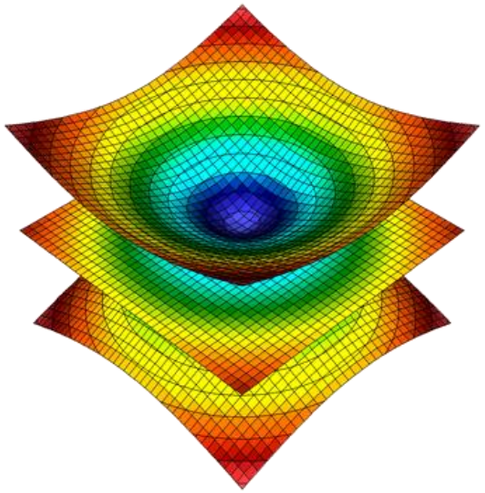


Scientific Visualization 210

ParaView and VisIt: *Scripting and Supercomputing Workflows*

KAUST Visualization Core Lab

James Kress

Workshop Site: wiki.vis.kaust.edu.sa/training

KAUST VISUALIZATION CORE LAB

Disclaimer

- Only KAUST students, faculty, staff, and those with existing projects on Shaheen or Ibex will be able to try the Shaheen and Ibex examples

- Everyone will be able to try the scripting workflows locally, which you can then translate for use on your own cluster/system

Workshop Setup

- Never logged in to Ibex before?
  - Do so now so that your scratch/user directory will have time to get setup
    - *ssh -X <username>@ilogin.ibex.kaust.edu.sa*
- Clone example repo on local machine
  - *git clone https://gitlab.kitware.com/jameskress/KAUST_Visualization_Vignettes*
    - ex00 - This script shows how to load a data set and then query information about the mesh, variables, and more
    - ex01 - This script shows how to create a screenshot and save it to disk
    - ex02 - This script shows how to take a series of screenshots while moving the camera and creating a movie
    - ex03 - This script shows how to animate the visualization of multiple iso surface values, showing different segments of a static data set
    - ex04 - This script shows how to animate the progress of streamlines in a flow field
    - ex05 - This script shows how to load and step through a multi time step file and take a screenshot per step
    - ex06 - This script shows the value of distributed computation, using a large data set to create a series of interesting visualizations of a cyclone simulation

Workshop Setup

mac machines

- Install ParaView --- 5.13.1
  - https://www.paraview.org/download/
  - Install XQuartz (X11)
    - https://www.xquartz.org/
- Install VisIt --- 3.4.1
  - https://visit-dav.github.io/visit-website/releases-as-tables/#latest
  - Install ffmpeg
    - https://www.ffmpeg.org/download.html
- Extra info
  - If you want to view ibex files locally without ‘scp’
    - Download and install fuse and sshfs: https://osxfuse.github.io/
      - Install instructions: https://sbgrid.org/corewiki/faq-sshfs.md
  - If multiple versions of VisIt are installed, we need to add a version command to local scripts in the examples later in the workshop (e.g. “-v 3.4.1”)

Workshop Setup

windows machines

- Install ParaView
  - https://www.paraview.org/download/
  - Install PuTTY
    - https://www.putty.org/
- Install VisIt
  - https://visit-dav.github.io/visit-website/releases-as-tables/#latest
  - Install ffmpeg
    - https://www.ffmpeg.org/download.html
      - Unzip this file by using any file archiver such as Winrar or 7z
      - Rename the extracted folder to ffmpeg and move it into the root of C: drive or location of your preference
      - Run the following in cmd: setx /m PATH "C:\ffmpeg\bin;%PATH%"
      - Reboot
- Extra info
  - Don't install VisIt in path with a space in it (`` '')
    - VisIt does not like this
  - I suggest running all the terminal examples in:
    - Ubuntu for Windows
      or
    - Visual Studio Code
  - If you want to view ibex files locally without 'scp'
    - Download and install SFTP Drive
      - https://www.nsoftware.com/sftp/drive/

Workshop Setup

linux machines

- Install ParaView
  - https://www.paraview.org/download/
- Install VisIt
  - https://visit-dav.github.io/visit-website/releases-as-tables/#latest
  - Install ffmpeg
    - https://www.ffmpeg.org/download.html
    - apt-get install ffmpeg

Workshop Notes

- Examples have been tested on the following:
  - Mac M Series
    - ParaView has an issue with ex04, investigating
  - Mac Intel
    - Everything runs
  - Linux Ubuntu 20
    - Everything runs
  - Windows
    - Everything runs
  - Ibex & Shaheen
    - Everything runs

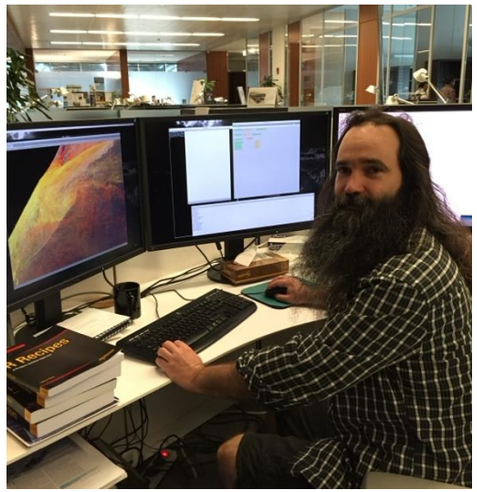
Visualization Core Lab

Overview of Facilities & Services

The Team

Dr. Sohaib Ghani
(LEAD STAFF SCIENTIST)

- VISUAL ANALYTICS
- INFORMATION VIS
- STATISTICAL ANALYSIS

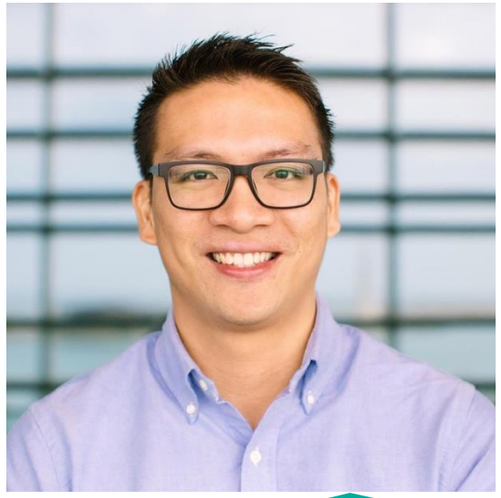


Thomas Theussl
SCIVIS

- SCIENTIFIC VISUALIZATION
- LARGE DATA ANALYSIS
- DISTRIBUTED VISUALIZATION

Dr. James Kress
HPC SCIVIS

- VISUALIZATION SOFTWARE
- HPC INSITU VISUALIZATION
- DISTRIBUTED VISUALIZATION



Dr. Ronell Sicat
VR/AR

- SCIENTIFIC VISUALIZATION
- VR DEVELOPMENT
- 3D RECONSTRUCTION

Dr. Didier Barradas
Data Scientist

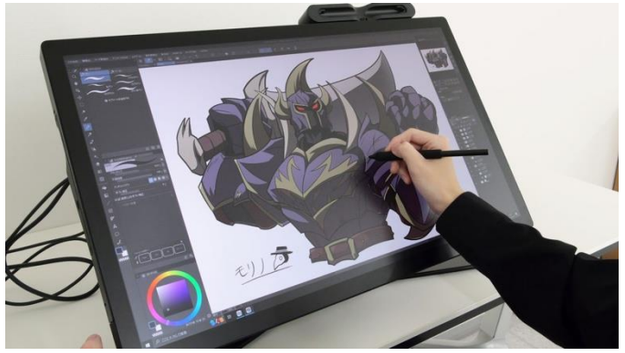
- DATA SCIENCE
- MACHINE LEARNING
- DEEP LEARNING

Dr. Abdelghafour Halimi
Data Scientist

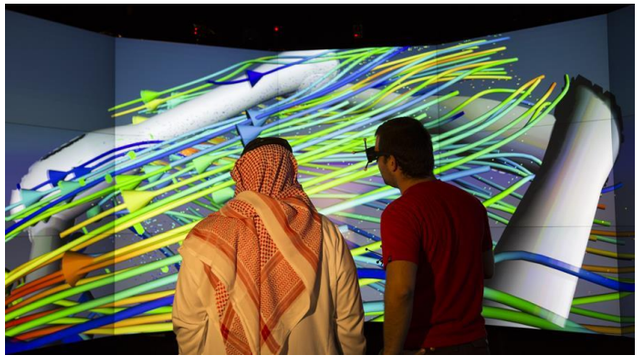
- Data Science
- Machine Learning
- Deep Learning

KVL Facilities

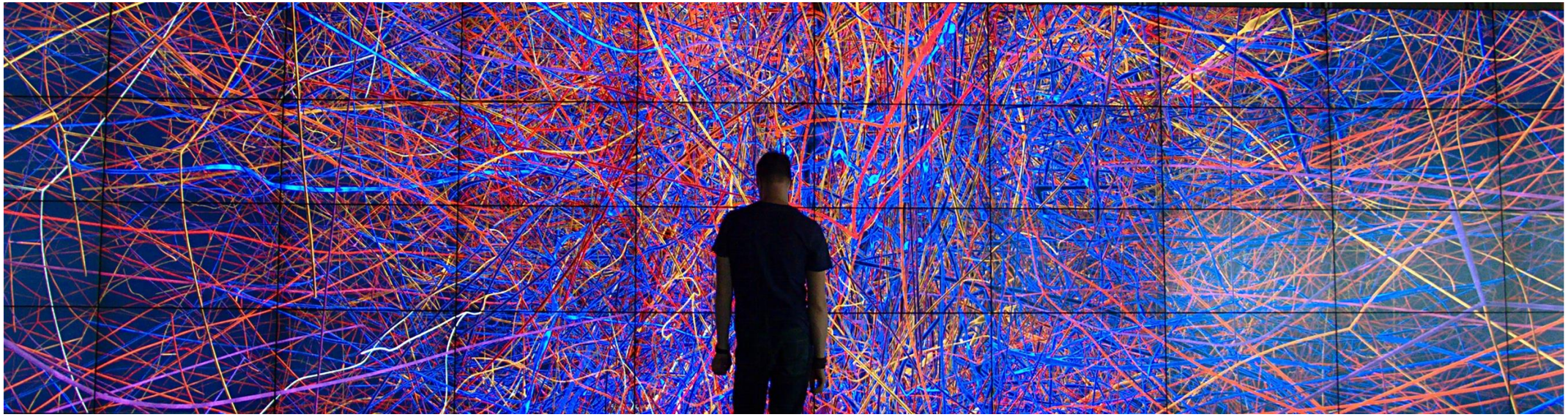
HMD’s



Segmentation Tablets



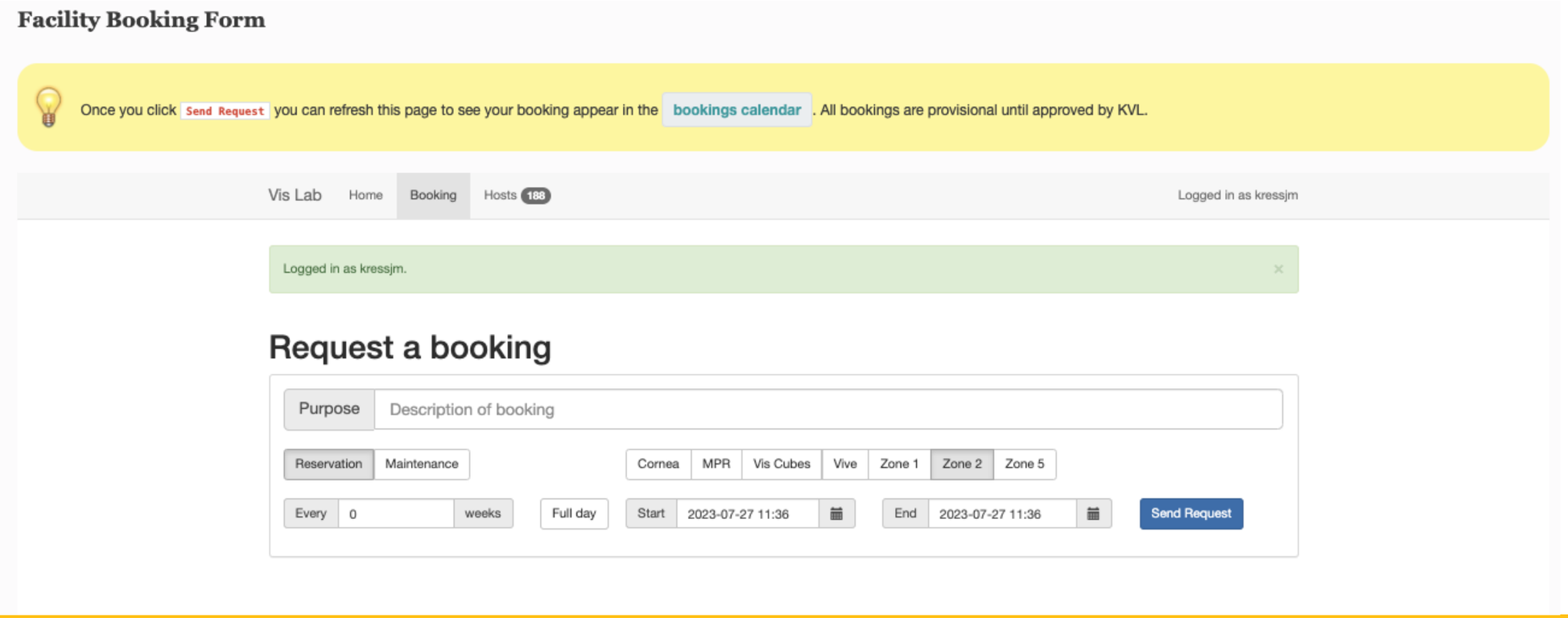
CUBES VR



ZONE 1/2 DISPLAY WALLS

Accessing KVL Facilities

- Book here (requires Portal Credentials):
  - https://wiki.vis.kaust.edu.sa/booking



Collaborating with KVL

- Standard Request
  - Load data ‘X’ in program ‘P’ to produce a visualization ‘V’
- Advanced Support
  - Investigative visualization –
    - Asking “why?” & “what?” of your data
- Collaboration
  - Work with you through your research and discovery cycle

Upcoming Training Events

Scientific Visualization Workshop Series Spring 2025

Date	Training Event	Speaker	Registration
~~January 28, 2025~~	~~Scientific Visualization 101: Amira & Avizo - An Introductory Hands-On Workshop~~	~~Thomas Theussl~~	~~Register~~
~~February 11, 2025~~	~~Scientific Visualization 101: Augmented and Virtual Reality for Data Visualization~~	~~Ronell Sicat~~	~~Register~~
February 18, 2025	Scientific Visualization 210: ParaView & VisIt ~ Scripting and Supercomputing Workflows	James Kress	Register

Data Science onboarding to Ibex Spring 2025

Date	Training Event	Speaker	Registration
~~February 4,2025~~	~~Data Science on-boarding on Ibex~~	~~Didier Barradas~~	~~Register~~

Introduction to Data Science Workshop Spring 2025

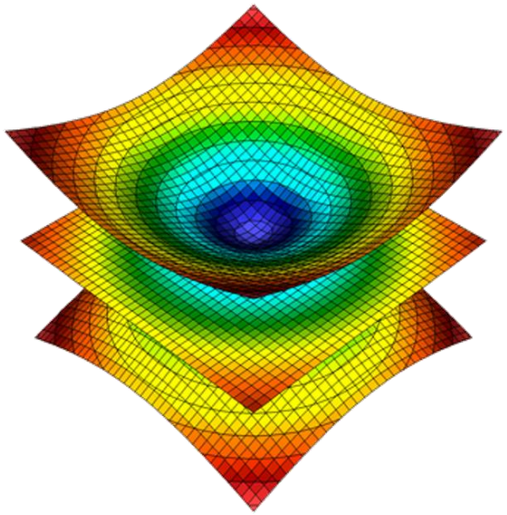
Date	Training Event	Speaker	Registration
April 9 ,2025	Introduction to Git for (Data) Scientists	Didier Barradas	Closed
April 10 ,2025	Introduction to PyTorch for (Data) Scientists	Didier Barradas	Closed

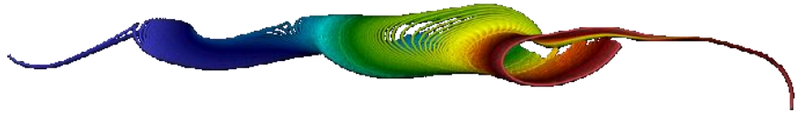
Workshop Goals

- Hands-on learning with ParaView and VisIt
  - Intermediate / advanced course
    - Scripting and workflows from desktop to HPC
  - Interactive sessions!
- Why ParaView and VisIt @ KAUST
  - Open source, scalable, multi-platform visualization applications with users worldwide
  - Available on all major computation resources at KAUST
    - Ibex and Shaheen
    - KVL Tiled-display walls

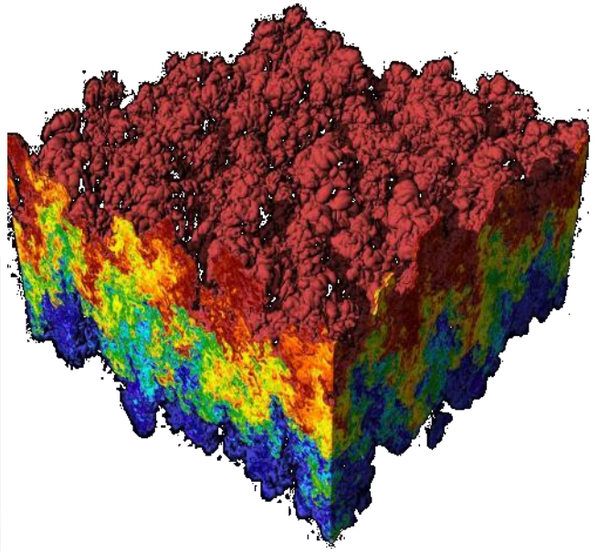
ParaView & VisIt

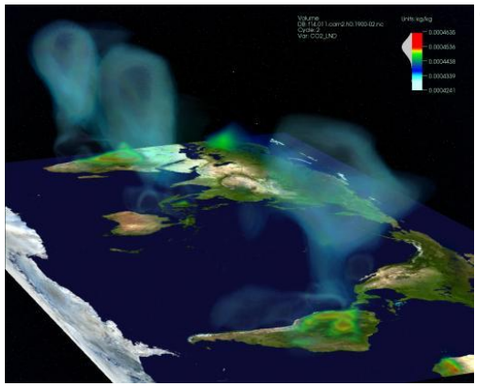
On Ibex and Shaheen



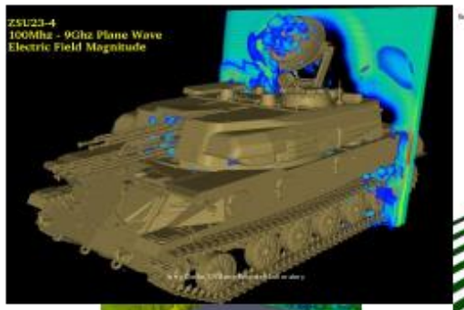


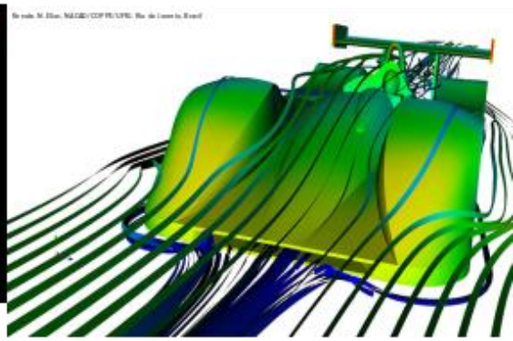
What are ParaView and VisIt?

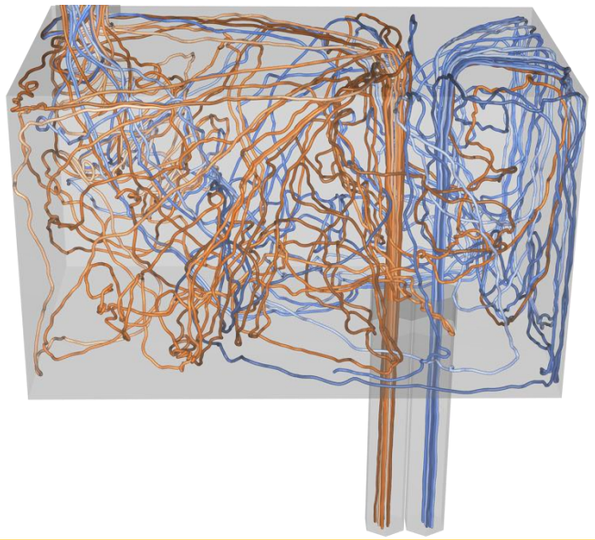


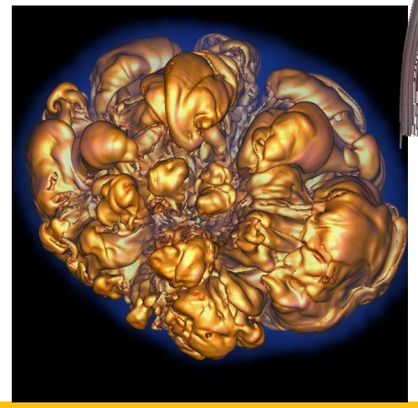


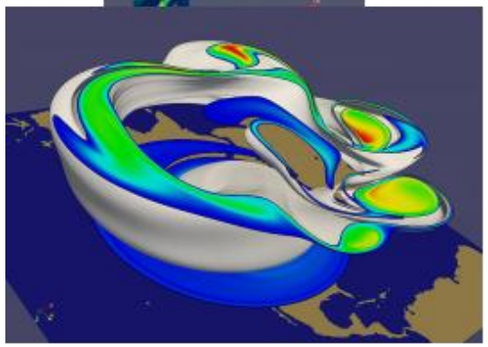
- Open-source turnkey application for data analysis and visualization of mesh-based data
- Infrastructure for parallel post-processing that scales from laptops to HPC clusters
- Built-in in situ capabilities

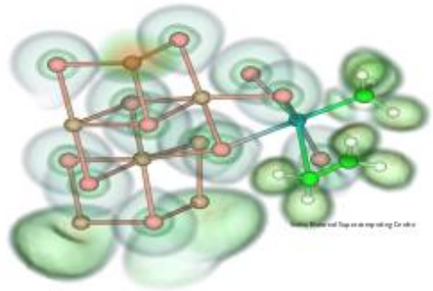












Source: Paraview Tutorial Slides

How Do I Obtain ParaView or VisIt?

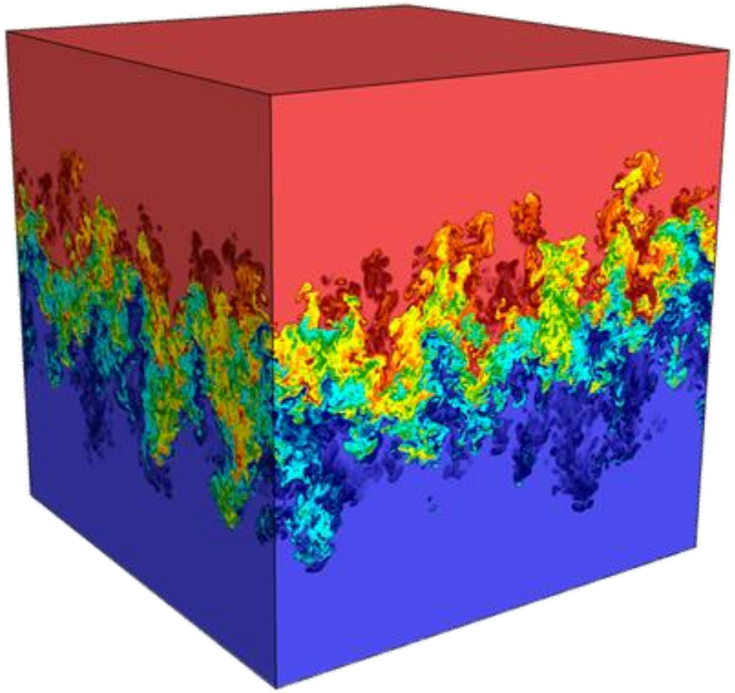
- Use an existing build:
  - For your Laptop or Workstation:
    - Binaries for Windows, OSX, and Linux (RHEL + Ubuntu)
      - https://visit-dav.github.io/visit-website/releases-as-tables/#latest
      - https://www.paraview.org/download/
  - KVL team manages builds on Ibex and Shaheen
- Build it yourself:
  - “build_visit” is a script that automates the process of building VisIt and its third-party dependencies. (docs: https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/building_visit/index.html)
  - https://gitlab.kitware.com/paraview/paraview-superbuild

Brief Look @ Core Concepts

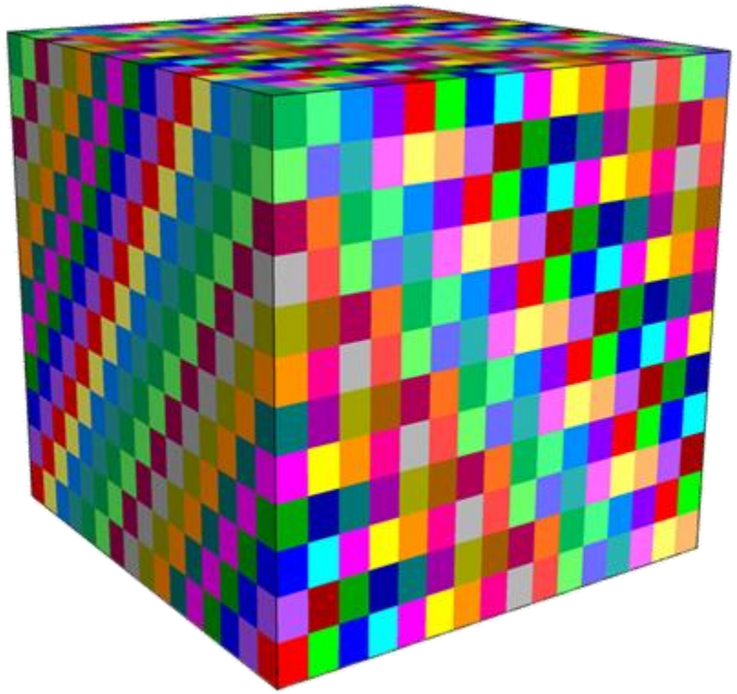
ParaView and VisIt Architecture

- **Plugin Architecture**
  - Custom File formats, Plots, Operators
  - Interface for custom GUIs in Python, C++ and Java
- **Python Interfaces**
  - Python scripting and batch processing
  - Data analysis via Python Expressions and Queries
- **In-Situ Coupling**
  - VisIt *Libsim*
  - ParaView Catalyst

ParaView and VisIt Use MPI for Distributed-Memory Parallelism

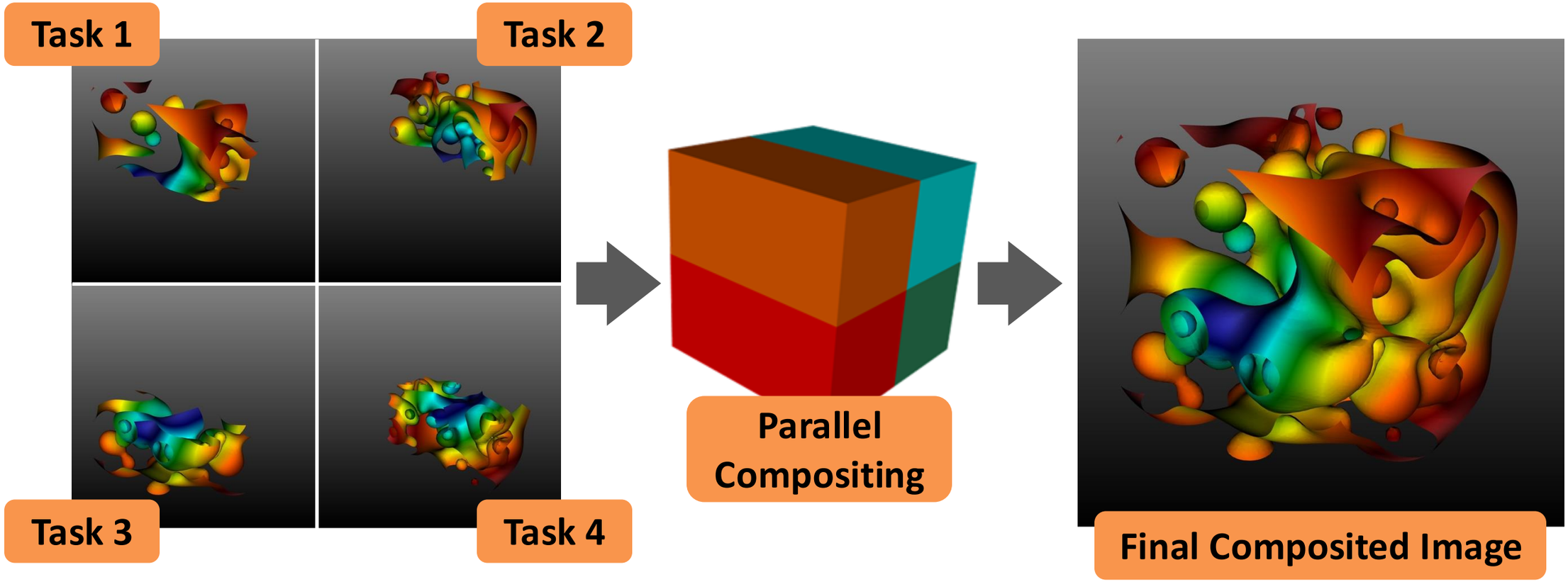


Full Dataset
(27 billion total elements)



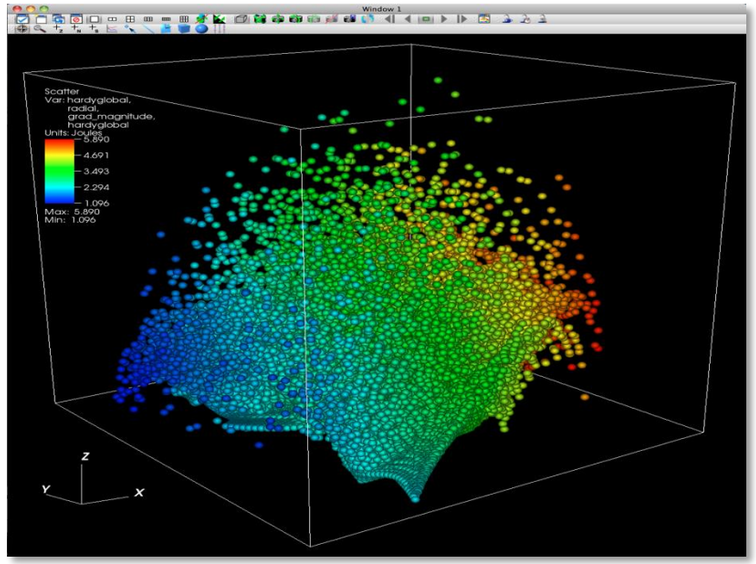
3072 sub-grids
(each 192x129x256 cells)

ParaView and VisIt Use Scalable Rendering



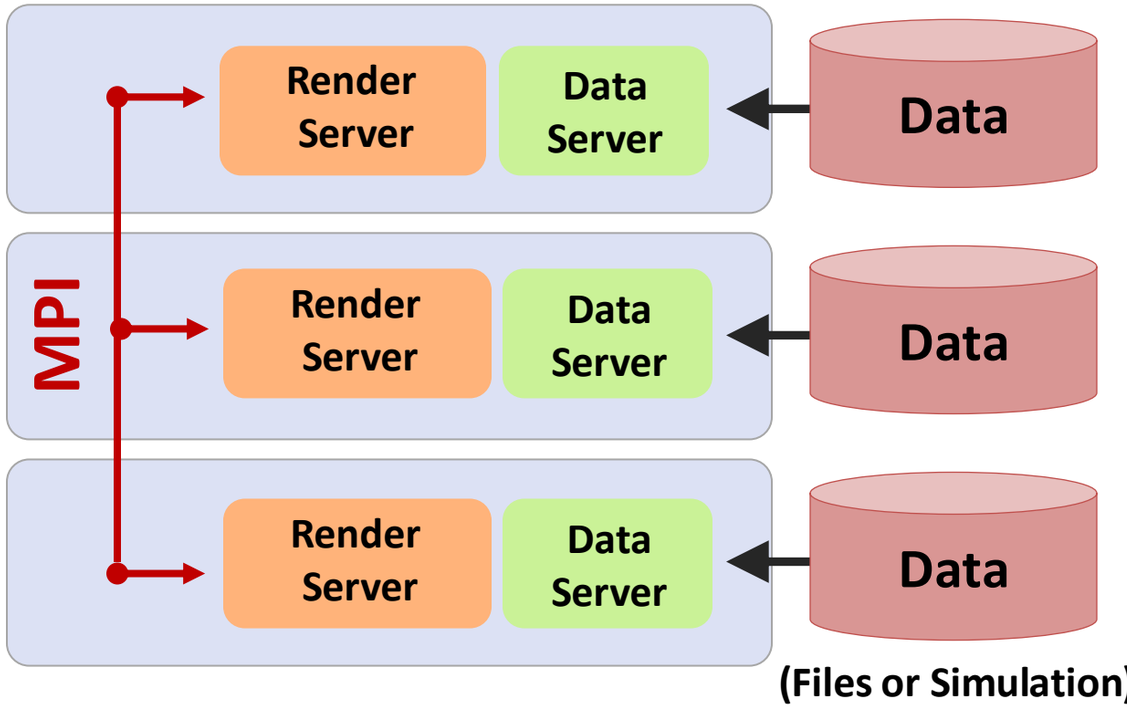
ParaView and VisIt Use a Client-Server Architecture

Client Computer



network connection

Remote System



Hands–On Session 1

Ibex/Shaheen Interactive Visualization Overview

Why use ParaView/VisIt on Ibex/Shaheen?

- Access to data generated w/out copying
- Can use distributed computation and rendering for very large data
- Ability to run scripted batch visualization
- Ability to run client-server mode
  - GUI runs locally, all computation is done remotely
  - Allows for fast GUI interactions and distributed computation

Download Example Repo on Ibex

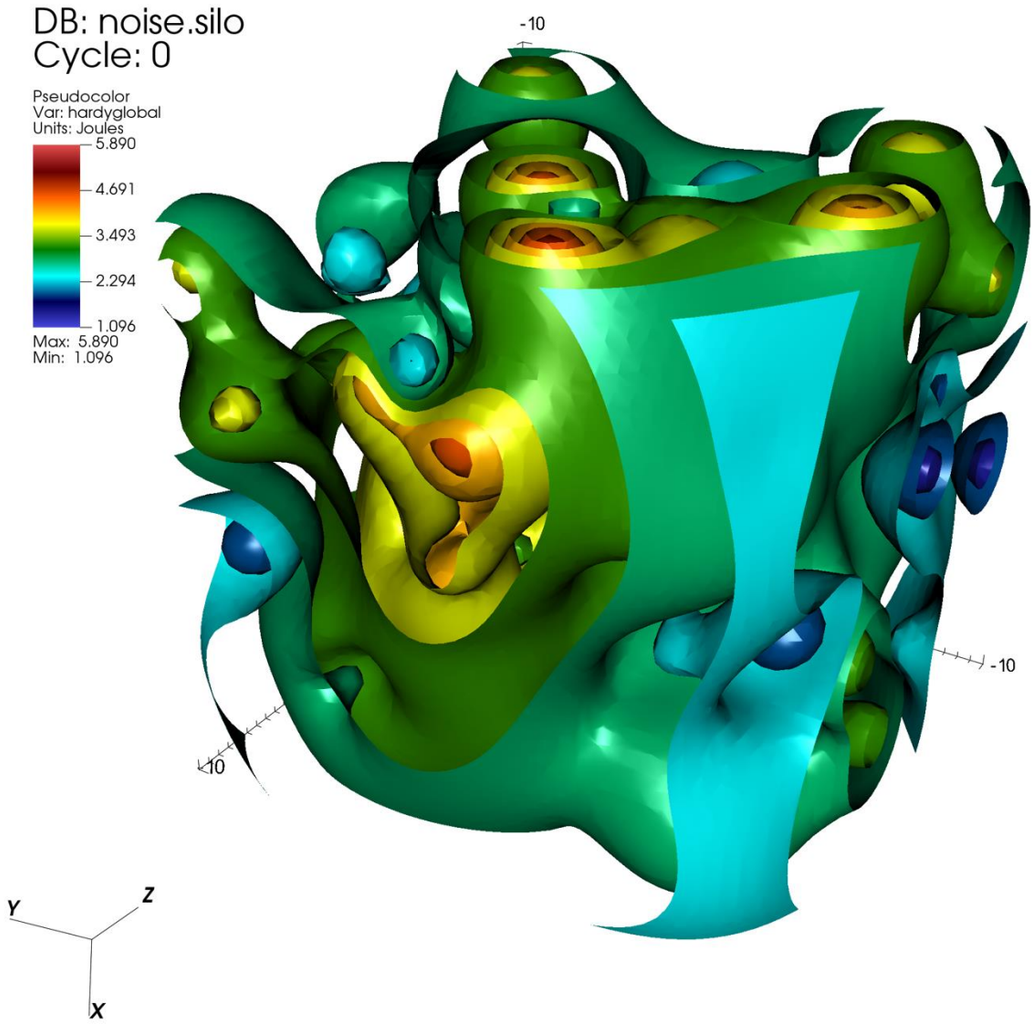
- Login to Ibex
  - *ssh <username>@ilogin.ibex.kaust.edu.sa*
- Navigate to scratch dir
  - *cd /ibex/scratch/<username>*

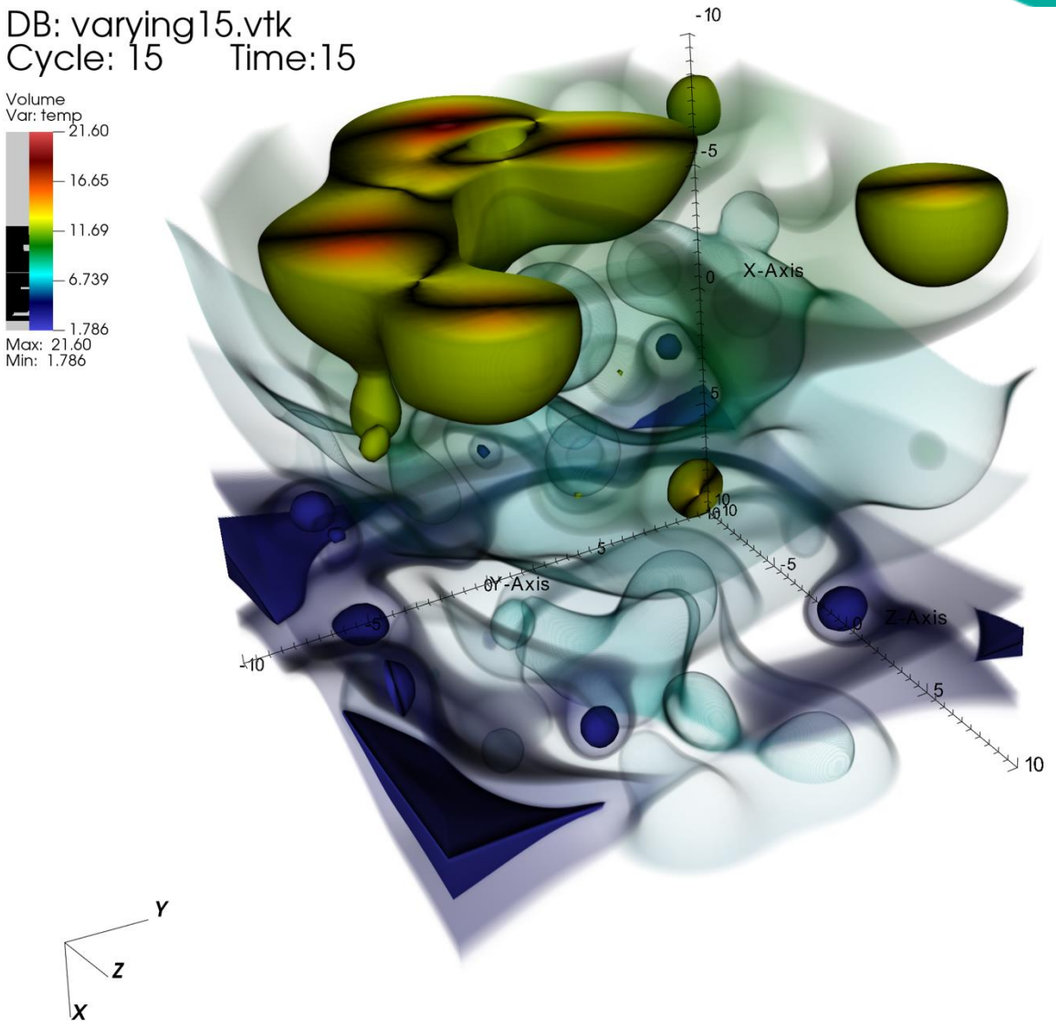
  Or, if you don't have a scratch
  - *cd /ibex/user/<username>*
- Clone repo
  - *git clone https://gitlab.kitware.com/jameskress/KAUST_Visualization_Vignettes.git*

Download Example Repo on Shaheen

- Login to Shaheen
  - *ssh <username>@shaheen.hpc.kaust.edu.sa*
- Navigate to scratch dir
  - *cd /ibex/scratch/<username>*
- Clone repo
  - *git clone https://gitlab.kitware.com/jameskress/KAUST_Visualization_Vignettes.git*

Repo Data


DB: noise.silo
Cycle: 0
Pseudocolor
Var: hardyglobal
Units: Joules
5.890
4.691
3.493
2.294
1.096
Max: 5.890
Min: 1.096
-10
-10
-10
Y
Z
X


DB: varying15.vtk
Cycle: 15 Time:15
Volume
Var: temp
21.60
16.65
11.69
6.739
1.786
Max: 21.60
Min: 1.786
-10
-5
0
5
10
X-Axis
Y-Axis
Z-Axis
Y
Z
X

Hands–On Session 1: Part I

Ibex/Shaheen Interactive Visualization with ParaView

Initially Accessing ParaView on Ibex

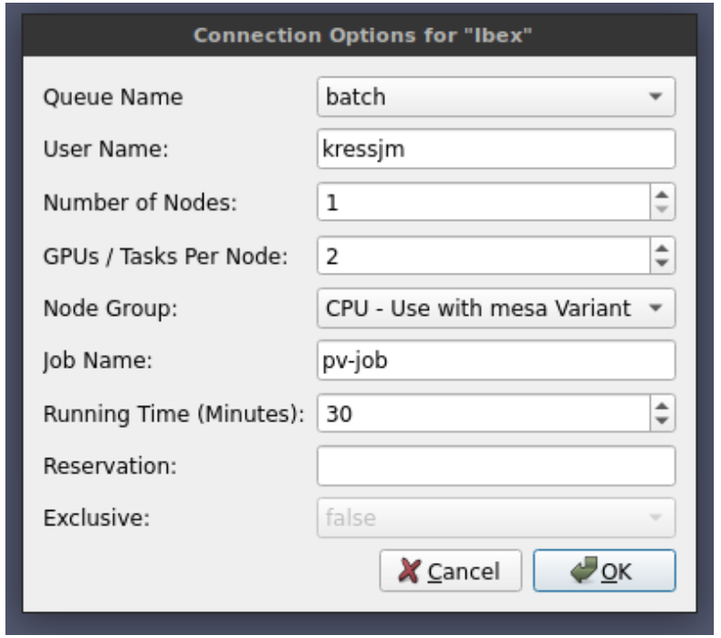
1. Check available ParaView versions on Ibex (use ***glogin***)

```
kressjm@login510-22:/home/kressjm$ module avail paraview

-------------------- /sw/csgv/modulefiles/applications ----------------------
paraview/5.11.1-openmpi4.0.3-egl
paraview/5.11.1-openmpi4.0.3-mesa(default)
```

2. Download/use the latest ParaView version that ***matches*** Ibex
3. If first time using ParaView on Ibex, load the KAUST profile
   1. **Save the following servers.pvsc file to your local computer:** *ibex_server*
   2. **Start ParaView:** select <File/Connect> to begin
   3. **Import Servers:** Click <Load Servers> button and find the servers.pvsc file

Using ParaView Interactively on Ibex

- Open **ParaView** on your local computer
- Go to: *<File/Connect>* or click the *<Connect>* button on the GUI
- Click the *<Ibex>* configuration and click connect
- Set connection options:
  - Enter <User Name>
  - Ensure *<Node Group>* is set to *"CPU"*
  - Click *"OK"*
- This will prompt you for your Ibex password, unless you have passwordless ssh setup
- Once specified, the server side of ParaView will be launched, and you can interact with your data (after the job launches and reaches to top of the Ibex queue)



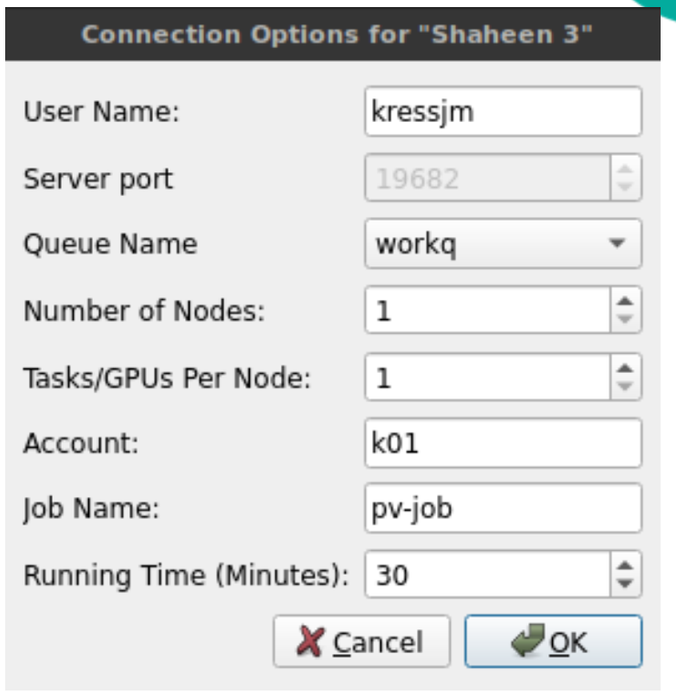
Initially Accessing ParaView on Shaheen

1. Check available ParaView versions on Shaheen

```
kressjm@login2:/home/kressjm$ module avail paraview

------------------------------------------------------------------------------ /sw/ex111genoa/modulefiles ---
paraview/5.13.1-egl          paraview/5.13.1-mesa(default)
```

2. Download/use the latest ParaView version that ***matches*** Shaheen
3. If first time using ParaView on Shaheen, load the KAUST profile
   1. **Save the following servers.pvsc file to your local computer:** *shaheen_server*
   2. **Start ParaView:** select <File/Connect> to begin
   3. **Import Servers:** Click <Load Servers> button and find the servers.pvsc file

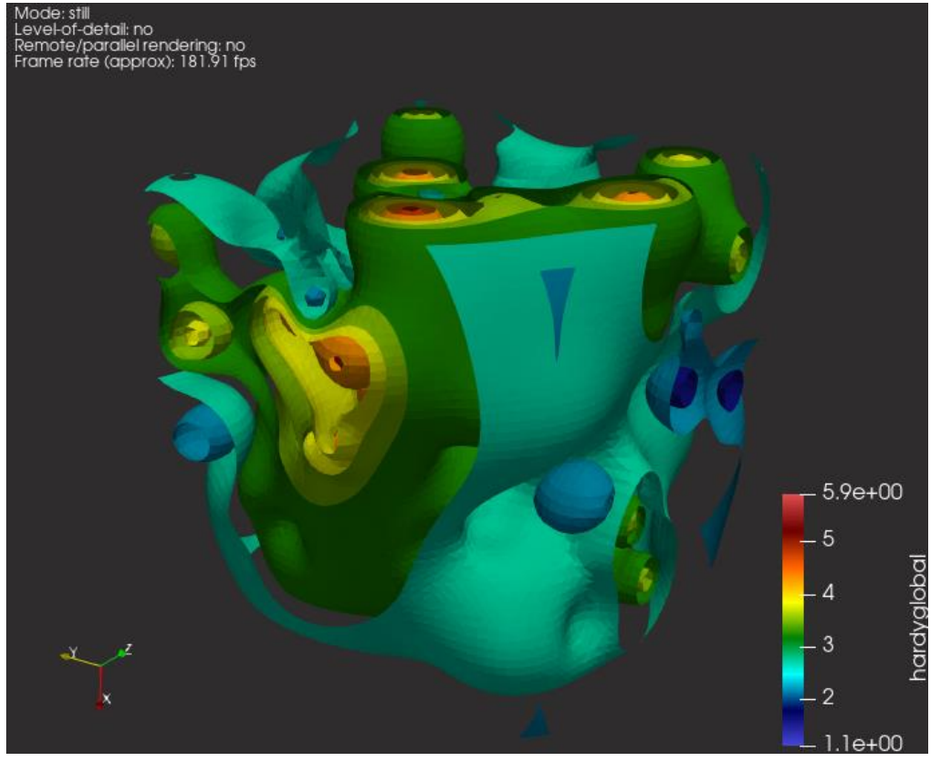
Using ParaView Interactively on Shaheen

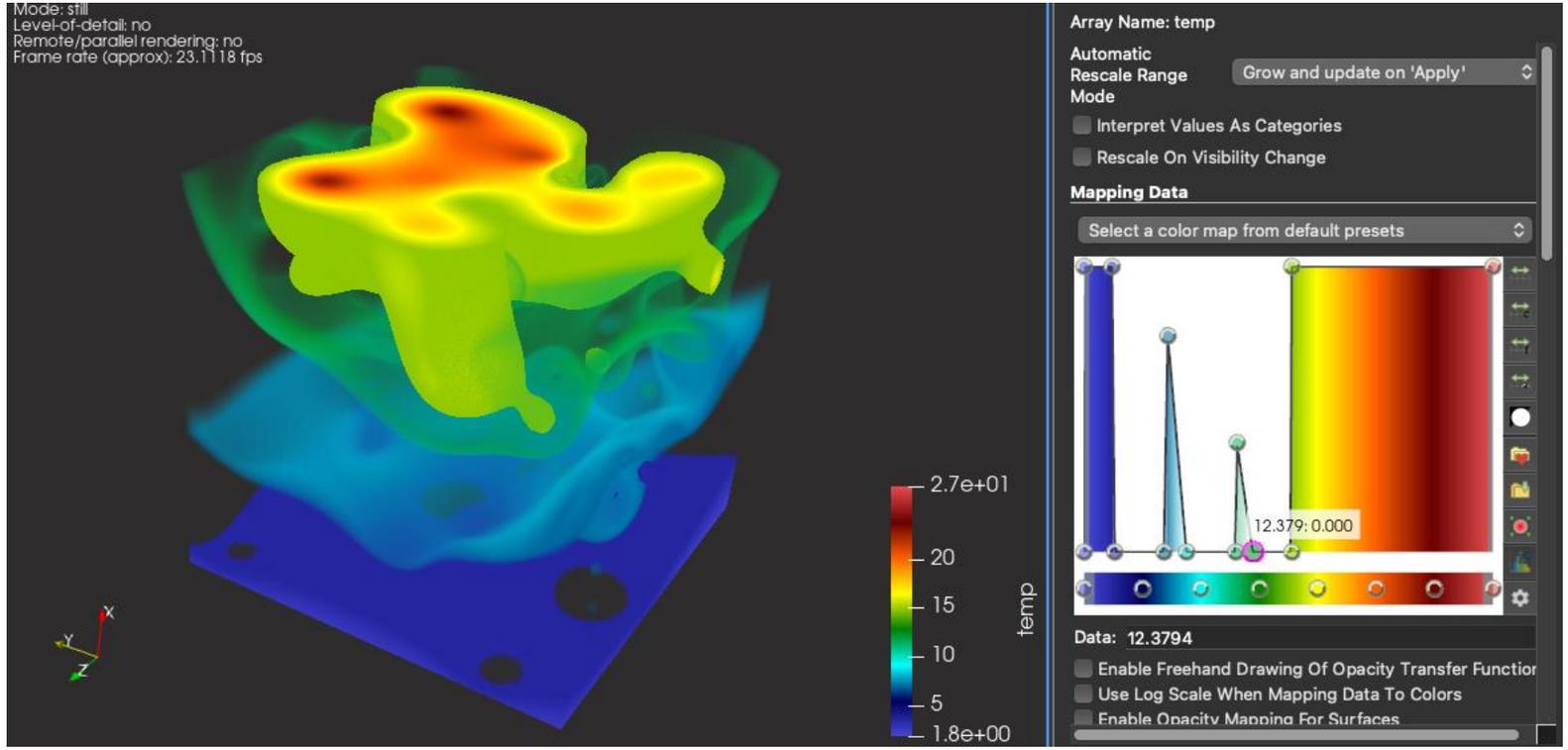


- Open **ParaView** on your local computer
- Go to: *<File/Connect>* or click the *<Connect>* button on the GUI
- Click the *<Shaheen 3>* configuration and click connect
- Set connection options:
  - Enter <User Name>
  - Set *<Queue Name>* is set to *"workq"*
  - *Enter your <Account>*
  - Click *"OK"*
- This will prompt you for your Shaheen password and OTP, unless you have passwordless ssh setup, then you just need OTP
- Once specified, the server side of ParaView will be launched, and you can interact with your data (after the job launches and reaches to top of the Shaheen queue)

Explore Example Repo Data Sets

- Load each of the example data sets and try different visualizations





Hands–On Session 1: Part II

Ibex/Shaheen Interactive Visualization with VisIt

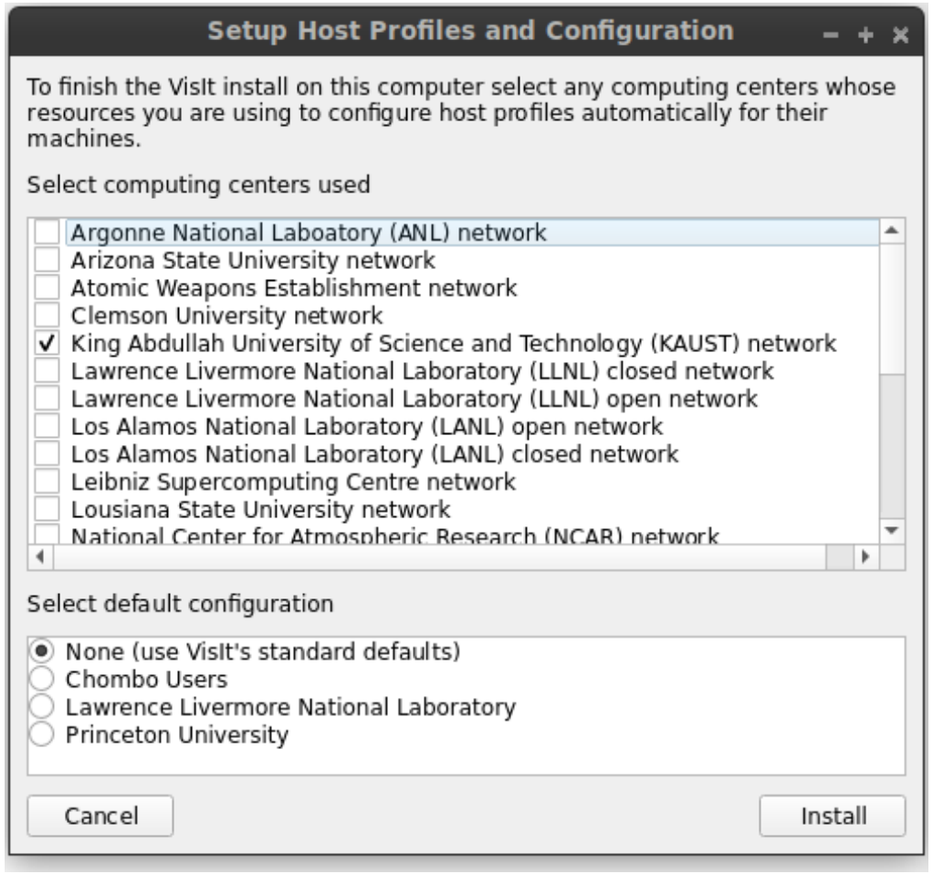
Accessing KAUST HPC Resources

- Must have an active/valid user account
- Load the KAUST profile
- Connect & Visualize

For instructions see:

- https://docs.hpc.kaust.edu.sa/soft_env/visualization/visit_overview.html

Note: The above process will not give you the Shaheen 3 host profile in VisIt versions 3.4.1 or older. For thos instances you will need to manually create the host profile using the information for the VisIt repository, located here: KAUST Shaheen 3 VisIt Host Profile.

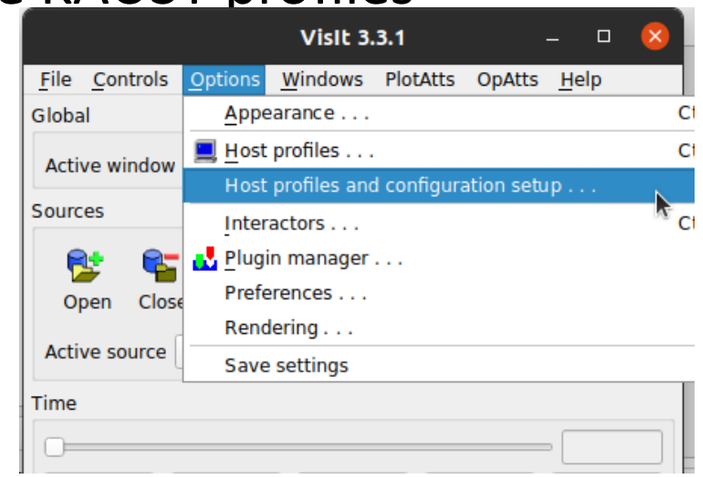


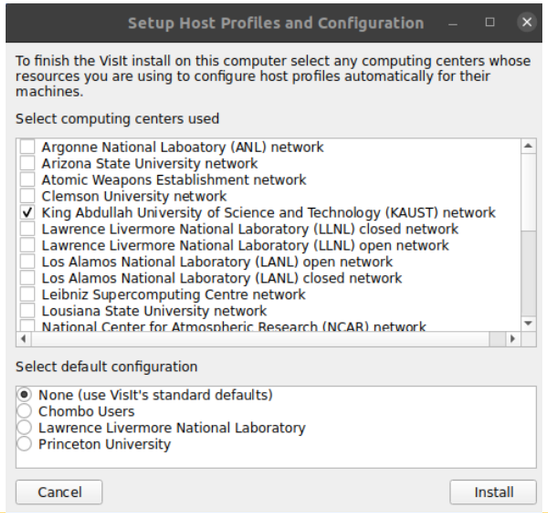
Initially Accessing VisIt on Ibex

1. Check available VisIt versions on Ibex (use ***ilogin***)

```
kressjm@login509-02-r:/home/kressjm$ module avail visit

---------------------- /sw/csi/modulefiles/applications ----------------------
visit/3.3.2
```

2. Download/use the latest VisIt version that ***matches*** Ibex
3. If first time using VisIt on Ibex, load the KAUST profiles
    1. Click *<Options/Host profiles and …>*
    2. Select KAUST network
    3. Click *<Install>*
    4. Save settings *<Options/Save Settings>*
    5. Relaunch VisIt

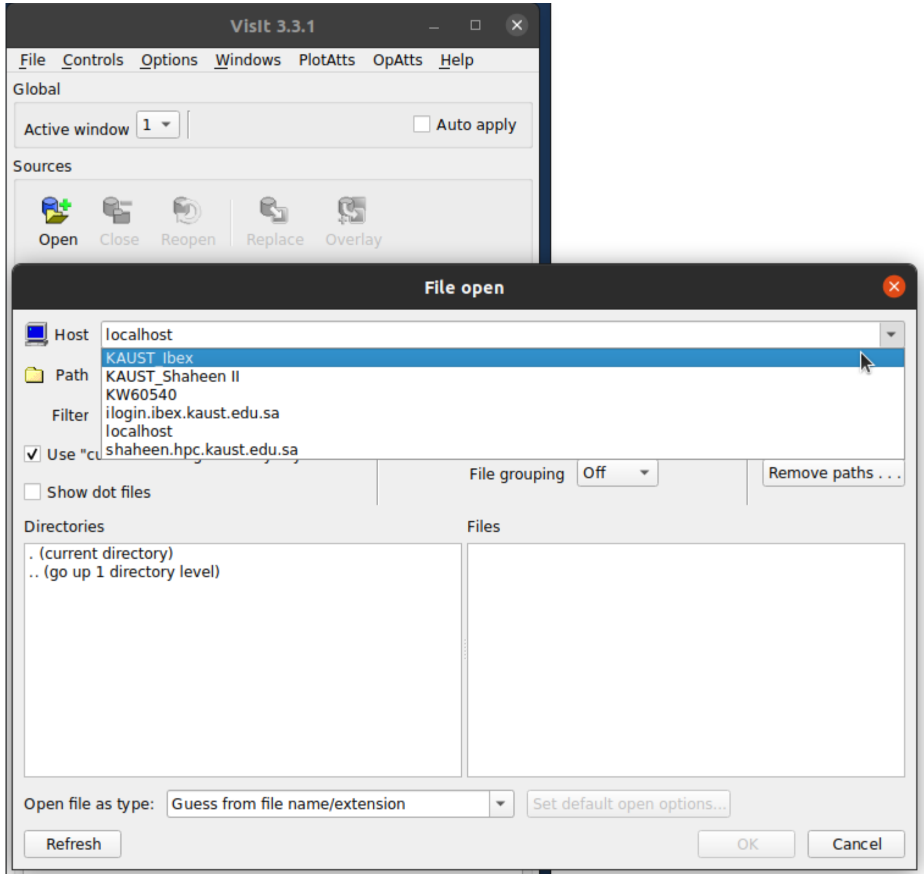




Using VisIt Interactively on Ibex

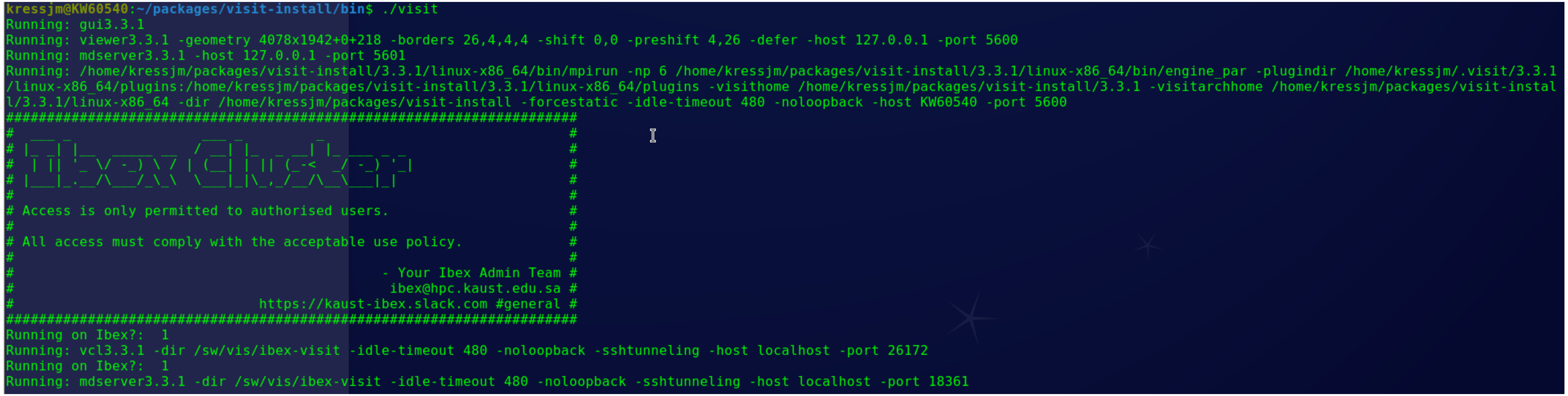
- Open **VisIt** on your local computer
- Go to: *<File/Open file>* or click the *<Open>* button on the GUI
- Click the *<Host>* dropdown menu on the *"File open"* window that popped up and choose *"Ibex"*
- This will prompt you for your Ibex password, unless you have passwordless ssh setup
- Navigate to the file you want to process
- Once you choose a file, you will be prompted for the number of nodes and processors you would like to use
- Once specified, the server side of VisIt will be launched, and you can interact with your data (after the job launches and reaches to top of the Ibex queue)

Using VisIt Interactively on Ibex Cont.

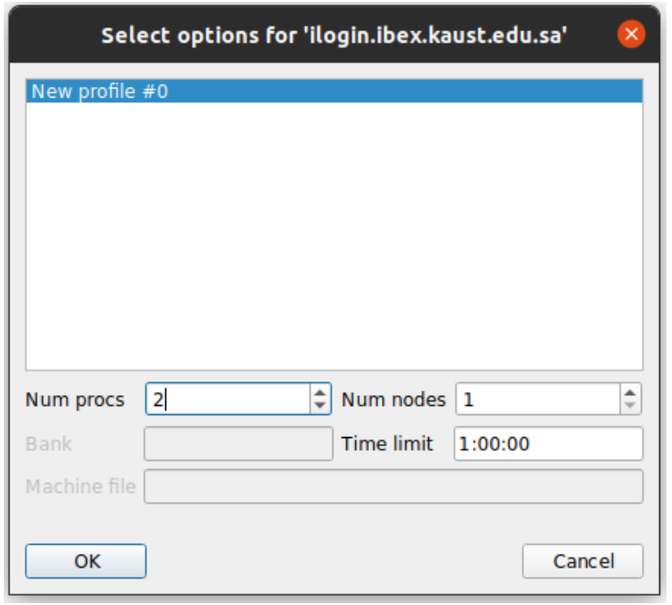


vcl – *VisIt Component Launcher (manages VisIt session)*

mdserver – *VisIt metadata server (interacts with GUI and databases)*



Using VisIt Interactively on Ibex Cont.




```
Running: /opt/slurm/cluster/ibex/install/bin/sbatch --export=HOME=/home/kressjm,LIBPATH=/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64/lib,LD_LIBRARY_PATH=/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64/lib/osmesa:/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64/lib/mesagl:/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64/lib:/sw/csi/gcc/8.2.0/el7.5_binary/lib64:/sw/vis/ibex-visit/bin/../3.3.1/linux-x86_64/lib,VISITHOME=/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1,VISITARCHHOME=/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64,VISITPLUGINDIR=/home/kressjm/.visit/3.3.1/linux-x86_64/plugins:/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64/plugins --partition=batch --time=1:00:00 --ntasks=2 --nodes=1 --tasks-per-node=2 /ibex/scratch/kressjm/visit.kaust.09:00:40
Submitted batch job 23496397
```

```
kressjm@login509-02-r:/ibex/scratch/kressjm$ cat visit.kaust.09\:00\:40
#!/bin/sh
cd /ibex/scratch/kressjm
ulimit -c 0
# Submitted on host login509-02-r
echo "LIBPATH=$LIBPATH"
echo "LD_LIBRARY_PATH=$LD_LIBRARY_PATH"
echo "VISITHOME=$VISITHOME"
echo "VISITARCHHOME=$VISITARCHHOME"
echo "VISITPLUGINDIR=$VISITPLUGINDIR"
srun --export=ALL --ntasks=2 --ntasks-per-node=2 /sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64/bin/engine_par -dir /sw/vis/ibex-visit -forcestatic -idle-timeout 480 -noloopback -sshtunneling -host login509-02-r -port 15602 -key 295fbdc83b814c55d533
```

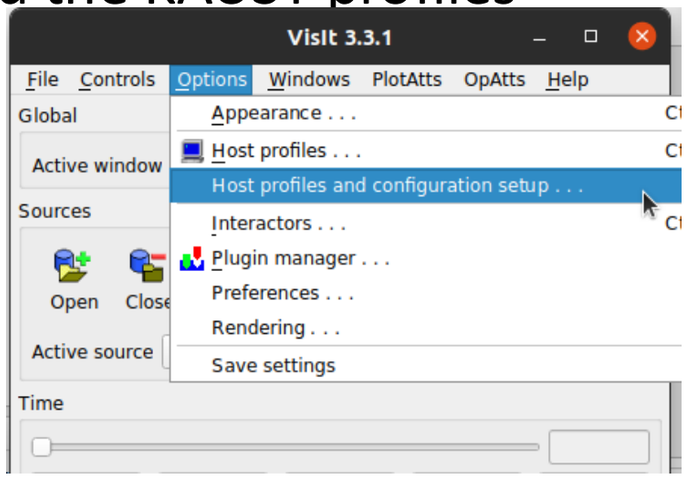
engine_par– *VisIt parallel computation engine*

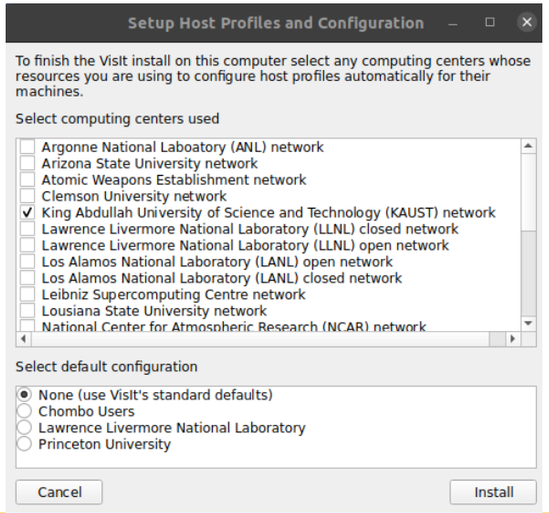
Initially Accessing VisIt on Shaheen

1. Check available VisIt versions on Shaheen

```
kressjm@login2:/home/kressjm$ module avail visit

------------------------------------------------------------------------------ /sw/ex111genoa/modulefiles --
visit/3.4.1
```

2. Download/use the latest VisIt version that ***matches*** Shaheen
3. If first time using VisIt on Shaheen, load the KAUST profiles
    1. Click *<Options/Host profiles and …>*
    2. Select KAUST network
    3. Click *<Install>*
    4. Save settings *<Options/Save Settings>*
    5. Relaunch VisIt



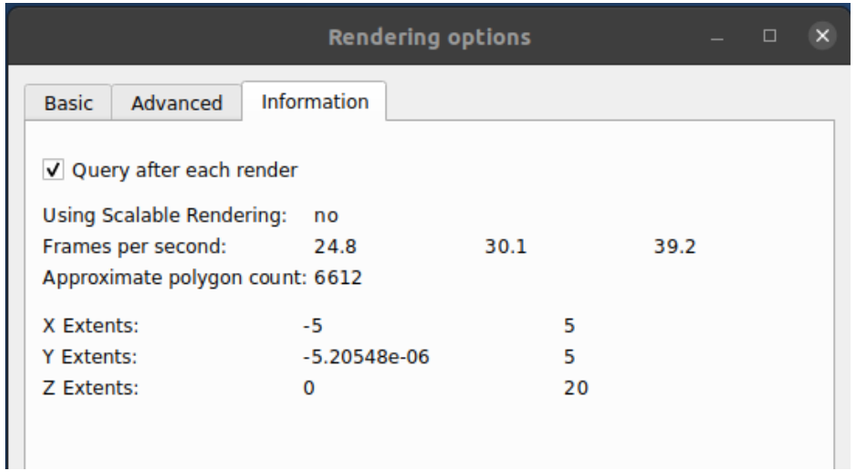


Using VisIt Interactively on Shaheen

- Open **VisIt** on your local computer
- Go to: *<File/Open file>* or click the *<Open>* button on the GUI
- Click the *<Host>* dropdown menu on the *"File open"* window that popped up and choose *"Shaheen 3"*
- This will prompt you for your Ibex password and OTP, unless you have passwordless ssh setup, then just the OTP
- Navigate to the file you want to process
- Once you choose a file, you will be prompted for the number of nodes, processors, and account ID
- Once specified, the server side of VisIt will be launched, and you can interact with your data (after the job launches and reaches to top of the Shaheen queue)

Explore Example Repo Data Sets

- Load each of the example data sets and try different visualizations
- Note on rendering
  - VisIt has two rendering modes
    - Transfer data to client for rendering
      - Done when data is small
    - Transfer images to client, rendering on the server
      - This is how VisIt can render extremely large data on clusters
      - This is called scalable rendering
      - You can turn on/off scalable rendering, see stats, and other options @ *<Options/Rendering>*



Hands–On Session 2: Part I

Scripting Visualization within ParaView

Download Example Repo Locally

- Navigate to your preferred local directory
- Clone repo
  - *git clone https://gitlab.kitware.com/jameskress/KAUST_Visualization_Vignettes.git*

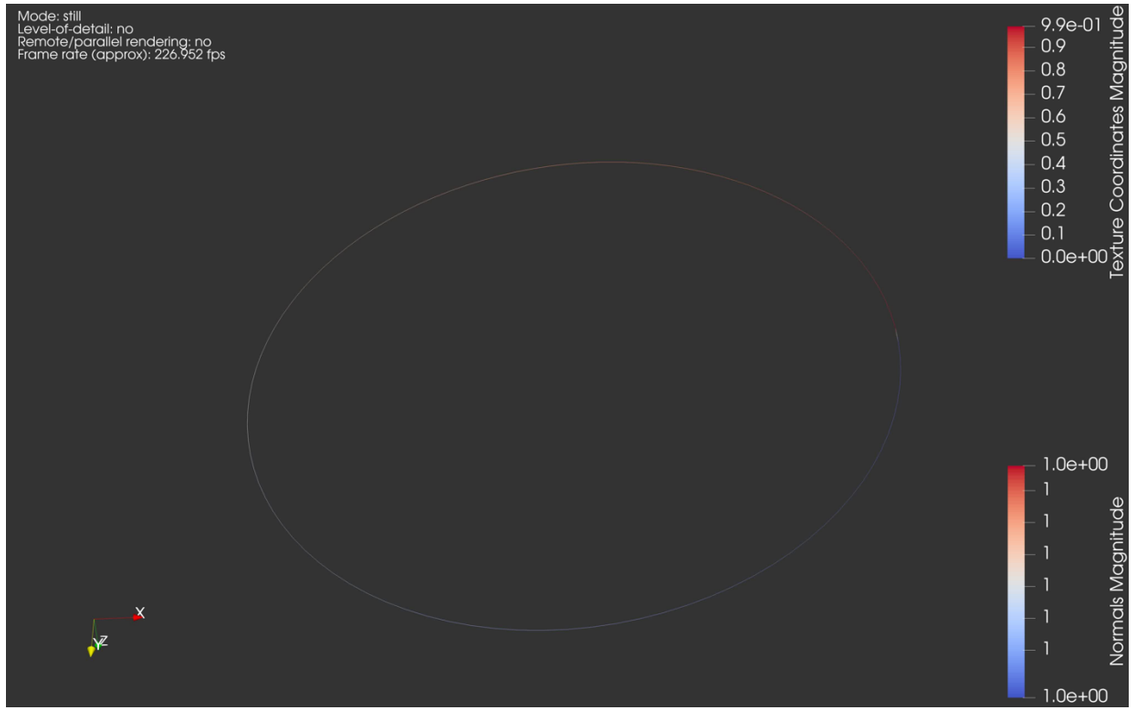
Using ParaView GUI and Python Simultaneously

- Open ParaView
  - Open Python shell: *<View/Python Shell>*

- *Go to ParaView Docs*
  - https://docs.paraview.org/en/latest/Tutorials/ClassroomTutorials/pythonAndBatchParaViewAndPython.html
  - We'll walk through some of the initial copy-paste examples

Running a Script Interactively in ParaView

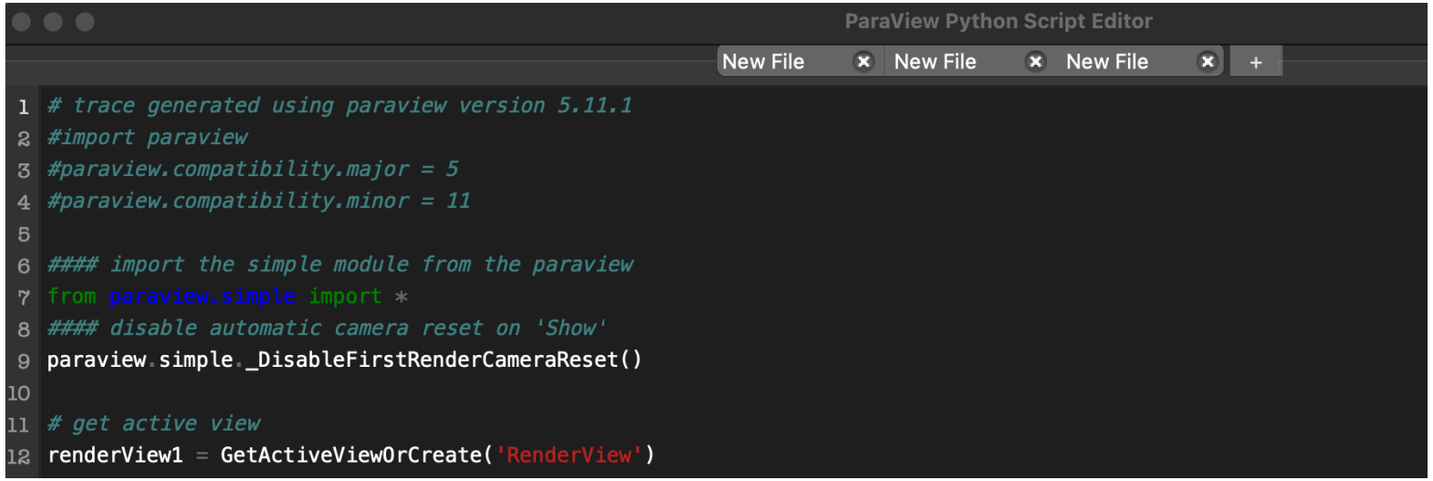
- Works just like the previous examples, but code is in a file
  - Use your favorite editor
  - Have more complicated multi-file scripts

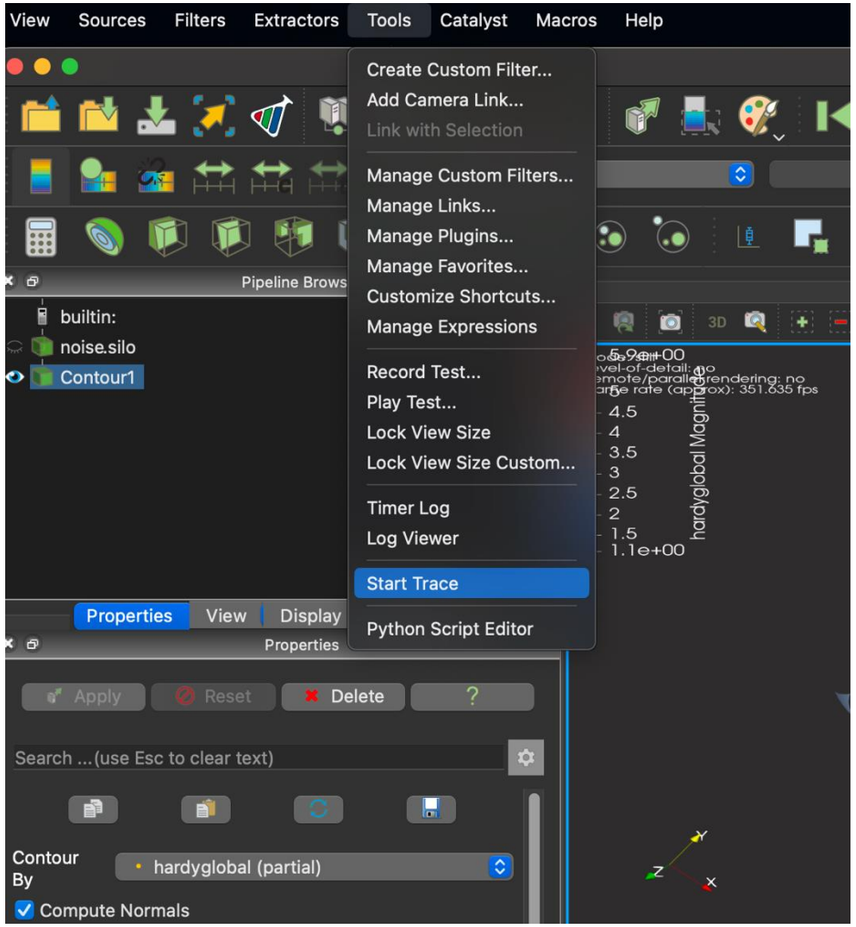


- Open the Python Shell
  - Click *<Run Script>*
  - Locate and run
    "/path/to/KAUST_Visualization_Vignettes/ParaView_Vignettes/ex02_pvAnimation/ex02_pvAnimation.py"

Tracing Your Actions

- Open ParaView
  - Start Trace: *<Tools/Start Trace>*
  - Interact with the GUI to do the vis you want
  - Stop Trace: *<Tools/Stop Trace>*
  - A lengthy trace will reproduce your actions



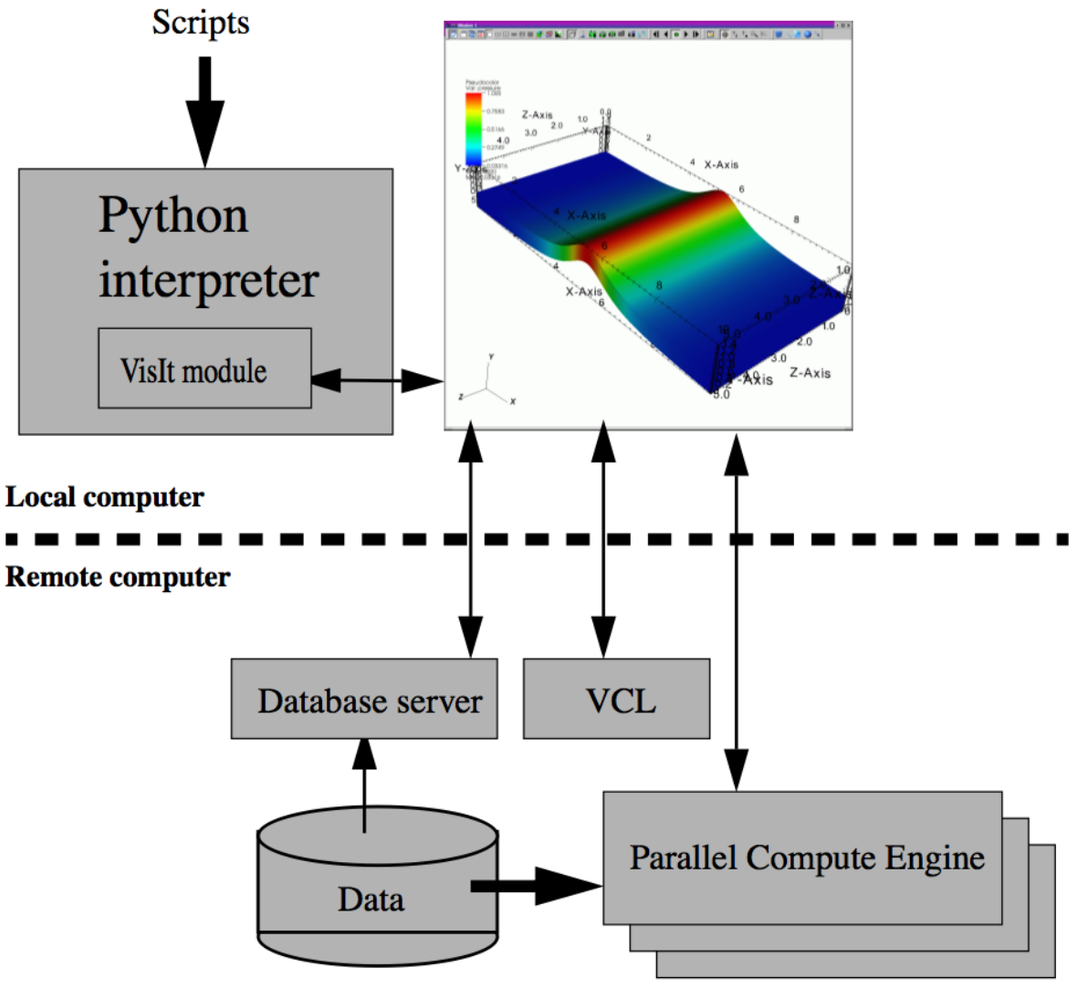


Hands–On Session 2: Part II

Scripting Visualization within VisIt

VisIt and Python

- VisIt can be used from python
  - *import sys*
  - *sys.path.append("/path/to/visit/<version>/<architecture>/lib/site-packages")*
    import visit
  - *visit.Launch()*
- Python can be used within VisIt



Using VisIt GUI and cli Simultaneously

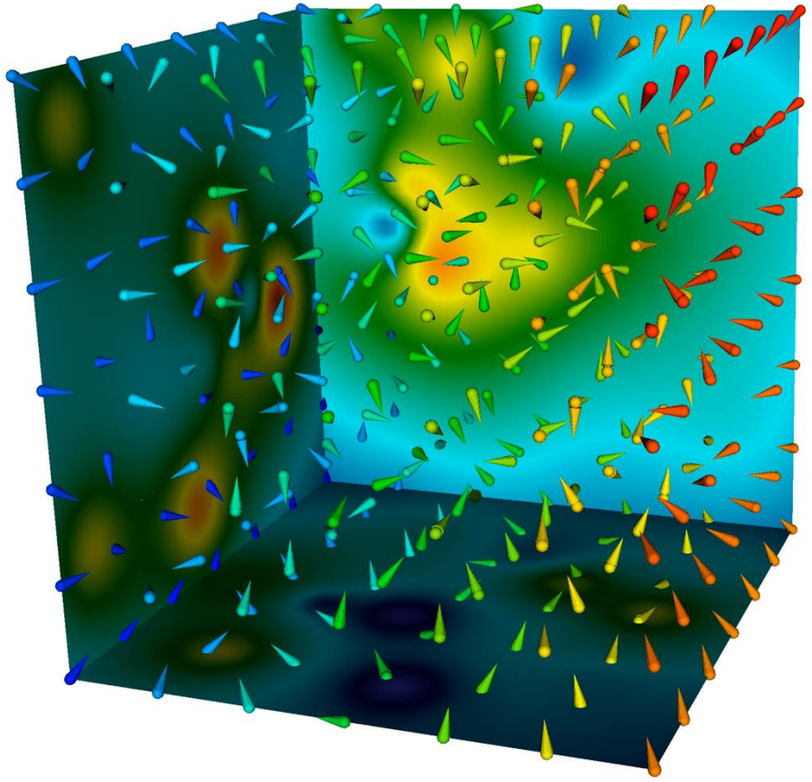
- Open VisIt
  - Open command window: *<Controls/Command>*

- *Go to VisIt Docs*
  - https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/tutorials/Scripting.html
  - We'll walk through some of the initial copy-paste examples

Running a Script Interactively in VisIt

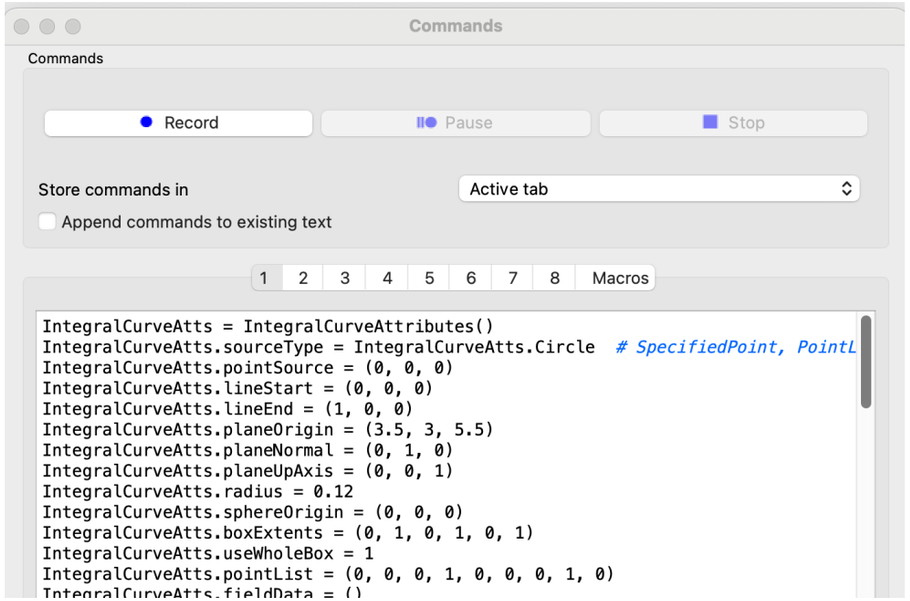
- Works just like the previous examples, but code is in a file
  - Use your favorite editor
  - Have more complicated multi-file scripts

- Enter the following in the cli and click *<Execute>*
  - Source("/path/to/KAUST_Visualization_Vignettes/VisIt_Vignettes/ex04_visitStreamlineAnimation/ex04_visitStreamlineAnimation.py")



Tracing Your Actions

- Open VisIt
  - Open command window: *<Controls/Command>*
  - Open an empty tab
  - Click *<Record>*
  - Interact with the GUI to do the vis you want
  - Click *<Stop>*
  - A lengthy trace will reproduce your actions
    - VisIt prints all possible options for your actions, so you can prune lots of the code away if you are not changing default options



Hands–On Session 3

Scripting Visualization from Command Line

Running Scripts without ParaView GUI

- Navigate to ParaView_Vignettes repo folder on your local computer
  - Run each of the examples (excluding *ex06*, data is too large for local use)
    - cd to individual example directory
    - Use pvpython or pvbatch and run the examples
      - pvbatch and pvpython are the same when running a script, except that pvbatch will run in parallel
      - *pvbatch ex00_pvConeStat.py*
      - *pvpython ex00_pvConeStat.py --verbosity=OFF (hides warnings we don't need)*

```
kressjm@KW-23567:~/Desktop/KAUST_Visualization_Vignettes/ParaView_Vignettes/ex00_pvQuery$ /Applications/ParaView-5.11.1.app/Contents/bin/pvpython ex00_pvConeStat.py
Running ParaView example script:  ex00_pvConeStat.py

Cone Resolution:  6
Cone Height:      1.0
Cone Radius:      0.5
Cone Center:      [0.0, 0.0, 0.0]
Cone Direction:   [1.0, 0.0, 0.0]

Finished ParaView example script

kressjm@KW-23567:~/Desktop/KAUST_Visualization_Vignettes/ParaView_Vignettes/ex00_pvQuery$ /Applications/ParaView-5.11.1.app/Contents/bin/pvbatch ex00_pvConeStat.py
Running ParaView example script:  ex00_pvConeStat.py

Cone Resolution:  6
Cone Height:      1.0
Cone Radius:      0.5
Cone Center:      [0.0, 0.0, 0.0]
Cone Direction:   [1.0, 0.0, 0.0]

Finished ParaView example script
```

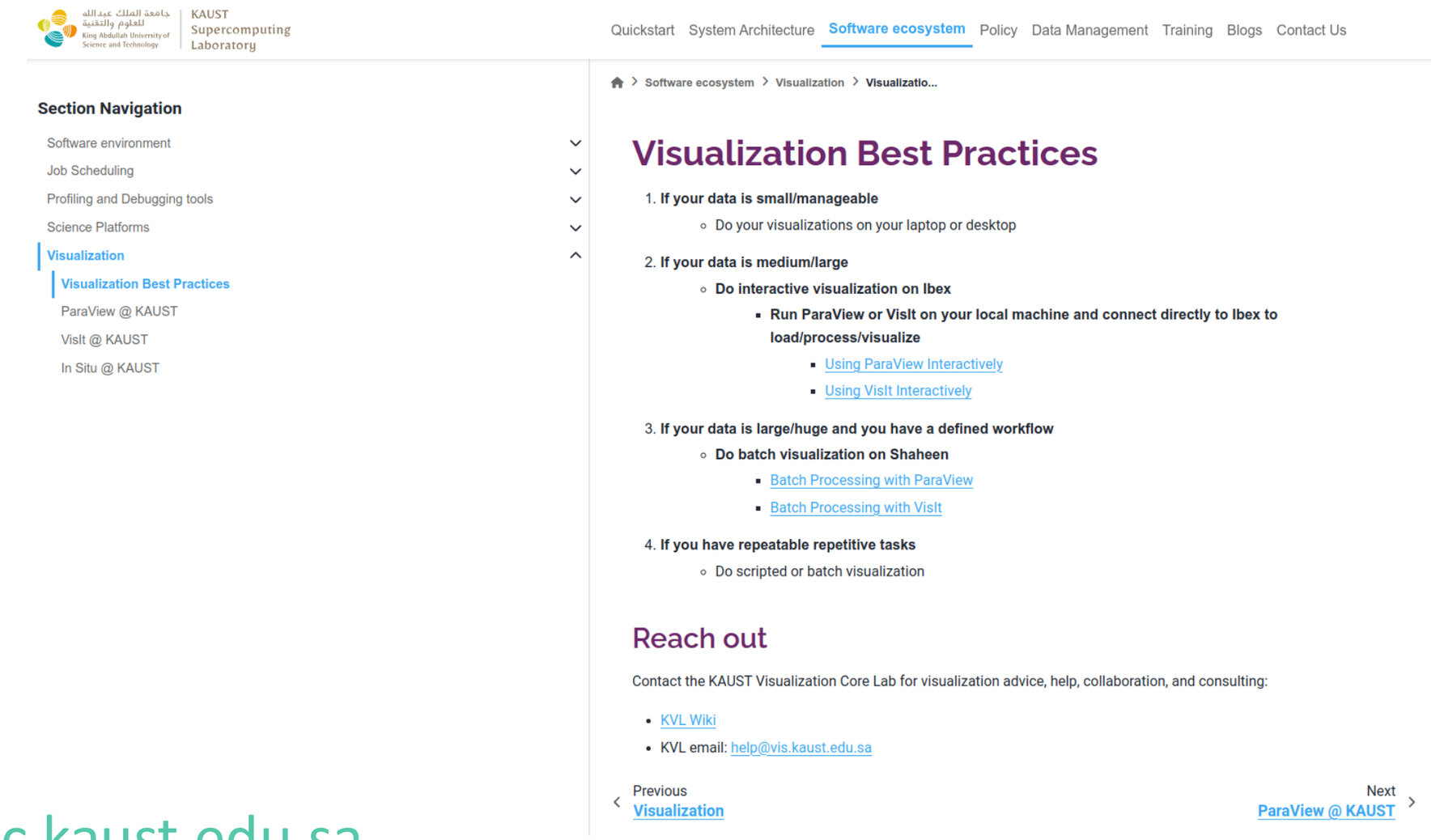
Running Scripts without VisIt GUI

- Navigate to VisIt_Vignettes repo folder on your local computer
  - Run each of the examples (excluding *ex06*, data is large for local use)
    - cd to individual example directory
    - *visit –nowin –cli –v 3.3.2 -s ex00 visitQuery.py*

```
kressjm@KW60540:~/packages/KAUST_Visualization_Vignettes/VisIt_Vignettes/ex00_visitQuery$ ../../../visit-install/bin/visit -cli -nowin -s ex00_visitQuery.py
Running: cli3.3.1 -nowin -s ex00_visitQuery.py
Running: viewer3.3.1 -nowin -noint -host 127.0.0.1 -port 5600
Running VisIt example script:  ex00_visitQuery.py

Running script from:  /home/kressjm/packages/KAUST_Visualization_Vignettes/VisIt_Vignettes/ex00_visitQuery
Running script locally, not launching a batch job

Running: mdserver3.3.1 -host 127.0.0.1 -port 5600
Running: /home/kressjm/packages/visit-install/3.3.1/linux-x86_64/bin/mpirun -np 6 /home/kressjm/packages/visit-install/3.3.1/linux-x86_64/bin/engine_par -plugindir /home/kressjm/.visit/3.3.1
/linux-x86_64/plugins:/home/kressjm/packages/visit-install/3.3.1/linux-x86_64/plugins -visithome /home/kressjm/packages/visit-install/3.3.1 -visitarchhome /home/kressjm/packages/visit-instal
l/3.3.1/linux-x86_64 -dir /home/kressjm/packages/visit-install -forcestatic -idle-timeout 480 -noloopback -host KW60540 -port 5600


3D surface area:  The total Surface Area is 2400 parsec^2
Average Value  :  The average value of hardyglobal is 3.27436 Joules
Centroid:         Centroid = (0.205405, 0.162072, -0.0195174)
GridInformation:  Grid 0: type=AVT_RECTILINEAR_MESH, dims={50,50,50}

MinMax:
hardyglobal -- Min = 1.09554 (node 105026 at coord <0.612245, -10, 7.14286>)
hardyglobal -- Max = 5.88965 (node 83943 at coord <7.55102, 1.42857, 3.46939>)


NumNodes:         The actual number of nodes is 125000.
NumZones:         The actual number of zones is 117649.
Volume:           The total Volume is 8000 parsec^3

Finished VisIt example script
```

Wrap-up

Visualization Best Practices



docs.hpc.kaust.edu.sa

Thanks!

Contacts:

help@vis.kaust.edu