Scientific Visualization 210

ParaView: *In Situ Visualization Using Catalyst*

KAUST Visualization Core Lab

James Kress

KAUST
VISUALIZATION
CORE LAB

Workshop Site: wiki.vis.kaust.edu.sa/training
Install ParaView 5.11.1: https://www.paraview.org/download/

Resources

Presenter/KVL Contact Info:

- James Kress: james.kress@kaust.edu.sa
- KVL website: wiki.vis.kaust.edu.sa
- General Inquiries: help@vis.kaust.edu.sa
- KVL Vis Repo: https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes

User Resources:

- User Guides:
  - https://docs.paraview.org/en/latest/
  - https://catalyst-in-situ.readthedocs.io/en/latest/index.html

Developer Resources:

- GitLab: https://gitlab.kitware.com/paraview/parview

Workshop Setup

- Never logged in to Ibex before?
  - Do so now so that your scratch directory will have time to get setup
    - `ssh -X <username>@glogin.ibex.kaust.edu.sa`
- Local installation of ParaView 5.11.1
- Download example data/slides
  - https://download.vis.kaust.edu.sa/pub/workshops/2024/SciVis210-Catalyst/
- That's all for now, we'll be using a module to access the sim, so no building required

KAUST CORE LABS

12 CORE LABS

270 HEADCOUNT

45 FIELDS OF EXPERTISE

MANAGEMENT AND CENTRAL OPERATIONS
29 Staff

ANALYTICAL CHEMISTRY
21 Staff

IMAGING AND CHARACTERIZATION
26 Staff

PLANT GROWTH
10 Staff

ANIMAL RESOURCES
1 Staff

LAB EQUIPMENT MAINTENANCE
27 Staff

RADIATION LABELING
1 Staff

BIOSCIENCE
25 Staff

NANOFABRICATION
19 Staff

SUPERCOMPUTING
18 Staff

COASTAL AND MARINE RESOURCES
50 Staff

PROTOTYPING AND PRODUCT DEVELOPMENT
38 Staff

VISUALIZATION
6 Staff

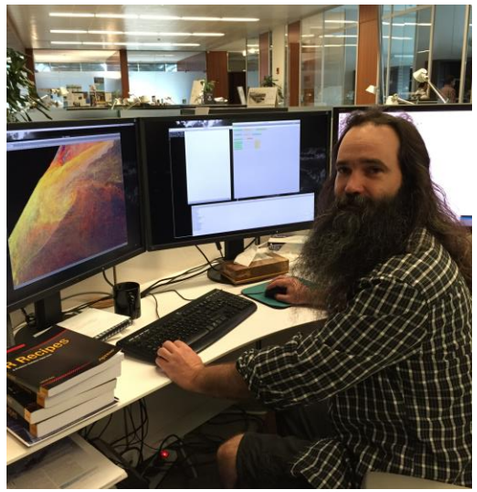
Visualization Core Lab

Overview of Facilities & Services

The Team

Dr. Sohaib Ghani
(LEAD STAFF SCIENTIST)

- VISUAL ANALYTICS
- INFORMATION VIS
- STATISTICAL ANALYSIS

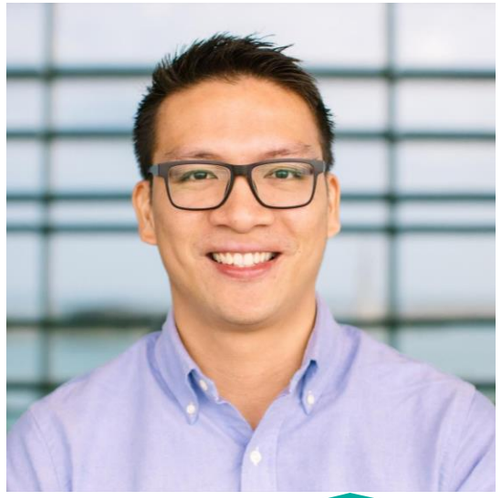


Thomas Theussl
SCIVIS

- 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

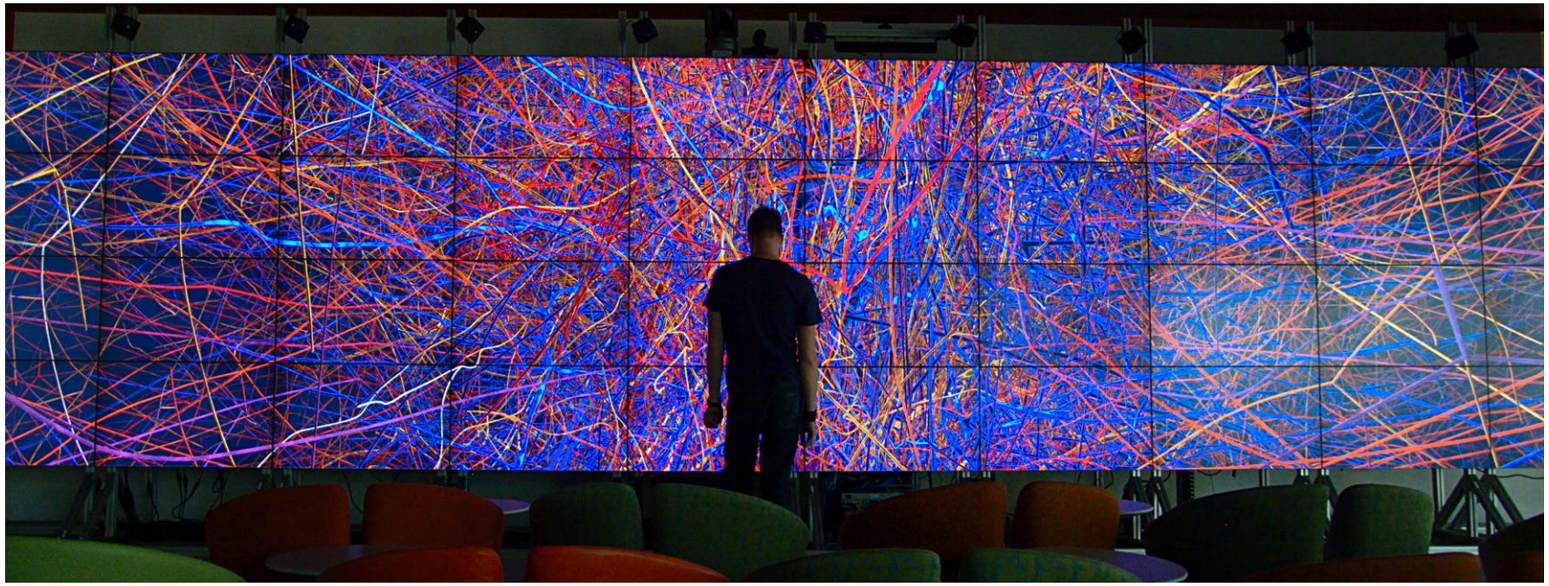
Dr. Didier Barradas
Data Scientist

- DATA SCIENCE
- MACHINE LEARNING
- DEEP LEARNING

Dr. Abdelghafour Halimi
Data Scientist

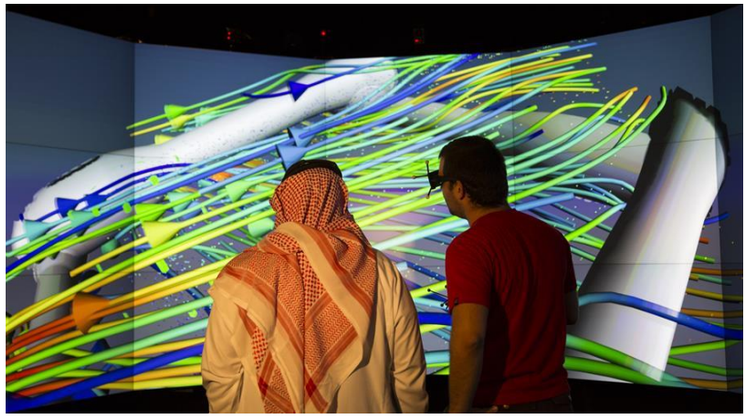
- Data Science
- Machine Learning
- Deep Learning

FACILITIES AND SPACES



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

HMD’s



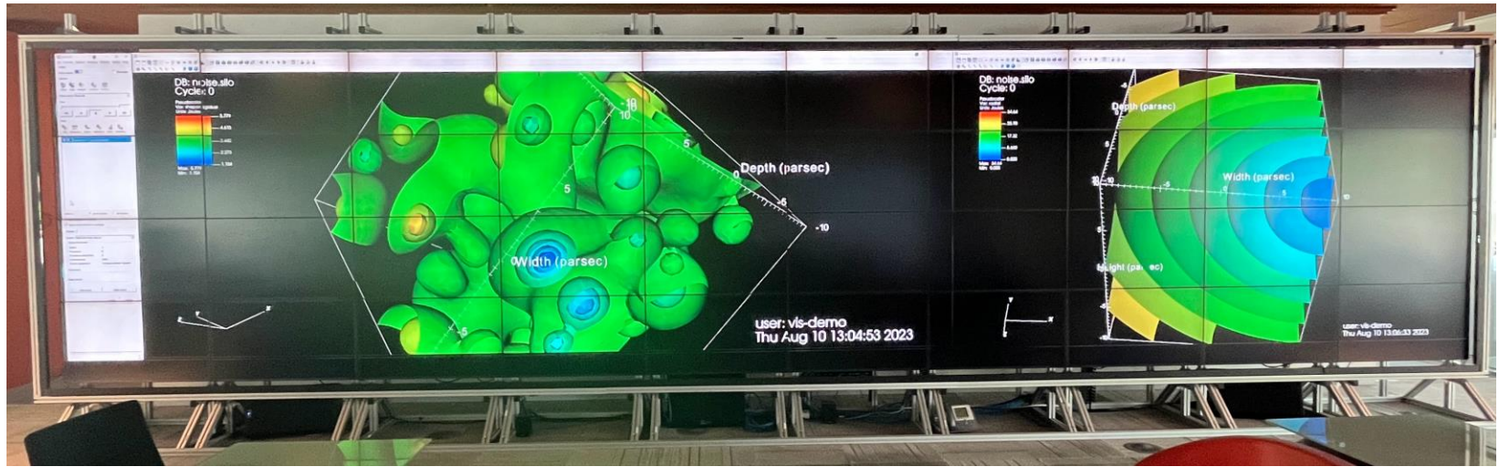
CUBES VR

ZONE 5 VR

MULTI-PURPOSE ROOM

Z2 Visualization and Collaboration

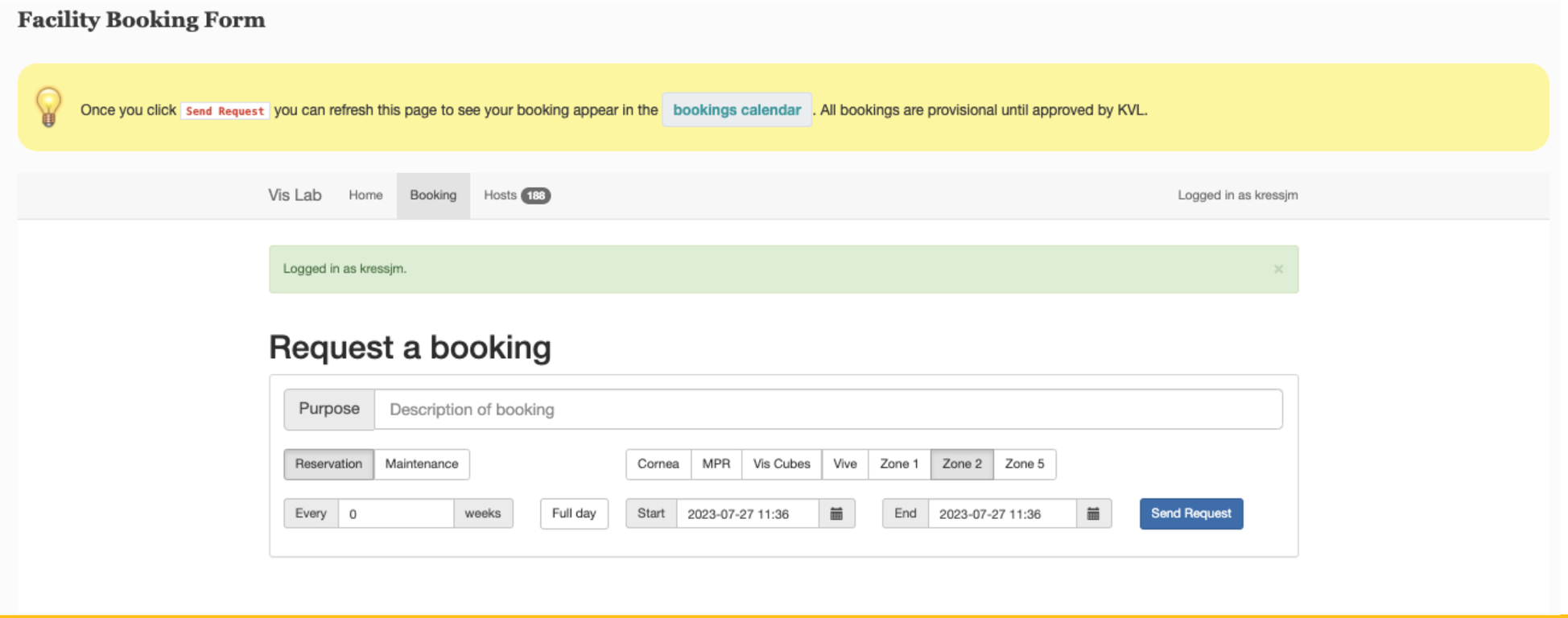
- **ParaView & VisIt on Z2**
  - Connect to Ibex for compute or other networked storage



- **Sage3 collaboration boards**
  - Software to enable teams of collaborators to work together with data in the form of data visualizations
  - https://sage3.sagecommons.org/

Accessing KVL Facilities

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



Upcoming Training Events

Scientific Visualization Workshop Series Spring 2024

Date	Training Event	Speaker	Registration
[redacted]			
February 20, 2024	Scientific Visualization 210: ParaView ~ In Situ Visualization using Catalyst	James Kress	Register Now
February 27, 2024	Scientific Visualization 101: Virtual Reality for Data Visualization	Ronell Sicat	Register Now

Edit

Avizo Workshop Series By Thermofisher and KVL, Spring 2024

Date	Training Event	Speaker	Registration
March 4, 2024	Scientific Visualization 101: Avizo (Day 1) ~ Introductory Level	Sarawuth Wantha	Register Now
March 5, 2024	Scientific Visualization 210: Avizo (Day 2) ~ Intermediate Level	Sarawuth Wantha	Register Now
March 6, 2024	Scientific Visualization 210: Avizo (Day 3) ~ Advanced Level	Sarawuth Wantha	Register Now

Edit

Hands-on AI Tools and Techniques Workshop Series (Arabic version) Spring 2024

Date	Training Event	Speaker	Registration
Sunday April 14, 2024	Introduction to Machine Learning	Abdelghafour Halimi	Closed
Thursday April 18, 2024	Introduction to Deep Learning	Abdelghafour Halimi	Closed

What is In Situ?

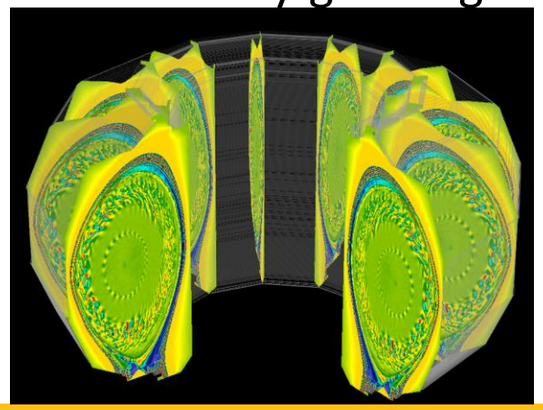
Why do we want/need it?

In Situ Visualization

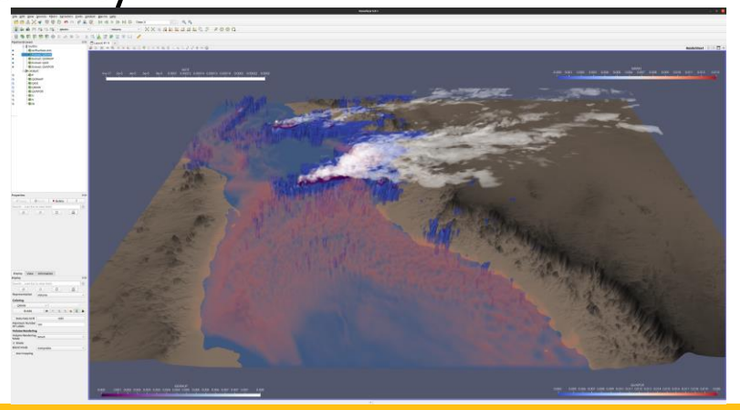
- What is in situ?
  - Produce visualization & analysis during an active simulation
  - Multiple ways in situ can be accomplished
- My application already does this, right?
  - Some applications do have visualizations built-in
- However,…
  - The goal of in situ visualization is to make visualization more adaptive, resilient, and familiar than coding in every possible visualization into a simulation
  - In situ is especially relevant to **HPC applications**

What is High Performance Computing (HPC)?

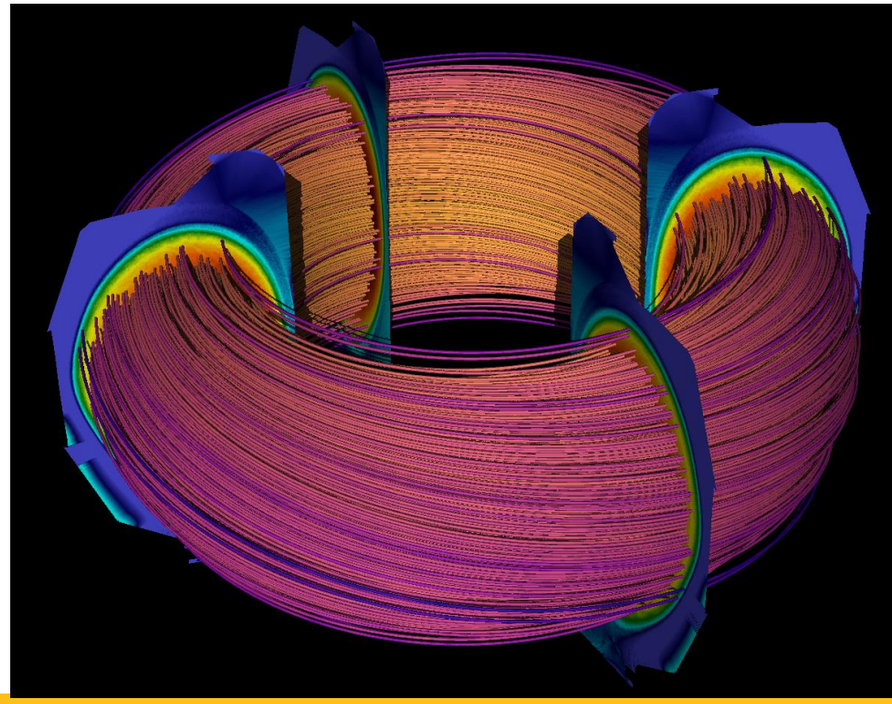
- Leveraging of interconnected processing units (Top500)
  - 50-billion-fold increase in computing power in 70 years
  - Performance measured in FLOPS *(floating-point operations per second)*
    - Human brain: 1-2 FLOPS
    - Smartphone: > 1 TeraFLOP (10^{12})
    - Frontier (top supercomputer in the world): 1.194 Exaflops (10^{18})
- Scientific simulations are large users of HPC
  - Constantly growing in complexity



Code: XGC1



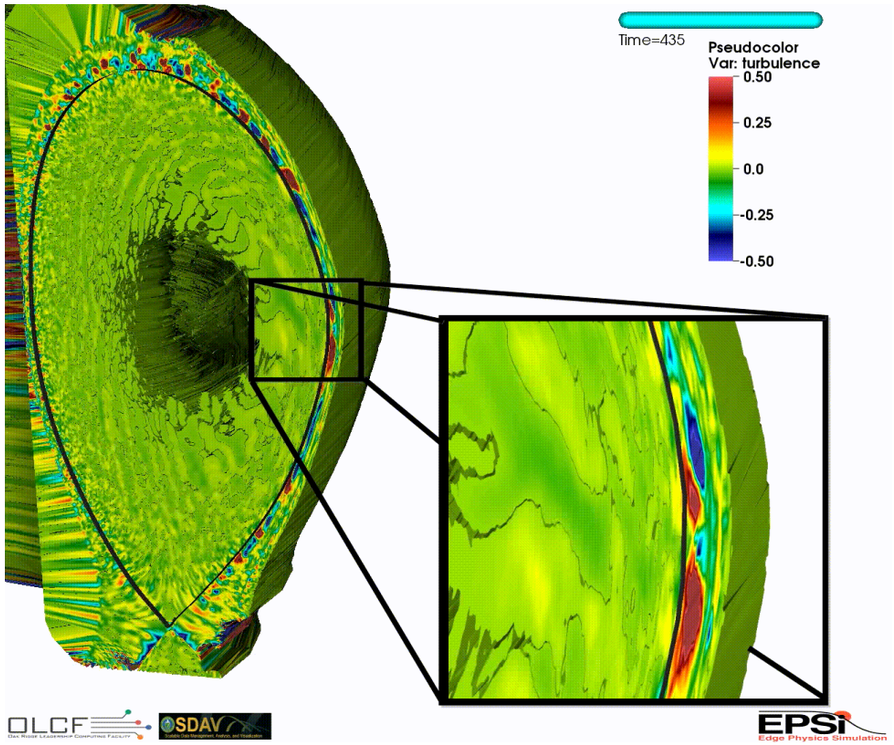
Code: WRF



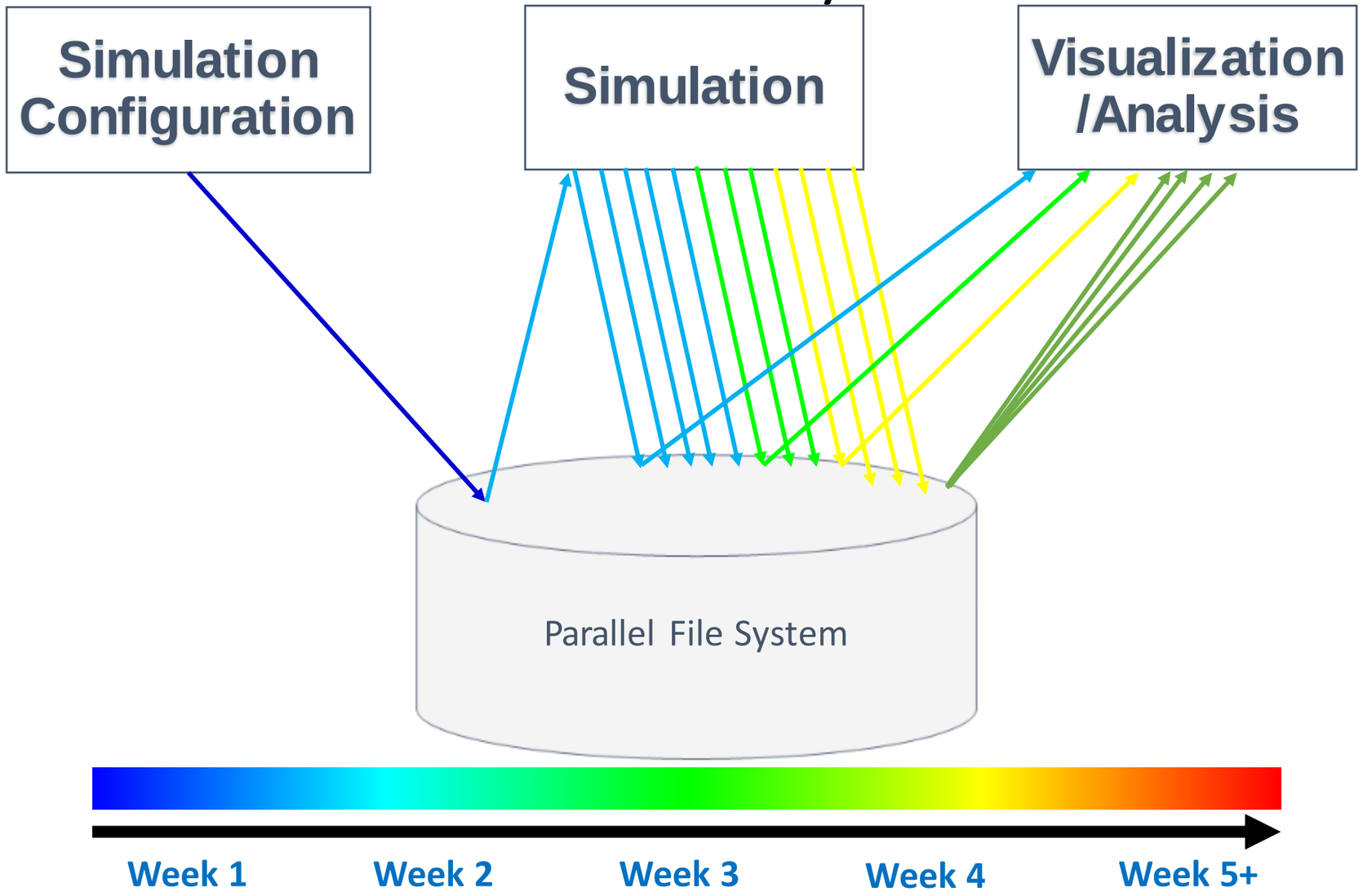
Code: XGC1

Visualization and Analysis in HPC

- Visualization enables:
  - Analytics
  - Locating the real physics
  - Public communication
  - and more

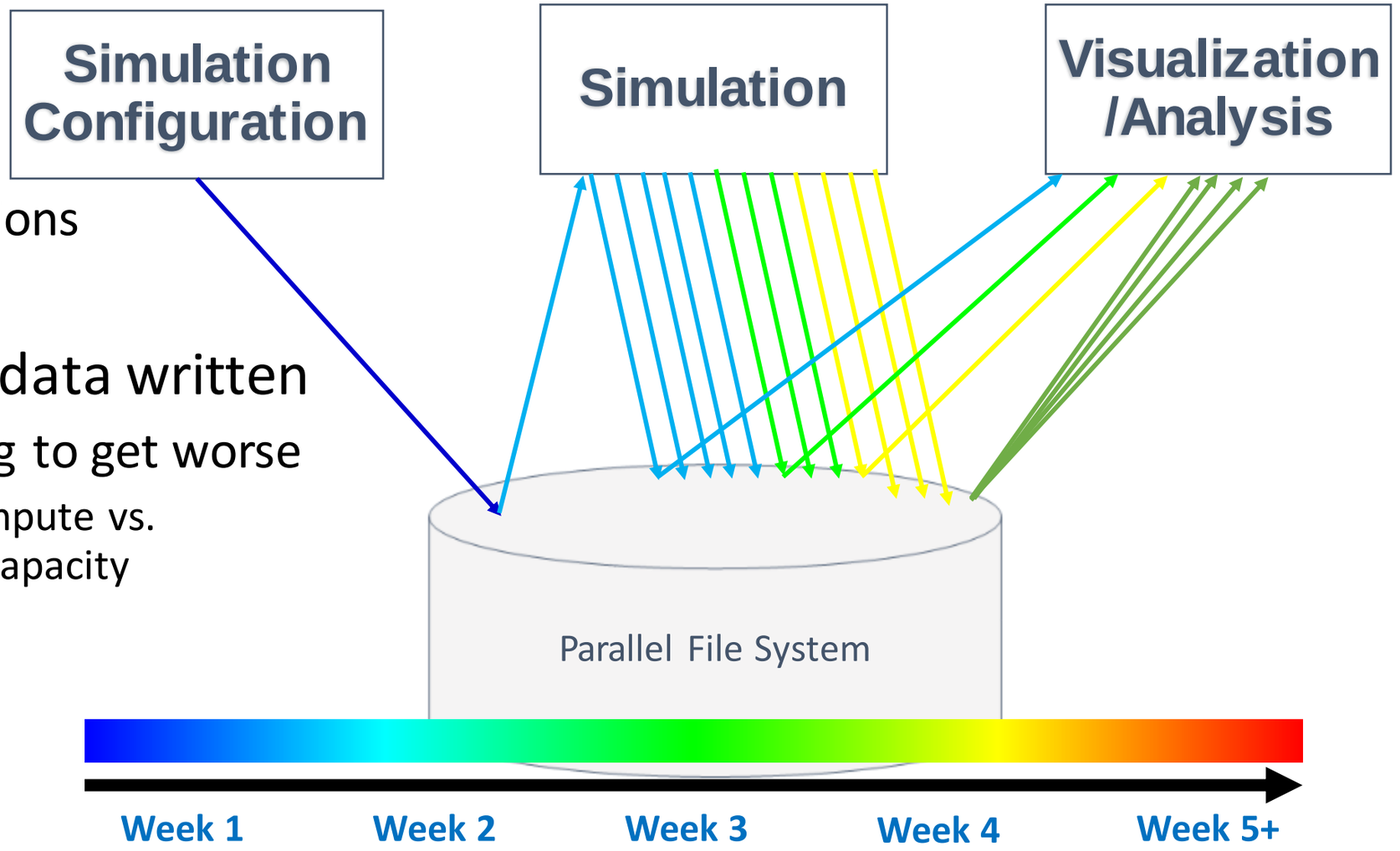


Traditional Post-hoc Analysis



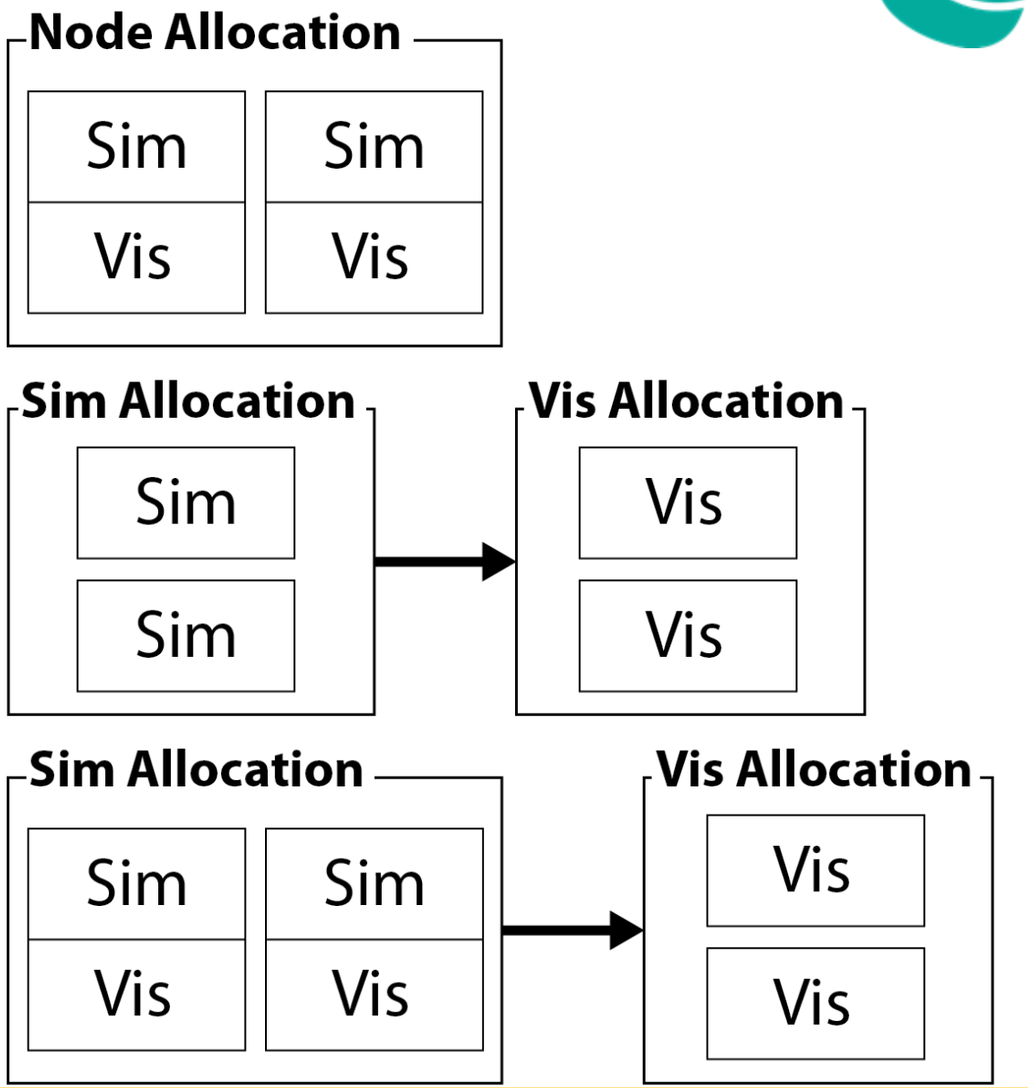
Problems with the Post-hoc Paradigm

- Missing discovery
  - Missing data
  - Infrequent visualizations
- Time and amount of data written
  - IO bottleneck is going to get worse
    - 500X increase in compute vs. 60X increase in I/O capacity

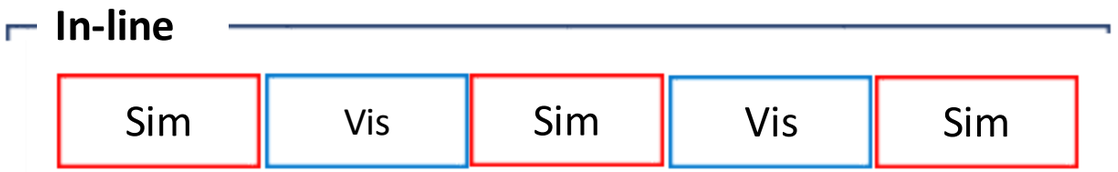


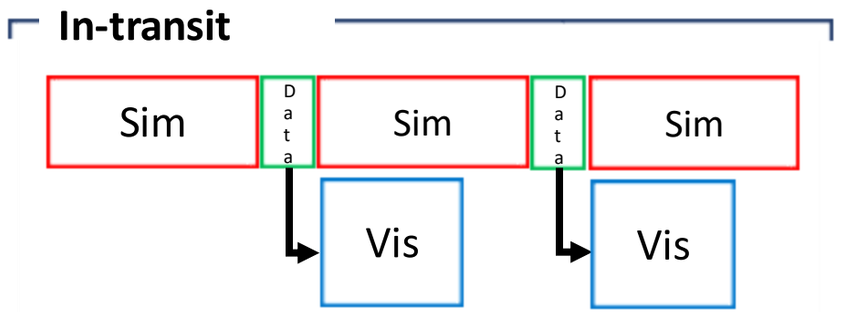
Common In Situ Configurations

- In-line *(Co-processing, tightly coupled)*
  - Simulation and visualization run in the same process using the same resources (*on-node*)
- In-transit *(Concurrent-processing, loosely coupled)*
  - Simulation transfers data to a separate set of visualization nodes (*off-node*)
- Hybrid coupling
  - Utilizing aspects of both in-line and in-transit



In-Line Vs. In-transit Visualization





Introduction to Catalyst

Catalyst History

- Starting with ParaView 5.9, Catalyst was revamped
  - Catalyst was split off to its own project (Catalyst API)
    - Catalyst is an API specification developed for simulations (and other scientific data producers) to analyze and visualize data in situ
  - ParaView has an implementation of the Catalyst API (ParaView Catalyst)
    - ParaView Catalyst exposes a simulations in-memory data, without writing data to disk, then uses interactive python pipelines to create visualization and analysis
    - Can modify pipelines without recompiling simulation
  - Other implementations exist that we are integrating into our miniapp
    - ADIOS2, Ascent

Catalyst

- The Catalyst API uses Conduit for describing data and other parameters which can be communicated between a simulation and Catalyst.
  - Conduit
    - Simplified Data Exchange for HPC Simulations
    - Conduit is an open source project from Lawrence Livermore National Laboratory that provides an intuitive model for describing hierarchical scientific data in C++, C, Fortran, and Python. It is used for data coupling between packages in-core, serialization, and I/O tasks.

ParaView Catalyst

- The Catalyst API comprises of 5 function calls that are used to pass data and control over to the Catalyst implementation from computational simulation codes:
  - `catalyst_initialize, catalyst_execute, catalyst_results, catalyst_finalize, and catalyst_about`
    - Each of these functions is passed a Conduit Node object.

- This is important if you will be adding Catalyst to a simulation, today however, we will simply be creating and using Catalyst scripts

Creating a Catalyst Script

- Demo
  - Load a representative data set in ParaView (***can.ex2***)
  - Create a pipeline to do your visualization
  - Save a script

KVL Visualization Vignettes

Miniapp (gray-scott simulation)

Visualization Vignettes

KVL › KAUST Visualization Vignettes › **Repository**

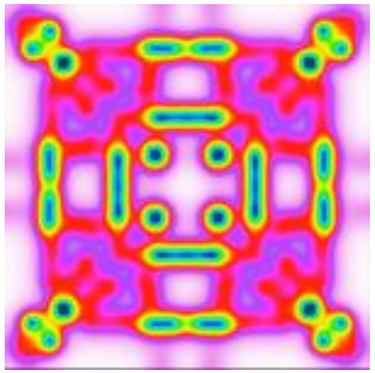
Add_miniapp | KAUST_Visualization_Vignettes | History | Find file | Clone

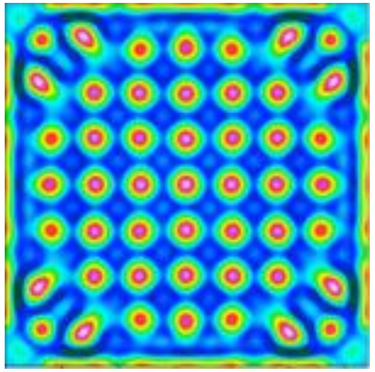
Merge branch 'Add_miniapp' of...
James Kress authored 1 week ago

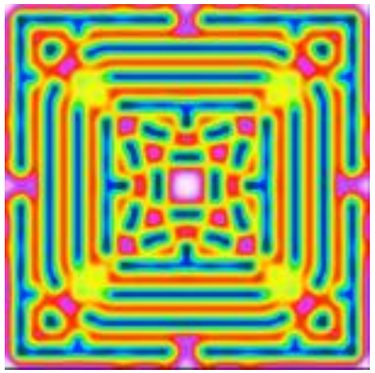
2b6bc400

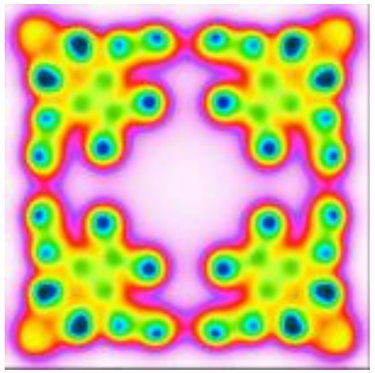
Name	Last commit	Last update
In_Situ_Vignettes	Adding initial visit example files.	1 year ago
Miniapps/gray-scott	Merge branch 'Add_miniapp' of https://gitl...	1 week ago
ParaView_Vignettes	Removing pv warning	4 months ago
Scripts	Updating documentation and repo organiz...	11 months ago
VisIt_Vignettes	Updating visit ibex script	5 months ago
data	Updating scripts for ibex.	6 months ago
README.md	Updating documentation and repo organiz...	11 months ago

Gray-Scott – *3D Reaction Diffusion Miniapp*









Miniapp Overview

- https://gitlab.kaust.edu.sa/kvl/KAUST_Visualization_Vignettes/-/tree/Add_miniapp/Miniapps/gray-scott

Name	Last commit	Last update
..		
common	Initial miniapp commit.X	3 months ago
configs	Initial work on a vtk only file writer.	1 week ago
img	Initial miniapp commit.X	3 months ago
simulation	Initial work on a vtk only file writer.	1 week ago
sites	Merge branch 'Add_miniapp' of https://gitlab.kaust.edu.sa/kvl/KAUST_Vi...	1 week ago
CMakeLists.txt	Initial work on a vtk only file writer.	1 week ago
README.md	Initial work on a vtk only file writer.	1 week ago

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Demonstration

Catalyst Workflows in Gray-Scott

Demo: Catalyst Workflows in Gray-Scott

- Output data to disk using catalyst_io
- Run Catalyst script without human-in-the-loop
- Run Catalyst live
  - Sim runs on Ibex
  - Catalyst runs on user's local computer

Hands-On

Creating Catalyst Scripts and Changing Simulation Parameters

Hands-On Setup

- *cd /ibex/scratch/<username>*
- *cp /sw/vis/ibex-gpu/KAUST_Visualization_Vignettes/Miniapps/gray-scott/configs/miniapp-settings/ibex-settings-catalyst-* .*
- *cp /sw/vis/ibex-gpu/KAUST_Visualization_Vignettes/Miniapps/gray-scott/configs/catalyst_scripts/catalyst-extract-* .*
- *cp /sw/vis/ibex-gpu/KAUST_Visualization_Vignettes/Miniapps/gray-scott/sites/ibex/* .*
- *export CATALYST_CLIENT=<your_IP>*

Hands-On with Catalyst

- Run an existing example and connect live
  - sbatch run-ibex.sbat
- Create a new catalyst script and run it
- Change the simulation parameters and run script
- …. Questions?

Thanks!

Contacts:

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help@vis.kaust.edu