



Scientific Visualization 210

ParaView and Visit: Scripting and Supercomputing Workflows

KAUST Visualization Core Lab

James Kress & Thomas Theussl

Workshop Site: <u>wiki.vis.kaust.edu.sa/training</u> Install VisIt 3.3.2: <u>https://visit-dav.github.io/visit-website/releases-as-tables/#latest</u> Install ParaView 5.11.1: <u>https://www.paraview.org/download/</u>



Resources

Presenter/KVL Contact Info:

- James Kress: james.kress@kaust.edu.sa
- KVL website: wiki.vis.kaust.edu.sa
- General Inquiries: <u>help@vis.kaust.edu.sa</u>
- KVL Vis Repo:

https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes

User Resources:

- User Guide:
 - <u>https://visit-sphinx-github-user-</u> manual.readthedocs.io/en/develop/
 - https://docs.paraview.org/en/latest/

Developer Resources:

- Github: <u>https://github.com/visit-dav/visit</u>
- GitLab: <u>https://gitlab.kitware.com/paraview/parview</u>





- Never logged in to Ibex before?
 - Do so now so that your scratch 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.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes.git
 - 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

mac machines

- Install ParaView
 - <u>https://www.paraview.org/download/</u>
 - Install XQuartz (X11)
 - https://www.xquartz.org/
- Install Vislt
 - <u>https://visit-dav.github.io/visit-website/releases-as-tables/#latest</u>
 - Install ffmpeg
 - <u>https://www.ffmpeg.org/download.html</u>
- Extra info
 - If you want to view ibex files locally without 'scp'
 - Download and install fuse and sshfs: https://osxfuse.github.io/
 - Install instructions: <u>https://sbgrid.org/corewiki/faq-sshfs.md</u>
 - 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 3.3.2")



windows machines

- Install ParaView
 - <u>https://www.paraview.org/download/</u>
 - Install PuTTY
 - <u>https://www.putty.org/</u>
- Install Visit
 - <u>https://visit-dav.github.io/visit-website/releases-as-tables/#latest</u>
 - Install ffmpeg
 - <u>https://www.ffmpeg.org/download.html</u>
 - 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
 - <u>or</u>
 - Visual Studio Code
 - If you want to view ibex files locally without 'scp'
 - Download and install SFTP Drive
 - <u>https://www.nsoftware.com/sftp/drive/</u>



linux machines

- Install ParaView
 - <u>https://www.paraview.org/download/</u>
- Install VisIt
 - https://visit-dav.github.io/visit-website/releases-as-tables/#latest
 - Install ffmpeg
 - <u>https://www.ffmpeg.org/download.html</u>
 - Use modules on KAUST machines
 - apt-get install ffmpeg



Workshop Notes



- Examples have been tested on the following:
 - Mac M1
 - Vislt has problems with offscreen rendering on the M1, is a future bug fix
 - ParaView has an issue with ex04, investigating
 - Mac Intel
 - Everything runs
 - Linux Ubuntu 20
 - Everything runs
 - Windows
 - 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	Dr. James Kress HPC SCIVIS	Dr. Ronell Sicat VR/AR	Dr. Didier Barradas Data Scientist	Dr. Abdelghafour Halimi Data Scientist
 SCIENTIFIC VISUALIZATION LARGE DATA ANALYSIS DISTRIBUTED VISUALIZATION 	 VISUALIZATION SOFTWARE HPC INSITU VISUALIZATION DISTRIBUTED VISUALIZATION 	 SCIENTIFIC VISUALIZATION VR DEVELOPMENT 3D RECONSTRUCTION 	 DATA SCIENCE MACHINE LEARNING DEEP LEARNING 	Data ScienceMachine LearningDeep Learning

FACILITIES AND SPACES



ZONE 1/2 DISPLAY WALLS: 2D/3D Analytics



HMD's







ZONE 5 VR



MULTI-PURPOSE ROOM



Z2 Visualization and Collaboration

- ParaView & Vislt on Z2
 - Connect to Ibex for compute or other networked storage





Sage3 collaboration boards

- Software to enable teams of collaborators to work together with data in the form of data visualizations
- <u>https://sage3.sagecommons.org/</u>

Accessing KVL Facilities



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

Facil	lity Booking Form		
	Once you click Send Request	you can refresh this page to see your booking appear in the bookings calendar . All bookings are provisional until approved by KVL.	
	١	Vis Lab Home Booking Hosts 188 Logged in as kressjr	n
		Logged in as kressjm.	
		Request a booking Purpose Description of booking Reservation Maintenance Cornea MPR Vis Cubes Vive Zone 1 Zone 2 Zone 5 Every 0 weeks Full day Start 2023-07-27 11:36 End 2023-07-27 11:36 End Send Request	

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 Fall 2023

Date	Training Event	Speaker	Registration
Sunday October 1, 2023	Scientific Visualization 101: Vielt - An Introductory Hands On Workshop	James Kross	Register New
Sunday October 8 2023	Scientific Visualization 210: ParaView & Vislt ~ Scripting and Supercomputing Workflows	James Kress & Thomas Theußl	S Register Now
Sunday October 22, 2023	Scientific Visualization 101: Avizo/Amira ~ An Introductory Hands-On Workshop	Thomas Theußl	S Register Now
Sunday October 29, 2023	Scientific Visualization 210: ParaView ~ A Plugin for Geometry Processing	Thomas Theußl	S Register Now
Sunday November 5, 2023	Scientific Visualization 210: Avizo and Ilastik for Image Segmentation and 3D Analysis	Ronell Sicat	S Register Now

Hands-on AI Tools and Techniques Workshop Series Fall 2023

Date	Training Event	Speaker	Registration
Tuesday Octobor 2, 2022	Introduction to Machine Learning	Abdelghafeur Halimi	C Register New
Tuesday October 10, 2023	Introduction to Deep Learning	Abdelghafour Halimi	S Register Now
Tuesday October 17, 2023	Data Visualization for Data Science	Abdelghafour Halimi	S Register Now

Edit

Data Science on Kaust HPC platforms Fall 2023

Date	Training Event	Speaker	Registration
Sunday November 20, 2023	S Data Science on-boarding on KSL platforms	DB & MS	S Register Now
Tuesday November 21, 2023	S Distributed Deep Learning on KSL platforms	DB & MS	S Register Now
Sunday November 22, 2023	S High Throughput Hyperparameter Optimization of ML/DL models on KSL platforms	DB & MS	S Register Now
Sunday November 23, 2023	S Introduction to Containers on KSL platforms	DB & MS & AH	S Register Now

Workshop Goals



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



ParaView & Vislt

On Ibex and Shaheen



What are ParaView and Vislt?

- 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 Vislt?

- 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
 - <u>https://www.paraview.org/download/</u>
 - KVL team manages builds on Ibex and Shaheen
 - IT Remote Workstations
- Build it yourself:
 - "build_visit" is a script that automates the process of building VisIt and its third-party dependencies. (docs: <u>https://visit-sphinx-github-user-</u> <u>manual.readthedocs.io/en/develop/building_visit/index.html</u>)
 - <u>https://gitlab.kitware.com/paraview/paraview-superbuild</u>



Brief Look @ Core Concepts

Paraview and Vislt 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

- Vislt *Libsim*
- ParaView Catalyst







ParaView and VisIt Use MPI for Distributed-Memory Parallelism







ParaView and Vislt Use Scalable Rendering



ParaView and Vislt Use a Client-Server Architecture



<u>Client Computer</u>

Parallel HPC Cluster





Hands–On Session 1

Ibex Interactive Visualization Overview

Why use ParaView and Vislt on Ibex?



- Access to data generated on Ibex or Shaheen 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 on Ibex
 - 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>
- Clone repo
 - git clone https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes.git

Repo Data





Hands–On Session 1: Part I

Ibex 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* lbex
- 3. If first time using ParaView on Ibex, load the KAUST profile
 - 1. Save the following servers.pvsc file to your local computer: <u>ibex_server</u>OR for Windows <u>ibex_server_windows</u>
 - 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 </bex-GPU> configuration and click connect
- Set connection options:
 - Can leave everything as default for today, just ensure <*Node Group>* is set to "CPU" and <*Module Variant>* is set to "openmpi4.0.3-mesa"
 - 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 lbex queue)

Explore Example Repo Data Sets

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





Hands–On Session 1: Part II

Ibex Interactive Visualization with Vislt

Initially Accessing Vislt on Ibex

1. Check available Vislt versions on Ibex

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

/sw/csi/modulefiles/applications

visit/3.3.2

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







Setup Host Profiles and Configuration

Using Vislt Interactively on Ibex

- Open Vislt 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 (for now, use 2 processes and 1 node)
- 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 Vislt Interactively on Ibex Cont.

vcl – Vi

mdserv

	Path KAUST_Shaheen II KAUST_Shaheen II KW60540 ilogin.ibex.kaust.edu.sa localhost V Use "cu shaheen.hpc.kaust.edu.sa F Show dot files F Directories F . (current directory) (go up 1 directory level)	File grouping Off Remove paths Files
slt Component Launcher (manages Vislt session) ver — Vislt metadata server (interacts with GUI and databases)	Open file as type: Guess from file name/extension Refresh	Set default open options OK Cancel
9540:~/packages/visit-install/bin\$./visit 13.3.1 ewer3.3.1 -geometry 4078x1942+0+218 -borders 26,4,4,4 -shift 0,0 -preshift 4,26 -defer - server3.3.1 -host 127.0.0.1 -port 5601 pme/kressjm/packages/visit-install/3.3.1/linux-x86_64/bin/mpirun -np 6 /home/kressjm/pac 64/plugins:/home/kressjm/packages/visit-install/3.3.1/linux-x86_64/plugins -visithome /h ux-x86_64 -dir /home/kressjm/packages/visit-install -forcestatic -idle-timeout 480 -nolo	host 127.0.0.1 -port 5600 ckages/visit-install/3.3.1/linux-x86_6 nome/kressjm/packages/visit-install/3. popback -host KW60540 -port 5600	54/bin/engine_par -plugindir /home/kressjm/.visit/3.3.1 .3.1 -visitarchhome /home/kressjm/packages/visit-instal
Image: manual distance of the second seco		
must comply with the acceptable use policy. # - Your Ibex Admin Team #		X
ibex@hpc.kaust.edu.sa # https://kaust-ibex.slack.com #general # ###################################	ost -port 26172 ocalhost -port 18361	

Global

Sources 1

Open

Active window 1 -

Host localhost

VisIt 3.3.1 File Controls Options Windows PlotAtts OpAtts Help

ę,

5

Auto apply

File open

ress1m@

/<mark>3.3.1/</mark>li

+####### unning ou unning on

Using Vislt Interactively on Ibex Cont.

Sel	ect optio	ns for 'ilo	gin.ibex.ka	ust.edu.sa	' 😣
New profile	#0				
Num procs	2		Num nodes	1	
Bank		•	Time limit	1:00:00	
Machine file					
OK	ſ				Cancol
UK	J				Lancel



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.202 2.02/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 2./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/linux-x86_64/lib/mesagl:/sw/vis/ibex-gpu.2022.02/visit-src/install/3.3.1/linux-x86_64/lib 5:/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/lib 5:/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 5:/sw/sited_batch_iob_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 "LD_LIBRARY_PATH=\$LIBPATH"
echo "LD_LIBRARY_PATH=\$LD_LIBRARY_PATH=\$LD_LIBRARY_PATH"
echo "VISITHOME=\$VISITHOME"
echo "VISITARCHHOME=\$VISITARCHHOME"
echo "VISITARCHHOME=\$VISITARCHHOME"
echo "VISITARCHHOME=\$VISITARCHHOME"
srun --export=ALL --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 -noloopba
ck -sshtunneling -host login509-02-r

engine_par– *VisIt parallel computation engine*

Explore Example Repo Data Sets

- Load each of the example data sets and try different visualizations
- Note on rendering
 - Vislt 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 Vislt 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>

	Rendering	options				×
Basic Advanced	Information					
✓ Query after each to Using Scalable Render Frames per second: Approximate polygor	render ering: no 24.8 n count: 6612	30.1		39.2		
X Extents:	-5		5			
Y Extents:	-5.20548e-06		5			
Z Extents:	0		20			



Hands–On Session 2: Part I

Scripting Visualization within ParaView



Download Example Repo Locally

- Navigate to your preferred dir
- Clone repo
 - git clone https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes.git



Using ParaView GUI and Python Simultaneously

- Open ParaView
 - Open Python shell: <View/Python Shell>
- Go to ParaView Docs
 - <u>https://docs.paraview.org/en/latest/Tutorials/ClassroomTutorials/</u> 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 Vislt

Vislt and Python

- Vislt 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 Vislt





Using Vislt GUI and cli Simultaneously

- Open Vislt
 - Open command window: <*Controls/Command*>
- Go to VisIt Docs
 - <u>https://visit-sphinx-github-user-</u> manual.readthedocs.io/en/develop/tutorials/Scripting.html
 - We'll walk through some of the initial copy-paste examples



Running a Script Interactively in Vislt

- 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_visitStre amlineAnimation.py")



Tracing Your Actions

- Open Vislt
 - 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



	Commands	
Commands		
Record	II Pause	Stop
Store commands in	Active tab	٥
Append commands to existing text	t	
1 2 IntegralCurveAtts = IntegralC IntegralCurveAtts.sourceType IntegralCurveAtts.lineStart =	3 4 5 6 7 8 Macros CurveAttributes() = IntegralCurveAtts.Circle <i># Specifi</i> e = (0, 0, 0) = (0, 0, 0)	edPoint, PointL
IntegralCurveAtts.lineEnd = ((1, 0, 0)	



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.pv
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 Vislt 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

NumZones: The actual number of zones is 11/649. Volume: The total Volume is 8000 parsec^3 Finished VisIt example script	1
NumNodes: The actual number of nodes is 125000.	
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>)	
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}	
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/plugins:/home/kressjm/packages/visit-install/3.3.1/linux-x86_64/plugins -visithome /home/kressjm/packages/visit-install/3.3.1 -visitarchh l/3.3.1/linux-x86_64 -dir /home/kressjm/packages/visit-install -forcestatic -idle-timeout 480 -noloopback -host KW60540 -port 5600	r -plugindir /home/kressjm/.visit/3.3.1 ome /home/kressjm/packages/visit-instal
Running script from: /home/kressjm/packages/KAUST_Visualization_Vignettes/VisIt_Vignettes/ex00_visitQuery Running script locally, not launching a batch job	
<pre>kressjm@KW60540:~/packages/KAUST_Visualization_Vignettes/VisIt_Vignettes/ex00_visitQuery\$//visit-install/bin/visit -cli -nowin -s ex00_visitQue 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</pre>	гу.ру



Demo

Scripting Visualization on Ibex

Access Data on Ibex



- Linux
 - scp –r <u>username@ilogin.ibex.kaust.edu.sa:/path/to/files</u> <local/destination>
 - Mount scratch locally as a folder:
 - sshfs <u>username@mover.ibex.kaust.edu.sa:/ibex/scratch/username</u> <local/destination>
- Mac
 - scp –r <u>username@ilogin.ibex.kaust.edu.sa:/path/to/files</u> <local/destination>
 - Mount scratch locally as a folder:
 - sshfs <u>username@mover.ibex.kaust.edu.sa:/ibex/scratch/username</u> <local/destination>
- Windows
 - scp –r <u>username@ilogin.ibex.kaust.edu.sa:/path/to/files</u> <local/destination>
 - Mount scratch locally as lettered drive:
 - Run SFTP Drive and connect: mover.ibex.kaust.edu.sa; drive path: /ibex/scratch/<username>



Running ParaView Examples on Ibex

- Login to Ibex
 - ssh -X <username>@glogin.ibex.kaust.edu.sa
 - module load paraview
- Navigate to example dir
 - cd /ibex/scratch/<username>/KAUST_Visualization_Vignettes/Paraview_Vignettes
- Run individual examples
 - cd ex00_pvQuery
 - sbatch ex00_ibex_runScript.sbat
 - View queue info: *squeue –u username*
 - When job finishes view results: *cat ex00.ibex.**.*out*
 - cd ex01_pvScreenshot
 - sbatch ex01_ibex_runScript.sbat
 - When job finishes view image: *display ex01_pvScreenshot.png*
 - ex02... etc.



Running Vislt Examples on Ibex

- Login to Ibex
 - ssh -X <username>@ilogin.ibex.kaust.edu.sa
 - module load visit
- Navigate to example dir
 - cd /ibex/scratch/<username>/KAUST_Visualization_Vignettes/Visit_Vignettes
- Run individual examples
 - cd ex00_visitQuery
 - sbatch ex00_ibex_runScript.sbat
 - View queue info: *squeue –u username*
 - When job finishes view results: *cat ex00.ibex.*.out*
 - cd ex01_visitScreenshot
 - sbatch ex01_ibex_runScript.sbat
 - When job finishes view image: *display output/ex01_visit000.png*
 - ex02... etc.

Parallelizing Bigger Problems

ex06_[pv/visit]LargeData.py

- Run: *fetchData.sh* to get data
- Visit
 - 1 node, 1 mpi process
 - real 4m23.610s
 - 8 nodes, 8 mpi processes
 - real 1m59.409s
 - 1 node, 8 mpi processes
 - real 1m46.211s
- ParaView
 - egl
 - 1 node, 1 mpi process, 32 cores 1 gpu
 - real 5m16.889s
 - 1 node, 1 mpi process, 32 cores 2 gpu
 - real 4m56.753s
 - mesa: don't volume render with mesa, transfer functions don't work properly, and it is slow
 - ~18 minutes on a beefy machine

Note: VisIt/ParaView timings are not directly comparable. VisIt is not using volume rendering, nor does it make use of GPU. Timings are meant to show how resources affect time-to-solution



~5 GB data files, expands to ~15 GB when loaded in VisIt/ParaView. The pipeline for this image uses ~59 GB of RAM





Wrap-up

October 3, 2023

Best Practices

How do I use ParaView or VisIt?

- If your data is small/manageable
 - Do your visualizations on your laptop, desktop, or IT Remote Workstation
- If your data is medium/large
 - Do interactive visualization on Ibex
 - Run it on your local machine and connect directly to Ibex to load/process/visualize
 - <u>https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/ParaView_Vignettes#using-paraview-interactively-on-ibex</u>
 - <u>https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/VisIt_Vignettes#using-visit-interactively-on-ibex</u>
- If your data is large/huge and you have a defined workflow
 - Do batch visualization on Shaheen
 - Look at example scripts and talk to us if you have questions
 - <u>https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/VisIt_Vignettes#expy</u>
 - <u>https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/ParaView_Vignettes#expy</u>
- If you have repeatable repetitive tasks
 - Do scripted or batch visualization







Thanks!

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