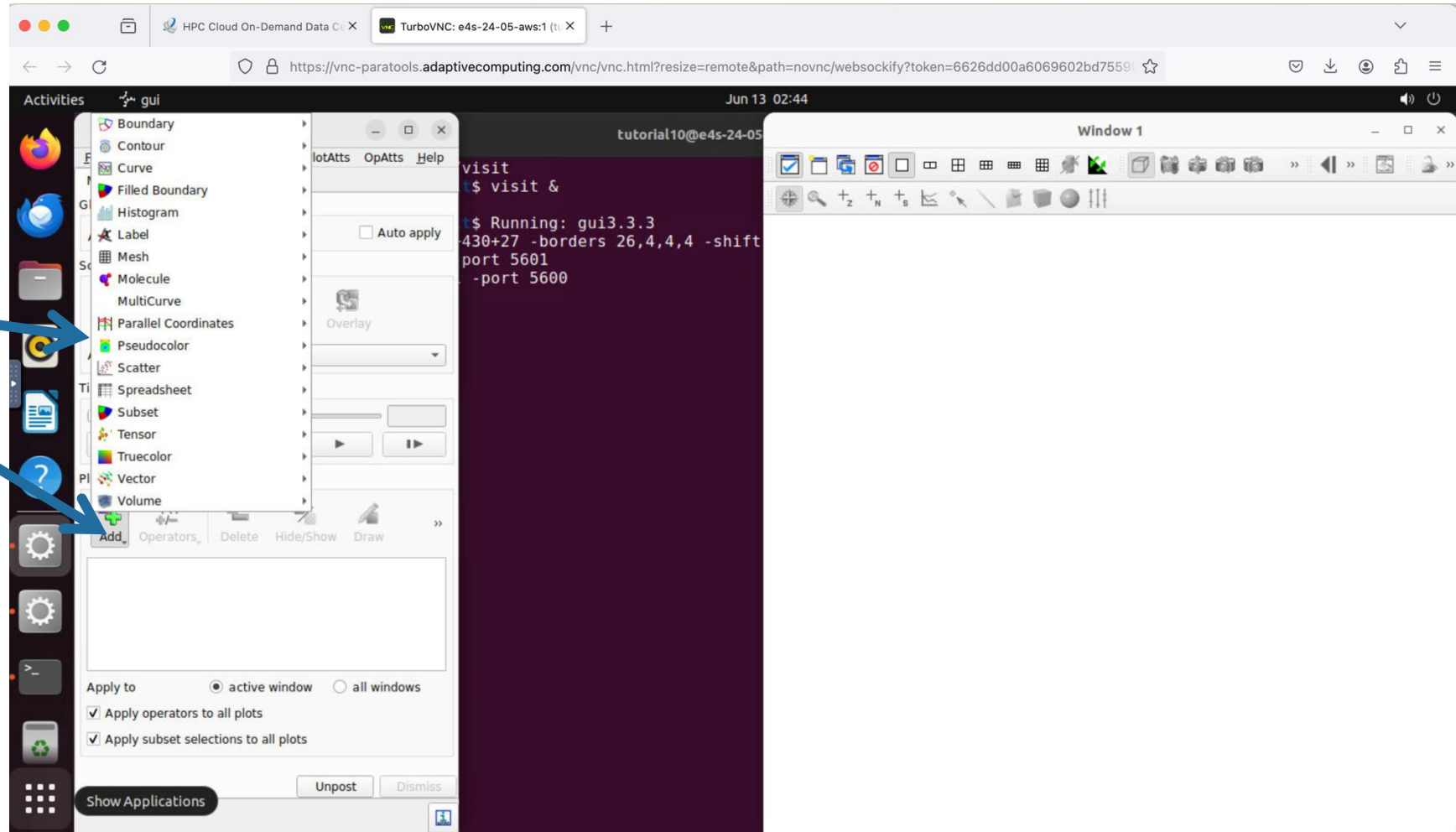


`cd ~/examples/visit`
`visit &`

Open `example.silo`

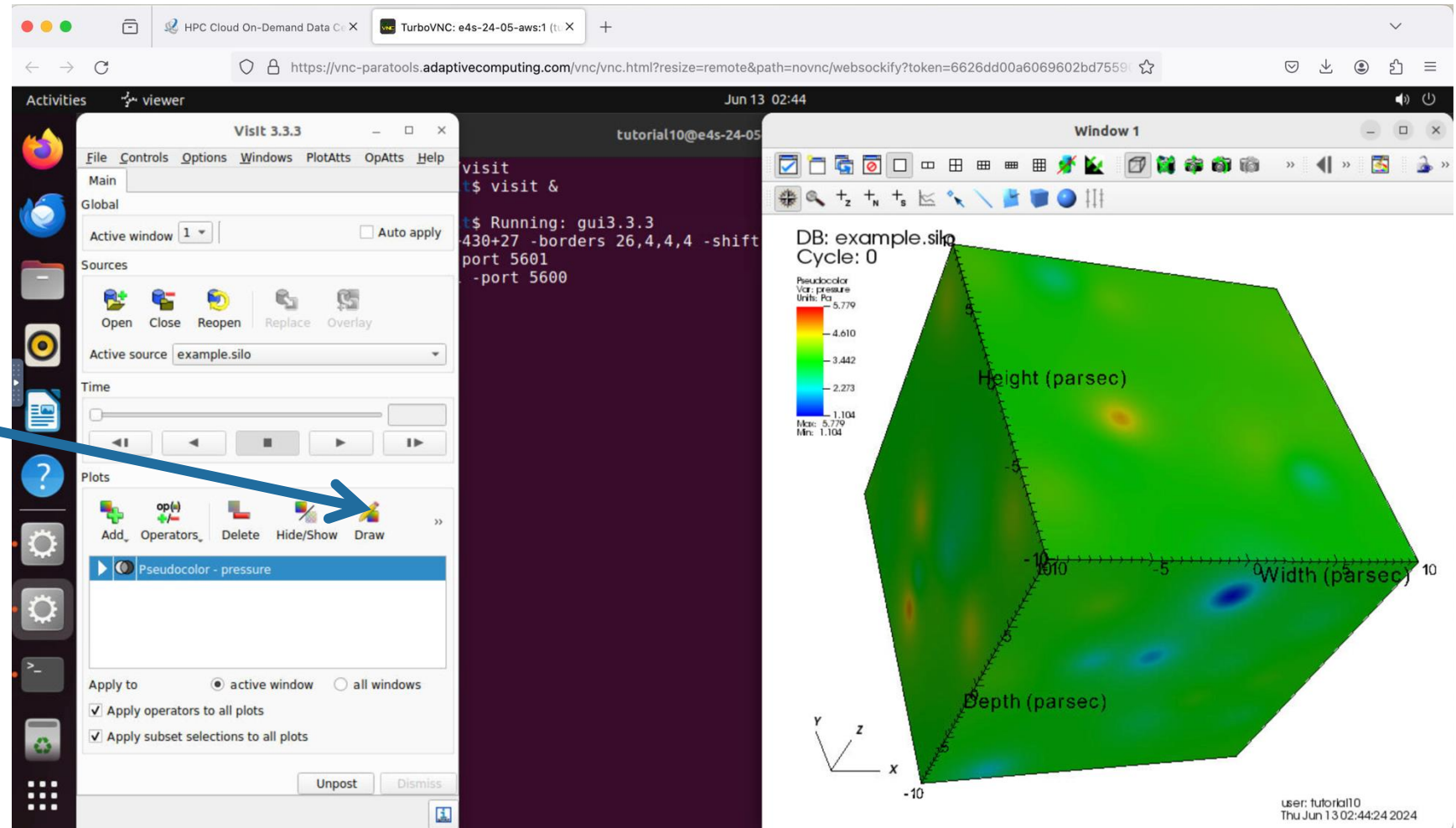
VisIt visualizer

Click Add
Add Pseudocolor ->
Pressure
Click Draw



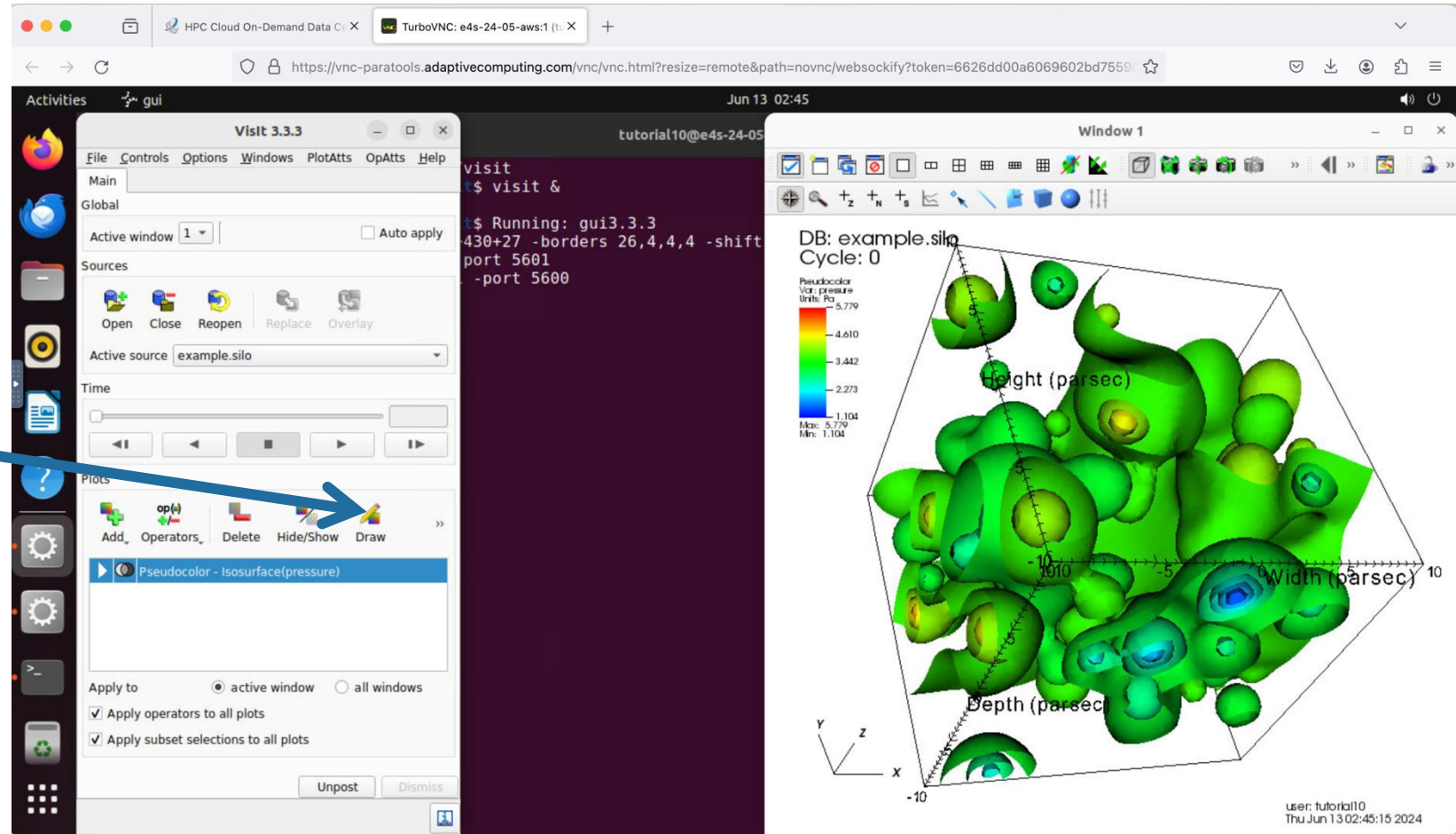
VisIt visualizer

Add Pseudocolor ->
Pressure
Click Draw
Rotate image

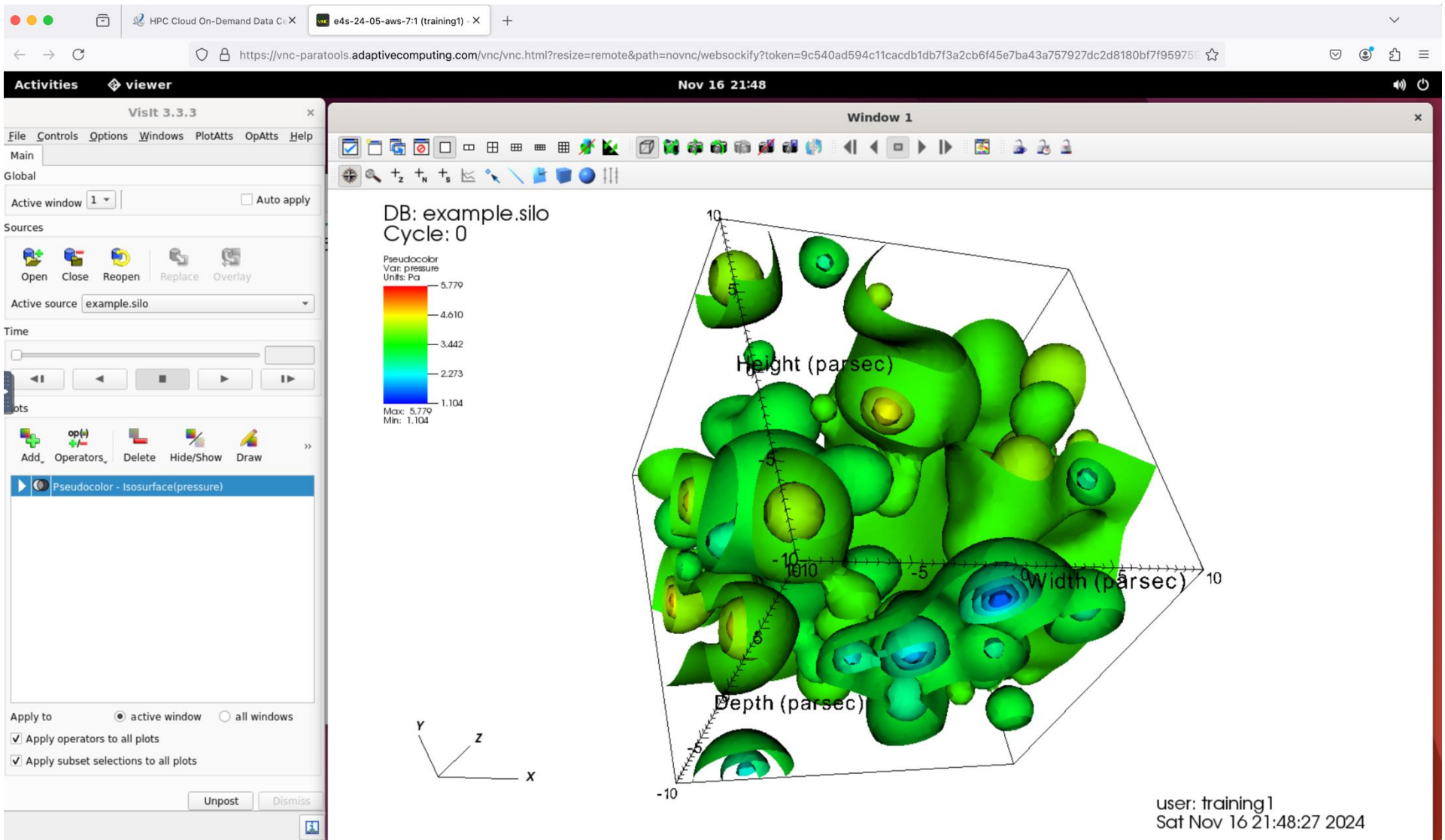


VisIt visualizer

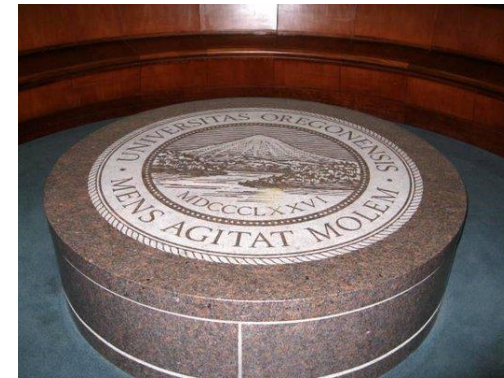
Add Operators ->
Isosurface
Click Draw
Rotate image



VisIt visualizer: 3D graphics check



Performance Research Laboratory, OACISS, University of Oregon



Support Acknowledgements

- US Department of Energy (DOE)
 - ANL
 - Office of Science contracts, ECP
 - SciDAC, LBL contracts
 - LLNL-LANL-SNL ASC/NNSA contract
 - Battelle, PNNL and ORNL contract
- NASA SBIR
- Department of Defense (DoD)
 - PETTT, HPCMP
- National Science Foundation (NSF)
 - SI2-SSI, Glassbox
- CEA, France
- Industry: AWS, AMD, IBM, ARM, Intel, NVIDIA
- Partners:
 - University of Oregon
 - The Ohio State University
 - ParaTools, Inc.
 - University of Tennessee, Knoxville
 - T.U. Dresden, GWT
 - Jülich Supercomputing Center



Acknowledgment

- This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Next-Generation Scientific Software Technologies program, under contract number DE-AC02-06CH11357. DOE SBIR DE-SC0022502.*



U.S. DEPARTMENT OF
ENERGY

Office of
Science

- <https://science.osti.gov/ascr>
- <https://pesoproject.org>
- <https://ascr-step.org>
- <https://hpsf.io>
- <https://www.energy.gov/technologytransitions/sbirsttr>



Thank you

<https://www.exascaleproject.org>

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.



Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.

