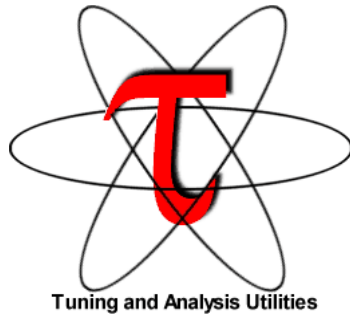


TAU Performance System® Hands-On



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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,thread -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 xzf /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
hpckurs08@cm2login4:~> ls /lrz/sys/courses/vihps/2024/material/tau/
workshop.tgz
hpckurs08@cm2login4:~> tar xzf /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
```

```
hpckurs08@cm2login4:~/workshop/NPB3.1/bin
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> cat reference.sbatch
#!/bin/bash
#SBATCH -o bt.%j.out
#SBATCH -e bt.%j.err
#SBATCH -J bt-A
#SBATCH --clusters=cm2_tiny
#SBATCH --partition=cm2_tiny
#SBATCH --reservation=hhps1s24
#SBATCH --nodes=2
#SBATCH --ntasks=16
#SBATCH --ntasks-per-node=8
#SBATCH --get-user-env
#SBATCH --time=00:05:00

# Benchmark configuration (disable load balancing with threads)
mpiexec -n $SLURM_NTASKS bt.A.16

hpckurs08@cm2login4:~/workshop/NPB3.1/bin> sbatch reference.sbatch
Submitted batch job 660933 on cluster cm2_tiny
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> █
```

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

```
hpckurs08@cm2login4:~/workshop/NPB3.1/bin
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

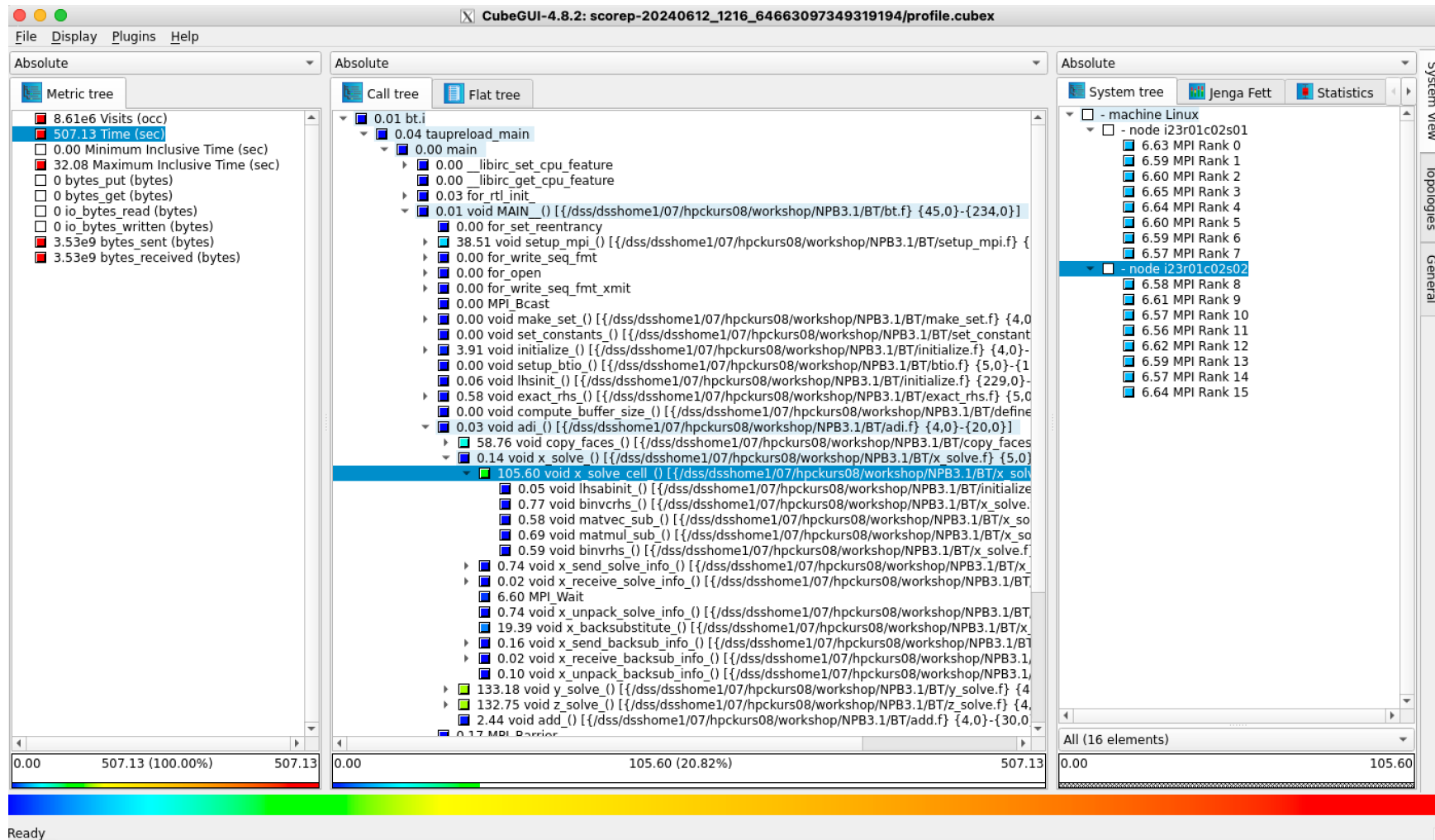
```
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> sbatch tau.sbatch
Submitted batch job 660935 on cluster cm2_tiny
hpckurs08@cm2login4:~/workshop/NPB3.1/bin> ls
bt.660933.err bt.660935.err bt.A.16 reference.sbatch rt.sh          select.tau  tau.sbatch.e660934
bt.660933.out bt.660935.out bt.i      r.sh              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
```

The screenshot displays the CubeGUI-4.8.2 interface for analyzing profile data. The main window is titled "CubeGUI-4.8.2: scorep.data/profile.cubex". It features four panels:

- Metric tree:** Shows a list of metrics with their values. The top metric is "8.61e6 Visits (occ)" and "646.70 Time (sec)". Other metrics include "0.00 Minimum Inclusive Time (sec)", "40.56 Maximum Inclusive Time (sec)", "0 bytes_put (bytes)", "0 bytes_get (bytes)", "0 io_bytes_read (bytes)", "0 io_bytes_written (bytes)", "3.53e9 bytes_sent (bytes)", and "3.53e9 bytes_received (bytes)".
- Call tree:** Shows a hierarchical view of function calls. The root is "0.01 bt.i", which contains "0.04 taupreload_main". Under "taupreload_main" is "0.00 main", which includes "0.00 __libc_set_cpu_feature", "0.00 __libc_get_cpu_feature", "0.03 for_rtl_init", and "0.01 void MAIN_()". The "MAIN_()" function includes "0.00 for_set_reentrancy", "179.10 void setup_mpi_()", "0.00 for_write_seq_fmt", "0.00 for_open", "0.00 for_write_seq_fmt_xmit", "0.01 MPI_Bcast", "0.00 void make_set_()", "0.00 void set_constants_()", "3.94 void initialize_()", "0.00 void setup_btio_()", "0.06 void lhsinit_()", "0.58 void exact_rhs_()", "0.00 void compute_buffer_size_()", "0.03 void adi_()", "57.67 void copy_faces_()", "0.14 void x_solve_()", "108.36 void x_solve_cell_()", "0.73 void x_send_solve_info_()", "0.02 void x_receive_solve_info_()", "6.43 MPI_Wait", "0.73 void x_unpack_solve_info_()", "19.39 void x_backsubstitute_()", and "0.15 void x_send_backsub_info_()".
- Flat tree:** Shows a flat view of the function calls, listing the same functions as the Call tree with their respective execution times.
- System tree:** Shows the system configuration, including the machine name "machine.Linux" and the MPI ranks used for the simulation, ranging from Rank 0 to Rank 15. The ranks are grouped by node: "- node i23r01c02s03" (Ranks 0-7) and "- node i23r01c02s04" (Ranks 8-15).

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 &
```



```
hpckurs08@cm2login4:~/workshop/NPB3.3-MZ-MPI/bin
hpckurs08@cm2login4:~/workshop/NPB3.3-MZ-MPI/bin> ls
bt.660936.i23r03c01s11.out  bt-mz.660937.out  reference.sbatch  traces          traces.otf2
bt-mz.660937.err          bt-mz_C.28       tau.sbatch       traces.def
hpckurs08@cm2login4:~/workshop/NPB3.3-MZ-MPI/bin> which vampir
/lrz/sys/courses/vihps/2024/tools/vampir/vampir-10.4.2/bin/vampir
hpckurs08@cm2login4:~/workshop/NPB3.3-MZ-MPI/bin> vampir traces.otf2 &
[1] 22460
hpckurs08@cm2login4:~/workshop/NPB3.3-MZ-MPI/bin> [Warning] QStandardPaths: XDG_RUNTIME_DIR not set, defaulting to '/gpfs/scratch/a2c06/hpckurs08/hpckurs08/runtime-hpckurs08'
```

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

The screenshot displays the Vampir application interface. On the left, a vertical timeline shows the execution of 14 ranks, each with two CPU threads (00 and 02). The trace is visualized as a series of colored bars representing different application components. A central dialog box is open, showing a list of application functions under the 'TAU_OPENMP' group. A context menu is visible over the list, with 'Set Random Colors' selected. The dialog box also includes a 'Color' column with color swatches and buttons for 'OK', 'Cancel', and 'Apply'. On the right side of the interface, a list of application components is visible, including various MPI and OpenMP functions with their respective ranks and thread IDs.

Name	Color
MPI	Red
Monitor	Blue
TAU_DEFAULT	Green
TAU_OPENMP	Orange

Search (Ctrl+F)

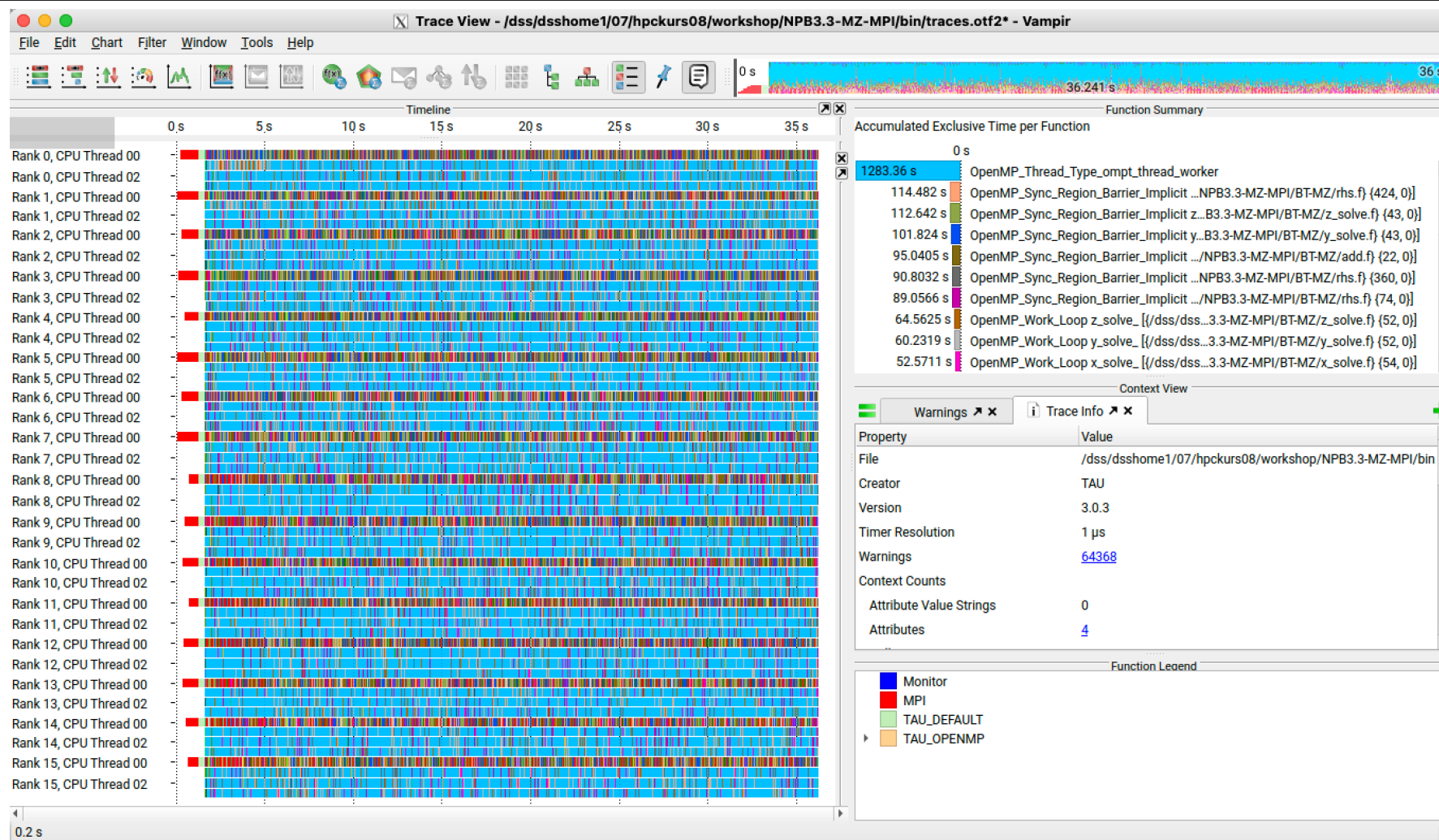
- OpenMP_Parallel_Region add_ [/{dss/dssh...rkshop/NPB3.3-MZ-MPI/BT-MZ/add.f} (22, 0)]
- OpenMP_Parallel_Region compute_rhs_ [/{dss/...orkshop/NPB3.3-MZ-MPI/BT-MZ/rhs.f} (28, 0)]
- OpenMP_Parallel_Region copy_x_face_ [/{dss/...p/NPB3.3-MZ-MPI/BT-MZ/exch_qbc.f} (247, 0)]
- OpenMP_Parallel_Region copy_x_face_ [/{dss/...p/NPB3.3-MZ-MPI/BT-MZ/exch_qbc.f} (258, 0)]
- OpenMP_Parallel_Region copy_y_face_ [/{dss/...p/NPB3.3-MZ-MPI/BT-MZ/exch_qbc.f} (207, 0)]
- OpenMP_Parallel_Region copy_y_face_ [/{dss/...p/NPB3.3-MZ-MPI/BT-MZ/exch_qbc.f} (218, 0)]
- OpenMP_Parallel_Region error_norm_ [/{dss/ds...} (27, 0)]
- OpenMP_Parallel_Region exact_rhs_ [/{dss/ds...p} (21, 0)]
- OpenMP_Parallel_Region initialize_ [/{dss/dss...o} (28, 0)]
- OpenMP_Parallel_Region rhs_norm_ [/{dss/dss...} (86, 0)]
- OpenMP_Parallel_Region x_solve_ [/{dss/dssh...h} (46, 0)]
- OpenMP_Parallel_Region y_solve_ [/{dss/dssh...h} (43, 0)]
- OpenMP_Parallel_Region z_solve_ [/{dss/dssh...h} (43, 0)]
- OpenMP_Sync_Region_Barrier_Implicit_L_comp... (74, 0)]
- OpenMP_Sync_Region_Barrier_Implicit_L_comp... (360, 0)]
- OpenMP_Sync_Region_Barrier_Implicit_L_comp... (424, 0)]
- OpenMP_Sync_Region_Barrier_Implicit_L_exact... (47, 0)]
- OpenMP_Sync_Region_Barrier_Implicit_L_exact... (218, 0)]

Legend:

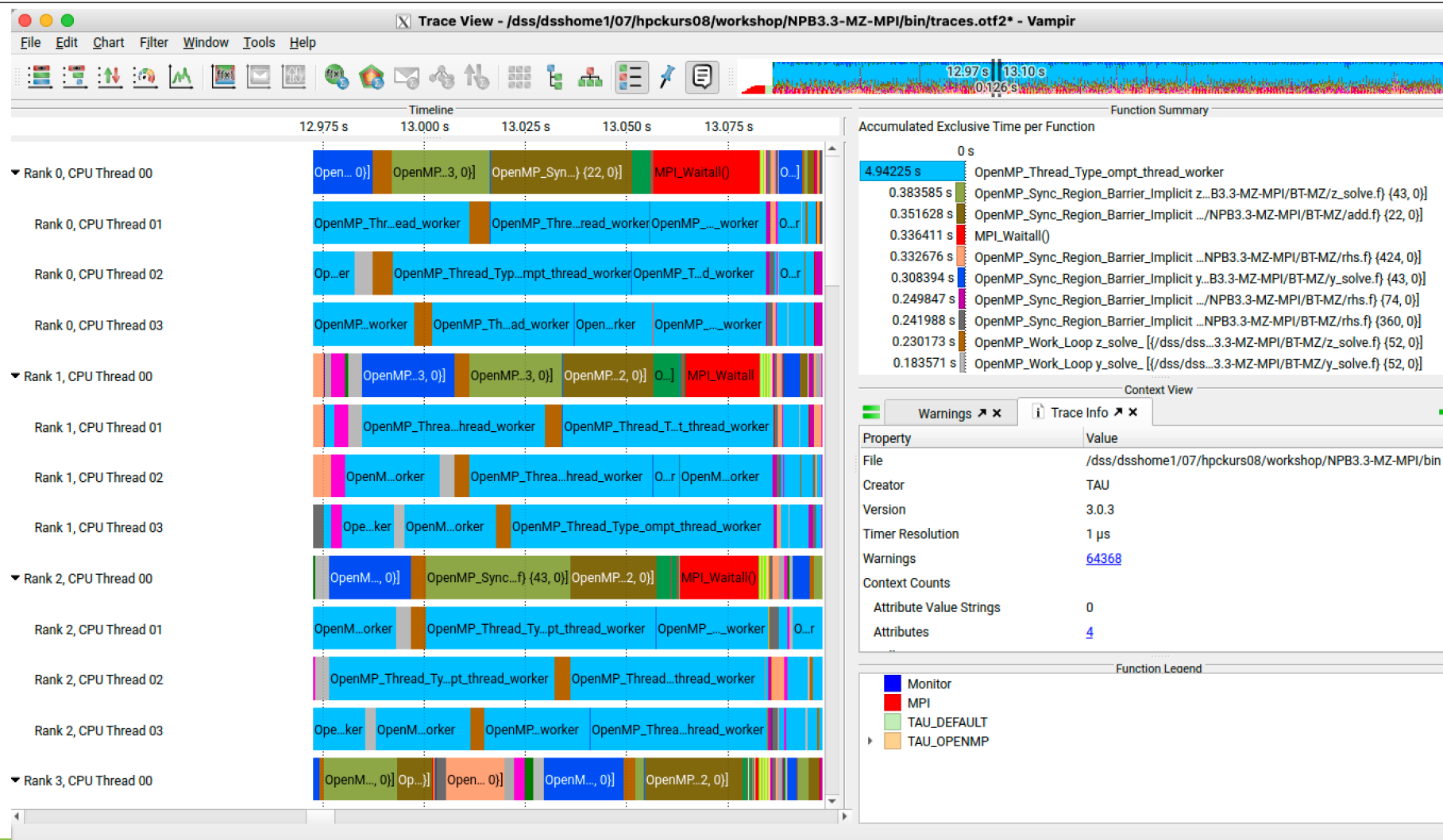
- Monitor (Blue)
- MPI (Red)
- TAU_DEFAULT (Green)
- TAU_OPENMP (Orange)

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

Cluster Manager

State	Name	Provider	Owner	Bursting	Nodes	Uptime
Down 1:53 6:24	e4s-24-05-oci	ORACLE Cloud Infrastructure	paratoolsadmin	off	2	N/A
Down 2:11 8:58	e4s-24-05-gcp	Google Cloud	paratoolsadmin	off	2	N/A
Down	e4s-24-05-azure	Microsoft Azure	paratoolsadmin	off	2	N/A
Down 2:46 5:21	e4s-24-05-arm	amazon web services	paratoolsadmin	off	2	N/A
Available 10:18 7:15	e4s-24-05-aws	amazon web services	paratoolsadmin	off	2	28 minutes

Rows per page: 10 1-6 of 6

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Click here

Adaptive Computing's ODDC: Go to Configuration tab

The screenshot displays the Adaptive Computing ODDC interface for a cluster named 'e4s-24-05-aws'. The interface is divided into several sections:

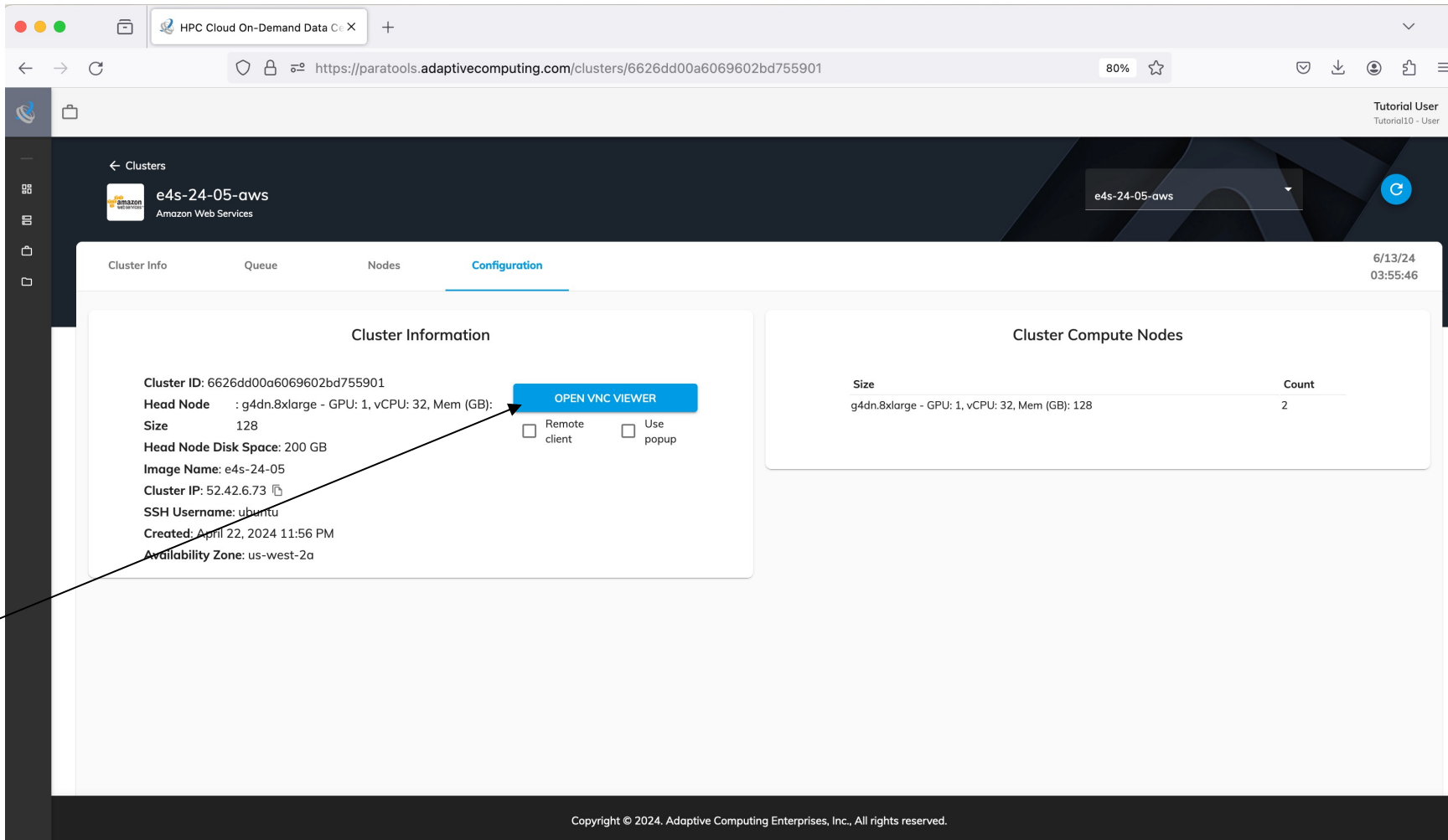
- Cluster Info:** Shows 'Jobs Submitted' as 0 (Total) and 'Blocked Jobs' as 0.
- Queue:** Shows 'Queue' as 0 (Running) and 'Total Jobs' as 0.
- Nodes:** Shows 'Nodes' as 2 (Available) and 'Total Nodes' as 2.
- Nodes Donut Chart:** A donut chart showing 2 Available Nodes (blue), 0 Busy Nodes (yellow), and 0 Down Nodes (orange).
- Workload:** A section for workload monitoring, currently empty.
- Activities Log:** A section for activities, currently empty.

The 'Configuration' tab is highlighted, and an arrow points to it from the text 'Click here' on the left. The interface also shows a sidebar with navigation options and a top navigation bar with the cluster name and a refresh button.

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Click here

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



The screenshot shows a web browser window displaying the ODDC configuration page for an AWS cluster. The browser address bar shows the URL: <https://paratools.adaptivecomputing.com/clusters/6626dd00a6069602bd755901>. The page title is "Clusters" and the cluster name is "e4s-24-05-aws". The "Configuration" tab is selected, showing the following information:

Cluster Information

- Cluster ID: 6626dd00a6069602bd755901
- Head Node : g4dn.8xlarge - GPU: 1, vCPU: 32, Mem (GB): 128
- Size: 128
- Head Node Disk Space: 200 GB
- Image Name: e4s-24-05
- Cluster IP: 52.42.6.73
- SSH Username: ubuntu
- Created: April 22, 2024 11:56 PM
- Availability Zone: us-west-2a

The "OPEN VNC VIEWER" button is highlighted with a blue background and a white arrow pointing to it. Below the button are two checkboxes: "Remote client" and "Use popup".

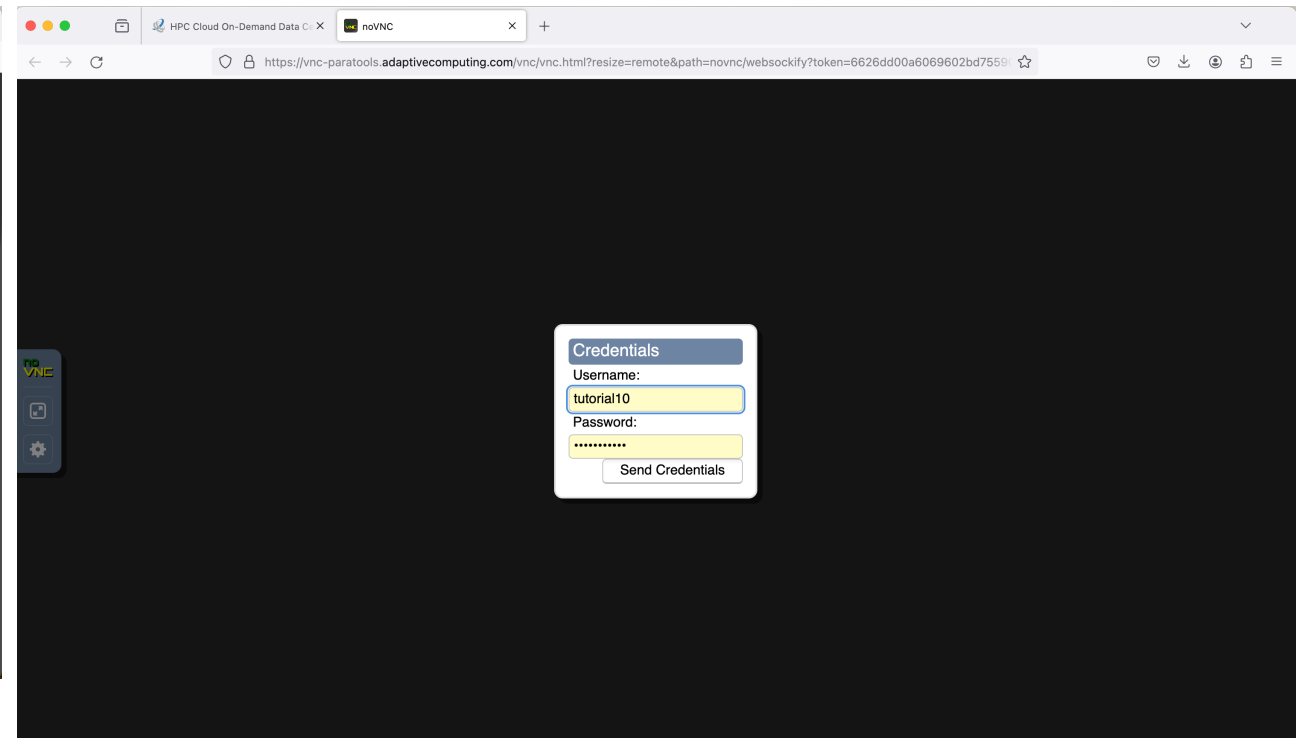
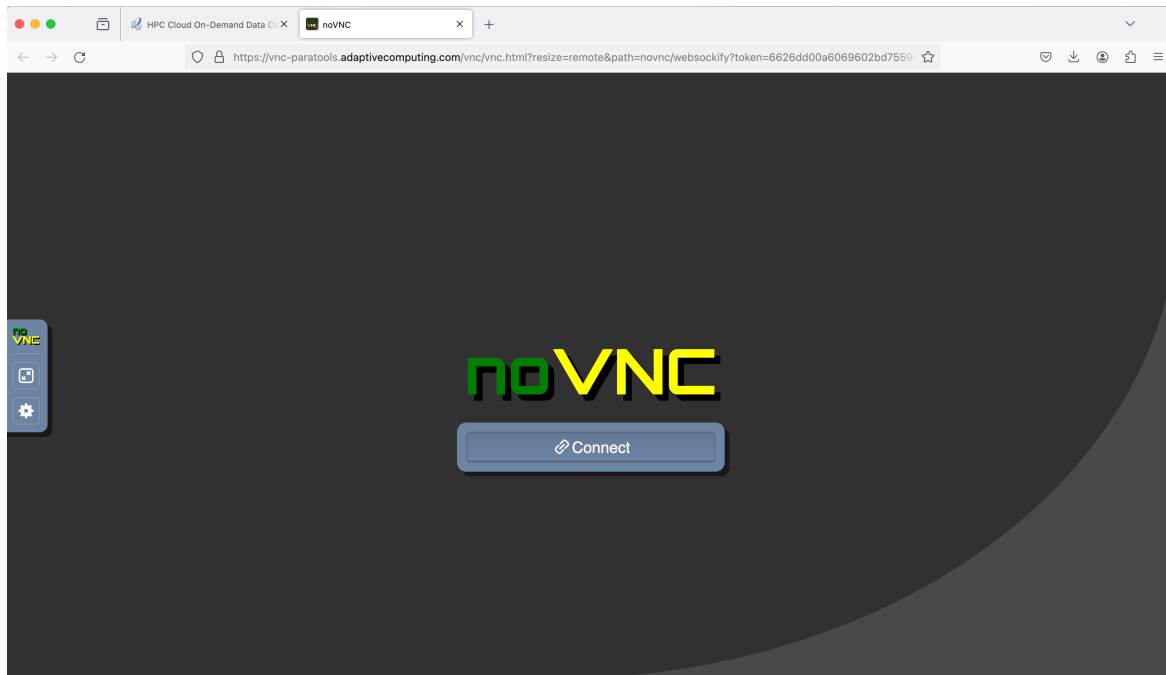
Cluster Compute Nodes

Size	Count
g4dn.8xlarge - GPU: 1, vCPU: 32, Mem (GB): 128	2

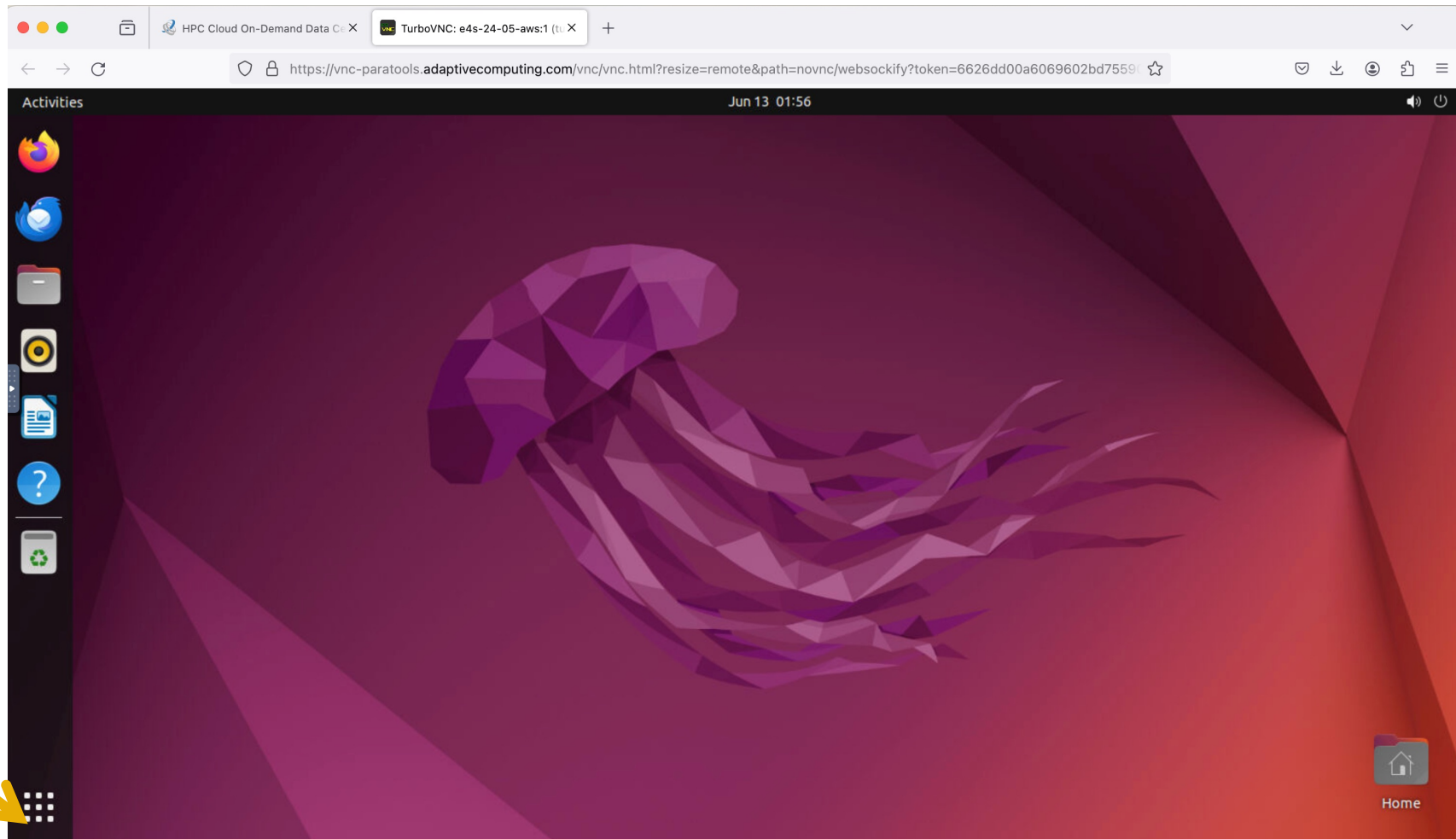
The page footer contains the text: "Copyright © 2024. Adaptive Computing Enterprises, Inc., All rights reserved."

Click here

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

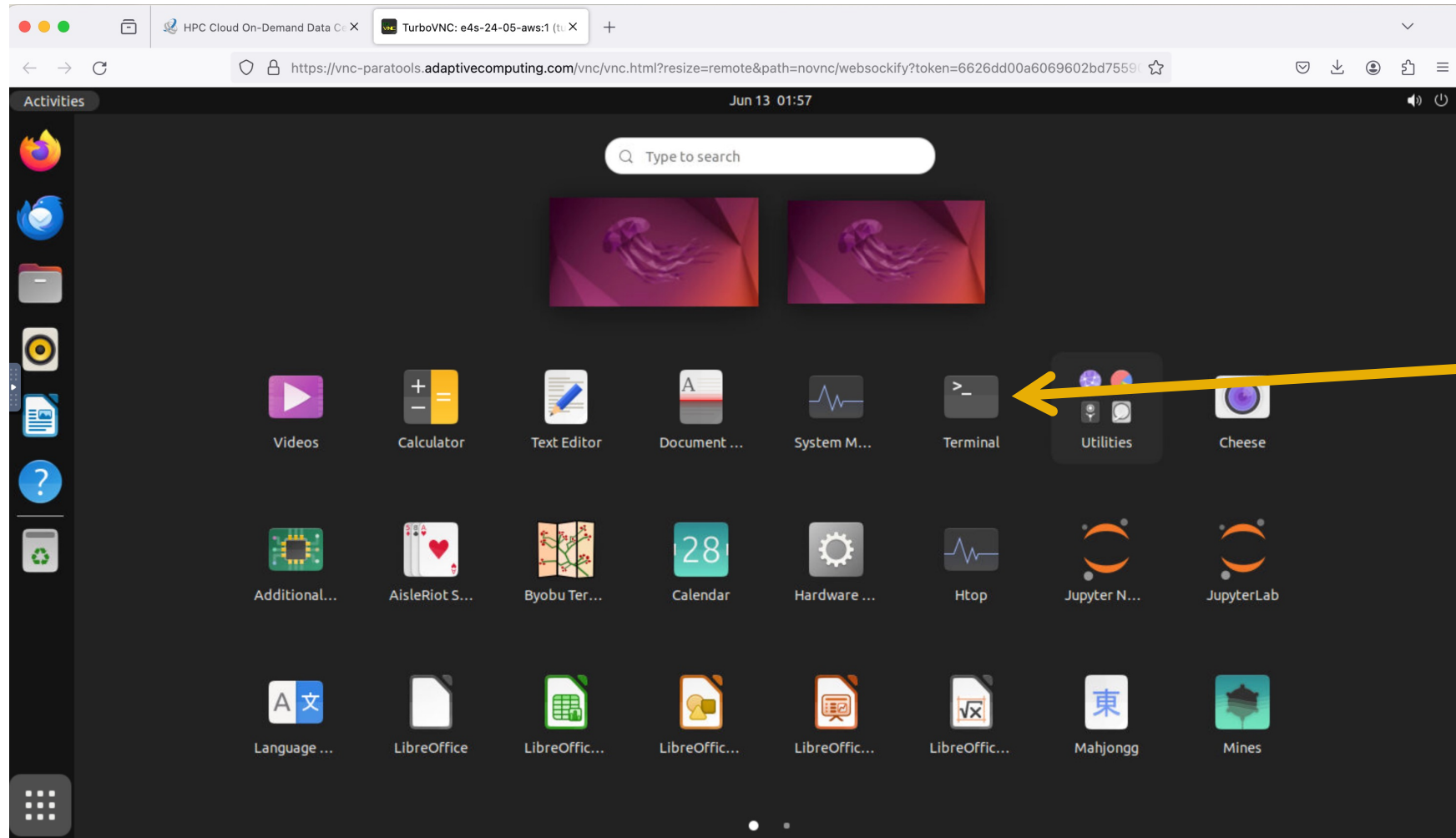


Remote Desktop from the ParaTools Pro for E4S image on AWS



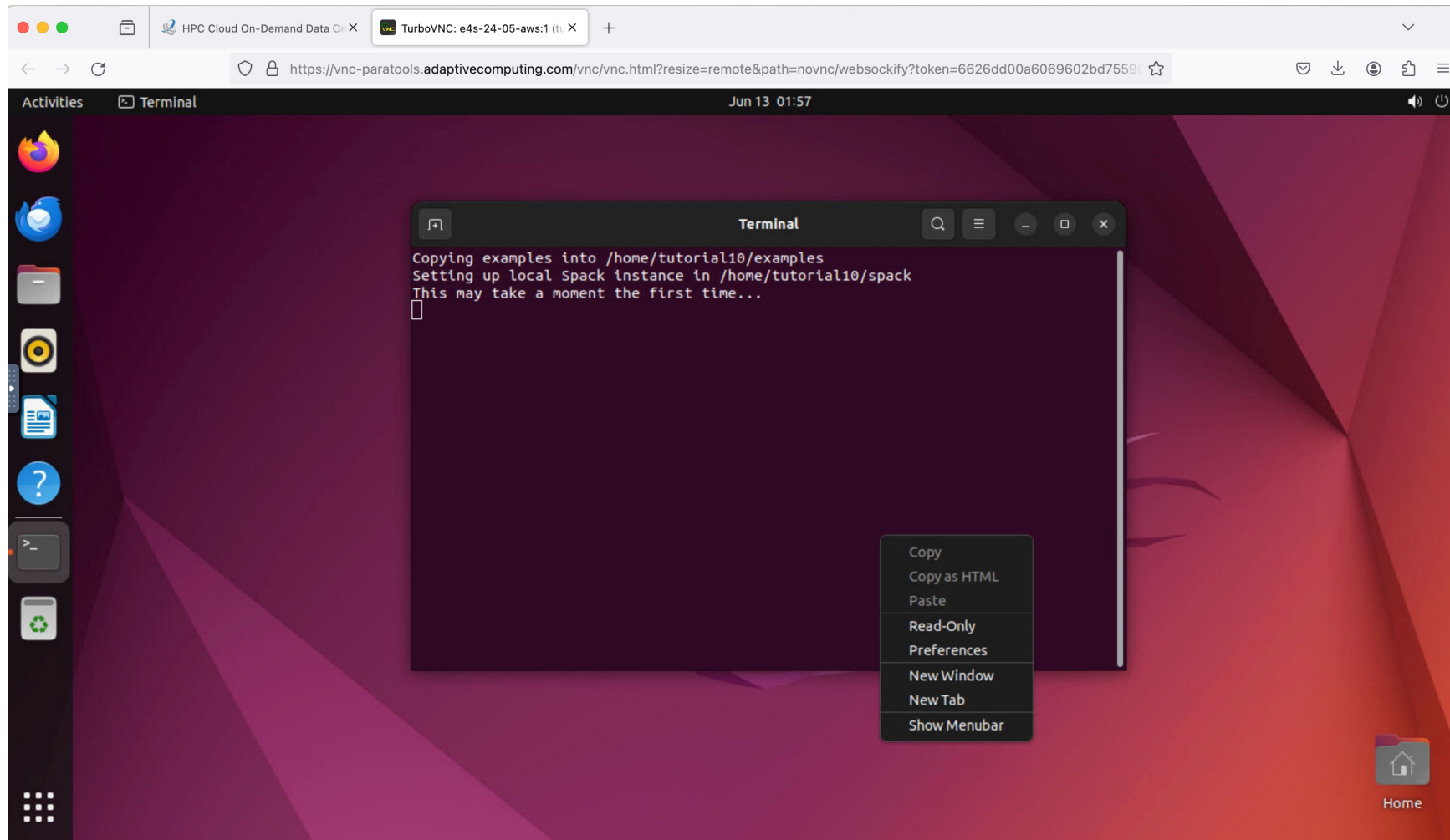
Click here

Launch Terminal in Remote Desktop

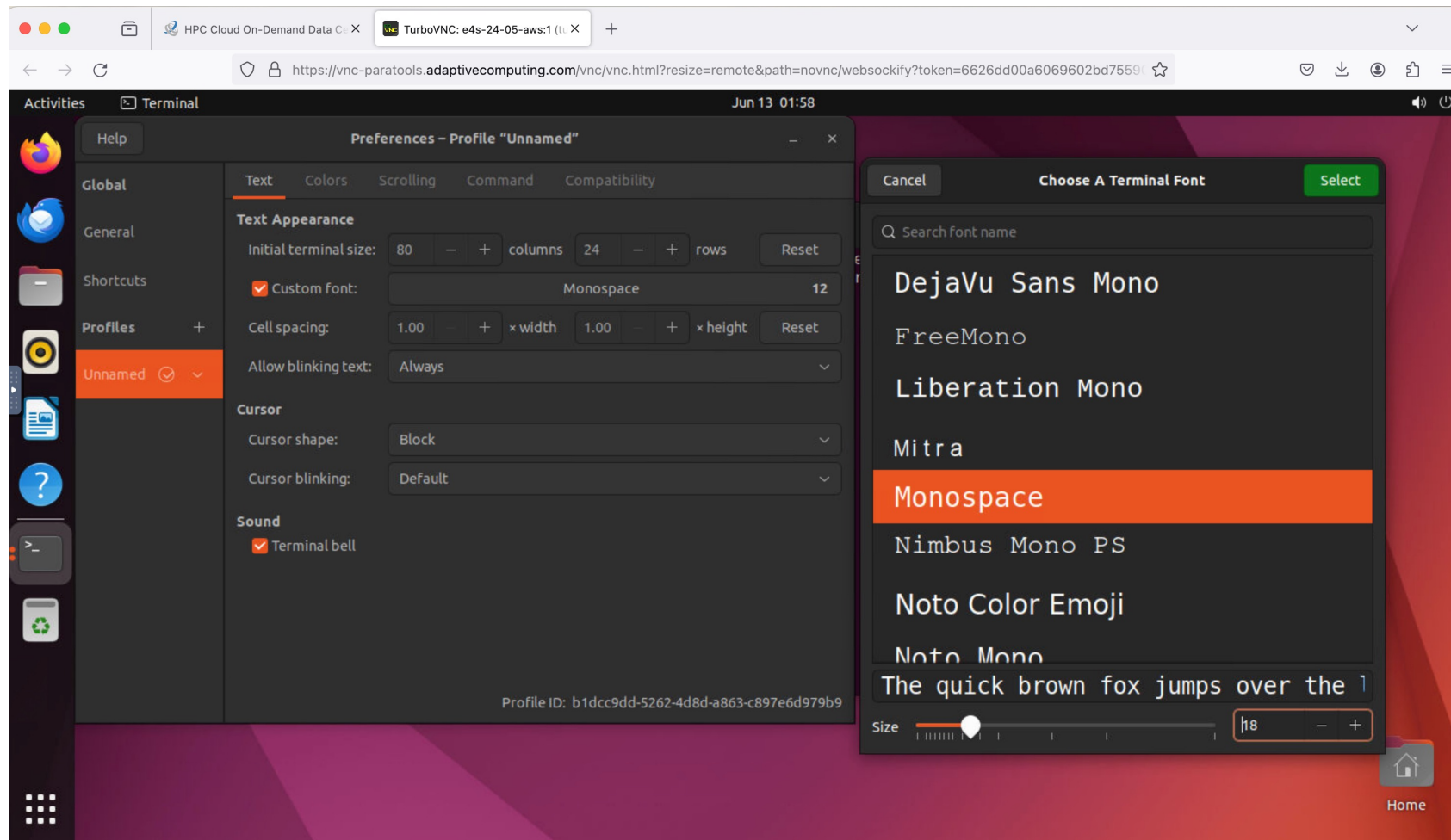


Click here

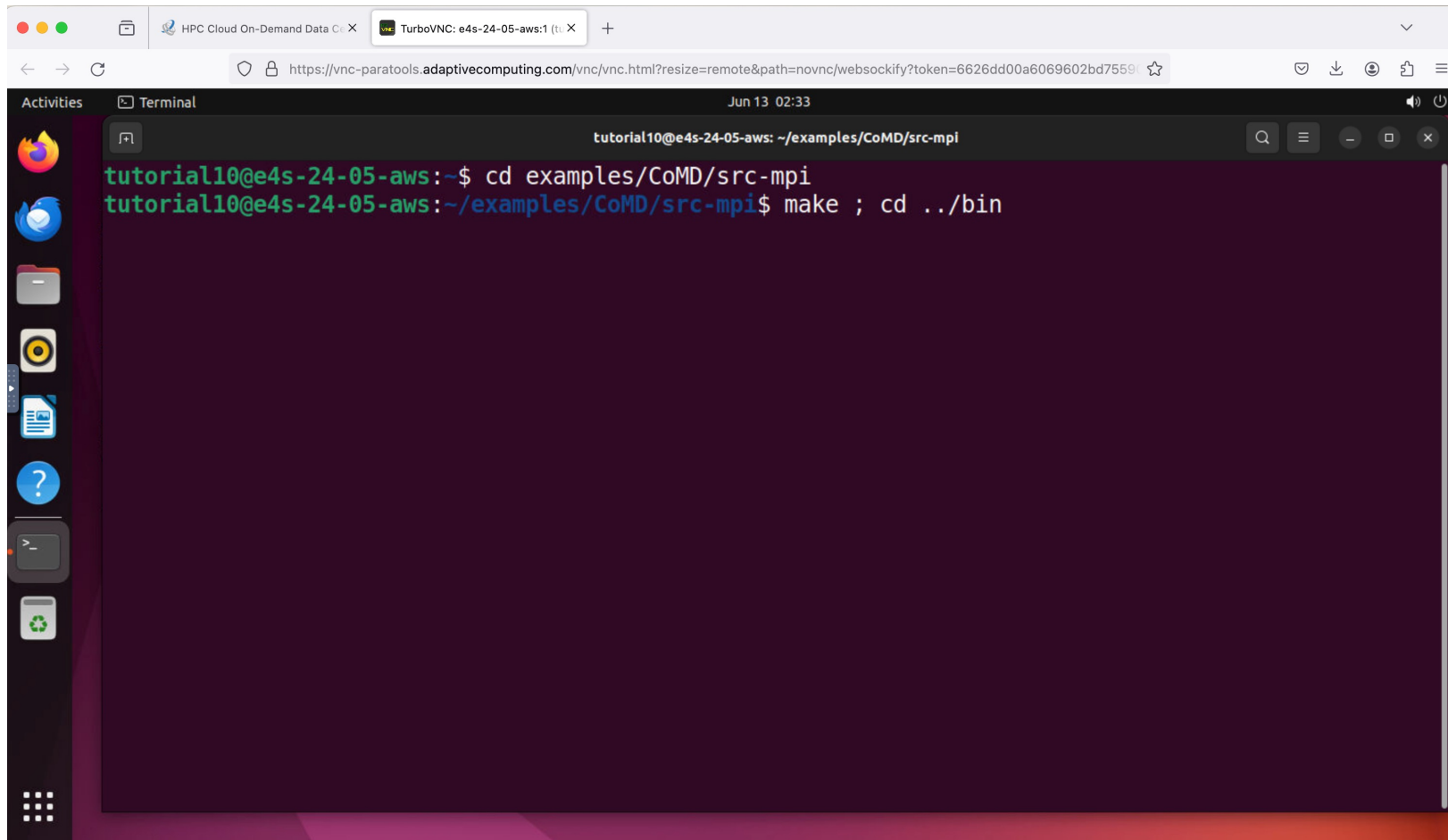
To increase font size right click and choose preferences



Choose font size after clicking Custom Font for Terminal



CoMD: TAU with event-based sampling (EBS)

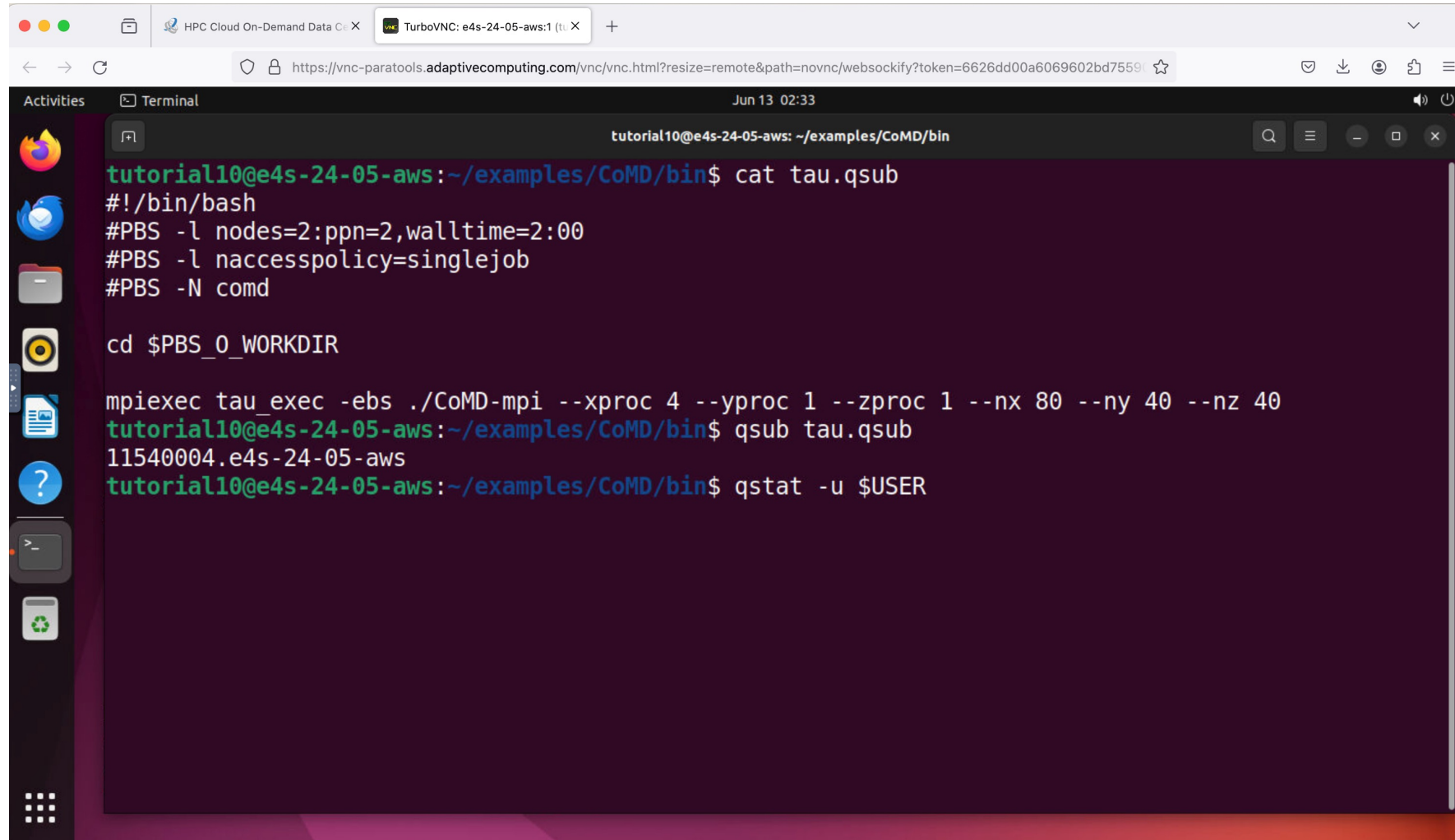


The screenshot shows a terminal window with the following content:

```
tutorial10@e4s-24-05-aws: ~$ cd examples/CoMD/src-mpi
tutorial10@e4s-24-05-aws:~/examples/CoMD/src-mpi$ make ; cd ../bin
```

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

CoMD: TAU with event-based sampling (EBS)



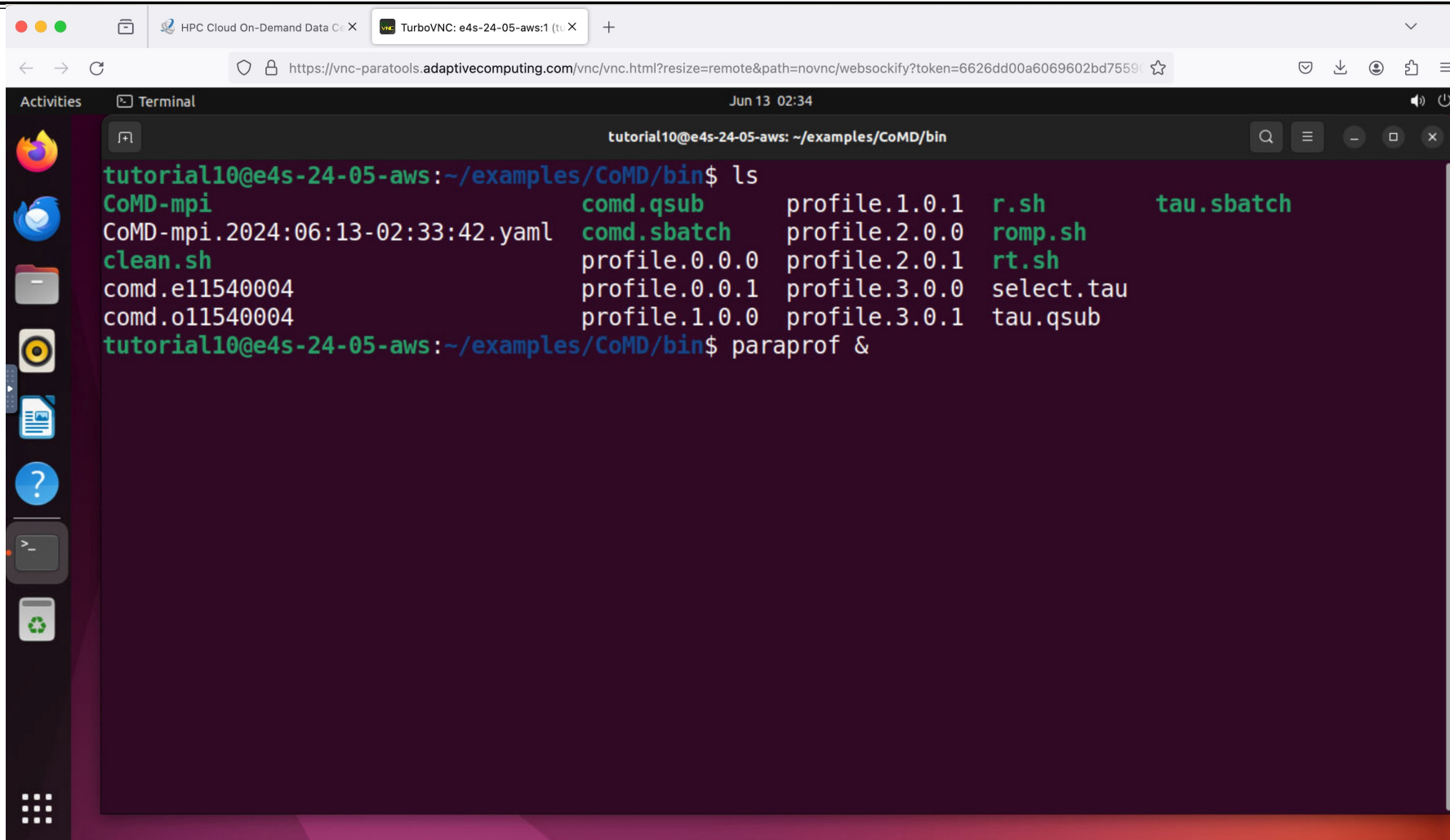
```
tutorial10@e4s-24-05-aws: ~/examples/CoMD/bin
tutorial10@e4s-24-05-aws:~/examples/CoMD/bin$ cat tau.qsub
#!/bin/bash
#PBS -l nodes=2:ppn=2,walltime=2:00
#PBS -l naccesspolicy=singlejob
#PBS -N comd

cd $PBS_0_WORKDIR

mpiexec tau_exec -ebs ./CoMD-mpi --xproc 4 --yproc 1 --zproc 1 --nx 80 --ny 40 --nz 40
tutorial10@e4s-24-05-aws:~/examples/CoMD/bin$ qsub tau.qsub
11540004.e4s-24-05-aws
tutorial10@e4s-24-05-aws:~/examples/CoMD/bin$ qstat -u $USER
```

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

CoMD: TAU's paraprof visualizer



The screenshot shows a terminal window with the following content:

```
tutorial10@e4s-24-05-aws: ~/examples/CoMD/bin
tutorial10@e4s-24-05-aws:~/examples/CoMD/bin$ ls
CoMD-mpi          comd.qsub         profile.1.0.1    r.sh             tau.sbatch
CoMD-mpi.2024:06:13-02:33:42.yaml  comd.sbatch      profile.2.0.0    romp.sh
clean.sh          profile.0.0.0    profile.2.0.1    rt.sh
comd.e11540004   profile.0.0.1    profile.3.0.0    select.tau
comd.o11540004   profile.1.0.0    profile.3.0.1    tau.qsub
tutorial10@e4s-24-05-aws:~/examples/CoMD/bin$ paraprof &
```

% paraprof &

CoMD: TAU's paraprof visualizer

The screenshot displays the TAU ParaProf Manager interface. The main window shows a list of trial fields for a specific application. A secondary window is open, showing a detailed view of thread statistics for Node 0, Thread 0. A yellow arrow points to the 'Show Thread Statistics Table' option in the context menu.

TrialField	Value
Name	bin/CoMD
Application ID	0
Experiment ID	0
Trial ID	0
CPU Cores	16
CPU MHz	3100.22
CPU Type	Intel(R)
CPU Vendor	Genuine
CPU Allowed	000000
CPU Allowed List	0-1
CWD	/home/t
Cache Size	36608 K
Command Line	./CoMD-
Ending Timestamp	171824
Executable	/home/t
File Type Index	1
File Type Name	TAU pro
Hostname	ac-5901
Local Time	2024-06
MPI Processor Name	ac-5901
Memories Allowed	000000
Memories Allowed List	0
Memory Size	130390
Node Name	ac-5901
OS Machine	x86_64
OS Name	Linux
OS Release	5.19.0-1029-aws
OS Version	#30~22.04.1-Ubuntu SMP Thu Jul ...
Starting Timestamp	1718246022396106

TAU: ParaProf: /home/tutorial10/examples/CoMD/bin

Metric: TIME
Value: Exclusive

Std. Dev. [Bar Chart]
Mean [Bar Chart]
Max [Bar Chart]
Min [Bar Chart]

node 0, thread 0 [Bar Chart]
node 0, thread 1 [Bar Chart]
node 1, thread 0 [Bar Chart]
node 1, thread 1 [Bar Chart]
node 2, thread 0 [Bar Chart]
node 2, thread 1 [Bar Chart]
node 3, thread 0 [Bar Chart]
node 3, thread 1 [Bar Chart]

Context Menu Options:

- Show Thread Bar Chart
- Show Thread Statistics Text Window
- Show Thread Statistics Table
- Show Thread Call Graph
- Show Thread Call Path Relations
- Show User Event Bar Chart
- Show User Event Statistics Window
- Show Context Event Window
- Show Metadata for Thread
- Add Thread to Comparison Window

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

TAU's ParaProf Profile Browser: Thread Statistics Table

TAU: ParaProf: Statistics for: node 0, thread 0 - /home/tutorial10/examples/CoMD/bin

Name	Exclusive TIME	Inclusive TIME	Calls	Child Calls
.TAU application	0	26.582	1	1
taupreload_main	26.174	26.582	1	1,255
[CONTEXT] taupreload_main	0	25.65	855	0
[SUMMARY] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c}]	24.27	24.27	809	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {198}]	4.8	4.8	160	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {209}]	3.78	3.78	126	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {199}]	3.66	3.66	122	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {189}]	2.76	2.76	92	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {202}]	1.98	1.98	56	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {193}]	1.56	1.56	52	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {208}]	1.47	1.47	49	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {207}]	1.38	1.38	46	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {224}]	0.66	0.66	22	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {206}]	0.63	0.63	21	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {223}]	0.39	0.39	13	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {185}]	0.27	0.27	9	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {210}]	0.24	0.24	8	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {220}]	0.18	0.18	6	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {214}]	0.15	0.15	5	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {181}]	0.12	0.12	4	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {175}]	0.09	0.09	3	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {159}]	0.06	0.06	2	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {187}]	0.06	0.06	2	0
[SAMPLE] IjForce [{/home/tutorial10/examples/CoMD/src-mpi/IjForce.c} {156}]	0.03	0.03	1	0
[SUMMARY] getBoxFromCoord [{/home/tutorial10/examples/CoMD/src-mpi/linkCells.c}]	0.36	0.36	12	0
[SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/libc.so.6	0.21	0.21	7	0
[SUMMARY] sortAtomsInCell [{/home/tutorial10/examples/CoMD/src-mpi/haloExchange}]	0.21	0.21	7	0
[SUMMARY] advancePosition [{/home/tutorial10/examples/CoMD/src-mpi/transport}]	0.12	0.12	4	0

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

The screenshot displays the TAU's ParaProf Profile Browser interface. On the left, a source code browser shows the C code for `ljForce.c`. The code includes nested loops for iterating over boxes and atoms, with a specific line (198) highlighted: `dr[m] = s->atoms->r[i0ff][m]-s->atoms->r[j0ff][m];`. On the right, a performance table provides detailed timing and call data for this line. The table has four columns: Exclusive TIME, Inclusive TIME, Calls, and Child Calls. The top row shows a total inclusive time of 26.582 seconds and 1 call. The table is color-coded by depth, with yellow for the top level and red for deeper levels.

Exclusive TIME	Inclusive TIME	Calls	Child Calls
0	26.582	1	1
26.174	26.582	1	1,255
0	25.65	855	0
24.27	24.27	809	0
4.8	4.8	160	0
3.78	3.78	126	0
3.66	3.66	122	0
2.76	2.76	92	0
1.98	1.98	66	0
1.56	1.56	52	0
1.47	1.47	49	0
1.38	1.38	46	0
0.66	0.66	22	0
0.63	0.63	21	0
0.39	0.39	13	0
0.27	0.27	9	0
0.24	0.24	8	0
0.18	0.18	6	0
0.15	0.15	5	0
0.12	0.12	4	0
0.09	0.09	3	0
0.06	0.06	2	0
0.06	0.06	2	0
0.03	0.03	1	0
0.36	0.36	12	0
0.21	0.21	7	0
0.21	0.21	7	0
0.12	0.12	4	0

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

The screenshot displays the TAU's ParaProf Profile Browser interface. On the left, a source code browser shows the C code for `ljForce.c`. The code includes nested loops for processing local boxes and atoms. The right pane shows a performance table with columns for Exclusive TIME, Inclusive TIME, Calls, and Child Calls. The table highlights the performance of line 198, which is `dr[m] = s->atoms->r[i0ff][m]-s->atoms->r[j0ff][m];`. The table shows that this line has an Exclusive TIME of 0.21 and an Inclusive TIME of 0.21, with 7 calls and 7 child calls.

Exclusive TIME	Inclusive TIME	Calls	Child Calls
0	26.582	1	1
26.174	26.582	1	1,255
0	25.65	855	0
24.27	24.27	809	0
4.8	4.8	160	0
3.78	3.78	126	0
3.66	3.66	122	0
2.76	2.76	92	0
1.98	1.98	66	0
1.56	1.56	52	0
1.47	1.47	49	0
1.38	1.38	46	0
0.66	0.66	22	0
0.63	0.63	21	0
0.39	0.39	13	0
0.27	0.27	9	0
0.24	0.24	8	0
0.18	0.18	6	0
0.15	0.15	5	0
0.12	0.12	4	0
0.09	0.09	3	0
0.06	0.06	2	0
0.06	0.06	2	0
0.03	0.03	1	0
0.36	0.36	12	0
0.21	0.21	7	0
0.21	0.21	7	0
0.12	0.12	4	0

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.

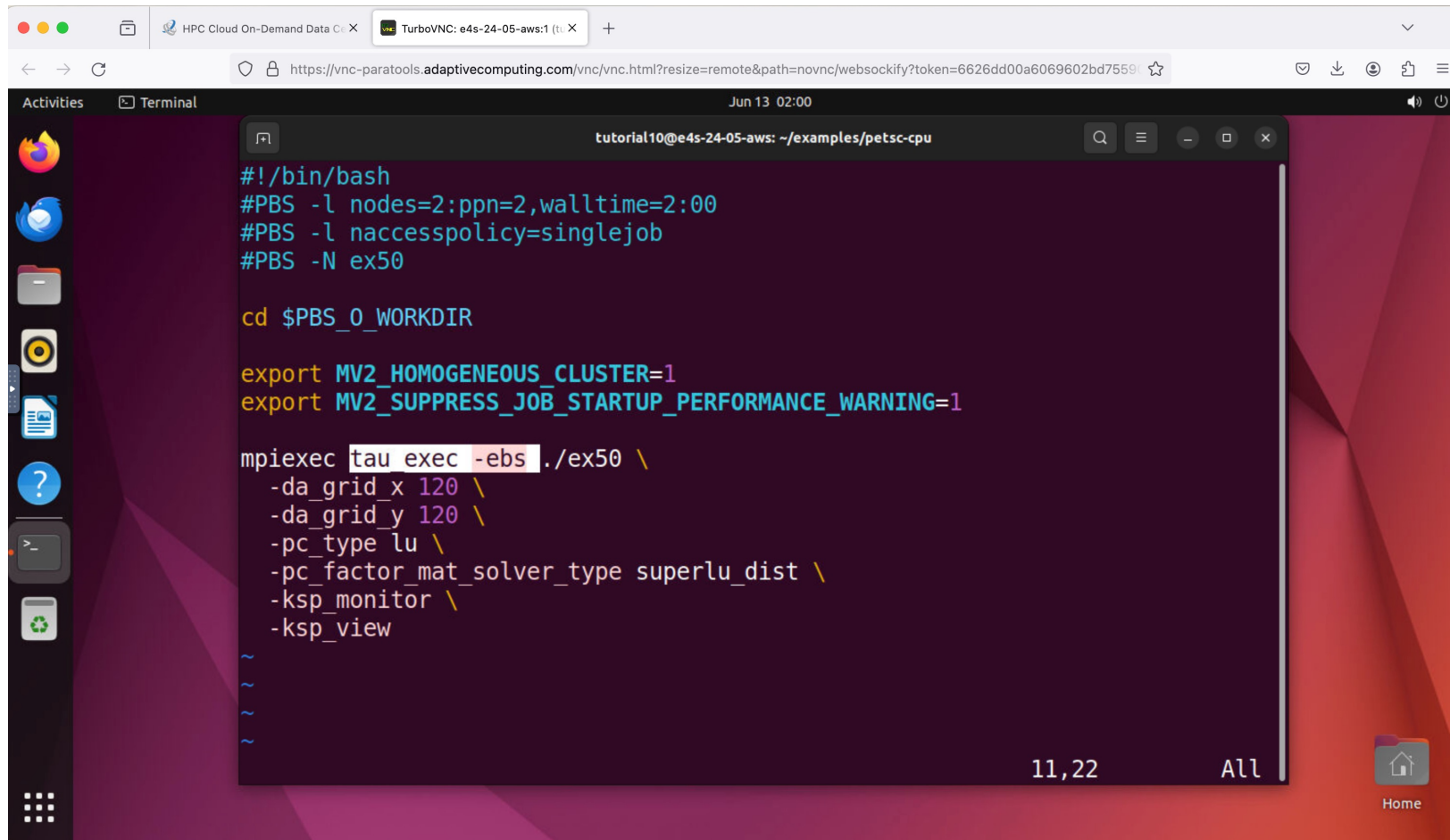
It is within five levels of for loops!

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



```
#!/bin/bash
#PBS -l nodes=2:ppn=2,walltime=2:00
#PBS -l naccesspolicy=singlejob
#PBS -N ex50

cd $PBS_O_WORKDIR

export MV2_HOMOGENEOUS_CLUSTER=1
export MV2_SUPPRESS_JOB_STARTUP_PERFORMANCE_WARNING=1

mpiexec tau_exec -ebs ./ex50 \
  -da_grid_x 120 \
  -da_grid_y 120 \
  -pc_type lu \
  -pc_factor_mat_solver_type superlu_dist \
  -ksp_monitor \
  -ksp_view
```

```
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

The screenshot shows a terminal window with the following content:

```
tutorial10@e4s-24-05-aws: ~/examples/petsc-cpu
-----
11540000.e4s-24-05-aws tutorial10 e4s-24-0 ex50          3795    2    4    --
   00:02:00 R   00:00:26
tutorial10@e4s-24-05-aws:~/examples/petsc-cpu$ qstat -u $USER
e4s-24-05-aws:
      Req'd      Elap
Job ID  Time      S  Time      Username  Queue   Jobname      SessID  NDS   TSK   Req'd
      Time      S  Time
-----
11540000.e4s-24-05-aws tutorial10 e4s-24-0 ex50          3795    2    4    --
   00:02:00 C          --
tutorial10@e4s-24-05-aws:~/examples/petsc-cpu$ ls
clean.sh      ex50.o11540000  profile.0.0.1  profile.2.0.0  profile.3.0.2
compile.sh    ex50.qsub       profile.0.0.2  profile.2.0.1  run-single-node.sh
ex50          ex50.sbatch    profile.1.0.0  profile.2.0.2  run-tau-oddc.sh
ex50.c        makefile        profile.1.0.1  profile.3.0.0
ex50.e11540000 profile.0.0.0  profile.1.0.2  profile.3.0.1
tutorial10@e4s-24-05-aws:~/examples/petsc-cpu$ paraprof &
```

qsub ex50.qsub
qstat -u \$USER

After it completes
ls
paraprof &

TAU's paraprof browser with PETSc performance profile

The screenshot shows the TAU ParaProf browser interface. The main window displays a tree view of performance events for node 0, thread 0. The table below shows the following data:

Name	Exclusive TIME	Inclusive TIME	Calls	Child C...
MPI_Init_thread()	2.701	2.701	1	0
Main Stage	1.615	3.629	1	284
[CONTEXT] Main Stage	0	1.567	12	0
[SAMPLE] MatLUFactorNumeric_SeqBAIJ_7_NaturalOrdering_inplace [{} /tmp/ubu	0.206	0.206	1	0
[SAMPLE] DMLabelView_Concrete_Ascii [{} /tmp/ubuntu/spack-stage/spack-sta	0.2	0.2	1	0
[SAMPLE] PetscDualSpaceSetUp_Lagrange [{} /tmp/ubuntu/spack-stage/spack	0.165	0.165	1	0
[SAMPLE] MatPreallocatorPreallocate_Preallocator [{} /tmp/ubuntu/spack-stagi	0.125	0.125	1	0
[SAMPLE] PCSetUp_GAMG [{} /tmp/ubuntu/spack-stage/spack-stage-petsc-3.21				
[SAMPLE] DMplexCreateSubmeshGeneric_Interpolated [{} /tmp/ubuntu/spack-s				
[SAMPLE] MatMult_MatMultAdd_SeqMAJ_Template [{} /tmp/ubuntu/spack-stage				
[SAMPLE] MatAXPY_Basic_Preallocate [{} /tmp/ubuntu/spack-stage/spack-stage				
[SAMPLE] ISView_General_HDF5 [{} /tmp/ubuntu/spack-stage/spack-stage-pets				
[SAMPLE] MatColoringCreateBipartiteGraph [{} /tmp/ubuntu/spack-stage/spack				
[SAMPLE] ScatterAndBOR_SignedChar_2_0 [{} /tmp/ubuntu/spack-stage/spack-				
[SAMPLE] ScatterAndinsert_SignedChar_2_1 [{} /tmp/ubuntu/spack-stage/spac				

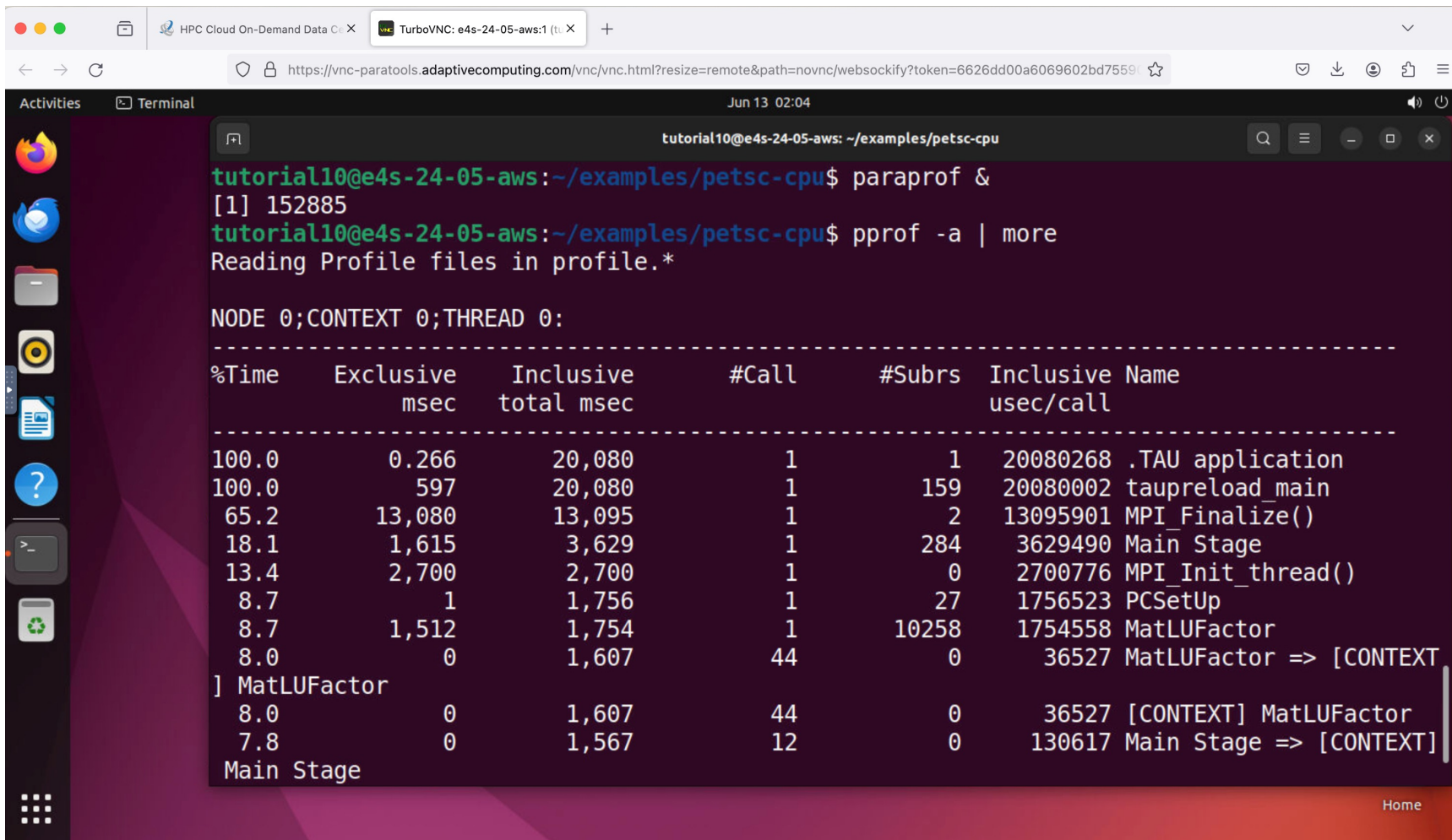
The context menu for 'MatLUFactor' includes the following options:

- Std. Dev.
- Mean
- Max
- Min
- node 0, thr... Show Thread Bar Chart
- node 0, thr... Show Thread Statistics Text Wind
- node 1, thr... Show Thread Statistics Table
- node 1, thr... Show Thread Call Graph
- node 2, thr... Show Thread Call Path Relations
- node 2, thr... Show User Event Bar Chart
- node 2, thr... Show User Event Statistics Window
- node 3, thr... Show Context Event Window
- node 3, thr... Show Metadata for Thread
- Add Thread to Comparison Window

paraprof

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

Using pprof: TAU's text based profile browser



```
tutorial10@e4s-24-05-aws: ~/examples/petsc-cpu
tutorial10@e4s-24-05-aws:~/examples/petsc-cpu$ paraprof &
[1] 152885
tutorial10@e4s-24-05-aws:~/examples/petsc-cpu$ pprof -a | more
Reading Profile files in profile.*

NODE 0;CONTEXT 0;THREAD 0:
-----
%Time   Exclusive   Inclusive   #Call   #Subrs   Inclusive Name
      msec    total msec
-----
100.0    0.266      20,080     1       1       20080268 .TAU application
100.0      597       20,080     1      159       20080002 taupreload_main
65.2    13,080     13,095     1       2       13095901 MPI_Finalize()
18.1     1,615     3,629     1      284       3629490 Main Stage
13.4     2,700     2,700     1       0       2700776 MPI_Init_thread()
8.7       1         1,756     1       27       1756523 PCSetUp
8.7     1,512     1,754     1    10258       1754558 MatLUFactor
8.0       0         1,607     44       0         36527 MatLUFactor => [CONTEXT
] MatLUFactor
8.0       0         1,607     44       0         36527 [CONTEXT] MatLUFactor
7.8       0         1,567     12       0        130617 Main Stage => [CONTEXT]
Main Stage
```

pprof -a | more

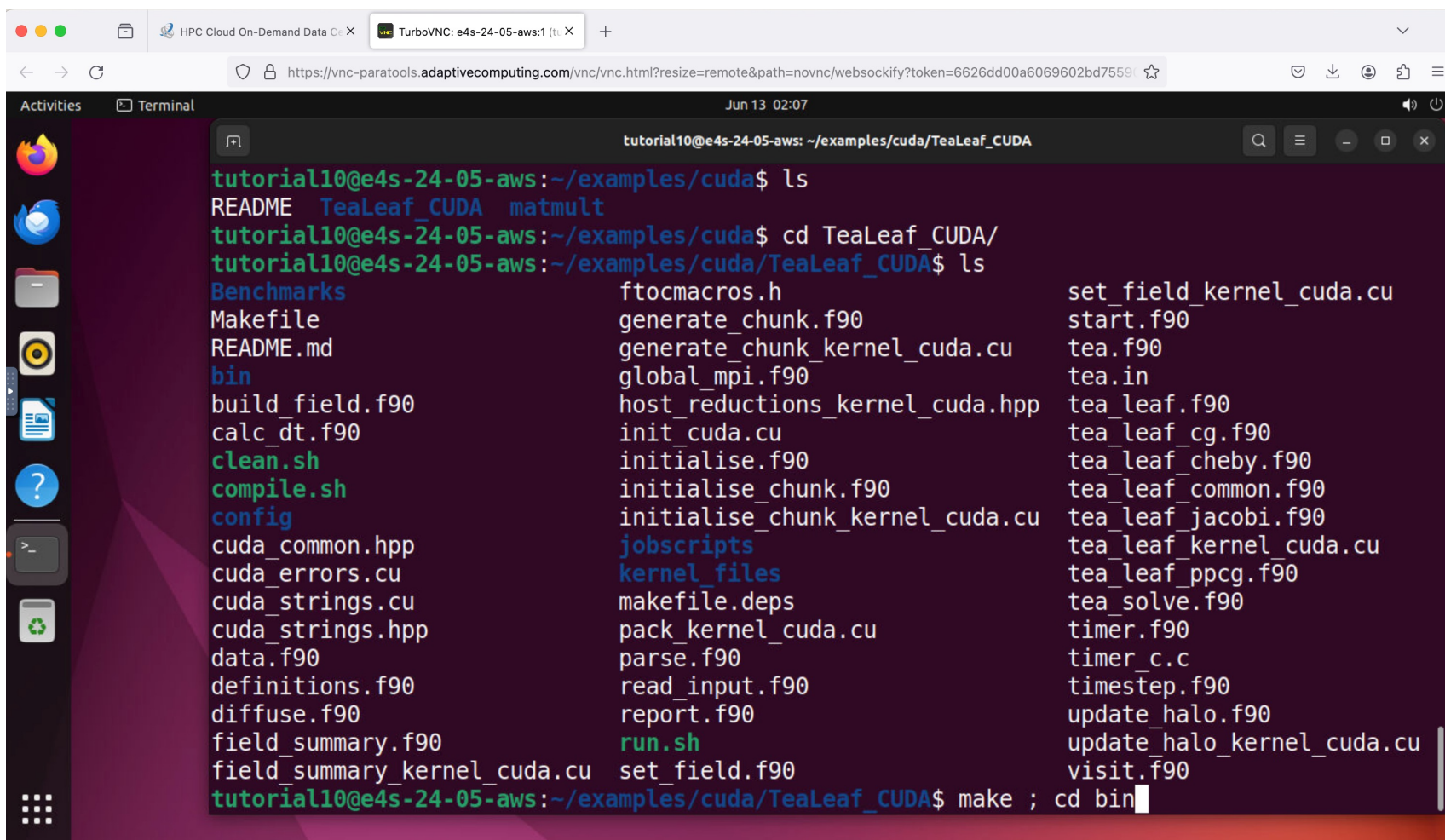
Here we see PETSc timers translated into TAU timers using the Perfstubs library.

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

TAU Exercise #5:

CUDA instrumentation using CUPTI (CUDA Profiling Tools Interface)

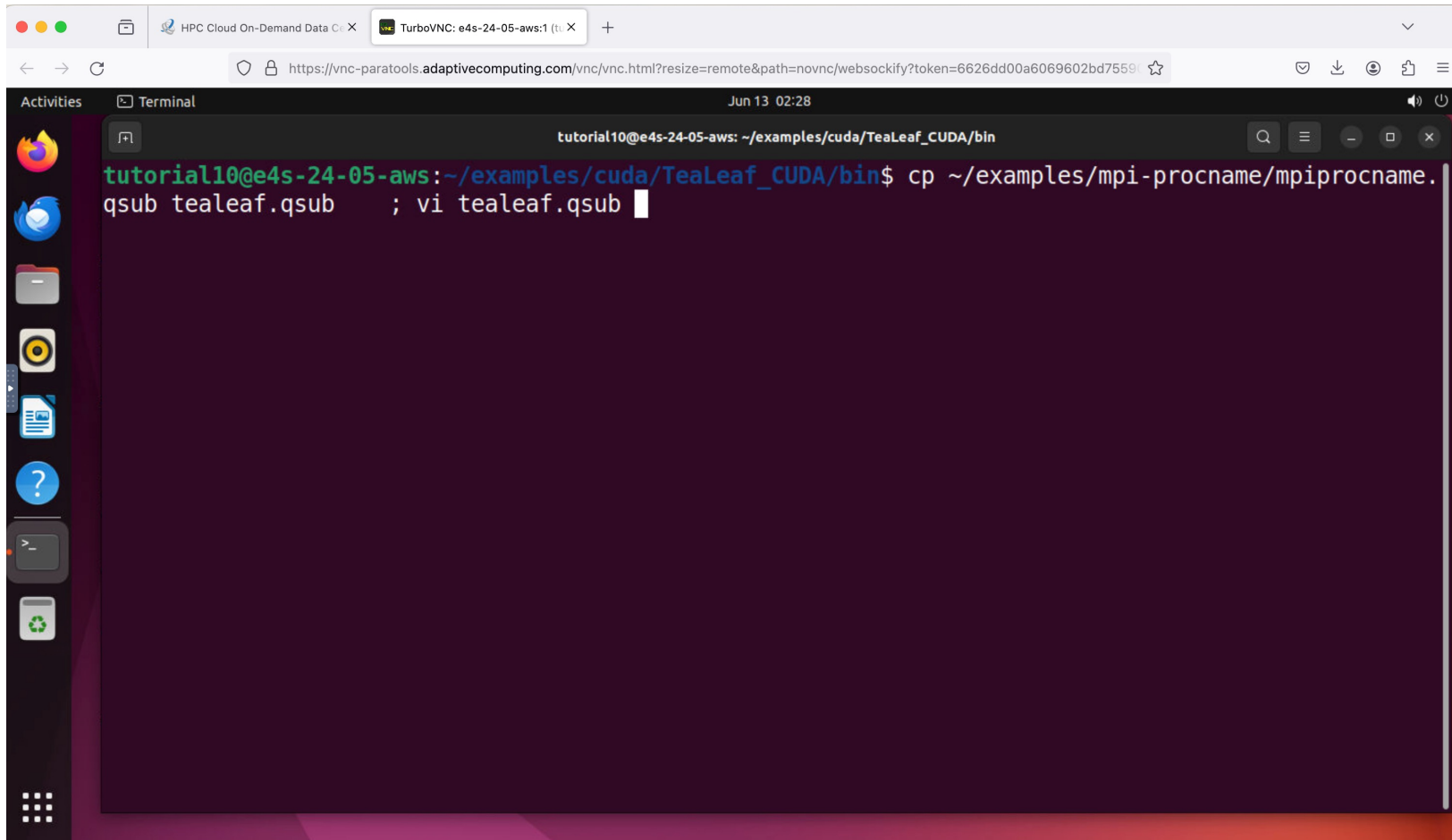
Compiling TeaLeaf_CUDA application



```
tutorial10@e4s-24-05-aws: ~/examples/cuda/TeaLeaf_CUDA
tutorial10@e4s-24-05-aws:~/examples/cuda$ ls
README  TeaLeaf_CUDA  matmult
tutorial10@e4s-24-05-aws:~/examples/cuda$ cd TeaLeaf_CUDA/
tutorial10@e4s-24-05-aws:~/examples/cuda/TeaLeaf_CUDA$ ls
Benchmarks          ftocmacros.h          set_field_kernel_cuda.cu
Makefile            generate_chunk.f90    start.f90
README.md          generate_chunk_kernel_cuda.cu  tea.f90
bin                global_mpi.f90       tea.in
build_field.f90    host_reductions_kernel_cuda.hpp  tea_leaf.f90
calc_dt.f90       init_cuda.cu         tea_leaf_cg.f90
clean.sh          initialise.f90       tea_leaf_cheby.f90
compile.sh        initialise_chunk.f90  tea_leaf_common.f90
config           initialise_chunk_kernel_cuda.cu  tea_leaf_jacobi.f90
cuda_common.hpp  jobscripts          tea_leaf_kernel_cuda.cu
cuda_errors.cu   kernel_files        tea_leaf_ppcg.f90
cuda_strings.cu  makefile.deps      tea_solve.f90
cuda_strings.hpp  pack_kernel_cuda.cu  timer.f90
data.f90         parse.f90           timer_c.c
definitions.f90  read_input.f90     timestep.f90
diffuse.f90     report.f90         update_halo.f90
field_summary.f90  run.sh            update_halo_kernel_cuda.cu
field_summary_kernel_cuda.cu  set_field.f90      visit.f90
tutorial10@e4s-24-05-aws:~/examples/cuda/TeaLeaf_CUDA$ make ; cd bin
```

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


Copying and editing a sample job submission script



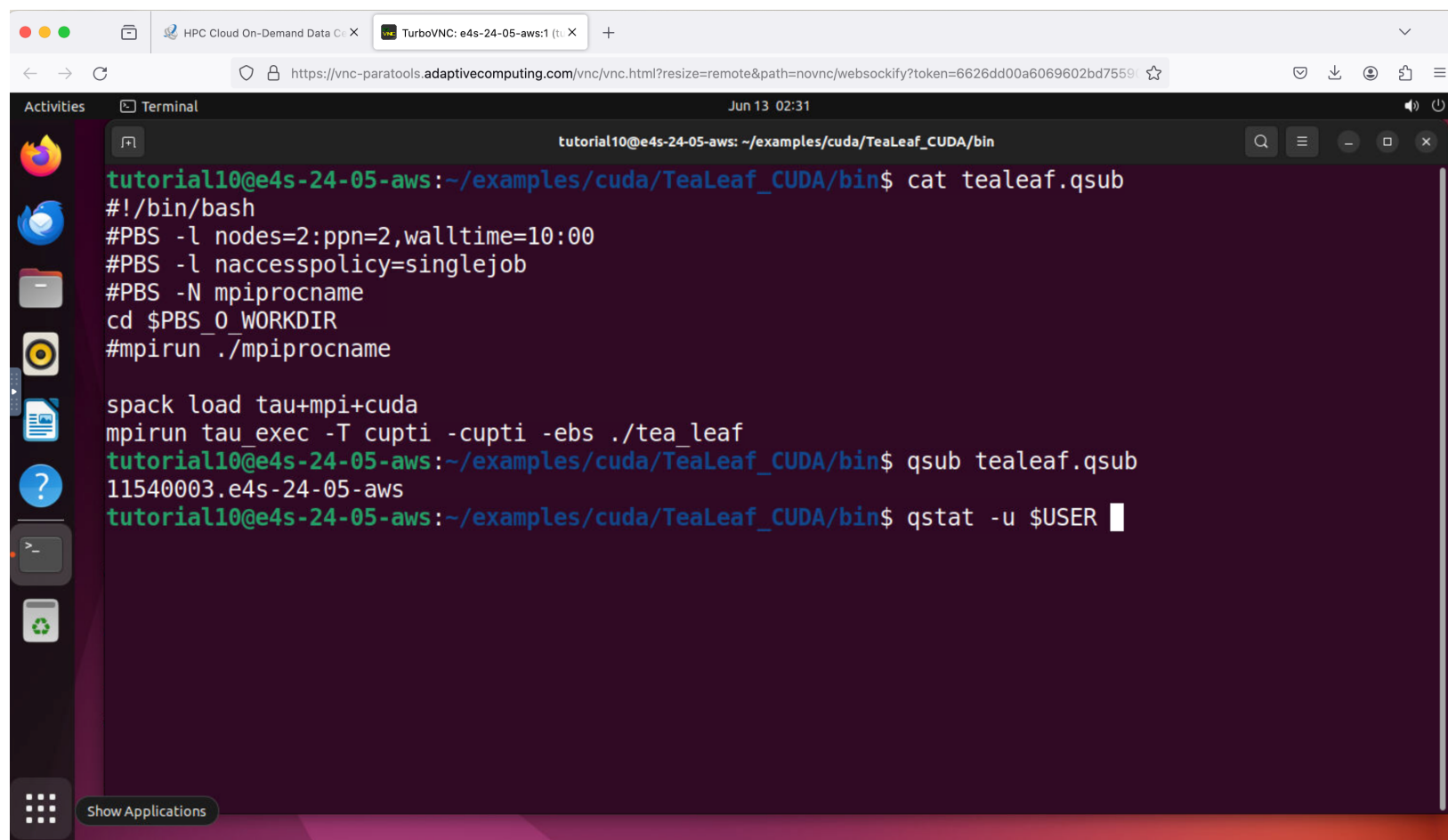
The screenshot shows a TurboVNC terminal window with the following content:

```
tutorial10@e4s-24-05-aws: ~/examples/cuda/TeaLeaf_CUDA/bin
tutorial10@e4s-24-05-aws: ~/examples/cuda/TeaLeaf_CUDA/bin$ cp ~/examples/mpi-procname/mpiprocname.qsub tealeaf.qsub ; vi tealeaf.qsub
```

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

```
vi tealeaf.qsub
```


Submit the CUDA job to run on four MPI ranks



```
tutorial10@e4s-24-05-aws: ~/examples/cuda/TeaLeaf_CUDA/bin
tutorial10@e4s-24-05-aws:~/examples/cuda/TeaLeaf_CUDA/bin$ cat tealeaf.qsub
#!/bin/bash
#PBS -l nodes=2:ppn=2,walltime=10:00
#PBS -l naccesspolicy=singlejob
#PBS -N mpiprocname
cd $PBS_0_WORKDIR
#mpirun ./mpiprocname

spack load tau+mpi+cuda
mpirun tau_exec -T cupti -cupti -ebs ./tea_leaf
tutorial10@e4s-24-05-aws:~/examples/cuda/TeaLeaf_CUDA/bin$ qsub tealeaf.qsub
11540003.e4s-24-05-aws
tutorial10@e4s-24-05-aws:~/examples/cuda/TeaLeaf_CUDA/bin$ qstat -u $USER
```

qsub tealeaf.qsub

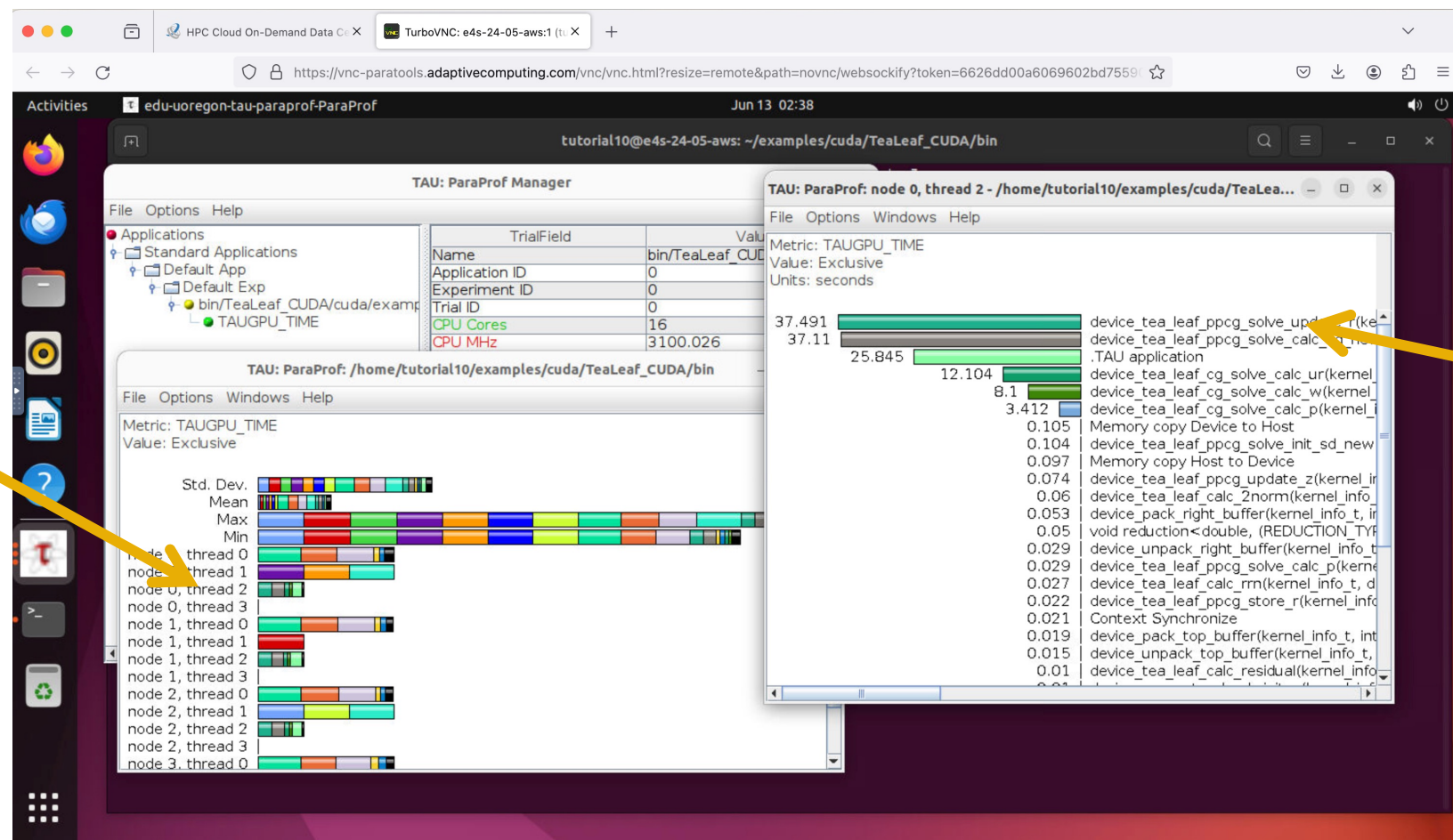
qstat -u \$USER

After it runs

paraprof &

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

Left click node 0, thread 2



CUDA kernels

TAU Exercise #6:

paraprof 3D display

TAU paraprof

The screenshot shows a terminal window with the following commands and output:

```
tutorial10@e4s-24-05-aws:~/examples/tau$ ls
demo.ppk  fetch.sh
tutorial10@e4s-24-05-aws:~/examples/tau$ paraprof demo.ppk &
[1] 309831
tutorial10@e4s-24-05-aws:~/examples/tau$
```

The TAU ParaProf Manager window displays a table of trial fields:

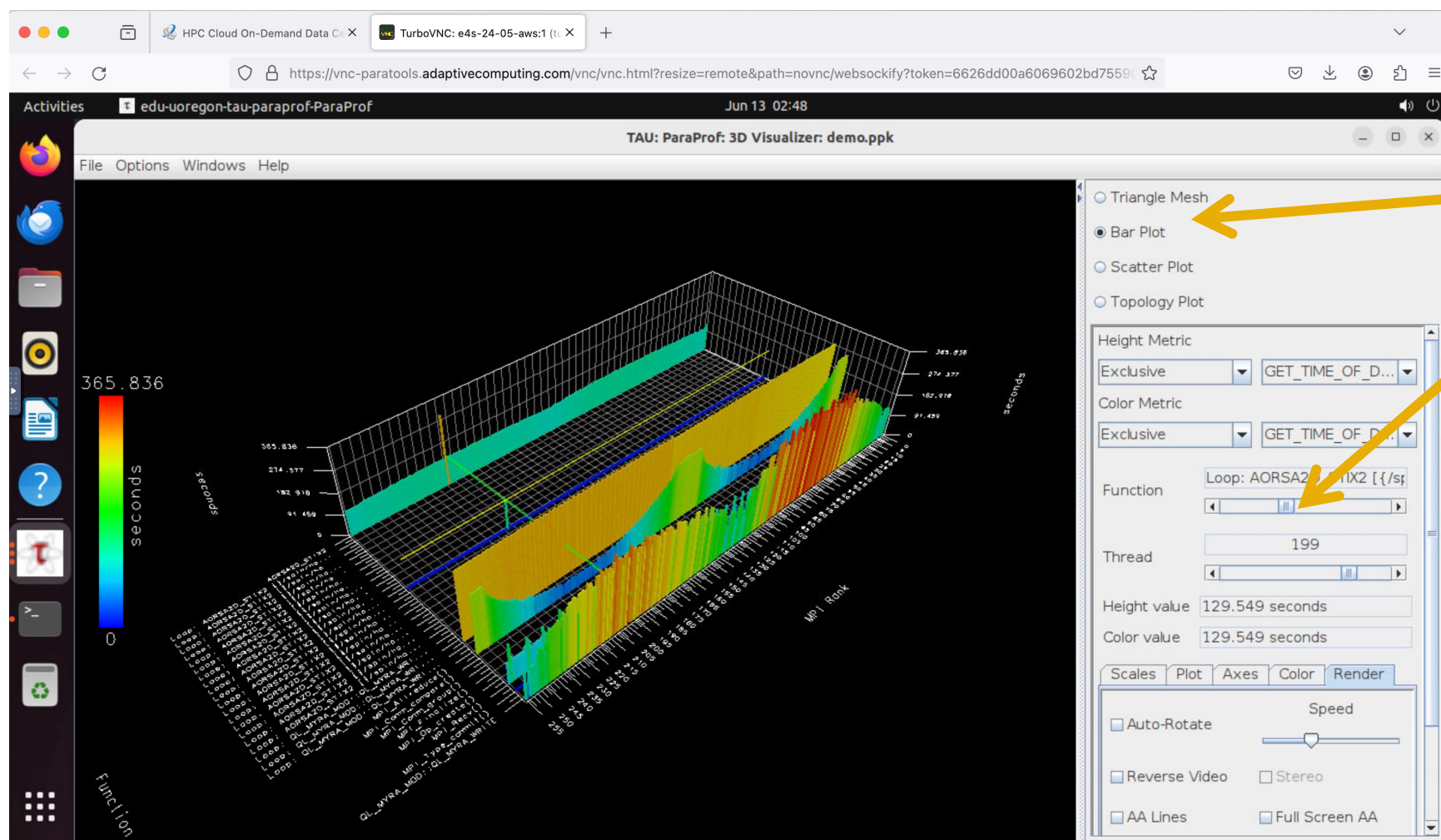
TrialField	
Name	demo.ppk
Application ID	0
Experiment ID	0
Trial ID	0
File Type Index	0
File Type Name	ParaProf Pa

The TAU ParaProf: demo.ppk window shows a 3D visualization of the application's performance. A yellow arrow points to the '3D Visualization' option in the 'Windows' menu.

cd ~/examples/tau
paraprof demo.ppk &

Choose 3D Visualization

TAU paraprof 3D visualization



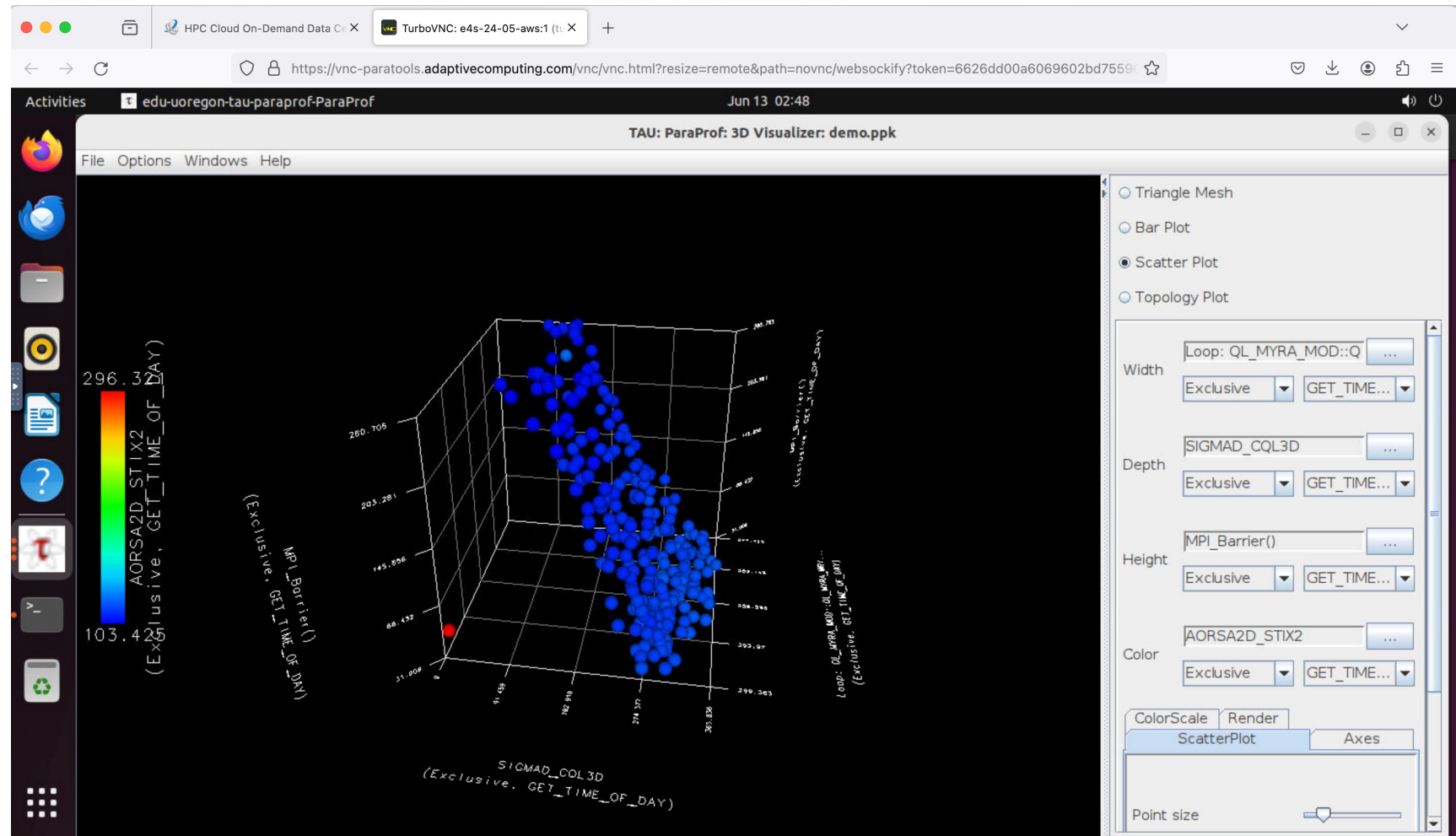
Choose Bar Plot and move

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

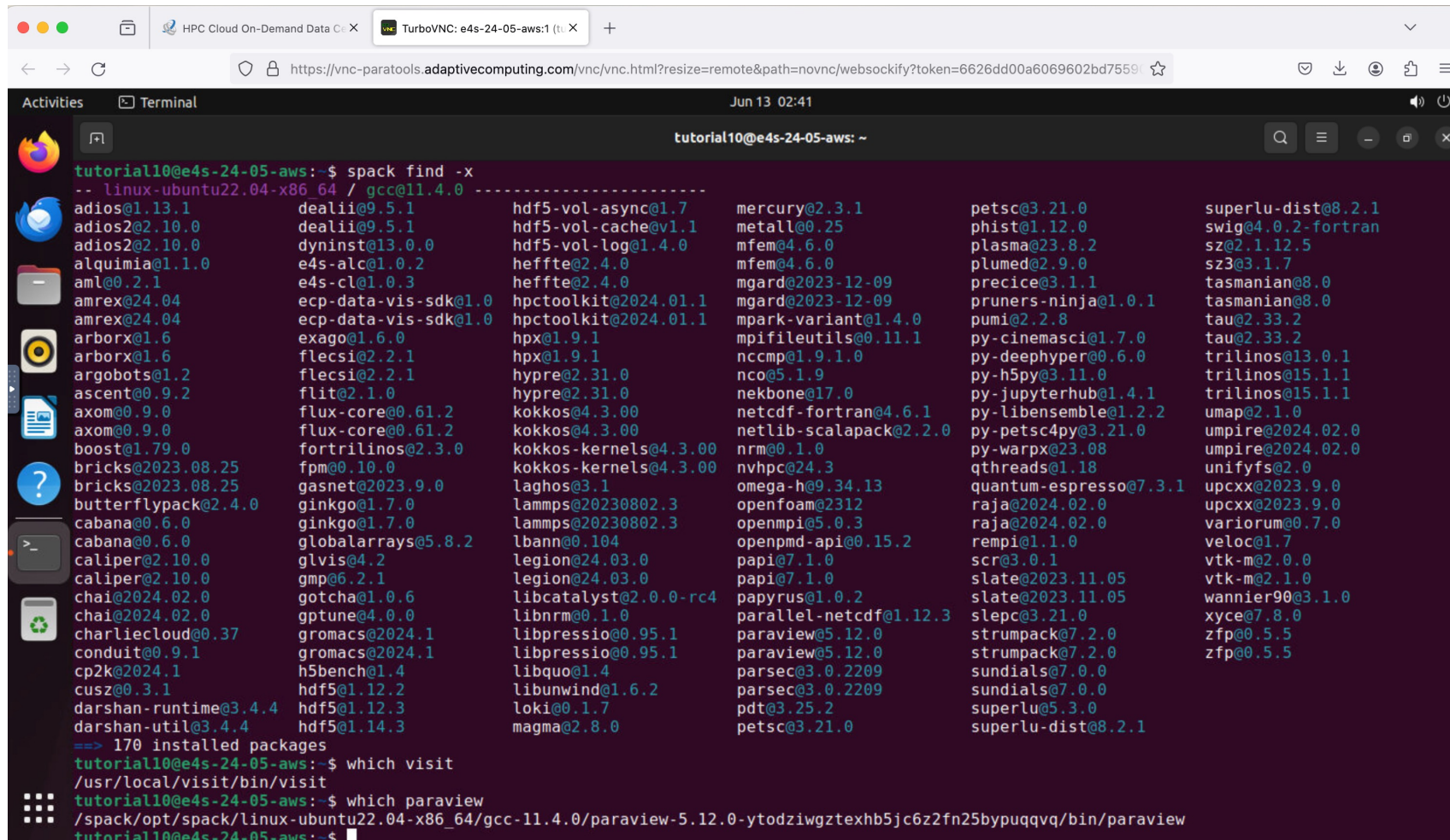
TAU paraprof: 3D Scatter Plot



Exercise #7

E4S: Extreme-scale Scientific Software Stack

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



```
tutorial10@e4s-24-05-aws: ~  
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           mfem@4.6.0        plumed@2.9.0      sz3@3.1.7  
aml@0.2.1        e4s-cl@1.0.3      heffte@2.4.0           mgard@2023-12-09  precice@3.1.1     tasmanian@8.0  
amrex@24.04      ecp-data-vis-sdk@1.0  hpctoolkit@2024.01.1  mgard@2023-12-09  pruners-ninja@1.0.1  tasmanian@8.0  
amrex@24.04      ecp-data-vis-sdk@1.0  hpctoolkit@2024.01.1  mpark-variant@1.4.0  pumi@2.2.8        tau@2.33.2  
arborx@1.6       exago@1.6.0       hpx@1.9.1              mpiutils@0.11.1   py-cinemasci@1.7.0  tau@2.33.2  
arborx@1.6       flecsi@2.2.1      hpx@1.9.1              nccmp@1.9.1.0     py-deepphyper@0.6.0  trilinos@13.0.1  
argobots@1.2     flecsi@2.2.1      hypre@2.31.0           nco@5.1.9          py-h5py@3.11.0     trilinos@15.1.1  
ascend@0.9.2     flit@2.1.0        kokkos@4.3.00          nekbone@17.0      py-jupyterhub@1.4.1  trilinos@15.1.1  
axom@0.9.0       flux-core@0.61.2  kokkos@4.3.00          netcdf-fortran@4.6.1  py-libensemble@1.2.2  umap@2.1.0  
axom@0.9.0       flux-core@0.61.2  kokkos@4.3.00          netlib-scalapack@2.2.0  py-petsc4py@3.21.0  umpire@2024.02.0  
boost@1.79.0     fortrilinos@2.3.0  kokkos-kernels@4.3.00  nrm@0.1.0          py-warp@23.08       umpire@2024.02.0  
bricks@2023.08.25  fpm@0.10.0        kokkos-kernels@4.3.00  nvhpc@24.3         qthreads@1.18       unifyfs@2.0  
bricks@2023.08.25  gasnet@2023.9.0   laghos@3.1              omega-h@9.34.13    quantum-espresso@7.3.1  upcxx@2023.9.0  
butterflypack@2.4.0  ginkgo@1.7.0      lammmps@20230802.3     openfoam@2312     raja@2024.02.0      upcxx@2023.9.0  
cabana@0.6.0     ginkgo@1.7.0      lammmps@20230802.3     openmpi@5.0.3     raja@2024.02.0      variorum@0.7.0  
cabana@0.6.0     globalarrays@5.8.2  lbann@0.104             openpmd-api@0.15.2  rempi@1.1.0         veloc@1.7  
caliper@2.10.0    glvis@4.2          legion@24.03.0          papi@7.1.0         scr@3.0.1           vtk-m@2.0.0  
caliper@2.10.0    gmp@6.2.1         legion@24.03.0          papi@7.1.0         slate@2023.11.05     vtk-m@2.1.0  
chai@2024.02.0   gotcha@1.0.6      libcatalyst@2.0.0-rc4  papyrus@1.0.2     slate@2023.11.05     wannier90@3.1.0  
chai@2024.02.0   gptune@4.0.0      libnrm@0.1.0           parallel-netcdf@1.12.3  slepc@3.21.0       xyce@7.8.0  
charliecloud@0.37  gromacs@2024.1    libpressio@0.95.1     paraview@5.12.0   strumpack@7.2.0     zfp@0.5.5  
conduit@0.9.1    gromacs@2024.1    libpressio@0.95.1     paraview@5.12.0   strumpack@7.2.0     zfp@0.5.5  
cp2k@2024.1      h5bench@1.4       libquo@1.4             parsec@3.0.2209    sundials@7.0.0      zfp@0.5.5  
cusz@0.3.1       hdf5@1.12.2       libunwind@1.6.2        parsec@3.0.2209    sundials@7.0.0      zfp@0.5.5  
darshan-runtime@3.4.4  hdf5@1.12.3      loki@0.1.7             pdt@3.25.2         superlu@5.3.0       superlu-dist@8.2.1  
darshan-util@3.4.4  hdf5@1.14.3      magma@2.8.0            petsc@3.21.0      superlu-dist@8.2.1  
==> 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-ytodziwgztxhb5jzc6z2fn25byuqqvq/bin/paraview  
tutorial10@e4s-24-05-aws:~$
```

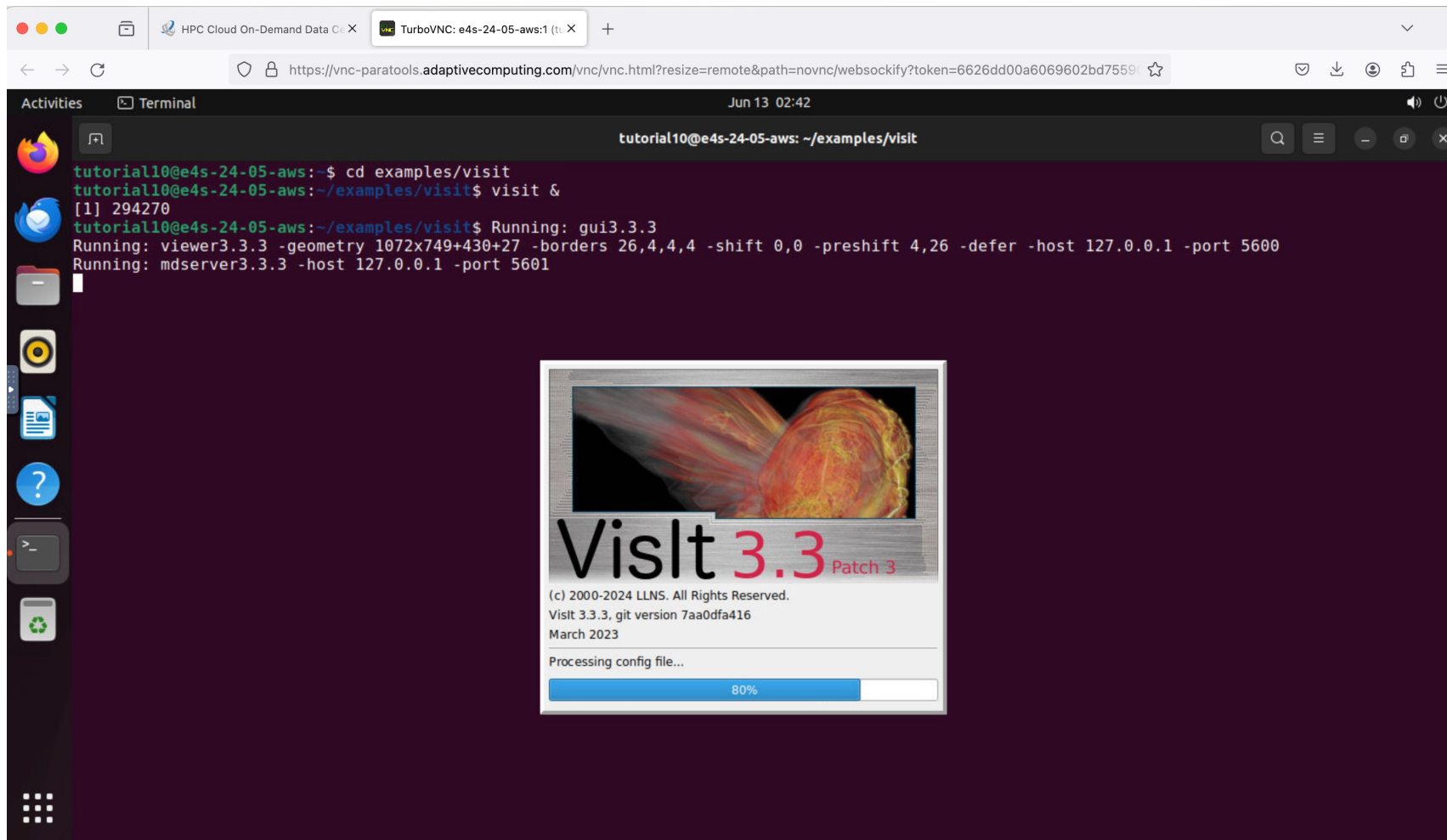
spack find -x

spack find

spack find +cuda

nvidia-smi

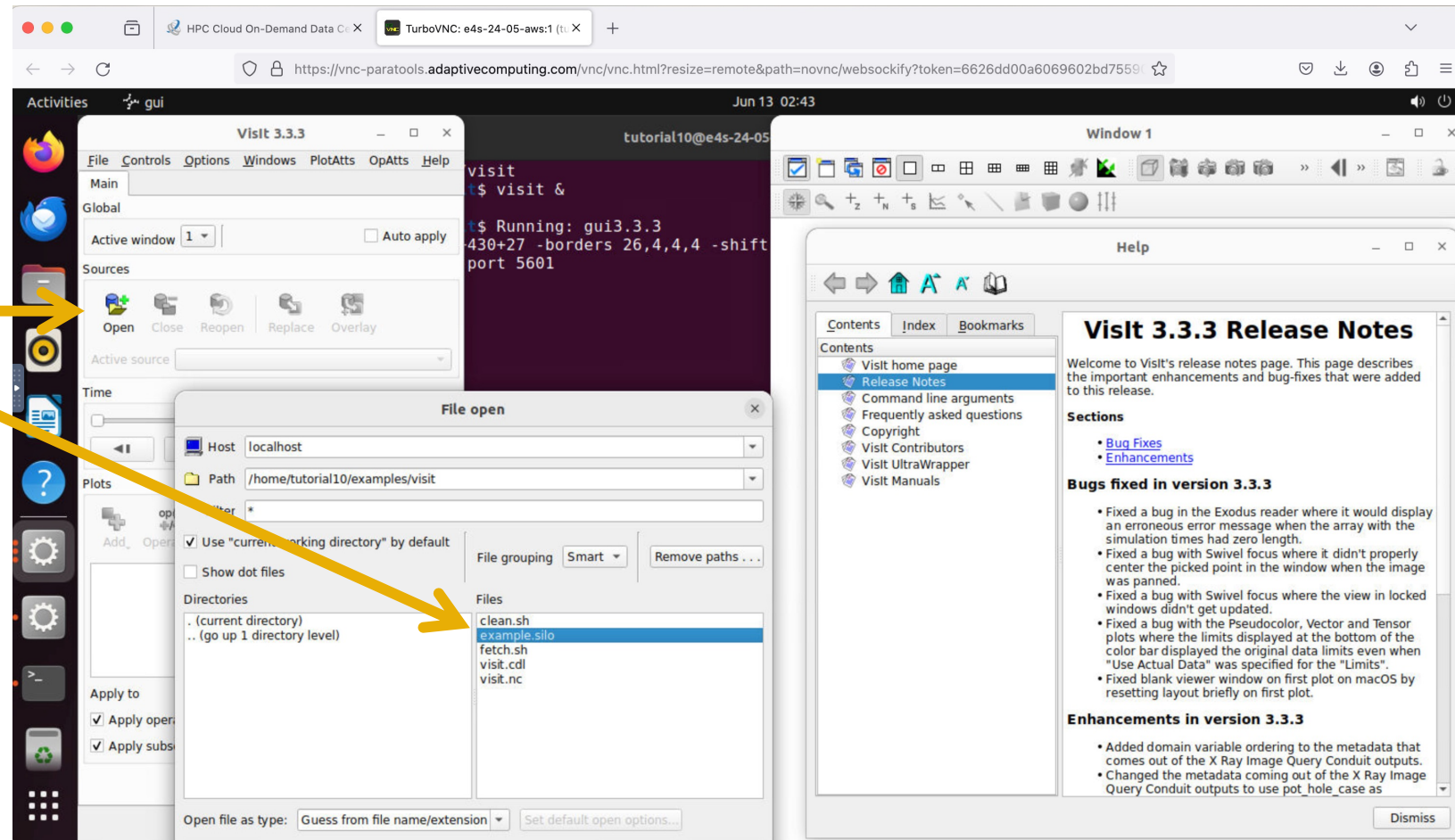
VisIt visualizer



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

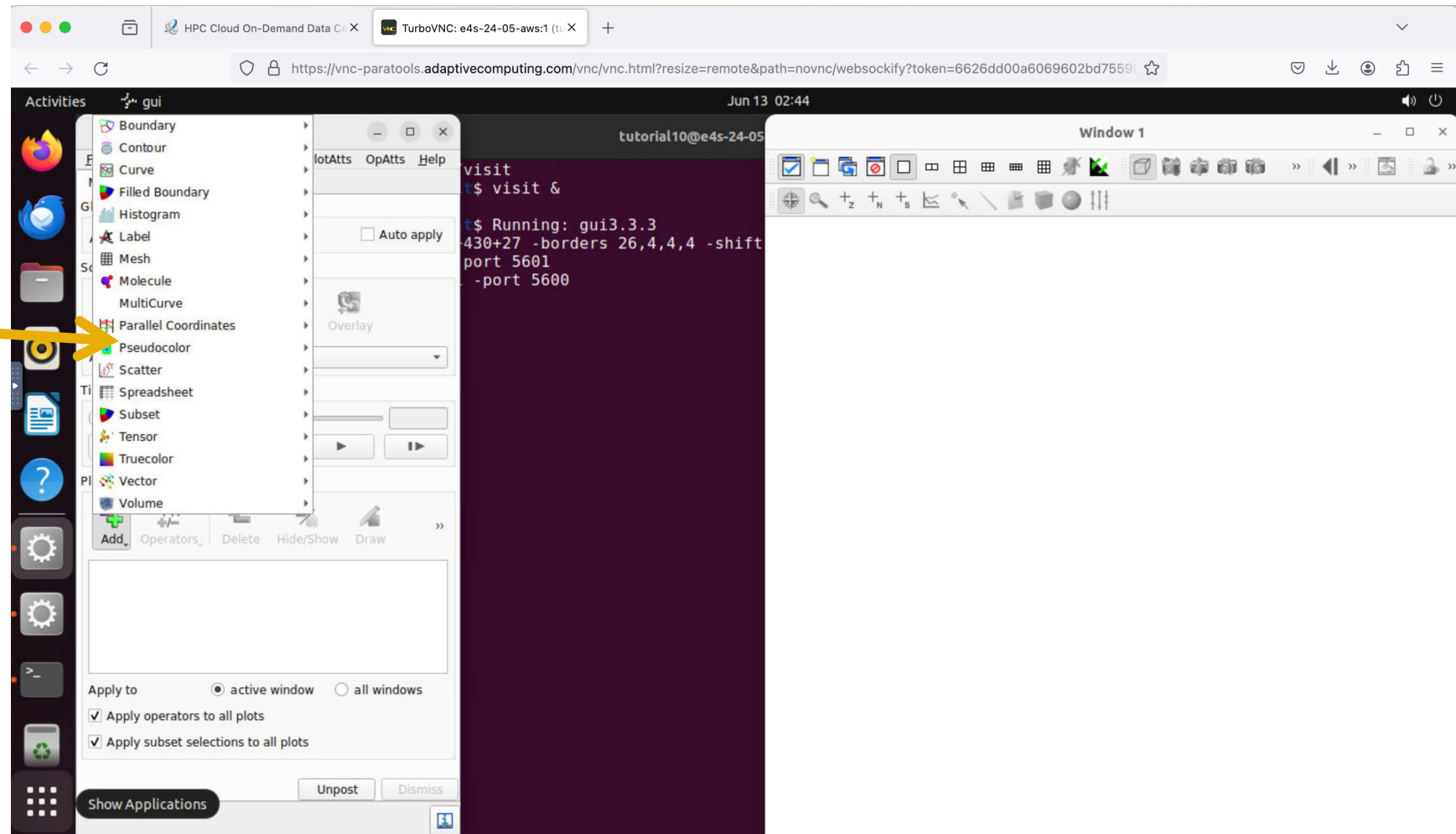

VisIt visualizer

Open example.silo



VisIt visualizer

Add Pseudocolor →
Pressure



VisIt visualizer

Add Pseudocolor →
Pressure
Click Draw
Rotate image

The screenshot displays the VisIt 3.3.3 interface within a TurboVNC session. The main window shows a 3D visualization of a pressure field. The plot area is titled "DB: example.silo" and "Cycle: 0". A color scale legend on the left indicates the pressure values, ranging from 1.104 (blue) to 5.779 (red). The plot is labeled with "Height (parsec)", "Width (parsec)", and "Depth (parsec)". The axes are labeled "x", "y", and "z". The status bar at the bottom right shows "user: tutorial10" and "Thu Jun 13 02:44:24 2024".

The interface includes a menu bar (File, Controls, Options, Windows, PlotAtts, OpAtts, Help) and a toolbar. The "Plots" section shows a list of plots, with "Pseudocolor - pressure" selected. The "Draw" button is highlighted with a yellow arrow. The "Apply to" section shows "active window" selected, and "Apply operators to all plots" and "Apply subset selections to all plots" are checked.

VisIt visualizer

Add Operators →
Isosurface
Click Draw
Rotate image

The screenshot displays the VisIt 3.3.3 interface within a TurboVNC session. The main window shows the 'Add Operators' menu, with 'Pseudocolor - Isosurface(pressure)' selected. The 'Active source' is 'example.silo'. The 'Apply to' options are set to 'active window', and 'Apply operators to all plots' and 'Apply subset selections to all plots' are checked. The 'Draw' button is highlighted. The 3D visualization window shows a complex, multi-lobed structure rendered in a green-to-yellow color scale, representing pressure. The axes are labeled 'Height (parsec)', 'Width (parsec)', and 'Depth (parsec)'. A color bar on the left indicates the pressure range from 1.104 to 5.779 Pa. The terminal window shows the command '\$ visit &' and the output '\$ Running: gui3.3.3 430+27 -borders 26,4,4,4 -shift port 5601 -port 5600'. The user is 'tutorial10' and the session is dated 'Thu Jun 13 02:45:15 2024'.

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Support Acknowledgments

- US Department of Energy (DOE)
 - Office of Science contracts, ECP
 - SciDAC, LBL contracts
 - LLNL-LANL-SNL ASC/NNSA contract
 - Battelle, PNNL contract
 - ANL, ORNL contract
- Department of Defense (DoD)
 - PETTT, HPCMP
- National Science Foundation (NSF)
 - Glassbox, SI-2
- NASA
- CEA, France
- Partners:
 - University of Oregon
 - ParaTools, Inc., ParaTools, SAS
 - The Ohio State University
 - University of Tennessee, Knoxville
 - T.U. Dresden, GWT
 - Juelich Supercomputing Center



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Acknowledgement

This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation's exascale computing imperative.

Acknowledgment

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR).



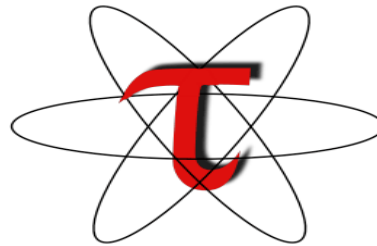
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