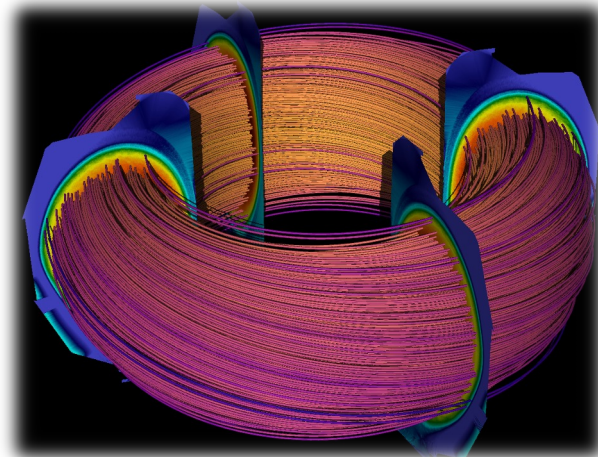


# HPC Visualization and In Situ Visualization at KAUST

## KAUST Visualization Core Lab

James Kress  
[james.kress@kaust.edu.sa](mailto:james.kress@kaust.edu.sa)

KVL website: [wiki.vis.kaust.edu.sa](http://wiki.vis.kaust.edu.sa)  
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جامعة الملك عبد الله  
للعلوم والتقنية  
King Abdullah University of  
Science and Technology

Core Labs and  
Research Infrastructure

# Visualization Core Lab

Overview of People & Services





# The Team



**Dr. Sohaib Ghani**  
(LEAD STAFF SCIENTIST)

- VISUAL ANALYTICS
- INFORMATION VIS
- STATISTICAL ANALYSIS



**Dr. Ronell Sicut**  
VR/AR

- SCIENTIFIC VISUALIZATION
- VR DEVELOPMENT
- 3D RECONSTRUCTION



**Dr. James Kress**  
HPC SCIVIS

- VISUALIZATION SOFTWARE
- HPC INSITU VISUALIZATION
- DISTRIBUTED VISUALIZATION



# The Team



Thomas Theussl  
SCIVIS

- SCIENTIFIC VISUALIZATION
- LARGE DATA ANALYSIS
- DISTRIBUTED VISUALIZATION



Dr. Didier Barradas  
Data Scientist

- DATA SCIENCE
- MACHINE LEARNING
- DEEP LEARNING

# Project Requests

- Standard Request
  - Load data 'X' in program 'P' to produce a visualization 'V'
- Advanced Support
  - “Investigative” Visualization
- Collaboration
  - Work with you through your research and discovery cycle
- Have an interest in HPC vis or in situ? Let me know!



# Upcoming Workshops at KVL

## Scientific Visualization Workshop Series

Fall 2022

Training Events	Date	Venue	Registration
<a href="#">Introduction to Scientific Visualization with VisIt</a>	9 Oct 2022, 1-5pm	Building 4 Level 5 Room 5220	<a href="#">Register</a>
<a href="#">Introduction to Scientific Visualization with Avizo</a>	24 Oct 2022 1-5 pm	TBA	TBA
<a href="#">Topological Analysis with ParaView and the Topology Toolkit (TTK)</a>	30 Oct 2022, 1-5pm	Building 4 Level 5 Room 5220	TBA
<a href="#">Image Segmentation and 3D Reconstruction using Ilastik and Avizo</a>	9 Nov 2022, 1-5 pm	Conference Room Between Bldgs. 2 and 3 (Auditorium 0215)	TBA

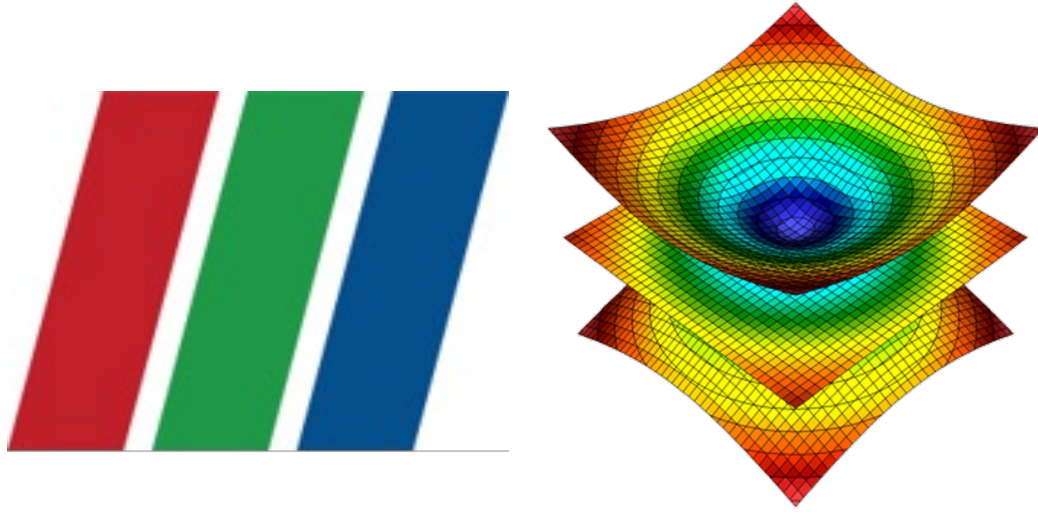
## Data Science Workshops

Fall 2022

### Introduction to Data Science Workshop Series

Training Events	Date	Venue	Registration
<a href="#">Introduction to Shell for (Data) Scientists</a>	2022-09-12, 2-4 pm AST	Level 0 Auditorium Between B4 and B5	<a href="#">Register Here</a>
<a href="#">Introduction to Conda for (Data) Scientists</a>	2022-09-21, 2-4 pm AST	Level 0 Auditorium Between B4 and B5	<a href="#">Register Here</a>
<a href="#">Introduction to Python for Data Science</a>	2022-10-10, 2-4 pm AST	Level 0 Auditorium Between B4 and B5	<a href="#">Register Here</a>





# ParaView & VisIt

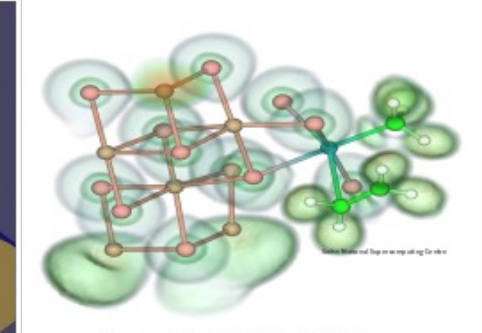
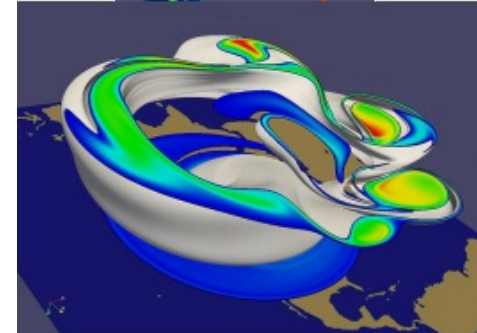
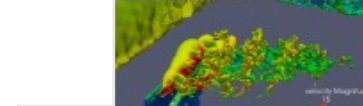
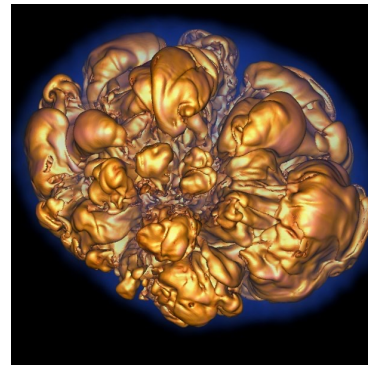
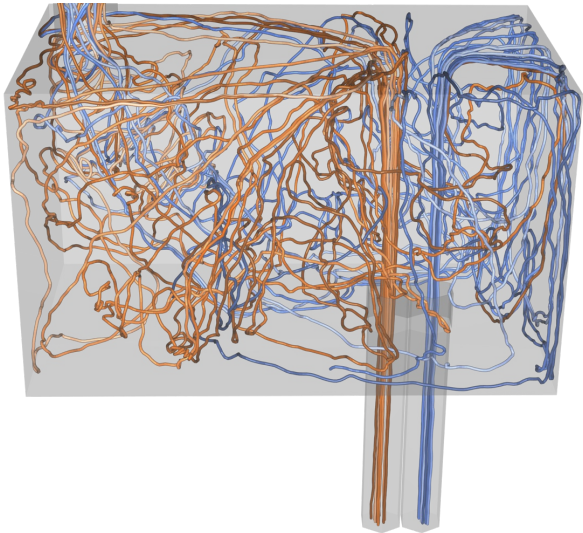
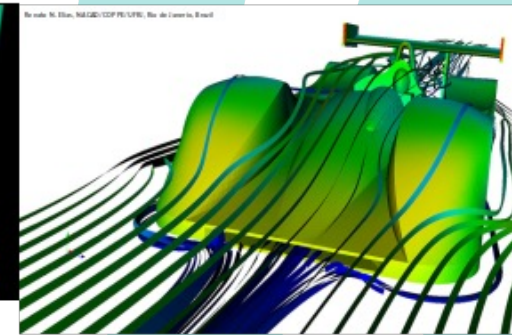
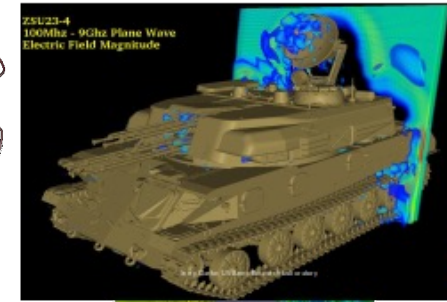
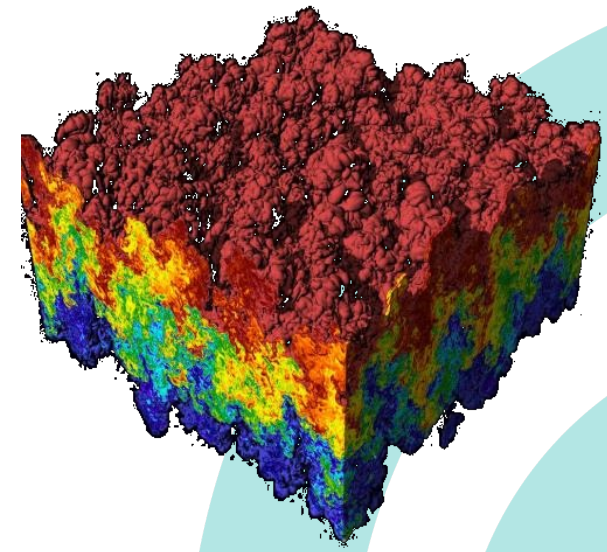
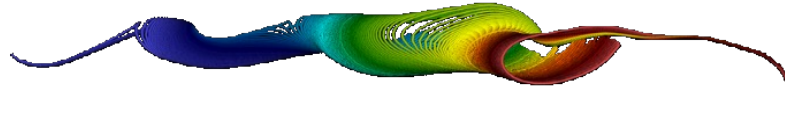
On Ibex and Shaheen





# 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





# 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
    - IT Remote Workstations
- 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://visit-sphinx-github-user-manual.readthedocs.io/en/develop/building_visit/index.html))
  - <https://gitlab.kitware.com/paraview/paraview-superbuild>

# 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
    - [https://gitlab.kaust.edu.sa/kvl/KAUST\\_Visualization\\_Vignettes/-/tree/master/ParaView\\_Vignettes#using-paraview-interactively-on-ibex](https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/ParaView_Vignettes#using-paraview-interactively-on-ibex)
    - [https://gitlab.kaust.edu.sa/kvl/KAUST\\_Visualization\\_Vignettes/-/tree/master/VisIt\\_Vignettes#using-visit-interactively-on-ibex](https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/VisIt_Vignettes#using-visit-interactively-on-ibex)
- If your data is large/huge and you have a defined workflow
  - Do batch visualization on Shaheen
    - [https://gitlab.kaust.edu.sa/kvl/KAUST\\_Visualization\\_Vignettes/-/tree/master/VisIt\\_Vignettes#expy](https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/VisIt_Vignettes#expy)
    - [https://gitlab.kaust.edu.sa/kvl/KAUST\\_Visualization\\_Vignettes/-/tree/master/ParaView\\_Vignettes#expy](https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/master/ParaView_Vignettes#expy)
- If you have repeatable repetitive tasks
  - Do scripted or batch visualization

# Scripting Examples

- KVL has a repo of simple examples of ParaView and VisIt scripting and the associated batch scripts to run on both Ibex and Shaheen
- Run scripts locally
  - `pvpython -force-offscreen-rendering ./stats.py`
  - `visit --nowin --cli --s stats.py`

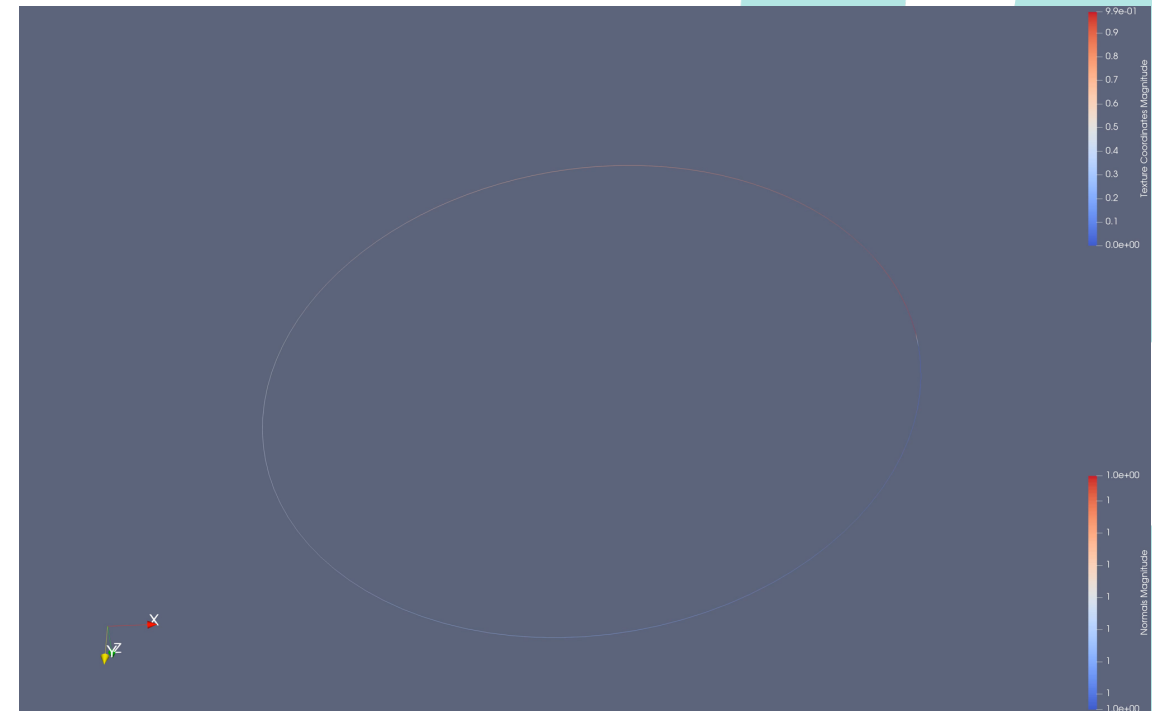
```

11 # Open file and add basic plot
12 OpenDatabase("localhost:../data/noise.silo", 0)
13 AddPlot("Pseudocolor", "hardyglobal", 1, 0)
14 DrawPlots()
15
16 # Query stats about data
17 SetQueryFloatFormat("%g")
18 print("\n")
19 print("3D surface area: ", Query("3D surface area"))
20 print("Average Value : ", Query("Average Value"))
21 print("Centroid:      ", Query("Centroid"))
22 print("GridInformation: ", Query("Grid Information"))
23 print("MinMax:        ", Query("MinMax", use_actual_data=1))
    
```

```

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>)
    
```





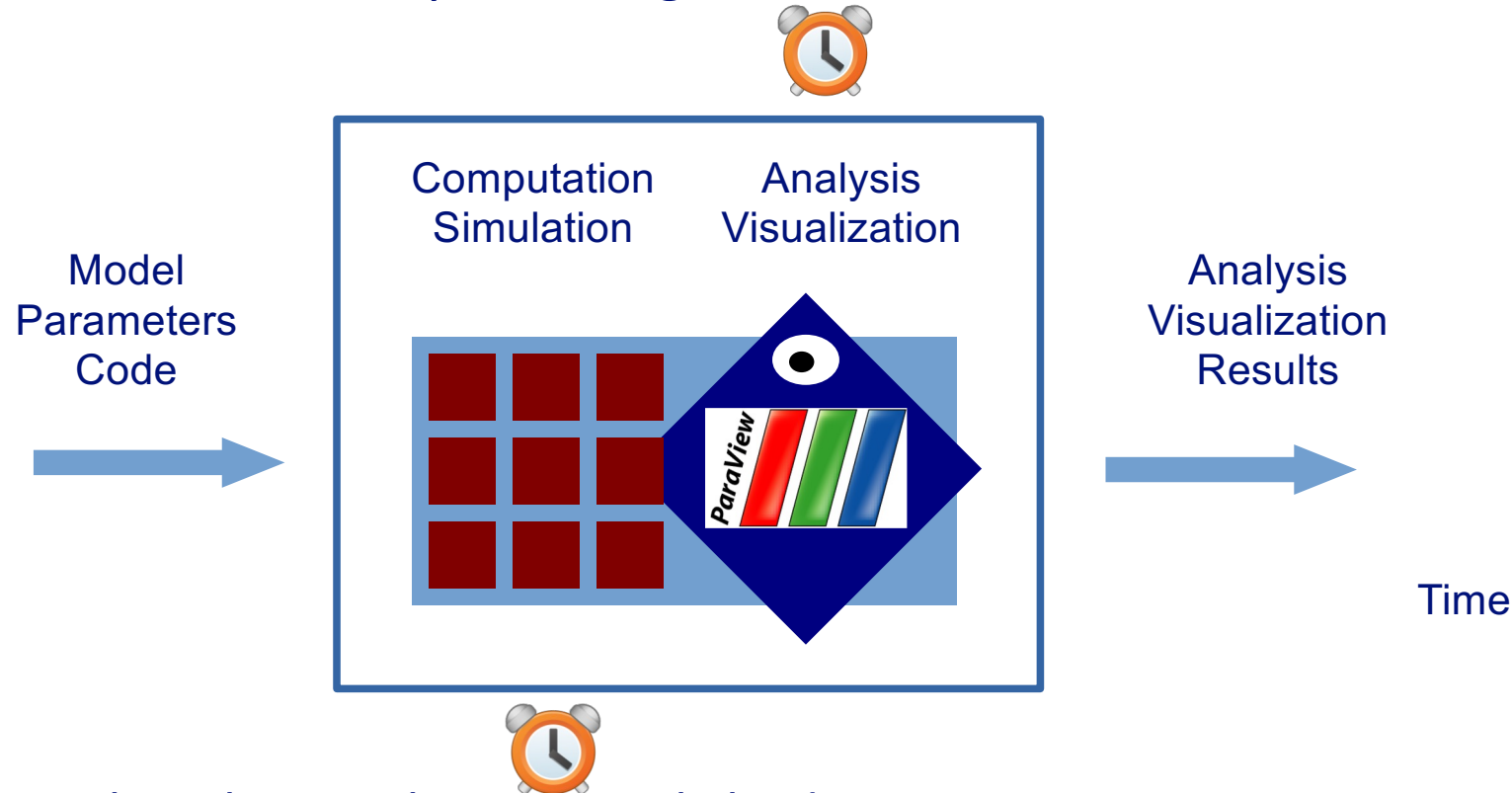
# In Situ Visualization

On Ibex and Shaheen



# What is In Situ Visualization?

- Produce visualization & analysis during the course of an active simulation



- Multiple ways that this can be accomplished

# Why Use In Situ Visualization?

- Faster simulations/More simulations
- Increase simulation resolution (time, spatial)
- Keep what you need
- Reduced I/O helps other users too
- Reduced storage keeps performance optimal





# Inshimtu

KVL has developed Inshimtu

- An in situ 'shim'
- Designed for existing, unmodified simulations
- Works with files written by simulation
- Uses Catalyst and ParaView vis-pipelines
- Low barrier to entry
  - Try-out in situ without commitment of creating a true in situ integration



# Cyclone Chapala 2015



# Bespoke In Situ

- If you are looking for a true in situ integration there are multiple options available
  - ADIOS2
    - A full data management solution.
    - Can aid in better I/O performance, in situ, data reduction
    - <https://adios2.readthedocs.io/en/latest/>
  - ParaView Catalyst / VisIt Libsim
    - Directly integrate ParaView or VisIt functionality into your simulation code
    - <https://catalyst-in-situ.readthedocs.io/en/latest/index.html>
    - <https://www.visitusers.org/index.php?title=VisIt-tutorial-in-situ>
  - Ascent
    - Ascent is a many-core capable flyweight in situ visualization and analysis infrastructure
    - <https://ascent.readthedocs.io/en/latest/>
  - VTK-m
    - VTK-m is a toolkit of scientific visualization algorithms for emerging processor architectures (many-core extension of VTK)
    - It is used by Ascent, but can be used with other libraries to enable in transit visualization
    - <https://m.vtk.org/>





# Thanks!

We can help! Contact us with HPC  
visualization / in situ questions

Contacts

[james.kress@kaust.edu.sa](mailto:james.kress@kaust.edu.sa)

[help@vis.kaust.edu.sa](mailto:help@vis.kaust.edu.sa)