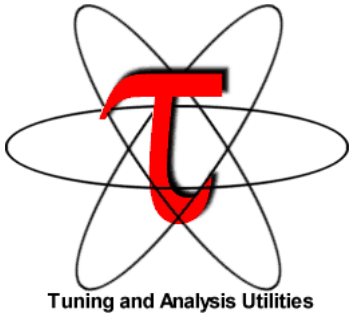
TAU Performance System® Hands-On



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University of Oregon

http://tau.uoregon.edu/TAU_TW45_Handson.pdf

TAU: Quickstart Guide

Profiling:

```
MPI: % mpirun -np 16 tau_exec -ebs ./a.out
```

- `Pthread:  % mpirun -np 16 tau_exec -T mpi,pthread -ebs ./a.out`
- `CUDA: % mpirun -np 16 tau_exec -T cupti,mpi -cupti -ebs ./a.out`
- `Score-P: % mpirun -np 16 tau_exec -T scorep,mpi ./a.out`

```
Analysis: % pprof -a -m | more;  % paraprof (GUI)
```

Tracing:

- `Vampir: MPI: % export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2`
  `% mpirun -np 16 tau_exec ./a.out; vampir traces.otf2 &`
- `Chrome/Jumpshot: % export TAU_TRACE=1; mpirun -np 64 tau_exec ./a.out`
  `% tau_treemerge.pl;`

```
Chrome: % tau_trace2json tau.trc tau.edf -chrome -ignoreatomic -o app.json
   Chrome browser: chrome://tracing   (Load -> app.json) or Perfetto.dev
```

- `Jumpshot: tau2slog2 tau.trc tau.edf -o app.slog2; jumpshot app.slog2`

TAU Hands-On

Hands-On Exercises on CoolMuc-2, LRZ

```
% ssh -Y loginid@lxlogin4.lrz.de
% ls /lrz/sys/courses/vihps/2024/material/tau/
workshop.tgz
% tar zxf /lrz/sys/courses/vihps/2024/material/tau/workshop.tgz
% cd workshop
% cat README
% cat handson.txt
% module use /lrz/sys/courses/vihps/2024/modulefiles/
% module load tau
% which tau_exec
/lrz/sys/courses/vihps/2024/tools/tau/tau-2.33.2/x86_64/bin/tau_exec
% which paraprof
/lrz/sys/courses/vihps/2024/tools/tau/tau-2.33.2/x86_64/bin/paraprof
```

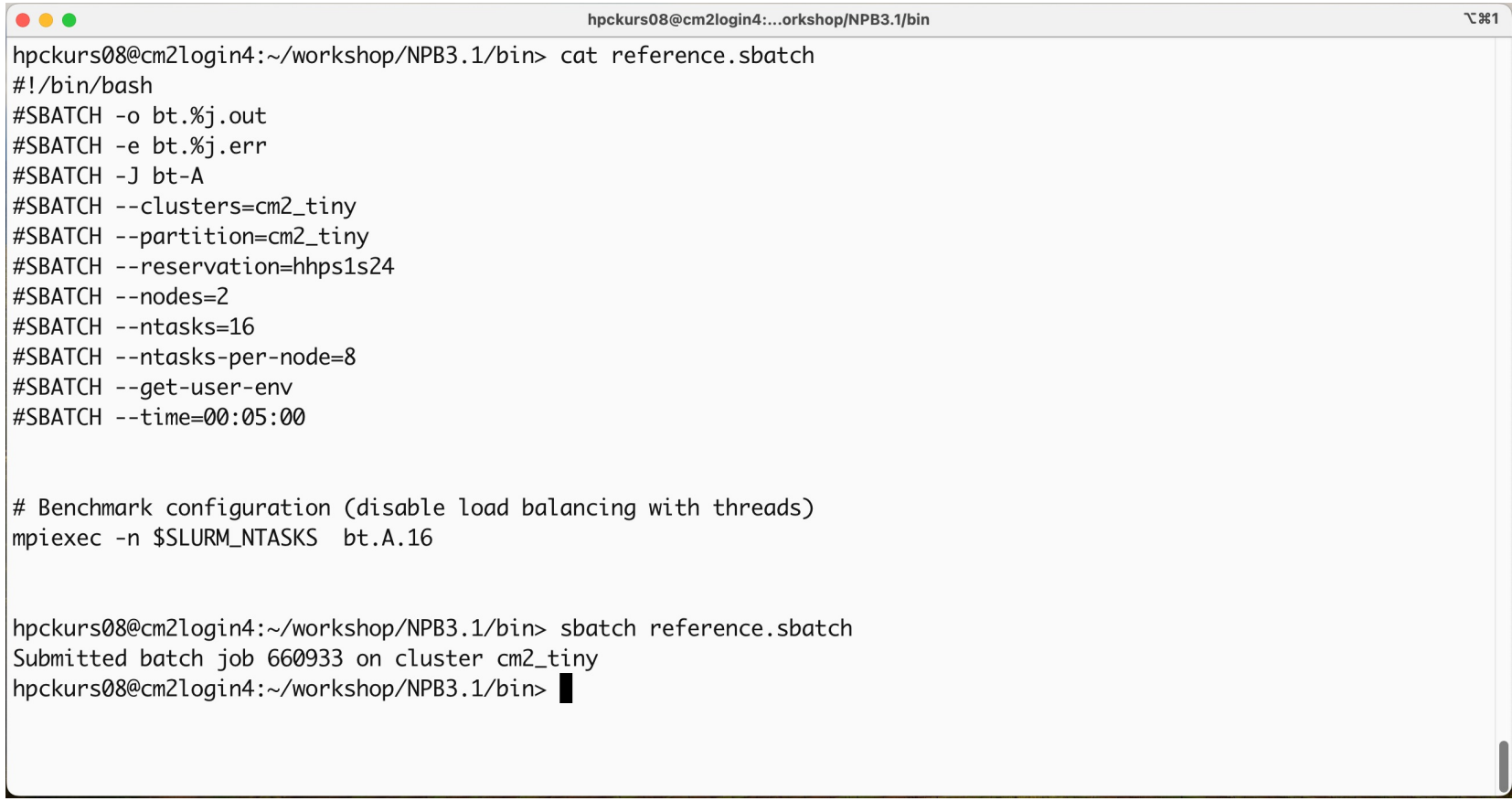
Hands-On Exercises on CoolMuc-2, LRZ

```
hpckurs08@cm2login4:~/workshop                                    ⌥⌘1
hpckurs08@cm2login4:~> ls /lrz/sys/courses/vihps/2024/material/tau/
workshop.tgz
hpckurs08@cm2login4:~> tar zxf /lrz/sys/courses/vihps/2024/material/tau/workshop.tgz
hpckurs08@cm2login4:~> cd workshop
hpckurs08@cm2login4:~/workshop> ls
handson.txt  NPB3.1  NPB3.3-MZ-MPI  README
hpckurs08@cm2login4:~/workshop> cat README
This directory contains some example codes for use in the TAU workshop.
--------------------------------------------------------------------------

Please follow along the hands-on using the handson.txt file. Also,
we recommend reading the README file in each subdirectory and trying the
commands to generate and analyze the data.

1) NPB3.1 - MPI application
2) NPB3.3-MZ-MPI - hybrid MPI and OpenMP Fortran codes.

Please
cat handson.txt
http://tau.uoregon.edu

- Sameer Shende (sameer@cs.uoregon.edu)
hpckurs08@cm2login4:~/workshop> cat handson.txt
```

TAU Exercise #1:
Binary instrumentation with DyninstAPI

Running NAS Parallel Benchmark BT

```
% cd workshop/NPB3.1
% make clean
% make
% cd bin
% cat reference.sbatch
% sbatch reference.sbatch
```



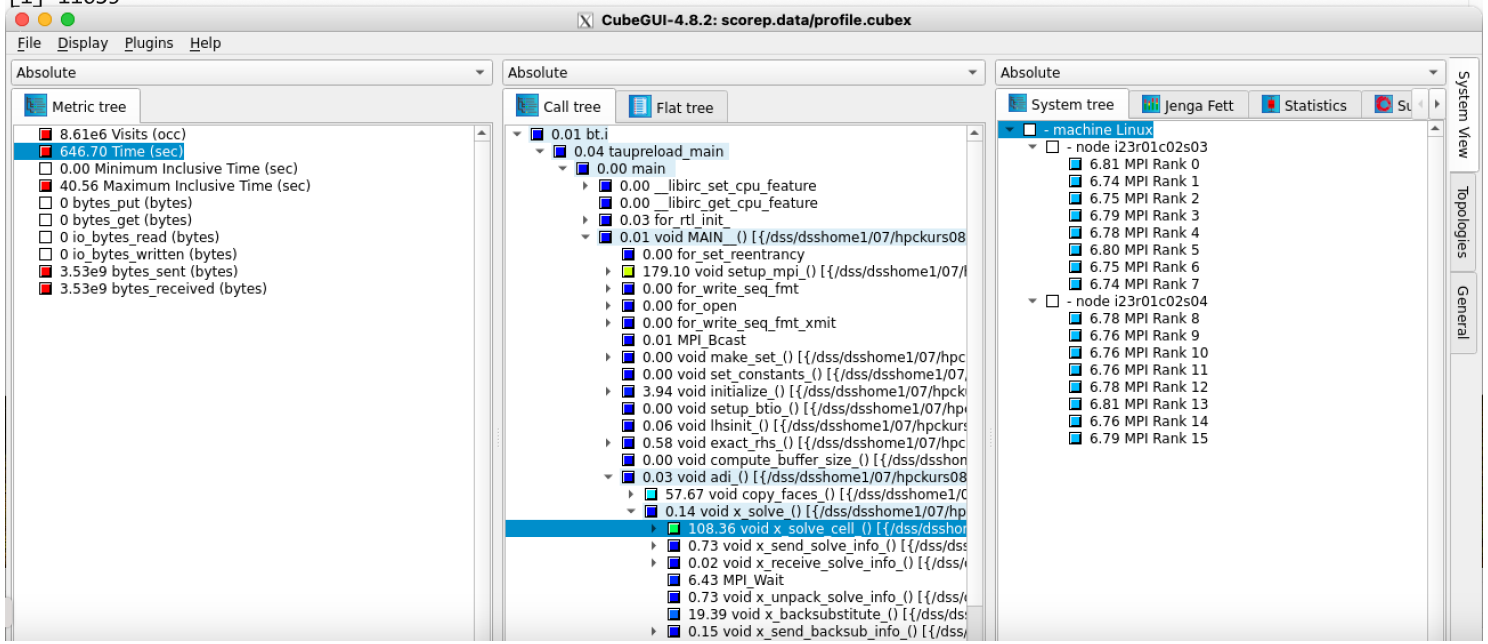
Using TAU's tau_run tool to instrument a binary with Score-P library

```
hpckurs08@cm2login4:...orkshop/NPB3.1/bin                    ⌥⌘1
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> ls
bt.660933.err  bt.660933.out  bt.A.16  reference.sbatch  r.sh  rt.sh  select.tau  tau.sbatch
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> module use /lrz/sys/courses/vihps/2024/modulefiles
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> module load tau
Loading tau/2.33.2
  Loading requirement: openjdk/11.0.12_7 papi/6.0.0.1-intel21 vampir/10.4.2 qt/5.15.2 cubegui/4.8.2
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> which tau_run
/lrz/sys/courses/vihps/2024/tools/tau/tau-2.33.2/x86_64/bin/tau_run
hpckurs08@cm2login4:~/workshop/NPB3.1/bin>
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> tau_run -T scorep ./bt.A.16 -o bt.i
./bt.A.16> Loading libTAUsh-intel-papi-mpi-pdt-scorep.so ...
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> ls
bt.660933.err  bt.660933.out  bt.A.16  bt.i  reference.sbatch  r.sh  rt.sh  select.tau  tau.sbatch
```

```
% tau_run –T scorep ./bt.A –o bt.i
% sbatch tau.sbatch
% cd scorep.data
% ls profile.cubex; cube profile.cubex &
```

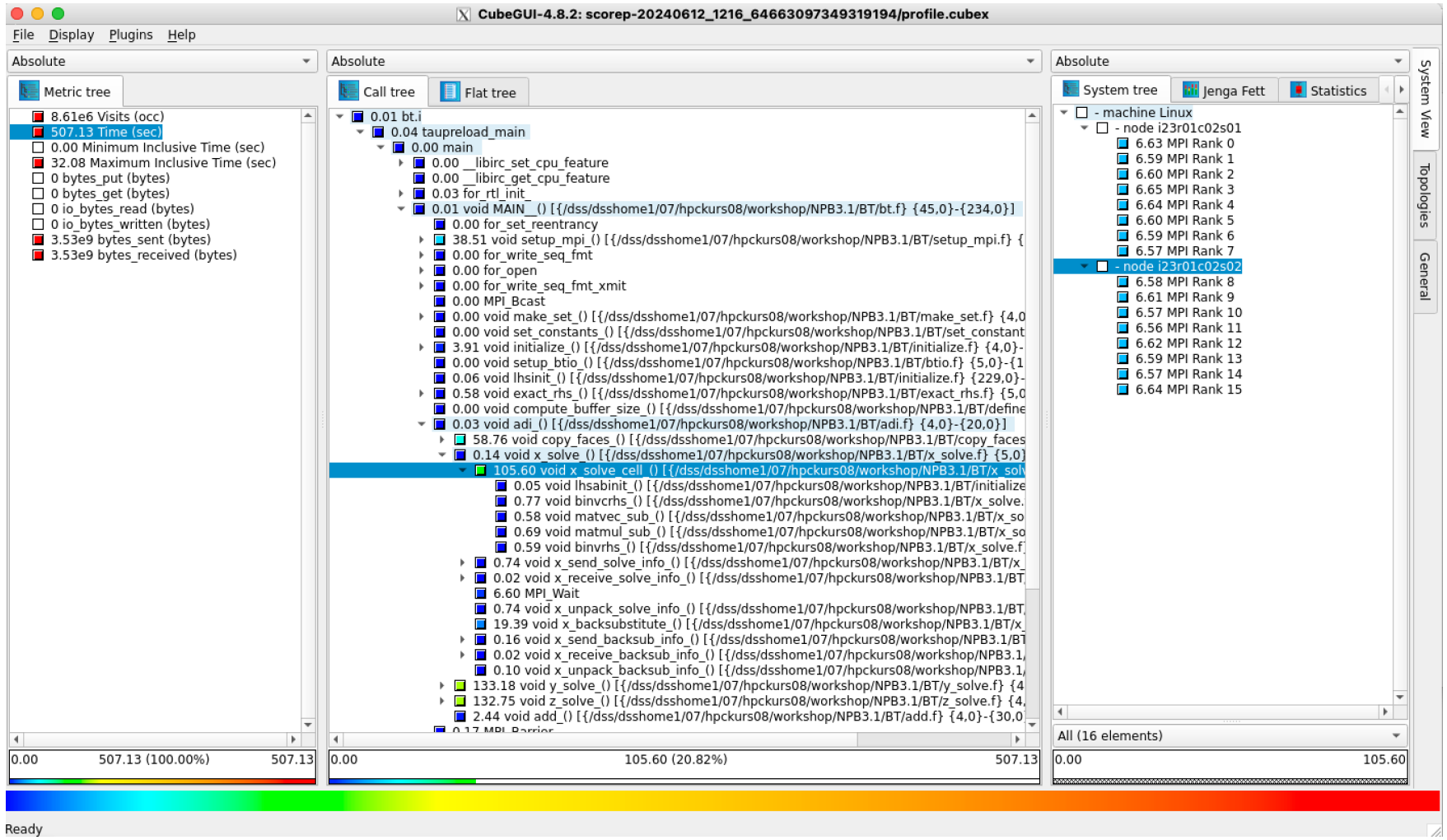
Running the instrumented binary to generate Score-P profile data

```
hpckurs08@cm2login4:....1/bin/scorep.data
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> sbatch tau.sbatch
Submitted batch job 660935 on cluster cm2_tiny
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> ls
bt.660933.err  bt.660935.err  bt.A.16  reference.sbatch  rt.sh        select.tau  tau.sbatch.e660934
bt.660933.out  bt.660935.out  bt.i     r.sh              scorep.data  tau.sbatch  tau.sbatch.o660934
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> cd scorep.data
hpckurs08@cm2login4:~/workshop/NPB3.1/bin/scorep.data> ls
MANIFEST.md  profile.cubex  scorep.cfg
hpckurs08@cm2login4:~/workshop/NPB3.1/bin/scorep.data> which cube
/lrz/sys/courses/vihps/2024/tools/cubegui/4.8.2/bin/cube
hpckurs08@cm2login4:~/workshop/NPB3.1/bin/scorep.data> cube profile.cubex &
[1] 11659
```



Note: compile with -g

Using CUBE to visualize Score-P data generate by TAU



NOTE:
No change to: source code or build system!

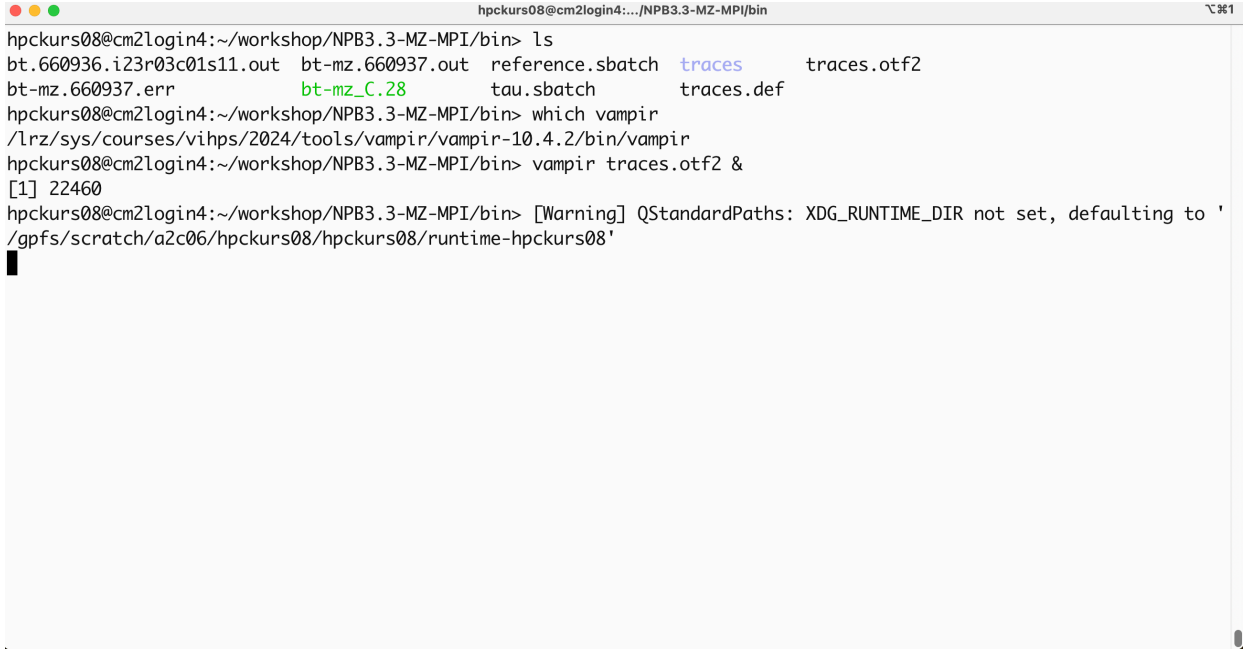
Rewriting the binary using tau_run and injecting Score-P to perform measurements!

TAU Exercise #2:

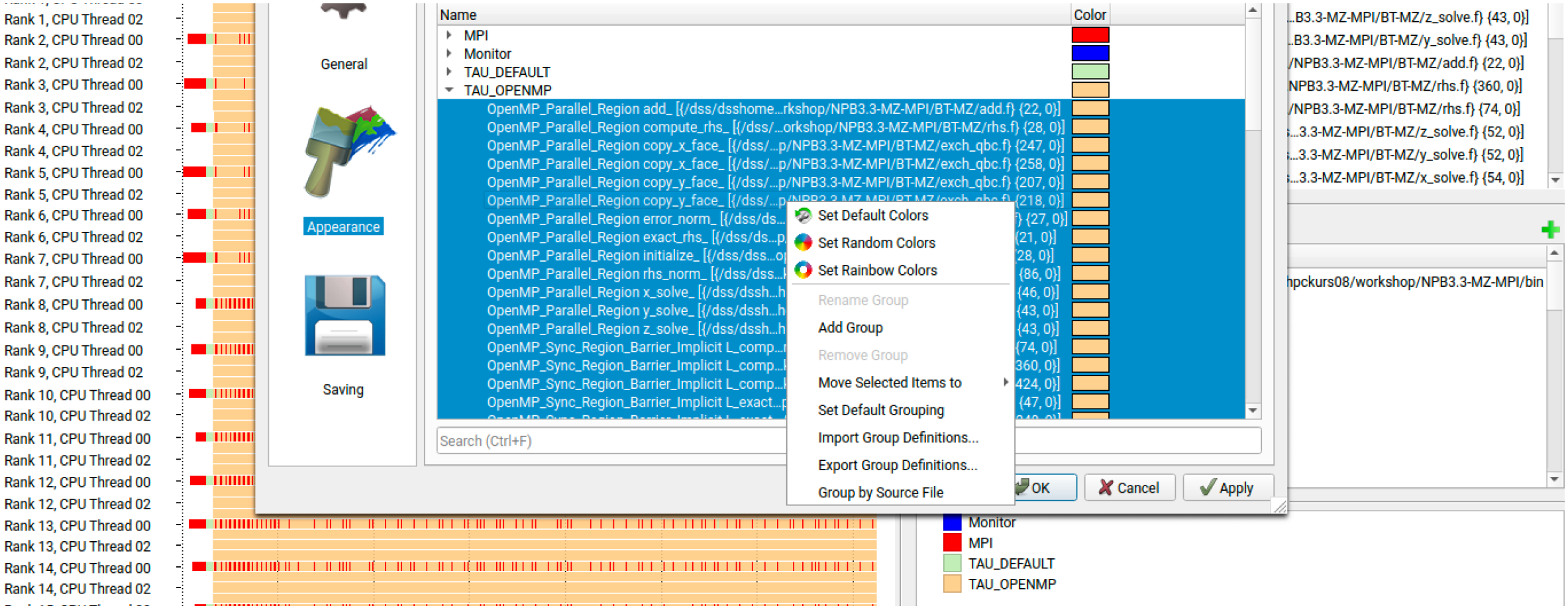
Generating OTF2 traces using MPI and OpenMP (OMPT)

Hands-On Exercises on CoolMuc-2, LRZ

```
% cd workshop/NPB3.3-MZ-MPI
% make clean
% make suite
% cd bin
% cat reference.sbatch
% sbatch reference.sbatch
% cat tau.sbatch
% sbatch tau.sbatch
# after it completes:
% module use
/lrz/sys/courses/vihps/2024/modulefiles/
% module load tau
% vampir traces.otf2 &
```

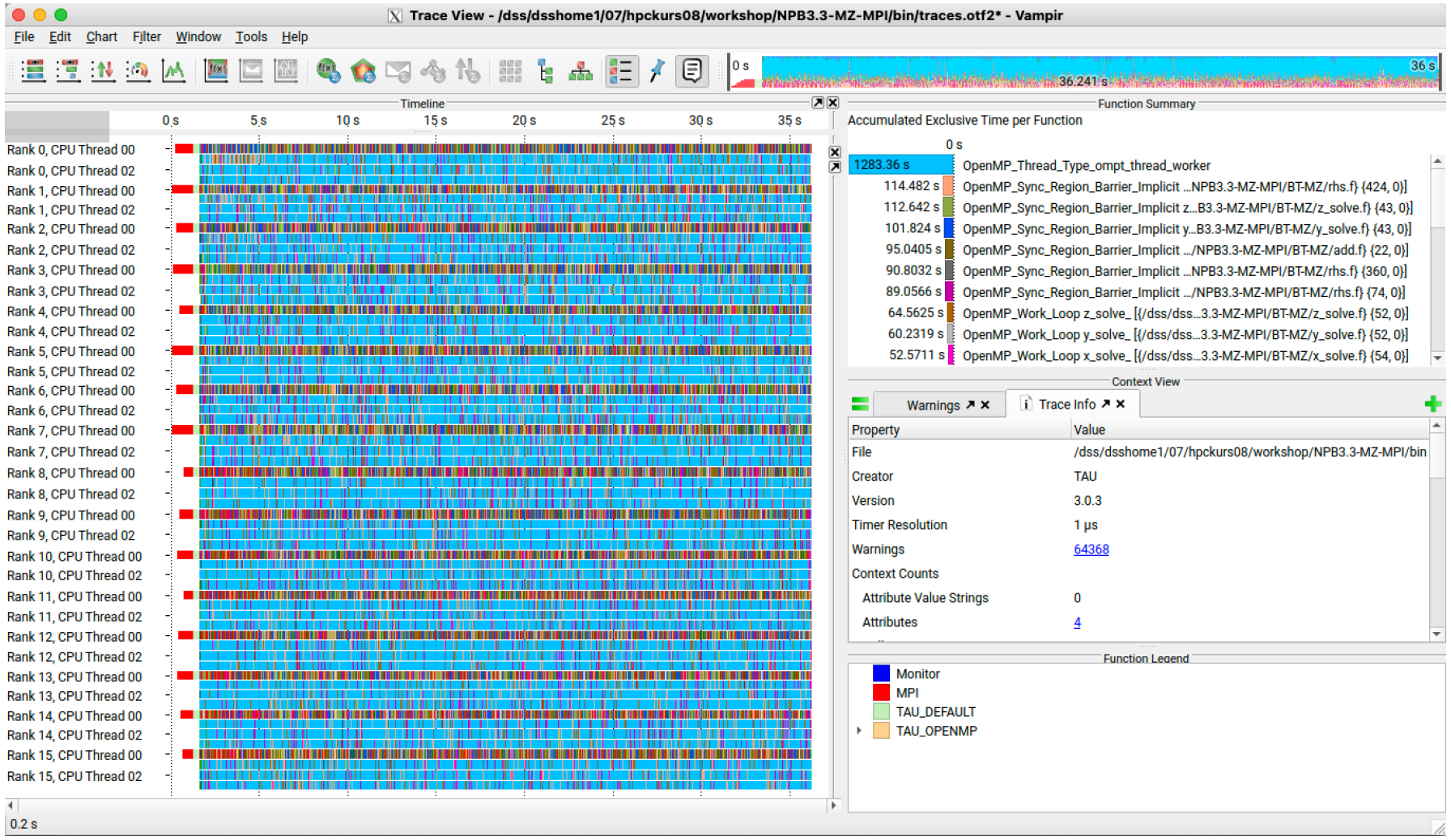


Visualizing OpenMP and MPI application traces using Vampir (from TU Dresden, Germany)

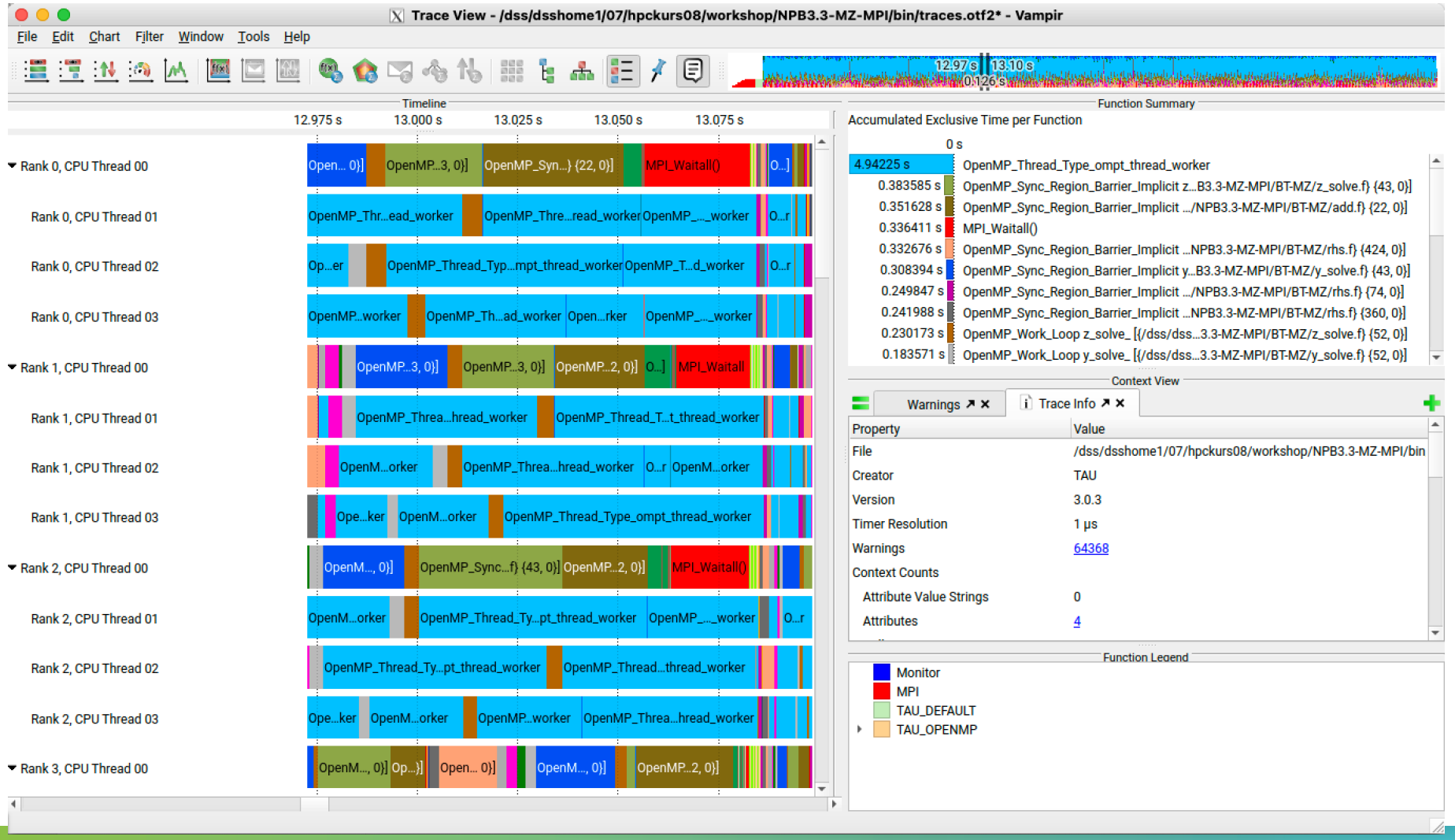


File –> Preferences –> Appearance –> Open TAU_OPENMP Multi–select all functions –> Set Random Colors

Vampir [TU Dresden]



Vampir showing OMPT and MPI data on a per-thread basis



NOTE:
No change to: source code or build system or binary!

Launching the job with tau_exec –T ompt

and generating OTF2 traces in TAU and visualizing with Vampir

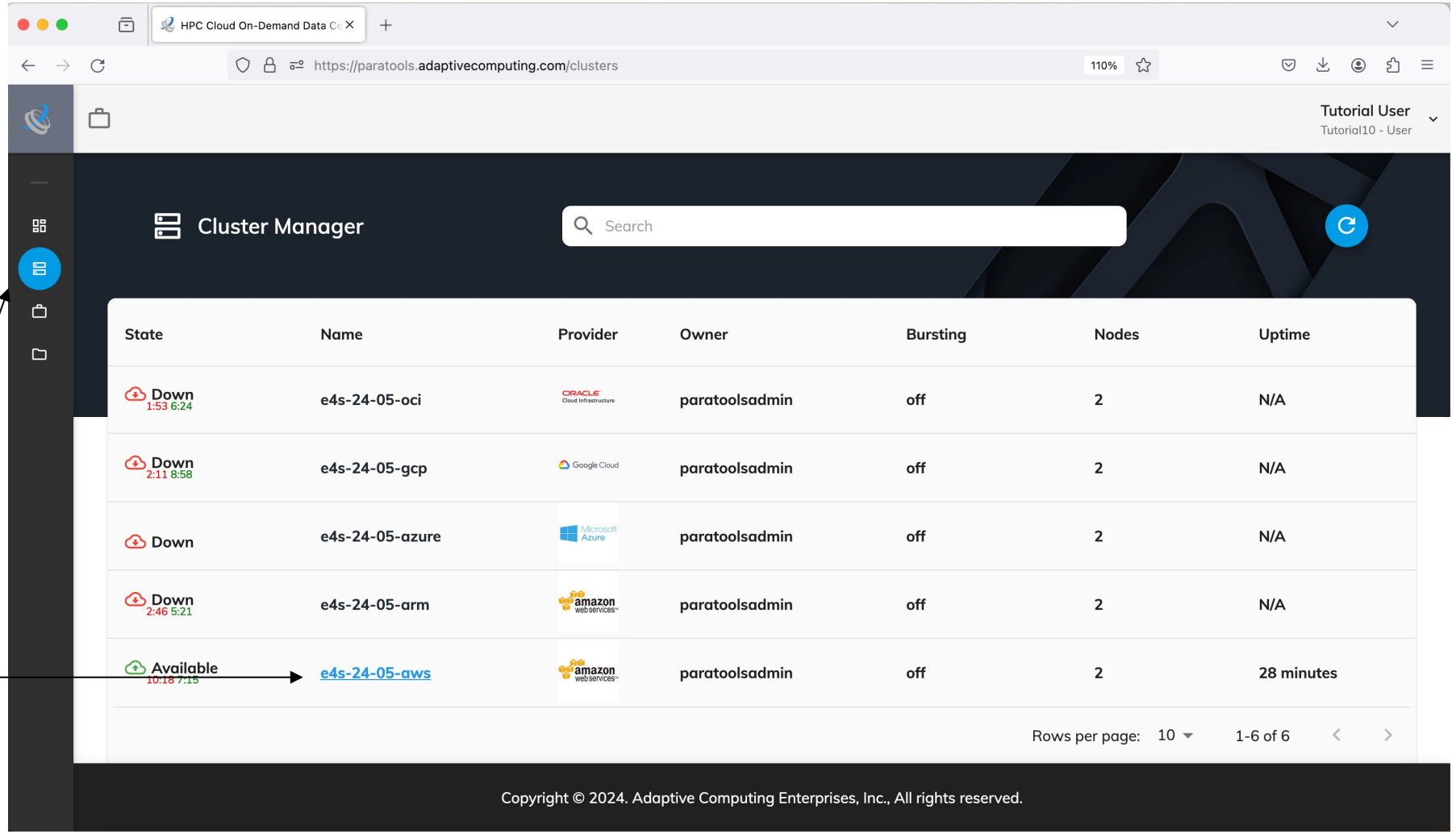
TAU Exercise #3:
Event Based Sampling (EBS)

Using ParaTools Pro for E4S image on AWS with Adaptive Computing's On-Demand Data Center (ODDC)

STEP 1: Go to https://tinyurl.com/e4stut

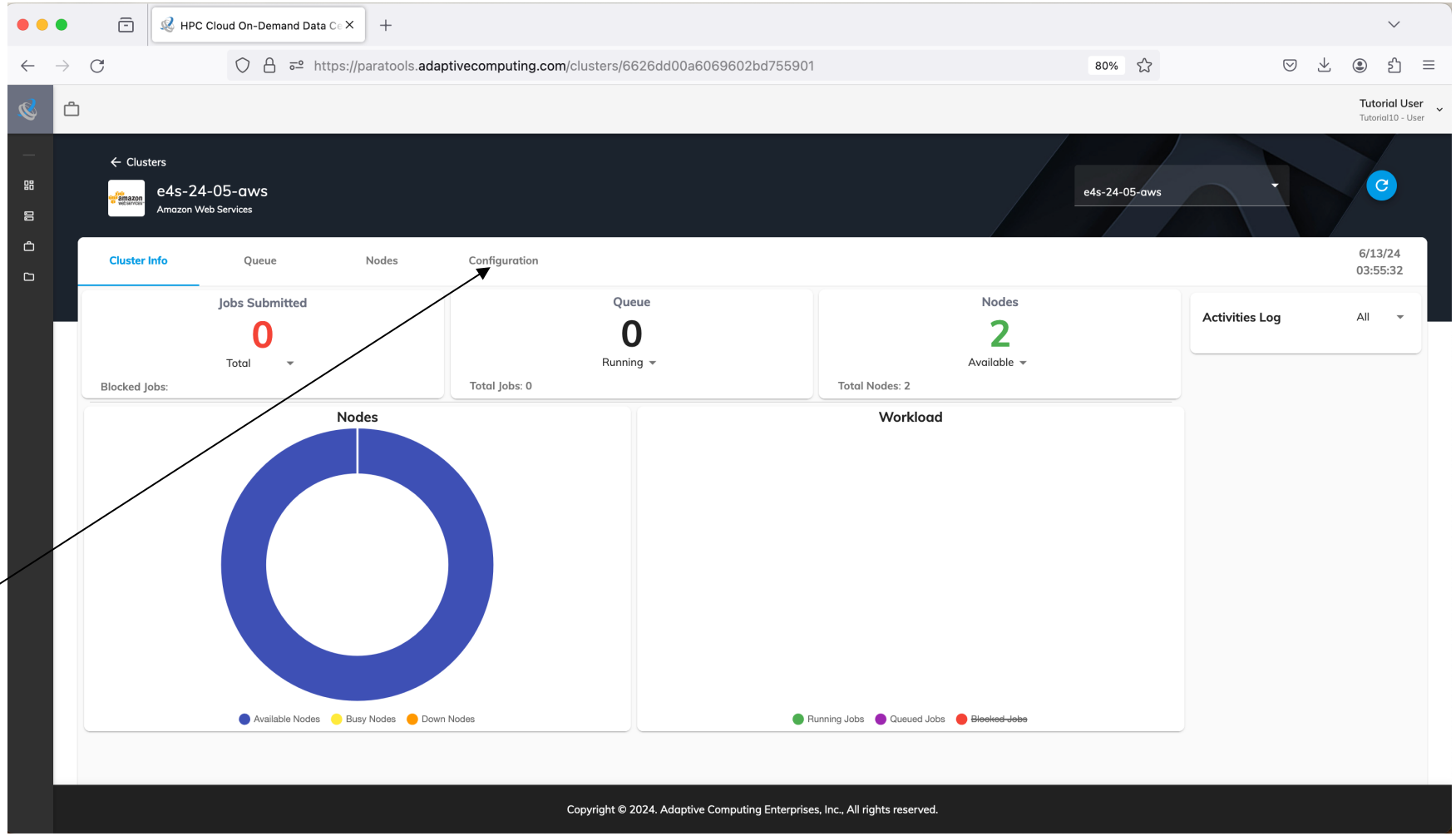
STEP 2: Reserve an instance and login to:
https://paratools.adaptivecomputing.com
with the credentials. Firefox recommended.

Adaptive Computing's ODDC: Go to Cluster Manager on the left



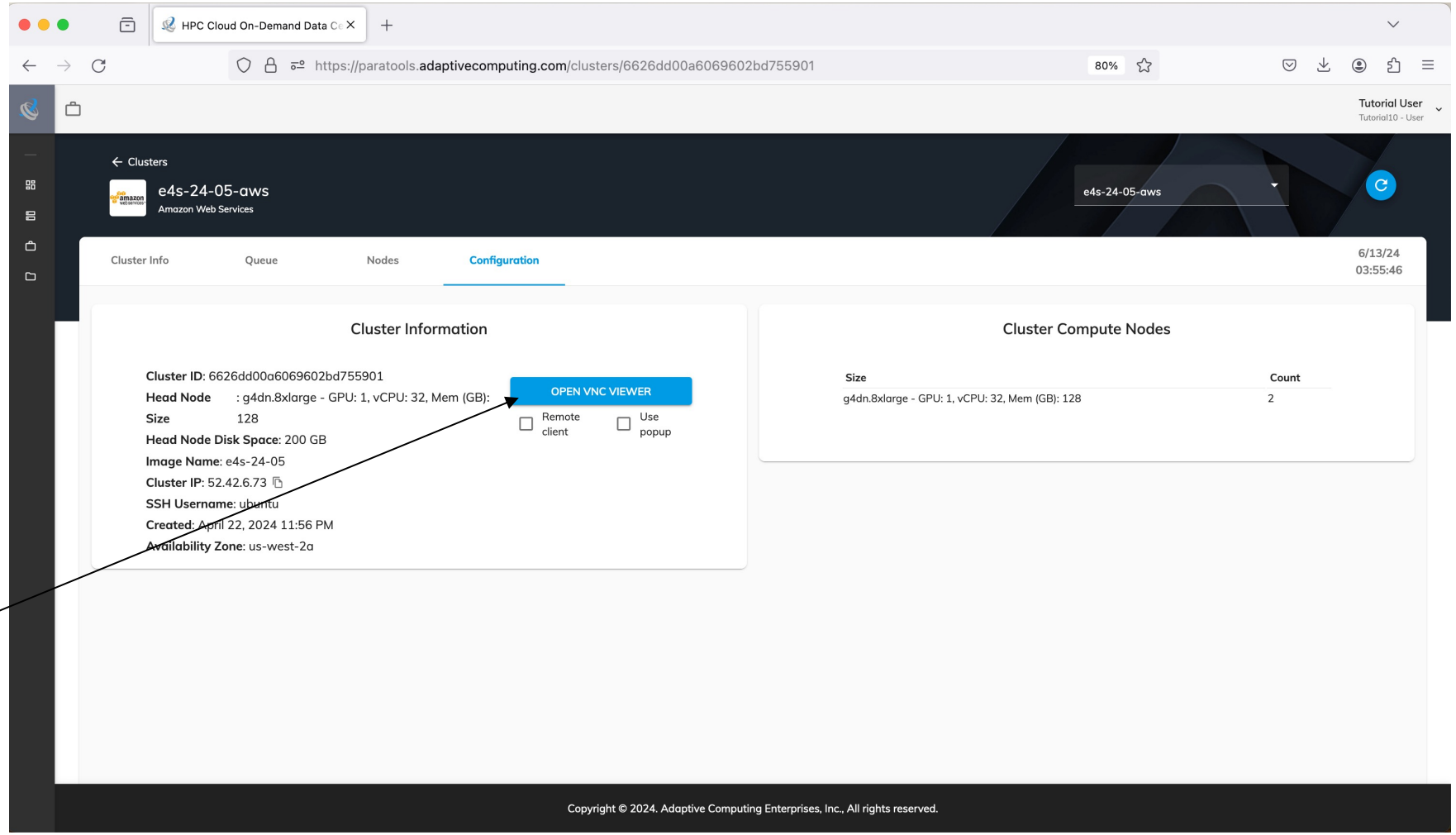
Click here

Adaptive Computing's ODDC: Go to Configuration tab



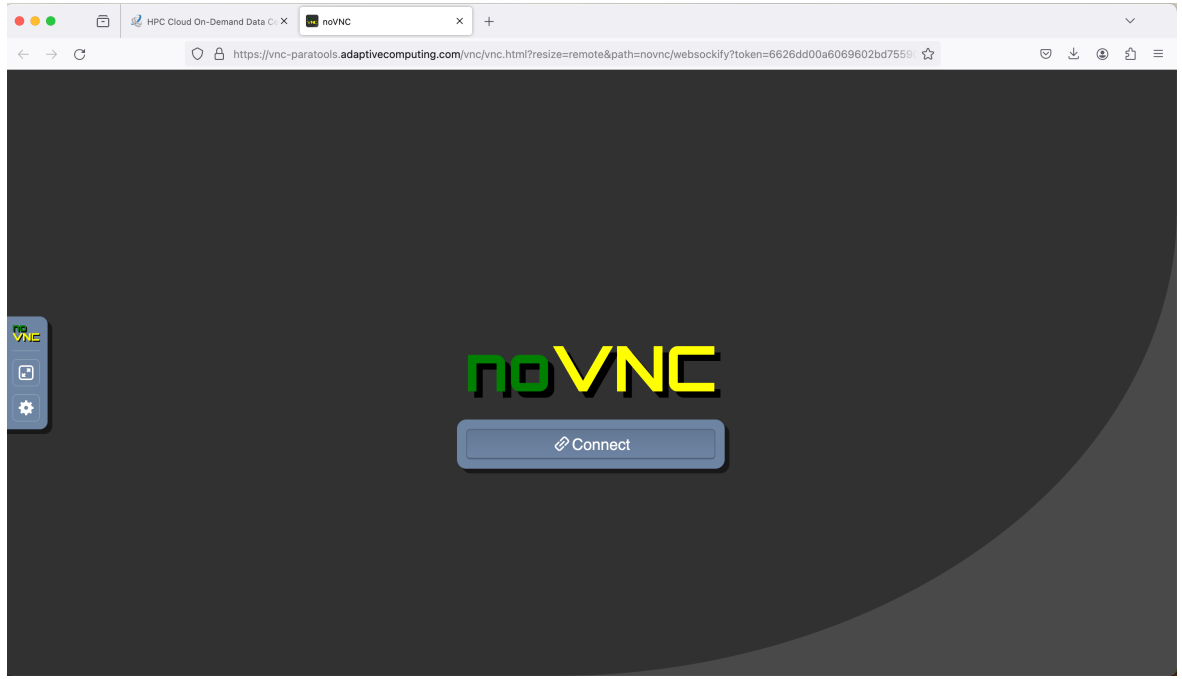
Click here

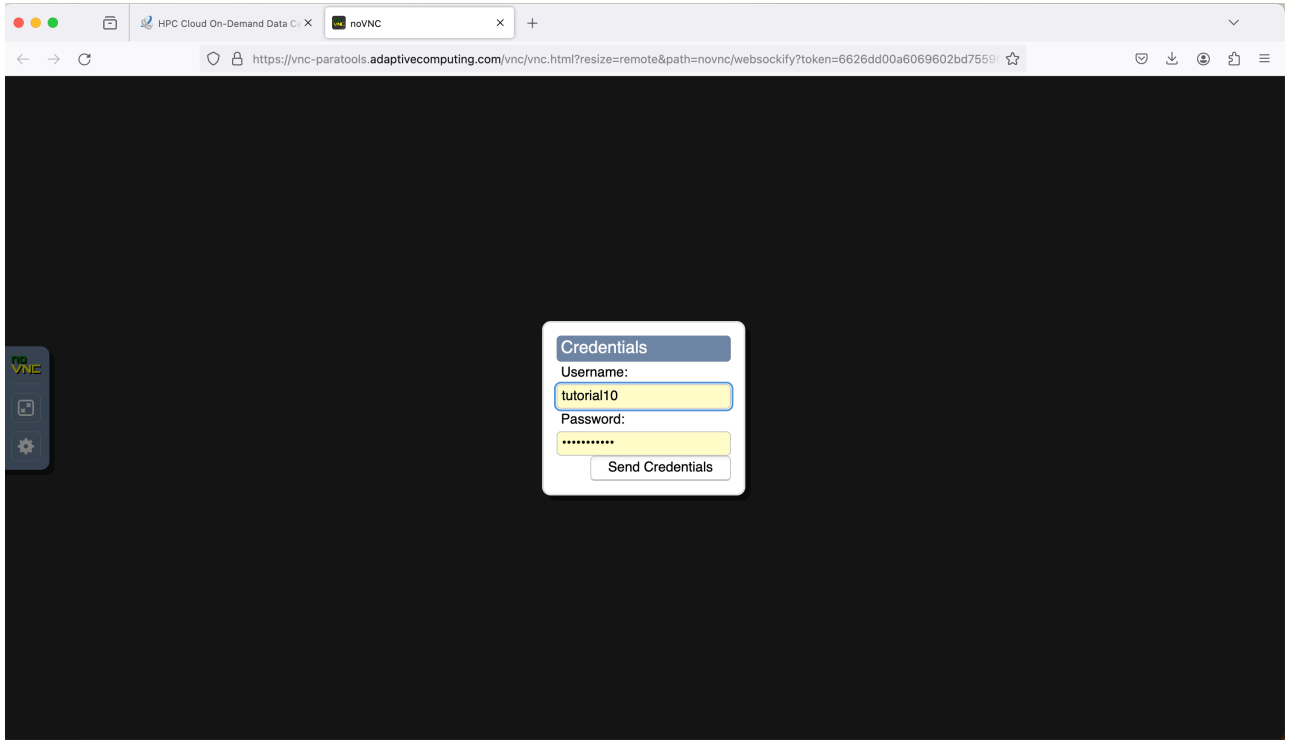
Launch VNC Viewer from ODDC's Configuration Tab for AWS cluster



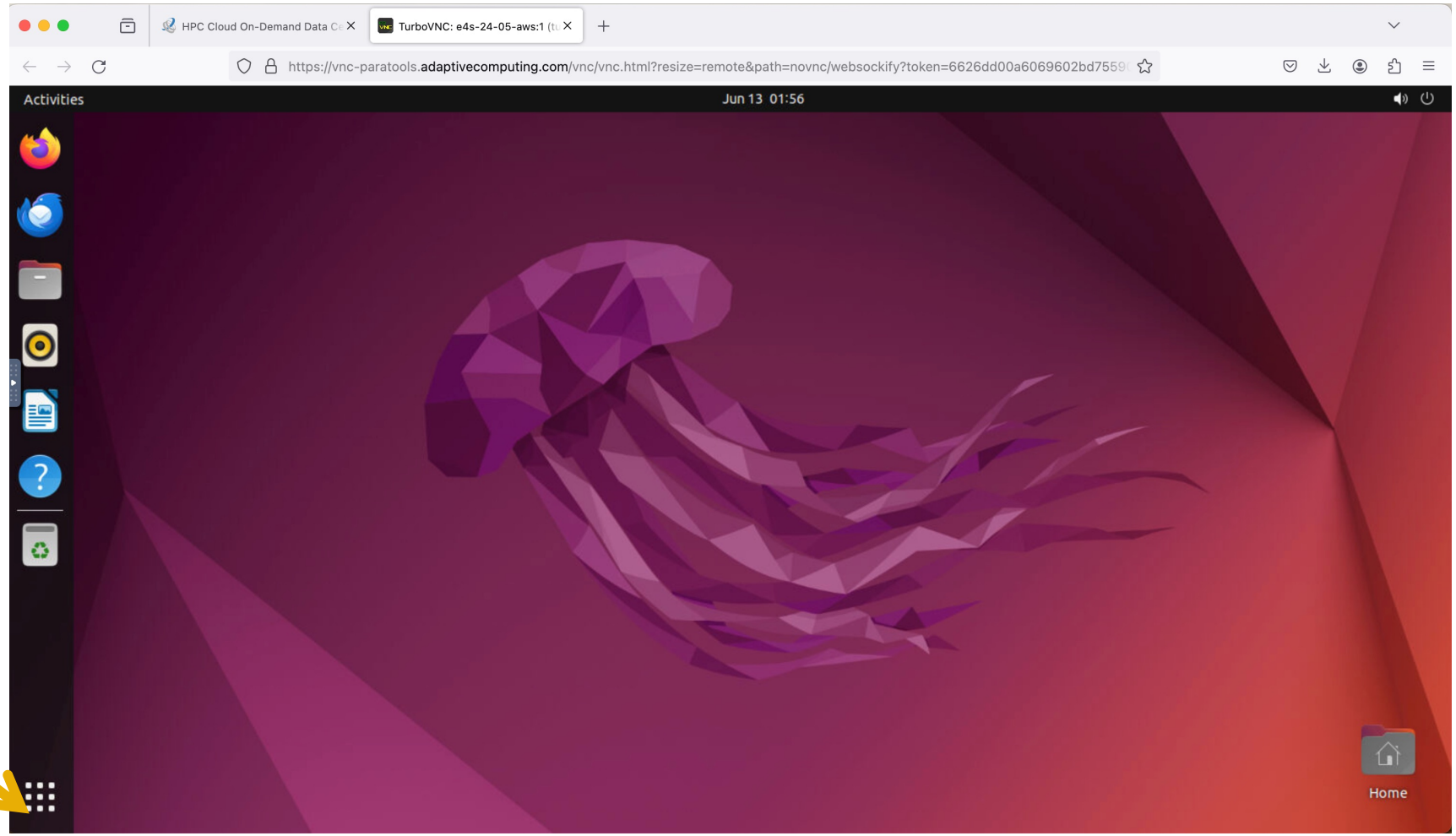
Click here

Authenticate after allowing pop-ups in browser (Firefox below)



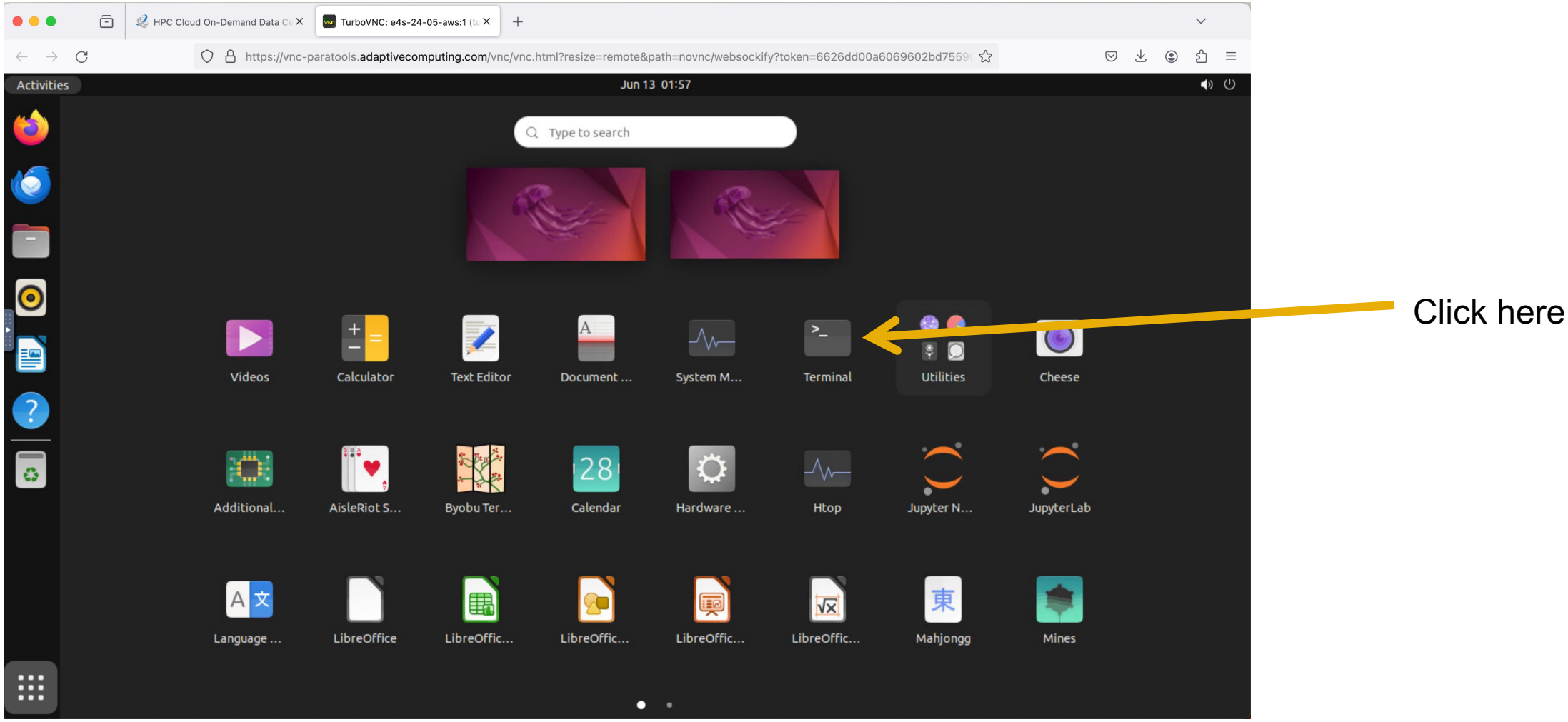


Remote Desktop from the ParaTools Pro for E4S image on AWS

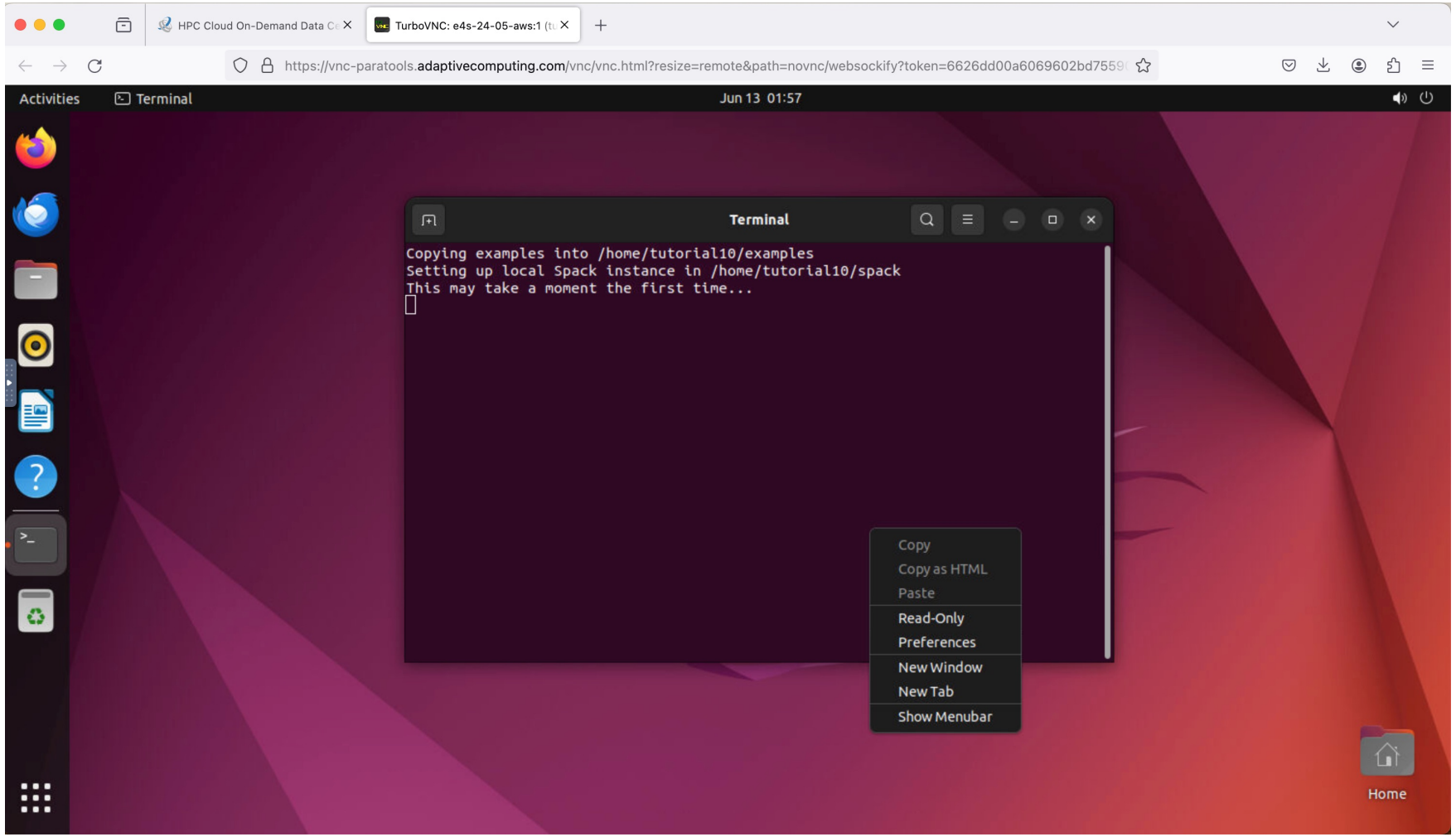


Click here

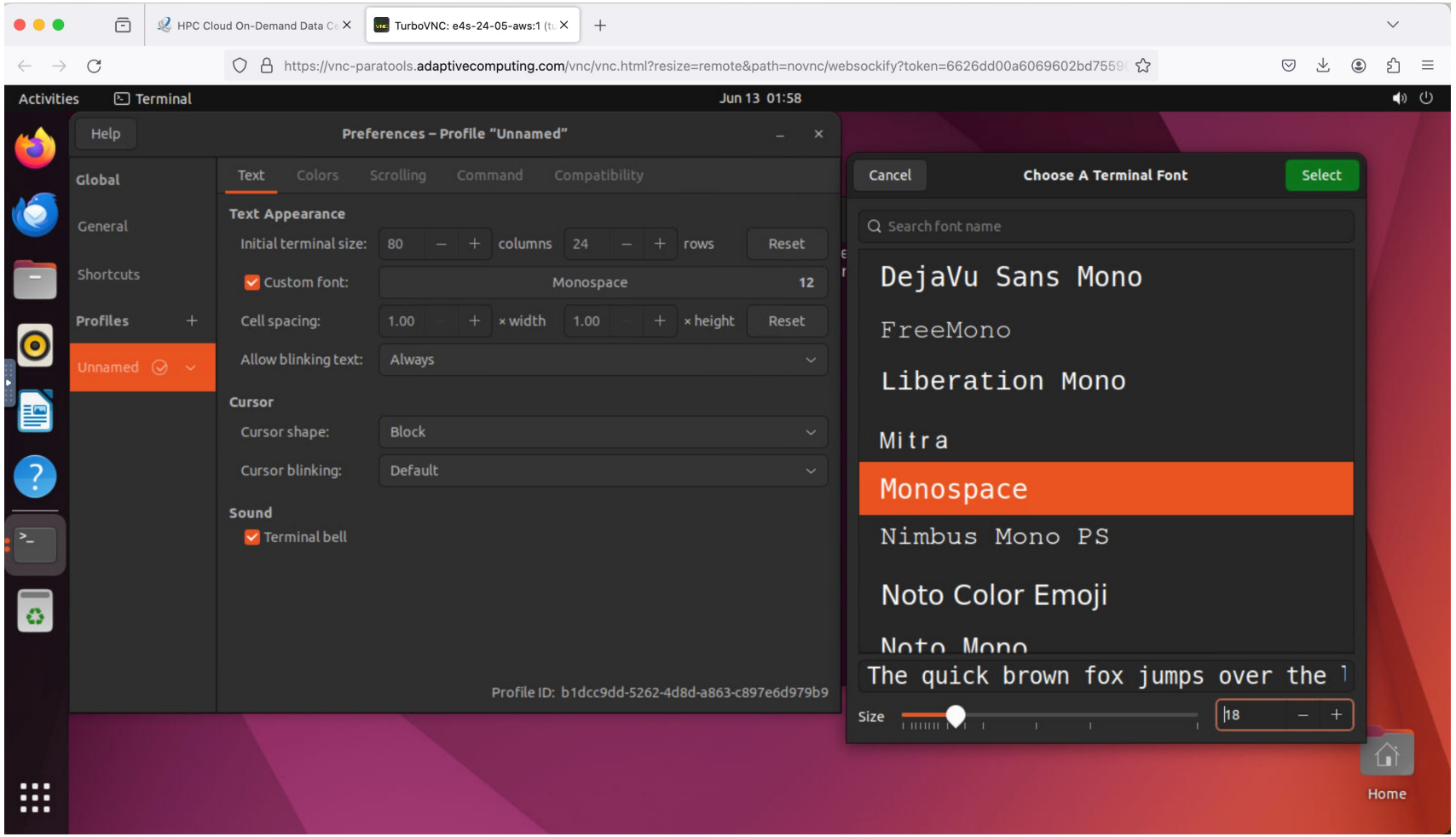
Launch Terminal in Remote Desktop



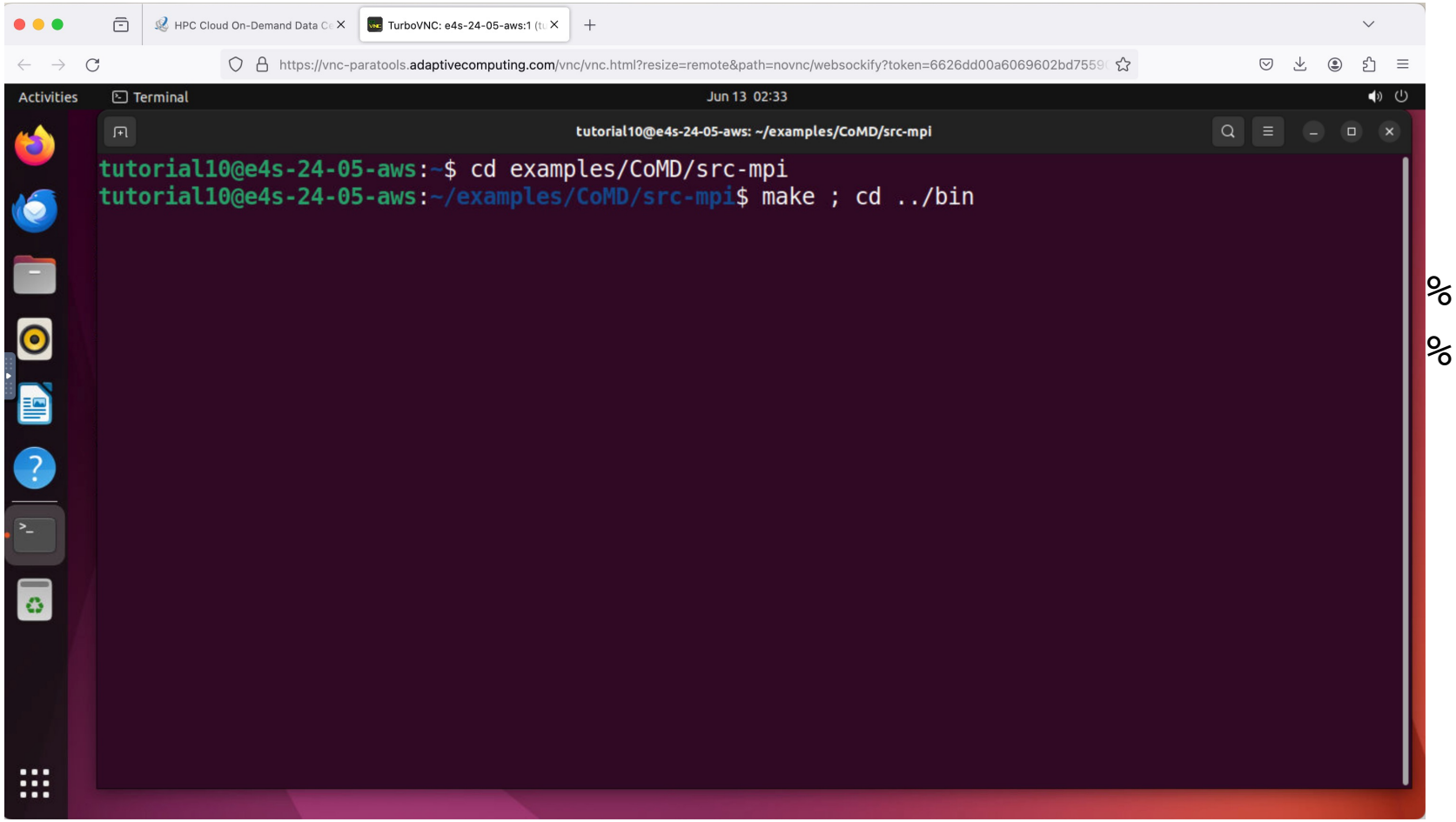
To increase font size right click and choose preferences



Choose font size after clicking Custom Font for Terminal

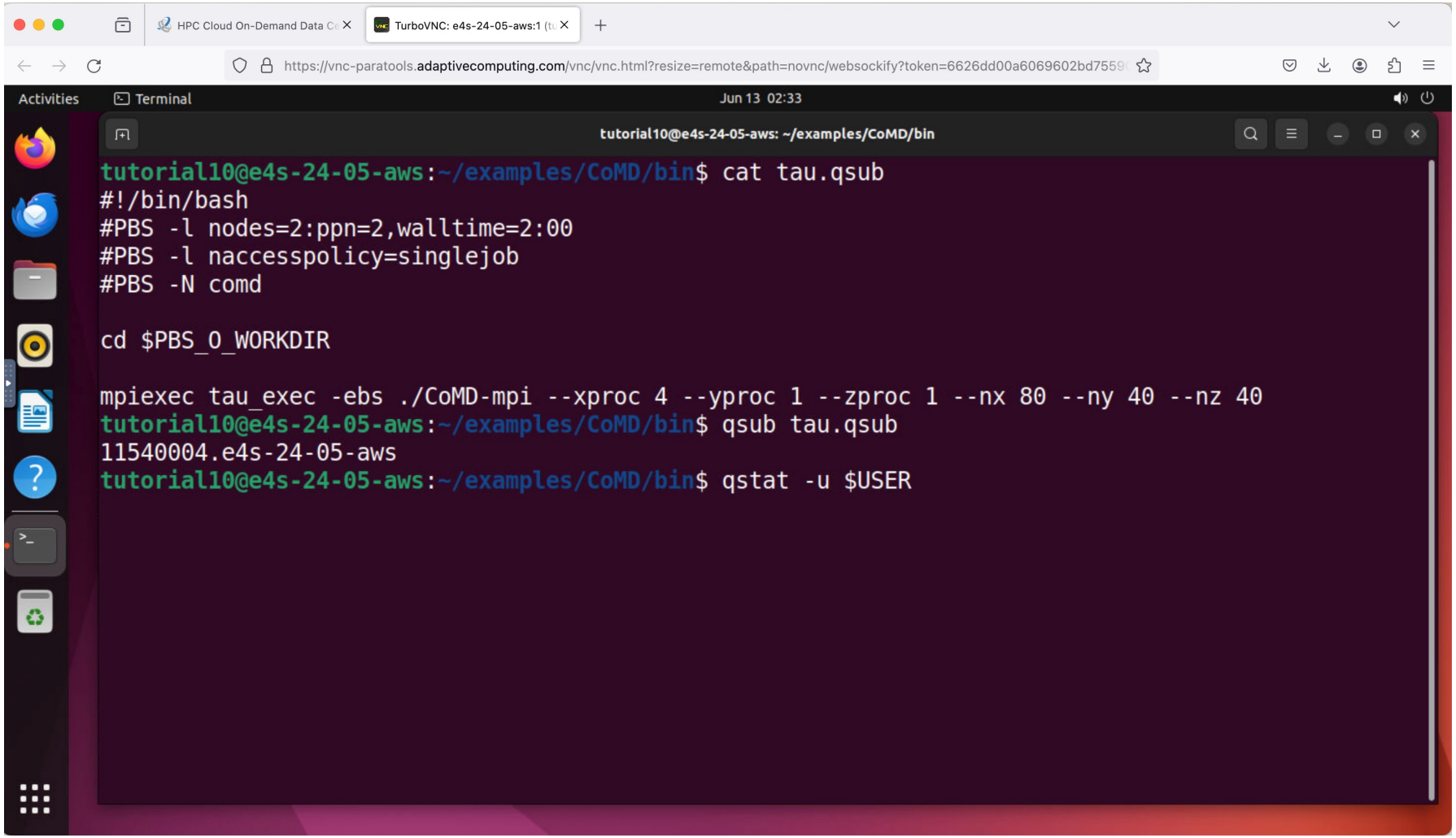


CoMD: TAU with event-based sampling (EBS)



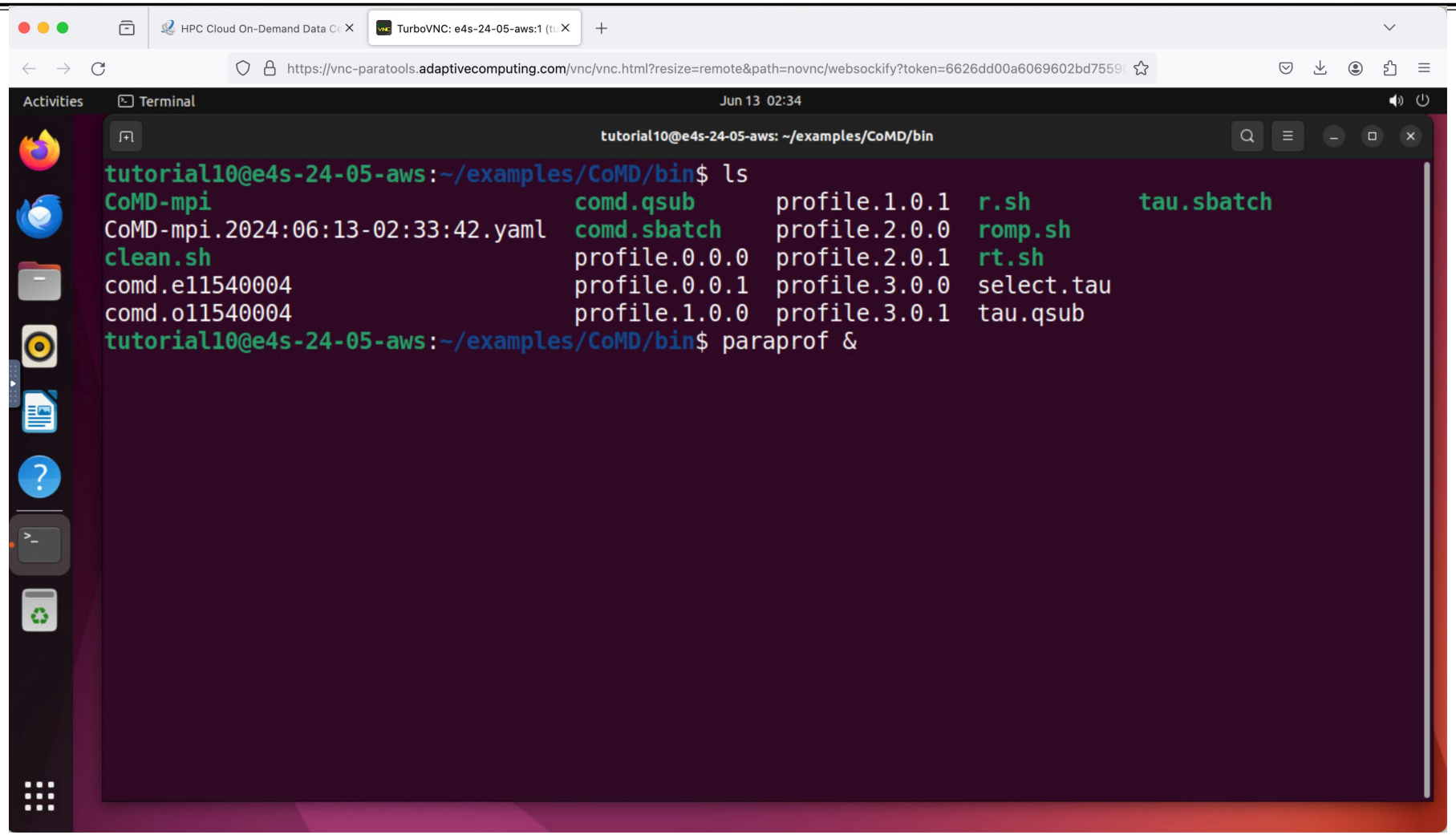

```
% cd examples/CoMD/src-mpi
% make; cd ../bin
```

CoMD: TAU with event-based sampling (EBS)



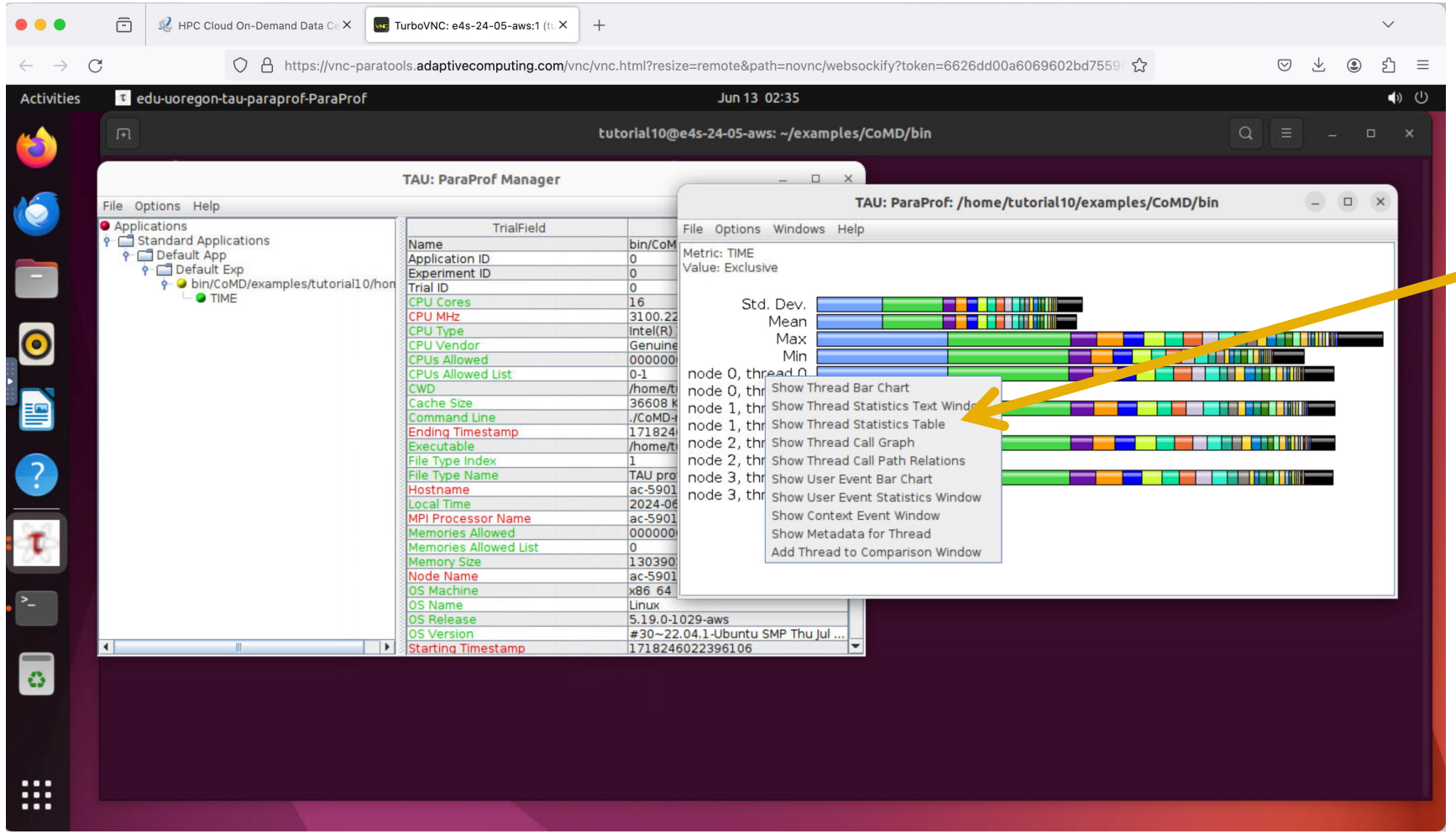

```
% qsub tau.qsub
% qstat –u $USER
```

CoMD: TAU's paraprof visualizer



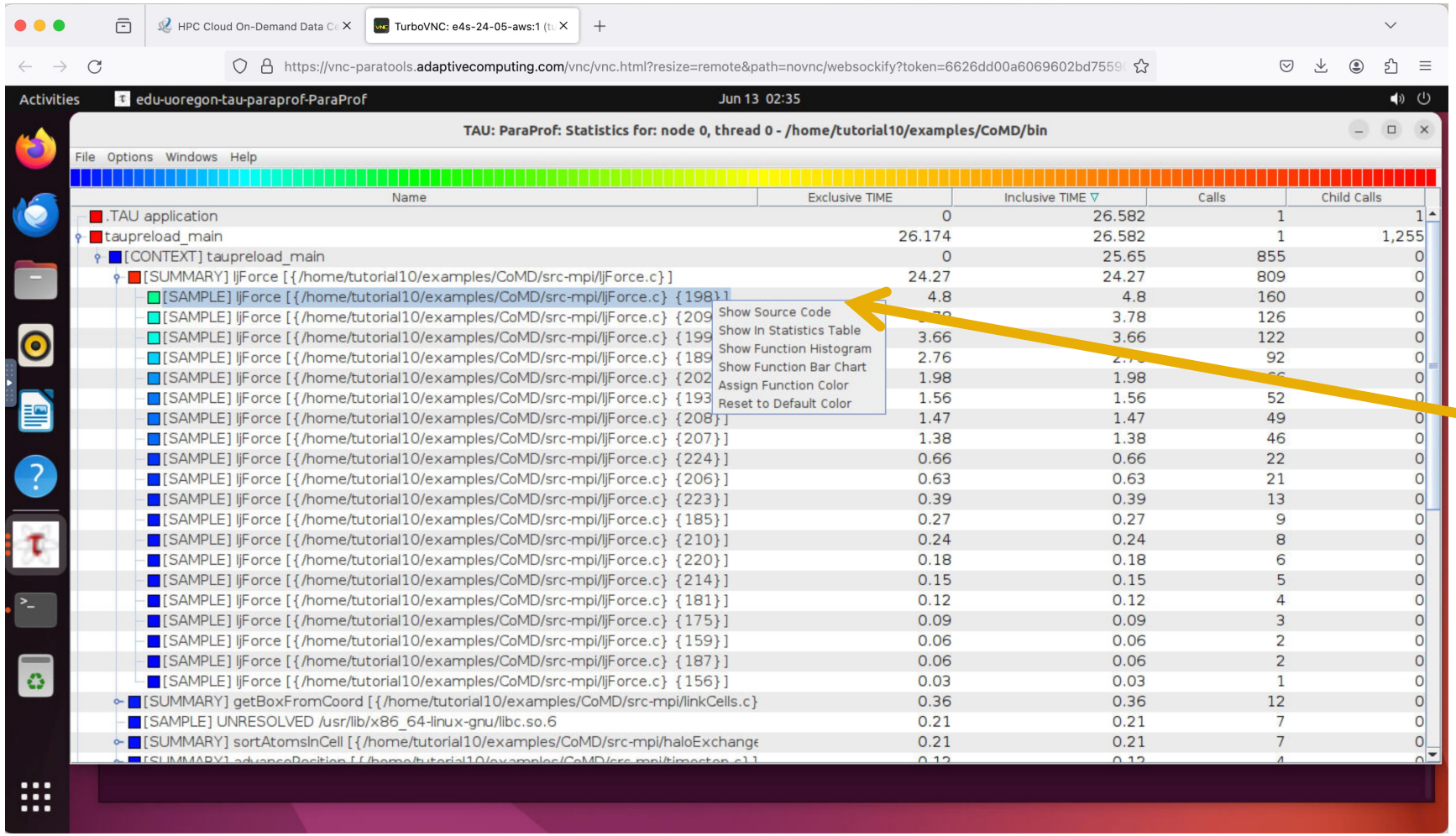

```
% paraprof &
```

CoMD: TAU's paraprof visualizer



Right click on Node 0, Thread 0 and choose Show Thread Statistics Table (third option)

TAU's ParaProf Profile Browser: Thread Statistics Table

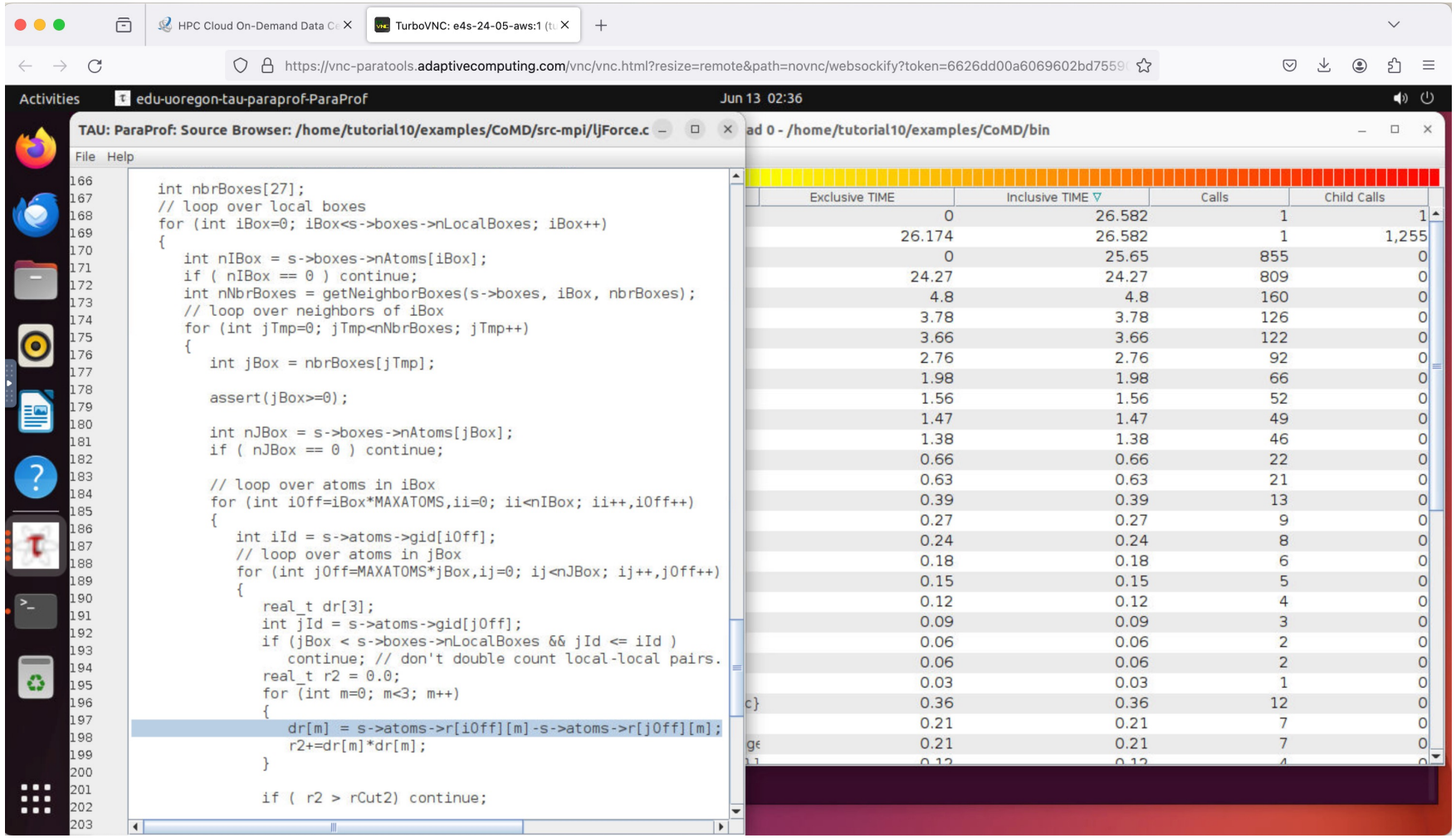


Click on columns to sort (e.g., Inclusive)

Expand nodes and right click on a sample and

Select "Show Source Code"

TAU's ParaProf Profile Browser: Source Code Browser



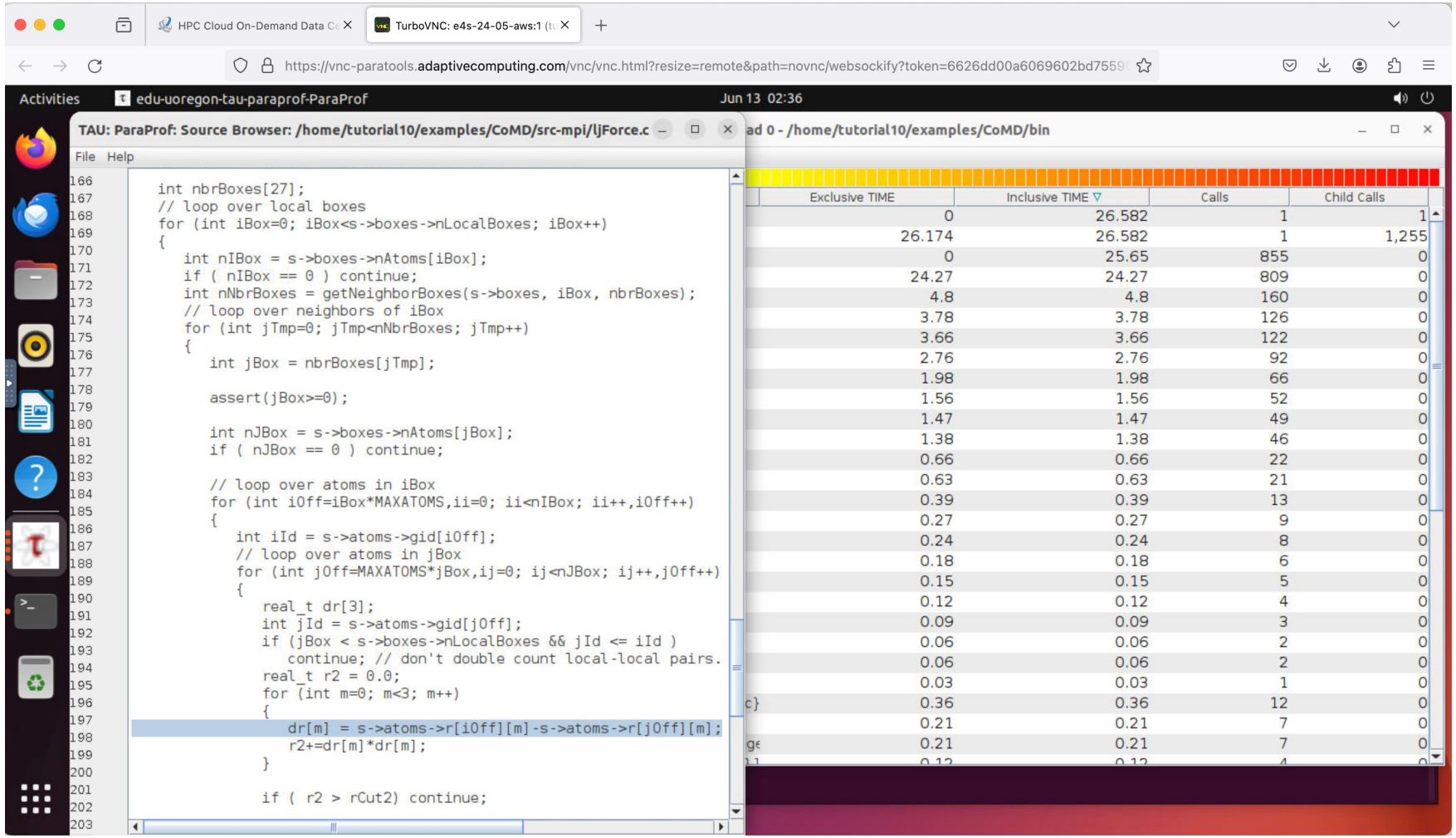

```
166   int nbrBoxes[27];
167   // loop over local boxes
168   for (int iBox=0; iBox<s->boxes->nLocalBoxes; iBox++)
169   {
170      int nIBox = s->boxes->nAtoms[iBox];
171      if ( nIBox == 0 ) continue;
172      int nNbrBoxes = getNeighborBoxes(s->boxes, iBox, nbrBoxes);
173      // loop over neighbors of iBox
174      for (int jTmp=0; jTmp<nNbrBoxes; jTmp++)
175      {
176         int jBox = nbrBoxes[jTmp];
177
178         assert(jBox>=0);
179
180         int nJBox = s->boxes->nAtoms[jBox];
181         if ( nJBox == 0 ) continue;
182
183         // loop over atoms in iBox
184         for (int iOff=iBox*MAXATOMS,ii=0; ii<nIBox; ii++,iOff++)
185         {
186            int iId = s->atoms->gid[iOff];
187            // loop over atoms in jBox
188            for (int jOff=MAXATOMS*jBox,ij=0; ij<nJBox; ij++,jOff++)
189            {
190               real_t dr[3];
191               int jId = s->atoms->gid[jOff];
192               if (jBox < s->boxes->nLocalBoxes && jId <= iId )
193                  continue; // don't double count local-local pairs.
194               real_t r2 = 0.0;
195               for (int m=0; m<3; m++)
196               {
197                  dr[m] = s->atoms->r[iOff][m]-s->atoms->r[jOff][m];
198                  r2+=dr[m]*dr[m];
199               }
200
201               if ( r2 > rCut2) continue;
202
203
```

The application spent 4.8 seconds in line 198 in ljForce.c in MPI rank 0. TAU collected 160 samples at this line of code.

It is within five levels of for loops!

There was no change to source code, build system, or the application binary!

TAU's ParaProf Profile Browser: Source Code Browser




```
166   int nbrBoxes[27];
167   // loop over local boxes
168   for (int iBox=0; iBox<s->boxes->nLocalBoxes; iBox++)
169   {
170      int nIBox = s->boxes->nAtoms[iBox];
171      if ( nIBox == 0 ) continue;
172      int nNbrBoxes = getNeighborBoxes(s->boxes, iBox, nbrBoxes);
173      // loop over neighbors of iBox
174      for (int jTmp=0; jTmp<nNbrBoxes; jTmp++)
175      {
176         int jBox = nbrBoxes[jTmp];
177
178         assert(jBox>=0);
179
180         int nJBox = s->boxes->nAtoms[jBox];
181         if ( nJBox == 0 ) continue;
182
183         // loop over atoms in iBox
184         for (int iOff=iBox*MAXATOMS,ii=0; ii<nIBox; ii++,iOff++)
185         {
186            int iId = s->atoms->gid[iOff];
187            // loop over atoms in jBox
188            for (int jOff=MAXATOMS*jBox,ij=0; ij<nJBox; ij++,jOff++)
189            {
190               real_t dr[3];
191               int jId = s->atoms->gid[jOff];
192               if (jBox < s->boxes->nLocalBoxes && jId <= iId )
193                  continue; // don't double count local-local pairs.
194               real_t r2 = 0.0;
195               for (int m=0; m<3; m++)
196               {
197                  dr[m] = s->atoms->r[iOff][m]-s->atoms->r[jOff][m];
198                  r2+=dr[m]*dr[m];
199               }
200
201               if ( r2 > rCut2) continue;
202
203
```

The application spent 4.8 seconds in line 198 in ljForce.c in MPI rank 0. TAU collected 160 samples at this line of code.

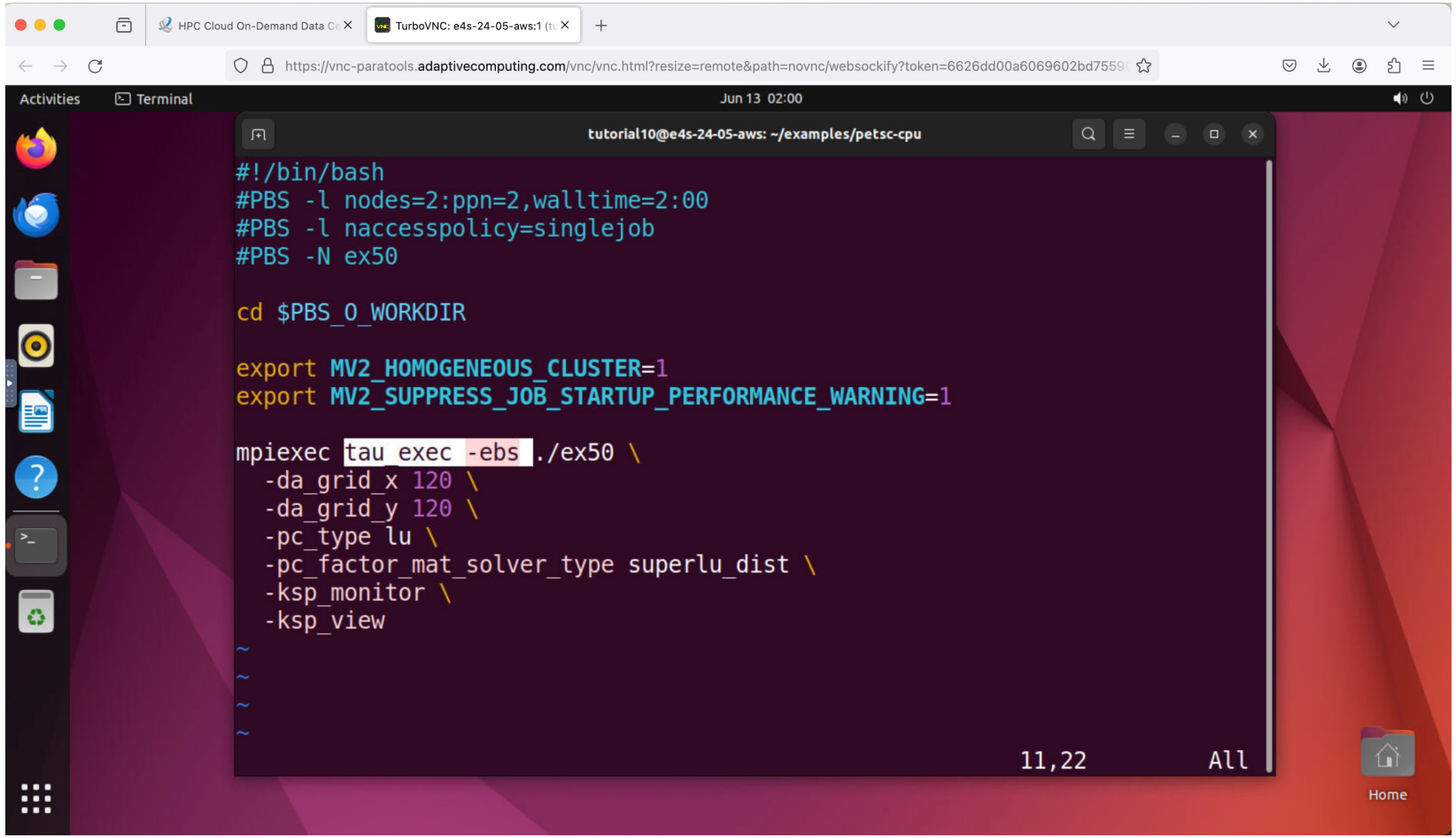
It is within five levels of for loops!

There was no change to source code, build system, or the application binary!

TAU Exercise #4:

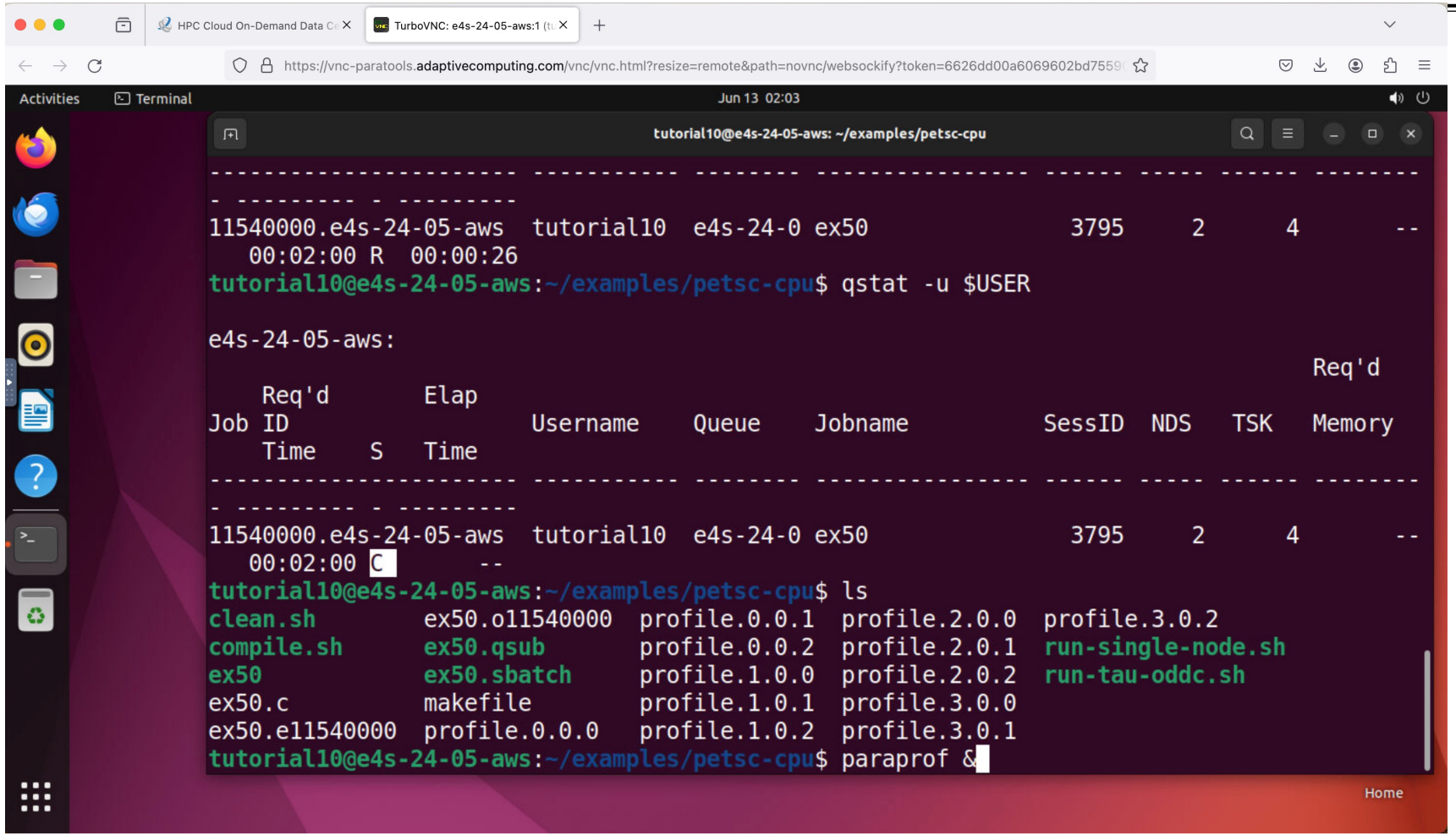
Instrumenting PETSc application using TAU's Perfstubs interface

Launching the binary using tau_exec –ebs




```
cd !~/examples/petsc-cpu
vi ex50.qsub

Add tau_exec –ebs
before ./ex50 in the
launch command. Save the
file.
```

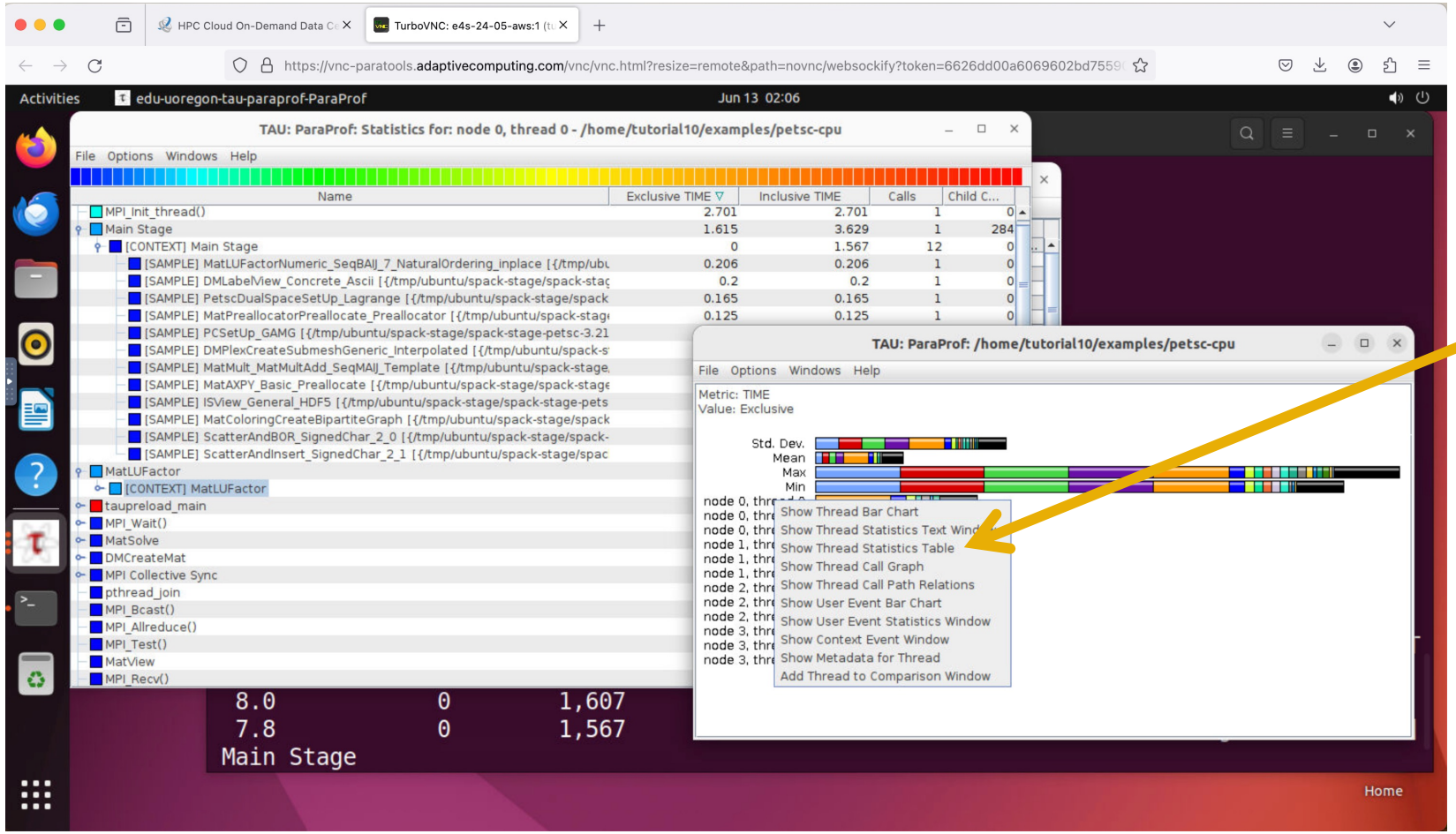
TAU's ParaProf Profile Browser: Source Code Browser



qsub ex50.qsub
qstat –u $USER

After it completes
ls
paraprof &

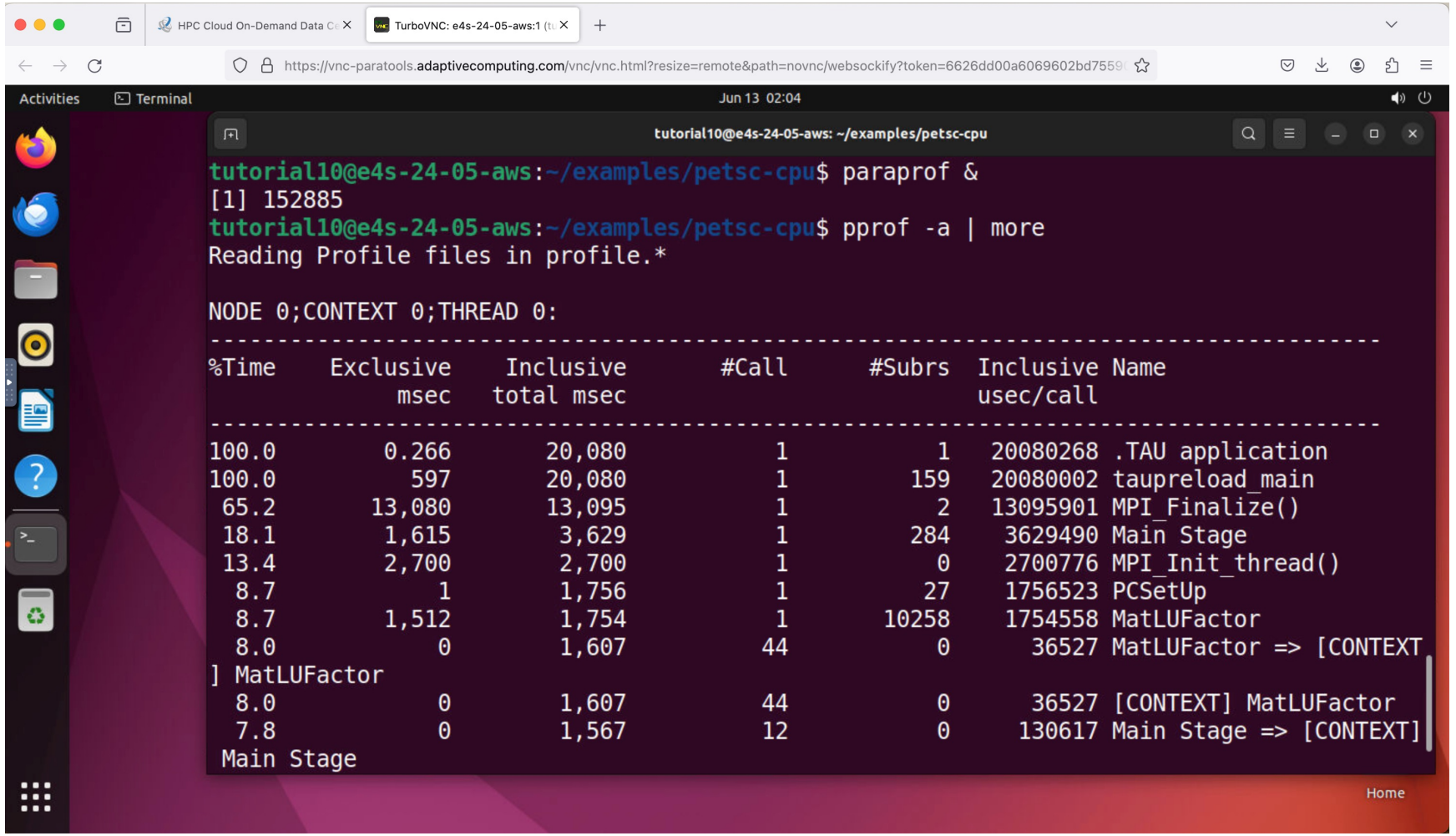
TAU's paraprof browser with PETSc performance profile



paraprof

Choose
Show thread statistics table
by right clicking on
node 0, thread 0.

Using pprof: TAU's text based profile browser



pprof –a | more

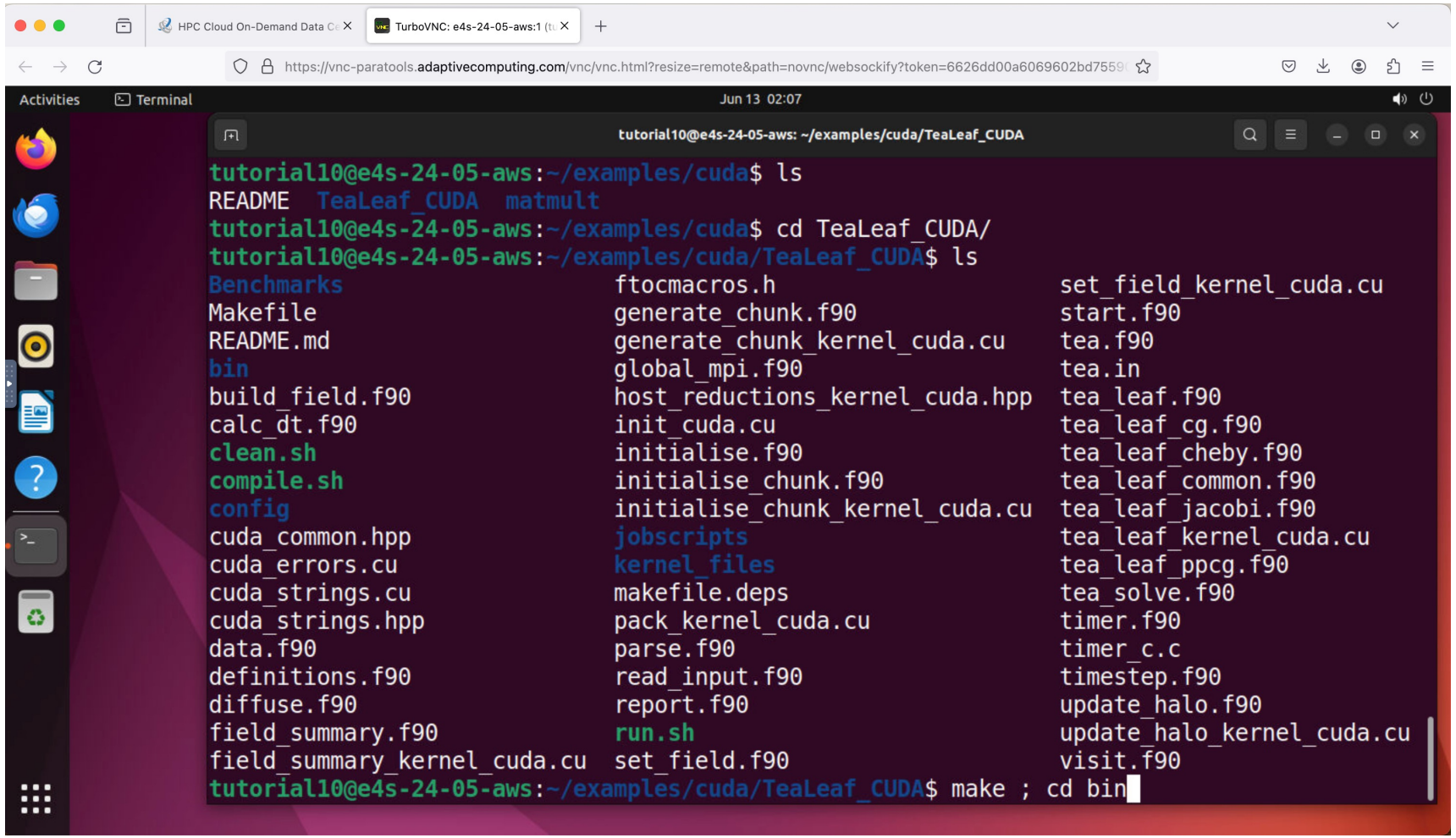
Here we see PETSc timers translated into TAU timers using the Perfstubs library.

No modification to the source, build system, or the binary!

TAU Exercise #5:

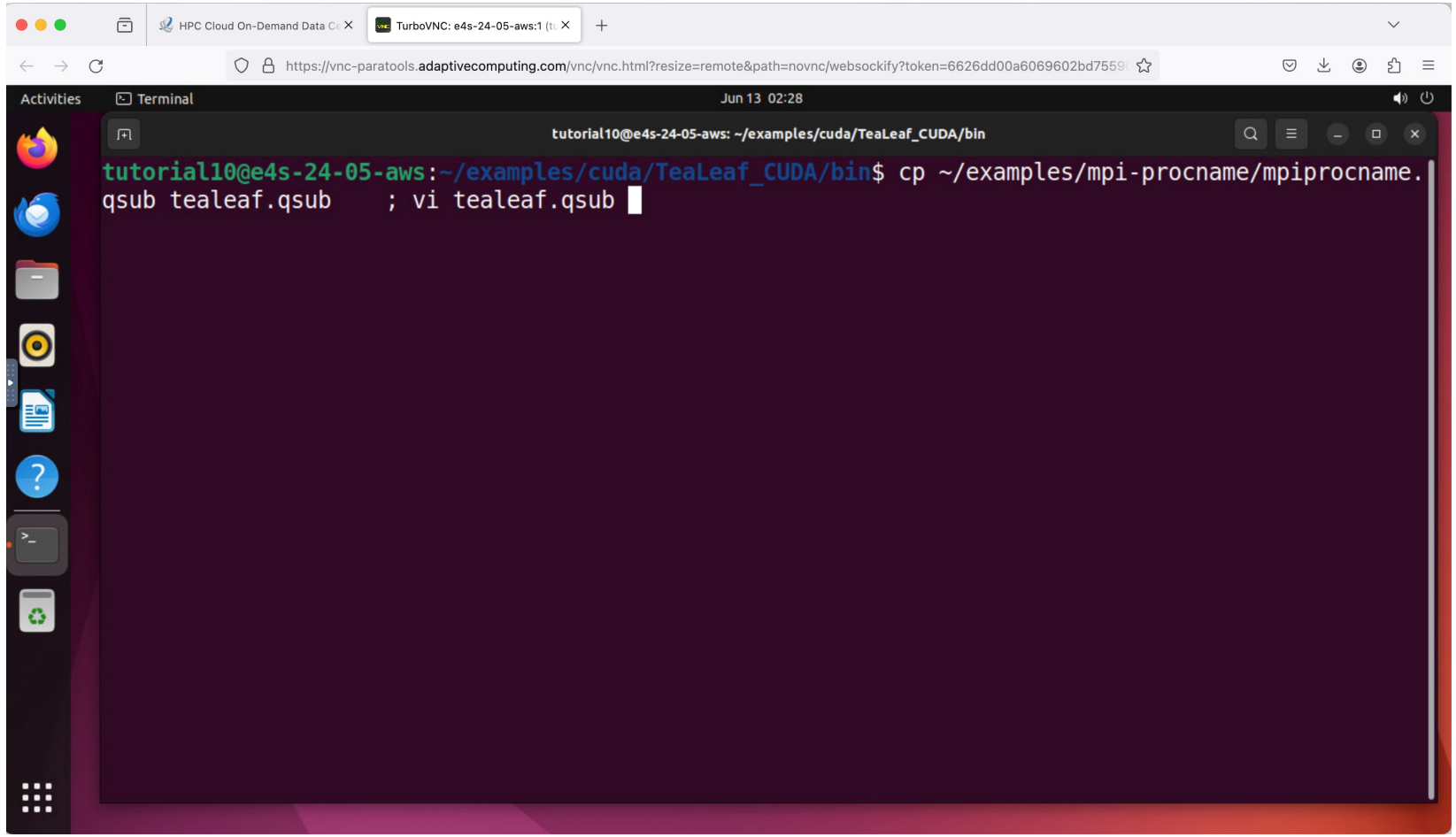
CUDA instrumentation using CUPTI (CUDA Profiling Tools Interface)

Compiling TeaLeaf_CUDA application



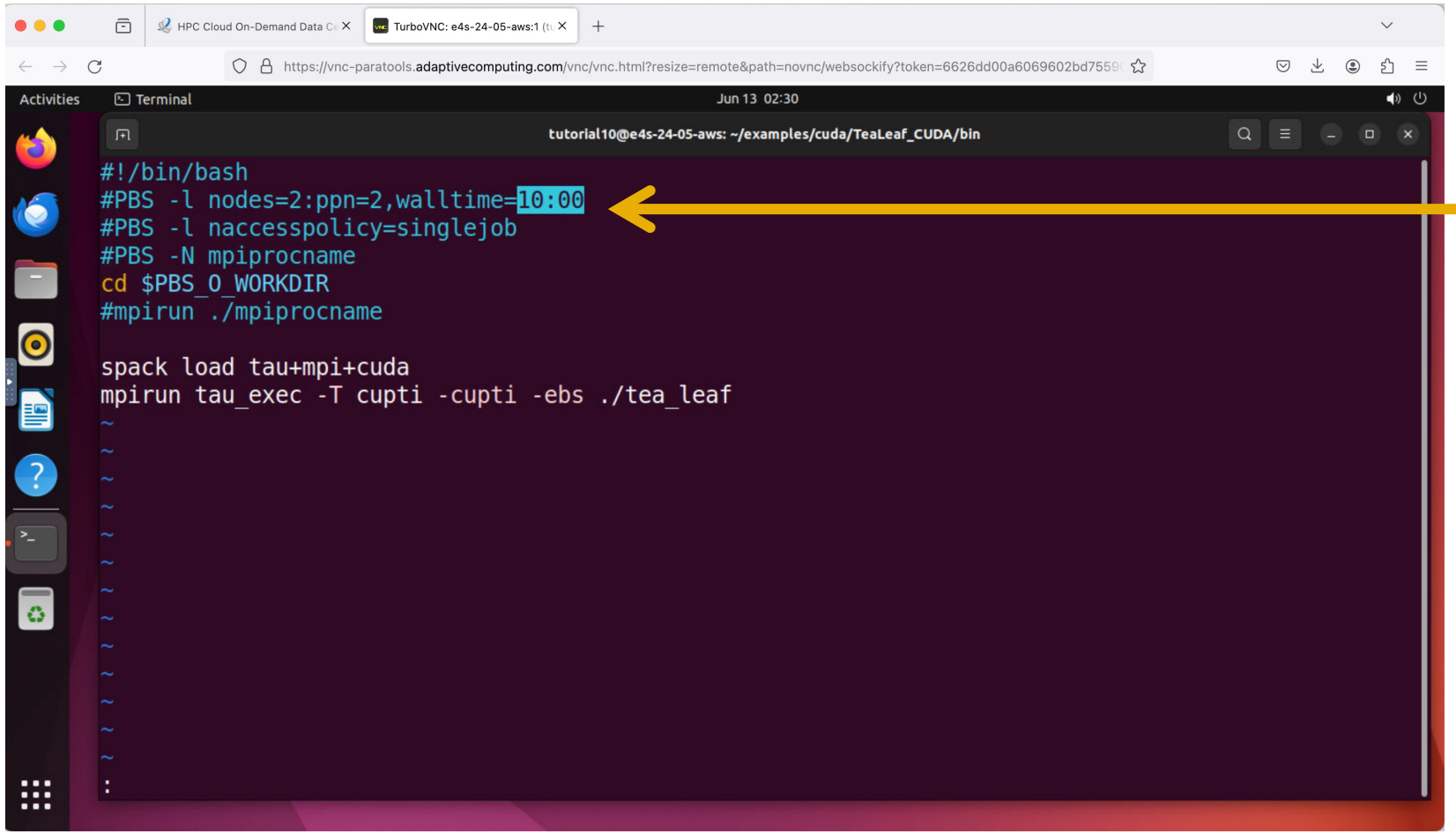

```
cd ~/examples/cuda
cd TeaLeaf_CUDA
ls
make
cd bin
```

Copying and editing a sample job submission script




```
cp ~/examples/mpi-procname/mpiprocname.qsub tealeaf.qsub

vi tealeaf.qsub
```

Editing the sample job submission script



Change the time from 1 minute to 10 minutes!

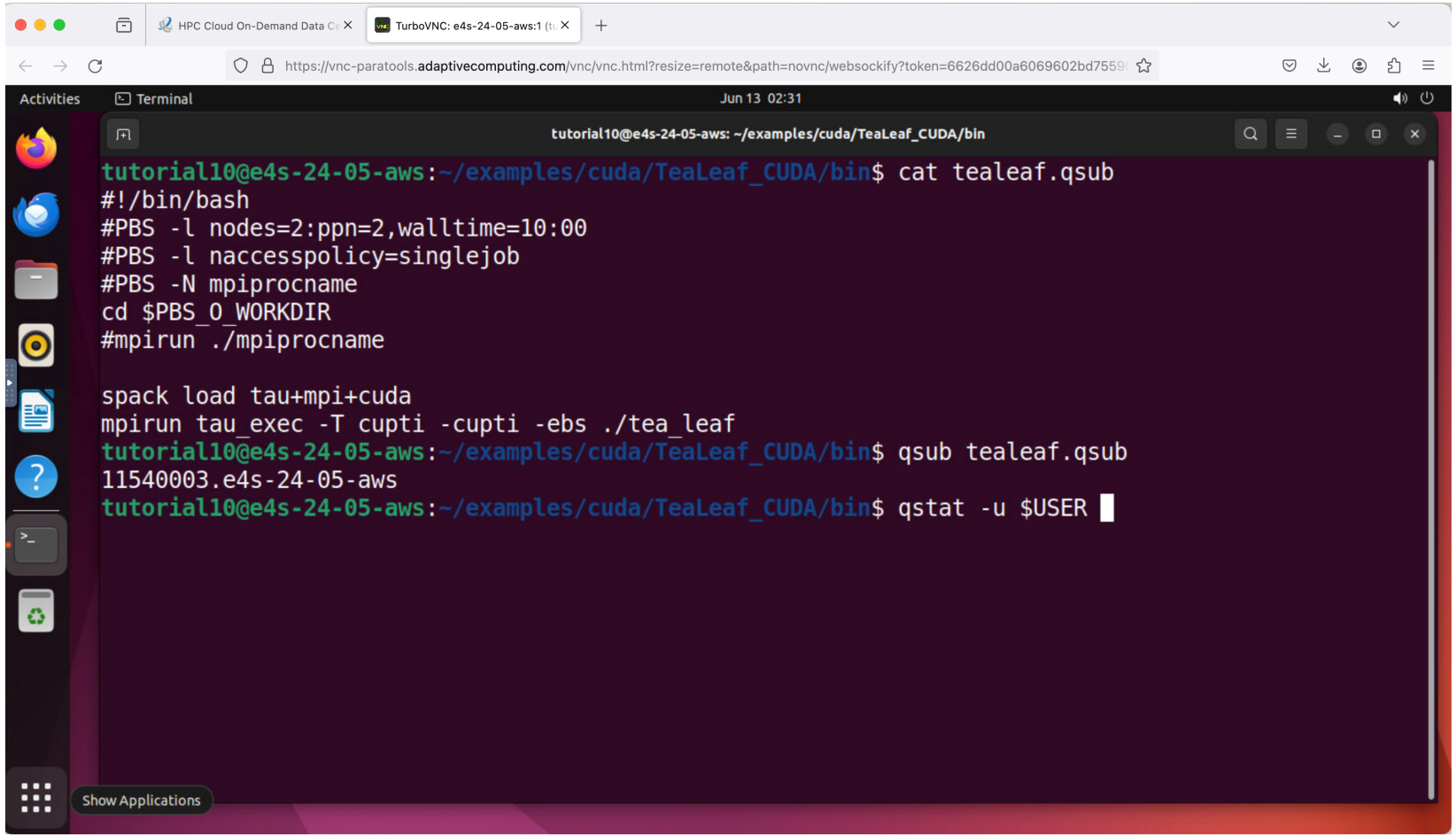
Comment out the mpiprocname launch

Add
spack load tau+mpi+cuda

Add
mpirun tau_exec –T cupti –cupti –ebs ./tea_leaf

Save the tealeaf.qsub file

Submit the CUDA job to run on four MPI ranks



qsub tealeaf.qsub

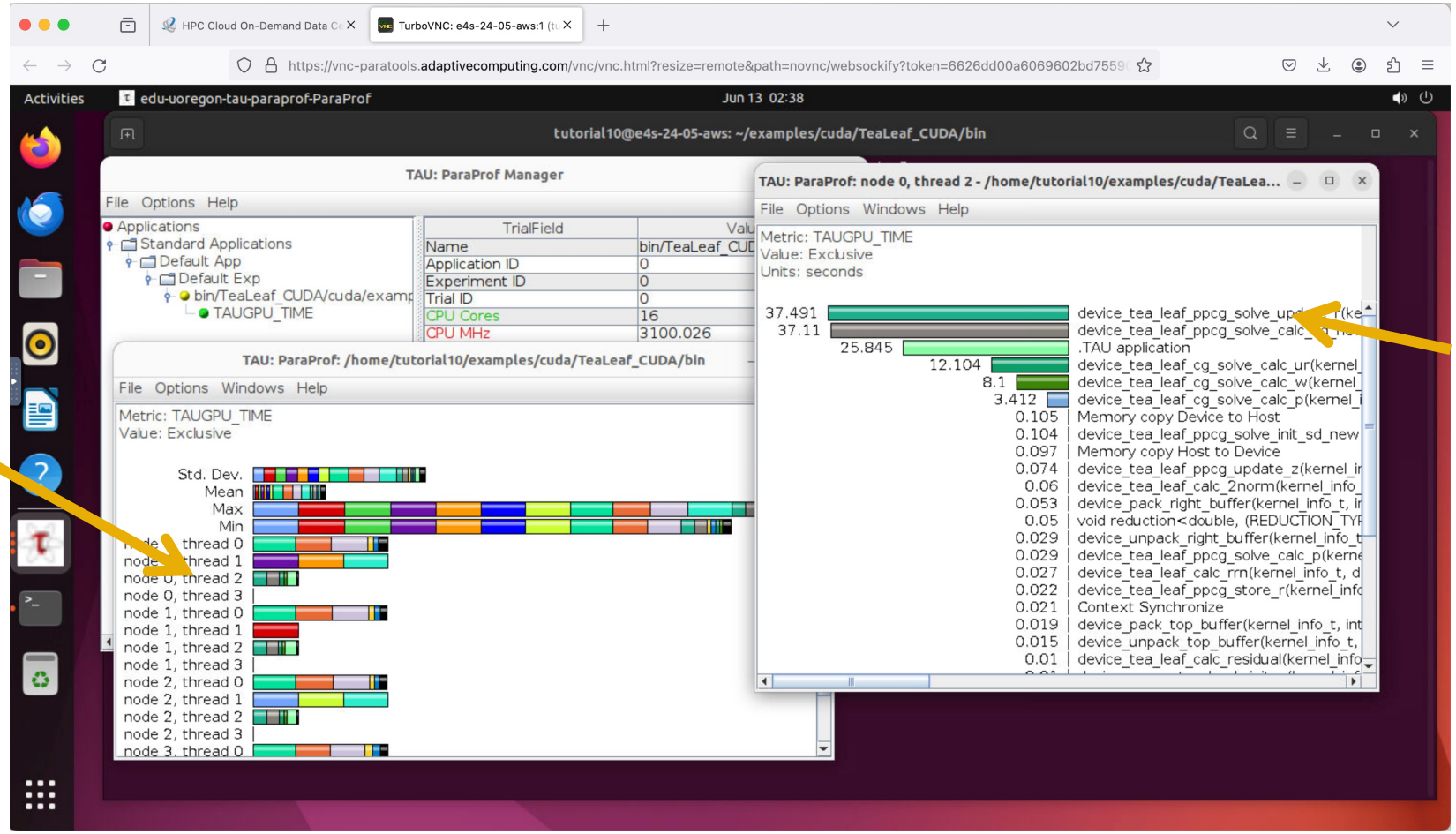
qstat –u $USER

After it runs

paraprof &

TAU's paraprof shows the time spent in individual CUDA kernels

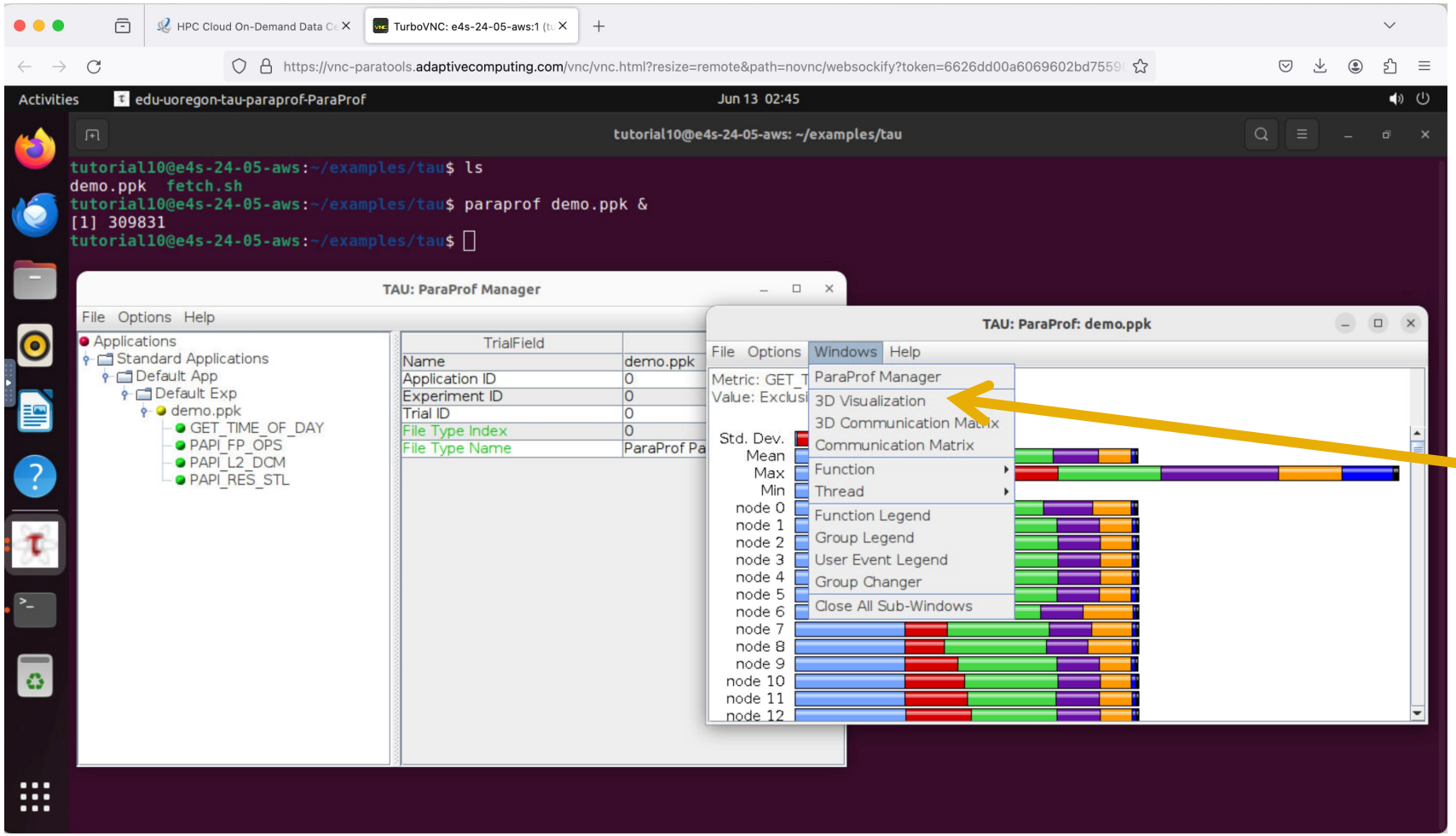
Left click node 0, thread 2



CUDA kernels

TAU Exercise #6:
paraprof 3D display

TAU paraprof

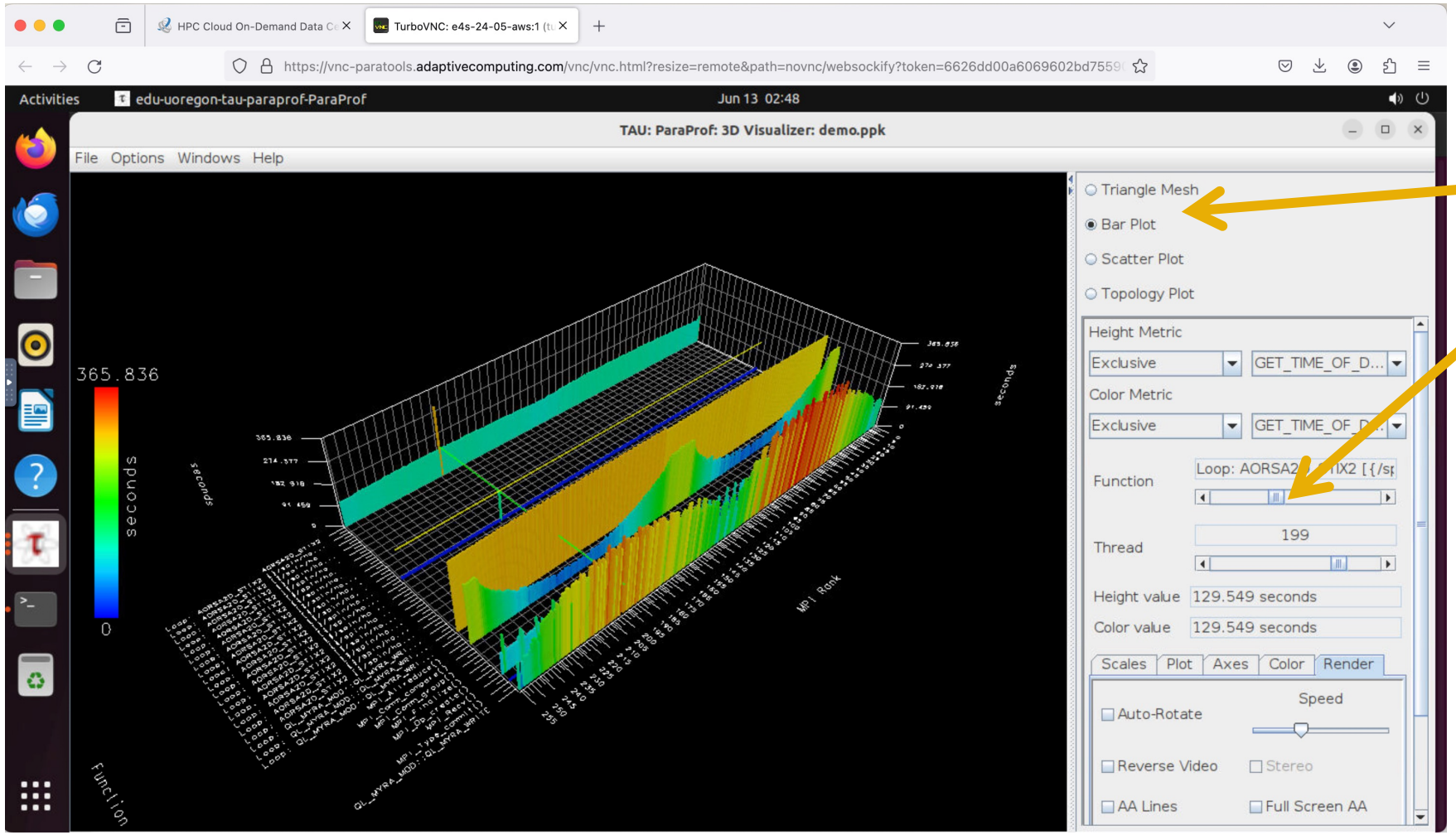


cd ~/examples/tau

paraprof demo.ppk &

Choose 3D Visualization

TAU paraprof 3D visualization



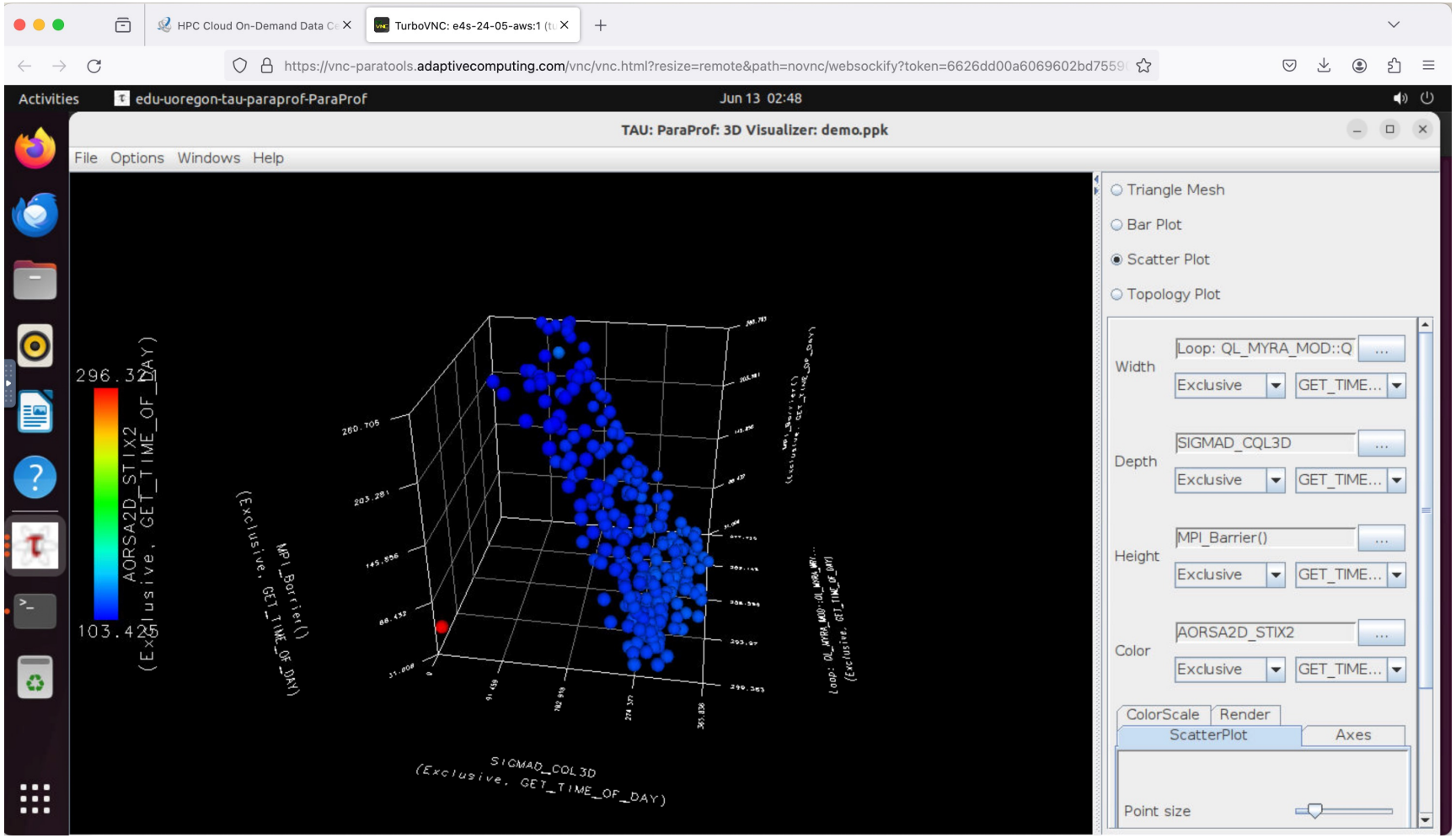
Choose Bar Plot and move

Function and Thread Sliders

First mouse button to rotate
Second mouse button to translate (left to right)
Scroll wheel (or +/- keys) to zoom in.

Try Scatter plot next

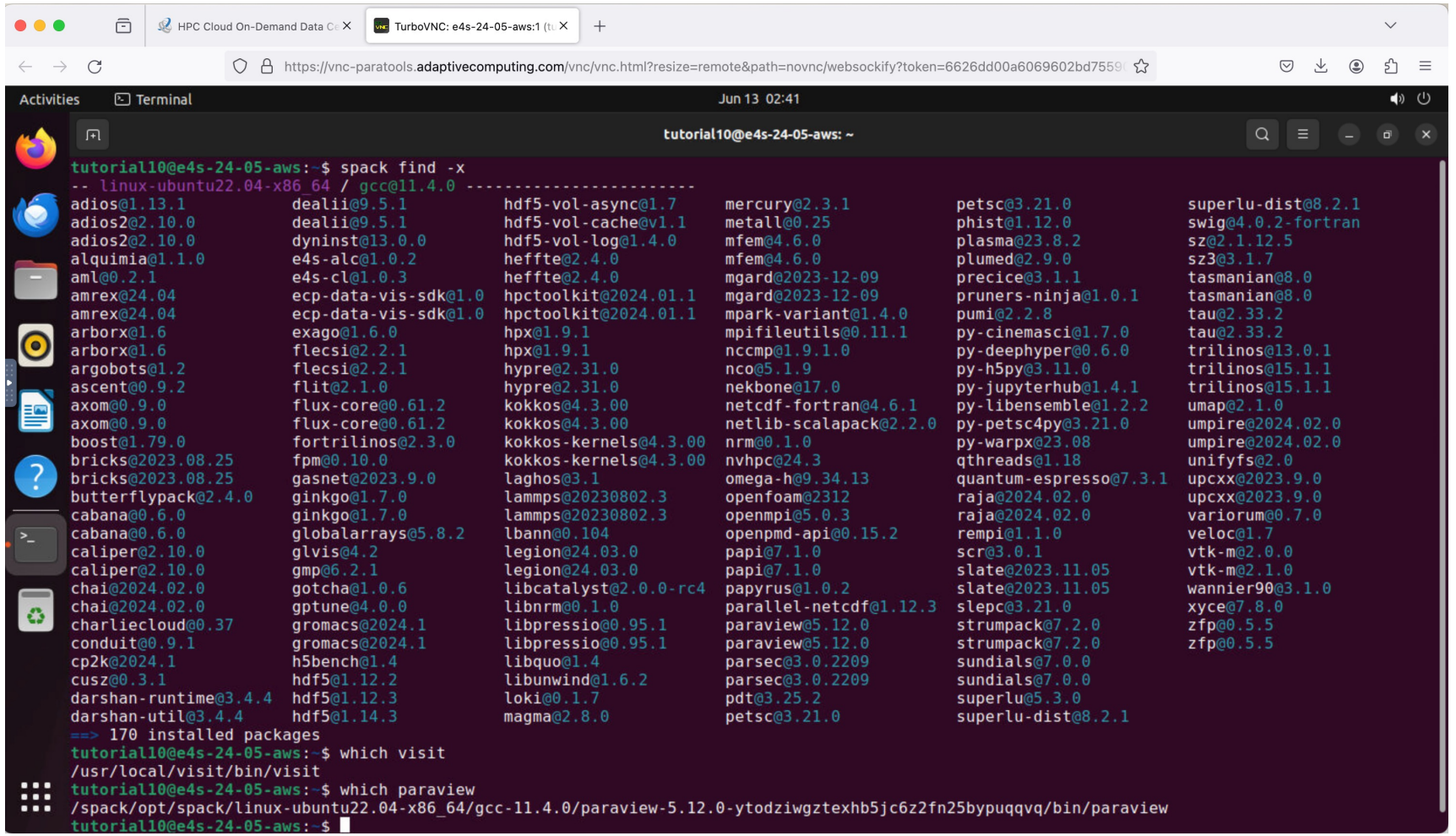
TAU paraprof: 3D Scatter Plot



Exercise #7

E4S: Extreme-scale Scientific Software Stack

Spack package manager [https://spack.io]

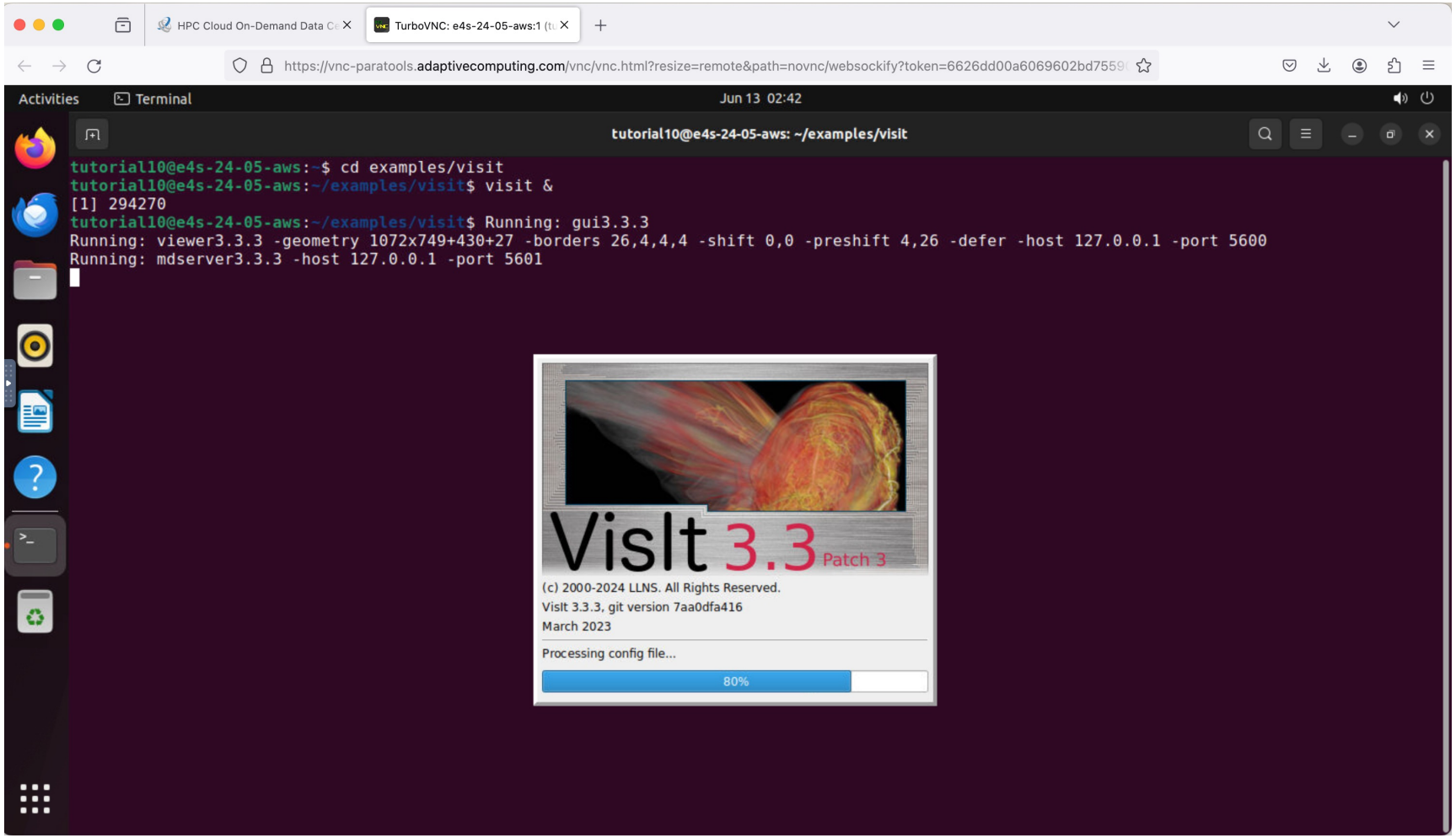


spack find –x
spack find

spack find +cuda

nvidia-smi

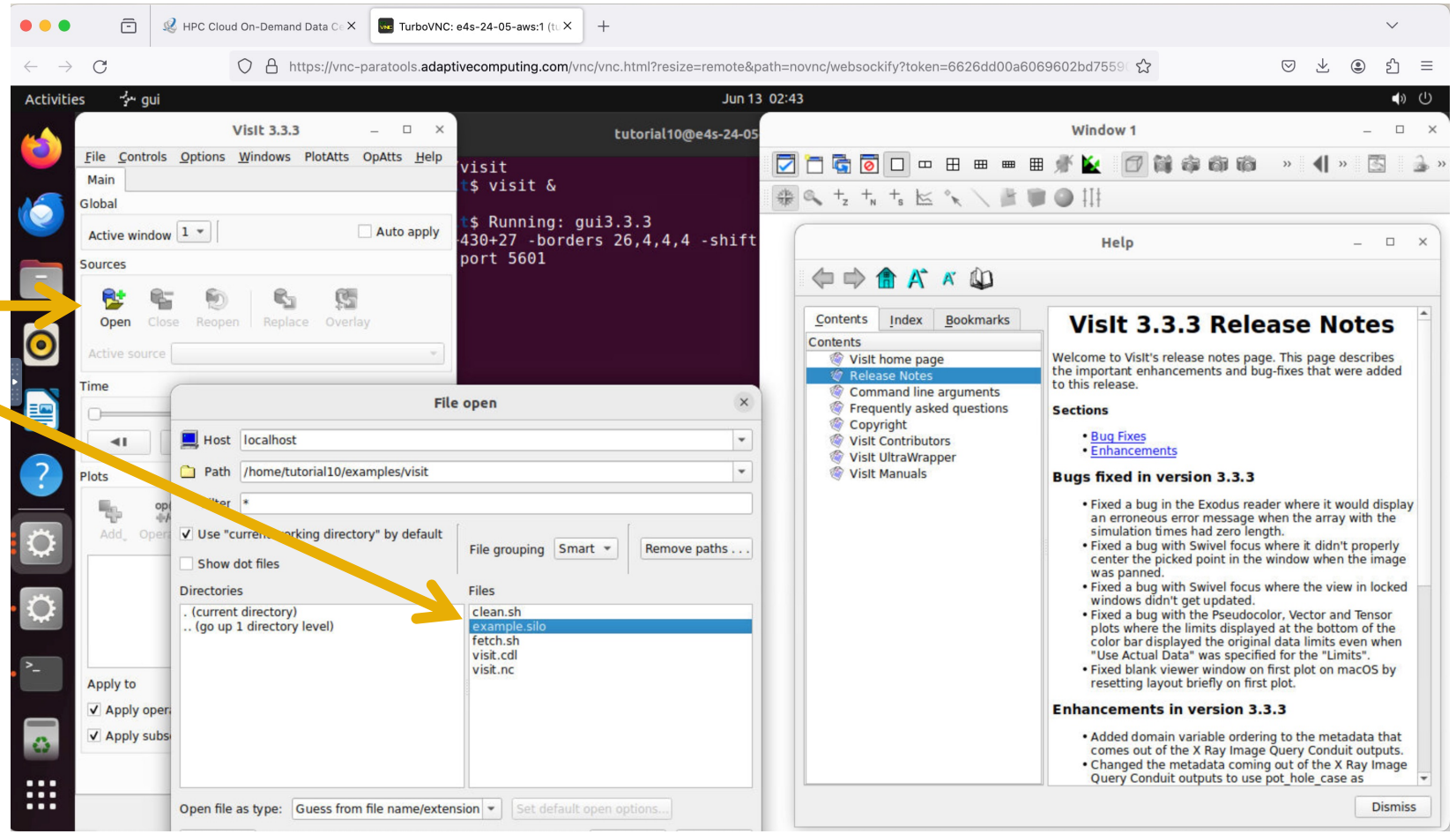
VisIt visualizer



cd ~/examples/visit
visit &

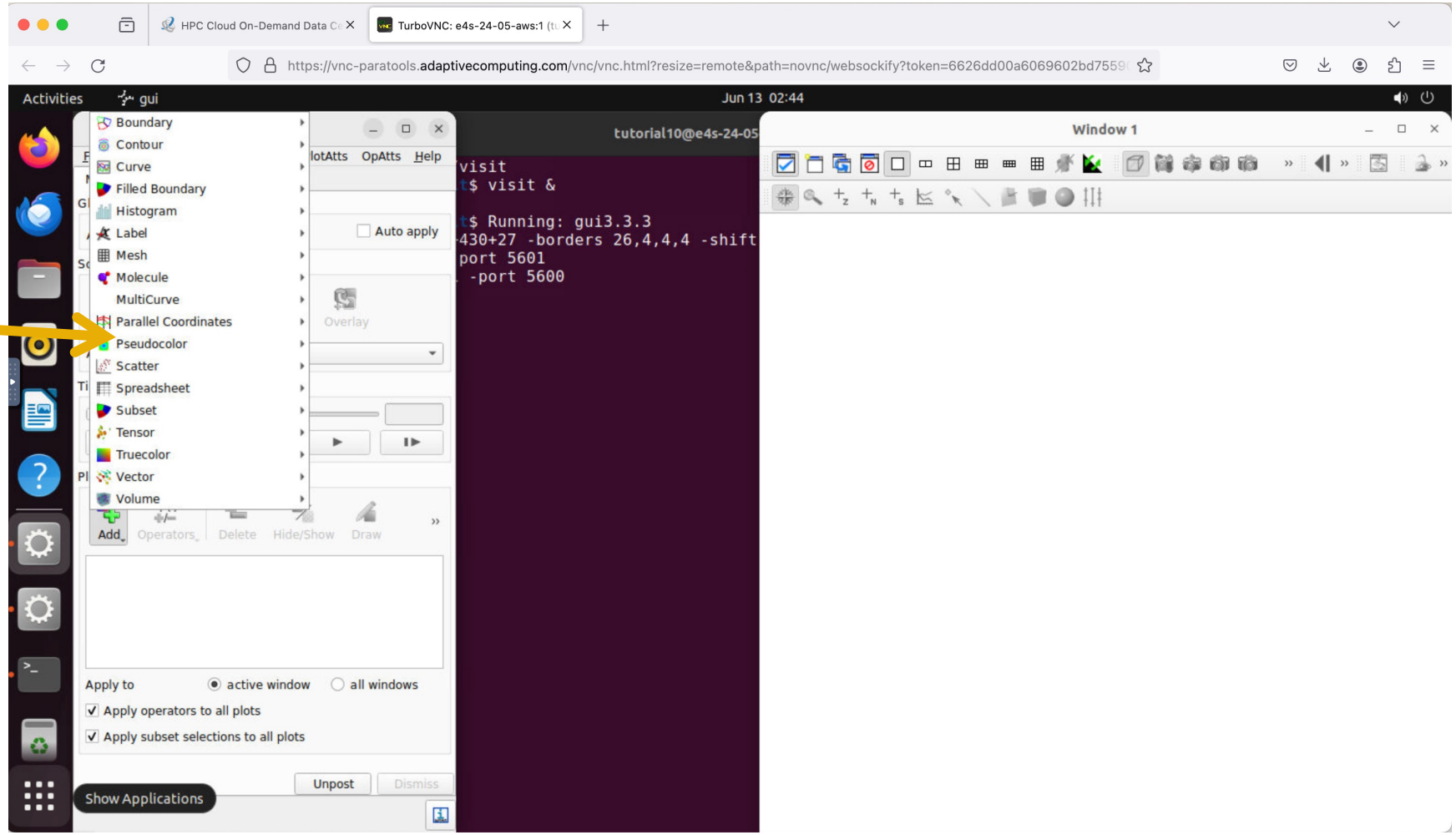
VisIt visualizer

Open example.silo



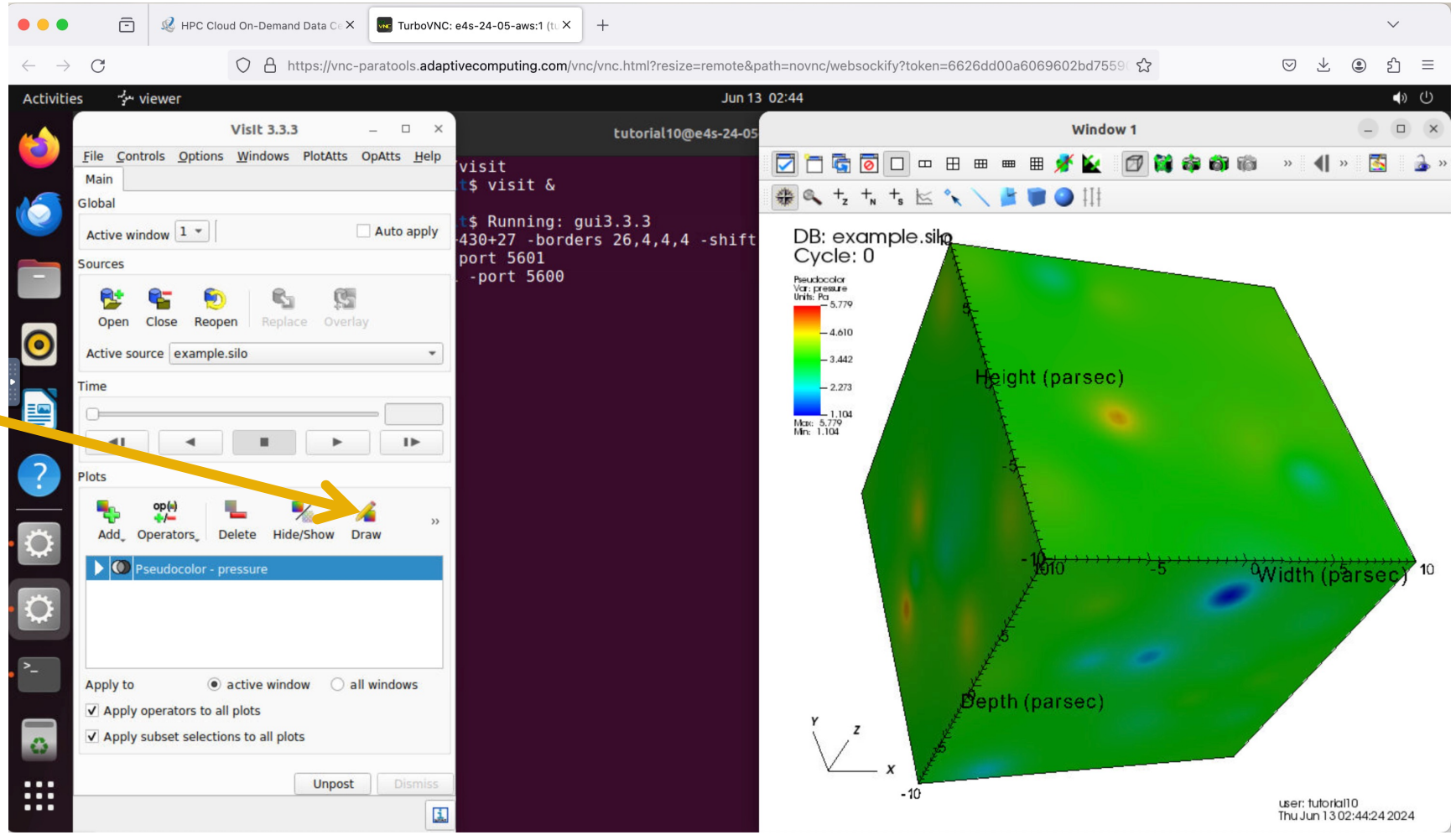
VisIt visualizer

Add Pseudocolor –>
Pressure



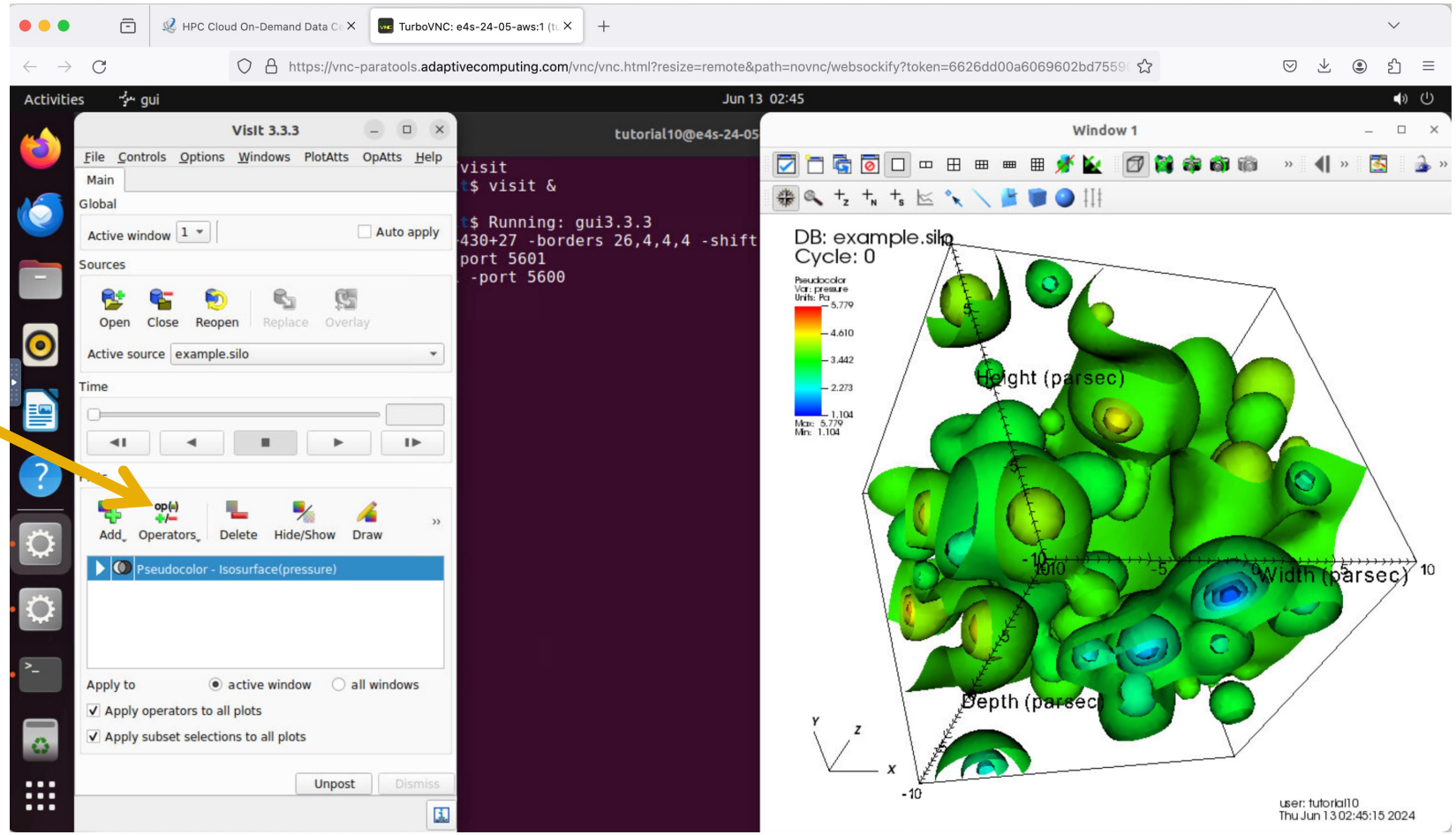
VisIt visualizer

Add Pseudocolor ->
Pressure
Click Draw
Rotate image



VisIt visualizer

Add Operators ->
Isosurface
Click Draw
Rotate image



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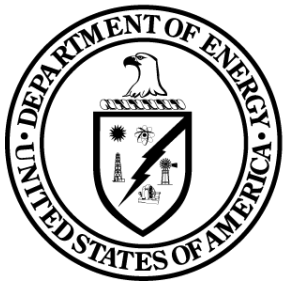

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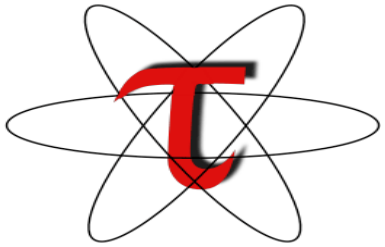
- https://science.osti.gov/ascr
- https://pesoproject.org
- https://ascr-step.org

Download TAU from U. Oregon



http://tau.uoregon.edu

http://www.hpclinux.com [LiveDVD, OVA]

https://e4s.io [Containers for Extreme-Scale Scientific Software Stack]

http://adaptivecomputing.com [ODDC with ParaTools Pro for E4S on cloud systems]

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