ADIOS 2.8: Storage and in situ I/O

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SC'22 Dallas, TX Nov 2022

Thanks to the many of my collaborators

- Hasan Abbasi
- Mark Ainsworth
- Chuck Atkins
- Vicente Bolea
- Phillipe Bonnet
- Michael Bussmann
- CS. Chang
- Jieyang Chen
- Hank Childs
- Jong Choi
- Michael Churchill
- Philip Davis
- Ciprian Docan
- Greg Eisenhauer
- Stephane Ethier
- Ana Gainaru
- Dmitry Ganyushin
- Kai Germaschewski
- Berk Geveci
- William Godoy
- Qian Gong
- Junmin Gu
- Kevin Huck
- Axel Huebl
- Chen Jin
- Mark Kim
- Brad King
- James Kress
- S.H. Ku
- Ralph Kube
- Tahsin Kurc
- Xin Liang
- Zhihong Lin
- Qing Liu
- Jay Lofstead
- Jeremy Logan
- Kshitij Mehta
- Ken Moreland
- Todd Munson
- Manish Parashar
- Franz Pöschel
- Dave Pugmire
- Anand Rangarajan
- Sanjay Ranka
- Caitlin Ross
- Nagiza Samatova
- Karsten Schwan
- Ari Shoshani
- Eric Suchyta
- Fred Suter
- Keichi Takahashi
- William Tang
- Roselyne Tchoua
- Nick Thompson
- Seiji Tsutsumi
- Ozan Tugluk
- Lipeng Wan
- Ruonan Wang
- Ben Whitney
- Matthew Wolf
- Kesheng Wu
- Bing Xie
- Fan Zhang
- Fang Zheng

Outline

- 8:30 Introduction to data management at extreme scale – Scott Klasky
- 9:15 ADIOS 2 concepts and API (C++, Python, F90) – Norbert Podhorszki
- 10:00 BREAK
- 10:30 ADIOS 2 API – Norbert Podhorszki
- 11:00 Hands on with ADIOS 2 – Files – Ana Gainaru
- 12:00 Lunch
- 1:30 ADIOS @ scale – Norbert Podhorszki
- 2:00 Introduction to Paraview + ADIOS + hands on Caitlin Ross
- 3:00 BREAK
- 3:30 Introduction to TAU and TAU + ADIOS – Kevin Huck
- 4:00 Hands on with TAU + ADIOS
- 4:15 Staging with ADIOS – hands 0n – Ana Gainaru
- 5:00 END

Introduction

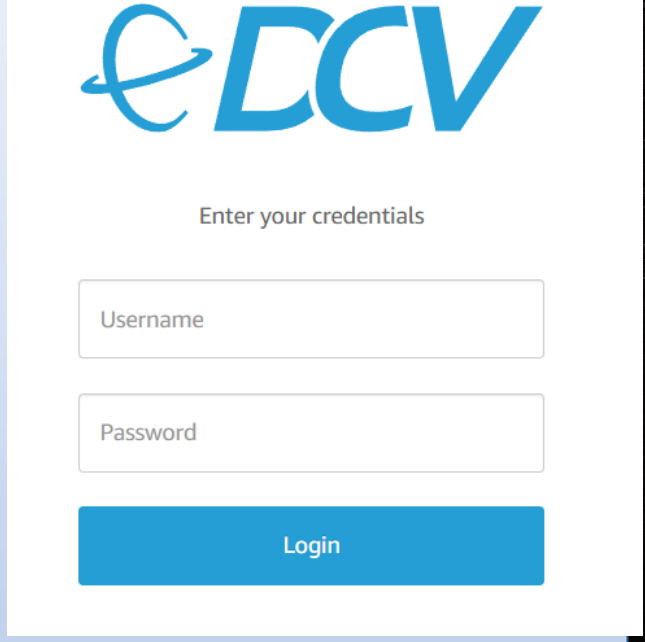
Login to a virtual machine

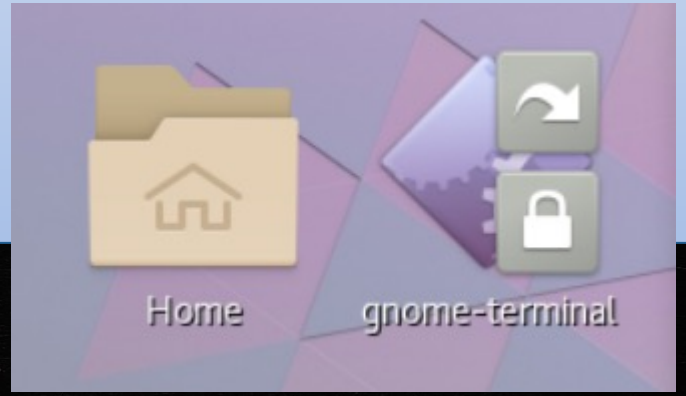
https://tut###.supercontainers.org:8443/#e4s

is a number assigned for you in this tutorial

Username: tutorial
Password: HPCLinux12!

Launch a couple of gnome-terminals





What should you get out of this tutorial

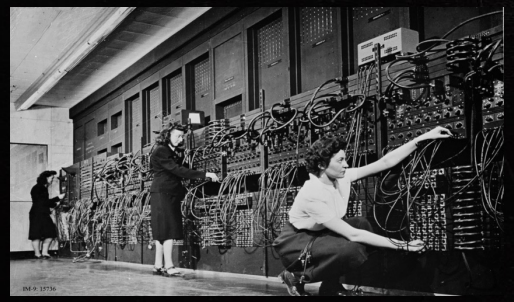
- Why you should use ADIOS
- What are the advantages of using ADIOS over other parallel I/O and in situ visualization frameworks
- How to use ADIOS
- How to get high performance using ADIOS
- How to use ADIOS for in situ analytics
- How to visualize data with Paraview for in situ and post processing of ADIOS-enabled codes
- How to use TAU with ADIOS and to visualize the TAU-ADIOS files

- What programming language should we focus this tutorial on for you? C++, Python, F90, C
- PLEASE ASK QUESTIONS!

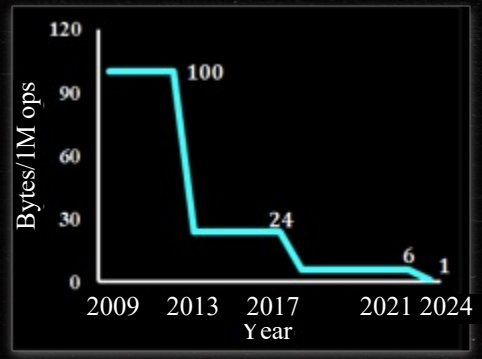
The data deluge

- Computing capability has increased by a factor of 10^{15} over the past 70 years
- Applications push the boundaries of data: e.g. Radio Astronomy
  - In 2022 the Vera C. Rubin Observatory in Chile will collect 20 terabytes/night as part of the Legacy Survey of Space and Time (LSST)
  - In 2028 the Square Kilometre Array, will generate 100 times that amount
- Filesystem/network bandwidth falls behind CPU/memory: Fewer bytes/operation

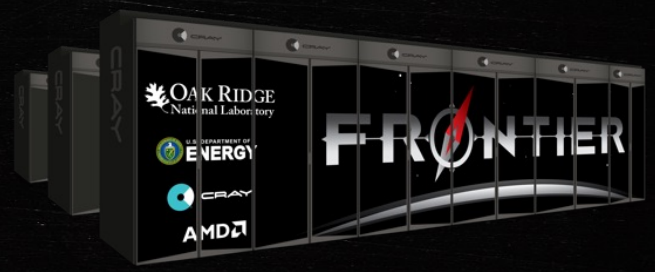
1943 , 5K Flops, Electronic Numerical Integrator And Computer – no filesystem



Filesystems continue to fall behind computing power



2022 , 2 Ex Flops, Frontier, LUSTRE filesystem



Supercomputing changes in the last 30 years

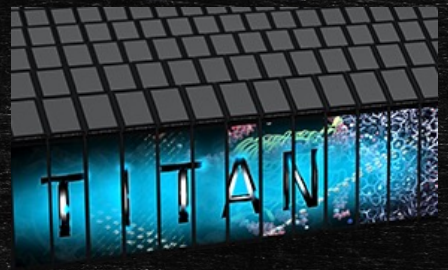
1988: Cray Y-MP:0.0000027 Pflops: Vector Processors, SSD for storage (13.6 GB/s)

1996:Cray T3E: 0.001 PFlops, massively parallel

1998: 0.0025 Pflops,ASCI Blue Mountain: shared memory across all procs

2002: Earth Simulator 0.040 Tflops, 50MW, vector procs

2009: Cray XT5: 2.5 Pflops: Multi-core, LUSTRE storage system



2013: Cray Titan: 27 Pflops , NVIDIA GPUs

2018: IBM Summit: 200 Pflops , NVIDIA GPUs

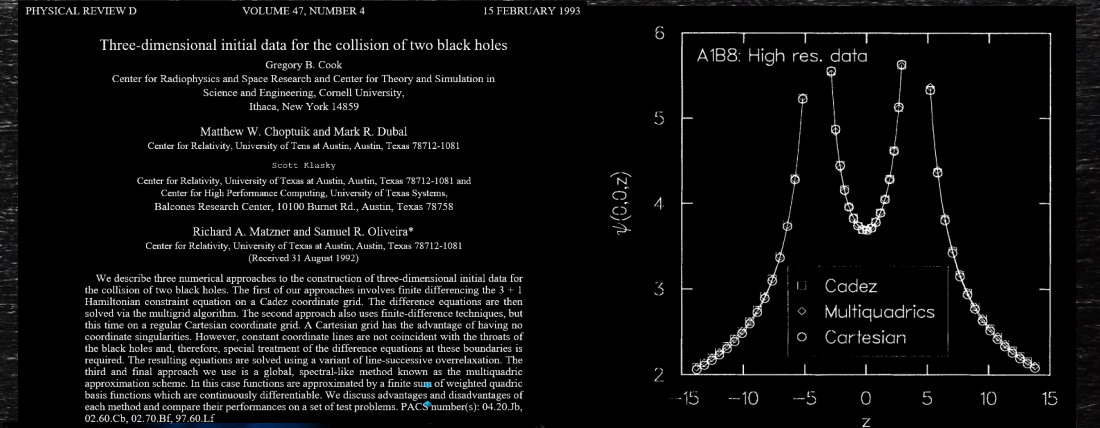
2022: Cray Frontier: 2000 Pflops , AMD GPUs, Burst Buffer Storage 10TB/s, long term at 4.6 TB/s

Observations:

- Ratio of Storage/Flops keeps getting worse
- I/O variability gets worse as systems scale
- New applications are running complex workflows with AI + HPC applications
- Experimental/Observational data is outpacing compute & storage

The vision: 1993, 2003

- 1993: Develop an efficient and accurate code to generate data for understanding the gravitational radiation from black hole coalescence
- 2003: Understand zonal flow in a fusion reactor
- Goals
  - Accelerate this process
  - Make the process predictable
  - Make the process adaptable
  - Make the process scalable as the complexity increases
  - Make the software easy-to-use
- Approach
  - Create long-term partnerships with some of the “most” data demanding applications in the world and create software solutions used around the world


PHYSICAL REVIEW D VOLUME 47, NUMBER 4 15 FEBRUARY 1993

Three-dimensional initial data for the collision of two black holes

Gregory B. Cook
Center for Radiophysics and Space Research and Center for Theory and Simulation in Science and Engineering, Cornell University, Ithaca, New York 14859

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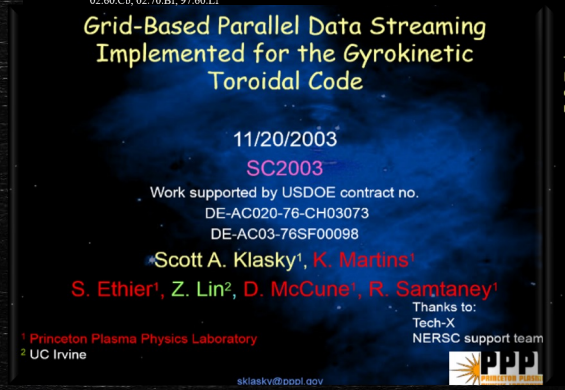
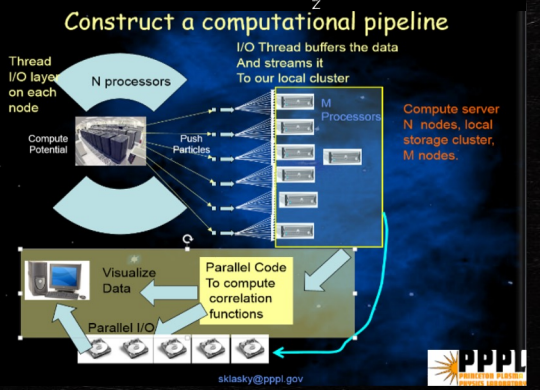
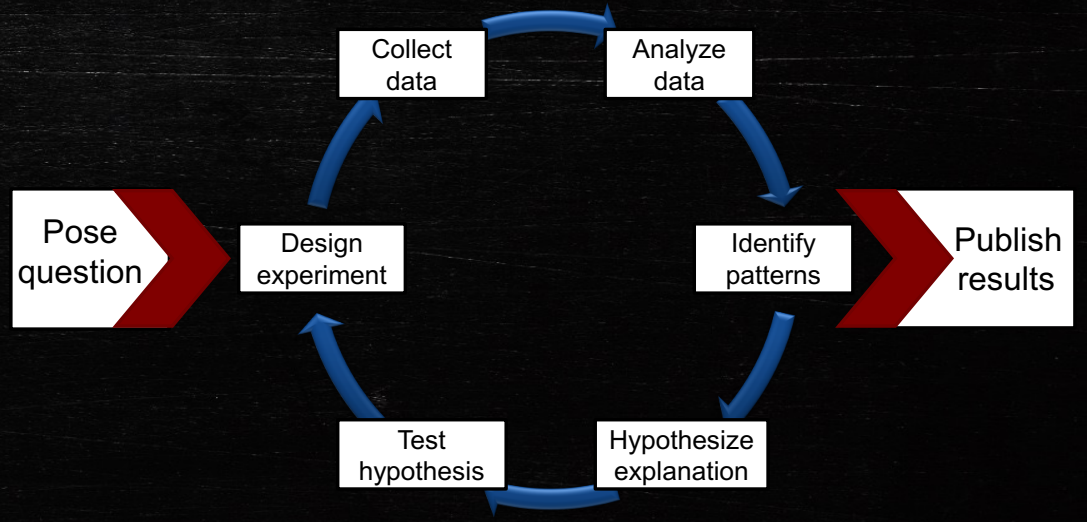
(Received 31 August 1992)

We describe three numerical approaches to the construction of three-dimensional initial data for the collision of two black holes. The first of our approaches involves finite differencing the 3 + 1 Hamiltonian constraint equation on a Cadez coordinate grid. The difference equations are then solved via the multigrid algorithm. The second approach also uses finite-difference techniques, but this time on a regular Cartesian coordinate grid. A Cartesian grid has the advantage of having no coordinate singularities. However, constant coordinate lines are not coincident with the throats of the black holes and, therefore, special treatment of the difference equations at these boundaries is required. The resulting equations are solved using a variant of line-successive overrelaxation. The third and final approach we use is a global, spectral-like method known as the multiquadric approximation scheme. In this case functions are approximated by a finite sum of weighted quadric basis functions which are continuously differentiable. We discuss advantages and disadvantages of each method and compare their performances on a set of test problems. PACS number(s): 04.20.Jb, 02.60.Cb, 02.70.Bf, 97.60.Lf





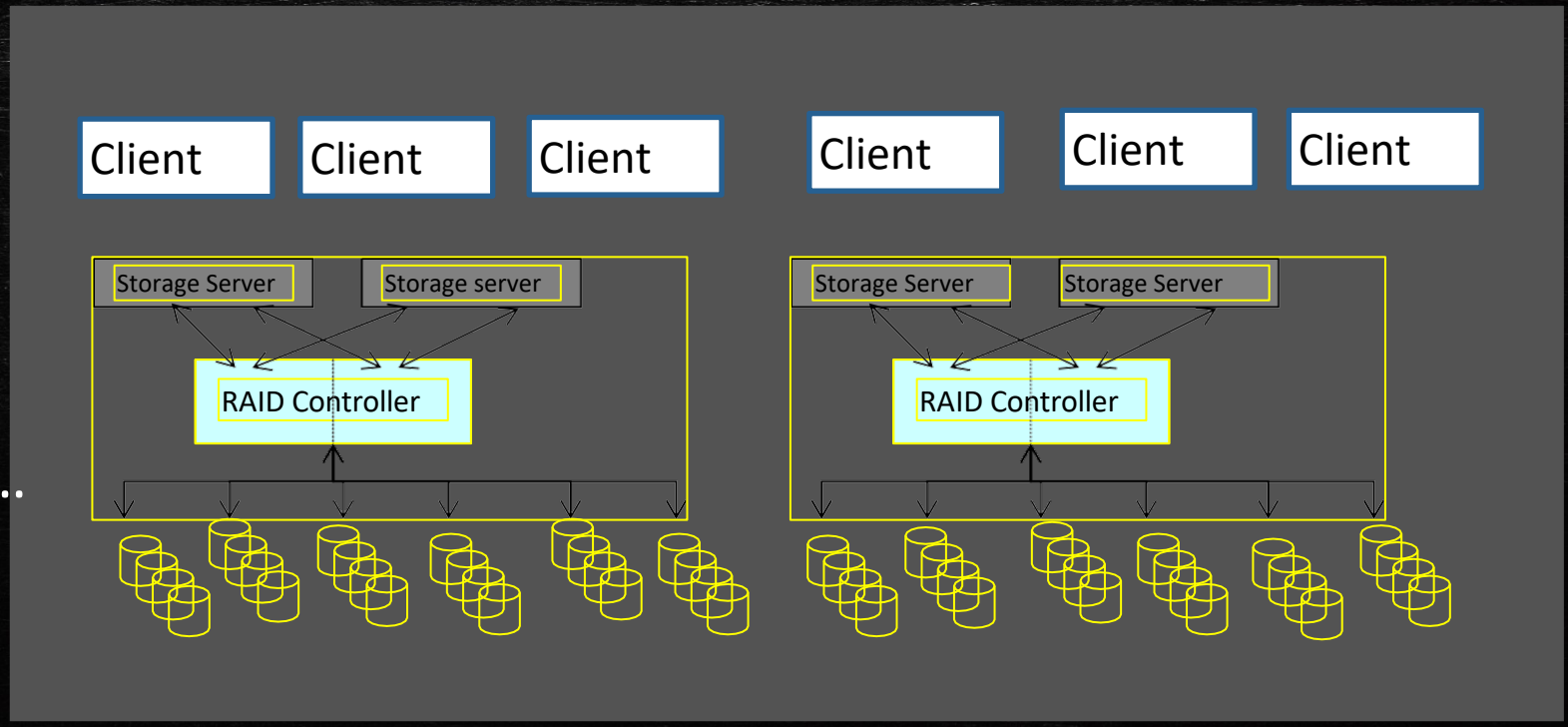


G. B. Cook, S. Klasky, et al., Three dimensional initial data for the collision of two black holes. Physical Review D 1993, 47, 1471. (98 citations)S. Klasky, S. Ethier, et al., Grid-based parallel data streaming implemented for the gyrokinetic toroidal code in Proceedings of the 2003 ACM/IEEE conference on Supercomputing, ACM, p. 24.

9

Storage System Choices

- Lustre
  - File system layered over objects (OSTS) on severs (OSS), which writes through a RAID controller on the OSTs. The OST hires the local file system
- IBM Spectrum Scale (GPFS)
- PanFS
- Ceph
- OrangeFS
- HDFS
- NVMe – on node, on servers, …

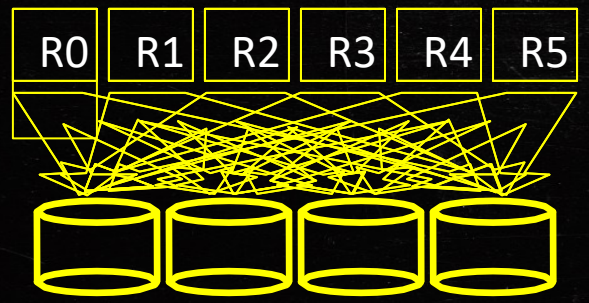


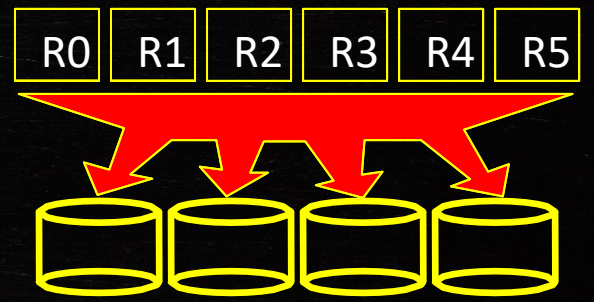
POSIX I/O

- POSIX is the IEEE Portable Operating System Interface for Computing Environments
- POSIX Contains: Files, directories, permissions, attributes through an API and a set of semantics for interacting with files, directories, …
- To optimize I/O you need to use the “correct” level of parallelism, but you need to be careful about
  - Knowing how you will stripe your data across a parallel file system
  - Knowing how you parallel file system will handle caching and locking
  - Knowing how to deal with data locality
  - Understanding how to map the parallel file system I/O requests to the network

MPI-IO

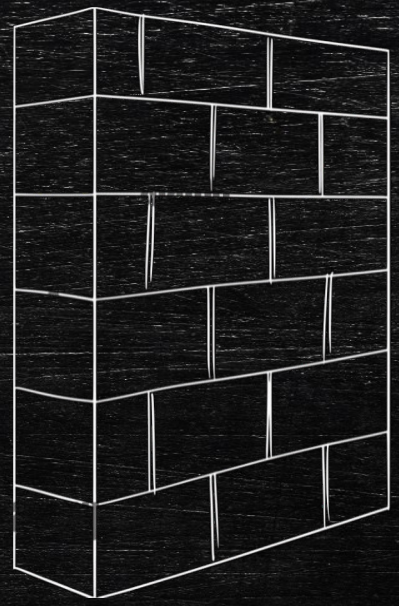
- A layer on top of POSIX – i.e. a stream of bytes in a file
- Features which contains many improvements over POSIX for parallel applications
  - Collective I/O
  - Noncontiguous I/O with MPI datatypes and file views
  - Nonblocking I/O
  - To manage parallelism
  - To reorganize data in distributed memory to serialized arrays on disk
- Contains ways to do this for independent and collective I/O





Users are hitting their head against to wall to deal with IO

- I/O needs to run
  - On HPC resources with Parallel File Systems
  - On HPC resources to connect multiple parallel writers with multiple parallel readers
  - Over the Wide Area Network
  - Over Local Area Network
  - On New storage devices, e.g., Burst Buffers, NVMe, DAOS,
  - Cloud Storage: HDFS
- And it must run efficiently
- And it needs to supports queries, at all scales



Some people want to

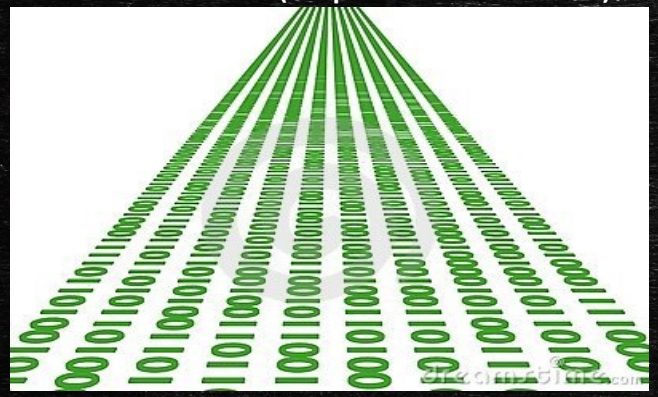
- Change the wall with a softer surface
- But… eventually it will still hurt!

Or… show them the light

Self Describing Data

- Raw data (byte streams) have little to no use without appropriate description
- Recovering actual information costs scale with the size of the data.
- Self-describing data: Raw data (expensive access) + Metadata (quick access, embedded).

Question:
What extra annotations do we add to the output to make it more valuable, without "greatly" effecting performance ?



Field	Value
Size	100
Min	0.00002352422
Max	1203213123.4542
Dimensions	{2,50}
Type	float
Name	"pressure"
Units	"KPa"

- **Cost:** metadata overhead. **Benefit:** make fast decisions based on metadata.
  - Example: Extract array bounds, min and max, are they physical? → Yes: analyze data, No: stop, debug
- Modern software self-describing components:
  - C++ STL containers → data + metadata: size, first and last iterators
  - Python numpy arrays →data + metadata: type, shape, element size
  - Self-describing data formats: JSON, XML schemas, HDF5, ADIOS BP, netCDF

Examples of Self Describing Files

MS-Word


```
<?mso-application progid="Word.Document"?>
<w:wordDocument xmlns:aml="http://schemas.microsoft.com/aml/2001/core"
xmlns:wpc="http://schemas.microsoft.com/office/word/2010/wordprocessingCanvas"
xmlns:cx="http://schemas.microsoft.com/office/drawing/2014/chartex"
xmlns:cx1="http://schemas.microsoft.com/office/drawing/2015/9/8/chartex"
xmlns:cx2="http://schemas.microsoft.com/office/drawing/2015/10/21/chartex"
xmlns:cx3="http://schemas.microsoft.com/office/drawing/2016/5/9/chartex"
xmlns:cx4="http://schemas.microsoft.com/office/drawing/2016/5/10/chartex"
xmlns:cx5="http://schemas.microsoft.com/office/drawing/2016/5/11/chartex"
xmlns:dt="uuid:C2F41010-65B3-11d1-A29F-00AA00C14882"
xmlns:mc="http://schemas.openxmlformats.org/markup-compatibility/2006"
xmlns:o="urn:schemas-microsoft-com:office:office" xmlns:v="urn:schemas-microsoft-
com:vml" xmlns:w10="urn:schemas-microsoft-com:office:word"
xmlns:w="http://schemas.microsoft.com/office/word/2003/wordml"
xmlns:wx="http://schemas.microsoft.com/office/word/2003/auxHint"
xmlns:wne="http://schemas.microsoft.com/office/word/2006/wordml"
xmlns:wsp="http://schemas.microsoft.com/office/word/2003/wordml/sp2"
xmlns:sl="http://schemas.microsoft.com/schemaLibrary/2003/core" w:macrosPresent="no"
w:embeddedObjPresent="no" w:ocxPresent="no" xml:space="preserve">
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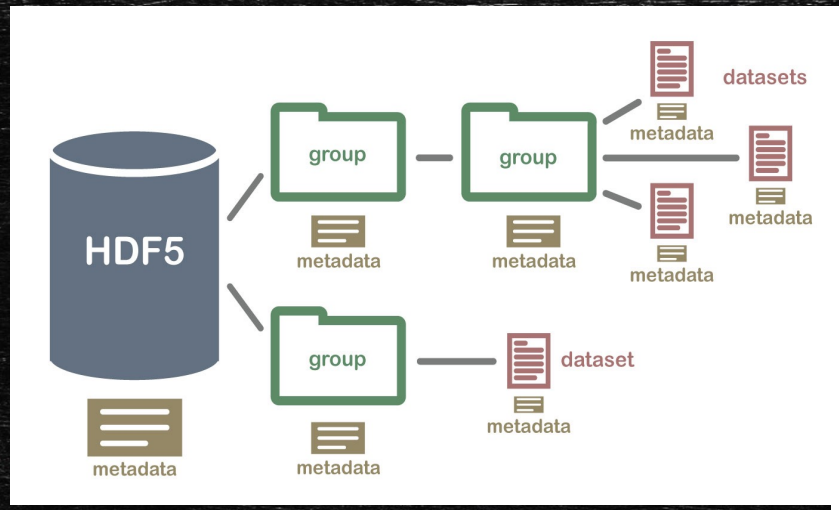
HDF5 (and netCDF4)



ADIOS

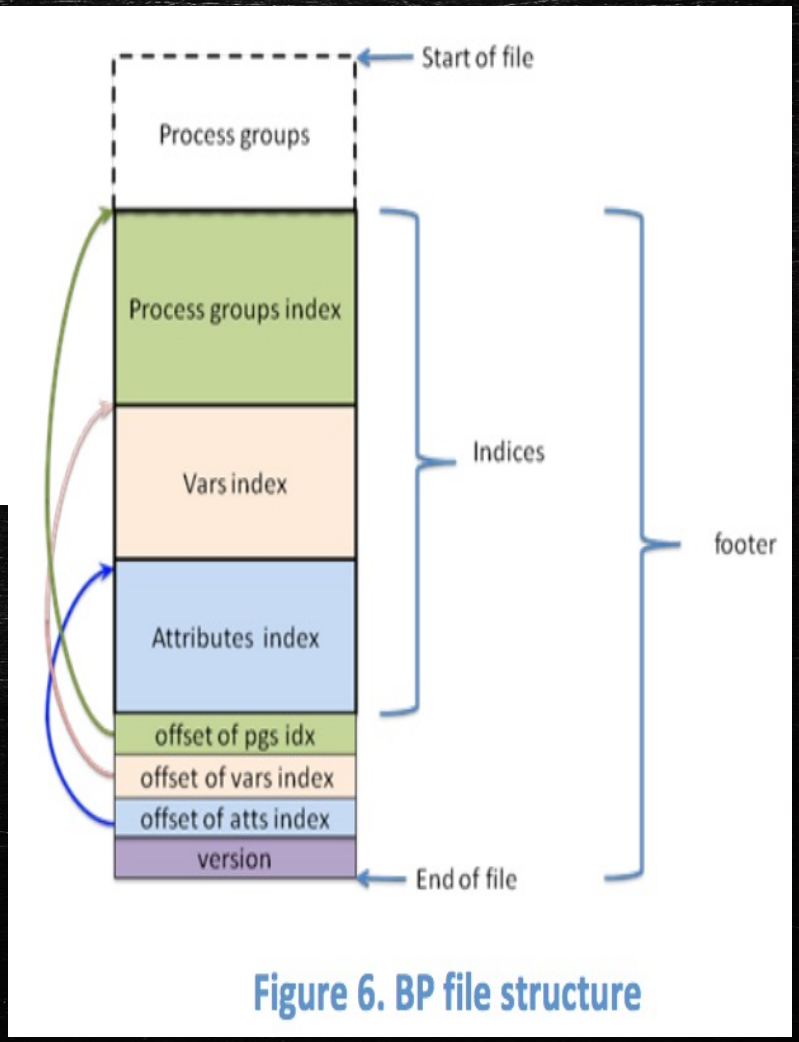


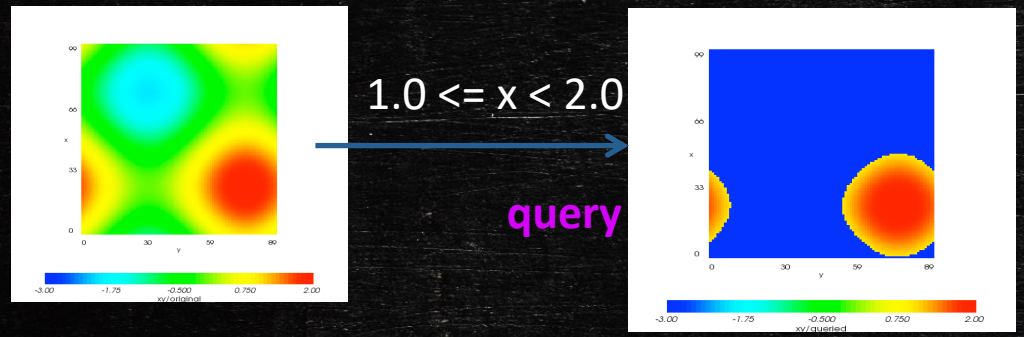
Figure 6. BP file structure

JPEG

JFIF file structure		
Segment	**Code**	**Description**
SOI	FF D8	Start of Image
JFIF-APP0	FF E0 *s1 s2* 4A 46 49 46 00 ...	see below
JFXX-APP0	FF E0 *s1 s2* 4A 46 58 58 00 ...	optional, see below
... additional marker segments (for example SOF, DHT, COM)		
SOS	FF DA	Start of Scan
	compressed image data	
EOI	FF D9	End of Image

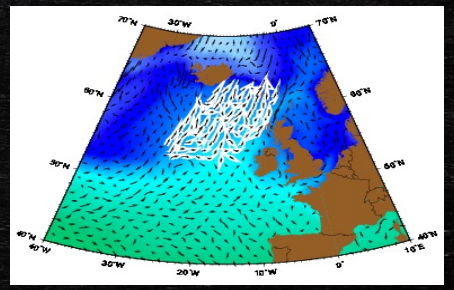
Useful for Queries

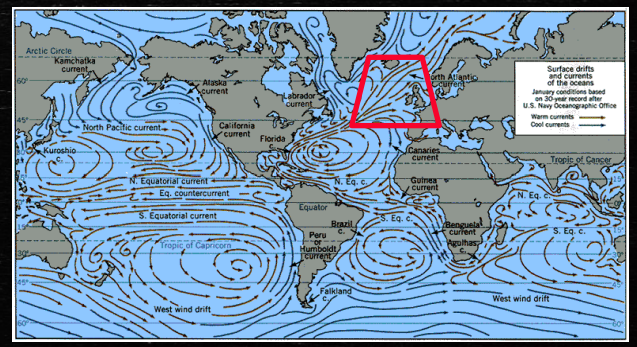
- Data analysis for decision-making is done on a “need to know” information basis
- Searching through the data is largely simplified by its self-descriptive nature
- Queries can be time constrained…give me the best information I can get in 1 hour
- Example: Extract “Var” (value range, region range, time range, ….) from large campaign simulations. Where “Var” is any physical variable → pressure, temperature, velocity, particle, energy

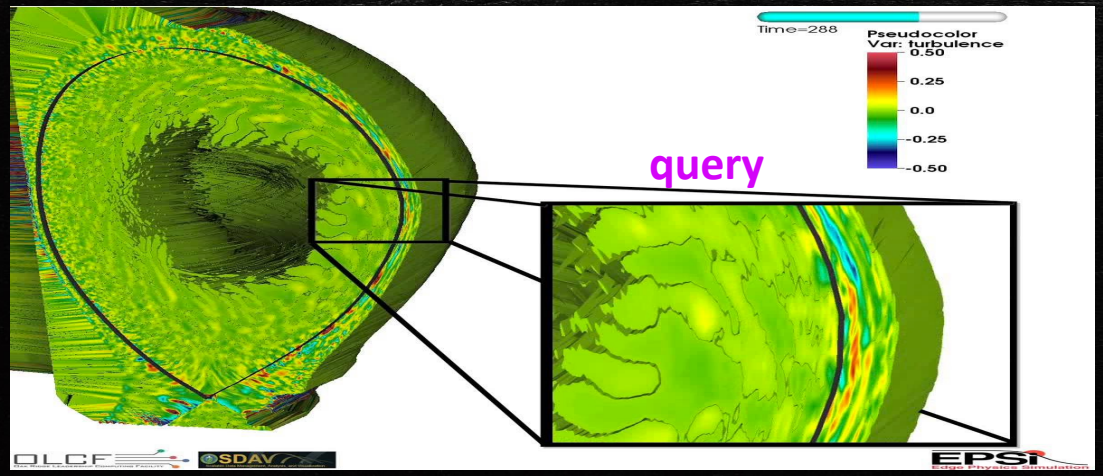


North-Atlantic Drift velocities averages Jan-Mar (miami.edu)

query







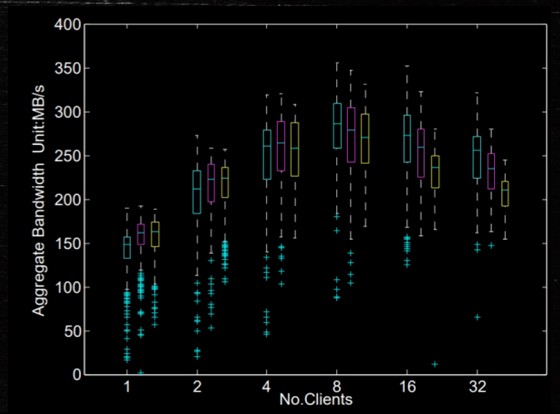
ADIOS: high-performance publisher/subscriber I/O framework

Vision

- Create an easy-to-use, high performance I/O abstraction to allow for on-line/off-line memory/file data subscription service
- Create a sustainable solution to work with multi-tier storage and memory systems

Research Details

- Declarative, publish/subscribe API is separated from the I/O strategy
- Multiple implementations (engines) provide functionality and performance
- Rigorous testing ensures portability
- Data reduction techniques are incorporated to decrease storage cost
- https://github.com/ornladios/ADIOS2



B. Xie, S. Klasky, et al. Characterizing output bottlenecks in a supercomputer. In High Performance Computing, Networking, Storage and Analysis (SC), 2012. Best Student paper nominee

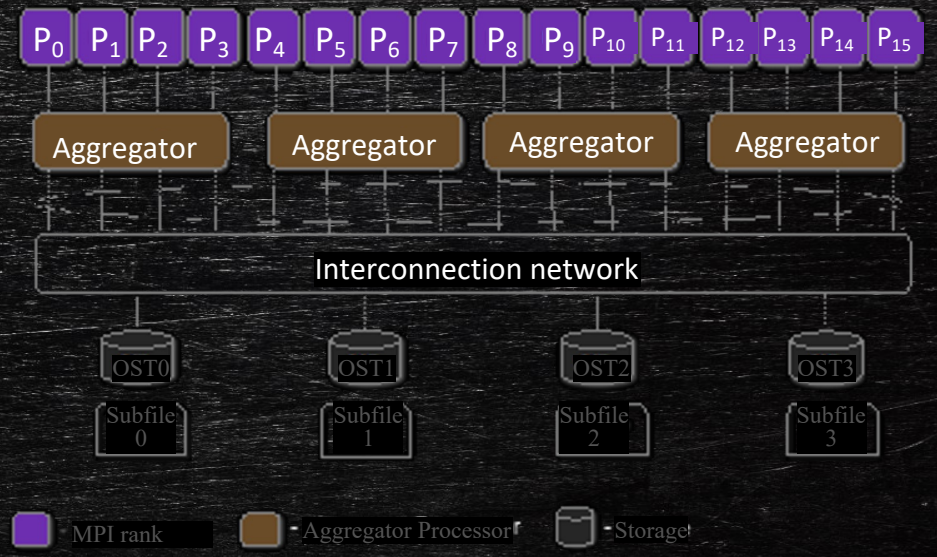
Godoy, W. F., Klasky, S. ,et al. (2020). ADIOS-2: The adaptable input output sys management. SoftwareX, 12, 100561.

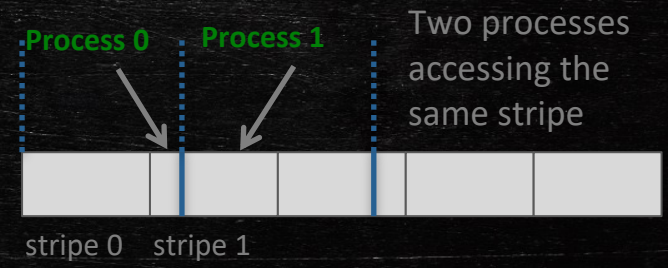
Why should you care about ADIOS

- ADIOS abstraction
  - ADIOS is about self describing I/O at scale
    - Scale – number of variables, number of ranks, data size, number of steps
    - Get/put… - there is nothing special about connecting multiple applications together compared to connecting through the storage system or connecting over the WAN
- ADIOS performance
  - ADIOS has been integrated into dozens of codes and has shown exceptional performance at scale on all different computational resources
- …

Optimizations for a parallel file system

- Avoid latency (of small writes): Buffer data for large bursts – use a type of self-describing log file format
- Avoid accessing a file system target from many processes at once
  - Aggregate to a small number of actual writers:
  - Avoid lock contention
  - Striping correctly & writing to subfiles
- Avoid global communication
- Topology-aware data movement that takes advantage of topology
  - Find the closest I/O node to each writer
  - Minimize data movement across racks/mid-planes



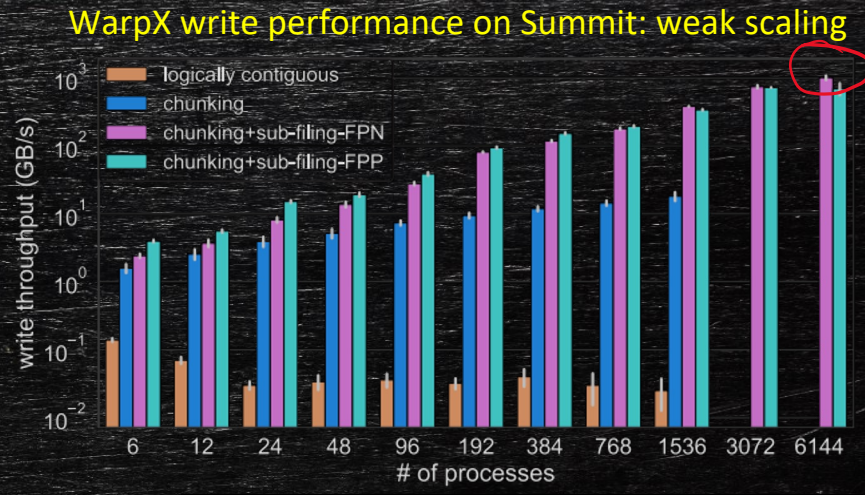


Application	Nodes/GPUs	Data Size/step	I/O speed
SPECFEM3D	3200/19200	250 TB	~2 TB/sec
GTC	512/3072	2.6 TB	~2 TB/sec
XGC	512/3072	64 TB	1.2 TB/sec
LAMMPS	512/3072	457 GB	1 TB/sec

Liu, Q., Klasky, S., et al. "Hello ADIOS: the challenges and lessons of developing leadership class I/O frameworks." Concurrency and Computation: Practice and Experience 26.7 (2014): 1453-1473.

Case study with the WarpX code

- How do we balance the write vs. read cost of a large scale HPC application such as WarpX?
  - Typical choices are to write to a logically contiguous file or chunk versions of this (e.g., HDF5) or to write separate chunks in many files (e.g., ADIOS-2) using one file per process (FPP) or one file per node (FPN)
- The challenge can be in optimizing reading
  - What is the most optimal organization?



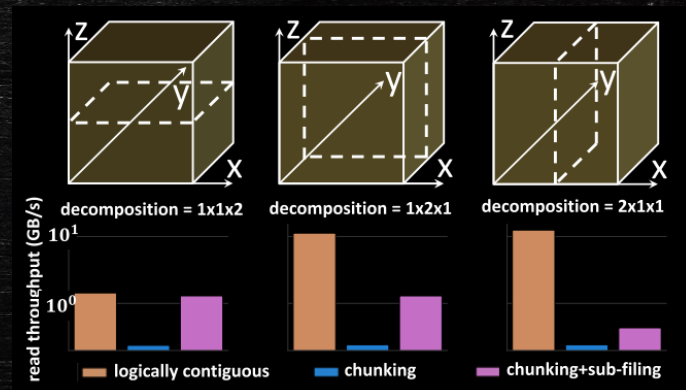
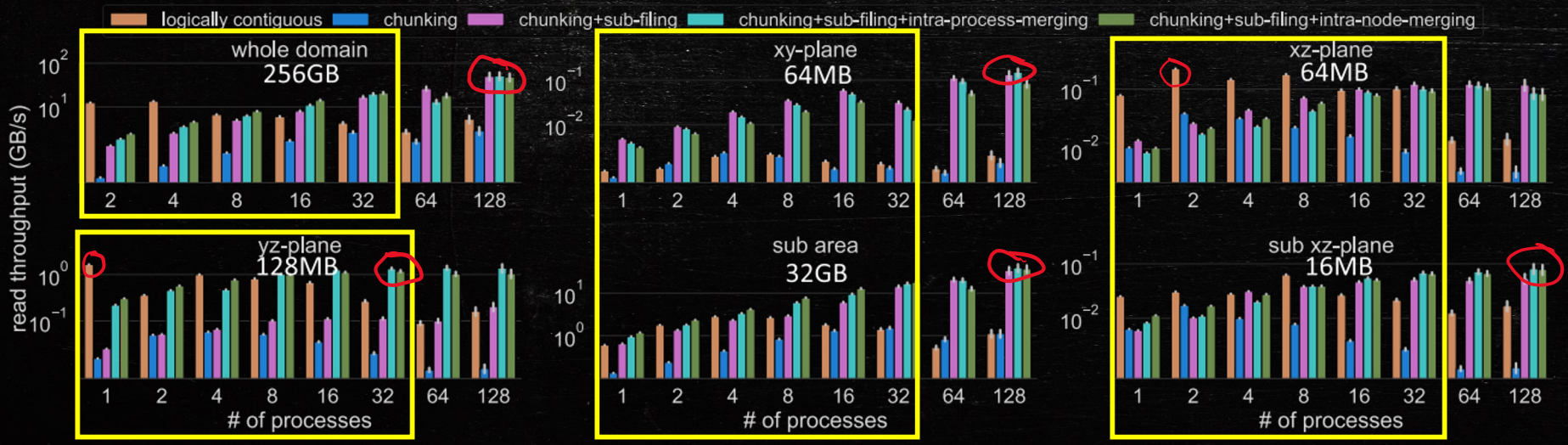
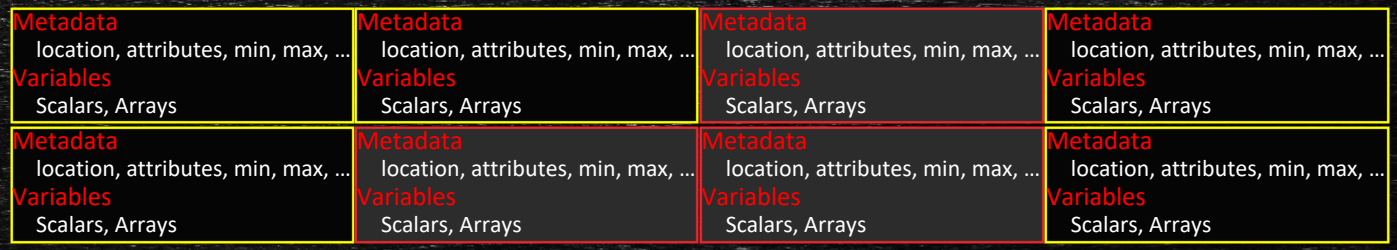


Fig. 5. Impact of decomposition schemes when reading.

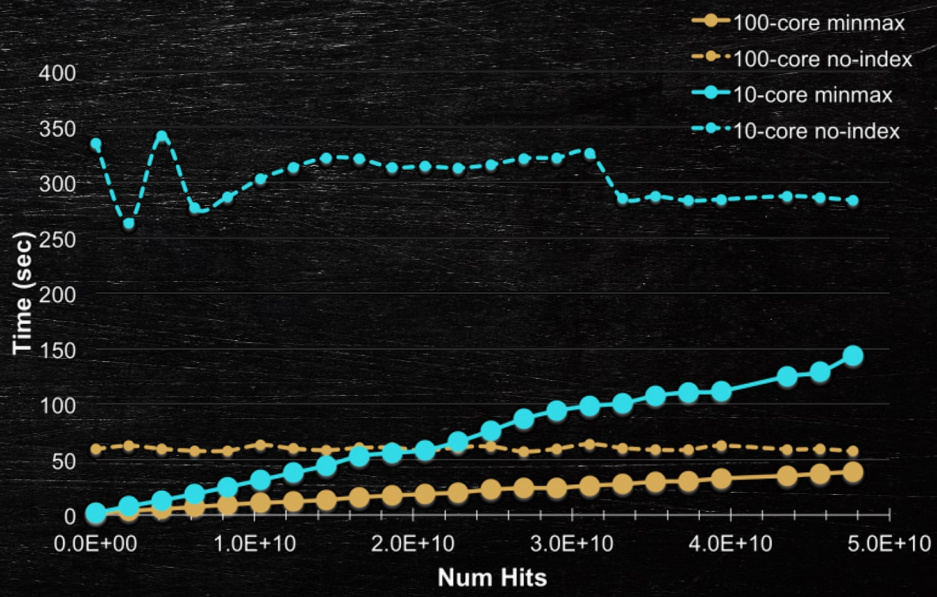


Wan, L., Huebl, A., Gu, J., Poeschel, F., Gainaru, A., Wang, R., ... & Klasky, S. (2021). Improving I/O performance for exascale applications through online data layout reorganization. IEEE Transactions on Parallel and Distributed Systems, 33(4), 878-890.

Querying Large Scientific Data Sets



- ADIOS writes metadata for each variable on each "chunk" of data
  - Currently it contains min/max, but it can include variance, mean, …
- Queries can contain 3 parts
  1. The selection box to limit the points considered
  2. The query conditions - in a form of query predicates connected with AND/OR operators
  3. The query output



- The chunks which satisfy the queries are returned to ADIOS and then the resultant data is given to the application.
  - This allows analysis tools to quickly query the data with no additional cost for storing indices
- Research is in optimizing the merge/split of chunks for Write/Read performance

Gu, J., Klasky, S., Podhorszki, N., Qiang, J., & Wu, K. (2018, March). Querying large scientific data sets with adaptable IO system ADIOS. In Asian Conference on Supercomputing Frontiers (pp. 51-69). Springer, Cham.

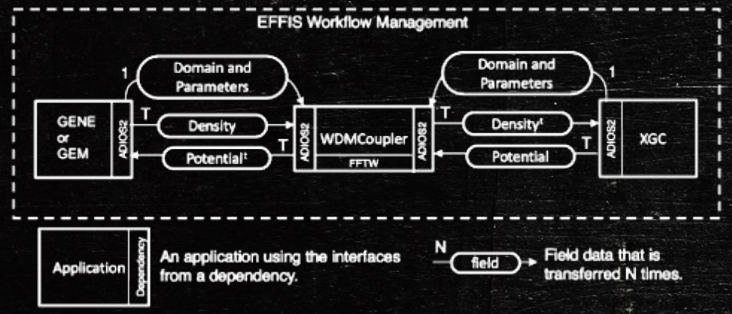
Q2C: Performance results from our recent integration progress

WDMApp

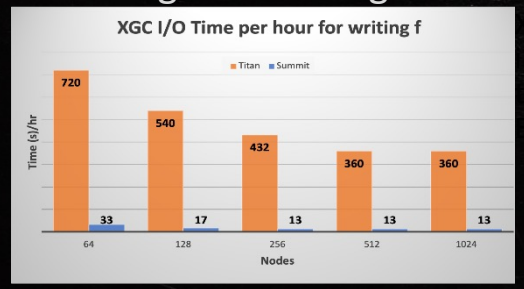
https://github.com/PrincetonUniversity/XGC-Devel

ADIOS main activities have been

1. Reduce the coupling time during communication between the coupler and the WDM codes



2. Reduce I/O overhead for C/R and writing out the large PDF data



XGC I/O time improvement since the beginning of ECP

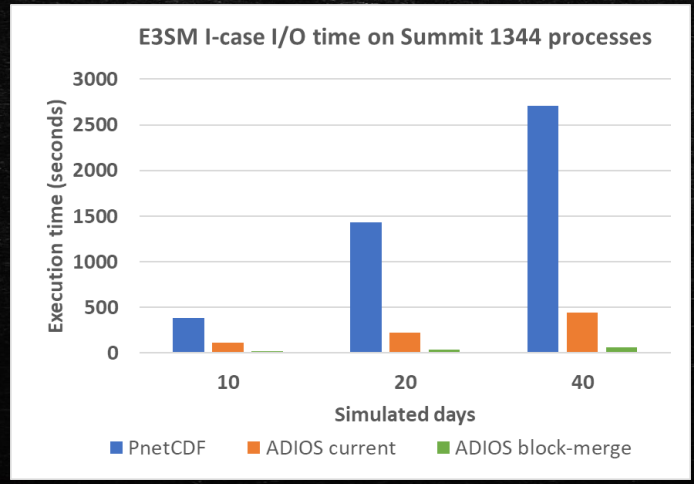
Contact: Amitava Bhattacharjee (PPPL)

E3SM-MMF

https://github.com/E3SM-Project/scorpio/tree/master

ADIOS BP4-based driver with block merging is integrated into master SCORPIO

- I-Case stresses IO
- Block-merging improves ADIOS performance

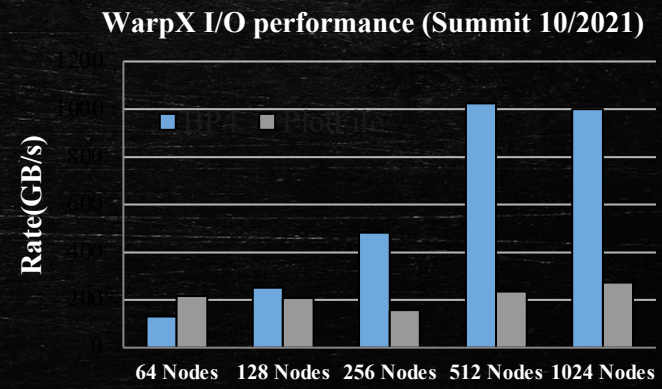


- Simulating 10, 20 and 40 days
- Writing data every simulated hour
- Run on Summit, 1344 MPI processes

Contact: Mark Taylor (SNL), I-Case Peter Thornton (ORNL)

WarpX

- Using ADIOS timesteps, WarpX improved simulation output times.
- WarpX, and in general, openPMD-api users can achieve high throughput for particle-mesh data in AMReX apps using ADIOS.



- WarpX on Summit, weak scaling
- 6 GPUs per node, up to 1024 nodes
- ADIOS vs. AMReX Plot files

Contact: Jean-Luc Vay, Axel Huebl (LBNL)

Why use ADIOS over other technologies

- Scalable performance
  - designed to be a parallel IO library,
  - one application can utilize the bandwidth of the entire file system (when running at large scale)
  - proven by users for many PBs datasets, tens of thousands of nodes, daylong runs, thousands of steps
- Scalable (distributed) compression routines
  - lossless and lossy, blosc, bzip2, zfp, sz, mgard
- Safe to append data into single dataset during run, at scale
  - new writes cannot corrupt existing data
  - entire output “step” is either in or not
  - application failure will not corrupt previously written data/file
- Able to read data from files being written
  - previous steps only, not the one under construction
  - stable semantics: data in a published step is always completely available

Why use ADIOS over other technologies

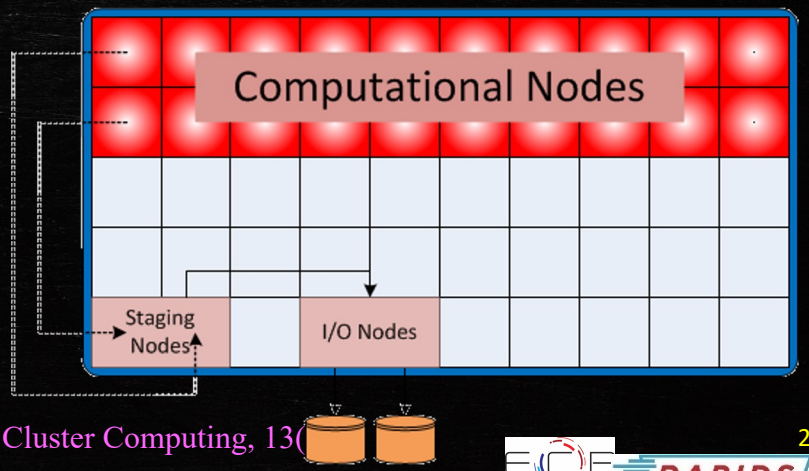
- Source code for file based persistent IO and in situ IO can be the same
  - Unified concepts and API around publishing/subscribing of "steps"
  - Easy to debug in situ pipelines using file-based streaming
- Empty/no-data pieces of a global space does not need to be written
  - Logically contiguous file formats require bytes in output for every cell, waste in writing time, data size and reading time

Why use ADIOS over other technologies

- Working in major HPC applications
  - For large/small levels of concurrency
  - For large/small volumes of data
  - Is fully self describing and has worked with applications writing and reading PBs of data
- Allows applications to specify what they want published/subscribed (write/read) and NOT how
  - Allows for SWMR and MWMR since the beginning of ADIOS (2005)
  - Allows for applications to stream and/or write to files with no changes
  - Allows for parallel compression decompression …

Introduction to staging

- Simplistic approach to staging
  - Decouple application performance from storage performance (burst buffer)
- Built on past work with threaded buffered I/O
  - Buffered asynchronous data movement with a single memory copy for networks which support RDMA, TCP, RUDP, or MPI
  - Application blocks for a very short time to copy data to outbound buffer
  - Data is moved asynchronously using server-directed remote reads
- Exploits network hardware for fast data transfer to remote memory
- Value added
  - Allows scientists to use a data-in-transit technique to write, reduce, analyze data
  - Can be used to couple multiple codes together
  - Can be used for asynchronous I/O



Abbasi, H., Klasky, S., et al., (2010). Datastager: scalable data staging services for petascale applications. Cluster Computing, 13(277-290.

Staging Options

Transfer mechanisms

- File based
- Network based on the same resource
  - RDMA (libfabric, UCX)
  - MPI (one sided, two sided)
  - TCP/ RUDP
- Memory references
- WAN data transfer
  - Files – GridFTP, scp, …
  - Streams – TCP, RUDP, RoCE

Placement options

- Same core
- Different cores/same node
- Different nodes
- Different resource (LAN)
- Different resource (WAN)
- Hybrid (mixture of options)

Scheduling options

- Fully synchronous
- Fully asynchronous
- Hybrid

Refactoring options

- Prioritize which data gets moved first

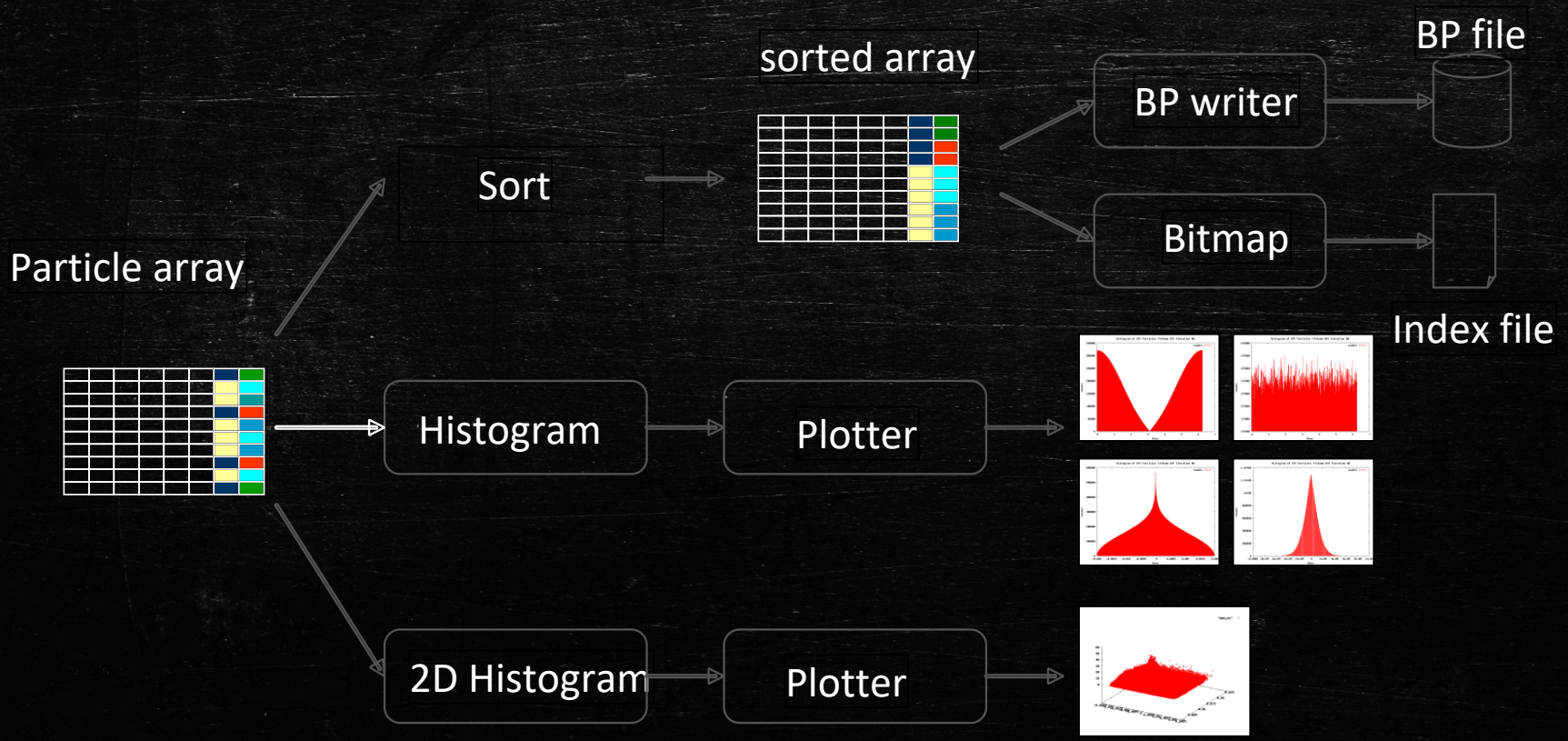
Storage options

- HDF5
- ADIOS-BP5, …

Gainaru, A., Klasky, S., et al., 2022, Understanding the Impact of Data Staging for Coupled Scientific Workflows , IEEE transactions on parallel and distributed systems. 2022.

I/O pipelines in staging

- Use the staging nodes and create a workflow in the staging nodes
- Mitigate performance impact of I/O of the GTC code by using asynchronous data movement
- Improve total simulation time by 2.7% , but we also improved the reading performance + analyzed the data + visualized the data

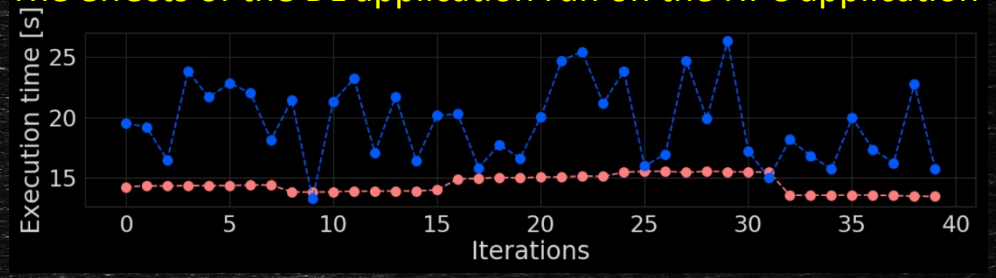


F. Zheng, S. Klasky, et al., "PreDatA - Preparatory Data Analytics on Peta-Scale Machines", IPDPS 2010.

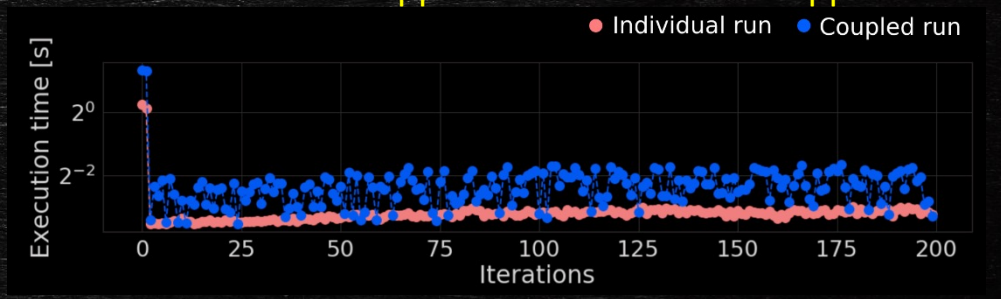
The movement for SDM for the convergence of HPC with AI

- Traditional simulations focused on scaling a single app
  - As they move to digital twins, they have been evolving into complex workflows which can mix simulations with AI
- The graphs show the cumulative execution times of a histopathology analysis pipeline that classifies image patches in WSIs to characterize tumor regions and lymphocyte distributions:
  - (Top) when multiple concurrent instances of the models are running in parallel, interference at the storage level causes a delay in the execution of each application shifting the distribution to the right
  - (Bottom) when streaming data directly to the consumer the I/O inference is decreased by 20%
- The results for analyzing 7,000 WSIs with the workflow using 500 concurrent instances on Summit is presented in the bottom: as we see, we can reduce congestion by streaming the data

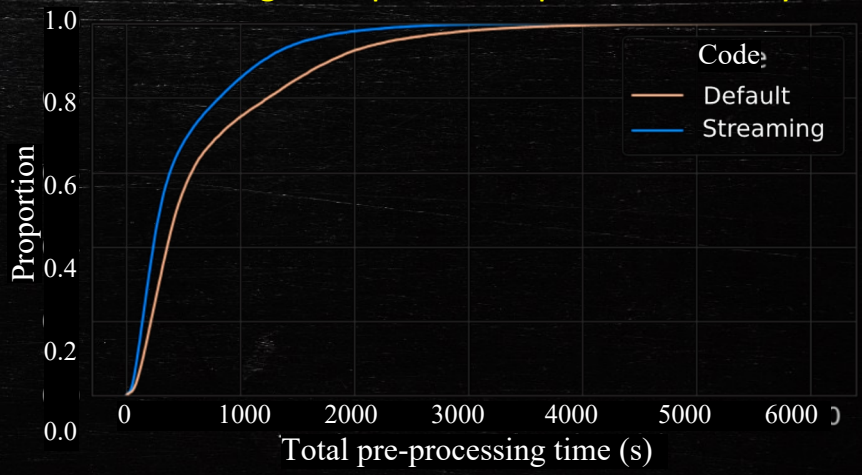
The effects of the DL application run on the HPC application



The effects of the HPC application run on the AI application



Use streaming to improve the performance by 20%

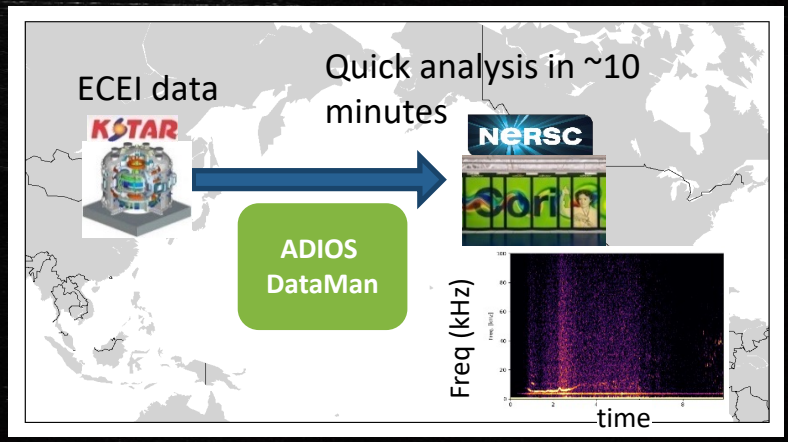


Gainaru, A., Klasky, S., et al., Framework for Automating the I/O of Deep Learning Methods in Biomedical Imaging Applications, submitted to IEE/ACM Transactions on computational biology and bioinformatics, 2022.

Using staging to establish capability for near-real time networked analysis of fusion experimental data (KSTAR)

Research and develop a streaming workflow framework, to enable near-real-time streaming analysis of KSTAR data on a US HPC

- Allow the framework to adopt ML/AI algorithms to enable adaptive near-real-time analysis on large data streams
- Created a framework to enable US fusion researchers to have broader and faster access to the KSTAR data, enabling
  - Faster analysis of data
  - Faster and autonomous utilization of ML/AI algorithms for incoming data
  - More informed steering of experiment
- Accomplishments
  - Created end-to-end Python framework, streams data using ADIOS over WAN (at rates > 4 Gbps), asynchronously processes on multiple workers with MPImulti-threading
  - Applied to KSTAR streaming data to NERSC Cori.
  - Reduces time for analysis from 12 hours to 10 minutes

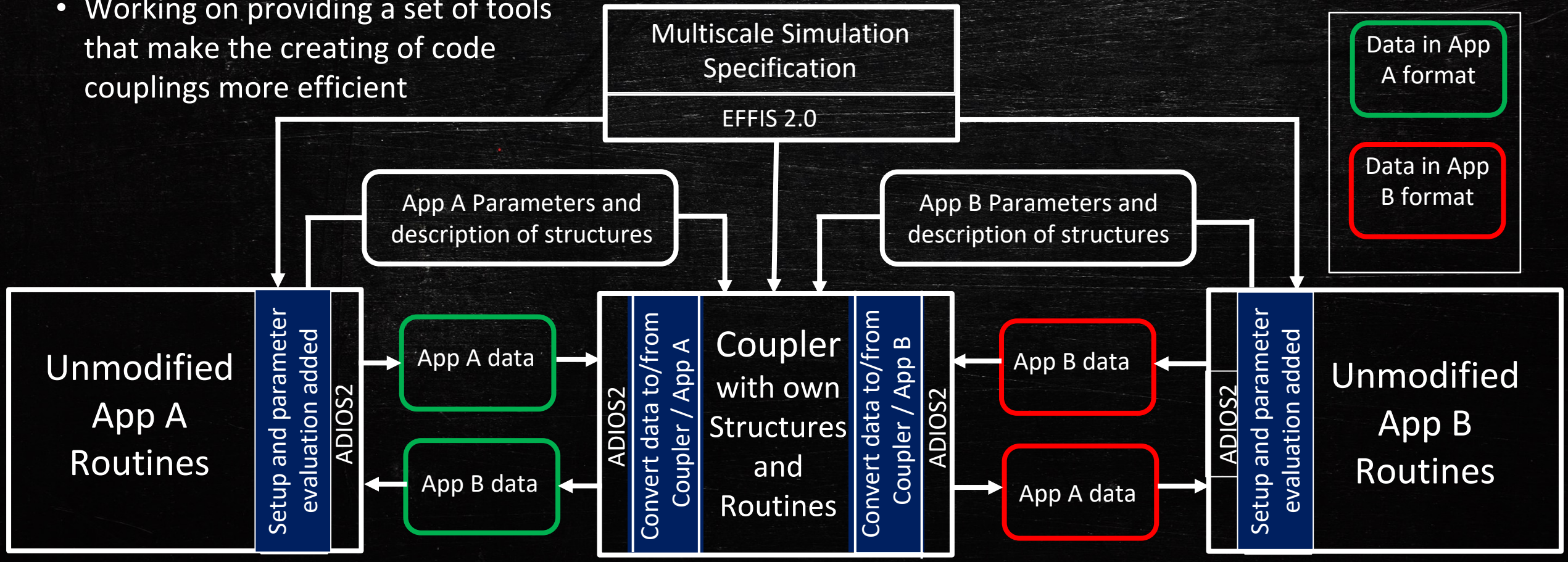


Churchill, Klasky, S., et al.(2021). A Framework for International Collaboration on ITER Using Large-Scale Data Transfer to Enable Near-Real-Time Analysis. Fusion Science and Technology, 77(2), 98-108.

Current/Future work: framework of WDM Coupler

Each coupling process involves defining the Multiscale Simulation Specification control box and replacing the shaded boxes (see fig. below for a two code coupling)

- Due to model and/or numerical methods mismatches a single coupler is not possible
- Working on providing a set of tools that make the creating of code couplings more efficient



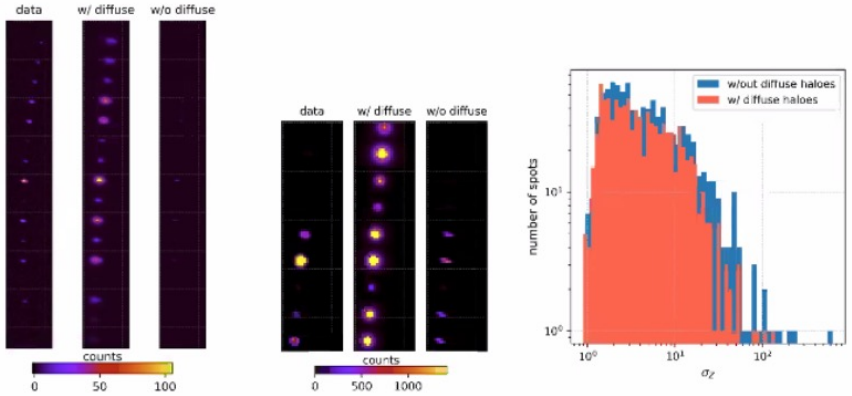
Suchyta, E., Klasky, S., et al. (2022). The Exascale Framework for High Fidelity coupled Simulations (EFFIS): Enabling whole device modeling in fusion science. *The International Journal of High Performance Computing Applications*, *36*(1), 106-128.

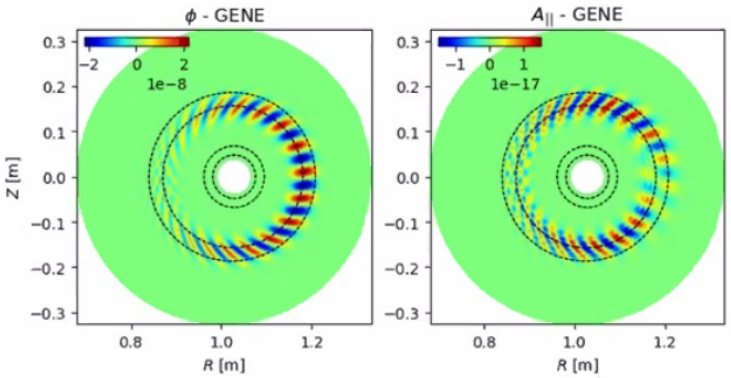
Integration: AD Teams Depend Heavily on ST Software to Meet KPPs

Kokkos

ExaFEL

nanoBragg code ported from Nvidia to AMD GPUs with minimal effort





ADIOS

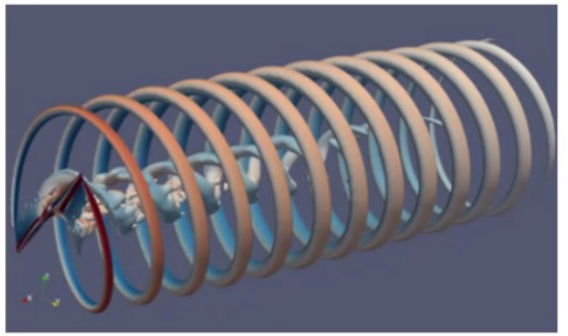
WDMApp

ADIOS enables in-memory coupling between GENE and XGC

hypre

ExaWind

hypre solve performance on AMD GPUs 30-40% faster than Summit



D. Kothe. ECP Annual meeting, 5/3/2022

DOE/ASCR Data Reduction

- Bill Spotz (ASCR)
  - Klasky, Najm, Thayer
- Main findings
- Data volumes and velocities from next generation experiments, observations and simulations require new R&D in data reduction

4 Priority Research Directions

1. Trust: Accuracy and Performance
2. Progressive Streaming
3. Feature Preserving
4. Platform Portability

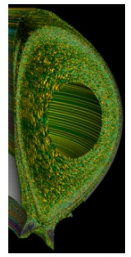
Data Reduction for Science: Brochure from the Advanced Scientific Computing Research Workshop

Scott Klasky, Oak Ridge National Laboratory
Jana Thayer, SLAC National Accelerator Laboratory
Habib Najm, Sandia National Laboratories

Publication date: April 15, 2021
Web DOI: 10.2171/1770192
DOE Office of Science Technical Contact: William Spotz (William.Spotz@science.doe.gov)

Introduction

The reduction of streaming and voluminous data sets while maintaining accurate representations of quantities of interest (QoIs) is a critical capability across the Office of Science (SC). SC-supported experiments, observations, and simulations produce data at volumes and velocities that are already overwhelming network, storage, and compute capabilities and their projected growth will greatly exacerbate this imbalance. The Advanced Scientific Computing Research program office held a virtual workshop in January 2021, bringing together 155 participants and 41 observers across experimental, observational, and computational application areas and research thrust areas in compression, reduced representations, experiment-specific triggers, filtering, and feature extraction/QoIs to identify priority research directions (PRD) leading to enhanced capabilities in data reduction. This workshop examined many scientific drivers, such as radio astronomy, fusion, combustion, climate, light sources, nuclear physics, and genomics, which are in desperate need for new Research & Development (R&D) in data reduction, because they currently risk ad hoc decisions that can limit the amount of knowledge gathered from SC facilities.



New workflows are beginning to emerge to both manage data and fully exploit the incredibly rich information produced by SC facilities. These data reduction workflows employ triggering, filtering, sampling, compression, reduced order modeling and feature detection. The workflows extend from observational/experimental devices to networks to remote and local storage to desktop and leadership computing facilities and require optimization across a diverse range of hardware.

In order for application scientists to trust data reduction methodologies, reduction techniques should be usable and adoptable by communities through best practices, benchmarks, data sharing, resource sharing, and through the development of tools that enable scientists to navigate these resources. The workshop focused on new R&D capabilities which can allow scientists to quantify the uncertainties in QoIs, along with preserving features to a specified tolerance. Furthermore, progressive techniques for streaming data need to be developed to enable scientists to make tradeoffs between the uncertainty, speed, and resource utilization. Since these workflows typically run on all types of

Home Agenda Presentations Contacts

Registration is Closed
Already Registered?

Data Reduction for Science Workshop

Sponsored by the U.S. Department of Energy,
Office of Advanced Scientific Computing Research
January 25, 26, and 28, 2021

The workshop will be held using a virtual format.

Scientific observations, experiments, and simulations are producing data at a rate beyond our capacity to store, analyze, stream, and archive. This data almost always contains redundancies and trivialities that hide the important information of interest to scientists. Of necessity, many research groups have already begun reducing the size of their data sets via techniques such as compression, reduced representations, experiment-specific triggers, filtering, and feature extraction. These efforts should be expanded to include mathematical rigor to ensure that quantities of interest are conserved, to be offered as services from scientific user facilities, to be integrated into scientific workflows, and to be implemented in a manner that inspires trust that the desired information is preserved. The purpose of this workshop is to:

- Bring together disparate communities of practice in the data reduction space to foster collaboration and improved understanding of the various techniques
- Outline requirements for data reduction techniques from domain scientists
- Highlight the relevant state-of-the-art in computer science and mathematics
- Identify priority research directions leading to enhanced capabilities in data reduction

Add to Calendar

U.S. DEPARTMENT OF ENERGY | Office of Science
ORAU
Oak Ridge Institute for Science and Education
Managed by ORAU for DOE

ORAU/ORISE Privacy Policy | Contract Acknowledgement

Support for Internet Explorer 11 will be ending soon. For the best experience using this site, we recommend using Google Chrome, Mozilla FireFox, or Microsoft Edge as your desktop browser.

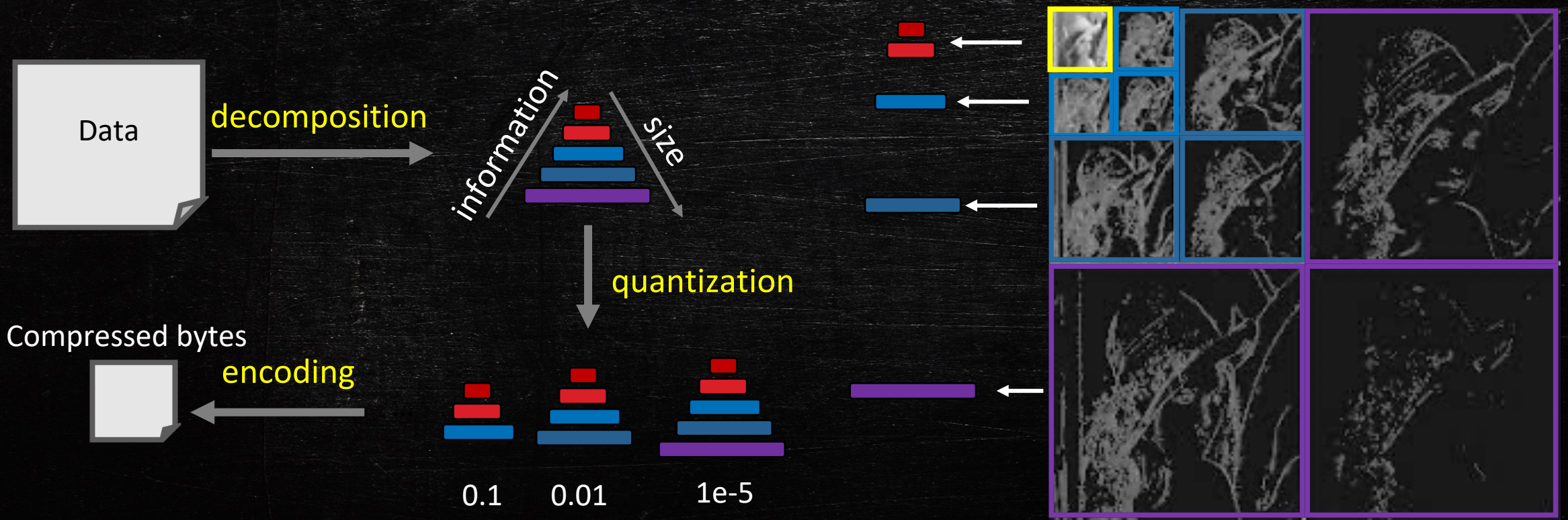
ADIOS + compression

- ADIOS has a very natural data layout which works well with parallel compression/decompression algorithms
- ADIOS contains
  - MGARD – a mathematical software framework based on MultiGrid which can reduce data with quantifiable error bounds on the data and linear QoIs
  - SZ
  - ZFP
  - BLOSC
  - BZip2
  - …

MGARD - Multi-Grid Adaptive Reduction of Data

MGARD is a transform-based compressor

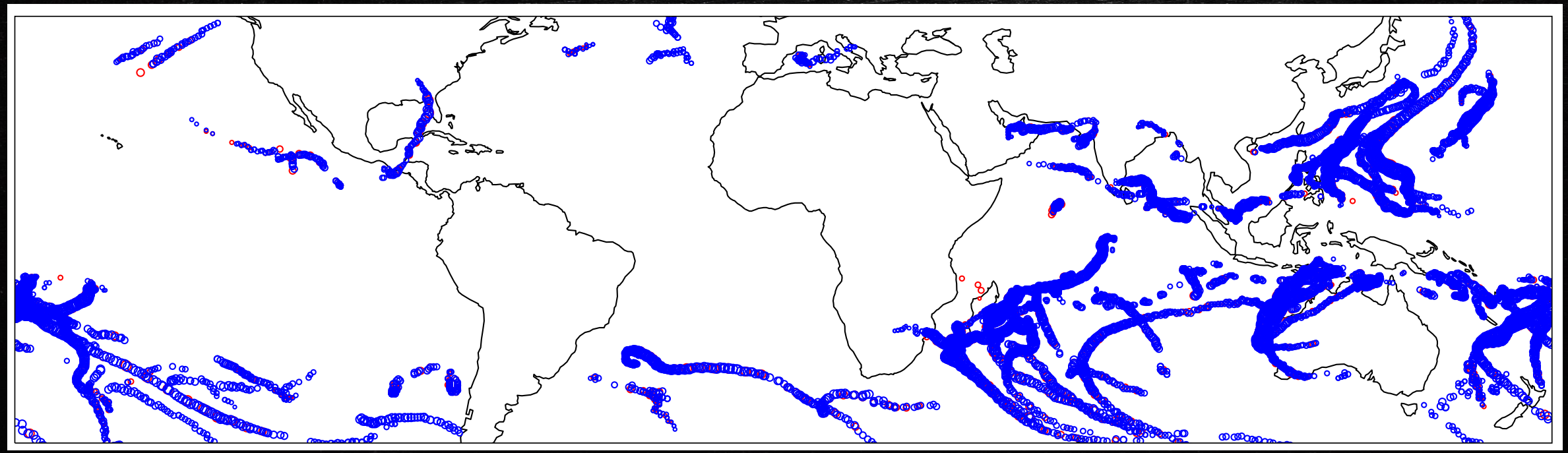
- multi-resolution, multi-precision



Similar to filtering Fourier coefficients, JPEG, wavelet methods

Improving the state of the art for Climate/E3SM

- By writing data at a higher frequency and reducing the overall storage footprint?
- 24X reduced data is more accurate for cyclone prediction c.f. non reduced



Application Impact

Dresden

Tel Aviv

Tokyo

Perth

Princeton

UMD

TAE

SNL

PPPL

ORNL

LBNL

Los Alamos

Seismic Tomography Workflow (PBs of data/run) [2.2 TB/s]

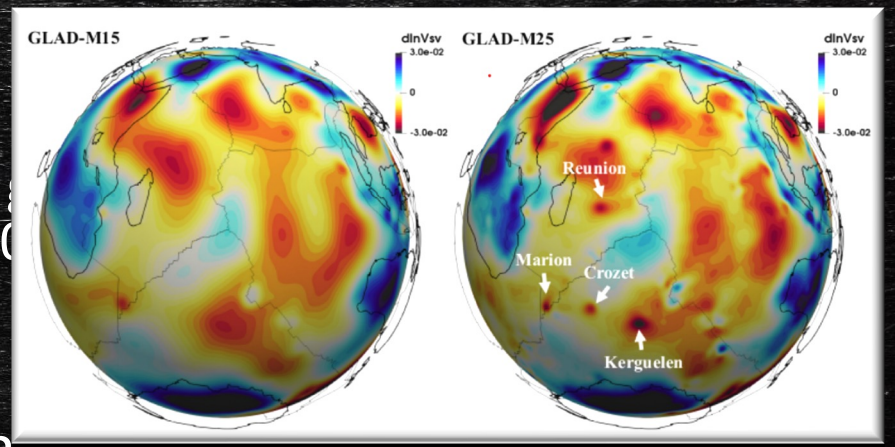
PI: Jeroen Tromp, Princeton

Scientific Achievement

- Most detailed **3-D model of Earth**'s interior showing the entire
  from the surface to the core–mantle boundary, a depth of 1,80

Significance and Impact

- Updated (transversely isotropic) global seismic model GLAD-M2
  used to simulate how seismic waves travel through the Earth. T
  are challenging even for leadership computer
- 7.5 PB of data is produced in a single workflow step
  - which is fully processed later in another step

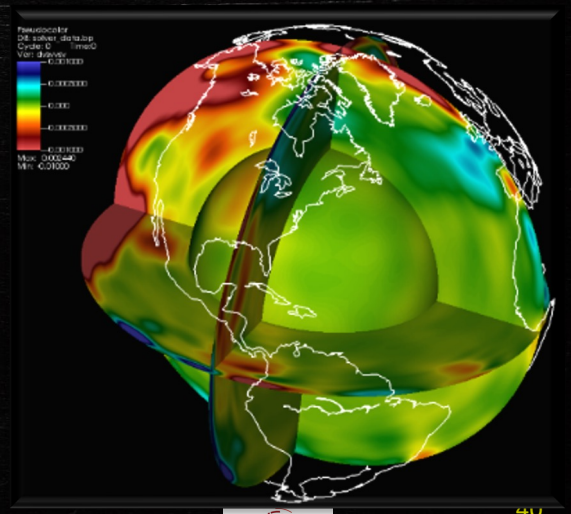


Map views at 250 km depth of vertically polarized shear wave speed perturbations in GLAD-M15 (2017) and GLAD-M25 (2020) in the Indian Ocean. New features have emerged in GLAD-M25, such as the Reunion, Marion, Kerguelen, Maldives, Seychelles, Cocos and Crozet hotspots.

Improvement by appending steps

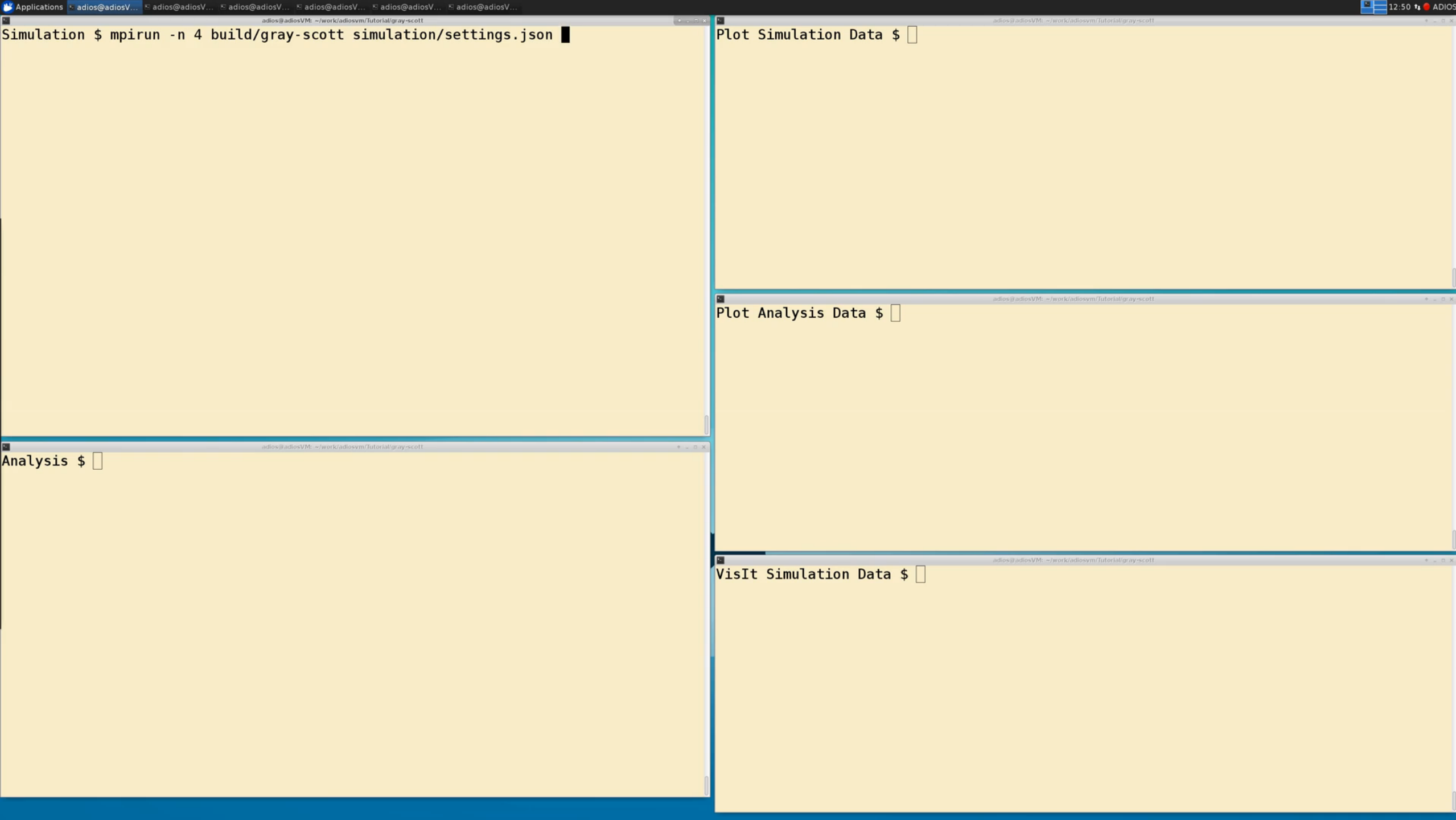
- 3200 nodes ensemble run, 19200 GPUs
- 50 tasks at once
- 5.2 TB per task in 133 steps
- 260 TB total per 50 tasks
- 7.5 PB per 1500 tasks (total run)

50 tasks, 133 steps, 3200 nodes	Time
No I/O	94s
BP3, one file per step	235s
BP4 one dataset per job 133x reduction in # of files	156s



Lei, Wenjie, et al. "Global adjoint tomography—model GLAD-M25." Geophysical Journal International 223.1 (2020): 1-21.

ECP RAPIDS


Applications
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12:50
ADIOS
adios@adiosVM: ~/work/adiosvm/Tutorial/gray-scott
Simulation $ mpirun -n 4 build/gray-scott simulation/settings.json
adios@adiosVM: ~/work/adiosvm/Tutorial/gray-scott
Plot Simulation Data $
adios@adiosVM: ~/work/adiosvm/Tutorial/gray-scott
Plot Analysis Data $
adios@adiosVM: ~/work/adiosvm/Tutorial/gray-scott
Analysis $
adios@adiosVM: ~/work/adiosvm/Tutorial/gray-scott
VisIt Simulation Data $

Outline

- 8:30 Introduction to data management at extreme scale – Scott Klasky
- 9:15 ADIOS 2 concepts and API (C++, Python, F90) – Norbert Podhorszki
- 10:00 BREAK
- 10:30 ADIOS 2 API – Norbert Podhorszki
- 11:00 Hands on with ADIOS 2 – Files – Ana Gainaru
- 12:00 Lunch
- 1:30 ADIOS @ scale – Norbert Podhorszki
- 2:00 Introduction to Paraview + ADIOS + hands on Caitlin Ross
- 3:00 BREAK
- 3:30 Introduction to TAU and TAU + ADIOS – Kevin Huck
- 4:00 Hands on with TAU + ADIOS
- 4:15 Staging with ADIOS – hands 0n – Ana Gainaru
- 5:00 END

ADIOS Concepts and C++ API

ADIOS Useful Information and Common tools

- ADIOS documentation: https://adios2.readthedocs.io/en/latest/index.html
- ADIOS Examples: https://adios2-examples.readthedocs.io/en/latest/
- ADIOS source code: https://github.com/ornladios/ADIOS2
  - Written in C++, wrappers for Fortran, Python, Matlab, C
  - Contains command-line utilities (bpls, adios_reorganize ..)
- This tutorial's code example (Gray-Scott): https://github.com/pnorbert/adiosvm.git
- Online help:
  - ADIOS2 GitHub Issues: https://github.com/ornladios/ADIOS2/issues

- Two movies showing the Tutorial for post-processing and on-line processing
- https://users.nccs.gov/~pnorbert/GrayScottPost.mp4
- https://users.nccs.gov/~pnorbert/GrayScottInsitu.mp4

ADIOS Approach: "How"

- I/O calls are of declarative nature in ADIOS
  - which process writes/reads what
    - add a local array into a global space (virtually)
  - EndStep() indicates that the user is done declaring all pieces that go into the particular dataset in that output step or what pieces each process gets
- I/O strategy is separated from the user code
  - aggregation, number of sub-files, target file-system hacks, and final file format not expressed at the code level
- This allows users
  - to choose the best method available on a system without modifying the source code
- This allows developers
  - to create a new method that's immediately available to applications
  - to push data to other applications, remote systems or cloud storage instead of a local filesystem

ADIOS basic concepts

- Self-describing Scientific Data
- Variables
  - multi-dimensional, typed, distributed arrays
  - single values
    - Global: one process, or Local: one value per process
- Attributes
  - static information
    - for humans or machines
  - global, or assigned to a variable

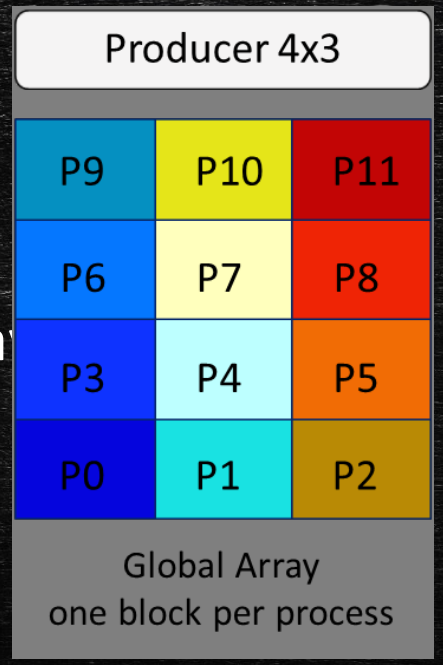
Self-describing Scientific Data

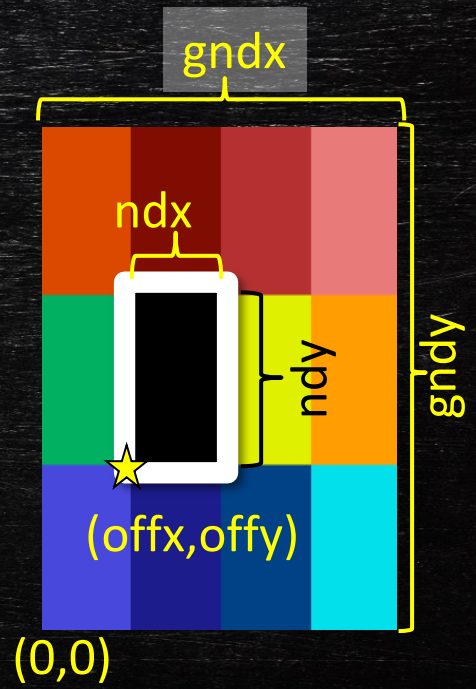
```
real     /fluid_solution/scalars/PREF                      scalar = 0
string   /fluid_solution/domain14/blockName/blockName      scalar = "rotor_flux_1_Main_Blade_skin"
integer  /fluid_solution/domain14/sol1/Rind                {6} = 2 / 2
real     /fluid_solution/domain14/sol1/Density             {8, 22, 52} = 0.610376 / 1.61812
real     /fluid_solution/domain14/sol1/VelocityX           {8, 22, 52} = -135.824 / 135.824
real     /fluid_solution/domain14/sol1/VelocityY           {8, 22, 52} = -277.858 / 309.012
real     /fluid_solution/domain14/sol1/VelocityZ           {8, 22, 52} = -324.609 / 324.609
real     /fluid_solution/domain14/sol1/Pressure            {8, 22, 52} = 1 / 153892
real     /fluid_solution/domain14/sol1/Nut                 {8, 22, 52} = -0.00122519 / 1
real     /fluid_solution/domain14/sol1/Temperature         {8, 22, 52} = 1 / 362.899
string   /fluid_solution/domain17/blockName/blockName      scalar = "rotor_flux_1_Main_Blade_shroudga

integer  /fluid_solution/domain17/sol1/Rind                {6} = 2 / 2
real     /fluid_solution/domain17/sol1/Density             {8, 8, 52} = 0.615973
real     /fluid_solution/domain17/sol1/VelocityX           {8, 8, 52} = -135.824
...
```

Global Array: data produced by multiple processes

- N-dimensional array
  - **Shape**
- Has a type (int32, double, etc.)
  - **Type**
- Blocks of data are written into the arra
  - **Start** (offset)
  - **Count** (size of block)





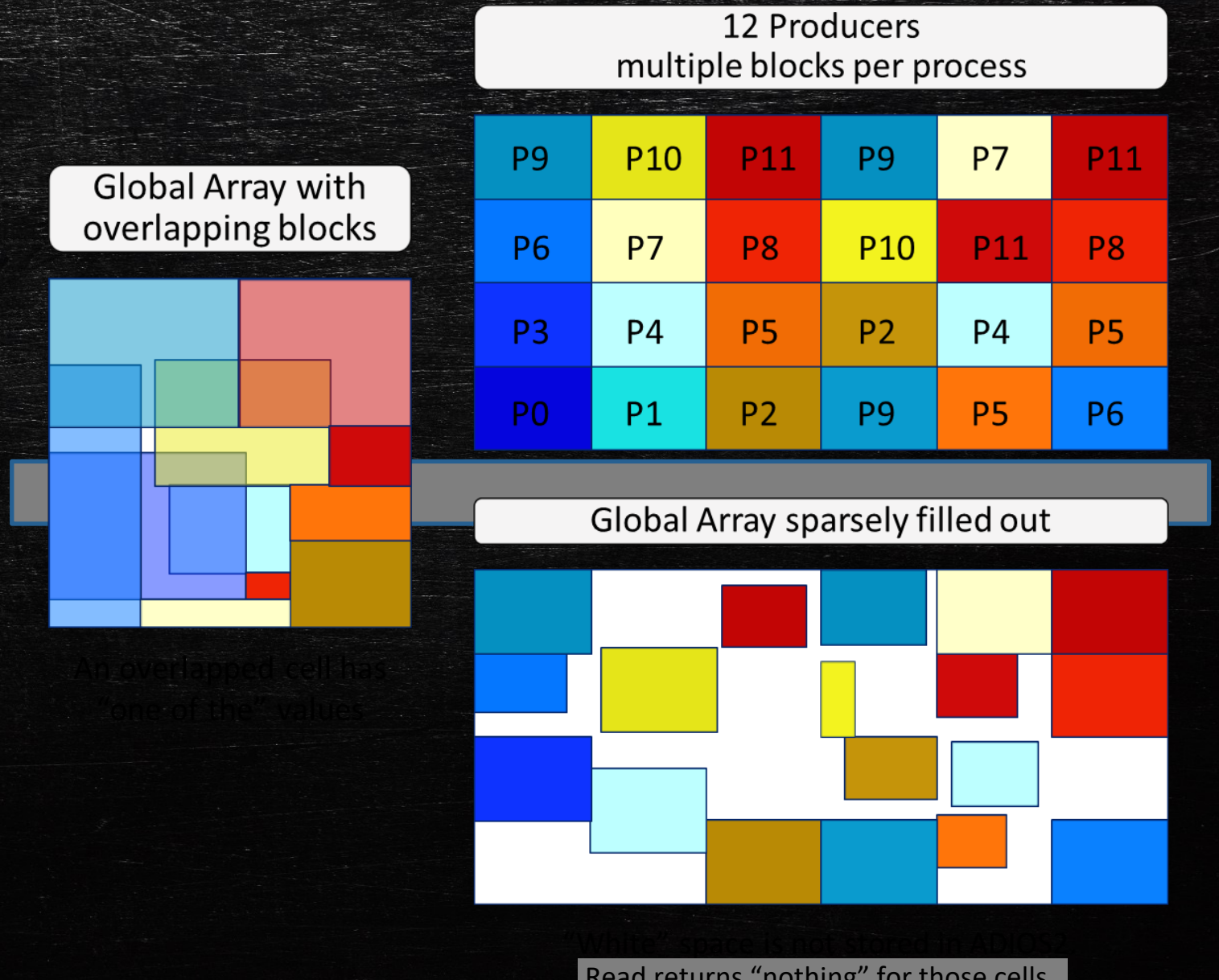
Shape = {gndx, gndy}

Start = {offx, offy}

Count = {ndx, ndy}

Global Array: data produced by multiple processes

- These are valid global arrays
  - One process can contribute more than one block
  - Some process may not write anything at all
  - Holes can be left in the global array
  - Overlapping of blocks is allowed



ADIOS basic concepts

- Step
  - Producer outputs a set of variables and attributes at once
    - This is an **ADIOS Step**
  - Producer iterates over computation and output steps
- Producer outputs multiple steps of data
  - e.g. into multiple, separate files, or into a single file
  - e.g. steps are transferred over network
- Consumer processes step(s) of data
  - e.g. one by one, as they arrive
  - e.g. all at once, reading everything from a file
    - not a scalable approach

ADIOS Steps: Rules and constraints

- Step is not necessarily tied to the application timesteps
  - a Step can be constructed over time
- Entire content of a Step is either completely written or not at all
- A new Step can be very different from the previous step
  - may contain a completely different set of variables
  - array sizes can change
  - array decomposition can change
- Consumer is guaranteed to have access to entire content of Step as long as it wants it
- Entire content of a Step must fit into the producer's memory as a copy

ADIOS coding basics

- Objects
  - ADIOS
  - Variable
  - Attribute
  - IO
    - a group object to hold all variable and attribute definitions that go into the same output/input step
    - settings for the output/input
    - settings may be given before running the application in a configuration file
  - Engine
    - the output/input stream
  - Operator
    - a compression, reduction, data transformation operator for output variables

ADIOS object

- The container object for all other objects
- Gives access to all functionality of ADIOS

```
#include <adios2.h>
adios2::ADIOS  adios(configfile, MPI communicator);
```

- Notes:
  - both arguments are optional
    - `adios(), adios("config.xml"), adios(comm)`
  - Normally use 1 config file and then have different communicators for each I/O target

ADIOS2-Examples/source/cpp/gray-scott/simulation/main.cpp

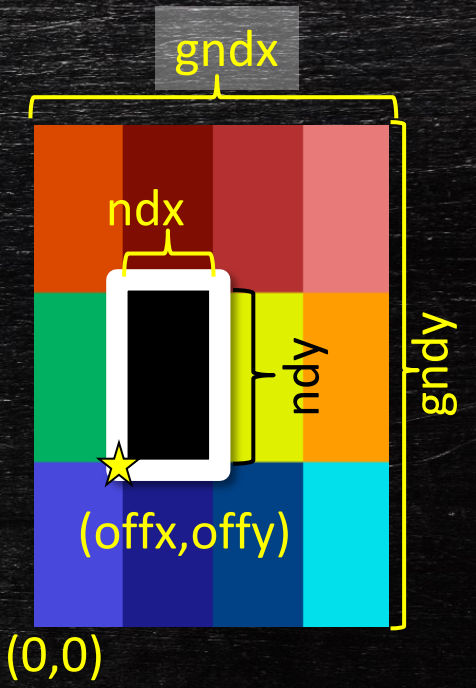
IO object

- Container for all variables and attributes that one wants to output or input at once
- Application settings for IO
- User run-time settings for IO – from configuration file (or input parameters)
  - a **name** is given to the IO object to identify it in the configuration

```
adios2::IO io = adios.DeclareIO("CheckpointRestart");
```

Variable

- N-dimensions
- Type
- Decomposition across many processors
  - global dimensions (Shape), local place (Start, Count)




```
adios2::Variable<double> &varT = io.DefineVariable<double>
(
    "T",                // name in output/input
    {gndx, gndy},       // Global dimensions (2D here)
    {offx, offy},       // starting offsets in global space
    {ndx, ndy}          // local size
);
```

  - C/C++/Python always row-major, Fortran/Matlab/R always column-major

Hint: if it's only checkpoint restart, just use global dimensions {NPROC, N}, local offsets {Rank, 0},

Engine object

- To perform the IO (for a single output step)

```
adios2::Engine writer =
io.Open("checkpoint.bp", adios2::Mode::Write);


writer.Put(varT, T.data());


writer.Close()
```

T is used in here!
Do not invalidate content of T before this!

Reading is similar, but we can read from any number of procs

```
adios2::IO io = adios.DeclareIO("CheckpointRestart");
adios2::Engine reader =
     io.Open("checkpoint.bp", adios2::Mode::Read);

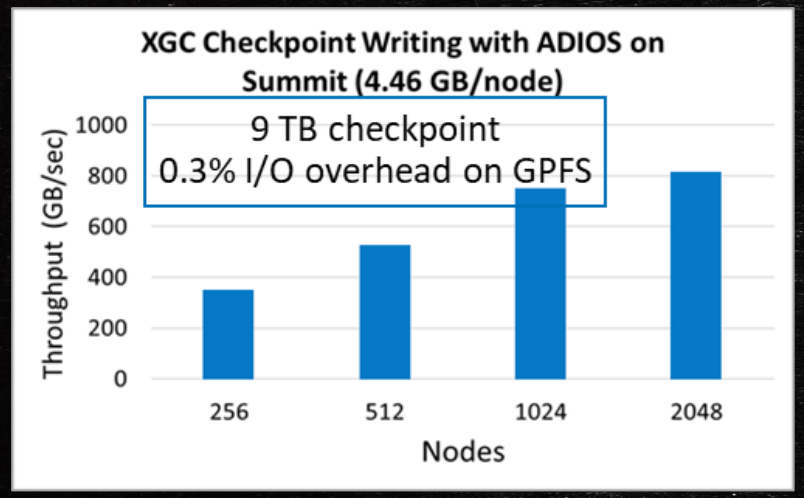

adios2::Variable<double> vT =
       io.InquireVariable<double>("T");
if (vT) {
   reader.Get(*vT, T.data());
}

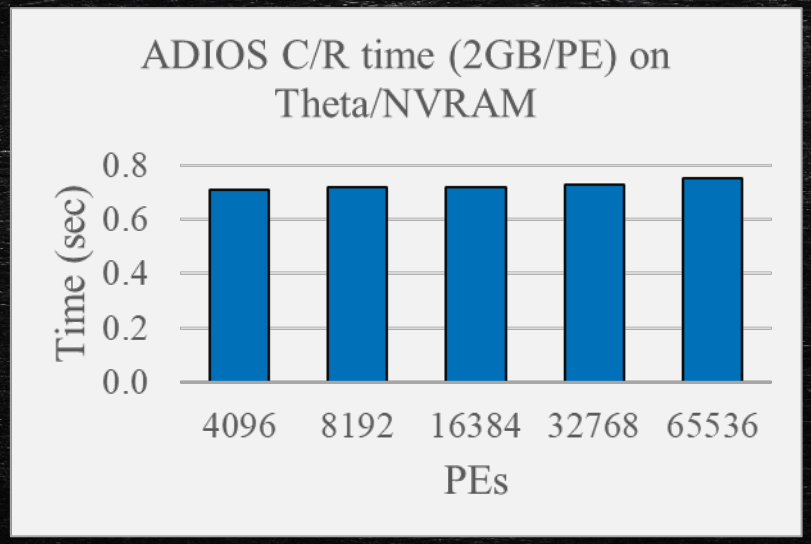
reader.Close()
```

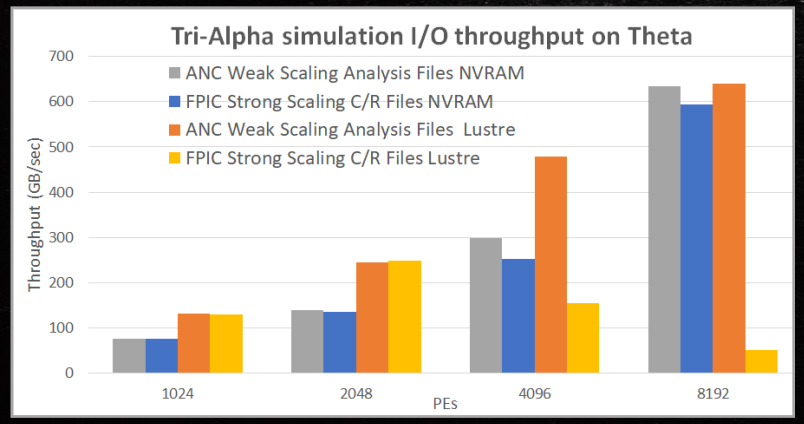
Reserve memory for T before this

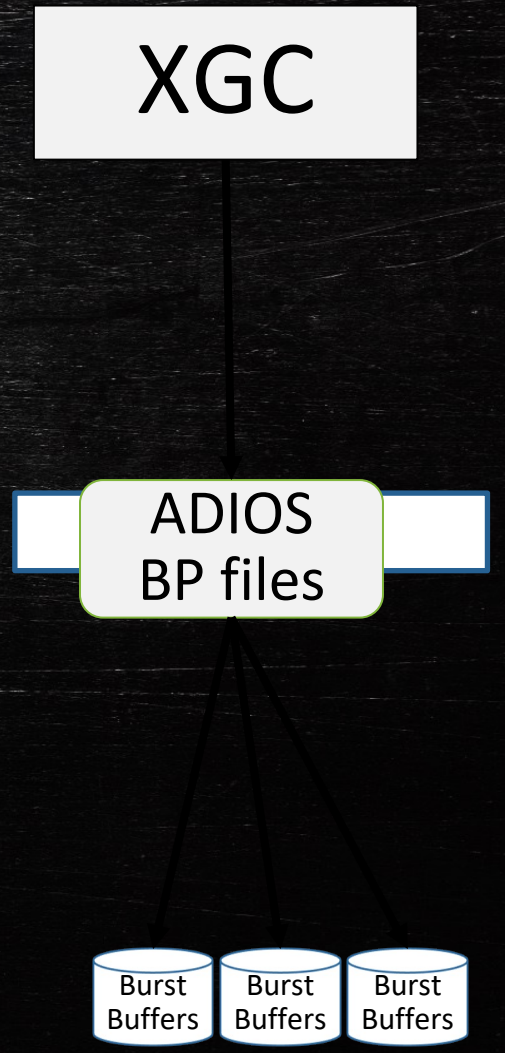
ADIOS APIs for self describing data output for C/R to NVRAM

- No changes to ADIOS APIs to write to Burst Buffers
  - The ADIOS-BP file format required no changes for C/R









Analysis/visualization data

```
adios2::IO io = adios.DeclareIO("Analysis_Data");
if (!io.InConfigFile()) {
    io.SetEngine("FileStream");
}
adios2::Variable<double> varT = io.DefineVariable<double>
(
    "Temperature",          // name in output/input
    {gndx,gndy,gndz},       // Global dimensions (3D here)
    {offx, offy, offz},     // starting offsets in global space
    {nx,ny,nz}              // local size
);
io.DefineAttribute<std::string>("unit", "C", "Temperature");
```

double	Temperature	10*{20, 30, 40} = 8.86367e-07 / 200
string	Temperature/unit	attr = "C"

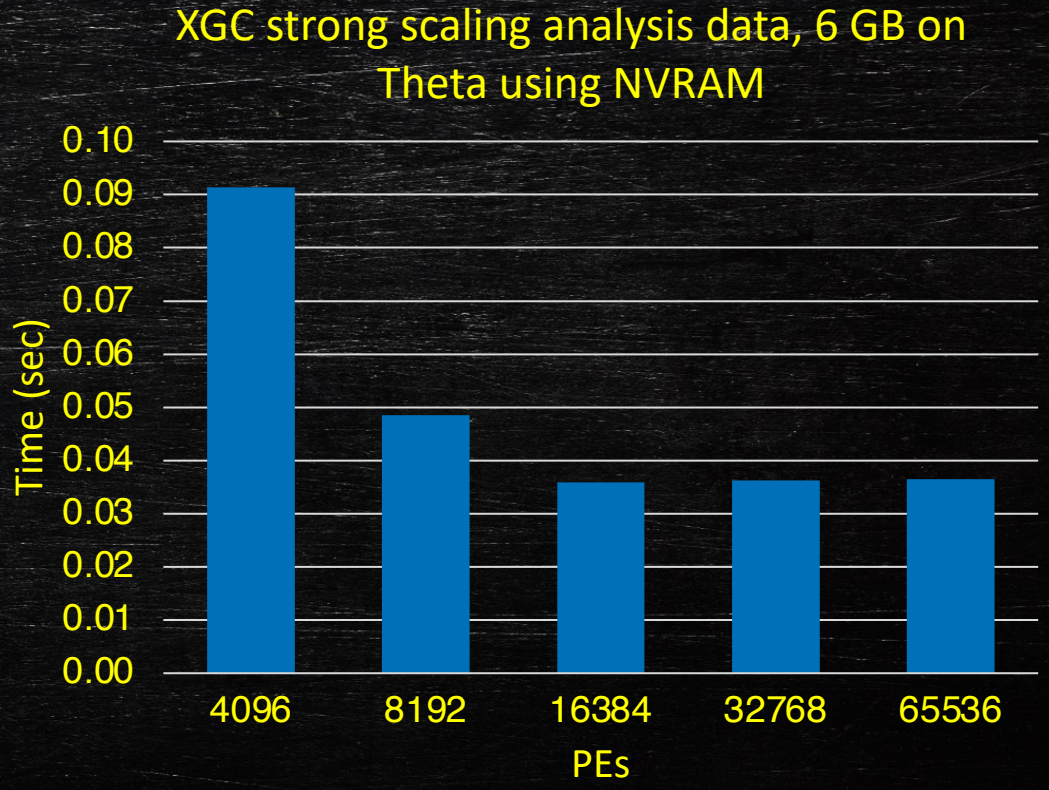
Engine object

- To perform the IO

```
adios2::Engine writer =
io.Open("analysis.bp",
        adios2::Mode::Write);


writer.BeginStep()
   writer.Put(varT, T.data());
writer.EndStep()


writer.Close()
```



Put API explained

```
engine.Put(varT, T.data())
```

- Equivalent to

```
engine.Put(varT, T.data(), adios2::Mode:Deferred)
```

- This does NOT do the I/O (to disk, stream, etc.) once put return.
- you can only reuse the data pointer after calling `engine.EndStep()`

```
engine.Put(varT, T.data(), adios2::Mode:Sync)
```

- This makes sure data is flushed or buffered before put returns
- Get() works the same way
- The default mode is deferred
- BP5 specific:
  - Large Deferred Put() is NOT buffered
  - Use Sync mode only when you need it (when you need to modify the data pointer before EndStep)

ADIOS engines – change from BP5 to HDF5

1. <io name="SimulationOutput">
2. <engine type="**BP5**"/>
3. </io>

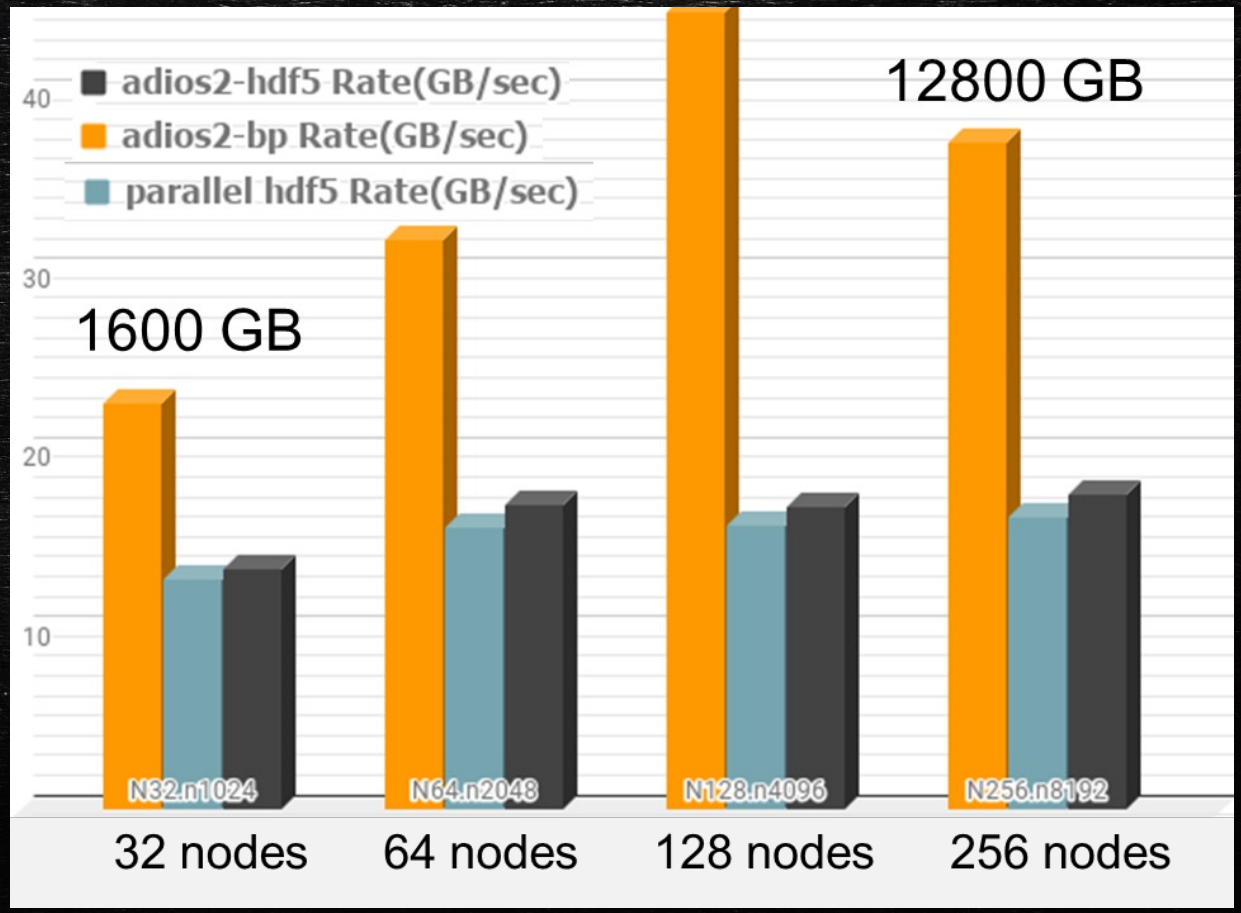
Change Engine name

1. <io name="SimulationOutput">
2. <engine type="**HDF5**"/>
3. </io>

- or in the source code

```
io.SetEngine("HDF5");
```

Cori + Lustre, for the heat equation



ADIOS Python API
Basically, the C++ API in Python

Python common

Serial python:

```
import numpy
import adios2

T = numpy.array(...)
```

Parallel python with MPI:

```
from mpi4py import MPI
import numpy
import adios2

T = numpy.array(...)
```

Python API start: ADIOS, IO and Engine objects

```
adios = adios2.ADIOS("adios2.xml")
adios = adios2.ADIOS("adios2.xml", comm, True)

io = adios.DeclareIO("SimulationOutput")
fr = io.Open("stream.bp", adios2.Mode.Read)

# adios2.Mode.Read – input stream step-by-step
# adios2.Mode.ReadRandomAccess – to see all steps at once (file)
# adios2.Mode.Write – to create an output stream
# adios2.Mode.Append – to append new steps to existing file

fr.Close()
```

Python API: Step-by-step reading

```
while True:
    status = fr.BeginStep()
    if status == adios2.StepStatus.EndOfStream:
        print("-- no more steps found --")
        break
    elif status == adios2.StepStatus.NotReady:
        sleep(1)
        continue
    elif status == adios2.StepStatus.OtherError:
        print("-- error with stream --")

    cur_step = fr.CurrentStep()
    ...
    fr.EndStep()
```

```
while True:
    status = fr.BeginStep()
    if status != adios2.StepStatus.OK:
        break
    cur_step = fr.CurrentStep()
    ...
    fr.EndStep()
```

Python Read API: List variables

```
vars_info = io.AvailableVariables()

for name, info in vars_info.items():
    print("variable_name: " + name)
    for key, value in info.items():
        print("\t" + key + ": " + value)
    print("\n")


# NOTE: list of variables may change
# from step to step
```

```
variable_name: T
    Type: double
    AvailableStepsCount: 2
    Max: 200
    SingleValue: false
    Min: 0
    Shape: 10, 16

variable_name: dT
    Type: double
    AvailableStepsCount: 2
    Max: 1.83797
    SingleValue: false
    Min: -1.78584
    Shape: 10, 16
```

Variable access, selection and read

- var = io.InquireVariable("U")
- shape = var.Shape()
  - E.g. [64, 64, 64]
- Allocate Numpy array for reading
  - data = numpy.empty([shape[1], shape[2]], dtype=np.float64)
- Selection to read: tuple of start and count (e.g. 2D slice of 3D array):
  - var.SetSelection([[int(shape[0]/2),0,0], [1,shape[1],shape[2]]])
- Read data now
  - fr.Get(var, data, adios2.Mode.Sync)

ADIOS Python API
File reading with ReadRandomAccess

Python API start: Engine objects

```
fr = io.Open("stream.bp", adios2.Mode.ReadRandomAccess)
vars_info = io.AvailableVariables()
ustep = int(vars_info["U"]["AvailableStepsCount"])
vu = io.InquireVariable("U")
vu.SetStepSelection([0, ustep])
print("Number of var 'step' steps after SetStepSelection =
{0}".format(vstep.Steps()))

# read first 4 elements of a 1D array A for all steps
nelems = 4
data = np.zeros([ustep*nelems],  dtype=np.float64)
vA.SetSelection([ [0], [4] ])
fr.Get(vA, data, adios2.Mode.Sync)
```

ADIOS Python High-level API

Python common

Sequential python script:

```
import numpy
import adios2

T = numpy.array(...)
```

Parallel python with MPI:

```
from mpi4py import MPI
import numpy
import adios2

T = numpy.array(...)
```

Python Read API: Open/close a file/stream

```
adios2.open(path, mode [, configFile, ioName])
adios2.open(path, mode, comm [, configFile, ioName])
fr.close()
```

Examples:

```
fr = adios2.open("data.bp", "r")
fr = adios2.open("data.bp", "r", "adios2.xml", "heat")

fr = adios2.open("data.bp", "r", mpicommunicator)
fr = adios2.open("data.bp", "r", mpicommunicator,
                 "adios2.xml", "heat")
fr.close()
```

Python Read API: List variables

```
vars_info = fr.available_variables()


for name, info in vars_info.items():
    print("variable_name: " + name)
    for key, value in info.items():
        print("\t" + key + ": " + value)
    print("\n")
```

```
variable_name: T
    Type: double
    AvailableStepsCount: 2
    Max: 200
    SingleValue: false
    Min: 0
    Shape: 10, 16

variable_name: dT
    Type: double
    AvailableStepsCount: 2
    Max: 1.83797
    SingleValue: false
    Min: -1.78584
    Shape: 10, 16
```

Python Read API: Read data from **file** -- Random access

```
fr.read(path[, start, count][, stepStart, stepCount])
```

Examples:

```
data = fr.read("T")
>>> data.shape
(10, 16)

data = fr.read("T", [0,0], [10,16])
>>> data.shape
(10, 16)

data = fr.read("T", [0,0], [10,16], 0, 2)
>>> data.shape
(2, 10, 16)
```

variable_name: **T**
- Type: double
- AvailableStepsCount: **2**
- Max: 200
- SingleValue: false
- Min: 0
- Shape: **10, 16**

Python Read API: Read data from **file/stream**

```
fr.read(path[, start, count][, endl=true])
```

Examples:

```
for step_fr in fr:
    data = step_fr.read("T")
    print("Shape: ", data.shape)
...
Shape:   (10, 16)
Shape:   (10, 16)
```

variable_name: **T**
Type: double
AvailableStepsCount: **2**
Max: 200
SingleValue: false
Min: 0
Shape: **10, 16**

ADIOS Fortran API

ADIOS Fortran API

- See documentation at https://adios2.readthedocs.io/en/latest/api_full/api_full.html#fortran-bindings
- See API source code in ADIOS2 source
  - bindings/Fortran/modules
  - https://github.com/ornladios/ADIOS2/tree/master/bindings/Fortran/modules

Writing with ADIOS I/O

Fortran variables

```
use adios2
implicit none
type(adios2_adios)      :: adios
type(adios2_io)         :: io
type(adios2_engine)     :: fh
type(adios2_variable)   :: var_T
type(adios2_attribute)  :: attr_unit, attr_desc
```

Writing with ADIOS I/O

```
call adios2_init (adios, "adios2.xml",  app_comm,
                  adios2_debug_mode_on, ierr)
call adios2_declare_io (io, adios, 'SimulationOutput', ierr )
...
call adios2_open (fh, io, filename, adios2_mode_write, ierr)
call adios2_define_variable (var_T, io, "T", adios2_type_dp,  &
                  2, shape_dims, start_dims, count_dims, &
                  adios2_constant_dims,  adios2_err )
```

```
call adios2_put (fh, var_T, T, adios2_err)
call adios_close (fh, adios_err)
...
call adios_finalize (rank, adios_err)
```

Multiple output steps:

```
call adios2_begin_step (fh, &
                  adios2_step_mode_append, &
                  0.0, istatus, adios2_err)
call adios2_put (fh, var_T, T_temp, adios2_err )
call adios2_end_step (fh, adios2_err)
```

Add attributes to output

```
call adios2_define_attribute(attr_unit, io, "unit", "C", "T", adios2_err)
```

Equivalent code in HDF5

```
call h5screate_simple_f(1, attrdim, aspace_id, err)
call h5tcopy_f(H5T_NATIVE_CHARACTER, atype_id, err)
call h5tset_size_f(atype_id, LEN_TRIM(“C”, err)
call h5acreate_f(dset_id, “unit”, atype_id, aspace_id, att_id, err)
call h5awrite_f(att_id, atype_id, “C, attrdim, err)
call h5aclose_f(att_id, err)
call h5sclose_f(aspace_id, err)
call h5tclose_f(atype_id, err)
```

Fortran Read API

```
integer(kind=8) :: adios, io, var, engine
call adios2_init(adios, MPI_COMM_WORLD, adios2_debug_mode_on, ierr)
call adios2_init_config(adios, "config.xml", MPI_COMM_WORLD,
                        adios2_debug_mode_on, ierr)
call adios2_declare_io(io, adios, 'SimulationOutput', ierr)
call adios2_open(engine, io, "data.bp", adios2_mode_read, ierr)
call adios2_inquire_variable(var, io, "T", ierr )
call adios2_variable_shape(var, ndim, dims, ierr)
call adios2_set_selection(var, ndims, sel_start, sel_count, ierr)
call adios2_begin_step(engine, adios2_step_mode_next_available, 0.0, ierr)
call adios2_get(engine, var, T, ierr)
call adios2_end_step(engine, ierr)
call adios2_close(engine, ierr)
call adios2_finalize(adios, ierr)
```

/home/adios/Tutorial/heat2d/fortran/analysis/heatAnalysis_adios2_file.F90

GPU

- GPU-aware
  - ADIOS variables will be associated with a memory space (Host, CUDA)
    - ADIOS can detect the memory space (5ns small penalty for every Put/Get)
    - If the `gpuData` is a Kokkos View the memory space is extracted from the View

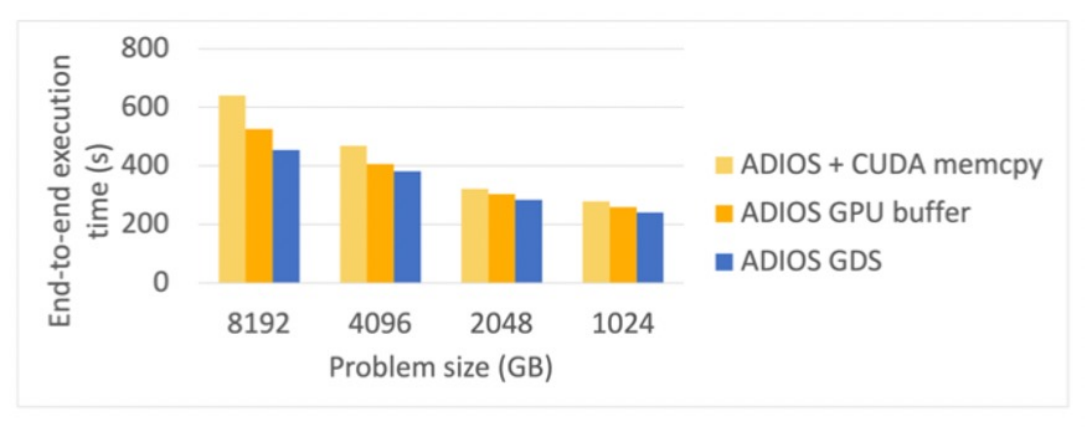
```
adios2::Engine bpWriter;
...
auto data = io.DefineVariable<float>("data",
shape, start, count);

bpWriter.Put(data, cpuData);

data.SetMemorySpace(adios2::MemorySpace::CUDA);
bpWriter.Put(data, gpuData);
```

ADIOS API to receive GPU buffers in Put/Get calls

- GDS (GPUDirect Storage)
  - NVIDIA GDS enables a direct data path
    - For direct memory access (DMA) transfers between GPU memory and storage
  - Experimental transport within ADIOS



Results for I/O benchmarking on Quadro RTX5000 GPU

DAOS

- Current support through the DFS API (DAOS File System) that provides a POSIX like API
  - you still see "files and directories" on a DAOS storage, can use **ls** and other tools
  - dfs is much faster than using a FUSE layer on top of DAOS to emulate a file system
  - ADIOS has a **transport** to write with DFS instead of POSIX (works with any BP engine)
    - C++: io.AddTransport("File", {{"Library", "DAOS"}});
    - XML:

```
<transport type="File">
    <parameter key="Library" value="DAOS"/>
</transport>
```

- In development: a native engine using DAOS Arrays and key-value stores
  - We still have not made up our minds about which abstraction between ADIOS process buffers and distributed arrays and multiple output steps to pick for representing them in DAOS Arrays. Our concern is scalability first and foremost.

Burst Buffer

- Node local NVMe/SSD
  1. ADIOS can output data to distributed storage without any extra option
     - .bp/data.X is a file on one of the local disk, .bp/md* are on process 0's local disk
     - General global reading is not supported – one must copy the entire dataset to a global file system
     - Reading locally available data is still possible
  2. BP4 engine implements the burst buffer functionality (store local, drain on the fly to target global file system)
     - See engine options: **string BurstBufferPath** and **bool BurstBufferDrain**
     - C++: io.AddParameter("BurstBufferPath", "/mnt/nvme/tmp");
     - XML: `<parameter key="BurstBufferPath" value="/mnt/nvme/tmp"/>`
  3. **IME** from **DDN** is a vendor supplied burst buffer solution. ADIOS has a **transport** to write to IME instead of a POSIX file system
     - C++: io.AddTransport("File", {{"Library", "IME"}});
     - XML:

```
<transport type="File">
        <parameter key="Library" value="IME"/>
</transport>
```

Building applications with ADIOS

Compile ADIOS2 codes

- CMake
  - Use MPI_C and ADIOS2 packages

```
CMakeLists.txt:
project(gray-scott C CXX)
find_package(MPI REQUIRED)
find_package(ADIOS2 REQUIRED)
add_definitions(-DOMPI_SKIP_MPICXX -DMPICH_SKIP_MPICXX)
...
target_link_libraries(gray-scott   adios2::cxx11_mpi   MPI::MPI_C)
```

  - Configure application by adding ADIOS installation to search path

```
cmake -DCMAKE_PREFIX_PATH="/opt/adios2"  <source_dir>
```

  - Available ADIOS2 targets: cxx11 c, fortran, cxx11_mpi, c_mpi, fortran_mpi

Compile ADIOS2 codes

- Makefile
  - Add ADIOS2 library paths to LD_LIBRARY_PATH
  - Use adios2_config tool to get compile and link options

```
ADIOS2_DIR = /opt/adios2/
ADIOS2_FINC=`${ADIOS2_DIR}/bin/adios2-config --fortran-flags`
ADIOS2_FLIB=`${ADIOS2_DIR}/bin/adios2-config --fortran-libs`
```

  - Codes that write and read

```
heatSimulation: heat_vars.F90 heat_transfer.F90 io_adios2.F90
	${FC}   -g -c -o heat_vars.o heat_vars.F90
	${FC}   -g -c -o heatSimulation.o heatSimulation.F90
	${FC}   -g -c -o io_adios2.o ${ADIOS2_FINC} io_adios2.F90
	${FC}   -g -o heatSimulation heatSimulation heat_vars.o io_adios2.o  ${ADIOS2_FLIB}
```

Configure and build the ADIOS2-Examples repository (example)

```
$ cd ~/ADIOS2-Examples/
$ mkdir -p build-cmake
$ cd build-cmake
$ cmake \
  -DCMAKE_INSTALL_PREFIX=/home/adios/Tutorial \
  -DCMAKE_PREFIX_PATH="/opt/adios2;/opt/hdf5-parallel/default;/opt/zfp/default;/opt/sz/default“ \
  -DCMAKE_BUILD_TYPE=RelWithDebInfo \
   ..
$ make -j 4
$ make install
$ cd /home/adios/Tutorial/share/adios2-examples/gray-scott

$ export PATH=$PATH:/home/adios/Tutorial/bin
$ export PYTHONPATH=/opt/adios2/lib/python3/dist-packages
$ export LD_LIBRARY_PATH=/opt/hdf5-1.13.0/parallel/lib::/opt/sz/default/lib:/opt/zfp/default/lib
```

Outline

- 8:30 Introduction to data management at extreme scale – Scott Klasky
- 9:15 ADIOS 2 concepts and API (C++, Python, F90) – Norbert Podhorszki
- 10:00 BREAK
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- 3:00 BREAK
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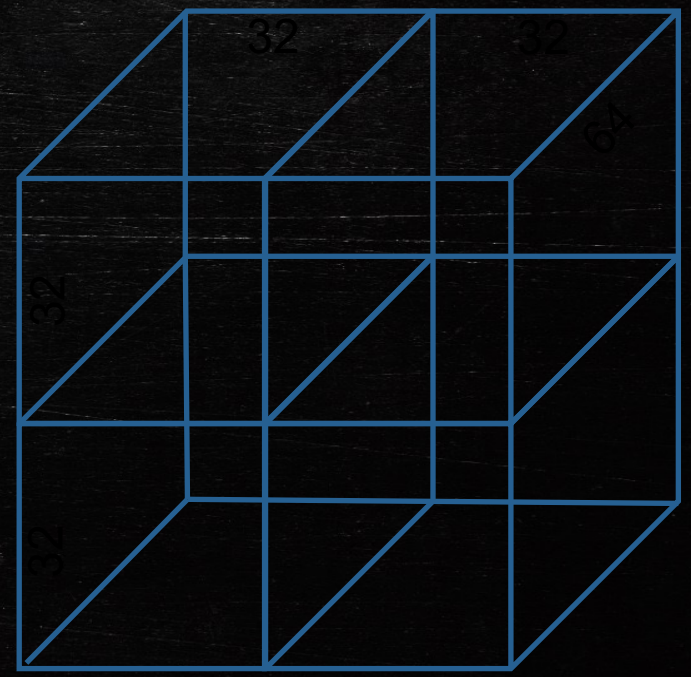
- 4:15 Staging with ADIOS – hands 0n – Ana Gainaru
- 5:00 END

Gray-Scott Example with **ADIOS:** **Write** Part

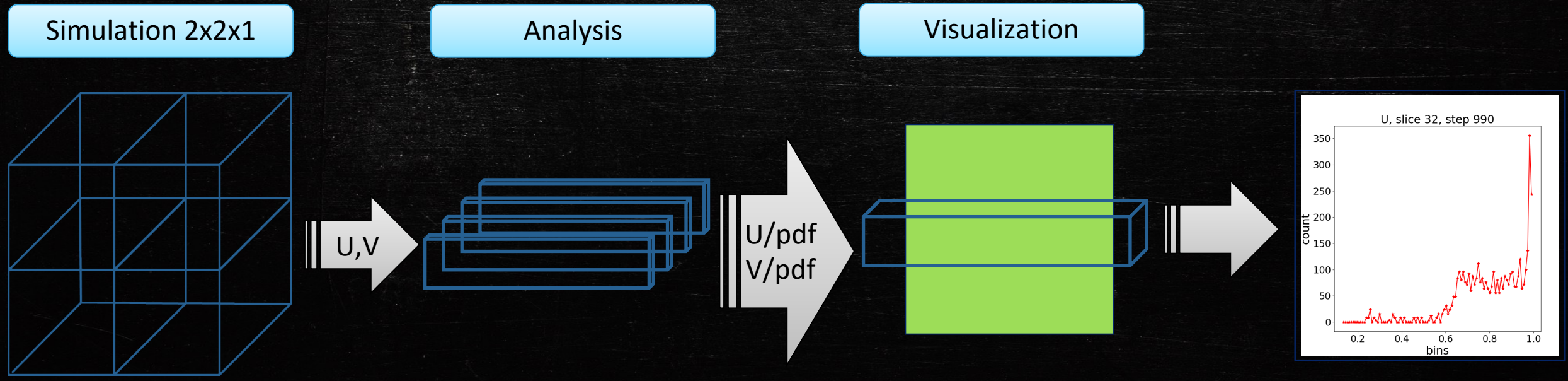
Gray-Scott Example

- In this example we start with a 3D code which writes 3D arrays, with a 3D domain decomposition, as shown in the figure.
  - Gray-Scott Reaction–diffusion system
  - https://en.wikipedia.org/wiki/Reaction%E2%80%93diffusion_system
  - https://github.com/ornladios/ADIOS2-Examples/tree/master/source/cpp/gray-scott
  - We write multiple time-steps, into a single output.
- For simplicity, we work on only 4 cores, arranged in a 2x2x1 arrangement.
- Each processor works on 32x32x64 subsets
- The total size of the output arrays = 4*64*64*64



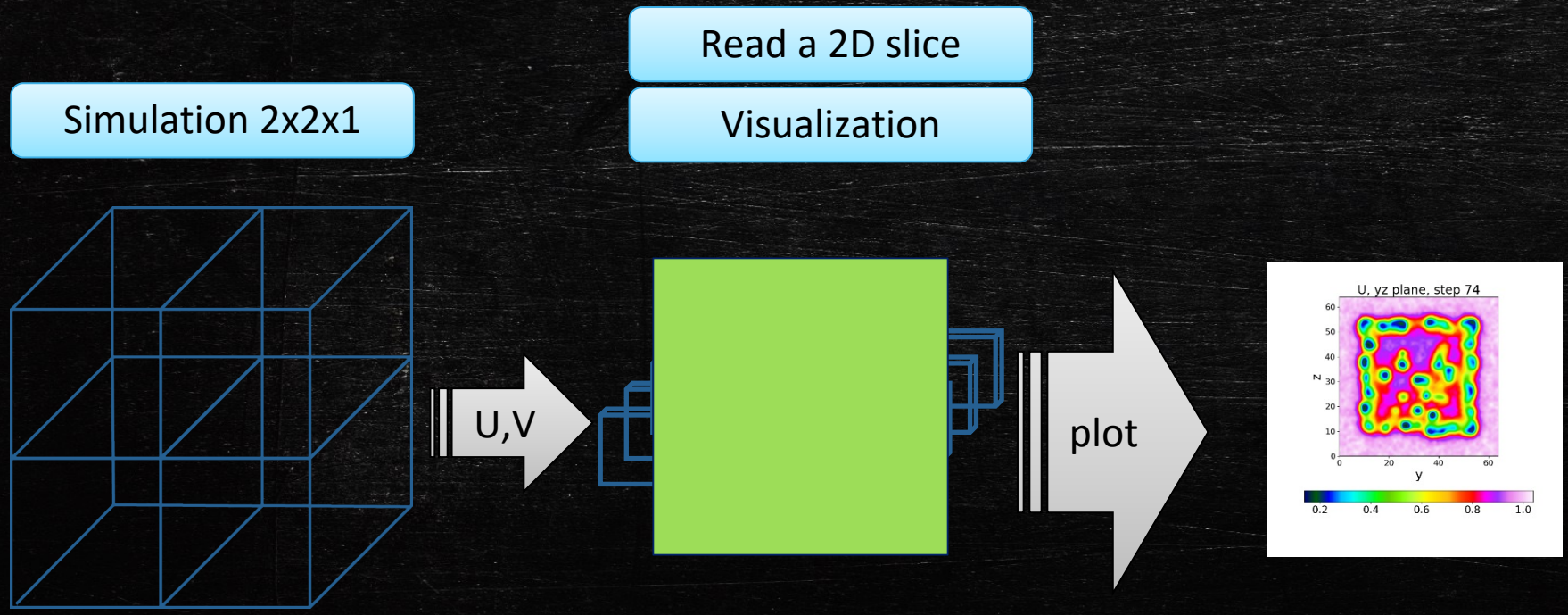
Analysis and visualization

- Read with a different decomposition (1D)
  - Calculate PDFs on a 2D slice of the 3D array
  - Read/Write U,V from M cores, arranged in a M x 1 x 1 arrangement.
- Plot U/pdf
  - image files



Visualization with plot/gsplot.py

- Read a 2D slice and plot it with matplotlib

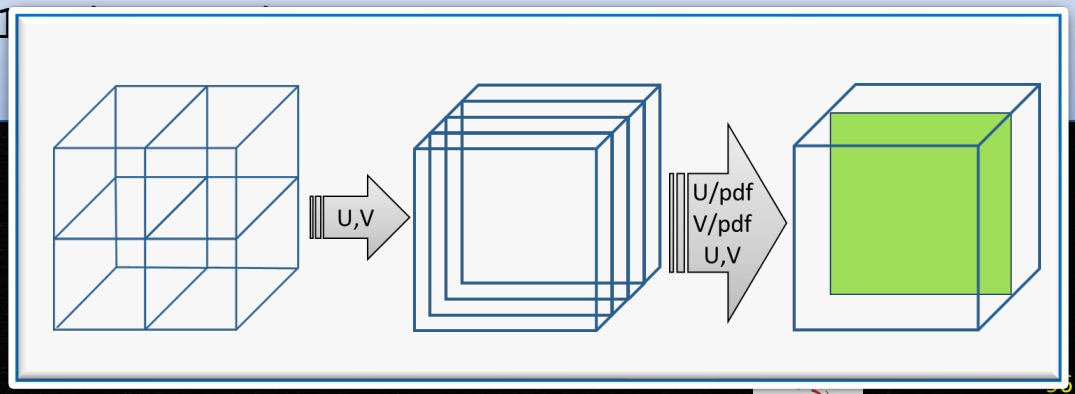


Goal by the end of the day: Running the example in situ

```
$ mpirun -n 4 adios2-gray-scott settings-staging.json
Simulation at step 10 writing output step     1
Simulation at step 20 writing output step     2
Simulation at step 30 writing output step     3
Simulation at step 40 writing output step     4
...
```

```
$ mpirun -n 1 adios2-pdf-calc gs.bp pdf.bp 100
PDF Analysis step 0 processing sim output step 0 sim compute step 10
PDF Analysis step 1 processing sim output step 1 sim compute step 20
PDF Analysis step 2 processing sim output step 2 sim compute step 30
...
```

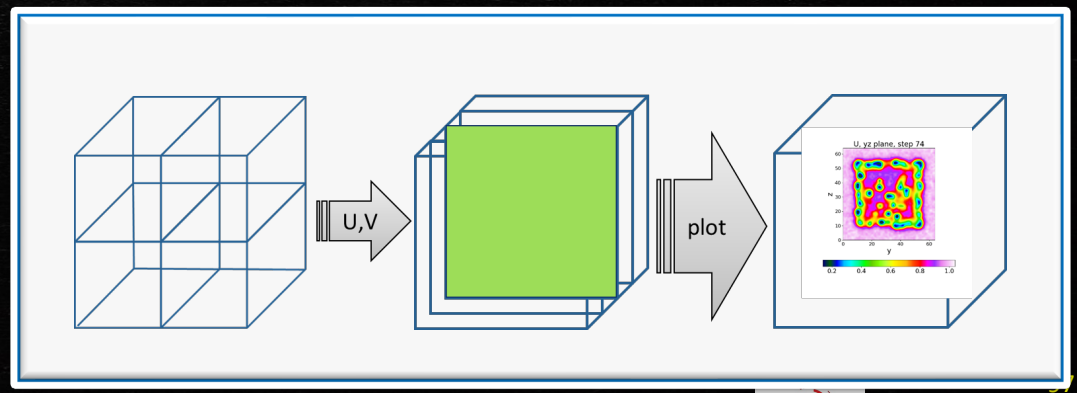
```
$ mpirun -n 1 python3 pdfplot.py -i pdf.bp
PDF Plot step 0 processing analysis step 0 simulation step 10
PDF Plot step 1 processing analysis step 1
...
```



Goal by the end of the exercise: Running the example in situ

```
$ mpirun -n 4 adios2-gray-scott settings-staging.json
Simulation at step 10 writing output step     1
Simulation at step 20 writing output step     2
Simulation at step 30 writing output step     3
Simulation at step 40 writing output step     4
...
```

```
$ mpirun -n 1 python3 gsplot.py -i gs.bp
GS Plot step 0 processing stream step 0 sim step 10 minmax=0.0765537..1.05494
GS Plot step 1 processing stream step 1 sim step 20 minmax=0.111669..1.05908
...
```



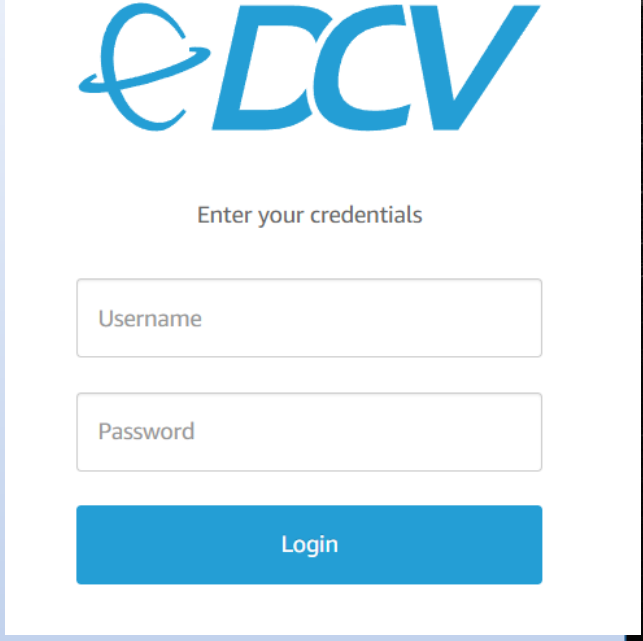
Login to a virtual machine

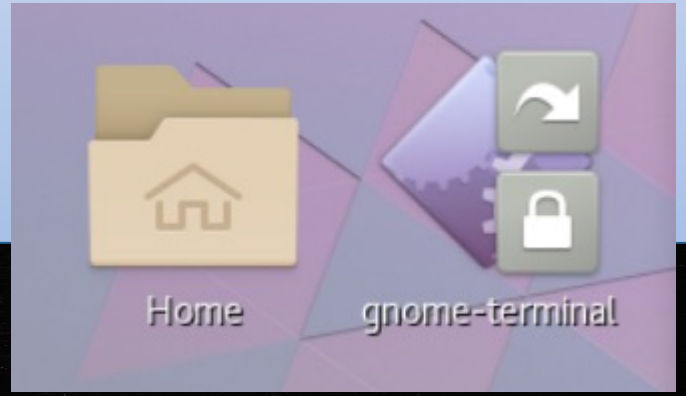
https://tut###.supercontainers.org:8443/#e4s

is a number assigned for you in this tutorial

Username: tutorial
Password: HPCLinux12!

Launch a couple of gnome-terminals





Configure the environment

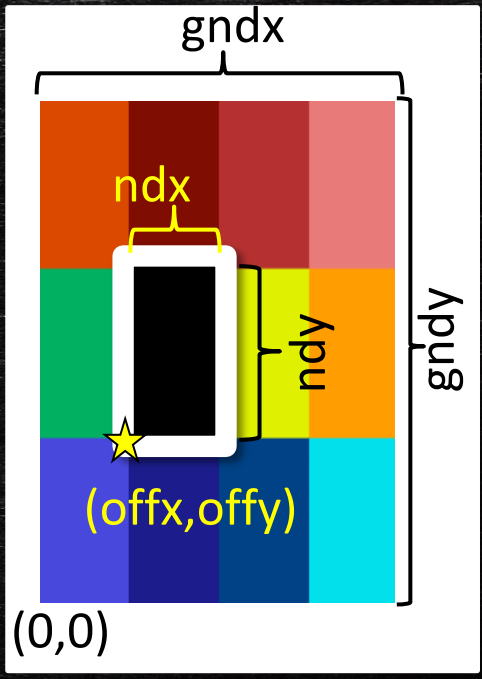
```
$ cd ~/adios2-tutorial-source
$ source ~/adios2-tutorial-source/adios2-tutorial-env.sh
$ cd ~/adios2-tutorial-source/ADIOS2-Examples/build/install/share/adios2-examples/gray-scott
```

Run the code

```
$ source ~/adios2-tutorial-source/adios2-tutorial-env.sh
$ cd ~/adios2-tutorial-source/ADIOS2-Examples/build/install/share/adios2-examples/gray-scott
$ mpirun -n 4 ../../../bin/adios2-gray-scott settings-files.json
Simulation writes data using engine type:              BP5
=========================================
grid:               64x64x64
steps:              1000
plotgap:            10
F:                  0.01
k:                  0.05
dt:                 2
Du:                 0.2
Dv:                 0.1
noise:              1e-07
output:             gs.bp
adios_config:       adios2.xml
process layout:     2x2x1
local grid size:    32x32x64
=========================================
Simulation at step 10 writing output step     1
Simulation at step 20 writing output step     2
...
$ du -hs *.bp
401M    gs.bp
```

Gray-Scott Global Array

- N-dimensions
- Type
- Decomposition across many processors
  - global dimensions (Shape), local place (Start, Count)



ADIOS2-Examples/source/cpp/gray-scott/simulation

main.cpp:

```
adios2::ADIOS adios(settings.adios_config, comm);
adios2::IO io = adios.DeclareIO("SimulationOutput");
```

writer.cpp:

```
var_u = io.DefineVariable<double>(
  "U",
  {settings.L, settings.L, settings.L},
  {sim.offset_z, sim.offset_y, sim.offset_x},
  {sim.size_z, sim.size_y, sim.size_x});
```

- Fortran/Matlab/R always column-major, C/C++/Python always row-major

bpls

- List content and print data from ADIOS2 output (.bp and .h5 files)
  - dimensions are reported in row-major order

```
$ bpls -la gs.bp
  double   Du        attr   = 0.2
  double   Dv        attr   = 0.1
  double   F         attr   = 0.01
  double   U         100*{64, 64, 64} = 0.0907898 / 1
  double   V         100*{64, 64, 64} = 0 / 0.674844
  double   dt        attr   = 2
  double   k         attr   = 0.05
  double   noise     attr   = 1e-07
  int32_t  step      100*scalar = 10 / 1000
```

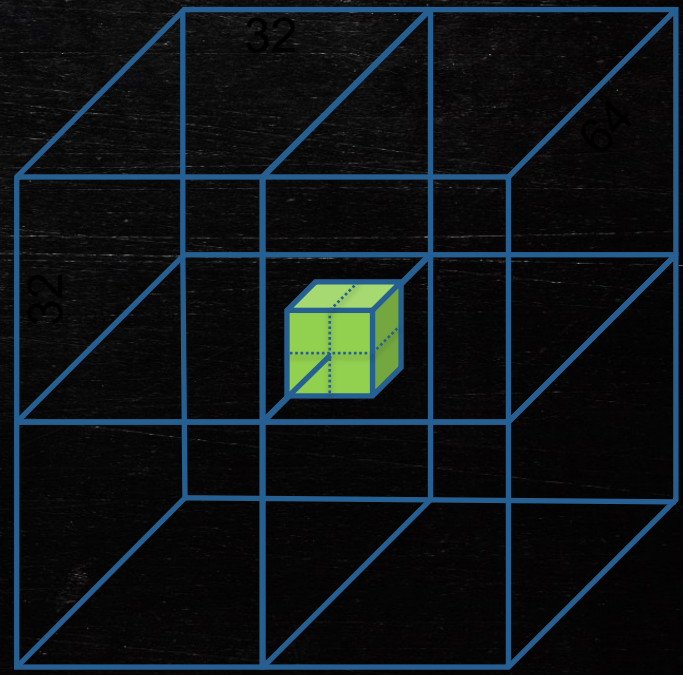
bpls (to show the decomposition of the array)

```
$ bpls -l -D gs.bp U
 double   U      100*{64, 64, 64} = 0.0907898 / 1
        step  0:
          block 0: [ 0:63,  0:31,  0:31] = 0.104002 / 1
          block 1: [ 0:63, 32:63,  0:31] = 0.104002 / 1
          block 2: [ 0:63,  0:31, 32:63] = 0.104002 / 1
          block 3: [ 0:63, 32:63, 32:63] = 0.104002 / 1
 ...
        step 99:
          block 0: [ 0:63,  0:31,  0:31] = 0.148308 / 0.998811
          block 1: [ 0:63, 32:63,  0:31] = 0.148302 / 0.998812
          block 2: [ 0:63,  0:31, 32:63] = 0.148335 / 0.998811
          block 3: [ 0:63, 32:63, 32:63] = 0.148302 / 0.998811
```

bpls to dump: 2x2x2 read with bpls

- Use bpls to read in the **center** 3D cube of the **last** output step

```
$ bpls gs.bp -d U -s "-1,31,31,31" -c "1,2,2,2" -n 2
double   U      100*{64, 64, 64}
   slice (99:99, 31:32, 31:32, 31:32)
    (99,31,31,31)    0.916973 0.916972
    (99,31,32,31)    0.916977 0.916975
    (99,32,31,31)    0.916974 0.916973
    (99,32,32,31)    0.916977 0.916976
```



- Note: bpls handles time as an extra dimension
- -s starting offset
  - first offset is the timestep, *-n to* count backwards
- -c size in each dimension
  - first value is how many steps
- -n how many values to print in one line

The ADIOS XML configuration file

- Describe runtime parameters for each IO grouping
  - select the Engine for writing
    - **BP5**, **HDF5**, **SST**
- see ~/Tutorial/share/adios2-examples/gray-scott/adios2.xml
- XML-free: engine can be selected in the source code as well

The runtime config file: adios2.xml

```
<?xml version="1.0"?>
<adios-config>

 <!--====================================
       Configuration for for Gray-Scott and GS Plot
     ====================================-->
  <io name="SimulationOutput">
    <engine type="BP5">
      <parameter key="OpenTimeoutSecs" value="10.0"/>
      <parameter key="NumAggregators" value="2"/>
    </engine>
  </io>
```

Engine types

BP5

BP4

HDF5

FileStream

SST

SSC

DataMan

```
  <!--====================================
       Configuration for PDF calc and PDF Plot
     ====================================-->

  <io name="PDFAnalysisOutput">
    <engine type="BP5">
    </engine>
  </io>

</adios-config>
```

The runtime config file: adios2.xml

adios2.xml

```
<?xml version="1.0"?>
<adios-config>

  <!--=====================================
      Configuration for for Gray-Scott and GS Plot
    =====================================-->
  <io name="SimulationOutput">
    <engine type="HDF5">
    </engine>
  </io>
```

Engine types
BP5
HDF5
FileStream
SST
SSC
DataMan

settings-files.json

```
{
    "L": 64,
    "Du": 0.2,
    "Dv": 0.1,
    "F": 0.01,
    "k": 0.05,
    "dt": 2.0,
    "plotgap": 10,
    "steps": 1000,
    "noise": 0.0000001,
    "output": "gs.bp",
    "checkpoint": false,
    "checkpoint_freq": 10,
    "checkpoint_output": "gs_ckpt.bp",
    "adios_config": "adios2.xml",
    "adios_span": false,
    "adios_memory_selection": false,
    "mesh_type": "image"
}
```

gs.h5

Run the code

```
$ cd ~/Tutorial/share/adios2-examples/gray-scott
$ mpirun -n 4 adios2-gray-scott settings-files.json
Simulation writes data using engine type:              HDF5
=========================================
grid:               64x64x64
steps:              1000
plotgap:            10
F:                  0.01
k:                  0.05
dt:                 2
Du:                 0.2
Dv:                 0.1
noise:              1e-07
output:             gs.bp
adios_config:       adios2.xml
process layout:     2x2x1
local grid size:    32x32x64
=========================================
Simulation at step 10 writing output step     1
Simulation at step 20 writing output step     2
...
$ du -hs *.h5
401M    gs.h5
```

List the content

```
$ h5ls -r gs.h5
/                        Group
/Step0                   Group
/Step0/U                 Dataset {64, 64, 64}
/Step0/V                 Dataset {64, 64, 64}
/Step0/step              Dataset {SCALAR}
/Step1                   Group
/Step1/U                 Dataset {64, 64, 64}
/Step1/V                 Dataset {64, 64, 64}
/Step1/step              Dataset {SCALAR}
...

$ h5ls -d gs.h5/Step1/U
```

bpls can read HDF5 files as well

```
$ bpls gs.bp -d U -s "-1,31,31,31" -c "1,2,2,2" -n 2
double   U      100*{64, 64, 64}
   slice (99:99, 31:32, 31:32, 31:32)
    (99,31,31,31)    0.916973 0.916972
    (99,31,32,31)    0.916977 0.916975
    (99,32,31,31)    0.916974 0.916973
    (99,32,32,31)    0.916977 0.916976
```

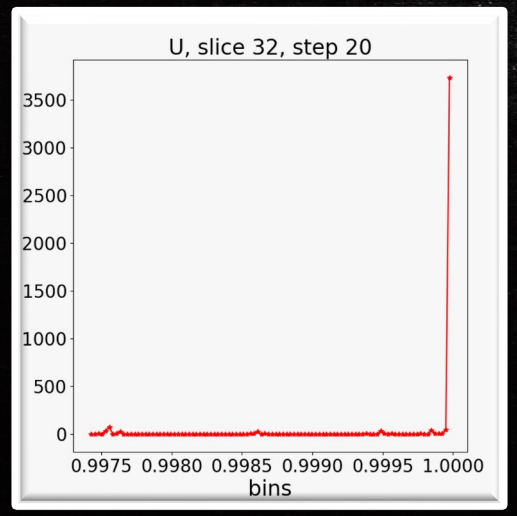
```
$ bpls gs.h5 -d U -s "-1,31,31,31" -c "1,2,2,2" -n 2
double   U      100*{64, 64, 64}
   slice (99:99, 31:32, 31:32, 31:32)
    (99,31,31,31)    0.916973 0.916972
    (99,31,32,31)    0.916977 0.916975
    (99,32,31,31)    0.916974 0.916973
    (99,32,32,31)    0.916977 0.916976
```

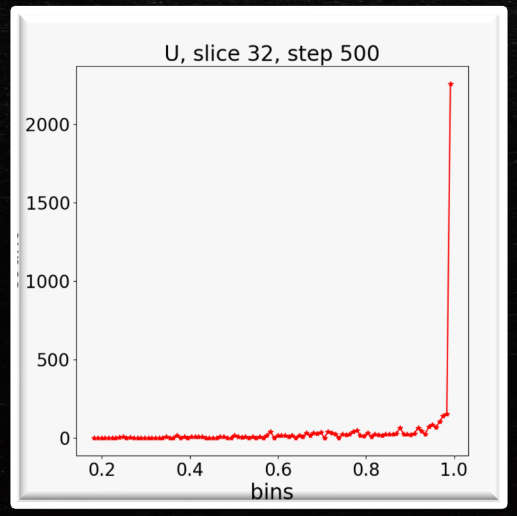
Compile and run the reader

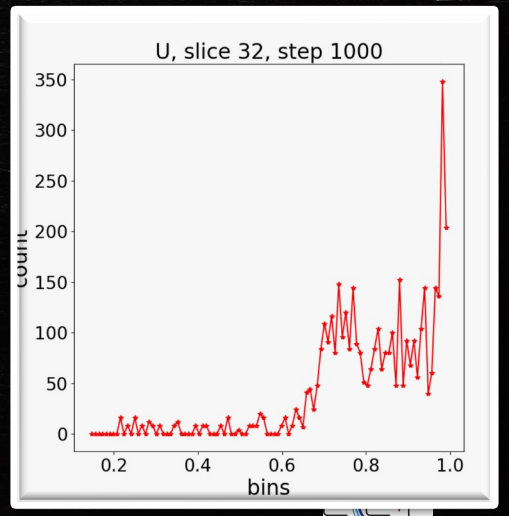
```
# make sure in adios2.xml, SimulationOutput's engine is set to BP5
# make sure in settings-files.json "output" is set to "gs.bp"
$ mpirun -n 3 ../../../bin/adios2-pdf-calc gs.bp pdf.bp 100
PDF analysis reads from Simulation using engine type:  BP5
PDF analysis writes using engine type:                 BP5
PDF Analysis step 0 processing sim output step 0 sim compute step 10
PDF Analysis step 1 processing sim output step 1 sim compute step 20
PDF Analysis step 2 processing sim output step 2 sim compute step 30
...
$ bpls -l  pdf.bp
  double   U/bins  100*{100} = 0.0908349 / 1
  double   U/pdf   100*{64, 100} = 0 / 4096
  double   V/bins  100*{100} = 0 / 0.668077
  double   V/pdf   100*{64, 100} = 0 / 4096
  int32_t  step    100*scalar = 10 / 1000
$ bpls -l  pdf.bp -D U/pdf
 double   U/pdf   100*{64, 100} = 0 / 4096
        step  0:
          block 0: [ 0:20,  0:99] = 0 / 894
          block 1: [21:41,  0:99] = 0 / 4096
          block 2: [42:63,  0:99] = 0 / 4096
        step  1:
```

Run the plotting script with file I/O

```
$ python3 pdfplot.py -i pdf.bp -o p
PDF Plot step 0 processing analysis step 0 simulation step 10
PDF Plot step 1 processing analysis step 1 simulation step 20
PDF Plot step 2 processing analysis step 2 simulation step 30
...
$ ls *.png
p00010_32.png  p00100_32.png  p00190_32.png ... p01000_32.png
$ eog . &
```

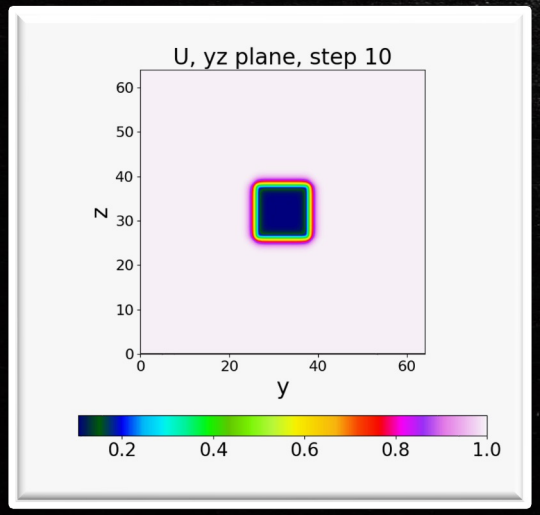


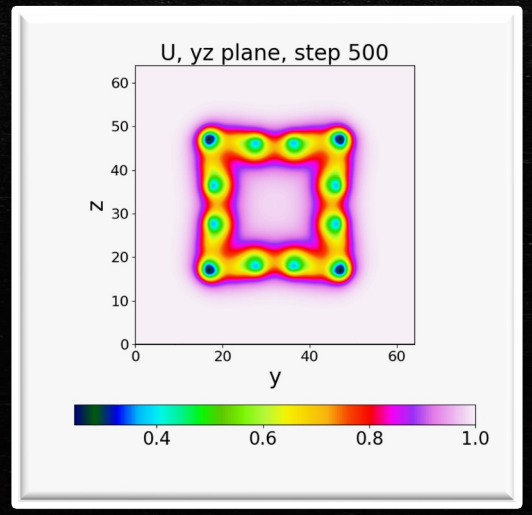


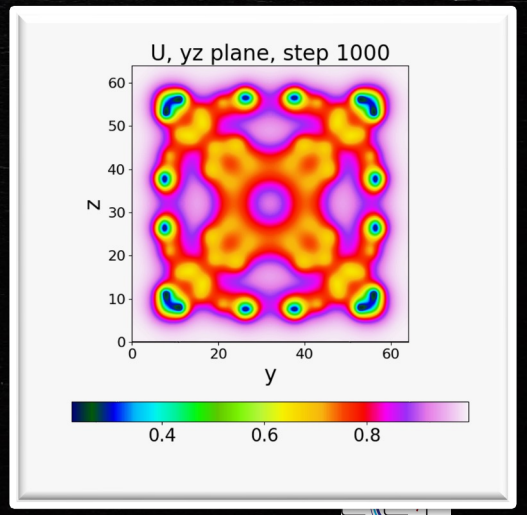


Run the plotting script with file I/O

```
$ python3 gsplot.py -i gs.bp -o g
PDF Plot step 0 processing analysis step 0 simulation step 10
PDF Plot step 1 processing analysis step 1 simulation step 20
PDF Plot step 2 processing analysis step 2 simulation step 30
...
$ ls g*.png
g00010_32.png  g00100_32.png  g00190_32.png ... g01000_32.png
$ eog . &
```







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How to scale ADIOS I/O

ADIOS Scaling for large parallel file systems

- There are a **few** options for changing the performance of ADIOS for your code on all HPC systems
  - Aggregation – choosing the number of sub-files for maximizing the filesystem bandwidth
  - Appending multiple steps into a single output for minimizing the filesystem metadata overhead
  - Asynchronous write with BP5 engine
  - Choosing the “best” ADIOS engine/storage system (staging, NVRAM-flush) for minimizing the variability

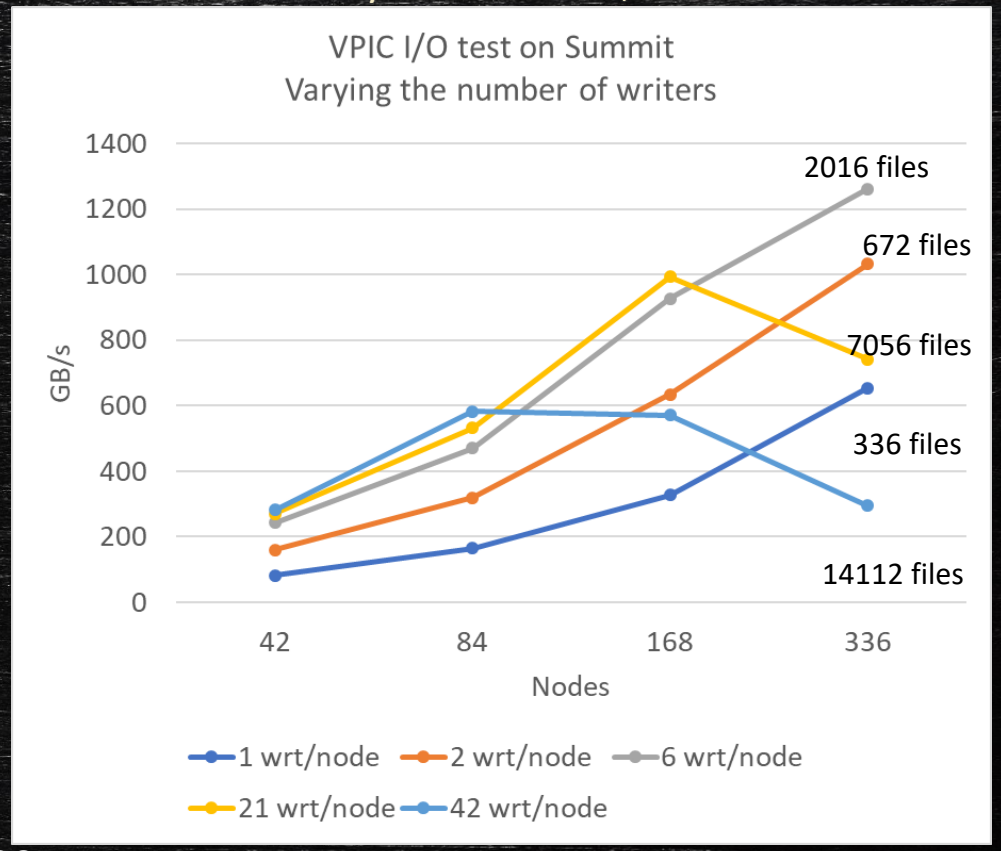
ADIOS Scaling for large parallel file systems: number of files

- Not good:
  - Single, global output file from many writers (or for many readers)
    - Bottleneck at file access
  - One file per process
    - Chokes the metadata server of the file system at create
    - Reading from different number of processes is very difficult
- Good:
  - Create K subfiles where K is proportioned to the capability of the file system, not the number of writers/readers
- ADIOS BP engine options
  - **NumAggregators**
  - **AggregatorRatio**
- ADIOS default settings
  - One file per compute node

```
<io name="SimulationOutput">
  <engine type="BP5">
    <parameter key="NumAggregators" value="2048"/>
  </engine>
</io>
```

Example: VPIC I/O test on Summit

chart courtesy of Junmin Gu, LBNL

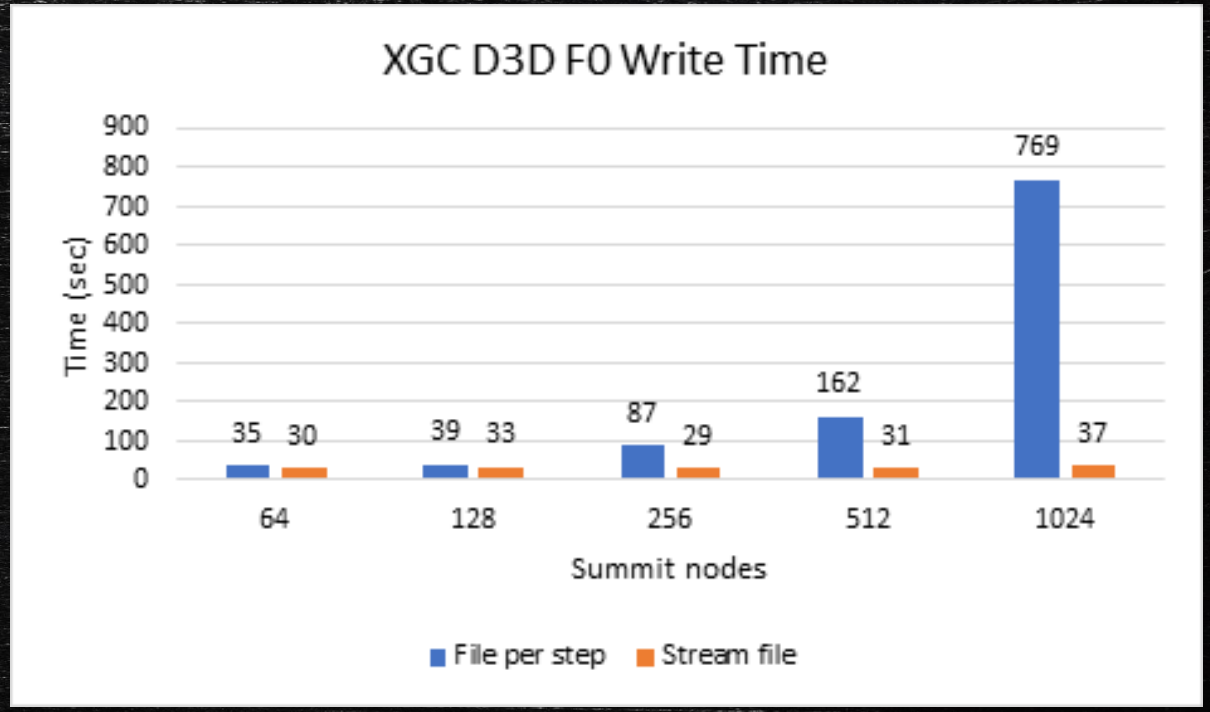


- A fixed aggregation ratio breaks down as we scale up the nodes
- Best options here:
  - 42 nodes – 42*42=1764 subfiles (1:1)
  - 84 nodes – 84*42=3528 subfiles (1:1)
  - 168 nodes – 168*21=3528 subfiles (1:2)
  - 336 nodes – 336*6=2016 subfiles (1:7)
- Summit general guidance
  - One subfile per GPU (6 per node) is a good start but apps usually have one MPI task/GPU, so keep the total number of subfiles below 4000

Application	Nodes/GPUs, 6 tasks/node	Data Size per step	I/O speed	ADIOS NumAggregators
SPECFEM3D_GLOBE	3200/19200	250 TB	~2 TB/sec	3200 (1:6 aggregation ratio)
GTC	512/3072	2.6 TB	~2 TB/sec	3072 (1:1 aggregation ratio)
XGC	512/3072	64 TB	1.2 TB/sec	1024 (1:3 aggregation ratio)
LAMMPS	512/3072	457 GB	1 TB/sec	512 (1:6 aggregation ratio)

ADIOS Scaling for large parallel file systems: number of steps

- Another aspect of number of files: number of output steps
- New output every step -> many files over the course of simulation
  - If the rate of steps stresses the file system, write performance will drop
  - Actually, the total time of creation of files will add up
- Appending multiple output steps into same file is better



XGC 100 output steps in 1245 second simulation, 40 GB per step (4TB total)

One file per node created in each step

Single output for all steps (one file per node)

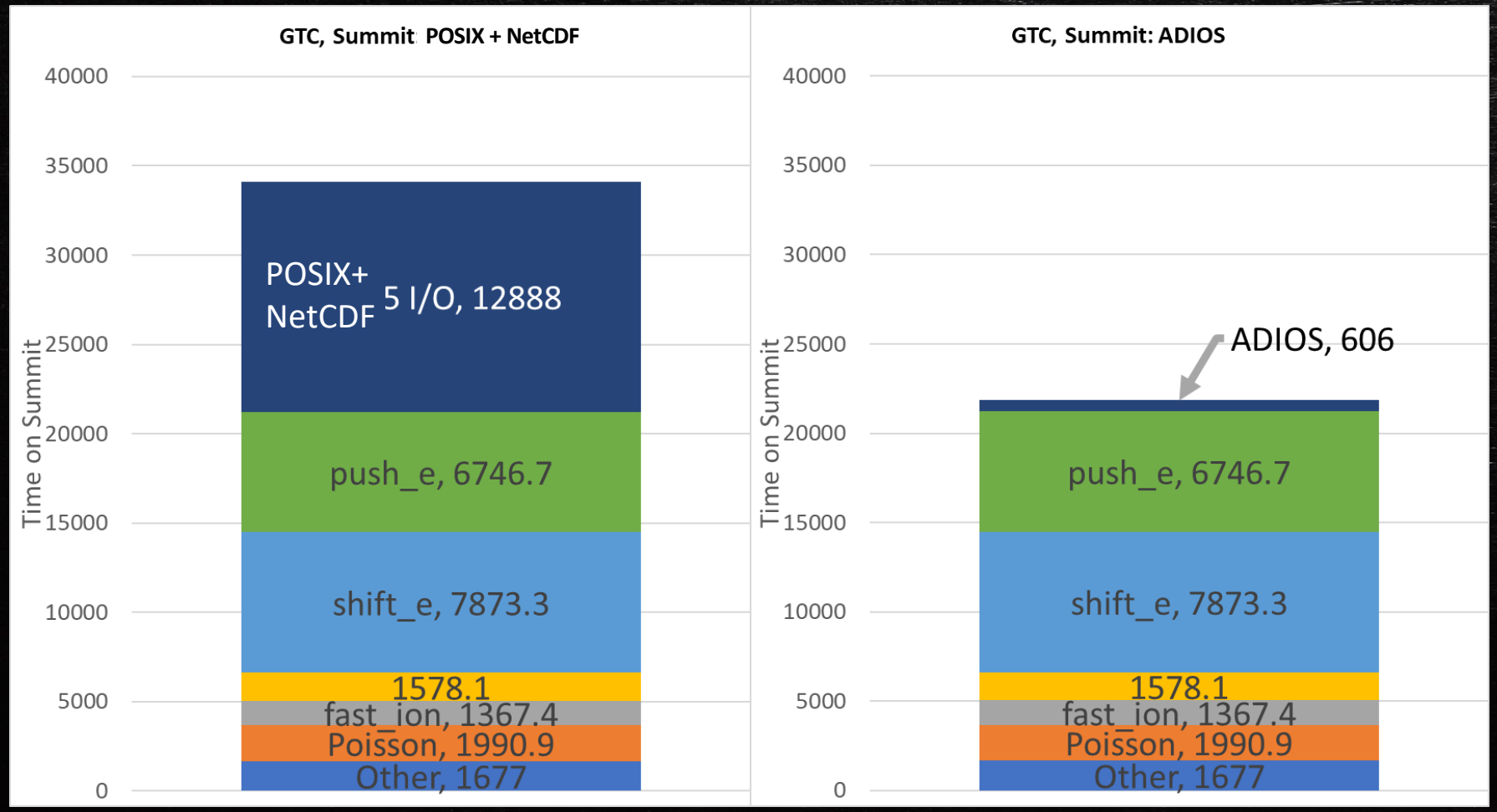
GTC Original I/O vs. ADIOS – Comparing the no. of files created

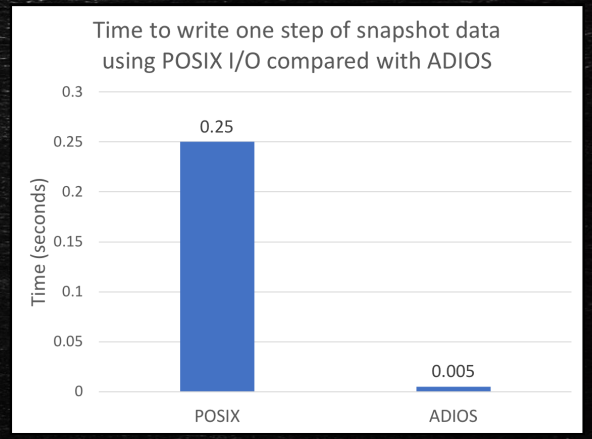
10k steps, 512 nodes (3072 ranks)

Data Category	Data Subcategory	Number of files in the original code	Number of files in the ADIOS container (1 writer per node)
diagnostics	equilibrium	1	1
diagnostics	data1d	1	1
diagnostics	history	1	1
snapshot	snapshot	**10,000** (1 file per step)	**1**
field data	phi3d	**32,000** (1 file every 10 steps per toroidal root)	**512** (1 file per node)
checkpoint	restart1	**2 * 3072** (1 file per rank)	**2 * 512** (1 file per node)

Optimized GTC, a fusion PIC code, I/O on Summit

PI: Zhihong Lin, UC Irvine





* average cost when measuring 10 000 steps

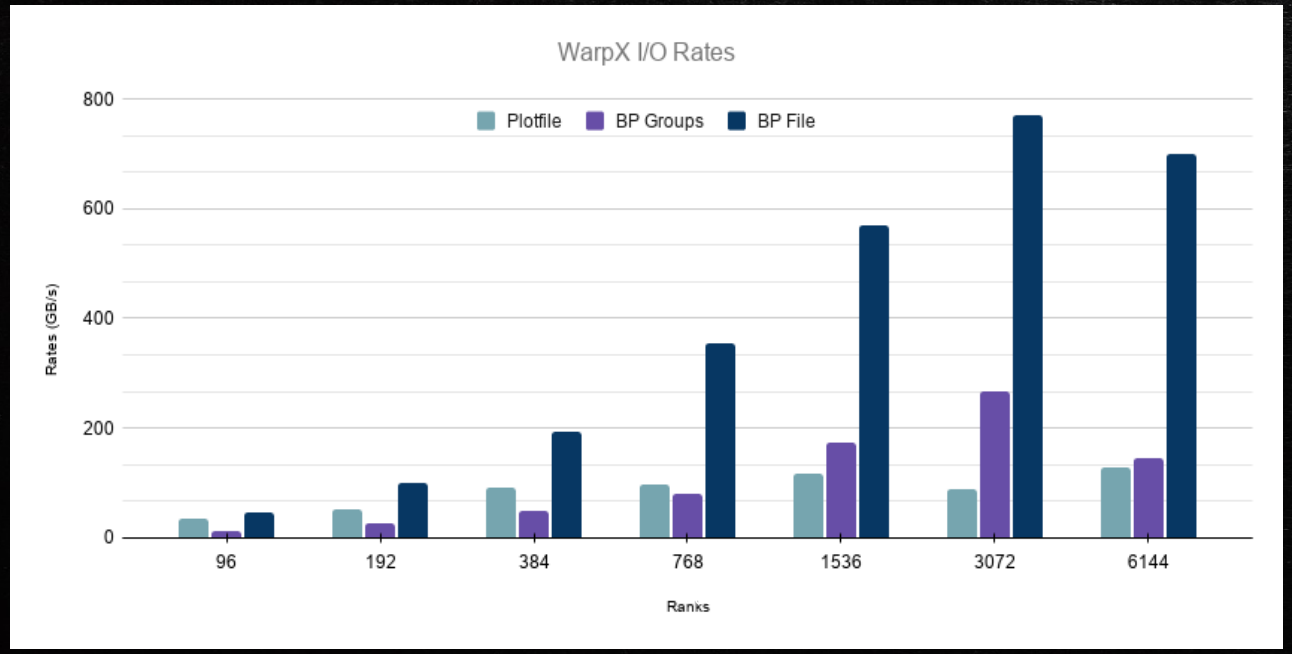
- Change to ADIOS I/O: Total simulation time reduced from 9.5 hours to 6.1 hours on 1024 nodes on Summit

WarpX example: appending + aggregation

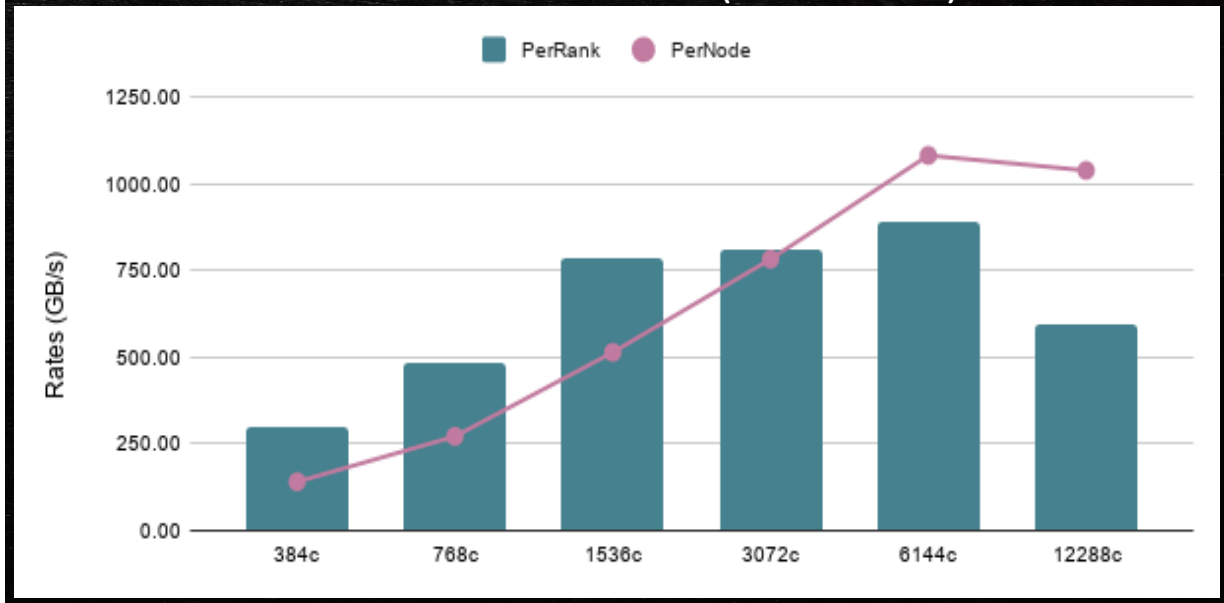
PI: Jean-Luc Vay, LBNL

- One file per compute node (6 processes on Summit)
- Better performance at 512 nodes and over
- One file per rank at smaller jobs

WarpX on Summit, Original vs
ADIOS new output per step vs
ADIOS single output



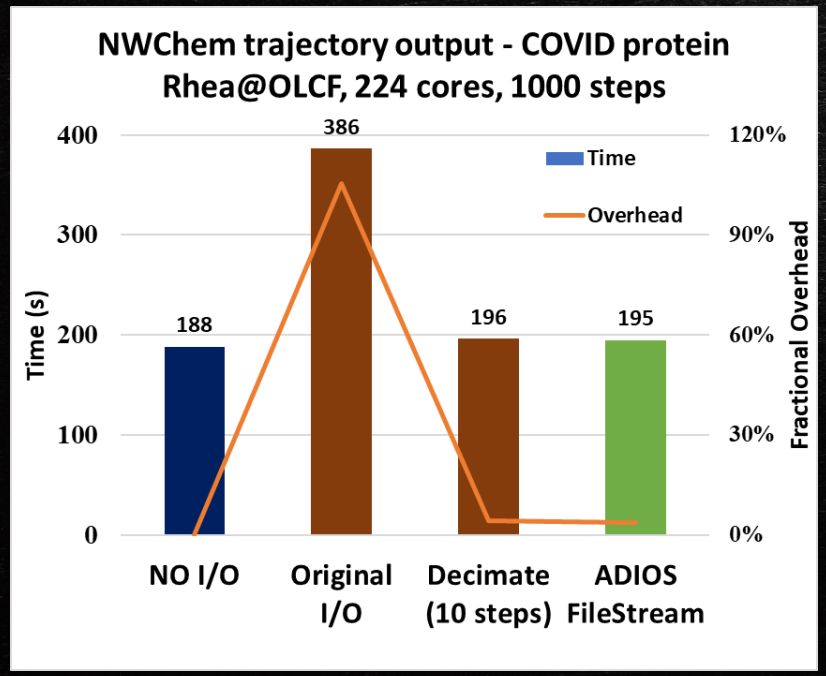
WarpX on Summit, 6 rank per node setup
240 TB on 1024 nodes (6144 cores)



240 TB on 1024 nodes (6144 cores)

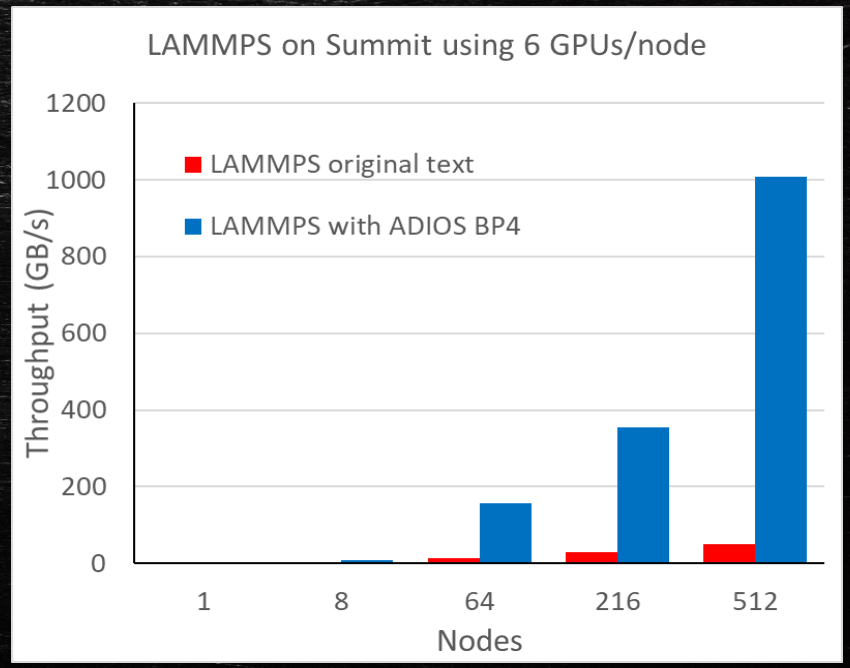
Single process I/O examples: NWChem, LAMMPS

- Moves data between processes as part of preparation for I/O
  - "I am doing POSIX/Fortran I/O on rank 0"
  - While gathering data, no one is writing
- Single file output – not utilizing available bandwidth



ADIOS can write all steps out with little cost (here every 0.2 seconds)

Summit 512 nodes
12B atoms, 5 TB

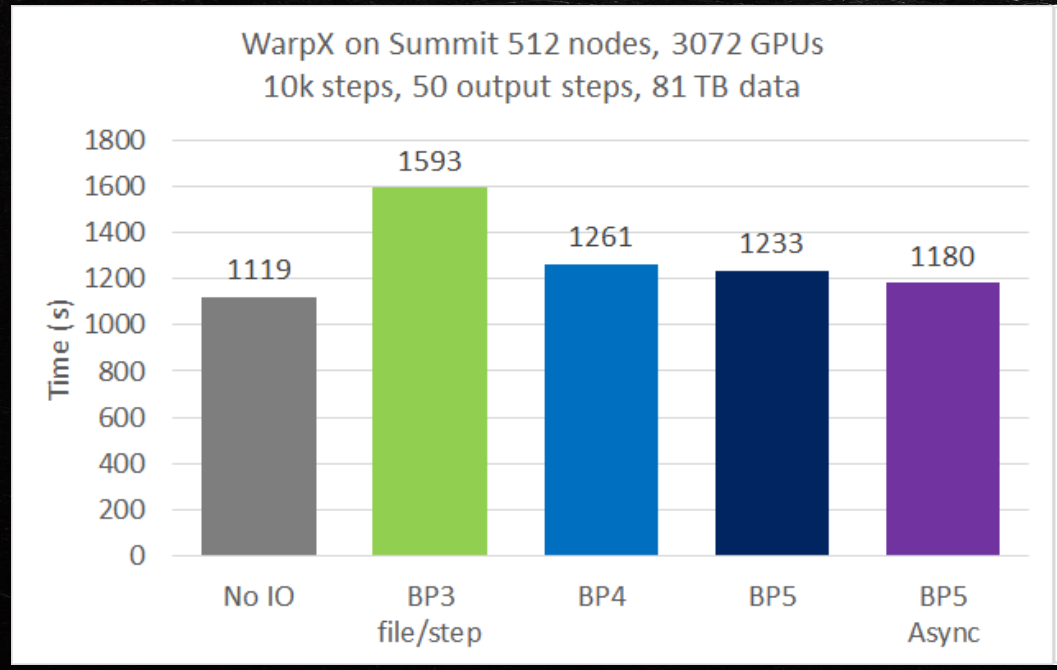


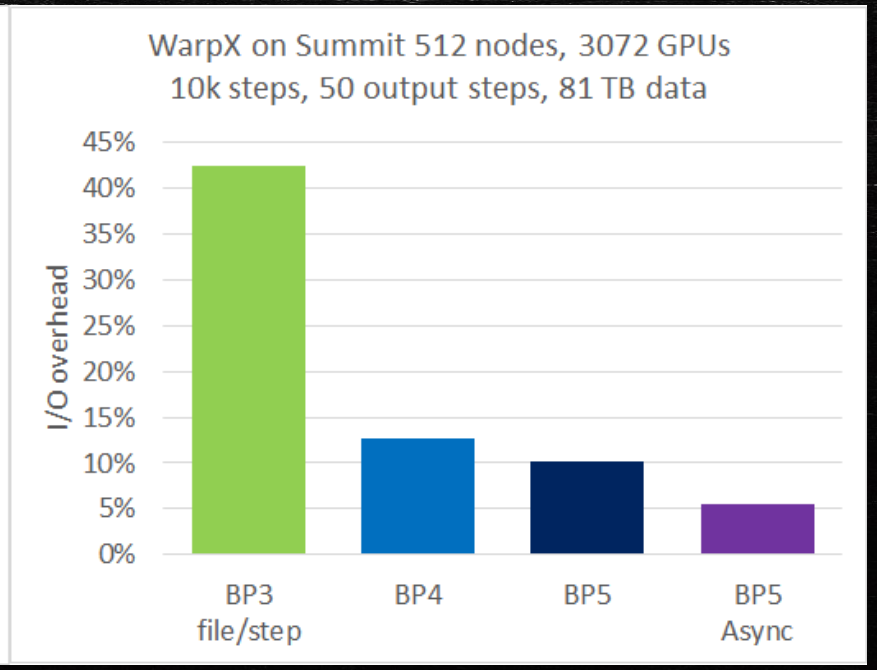
https://github.com/lammps/lammps/tree/master/src/USER-ADIOS

- USER-ADIOS package in LAMMPS for dump commands
  dump atom/adios dump custom/adios
- Output goes into an I/O stream
  BP4 file by default Can use staging engines

Asynchronous write to storage (BP5 engine, 2.8.0 release)

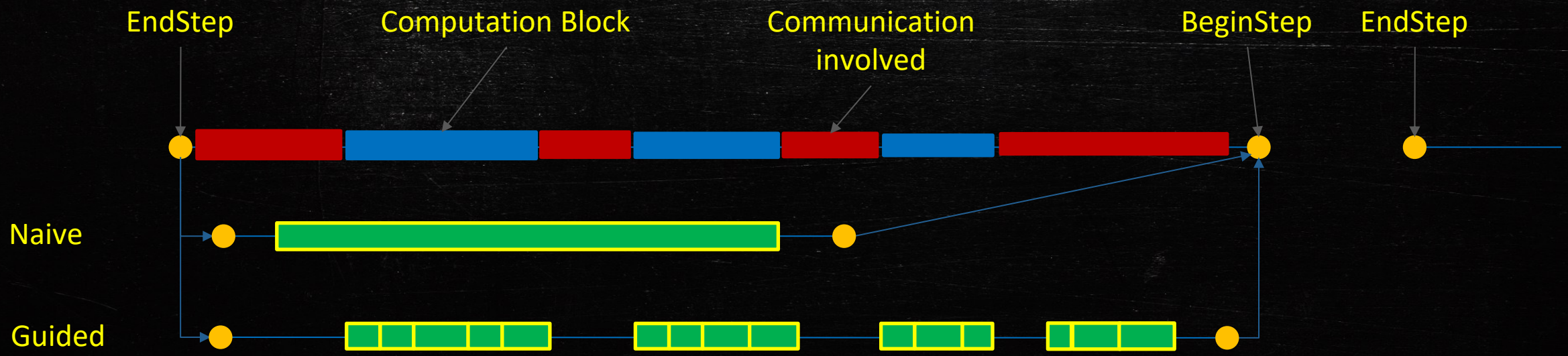
- User friendly On/Off option
  - No need to modify the user code
- Only data writing is async, metadata gathering and writing is still sync
- Don’t have too much experience with this yet





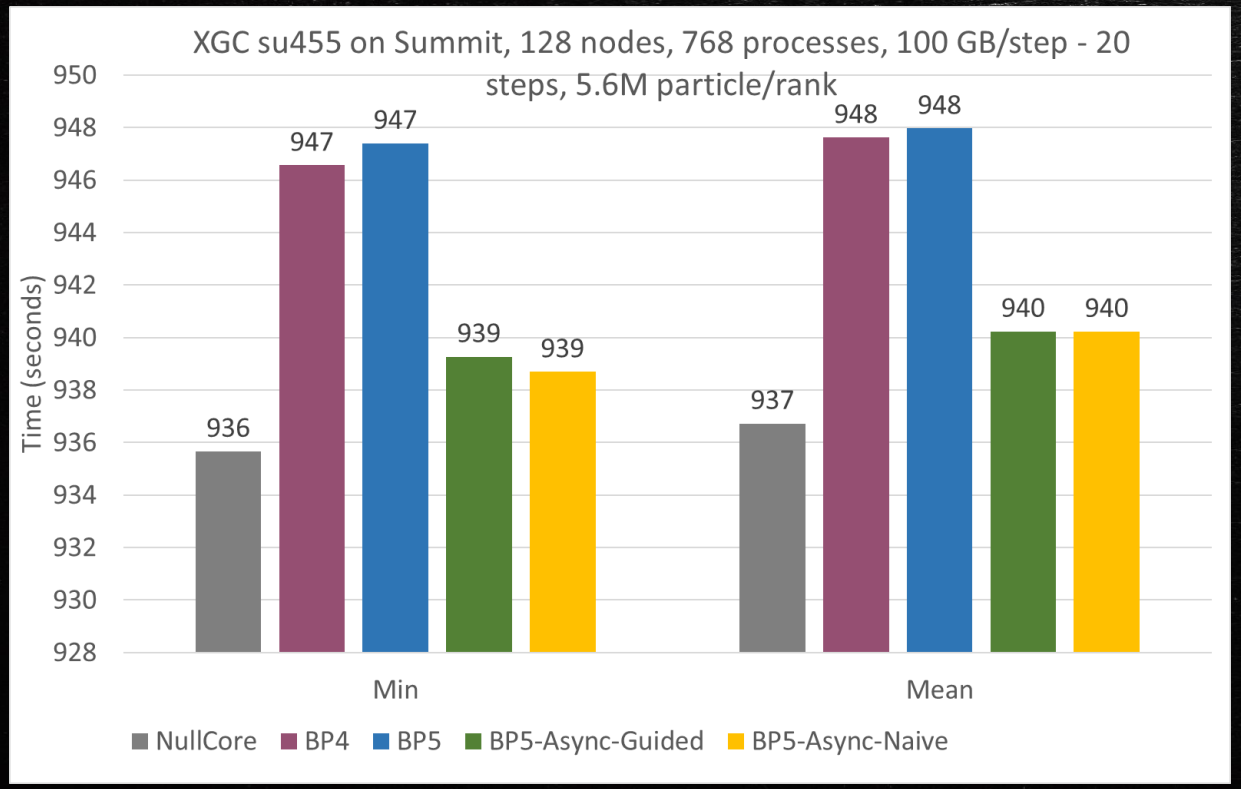
Async strategies

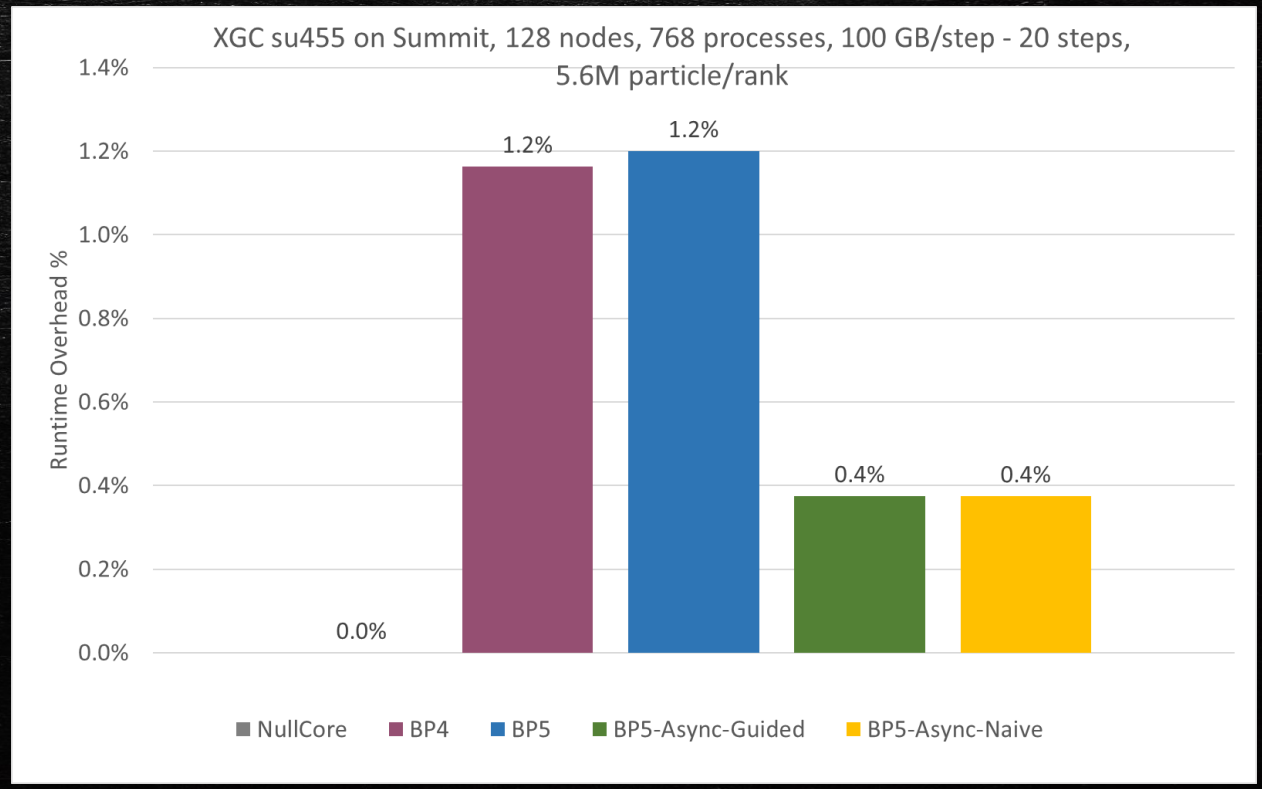
- Naive
  - dump data without thinking
- Guided
  - Application augmented with EnterComputationBlock/ExitComputationBlock pairs
  - Attempt writing during computation blocks
  - Naïve dump when running out of (forecasted) computation blocks



Async IO with XGC only small data

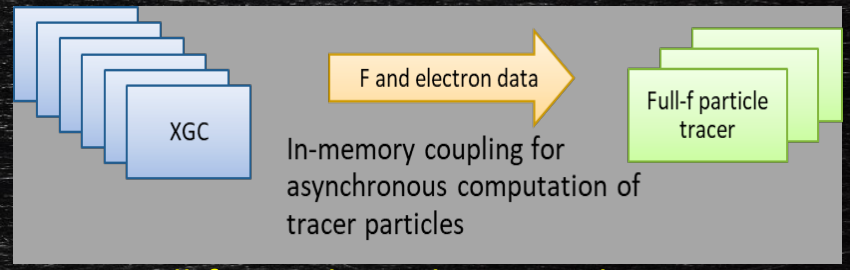
- This is a small D3D run case and quick test



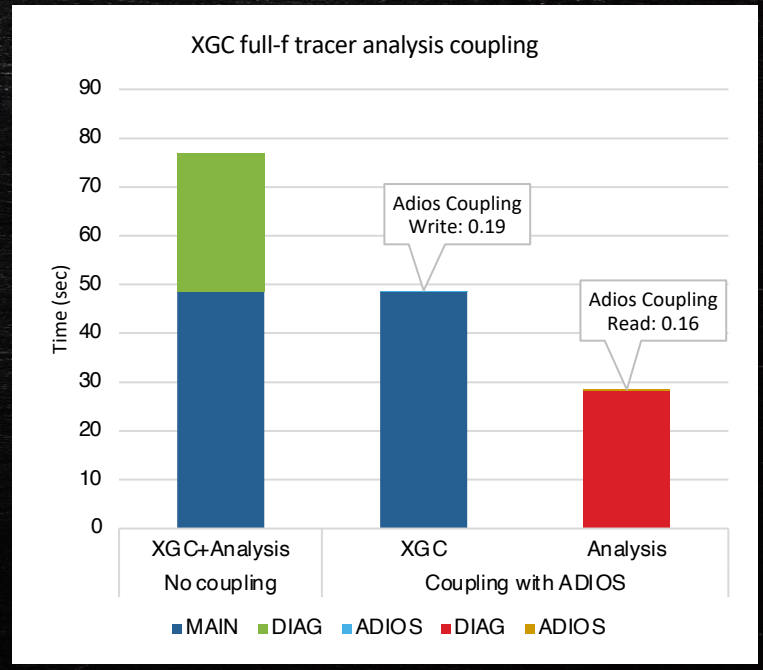


Staging use case: off-load non-scaling code part

- Tracer particle analysis enables understanding of the transport characteristics spanning the pedestal and scrape-off layer
- It is costly to perform and is communication-heavy
- Asynchronously stage data to the tracer particle analysis running on additional nodes
  - Coupled data size: f0(95 GB) + E_rho/pot_rho(1.4GB)
- Reduced 36% of the XGC iteration time by using asynchronous services (only 0.4% time-overhead for coupling data)



Full-f particle analysis coupling



Full-f coupling performance on Summit with ADIOS using 4/1024 extra nodes

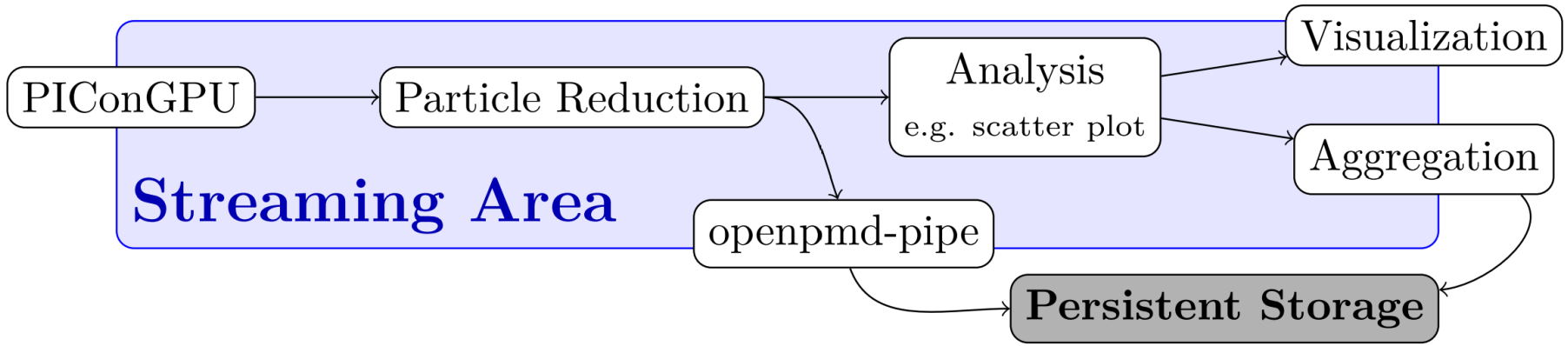
Choi, J. Y., Chang, C. S., Dominski, J., Klasky, Churchill, M., S., Merlo, G., Suchyta, E., ... & Wood, C. "Coupling exascale multiphysics applications: Methods and lessons learned". IEEE e-Science, 2018.

HBPS High-fidelity Boundary Plasma Simulation

How to get beyond the storage bandwidth limit

Staging performance

Vision: Loosely coupled data processing pipeline



→ Streaming I/O between application bypasses I/O bottleneck

Slides from Franz Poeschl at SMC21
Transitioning from file-based HPC workflows to streaming data pipelines with openPMD and ADIOS2

Staging performance: openPMD example

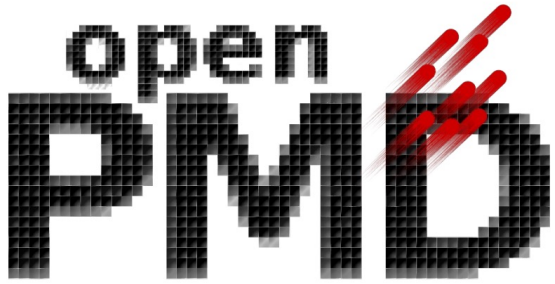
openPMD is *not* a file format but

- an object-oriented markup
- meta data naming convention

Self-describing, **data format agnostic** standard for **frictionless exchange** of **particle-mesh data**

Flagship implementation: **openPMD-api**:

- Describe particle-mesh data in a unified way
- API in C++ and Python (upcoming: Julia)
- Flexibly store to / read from interchangeable backends:
  - ADIOS1/2
  - HDF5
  - JSON (serial only)



https://github.com/openPMD/openPMD-standard

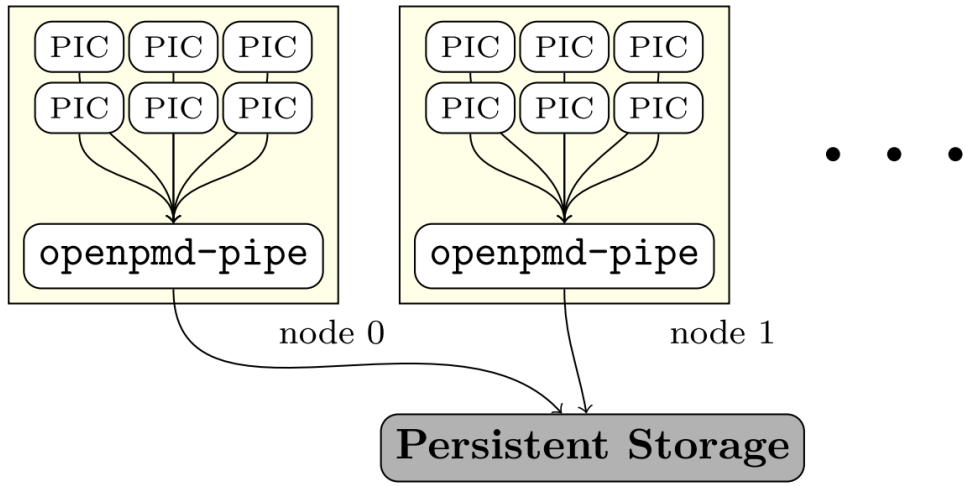
Staging performance

A simple use for streaming: Asynchronous I/O

A simple low-effort application for streaming:

- **Goal:** accelerate simulate-dump workflow
- **Assumption:** IO routines block other parts of the simulation
- **Solution:** Asynchronously launch a second application
  (`openpmd-pipe.py` – compare UNIX pipes)
  → Reads from stream, writes to disk
- **Effect:** Hides (not reduces!) disk IO times

No changes in the code required

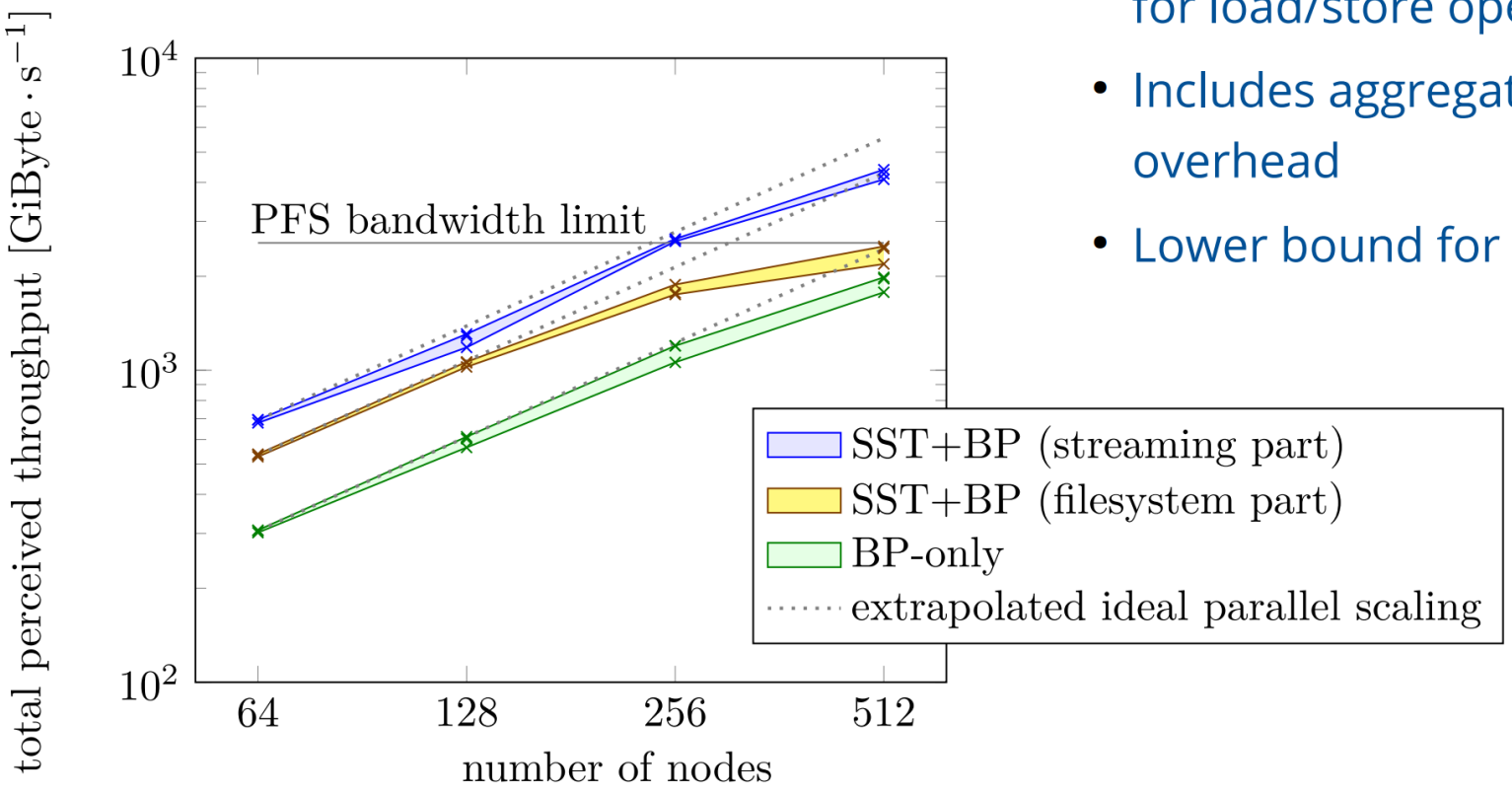


→ Compare this setup *(stream+file)* against regular BP output *(file-only)*

```
> openpmd-pipe.py --infile stream.sst --outfile dump.bp
```

Staging performance

High throughput of Infiniband Streaming on Summit

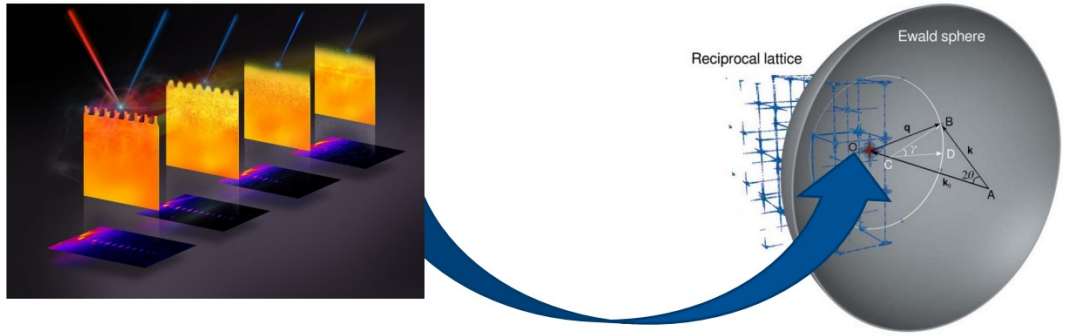


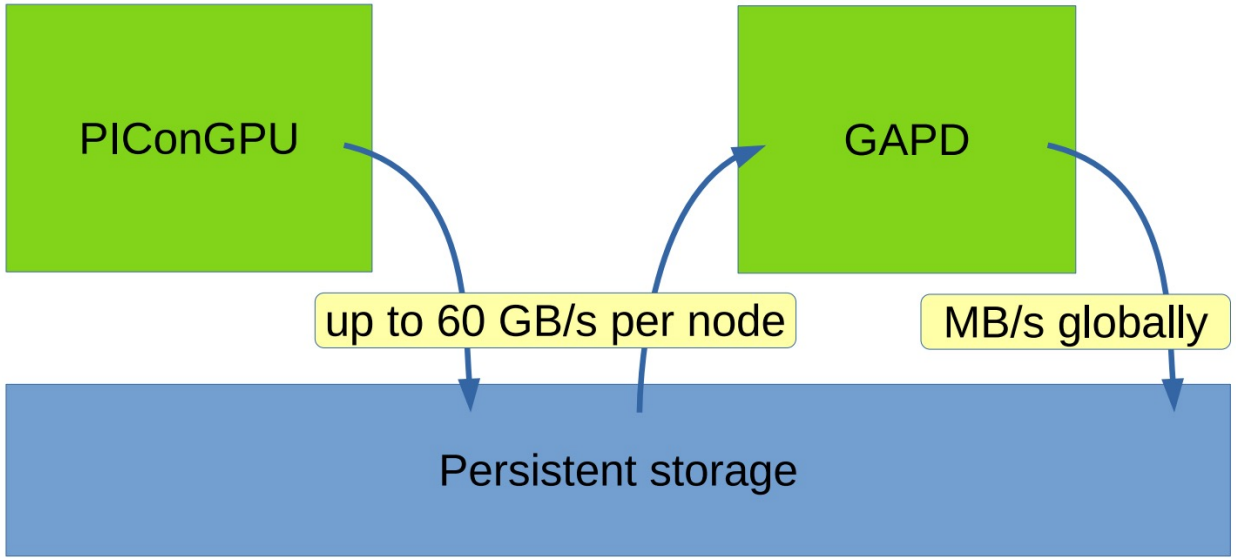
Perceived throughput:

- Based on time measured in application for load/store operation
- Includes aggregation and communication overhead
- Lower bound for precise throughput

Staging performance

Circumvent I/O bottleneck by loose coupling



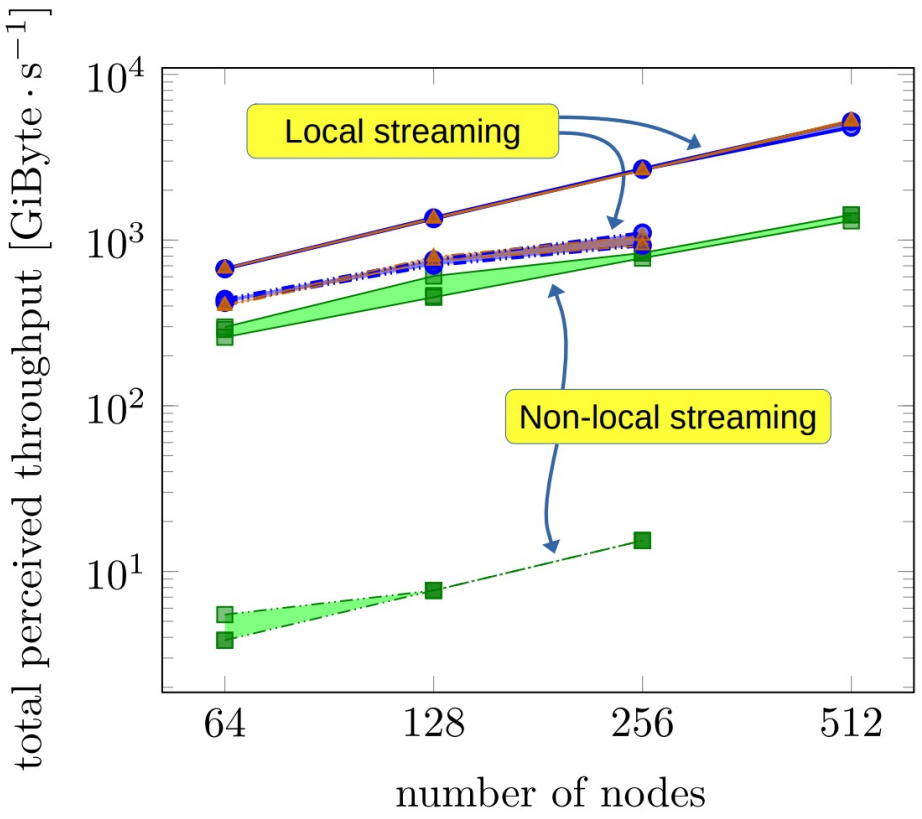


- Simulation pipeline: PIConGPU → GAPD
- Data description in openPMD is **independent of implementation**
- Use legacy, file-IO based implementations, but toggle a **streaming-aware backend**
- **GAPD**:
  Scattering analysis that relies only on particle data
  → Field data need not be sent
- Only **store the final result persistently**

J. C. E, L. Wang, S. Chen, Y. Y. Zhang and S. N. Luo. “GAPD: a GPU- accelerated atom-based polychromatic diffraction simulation code”. In: Journal of Synchrotron Radiation 25.2 (Mar. 2018), pp. 604–611.

Staging performance

For good throughput:
Local streaming patterns, Infiniband/RDMA



Local streaming:
Distribute data chunks only within a node (alternatively: to neighboring nodes)

Non-local streaming:
Distribute data chunks globally, optimize for balance and alignment

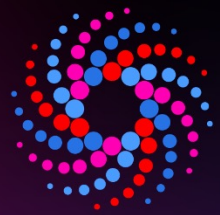
Straight lines:
Infiniband/RDMA

Dashed lines:
WAN/sockets

Takeaway:
- RDMA necessary for HPC
- Reasonable scaling with RDMA
- SST: no benefit from keeping communication strictly within a node
- SST: number of communication partners for each single instance decisive

Outline

- 8:30 Introduction to data management at extreme scale – Scott Klasky
- 9:15 ADIOS 2 concepts and API (C++, Python, F90) – Norbert Podhorszki
- 10:00 BREAK
- 10:30 ADIOS 2 API – Norbert Podhorszki
- 11:00 Hands on with ADIOS 2 – Files – Ana Gainaru
- 12:00 Lunch
- 1:30 ADIOS @ scale – Norbert Podhorszki
- 2:00 Introduction to Paraview + ADIOS + hands on Caitlin Ross
- 3:00 BREAK
- 3:30 Introduction to TAU and TAU + ADIOS – Kevin Huck
- 4:00 Hands on with TAU + ADIOS
- 4:15 Staging with ADIOS – hands 0n – Ana Gainaru
- 5:00 END



Paraview

SC'22 Dallas, TX Nov 2022

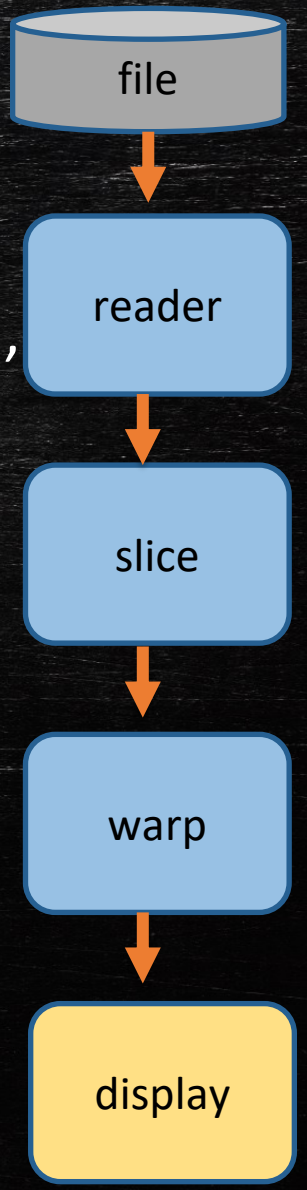
Caitlin Ross <caitlin.ross@kitware.com>

ParaView

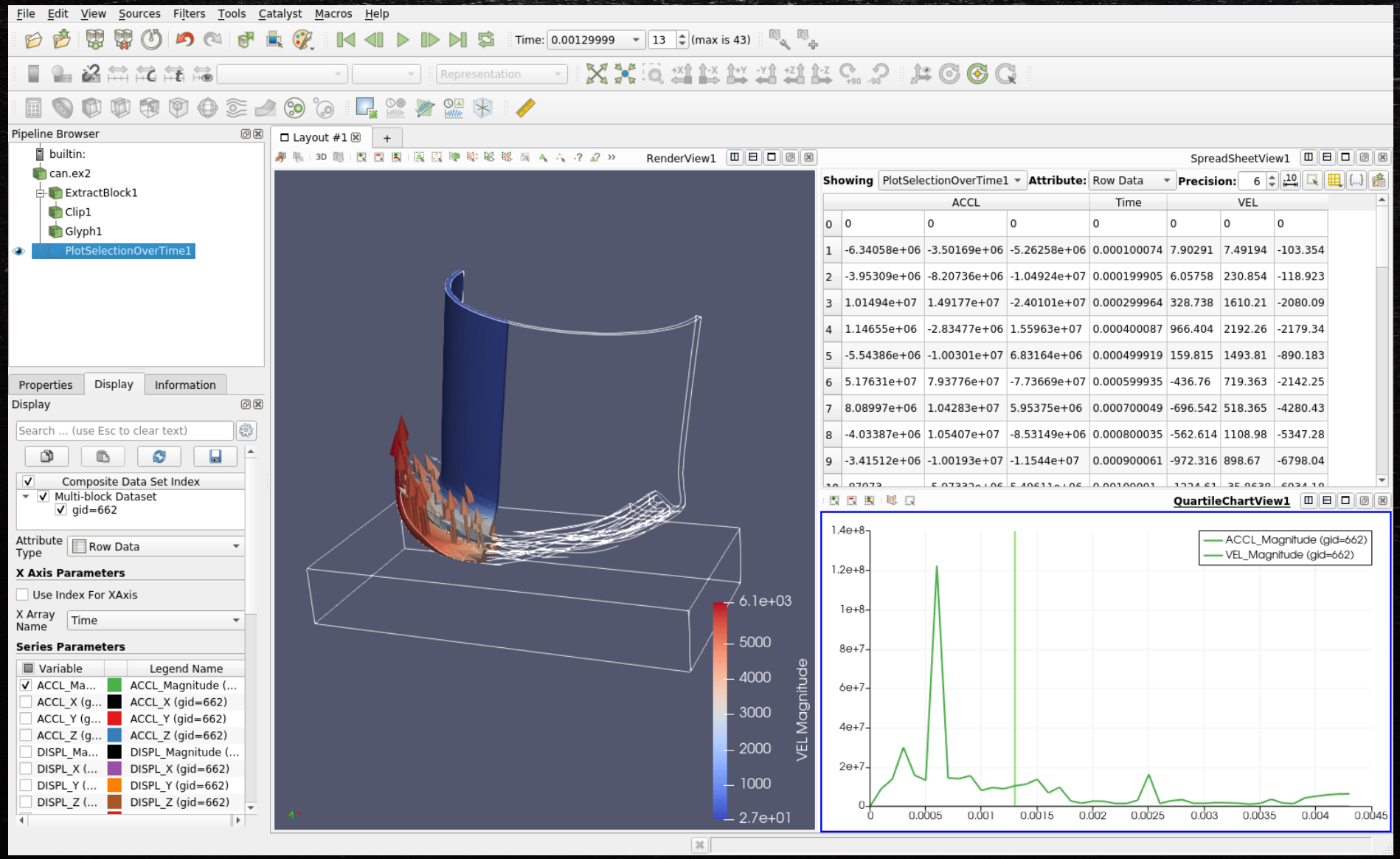
- Open-source software for visualization of large-scale scientific data
  - Supported by an active user and developer community
- Leverages parallel data processing and rendering to enable interactive visualization for extremely large datasets
  - Scales from laptops to supercomputers
  - Client/server: run the ParaView server on a supercomputer and connect the client on your laptop to it
- Can be extended and customized as necessary
- Supports scripting and batch processing using Python

ParaView's Visualization Pipeline

- Read in data
  - Many different file formats supported
  - Handles structured, unstructured, polygonal, graph, time-varying data,
- Build a pipeline to process your data
  - Choose from a number of different filters
  - Tune filter parameters
- Can save results in a variety of formats



ParaView User Interface



Python Scripting with ParaView

- Two Python APIs
  - Python wrapping allows direct access to proxies and their properties
  - paraview.simple module has helper methods that simplifies the API
    - from paraview.simple import *
- Why use Python scripting?
  - Running in batch mode
    - Set up your script on a small representative dataset locally
    - Then use the script on real data on supercomputer

Built-in Python Interpreters

- Shell in GUI
  - Can save trace of actions taken in GUI (e.g., setting up filters)
  - Visual feedback from running shell commands make it easiest place to learn ParaView's Python API
- pvpython
  - meant for interactive scripts
- pvbatch
  - For batch processing
  - Can be run in parallel with MPI
  - Cannot interact with it
- All three have the python path set automatically

Creating a Simple Visualization

- Create a cone
  - `>>> myCone = Cone()`
- Get docs on properties
  - `>>> help(myCone)`
- Examine a property
  - `>>> myCone.Center`
- Change a property
  - `>>> myCone.Center = [0, 0, 1]`
- Show the Result
  - `>>> Show(myCone)`
  - `>>> Render()`
- Add a filter
  - `>>> clip1 = Clip()`
- List properties
  - `>>> clip1.ListProperties()`
- Change a property
  - `>>> clip1.ClipType.Normal = [0,1,0]`
- Show the filter, hide the cone
  - `>>> Show(clip1)`
  - `>>> Hide(myCone)`
  - `>>> Render()`

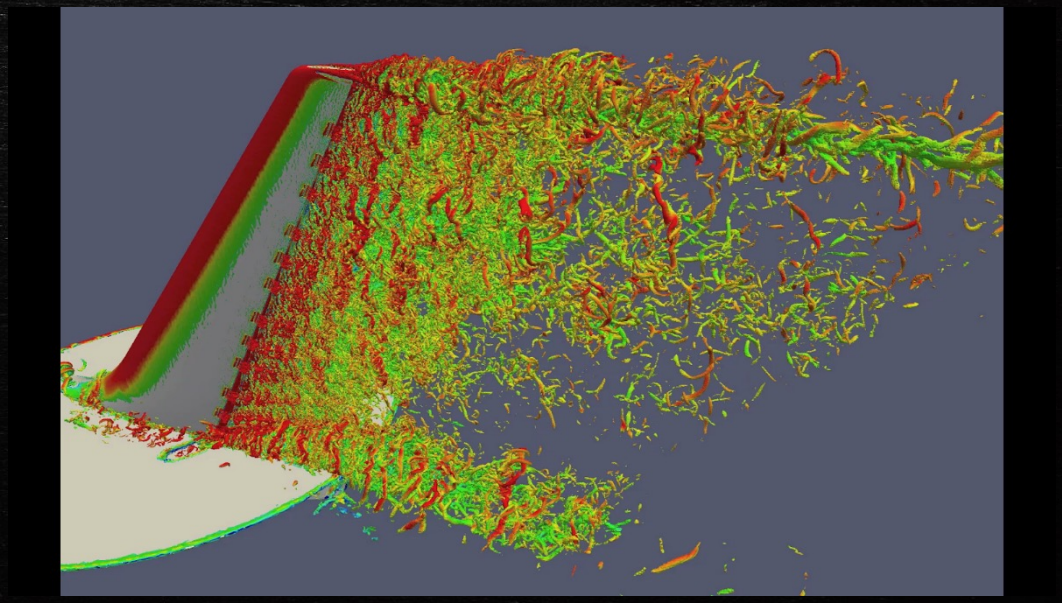
Post-hoc vs In situ analysis

- Post-hoc
  - Configure simulation
  - Run simulation
  - Wait for data
  - Analyze data
- Limitations
  - I/O bottleneck
  - Limited feedback before the end of simulation

- In situ
  - Configure simulation
  - Run simulation
  - Analyze data while results are in memory
  - Visualization/analysis output is smaller than raw data

ParaView Catalyst

- Provides in situ data analysis and visualization capabilities for ParaView
- Write a Python script with your pipeline and perform batch processing on each time step
- Can also connect to the simulation with Catalyst Live from the ParaView GUI for interactive in situ visualization
  - Can pause simulation to investigate
  - Then resume simulation



Catalyst Workflow

- Get representative data
  - First timestep or a toy case
- Set up the analysis in ParaView
- Export Python script
- Manually modify script as necessary
- Start Simulation

Catalyst 2.0 Features

- ABI Compatibility
  - Can build your simulation against the Catalyst2 stub library
    - Lightweight library, easy to build
    - At runtime can use the ParaView Catalyst implementation

Reading ADIOS data in ParaView with Fides

- ParaView contains a reader called Fides that can be used to load your ADIOS data
- Fides provides a schema for mapping ADIOS Variables to VTK-m ArrayHandles
- Data model described in JSON
  - Describe mesh and fields
  - No need to write adaptors
  - Don’t need to modify how ADIOS writes your data
- User guide: https://fides.readthedocs.io/

```
"VTK_Structured_Grid": {
  "data_sources": [{
    "name": "source",
    "filename_mode": "input" }],
  "coordinate_system" : {
    "array" : {
      "array_type" : "basic",
      "data_source": "source",
      "variable" : "points",
      "is_vector" : "true",
      "static" : true }},
  "cell_set": {
    "cell_set_type" : "structured",
      "dimensions" : {
        "source" : "variable_dimensions",
        "data_source": "source",
        "variable" : "density" }},
  "fields": [{
      "name": "density",
      "association": "points",
      "array" : {
        "array_type" : "basic",
        "data_source": "source",
        "variable" : "density" }}]}
```

Fides Schema

```
"data_sources": [{
  "name": "source",
  "filename_mode": "input" }],
```

- Specify one or more **data_sources**
  - Each data source is an ADIOS file/stream
  - **name** lets you refer to it elsewhere in the data model
  - **filename_mode** should be set to “input” in most cases
- Supports multiple sources may be used
  - e.g., the mesh may be written to one file and fields written to another

Fides Schema

- **coordinate_system** and **cell_set** define the mesh
  - Can specify the mesh arrays are **static**, so Fides will cache the mesh details and not read it on every time step
  - **data_source** points back to a defined data source
  - **variable** is the name of the ADIOS variable
- **coordinate_system**
  - Can be **basic**, **uniform_point_coordinates**, or **cartesian_product**
- **cell_set**
  - Can be **structured**, **explicit**, or **single_type**

```
"coordinate_system" : {
  "array" : {
    "array_type" : "basic",
    "data_source": "source",
    "variable" : "points",
    "is_vector" : "true",
    "static" : true }},
"cell_set": {
  "cell_set_type" : "structured",
    "dimensions" : {
      "source" : "variable_dimensions",
      "data_source": "source",
      "variable" : "density" }},
```

Fides Schema

```
"fields": [{
    "name": "density",
    "association": "points",
    "array" : {
      "array_type" : "basic",
      "data_source": "source",
      "variable" : "density" }}]}
```

- **fields**
  - specify any ADIOS variables you would like read as field data
  - **association** should be either “points” or “cells”
  - array_type will usually be “basic”, but there are some other options to support special cases such as the XGC simulation
  - **variable** is the name of the ADIOS Variable, while name can be a different **name** if you prefer

Fides Schema

- It's also possible to add some ADIOS Attributes with metadata and Fides will generate the data model for you
- For instance, if you have a uniform grid, you can specify the following attributes
  - **Fides_Data_Model**: "uniform"
  - **Fides_Origin**: [x, y, z]
  - **Fides_Spacing**: [x, y, z]
- For fields, it's also possible to use wildcard fields, so you don't have to specify every field
  - **Fides_Variable_List**: vector of variable names
  - **Fides_Variable_Associations**: vector of variable associations

```
"fields": [
    {
        "variable_list_attribute_name": "Fides_Variable_List",
        "variable_association_attribute_name": "Fides_Variable_Associations",
        "array": {
            "array_type": "basic",
            "data_source": "source",
            "variable": ""
        }
    }
]
```

Fides and ParaView Catalyst

- As of ParaView 5.11, the Fides reader has been integrated into ParaView Catalyst
- To use this feature, use the ADIOS engine plugin ParaViewADIOSInSituEngine
  - To get the engine plugin, build ADIOS with the Catalyst stub library: https://gitlab.kitware.com/paraview/catalyst
  - This engine plugin is used like other ADIOS engines
  - No need to instrument your code with calls to the Catalyst API – this engine handles that for you

Resources

- ParaView
  - User Guide: https://docs.paraview.org/en/latest/
  - Self-directed tutorial: https://docs.paraview.org/en/latest/Tutorials/index.html
  - Forum: https://discourse.paraview.org/
- Fides
  - User Guide: https://fides.readthedocs.io/en/latest/
  - Using Fides with ParaView: https://fides.readthedocs.io/en/latest/paraview/paraview.html

Configure the environment

```
$ cd ~/adios2-tutorial-source
$ source ~/adios2-tutorial-source/adios2-tutorial-env.sh
$ cd ~/adios2-tutorial-source/ADIOS2-Examples/build/install/share/adios2-examples/gray-scott
```

- ParaView is in PATH, so you can open by just typing paraview

Hands-on Demo: Visualizing Gray Scott with ParaView (Post-hoc)

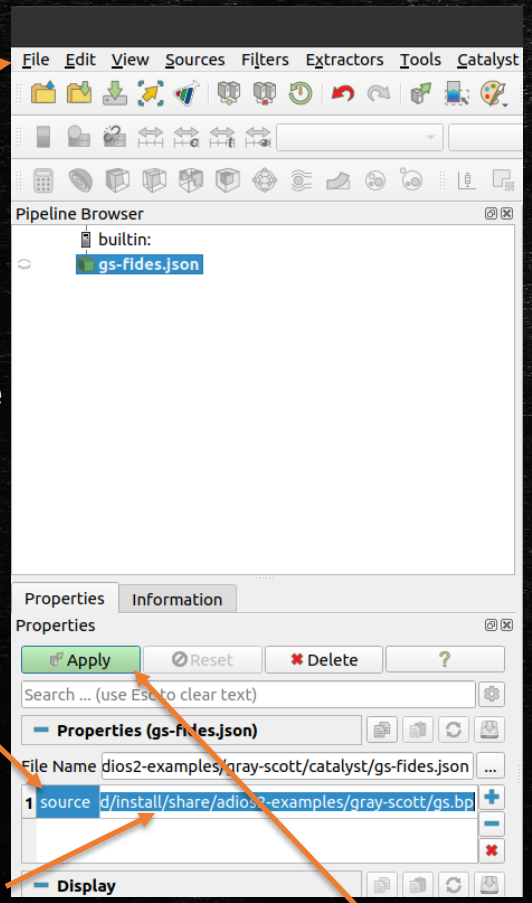
- Opening BP file with a Fides JSON data model file

1. Open JSON file

2. Add data source name from JSON file

```
"VTK-Cartesian-grid": {
  "data_sources": [
    {
    "name": "source",
    "filename_mode": "input"
    }
  ],
```

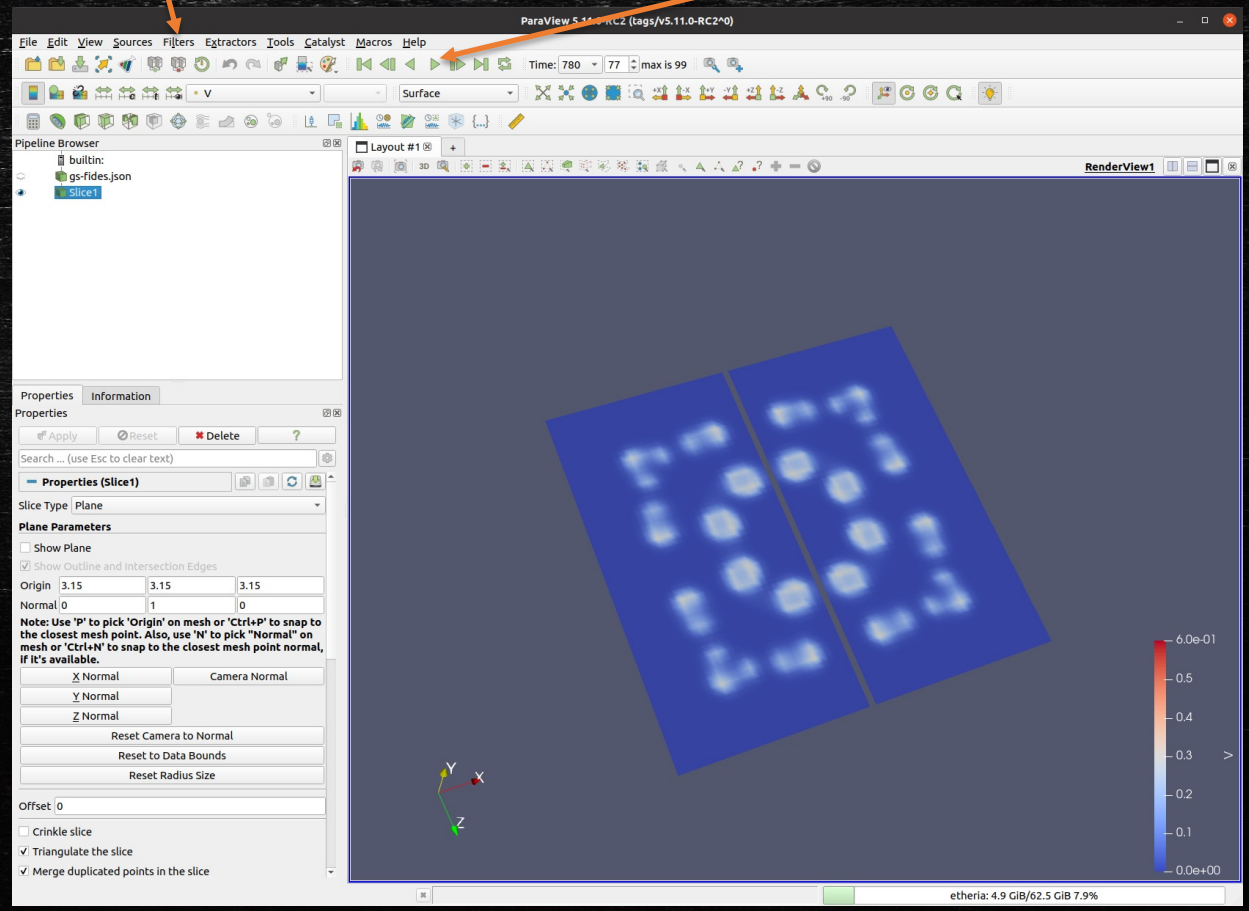
3. Add path to bp file



4. Click ”Apply”

5. Add desired filters

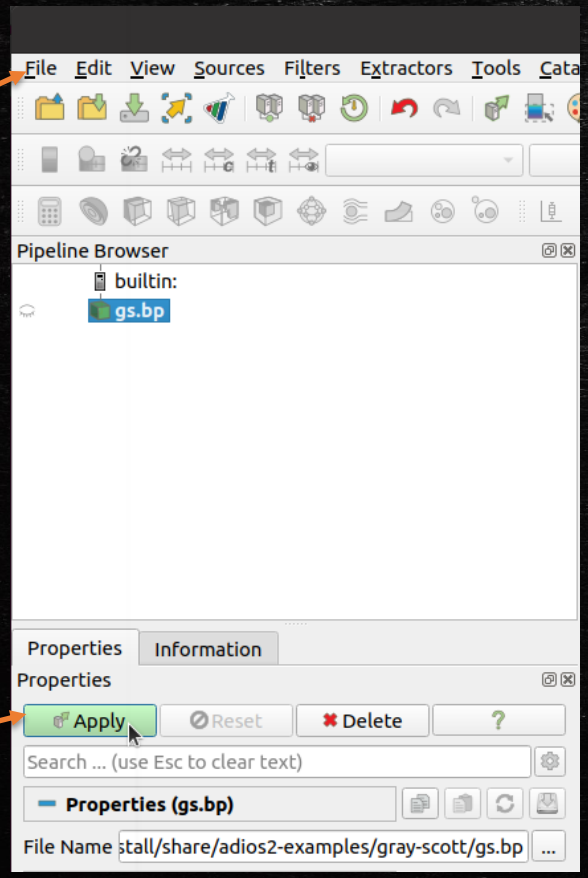
6. Play animation



Hands-on Demo: Visualizing Gray Scott with ParaView (Post-hoc)

- Easier approach: Opening BP file directly

1. Open BP file



2. Click ”Apply”

3. Can now add filters, play animation, etc

- Requires writing Fides metadata in ADIOS attributes
- From simulation/writer.cpp constructor:

```
// add attributes for Fides
io.DefineAttribute<std::string>("Fides_Data_Model", "uniform");
double origin[3] = {0.0, 0.0, 0.0};
io.DefineAttribute<double>("Fides_Origin", &origin[0], 3);
double spacing[3] = {0.1, 0.1, 0.1};
io.DefineAttribute<double>("Fides_Spacing", &spacing[0], 3);
io.DefineAttribute<std::string>("Fides_Dimension_Variable", "U");

std::vector<std::string> varList = {"U", "V"};
std::vector<std::string> assocList = {"points", "points"};
io.DefineAttribute<std::string>("Fides_Variable_List", varList.data(), varList.size());
io.DefineAttribute<std::string>("Fides_Variable_Associations", assocList.data(), assocList.size());
```

```
[tutorial@ip-172-31-37-244 gray-scott]$ bpls gs.bp/ -Ad
  double   Du                              attr   = 0.2
  double   Dv                              attr   = 0.1
  double   F                               attr   = 0.01
  string   Fides_Data_Model                attr   = "uniform"
  string   Fides_Dimension_Variable        attr   = "U"
  double   Fides_Origin                    attr   = {0, 0, 0}
  double   Fides_Spacing                   attr   = {0.1, 0.1, 0.1}
  string   Fides_Variable_Associations     attr   = {"points", "points"}
  string   Fides_Variable_List             attr   = {"U", "V"}
```

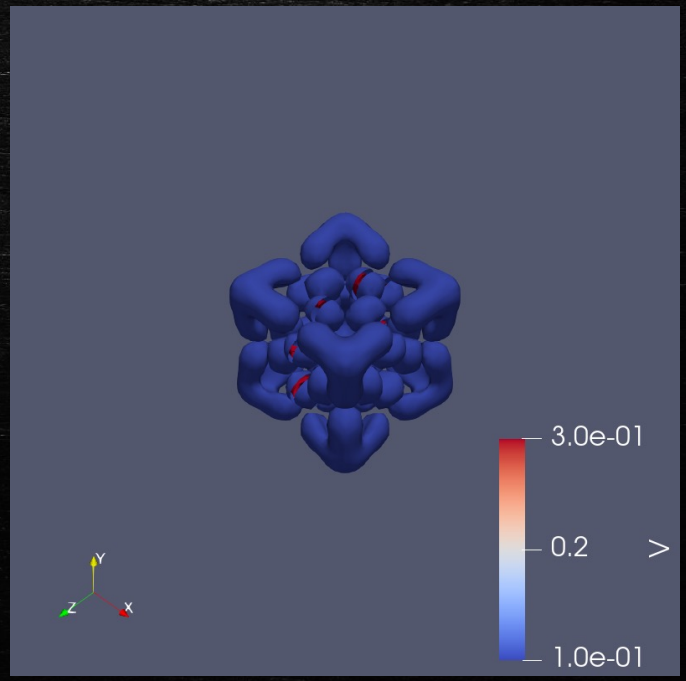
Hands-on Demo: Visualizing Gray Scott with ParaView (Post-hoc)

- Batch visualization with a Python script (not using the GUI)
- Run:

$ mpirun -n 2 pvbatch --force-offscreen-rendering catalyst/gs-pipeline.py –j catalyst/gs-fides.json –b gs.bp

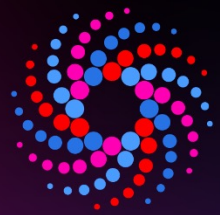
- You'll see output-XXXXX.png files in the directory

```
at 11:27:45 with caitlin.ross in share/adios2-examples/gray-scott took 22s
→ ls
adios2-fides-staging.xml  output-00014.png  output-00038.png  output-00062.png  output-00086.png
adios2-inline-plugin.xml  output-00015.png  output-00039.png  output-00063.png  output-00087.png
adios2.xml                output-00016.png  output-00040.png  output-00064.png  output-00088.png
catalyst                  output-00017.png  output-00041.png  output-00065.png  output-00089.png
ckpt.bp                   output-00018.png  output-00042.png  output-00066.png  output-00090.png
cleanup.sh                output-00019.png  output-00043.png  output-00067.png  output-00091.png
datasets                  output-00020.png  output-00044.png  output-00068.png  output-00092.png
decomp.py                 output-00021.png  output-00045.png  output-00069.png  output-00093.png
gs.bp                     output-00022.png  output-00046.png  output-00070.png  output-00094.png
gsplot.py                 output-00023.png  output-00047.png  output-00071.png  output-00095.png
output-00000.png          output-00024.png  output-00048.png  output-00072.png  output-00096.png
output-00001.png          output-00025.png  output-00049.png  output-00073.png  output-00097.png
output-00002.png          output-00026.png  output-00050.png  output-00074.png  output-00098.png
output-00003.png          output-00027.png  output-00051.png  output-00075.png  output-00099.png
output-00004.png          output-00028.png  output-00052.png  output-00076.png  pdfplot.py
output-00005.png          output-00029.png  output-00053.png  output-00077.png  README.md
output-00006.png          output-00030.png  output-00054.png  output-00078.png  settings-files.json
output-00007.png          output-00031.png  output-00055.png  output-00079.png  settings-inline.json
output-00008.png          output-00032.png  output-00056.png  output-00080.png  settings-staging.json
output-00009.png          output-00033.png  output-00057.png  output-00081.png  visit-bp4.session
output-00010.png          output-00034.png  output-00058.png  output-00082.png  visit-bp4.session.gui
output-00011.png          output-00035.png  output-00059.png  output-00083.png  visit-sst.session
output-00012.png          output-00036.png  output-00060.png  output-00084.png  visit-sst.session.gui
output-00013.png          output-00037.png  output-00061.png  output-00085.png
```



Outline

- 8:30 Introduction to data management at extreme scale – Scott Klasky
- 9:15 ADIOS 2 concepts and API (C++, Python, F90) – Norbert Podhorszki
- 10:00 BREAK
- 10:30 ADIOS 2 API – Norbert Podhorszki
- 11:00 Hands on with ADIOS 2 – Files – Ana Gainaru
- 12:00 Lunch
- 1:30 ADIOS @ scale – Norbert Podhorszki
- 2:00 Introduction to Paraview + ADIOS + hands on Caitlin Ross
- 3:00 BREAK
- 3:30 Introduction to TAU and TAU + ADIOS – Kevin Huck
- 4:00 Hands on with TAU + ADIOS
- 4:15 Staging with ADIOS – hands 0n – Ana Gainaru
- 5:00 END



The TAU Performance System

Kevin Huck, Sameer Shende, Allen Malony

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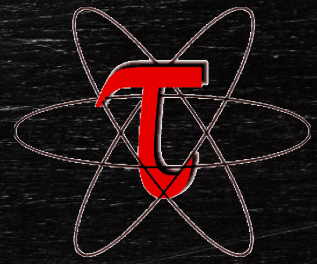
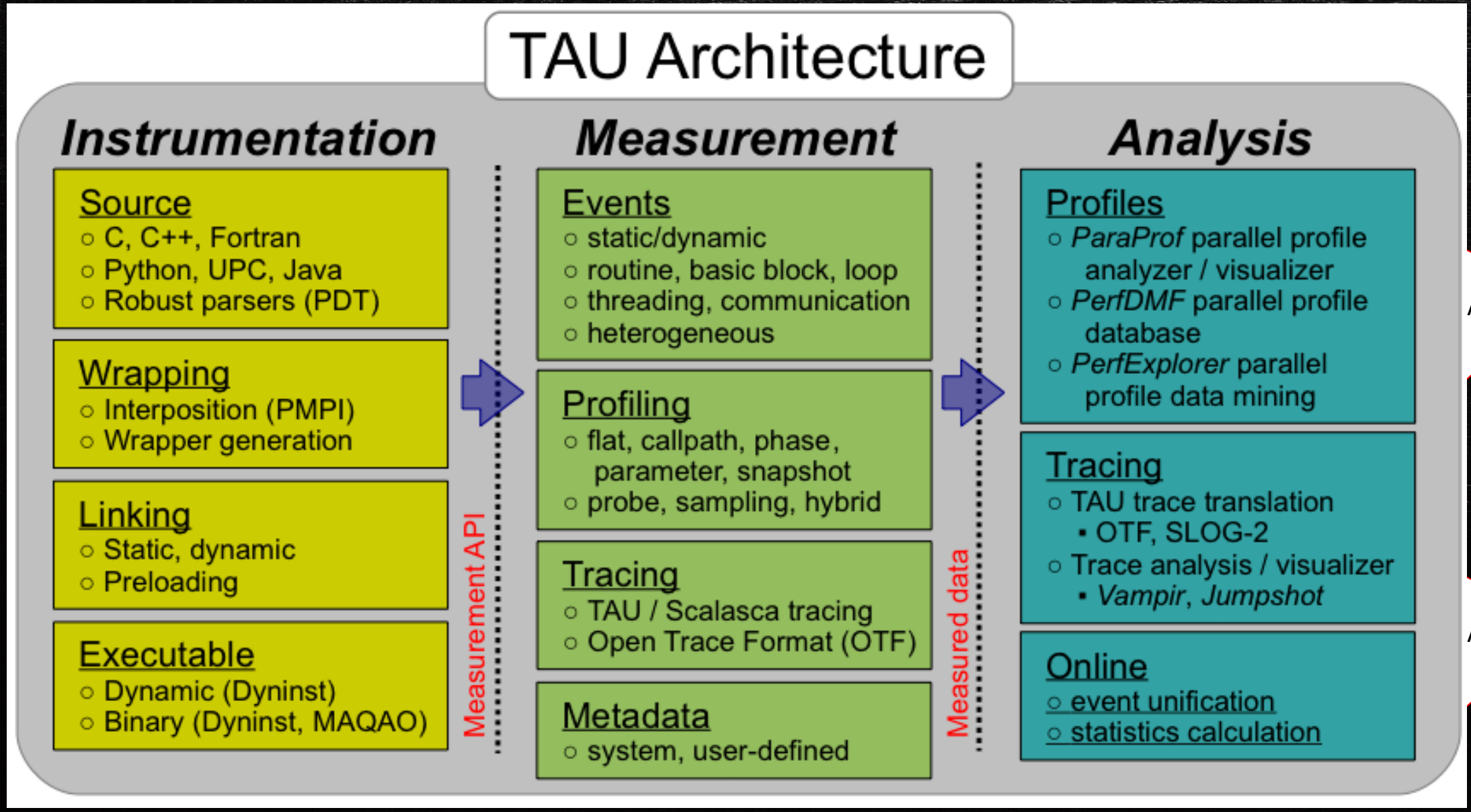
http://tau.uoregon.edu

TAU : brief overview



- Tuning and Analysis Utilities (28+ year project)
- Integrated performance toolkit:
  - Multi-level performance instrumentation
  - Highly configurable
  - Widely ported performance profiling / tracing system
  - Portable (java, python) visualization / exploration / analysis tools
- Supports all major HPC programming models
  - MPI/SHMEM, OpenMP/ACC, CUDA, HIP, OneAPI, Kokkos...

TAU : brief overview

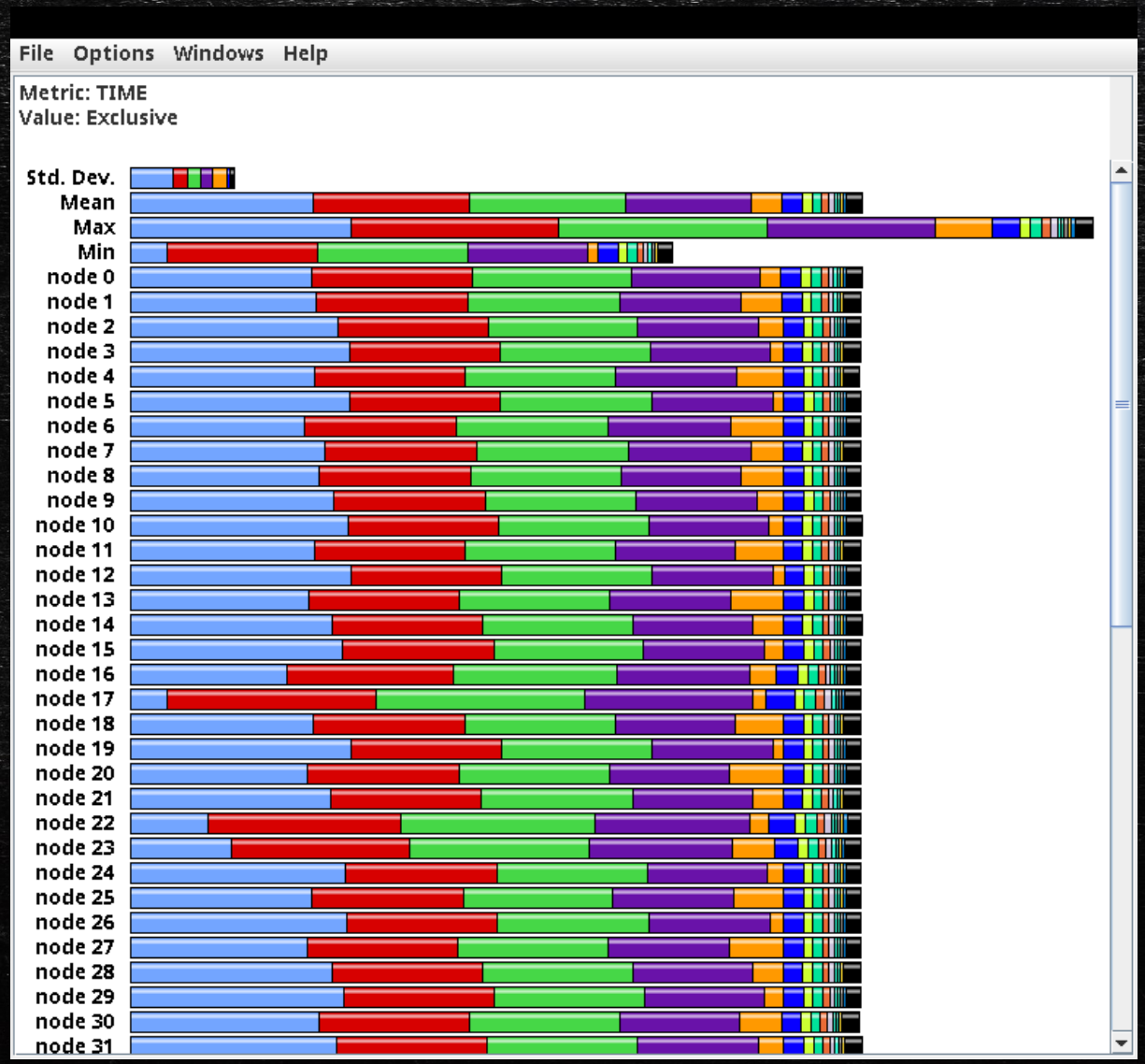


New!
ADIOS2
BP4

New!
ADIOS2
SST

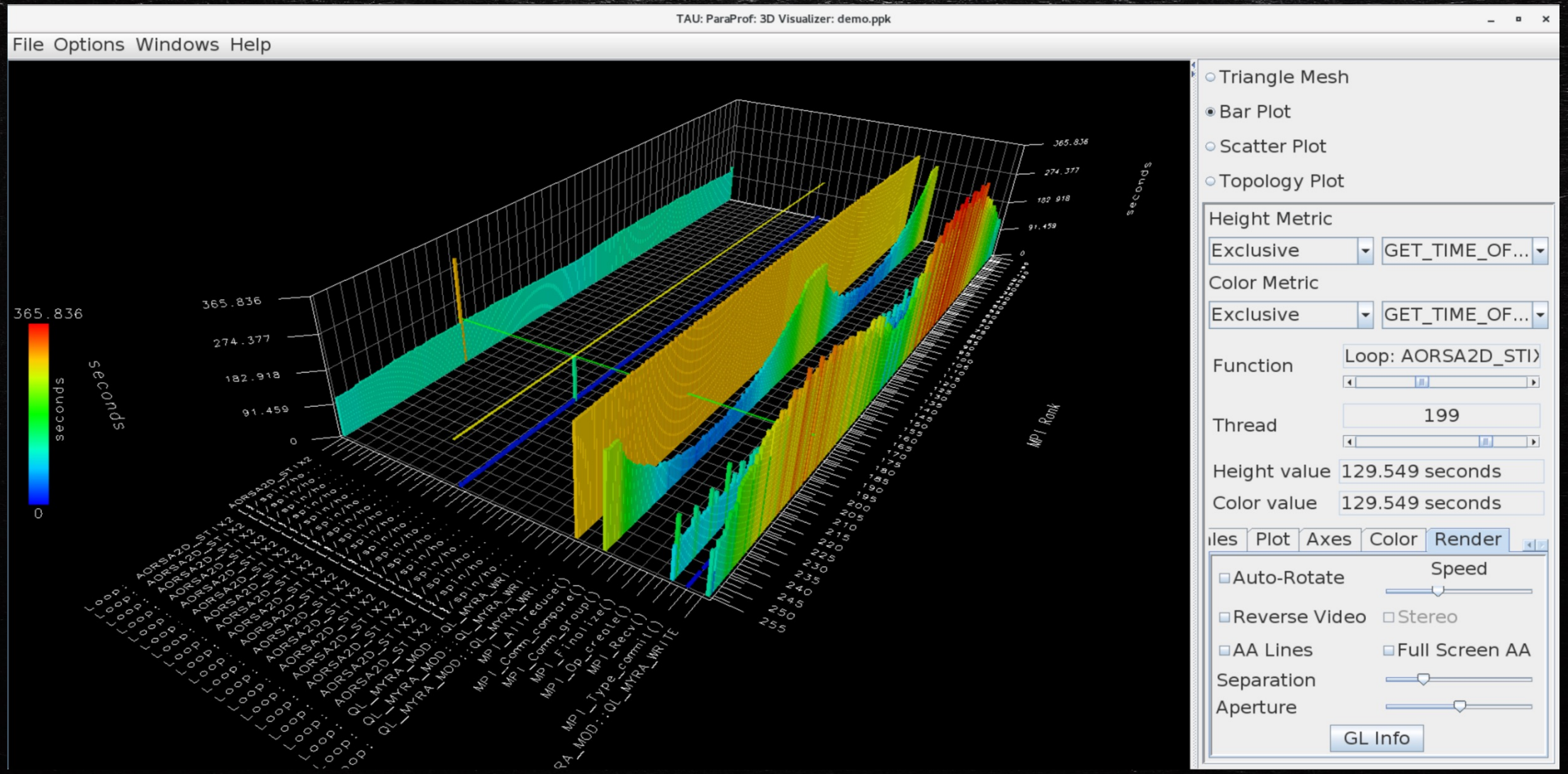
ParaProf Profile Browser

```
% paraprof
```

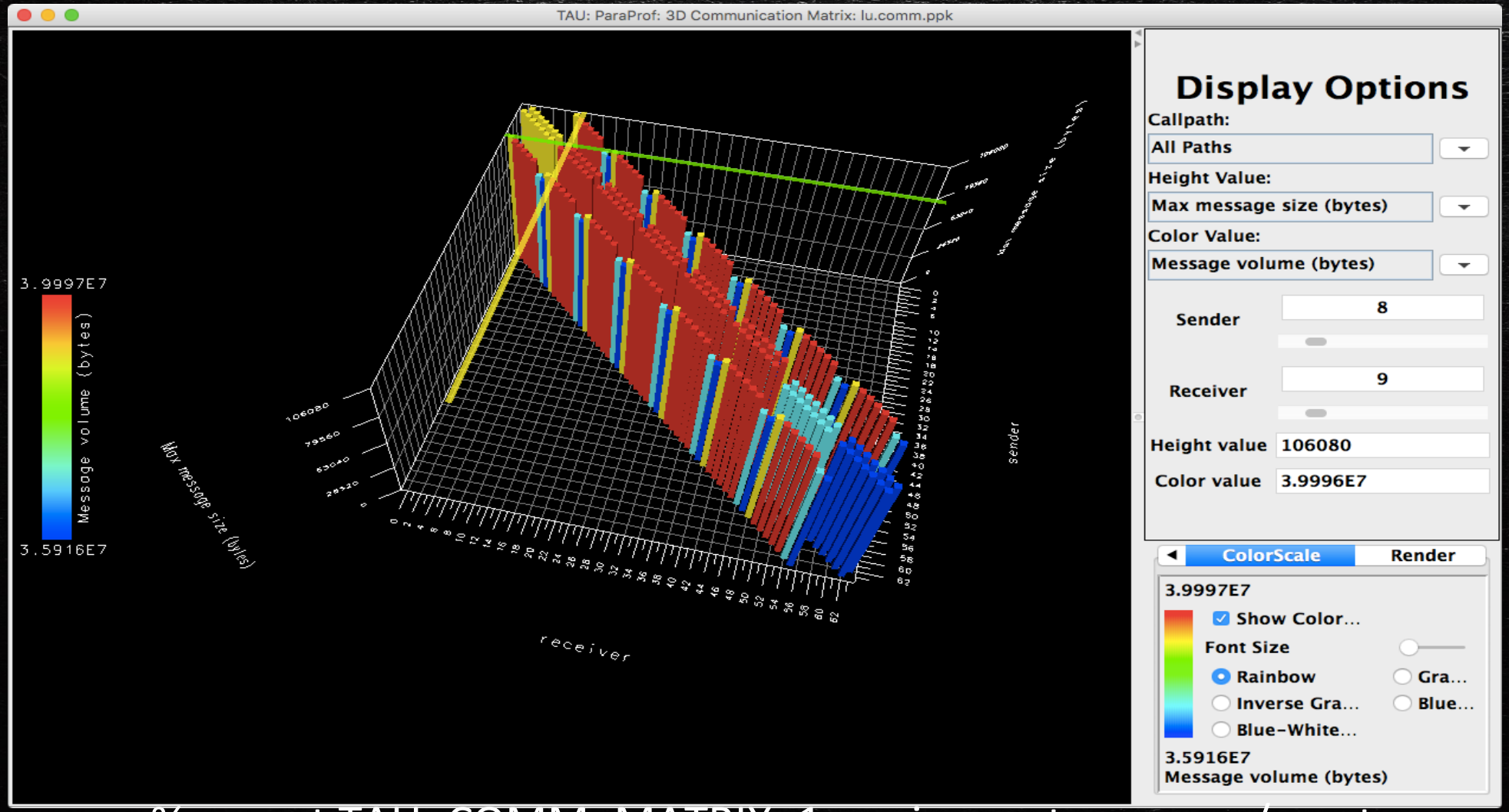


Each line is a different process/thread of execution, each color is a different function

ParaProf 3D Profile Browser



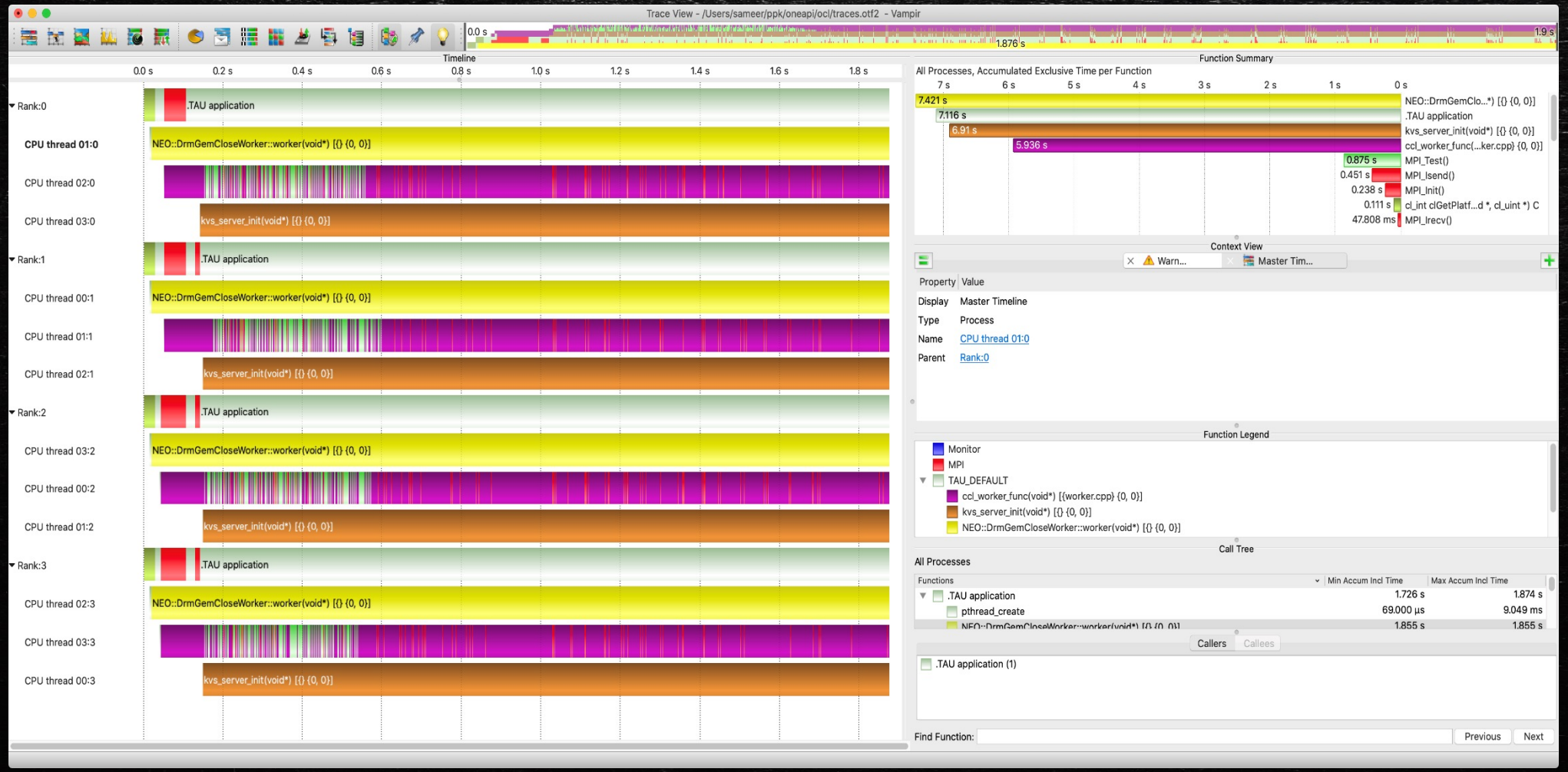
TAU – 3D Communication Window



% export TAU_COMM_MATRIX=1; mpirun … tau_exec ./a.out

% paraprof ; Windows -> 3D Communication Matrix

TAU and Vampir [TU Dresden]: Intel oneAPI OpenCL



% export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2

% mpirun –np 4 tau_exec –T level_zero –opencl ./a.out

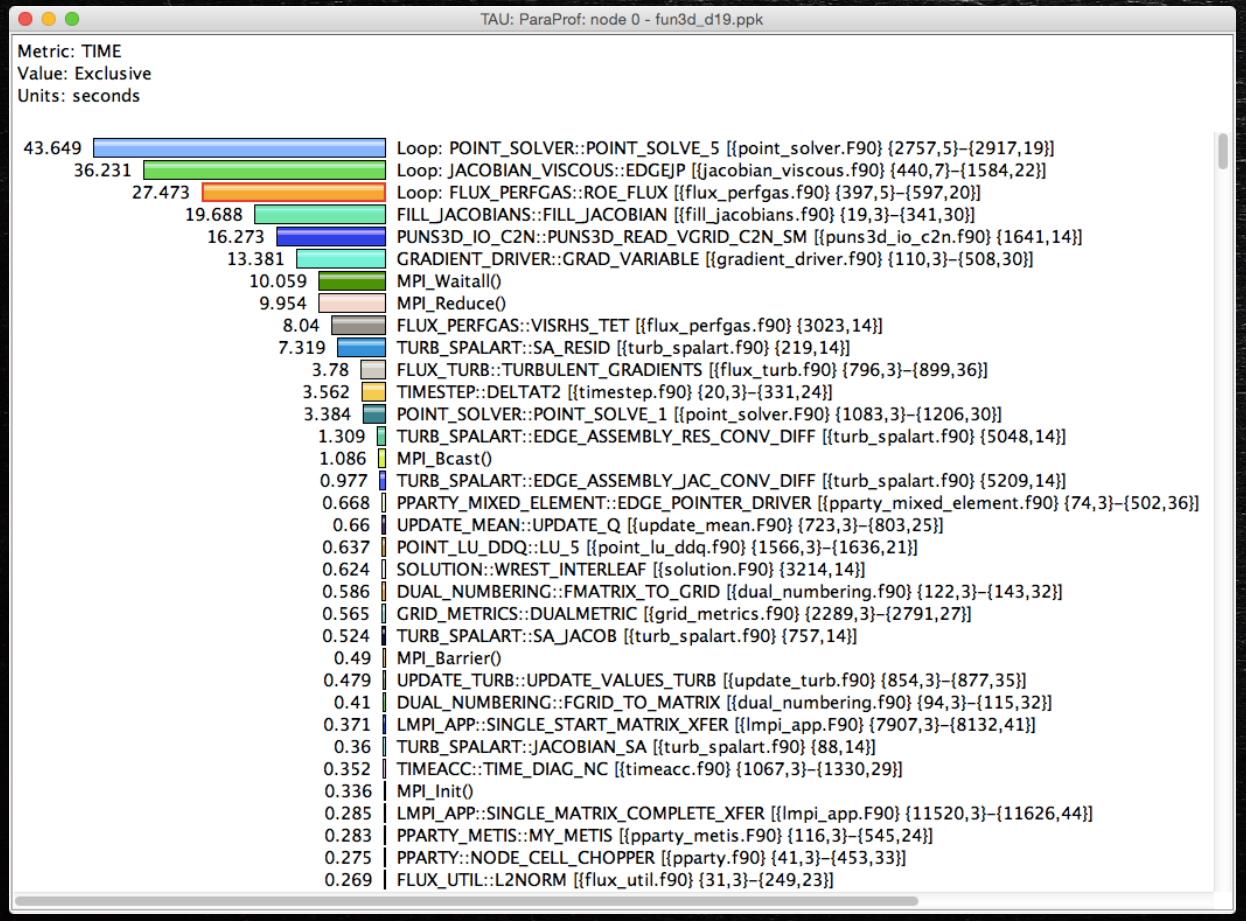
Performance Measurement

- **Timers**
  - Requires instrumentation of some kind
    - Manual, automated
    - Source, compiler provided, binary
    - Library callbacks, API wrappers, weak symbol replacement
  - Simple to implement
- **Sampling**
  - Requires specialized system libraries / support
    - Periodic signals, signal handler
  - No modification to executable/library needed
  - Potential to interfere with system support (signal handlers)

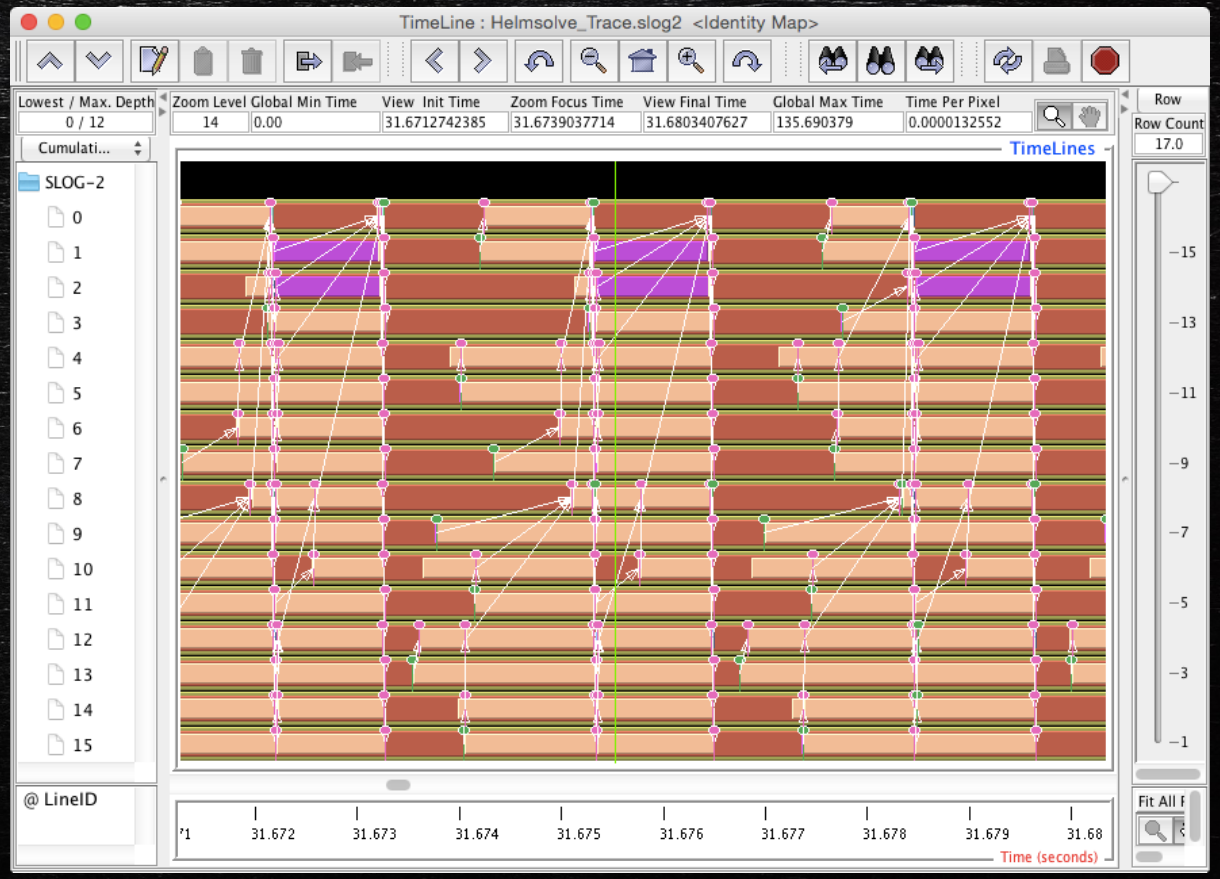
Profiling and Tracing

- **Profiling**: how much time was spent in each measured function on each thread in each process?
  - Collapses the time axis
  - No ordering or causal event information
  - Small summary per thread/process, regardless of execution time – only grows with number of timers & threads/processes
- **Tracing**: record all function entry & exit events on a timeline
  - Detailed view of what happened
  - The longer the program runs, the bigger the trace

Profiling and Tracing



Profiling shows you **how much** (total) time was spent in each routine



Tracing shows you **when** the events take place on a timeline

Integrating TAU

Compile Time

- Compile with TAU compiler wrappers (see next slides)
- Link with TAU libraries

Runtime

- Execute with `tau_exec`
- Preloads the TAU shared object library and instantiates measurement support for different models
- More later…

Instrumentation Approaches

- Manual
  - Add TAU API calls to the code by hand: https://www.cs.uoregon.edu/research/tau/docs/newguide/bk05rn01.html
- Automated:
  - PDT – optional TAU configuration
  - Compiler based instrumentation – comes with TAU
  - LLVM plugin – comes with TAU
  - Binary instrumentation - using Dyninst, PIN, or MAQAO
    - Optional TAU configuration, not covered in this tutorial
- PerfStubs API: https://github.com/UO-OACISS/perfstubs

Sampling

- Run the application with `tau_exec -ebs`
  - Preloads the TAU library, instantiates a signal handler and periodic interrupt to process the signal
  - The signal handler will record the current instruction pointer, all requested metrics, and optionally unwind the callstack
  - At the end of execution, all addresses are resolved to symbols in the application using binutils/libdwarf
- Some things that help:
  - For best support, build application with debug (-g) - all other optimizations are fine

Using TAU's Runtime Preloading Tool: tau_exec

- <mpirun> `tau_exec -T` <config> <options> <executable>
- `tau-config --list-matching` <mpi/serial> will show available configs
- Preload a wrapper that intercepts the runtime calls and substitutes with another (using dlsym() or weak symbol replacement)
  - MPI
  - OpenMP
  - POSIX I/O
  - Memory allocation/deallocation routines
  - Wrapper library for an external package
- No modification to the binary executable
- Enable other TAU options (communication matrix, OTF2, event-based sampling)

Sampled Measurement

Instrumentation example:

```
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0          21        1,538           1           1    1538547 .TAU application
 98.6       0.078        1,517           1           9    1517236 int main(int, char **) C [{simple.c} {49,1}-{63,1}]
 97.1       1,494        1,494           1           0    1494336 void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}]
  1.3          20           20           3           0       6813 double **allocateMatrix(int, int) C [{simple.c} {10,1}-{17,1}]
  0.1           2            2           2           0       1129 void init(double **) C [{simple.c} {28,1}-{35,1}]
  0.0       0.125        0.125           3           0         42 void freeMatrix(double **, int) C [{simple.c} {19,1}-{25,1}]
```

Sampling example:

```
[khuck@instinct:~/src/tau2/examples/simple$ make
gcc    -g -O2  -no-pie -c simple.c -o simple.o
gcc    -g -O2  -no-pie  simple.o -o simple
[khuck@instinct:~/src/tau2/examples/simple$ tau_exec -T serial -ebs ./simple
c[9][9] = 367967744.000000
[khuck@instinct:~/src/tau2/examples/simple$ pprof -a | grep -v CONTEXT
Reading Profile files in profile.*

---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0       1,730        1,730           1           0    1730983 .TAU application
 84.9       1,469        1,469          49           0      30000 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {43}]
 13.9         240          240           8           0      30003 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {42}]
```

Both *more* and *less* information at the same time…

Sampled Measurement

```
khuck@instinct:~/src/tau2/examples/simple$ make
gcc    -g -O2  -no-pie -c simple.c -o simple.o
gcc    -g -O2  -no-pie  simple.o -o simple
khuck@instinct:~/src/tau2/examples/simple$ tau_exec -T serial -ebs ./simple
c[9][9] = 367967744.000000
khuck@instinct:~/src/tau2/examples/simple$ pprof -a | grep -v CONTEXT
Reading Profile files in profile.*

---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0       1,730       1,730           1           0    1730983 .TAU application
 84.9       1,469       1,469          49           0      30000 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {43}]
 13.9         240         240           8           0      30003 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {42}]
```

```
37 /* Perform matrix multiply */
38 void compute(double **a, double **b, double **c) {
39     int i,j,k;
40     for (i=0; i < SIZE; i++) {
41         for(j=0; j < SIZE; j++) {
42             for (k=0; k < SIZE; k++) {
43                 c[i][j] += a[i][k] * b[k][j];
44             }
45         }
46     }
47 }
```

14% spent here

85% spent here

Simple Transformation – loop inversion

```
37 /* Perform matrix multiply */
38 void compute(double **a, double **b, double **c) {
39     int i,j,k;
40     for (i=0; i < SIZE; i++) {
41         for(j=0; j < SIZE; j++) {
42             for (k=0; k < SIZE; k++) {
43                 c[i][j] += a[i][k] * b[k][j];
44             }
45         }
46     }
47 }
```

```
37 /* Perform matrix multiply */
38 void compute(double **a, double **b, double **c) {
39     int i,j,k;
40     for (i=0; i < SIZE; i++) {
41         for (k=0; k < SIZE; k++) {
42             for(j=0; j < SIZE; j++) {
43                 c[i][j] += a[i][k] * b[k][j];
44             }
45         }
46     }
47 }
```

Reduced from 1.73 seconds

```
khuck@instinct:~/src/tau2/examples/simple$ make
gcc    -g -O2  -no-pie -c simple.c -o simple.o
gcc    -g -O2  -no-pie  simple.o -o simple
khuck@instinct:~/src/tau2/examples/simple$ tau_exec -T serial -ebs ./simple
c[9][9] = 367967744.000000
khuck@instinct:~/src/tau2/examples/simple$ pprof -a | grep -v CONTEXT
Reading Profile files in profile.*

---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0          976          976           1           0     976578 .TAU application
 70.7          690          690          23           0      30001 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {43}]
 27.6          269          269           9           0      29997 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {42}]
```

Both together!

Timers

```
khuck@instinct:~/src/tau2/examples/simple$ tau_exec -T serial -ebs ./simple
c[9][9] = 367967744.000000
khuck@instinct:~/src/tau2/examples/simple$ pprof -a | grep -v CONTEXT
Reading Profile files in profile.*

---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0          18        1,611           1           1    1611909 .TAU application
 98.9       0.116        1,593           1           6    1593593 int main(int, char **) C [{simple.c} {49,1}-{63,1}]
 97.6       1,572        1,572           1           0    1572560 void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}]
 67.0       1,079        1,079          36           0      30000 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {43}]
 29.8         480          480          16           0      30000 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {42}]
  1.9          30           30           1           0      30018 [SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/libc-2.31.so
  1.2          18           18           3           0       6198 double **allocateMatrix(int, int) C [{simple.c} {10,1}-{17,1}]
  0.1           2            2           2           0       1161 void init(double **) C [{simple.c} {28,1}-{35,1}]
```

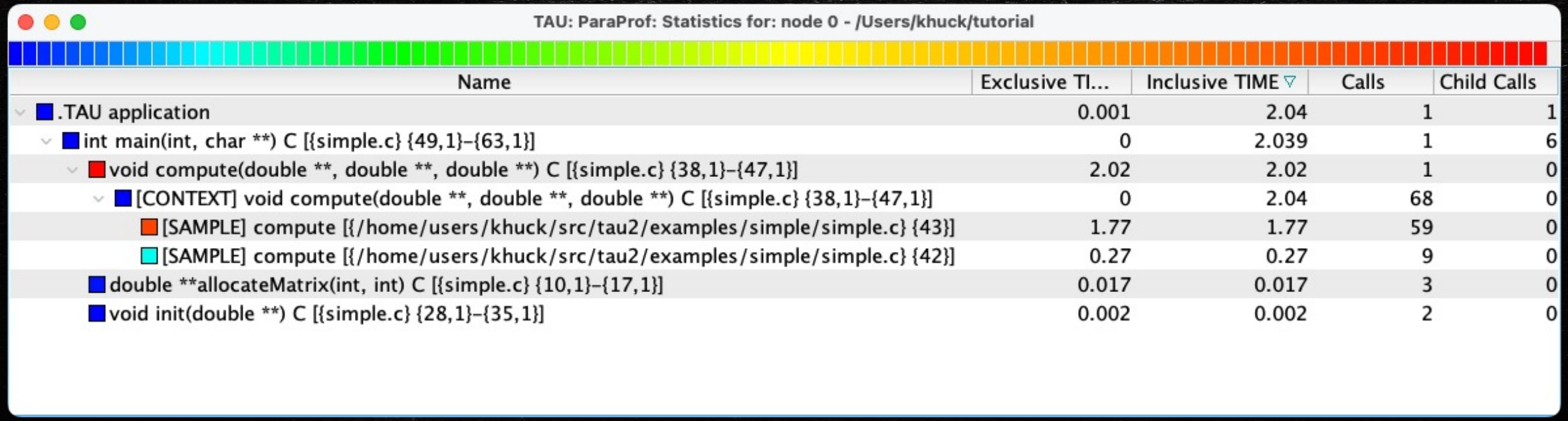
Samples

...with callpath profiling

```
khuck@instinct:~/src/tau2/examples/simple$ TAU_CALLPATH=1 TAU_CALLPATH_DEPTH=100 tau_exec -T serial -ebs ./simple
c[9][9] = 367967744.000000
khuck@instinct:~/src/tau2/examples/simple$ pprof -a
Reading Profile files in profile.*

NODE 0;CONTEXT 0;THREAD 0:
---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0           1        2,040           1           1    2040179 .TAU application
100.0           0        2,040          68           0      30000 .TAU application => int main(int, char **) C [{simple.c} {49,1}-{63,1}] => void compute(double **
, double **, double **) C [{simple.c} {38,1}-{47,1}] => [CONTEXT] void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}]
100.0           0        2,040          68           0      30000 [CONTEXT] void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}]
 99.9        0.15        2,038           1           6    2038709 .TAU application => int main(int, char **) C [{simple.c} {49,1}-{63,1}]
 99.9        0.15        2,038           1           6    2038709 int main(int, char **) C [{simple.c} {49,1}-{63,1}]
 99.0       2,019        2,019           1           0    2019510 .TAU application => int main(int, char **) C [{simple.c} {49,1}-{63,1}] => void compute(double **
, double **, double **) C [{simple.c} {38,1}-{47,1}]
 99.0       2,019        2,019           1           0    2019510 void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}]
 86.8       1,769        1,769          59           0      30000 .TAU application => int main(int, char **) C [{simple.c} {49,1}-{63,1}] => void compute(double **
, double **, double **) C [{simple.c} {38,1}-{47,1}] => [CONTEXT] void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}] => [SAMPLE] compute [{/
home/users/khuck/src/tau2/examples/simple/simple.c} {43}]
 86.8       1,769        1,769          59           0      30000 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {43}]
 13.2         270          270           9           0      30001 .TAU application => int main(int, char **) C [{simple.c} {49,1}-{63,1}] => void compute(double **
, double **, double **) C [{simple.c} {38,1}-{47,1}] => [CONTEXT] void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}] => [SAMPLE] compute [{/
home/users/khuck/src/tau2/examples/simple/simple.c} {42}]
 13.2         270          270           9           0      30001 [SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {42}]
  0.8          16           16           3           0       5562 .TAU application => int main(int, char **) C [{simple.c} {49,1}-{63,1}] => double **allocateMatri
x(int, int) C [{simple.c} {10,1}-{17,1}]
  0.8          16           16           3           0       5562 double **allocateMatrix(int, int) C [{simple.c} {10,1}-{17,1}]
  0.1           2            2           2           0       1182 .TAU application => int main(int, char **) C [{simple.c} {49,1}-{63,1}] => void init(double **) C
 [{simple.c} {28,1}-{35,1}]
  0.1           2            2           2           0       1182 void init(double **) C [{simple.c} {28,1}-{35,1}]
```

…easier to view in ParaProf



Name	Exclusive TI...	Inclusive TIME ▽	Calls	Child Calls
.TAU application	0.001	2.04	1	1
int main(int, char **) C [{simple.c} {49,1}-{63,1}]	0	2.039	1	6
void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}]	2.02	2.02	1	0
[CONTEXT] void compute(double **, double **, double **) C [{simple.c} {38,1}-{47,1}]	0	2.04	68	0
[SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {43}]	1.77	1.77	59	0
[SAMPLE] compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {42}]	0.27	0.27	9	0
double **allocateMatrix(int, int) C [{simple.c} {10,1}-{17,1}]	0.017	0.017	3	0
void init(double **) C [{simple.c} {28,1}-{35,1}]	0.002	0.002	2	0

Other measurement support

- Many programming models provide “hooks” for tools
- Often, instrumentation isn’t necessary!
  - **MPI**, SHMEM, Charm++
  - Pthreads, **OpenMP**, Kokkos
  - CUDA, **HIP/ROCm**, OneAPI, OpenACC, OpenCL, OpenMP offload
  - Python
  - Wrappers: POSIX, Chapel, UPC, memory, ARMCI, GASNet…
  - Java

Other TAU features

- Binary instrumentation
  - Dyninst, MAQAO, PIN
- Hardware counter support
  - PAPI, LIKWID
- Tracing support (native or converters)
  - Vampir (OTF2), Perfetto (JSON), Jumpshot (SLOG2), …
- Plugins
  - OS/HW monitoring, ADIOS2, SOS, Mochi, SQLite3, …

OpenMP

- https://www.openmp.org
- Pragma-based language extension to facilitate threading
- OpenMP 5.0 standard includes OpenMP Tools (OMPT/OMPD) specification for providing callbacks from the runtime to performance/debugging tools
- Provided by Intel, LLVM, IBM compilers
- GCC can use drop-in replacement (LLVM 8.0 runtime)
- TAU provides OPARI legacy support (when using PDT)

Adding OpenMP

```
37 /* Perform matrix multiply */
38 void compute(double **a, double **b, double **c) {
39     int i,j,k;
40 #pragma omp parallel for
41     for (i=0; i < SIZE; i++) {
42         for(j=0; j < SIZE; j++) {
43             for (k=0; k < SIZE; k++) {
44                 c[i][j] += a[i][k] * b[k][j];
45             }
46         }
47     }
48 }
```

If OMP_NUM_THREADS=4, SIZE=1024, then iteration space will be split into 4 of chunk size 256 each – 4x speedup

Compiling, Running, Reporting

```
khuck@instinct:~/src/tau2/examples/simple$ make
TAU_MAKEFILE=/storage/users/khuck/src/tau2/x86_64/lib/Makefile.tau-ompt-pdt-openmp tau_cc.sh -optShared -optQuiet -g -O2 -fopenmp  -no-pie -c simple.c -o simple.o
TAU_MAKEFILE=/storage/users/khuck/src/tau2/x86_64/lib/Makefile.tau-ompt-pdt-openmp tau_cc.sh -optShared -optQuiet -g -O2 -fopenmp  -no-pie  simple.o -o simple
khuck@instinct:~/src/tau2/examples/simple$ export OMP_NUM_THREADS=2
khuck@instinct:~/src/tau2/examples/simple$ ./simple
c[9][9] = 367967744.000000
khuck@instinct:~/src/tau2/examples/simple$ pprof -s -a
Reading Profile files in profile.*

FUNCTION SUMMARY (total):
---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0          18        1,787           2           2     893950 .TAU application
 97.2       1,738        1,738           2           1     869314 OpenMP_Implicit_Task
 50.3       0.078          899           1           9     899006 int main(int, char **) C [{simple.c} {50,1}-{64,1}]
 49.0           6          875           1           1     875235 void compute(double **, double **, double **) C [{simple.c} {38,1}-{48,1}]
 48.7       0.012          870           1           1     870224 OpenMP_Thread_Type_ompt_thread_worker
 48.6       0.131          868           1           1     868546 OpenMP_Parallel_Region compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {51, 0}]
  1.2          21           21           3           0       7012 double **allocateMatrix(int, int) C [{simple.c} {10,1}-{17,1}]
  0.1           2            2           2           0       1071 void init(double **) C [{simple.c} {28,1}-{35,1}]
  0.0       0.516        0.516           3           0        172 void freeMatrix(double **, int) C [{simple.c} {19,1}-{25,1}]
  0.0       0.012        0.012           1           0         12 OpenMP_Sync_Region_Barrier compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {51, 0}]

FUNCTION SUMMARY (mean):
---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0           9          893           1           1     893950 .TAU application
 97.2         869          869           1         0.5     869314 OpenMP_Implicit_Task
 50.3       0.039          449         0.5         4.5     899006 int main(int, char **) C [{simple.c} {50,1}-{64,1}]
 49.0           3          437         0.5         0.5     875235 void compute(double **, double **, double **) C [{simple.c} {38,1}-{48,1}]
 48.7       0.006          435         0.5         0.5     870224 OpenMP_Thread_Type_ompt_thread_worker
 48.6      0.0655          434         0.5         0.5     868546 OpenMP_Parallel_Region compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {51, 0}]
  1.2          10           10         1.5           0       7012 double **allocateMatrix(int, int) C [{simple.c} {10,1}-{17,1}]
  0.1           1            1           1           0       1071 void init(double **) C [{simple.c} {28,1}-{35,1}]
  0.0       0.258        0.258         1.5           0        172 void freeMatrix(double **, int) C [{simple.c} {19,1}-{25,1}]
  0.0       0.006        0.006         0.5           0         12 OpenMP_Sync_Region_Barrier compute [{/home/users/khuck/src/tau2/examples/simple/simple.c} {51, 0}]
```

Compiler flag to Enable OpenMP

Thread lifetime

Worker lifetime

Region

Synchronization

MPI Support

- MPI standard includes tool support
  - MPI_* functions are thin, weak wrappers around PMPI_* API
  - Tools create their own wrappers to replace them and intercept MPI calls
  - Tool library is preloaded or linked ahead of MPI library(ies)
  - Example:

```
int MPI_Barrier(MPI_Comm comm) {
    int returnVal;

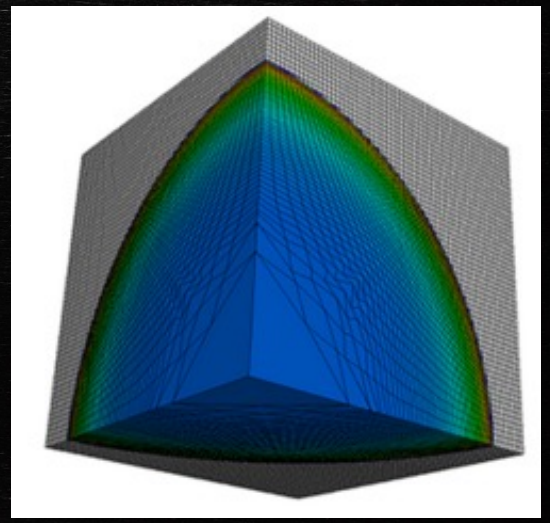
    TAU_PROFILE_TIMER(tautimer, "MPI_Barrier()",  " ", TAU_MESSAGE);
    TAU_PROFILE_START(tautimer);

    returnVal = PMPI_Barrier( comm );

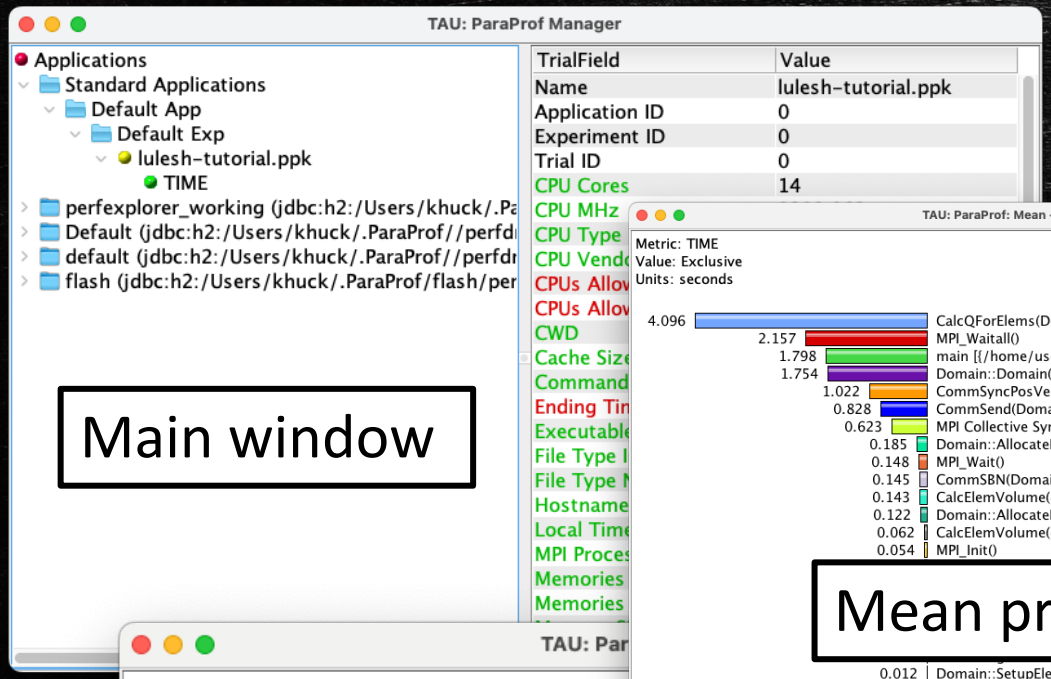
    TAU_PROFILE_STOP(tautimer);
    return returnVal;
}
```

MPI example – Lulesh

- Lulesh 2.0.3 https://asc.llnl.gov/codes/proxy-apps/lulesh
- “The Shock Hydrodynamics Challenge Problem was originally defined and implemented by LLNL as one of five challenge problems in the DARPA UHPC program and has since become a widely studied proxy application in DOE co-design efforts for exascale.”
- C++, Serial, OpenMP, MPI
- CUDA, OpenACC, OpenCL, other models

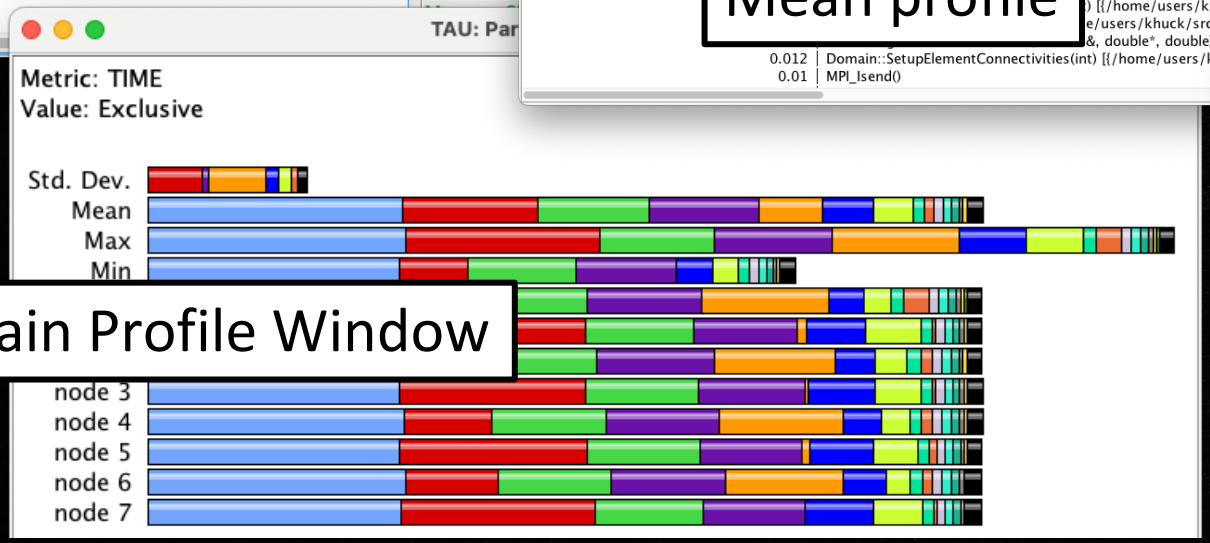


Lulesh Profile - ParaProf

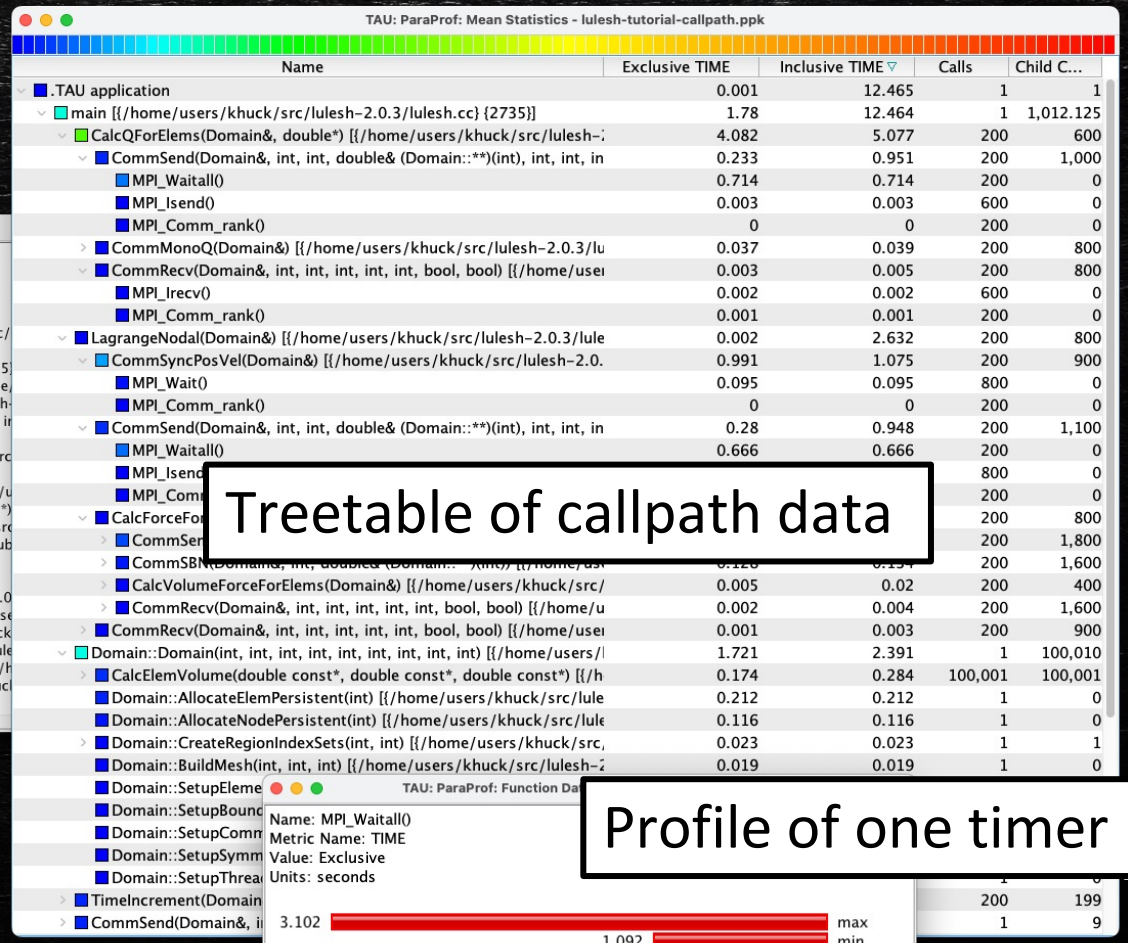


Main window

Mean profile



Main Profile Window



Treetable of callpath data

Profile of one timer

Lulesh Trace – Vampir

Measuring HIP kernel performance

- Hip-stream – small program with 4+ kernel

```
[khuck@login2.crusher add4]$ ./gpu-stream-hip
GPU-STREAM
Version: 1.0
Implementation: HIP
GridSize: 26214400 work-items
GroupSize: 1024 work-items
Operations/Work-item: 1
Precision: double

Running kernels 10 times
Array size: 200.0 MB (=0.2 GB) 0 bytes padding
Total size: 1000.0 MB (=1.0 GB)
Using HIP device  (compute_units=110)
Driver: 50013601
d_a=0x7f0cb0000000
d_b=0x7f0ca0000000
d_c=0x7f0c90000000
d_d=0x7f0c80000000
d_e=0x7f0c70000000
Function    MBytes/sec  Min (sec)   Max         Average
Copy        1331503.944 0.00032     0.00032     0.00032
Mul         1332392.192 0.00031     0.00032     0.00032
Add4        1196944.446 0.00088     0.00089     0.00088
Triad       1256501.941 0.00050     0.00051     0.00050
GEOMEAN     1278064.946
```

Program output

```
*-----------------------------------------------------------------------
* Copyright 2015: Tom Deakin, Simon McIntosh-Smith, University of Bristol HPC
* Based on John D. McCalpin's original STREAM benchmark for CPUs
*-----------------------------------------------------------------------
```

```
template <typename T> __global__ void copy(const T * a, T * c) {
    const int i = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
    c[i] = a[i];
}

template <typename T> __global__ void mul(T * b, const T * c) {
    const T scalar = 3.0;
    const int i = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
    b[i] = scalar * c[i];
}

template <typename T> __global__ void
add(const T * a, const T * b, const T *d, const T *e, T * c) {
    const int i = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
    c[i] = a[i] + b[i] + d[i] + e[i];
}

template <typename T> __global__ void
triad(T * a, const T * b, const T * c) {
    const T scalar = 3.0;
    const int i = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
    a[i] = b[i] + scalar * c[i];
}
```

HIP kernels

Measuring HIP kernel performance

- Just add **`tau_exec`** and arguments to the command (between srun/mpirun and application when applicable)
- **`tau-config`** shows available configs

"use serial,rocprofiler configuration with HIP/ROCm support enabled"

```
[khuck@login2.crusher add4]$ tau_exec -T serial,rocprofiler -rocm ./gpu-stream-hip
GPU-STREAM
Version: 1.0
Implementation: HIP
GridSize: 26214400 work-items
GroupSize: 1024 work-items
Operations/Work-item: 1
Precision: double

Running kernels 10 times
Array size: 200.0 MB (=0.2 GB) 0 bytes padding
Total size: 1000.0 MB (=1.0 GB)
Using HIP device   (compute_units=110)
Driver: 50013601
d_a=0x7f48e0000000
d_b=0x7f48d0000000
d_c=0x7f47b0000000
d_d=0x7f47a0000000
d_e=0x7f4790000000
Function    MBytes/sec  Min (sec)   Max         Average
Copy        1320624.685 0.00032     0.00032     0.00032
Mul         1321623.393 0.00032     0.00032     0.00032
Add4        1217965.813 0.00086     0.00088     0.00087
Triad       1254042.504 0.00050     0.00051     0.00051
GEOMEAN     1277787.457
```

Pprof output, timers

```
[khuck@login2.crusher add4]$ pprof
Reading Profile files in profile.*

NODE 0;CONTEXT 0;THREAD 0:
---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0        1,031        1,031           1           1    1031765 .TAU application
  0.0         0.03         0.03           1           0         30 pthread_create

NODE 0;CONTEXT 0;THREAD 1:
---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0            1          479           1           1     479989 .TAU application
 99.6          478          478           1           0     478248 [PTHREAD] _ZN4rocr2os16ThreadTrampolineEPv

NODE 0;CONTEXT 0;THREAD 2:
---------------------------------------------------------------------------------------
%Time    Exclusive    Inclusive       #Call      #Subrs  Inclusive Name
              msec   total msec                          usec/call
---------------------------------------------------------------------------------------
100.0        0.638           20           1          40      20298 .TAU application
 42.4            8            8          10           0        861 void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
 24.2            4            4          10           0        492 void triad<double>(double*, double const*, double const*) [clone .kd]
 15.1            3            3          10           0        307 void copy<double>(double const*, double*) [clone .kd]
 15.1            3            3          10           0        306 void mul<double>(double*, double const*) [clone .kd]
---------------------------------------------------------------------------------------
```

Main Thread

Rocprofiler Thread

Device activity

Pprof output, counters

Counters for measuring register pressure and occupancy

```
USER EVENTS Profile :NODE 0, CONTEXT 0, THREAD 2
---------------------------------------------------------------------------------------
NumSamples   MaxValue   MinValue  MeanValue  Std. Dev.  Event Name
---------------------------------------------------------------------------------------
        10  2.621E+07  2.621E+07  2.621E+07          0  Grid Size : void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
        10  2.621E+07  2.621E+07  2.621E+07          0  Grid Size : void copy<double>(double const*, double*) [clone .kd]
        10  2.621E+07  2.621E+07  2.621E+07          0  Grid Size : void mul<double>(double*, double const*) [clone .kd]
        10  2.621E+07  2.621E+07  2.621E+07          0  Grid Size : void triad<double>(double*, double const*, double const*) [clone .kd]
        10          0          0          0          0  LDS Memory Size : void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
        10          0          0          0          0  LDS Memory Size : void copy<double>(double const*, double*) [clone .kd]
        10          0          0          0          0  LDS Memory Size : void mul<double>(double*, double const*) [clone .kd]
        10          0          0          0          0  LDS Memory Size : void triad<double>(double*, double const*, double const*) [clone .kd]
        10         32         32         32          0  Scalar Register Size (SGPR) : void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
        10         24         24         24          0  Scalar Register Size (SGPR) : void copy<double>(double const*, double*) [clone .kd]
        10         24         24         24          0  Scalar Register Size (SGPR) : void mul<double>(double*, double const*) [clone .kd]
        10         24         24         24          0  Scalar Register Size (SGPR) : void triad<double>(double*, double const*, double const*) [clone .kd]
        10          0          0          0          0  Scratch Memory Size : void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
        10          0          0          0          0  Scratch Memory Size : void copy<double>(double const*, double*) [clone .kd]
        10          0          0          0          0  Scratch Memory Size : void mul<double>(double*, double const*) [clone .kd]
        10          0          0          0          0  Scratch Memory Size : void triad<double>(double*, double const*, double const*) [clone .kd]
        10          8          8          8          0  Vector Register Size (VGPR) : void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
        10          4          4          4          0  Vector Register Size (VGPR) : void copy<double>(double const*, double*) [clone .kd]
        10          4          4          4          0  Vector Register Size (VGPR) : void mul<double>(double*, double const*) [clone .kd]
        10          4          4          4          0  Vector Register Size (VGPR) : void triad<double>(double*, double const*, double const*) [clone .kd]
        10       1024       1024       1024          0  Work Group Size : void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
        10       1024       1024       1024          0  Work Group Size : void copy<double>(double const*, double*) [clone .kd]
        10       1024       1024       1024          0  Work Group Size : void mul<double>(double*, double const*) [clone .kd]
        10       1024       1024       1024          0  Work Group Size : void triad<double>(double*, double const*, double const*) [clone .kd]
        10       5952       5952       5952          0  fbarrier count : void add<double>(double const*, double const*, double const*, double const*, double*) [clone .kd]
        10       3392       3392       3392          0  fbarrier count : void copy<double>(double const*, double*) [clone .kd]
        10       4672       4672       4672          0  fbarrier count : void mul<double>(double*, double const*) [clone .kd]
        10          0          0          0          0  fbarrier count : void triad<double>(double*, double const*, double const*) [clone .kd]
---------------------------------------------------------------------------------------
```

ParaProf view of same data

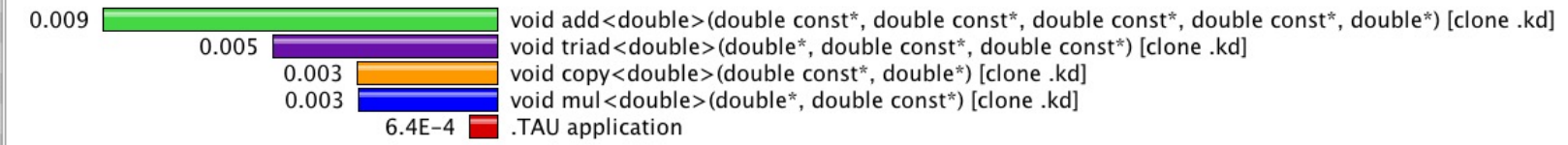
TAU: ParaProf: Context Events for: node 0, thread 2 - add4.ppk

Name	NumSamp...	MaxValue	MinValue	MeanVal...	Std. Dev.
void add<double>(double const*, double const*, double const*, double cor					
Grid Size	10	26,214,400	26,214,400	26,214,400	0
LDS Memory Size	10	0	0	0	0
Scalar Register Size (SGPR)	10	32	32	32	0
Scratch Memory Size	10	0	0	0	0
Vector Register Size (VGPR)	10	8	8	8	0
Work Group Size	10	1,024	1,024	1,024	0
fbarrier count	10	5,952	5,952	5,952	0
void copy<double>(double const*, double*) [clone .kd]					
Grid Size	10	26,214,400	26,214,400	26,214,400	0
LDS Memory Size	10	0	0	0	0
Scalar Register Size (SGPR)	10	24	24	24	0
Scratch Memory Size	10	0	0	0	0
Vector Register Size (VGPR)	10	4	4	4	0
Work Group Size	10	1,024	1,024	1,024	0
fbarrier count	10	3,392	3,392	3,392	0
void mul<double>(double*, double const*) [clone .kd]					
Grid Size	10	26,214,400	26,214,400	26,214,400	0
LDS Memory Size					
Scalar Register Size (SGPR)					
Scratch Memory Size					
Vector Register Size (VGPR)					
Work Group Size					
fbarrier count					
void triad<double>(double*, double const*, double const*) [clone .kd]					
Grid Size					
LDS Memory Size					
Scalar Register Size (SGPR)					
Scratch Memory Size					
Vector Register Size (VGPR)					

VERY helpful for understanding **register pressure** and **occupancy**

TAU: ParaProf: node 0, thread 2 - add4.ppk

Metric: TAUGPU_TIME
Value: Exclusive
Units: seconds



Tracing support uses Roctracer

```
$ TAU_TRACE=1 TAU_TRACE_FORMAT=otf2 tau_exec -T serial,roctracer ./gpu-stream-hip
```

Each device has 2-3 virtual threads:
1) kernels,
2) memory transfers
3) synchronization
(prevents overlapping timers)

tau_exec command reference

- Uninstrumented execution
  - % mpirun -np 256 ./a.out
- Track GPU operations
  - % mpirun –np 256 tau_exec –l0 ./a.out
  - % mpirun –np 256 tau_exec –opencl ./a.out
  - % mpirun –np 256 tau_exec –openacc ./a.out
  - % mpirun –np 256 tau_exec –cupti ./a.out
  - % mpirun –np 256 tau_exec –rocm ./a.out
- Track MPI performance
  - % mpirun -np 256 tau_exec ./a.out
- Track I/O, and MPI performance (MPI enabled by default)
  - % mpirun -np 256 tau_exec -io ./a.out
- Track OpenMP and MPI execution (using OMPT for Intel v19+ or Clang 8+)
  - % export TAU_OMPT_SUPPORT_LEVEL=full;
  - % mpirun –np 256 tau_exec –T ompt,mpi -ompt ./a.out
- Track memory operations
  - % export TAU_TRACK_MEMORY_LEAKS=1
  - % mpirun –np 256 tau_exec –memory_debug ./a.out (bounds check)
- Use event based sampling (compile with –g)
  - % mpirun –np 256 tau_exec –ebs ./a.out
  - Also export TAU_METRICS=TIME,PAPI_L1_DCM… -ebs_resolution=<file | function | line>
- Non-MPI execution: use –T serial
  - % tau_exec –T serial,level_zero –l0 –ebs ./a.out

TAU Runtime Environment Variables

Environment Variable	Default	Description
TAU_TRACE	0	Setting to 1 turns on tracing
TAU_CALLPATH	0	Setting to 1 turns on callpath profiling
TAU_TRACK_MEMORY_FOOTPRINT	0	Setting to 1 turns on tracking memory usage by sampling periodically the resident set size and high water mark of memory usage
TAU_TRACK_POWER	0	Tracks power usage by sampling periodically.
TAU_CALLPATH_DEPTH	2	Specifies depth of callpath. Setting to 0 generates no callpath or routine information, setting to 1 generates flat profile and context events have just parent information (e.g., Heap Entry: foo)
TAU_SAMPLING	1	Setting to 1 enables event-based sampling.
TAU_TRACK_SIGNALS	0	Setting to 1 generate debugging callstack info when a program crashes
TAU_COMM_MATRIX	0	Setting to 1 generates communication matrix display using context events
TAU_THROTTLE	1	Setting to 0 turns off throttling. Throttles instrumentation in lightweight routines that are called frequently
TAU_THROTTLE_NUMCALLS	100000	Specifies the number of calls before testing for throttling
TAU_THROTTLE_PERCALL	10	Specifies value in microseconds. Throttle a routine if it is called over 100000 times and takes less than 10 usec of inclusive time per call
TAU_CALLSITE	0	Setting to 1 enables callsite profiling that shows where an instrumented function was called. Also compatible with tracing.
TAU_PROFILE_FORMAT	Profile	Setting to “merged” generates a single file. “snapshot” generates xml format
TAU_METRICS	TIME	Setting to a comma separated list generates other metrics. (e.g., ENERGY,TIME,P_VIRTUAL_TIME,PAPI_FP_INS,PAPI_NATIVE_<event>:<subevent>)

TAU Runtime Environment Variables

Environment Variable	Default	Description
TAU_TRACE	0	Setting to 1 turns on tracing
TAU_TRACE_FORMAT	Default	Setting to “otf2” turns on TAU’s native OTF2 trace generation (configure with –otf=download)
TAU_EBS_UNWIND	0	Setting to 1 turns on unwinding the callstack during sampling (use with tau_exec –ebs or TAU_SAMPLING=1)
TAU_EBS_RESOLUTION	line	Setting to “function” or “file” changes the sampling resolution to function or file level respectively.
TAU_TRACK_LOAD	0	Setting to 1 tracks system load on the node
TAU_SELECT_FILE	Default	Setting to a file name, enables selective instrumentation based on exclude/include lists specified in the file.
TAU_OMPT_SUPPORT_LEVEL	basic	Setting to “full” improves resolution of OMPT TR6 regions on threads 1.. N-1. Also, “lowoverhead” option is available.
TAU_OMPT_RESOLVE_ADDRESS_EAGERLY	1	Setting to 1 is necessary for event based sampling to resolve addresses with OMPT. Setting to 0 allows the user to do offline address translation.

For more info…

- https://tau.uoregon.edu
- https://github.com/UO-OACISS/tau2
- https://github.com/UO-OACISS/tau2/wiki
- https://github.com/UO-OACISS/tau2/wiki/Frequently-Asked-Questions-%28FAQ%29
- Email tau-bugs@cs.uoregon.edu

ADIOS2 Output

- As discussed, **`tau_exec`** is the execution wrapper to attach ”inject” or ”attach” TAU to the application
- TAU comes with a plugin API (see Malony, Allen D., et al. "A plugin architecture for the TAU performance system”, *ICPP*, 2019.)
  - Code is executed at TAU events (timer start/stop, profile dump, program start/stop, etc.), or periodically
  - TAU comes with an ADIOS2 plugin that will write the profile data to ADIOS2 instead of TAU profile files

ADIOS2 plugin events

- PostInit – after MPI_Init, initialize ADIOS2 for writing
- Dump – when the “Tau_dump()” function is called, update all available profile statistics, write to ADIOS2
- PreEndOfExecution – before MPI_Finalize is executed, perform any final unification and write and close
- EndOfExecution – cleanup

Using the ADIOS2 plugin

- Just add the **`-adios2`** flag to tau_exec
- Useful environment variables
  - **`TAU_ADIOS2_PERIODIC`**: yes/true/on/1 – tells the plugin to write output periodically and asynchronously, (defaults to **`false`**)
  - **`TAU_ADIOS2_PERIOD`**: number in microseconds (default 2,000,000)
  - **`TAU_ADIOS2_ONE_FILE`**: write one ADIOS2 file, or each MPI rank writes their own (defaults to **`true`**)
  - **`TAU_ADIOS2_FILENAME`**: defaults to **`tauprofile-<executable name>.bp`** (can specify path with TAU **`$PROFILEDIR`** env var)
  - **`TAU_ADIOS2_ENGINE`**: (defaults to **`BPFile`**)
  - **`TAU_ADIOS2_CONFIG_FILE`**: for specifying all ADIOS2 settings (default: **`./adios2.xml`**)

What data is stored?

- TAU Metadata stored as ADIOS2 attributes (strings)
- TAU Counters
  - Bytes sent, GPU registers used, etc.
- TAU Timers
  - Time in foo(), bar(), etc.

Metadata examples (bpls -A -d)

```
[khuck@Kevins-Air xgc % $HOME/src/ADIOS2/install/bin/bpls -A -d tauprofile-xgc-es-cpp-gpu-checkpoint.bp | head -n 40 ]
  string   TAU:0:0:MetaData:CPU Cores                          attr   = "64"
  string   TAU:0:0:MetaData:CPU MHz                            attr   = "1894.426"
  string   TAU:0:0:MetaData:CPU Type                           attr   = "AMD EPYC 7A53 64-Core Processor"
  string   TAU:0:0:MetaData:CPU Vendor                         attr   = "AuthenticAMD"
  string   TAU:0:0:MetaData:CPUs Allowed                       attr   = "00000000,00000000,00000000,000000ff"
  string   TAU:0:0:MetaData:CPUs Allowed List                  attr   = "0-7"
  string   TAU:0:0:MetaData:CRAY_CORE_ID                       attr   = "3"
  string   TAU:0:0:MetaData:CWD                                attr   = "/gpfs/alpine/fus123/proj-shared/khuck/FOM_
run/WeakScalingESFrontier/rundir_2_planes_check_tau_adios2"
  string   TAU:0:0:MetaData:Cache Size                         attr   = "512 KB"
  string   TAU:0:0:MetaData:Command Line                       attr   = "/ccs/home/khuck/ECP-WDM/ecp-wdm-coe/crushe
r_rocm5.2.0/build/xgc.princeton/bin/xgc-es-cpp-gpu"
  string   TAU:0:0:MetaData:Cpus_allowed_list                  attr   = "0-7"
  string   TAU:0:0:MetaData:Executable                         attr   = "/autofs/nccs-svm1_home1/khuck/ECP-WDM/ecp-
wdm-coe/crusher_rocm5.2.0/build/xgc.princeton/bin/xgc-es-cpp-gpu"
  string   TAU:0:0:MetaData:Hostname                           attr   = "crusher047"
  string   TAU:0:0:MetaData:Local Time                         attr   = "2022-10-05T19:26:33-04:00"
  string   TAU:0:0:MetaData:MPI Comm World Rank                attr   = "0"
  string   TAU:0:0:MetaData:MPI Comm World Size                attr   = "256"
  string   TAU:0:0:MetaData:MPI Host Name                      attr   = "crusher047"
  string   TAU:0:0:MetaData:MPI Processor Name                 attr   = "crusher047"
  string   TAU:0:0:MetaData:MPI Unique Hosts                   attr   = "1"
  string   TAU:0:0:MetaData:Memories Allowed                   attr   = "00000000,0000000f"
  string   TAU:0:0:MetaData:Memories Allowed List              attr   = "0-3"
  string   TAU:0:0:MetaData:Memory Size                        attr   = "526858456 kB"
  string   TAU:0:0:MetaData:Mems_allowed_list                  attr   = "0-3"
  string   TAU:0:0:MetaData:Node Name                          attr   = "crusher047"
  string   TAU:0:0:MetaData:OS Machine                         attr   = "x86_64"
  string   TAU:0:0:MetaData:OS Name                            attr   = "Linux"
  string   TAU:0:0:MetaData:OS Release                         attr   = "5.3.18-150300.59.68_11.0.76-cray_shasta_c"
  string   TAU:0:0:MetaData:OS Version                         attr   = "#1 SMP Sun May 29 15:23:06 UTC 2022 (2104b
1c)"
  string   TAU:0:0:MetaData:Starting Timestamp                 attr   = "1665012393419330"
```

Timer Examples (bpls -l)

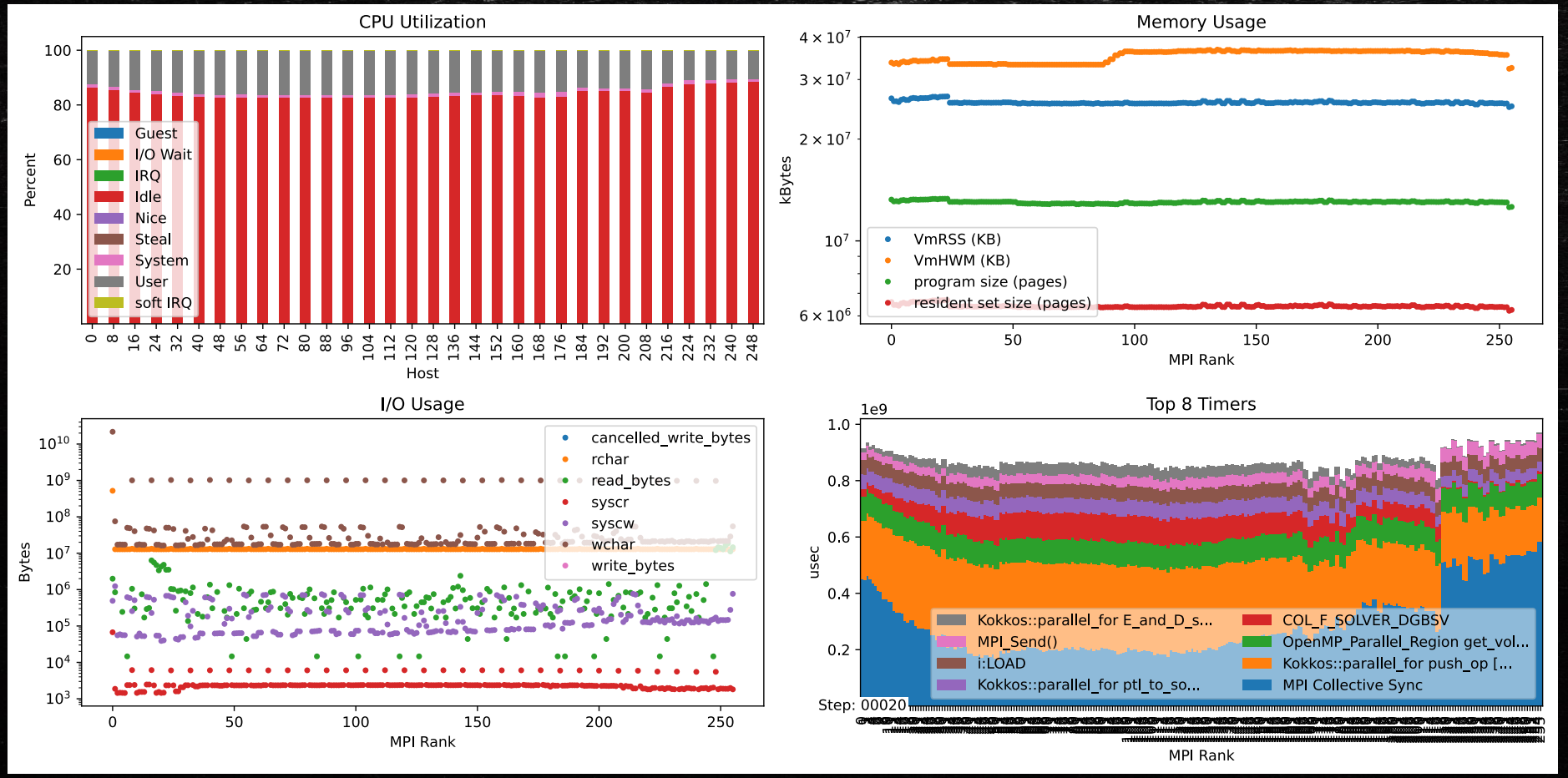
```
double   .TAU application / Calls
double   .TAU application / Exclusive TIME
double   .TAU application / Inclusive TIME
double   ADD_F0_ANALYTIC / Calls
double   ADD_F0_ANALYTIC / Exclusive TIME
double   ADD_F0_ANALYTIC / Inclusive TIME
double   ADIOS_WRITE_RESTART / Calls
double   ADIOS_WRITE_RESTART / Exclusive TIME
double   ADIOS_WRITE_RESTART / Inclusive TIME
double   ADIOS_WRITE_RESTARTF0 / Calls
double   ADIOS_WRITE_RESTARTF0 / Exclusive TIME
double   ADIOS_WRITE_RESTARTF0 / Inclusive TIME
double   ASSIGN_TO_TMP / Calls
double   ASSIGN_TO_TMP / Exclusive TIME
double   ASSIGN_TO_TMP / Inclusive TIME
double   BP4Writer::AggregateWriteData / Calls
double   BP4Writer::AggregateWriteData / Exclusive TIME
double   BP4Writer::AggregateWriteData / Inclusive TIME
double   BP4Writer::BeginStep / Calls
double   BP4Writer::BeginStep / Exclusive TIME
double   BP4Writer::BeginStep / Inclusive TIME
double   BP4Writer::Close / Calls
double   BP4Writer::Close / Exclusive TIME
double   BP4Writer::Close / Inclusive TIME
double   BP4Writer::EndStep / Calls
double   BP4Writer::EndStep / Exclusive TIME
double   BP4Writer::EndStep / Inclusive TIME
double   BP4Writer::Flush / Calls
double   BP4Writer::Flush / Exclusive TIME
double   BP4Writer::Flush / Inclusive TIME
double   BP4Writer::Open / Calls
double   BP4Writer::Open / Exclusive TIME
double   BP4Writer::Open / Inclusive TIME
double   BP4Writer::PerformPuts / Calls
double   BP4Writer::PerformPuts / Exclusive TIME
double   BP4Writer::PerformPuts / Inclusive TIME
double   BP4Writer::PopulateMetadataIndexFileContent / Calls
double   BP4Writer::PopulateMetadataIndexFileContent / Exclusive TIME
double   BP4Writer::PopulateMetadataIndexFileContent / Inclusive TIME
```

Counter Examples (bpls -l)

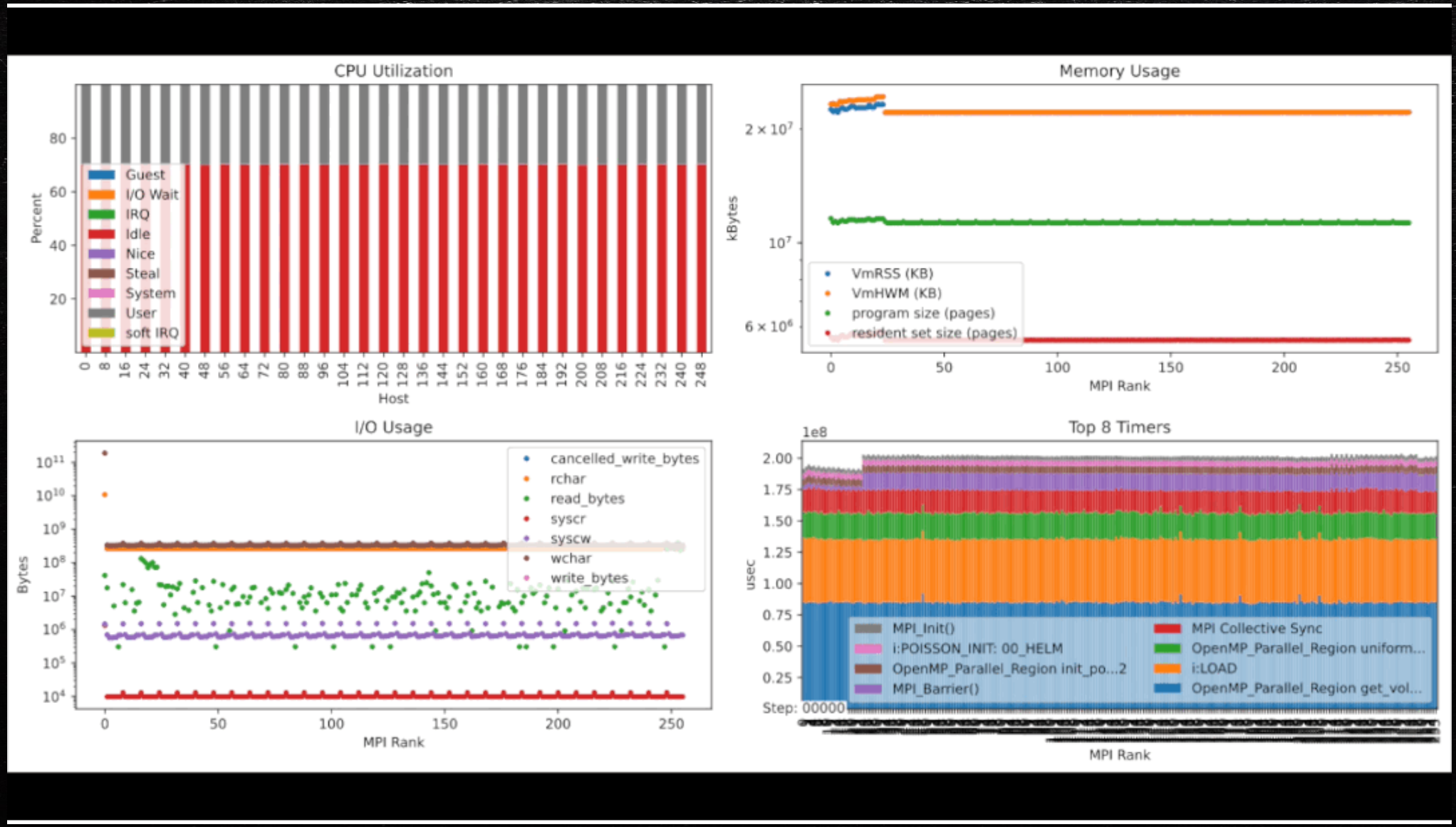
```
  double   Memory Footprint (VmRSS) (KB) / Max
  double   Memory Footprint (VmRSS) (KB) / Mean
  double   Memory Footprint (VmRSS) (KB) / Min
  double   Memory Footprint (VmRSS) (KB) / Num Events
  double   Memory Footprint (VmRSS) (KB) / Sum Squares
  double   Message size for all-gather / Max
  double   Message size for all-gather / Mean
  double   Message size for all-gather / Min
  double   Message size for all-gather / Num Events
  double   Message size for all-gather / Sum Squares
  double   Message size for all-reduce / Max
  double   Message size for all-reduce / Mean
  double   Message size for all-reduce / Min
  double   Message size for all-reduce / Num Events
  double   Message size for all-reduce / Sum Squares
  double   Message size for all-to-all / Max
  double   Message size for all-to-all / Mean
  double   Message size for all-to-all / Min
  double   Message size for all-to-all / Num Events
  double   Message size for all-to-all / Sum Squares
  double   Message size for broadcast / Max
  double   Message size for broadcast / Mean
  double   Message size for broadcast / Min
  double   Message size for broadcast / Num Events
  double   Message size for broadcast / Sum Squares
  double   Message size for gather / Max
  double   Message size for gather / Mean
  double   Message size for gather / Min
  double   Message size for gather / Num Events
  double   Message size for gather / Sum Squares
  double   Message size for reduce / Max
  double   Message size for reduce / Mean
  double   Message size for reduce / Min
  double   Message size for reduce / Num Events
  double   Message size for reduce / Sum Squares
  double   Message size for scan / Max
  double   Message size for scan / Mean
  double   Message size for scan / Min
  double   Message size for scan / Num Events
```

Visualizing the data

- Using ADIOS2 Python API, we can read the data and visualize it



Monitoring of application data

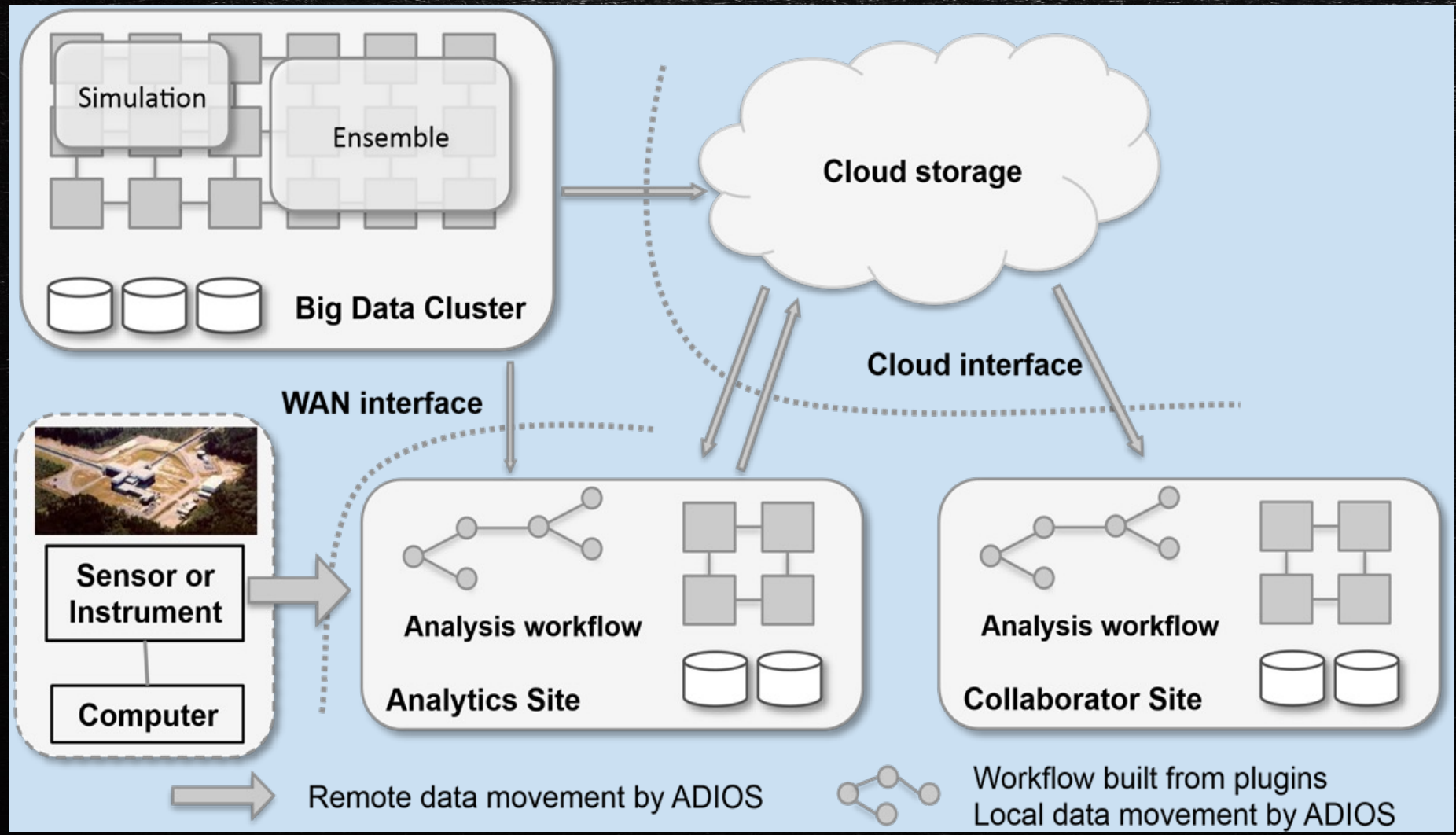


Current/Previous Acknowledgements

Outline

- 8:30 Introduction to data management at extreme scale – Scott Klasky
- 9:15 ADIOS 2 concepts and API (C++, Python, F90) – Norbert Podhorszki
- 10:00 BREAK
- 10:30 ADIOS 2 API – Norbert Podhorszki
- 11:00 Hands on with ADIOS 2 – Files – Ana Gainaru
- 12:00 Lunch
- 1:30 ADIOS @ scale – Norbert Podhorszki
- 2:00 Introduction to Paraview + ADIOS + hands on Caitlin Ross
- 3:00 BREAK
- 3:30 Introduction to TAU and TAU + ADIOS – Kevin Huck
- 4:00 Hands on with TAU + ADIOS
- 4:15 Staging with ADIOS – hands 0n – Ana Gainaru
- 5:00 END

Vision: building scientific collaborative applications

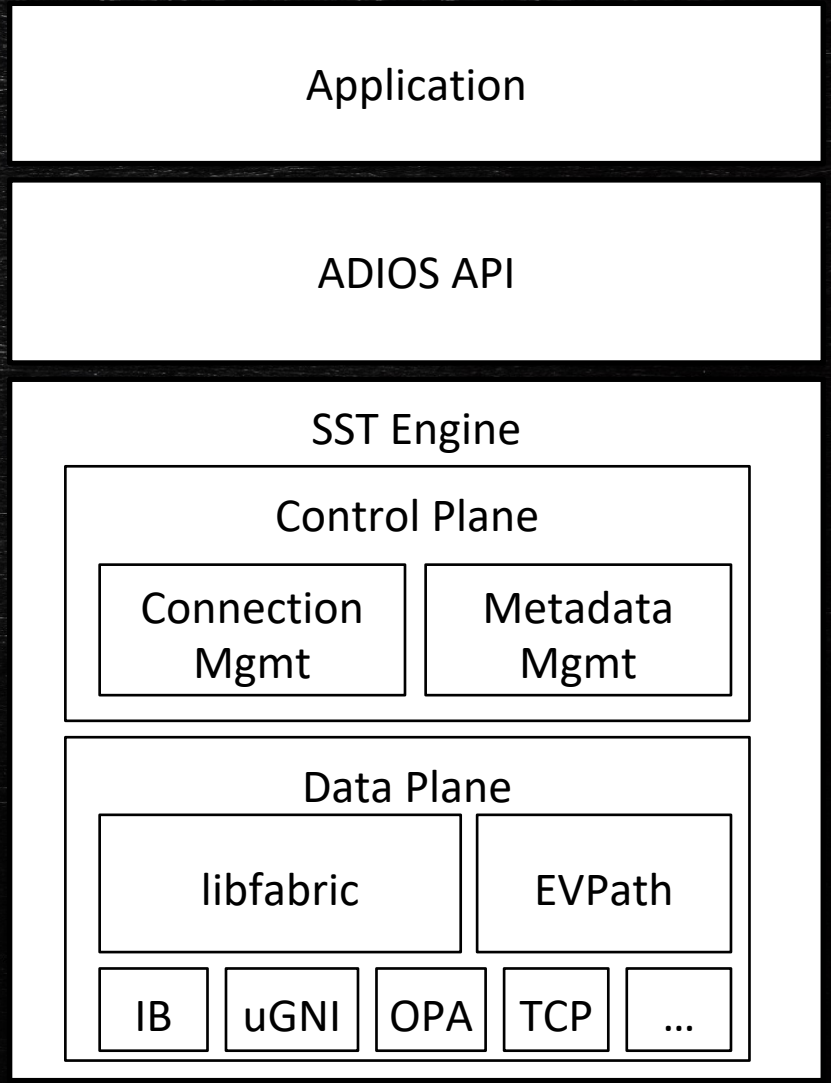


Data Staging in ADIOS

- Sustainable Staging Transport (SST)
  - In-situ infrastructure for staging in a streaming-like fashion using RDMA, SOCKETS
- DataMan
  - WAN transfers using sockets and ZeroMQ
- SSC (Staging for Strong Coupling)
  - One-sided MPI for strong coupling of codes
- Inline
  - Traditional in-situ execution of consumer code

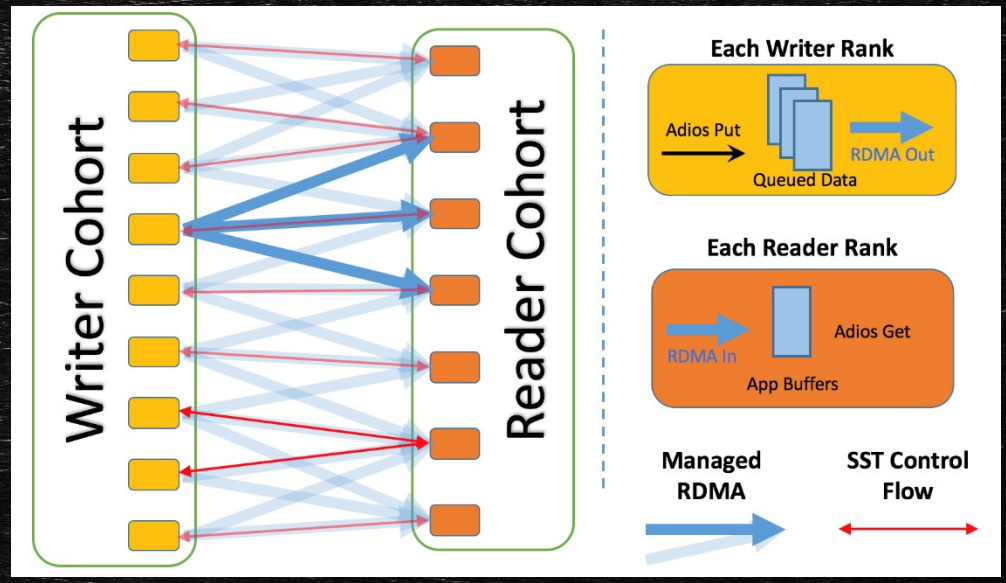
Sustainable Staging Transport (SST)

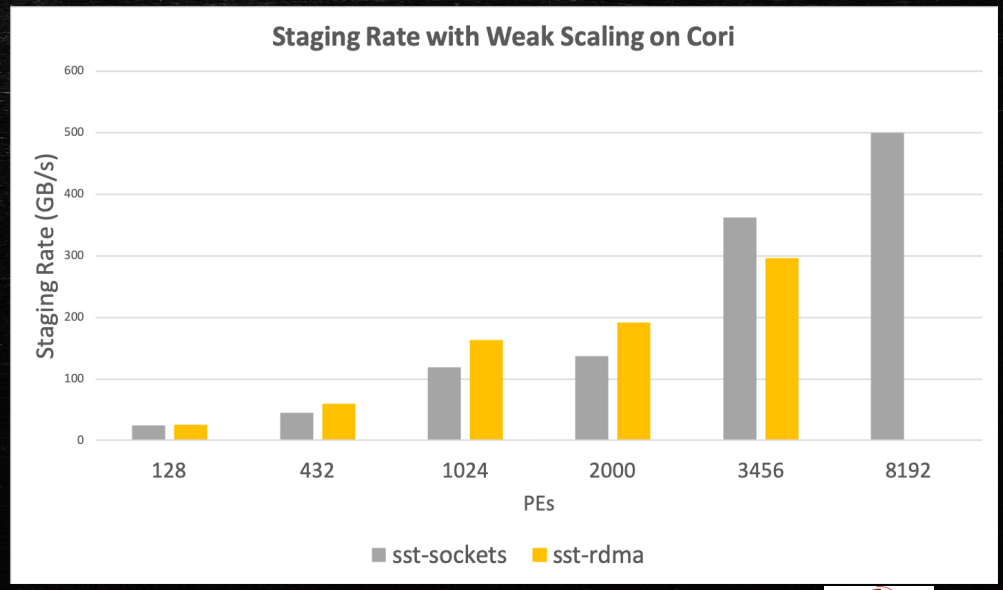
- Direct coupling between data producers and consumers for in-situ/in-transit processing
- Designed for portability and reliability.
- Control Plane
  - Manages meta-data and control using a message-oriented protocol
  - Inherits concepts from Flexpath, DIMES, uses EVPath
  - Allows for dynamic connections, multiple readers and complex flow control management
- Data Plane
  - Exchange data using RDMA
  - Responsible for resource management for data transfer
  - Uses libfabric for portable RDMA support
  - Threaded to overlap communication with computation and for asynchronous progress monitoring
  - Modular interface with the control plane supports alternative data plane implementations



Sustainable Staging Transport (SST)

- Data is staged in writer ranks' memory.
  - Metadata is propagated to subscribed readers, reader ranks perform indexing locally.
  - Metadata structure is optimized for single writer, N reader workflows.
  - Supports late joining/early leaving readers.
- Modular design
  - Well-encapsulated interface between DP and CP.
  - Multiple inter-changeable DP implementations.
- RDMA for asynchronous transfer
  - Currently tested and performant for GNI, IB (verbs), OPA (verbs/psm2).





SSC (Staging for Strong Coupling)

- An ADIOS 2 engine using MPI for portability and performance

- Features
  - Use a combination of one-sided MPI and two-sided MPI methods for flexibility and performance.
  - Use threads and non-blocking MPI methods to hide communication time.
  - Optimized for fixed I/O pattern – push data to consumer

- Target Applications
  - XGC, Gene, or Gem (Edge-core strong coupling)
  - Other ECP applications requiring strong coupling or always-on in-situ analysis/visualization

DataMan

- An ADIOS 2 engine subroutine designed for wide area network data transfer, data staging, near-real-time data reduction and remote in-situ processing
- Designed with following principles:
  - Flexibility: allowing transport layer switching (ADIOS BP file, ZeroMQ, google-rpc etc.)
  - Versatility: supporting various workflow modes (p2p, query, pub/sub, etc.)
  - Adaptability: allowing adaptive data compression based on near-real-time decision making
  - Extendibility: taking advantage of all ADIOS transports and operators, and other potential third-party libraries. For example, DataMan can use ZFP, Bzip, SZ that have been built into ADIOS, as well as any compression techniques that will be built into ADIOS in future.
- Features
  - Step aggregation to improve data rate, by sacrificing latency.
  - Lossy compression to reduce data size to be transferred, by sacrificing latency and precision.
  - Fast mode to improve latency and data rate, by sacrificing reliability.
  - Combinations of features above to achieve a certain set of performance requirements.
- Target Applications:
  - ECP applications requiring wide area network data transfer and adaptive data reduction
  - Square Kilometer Array observational data
  - KSTAR fusion experimental data

DataMan: Supports three workflow modes

- Push
  - Sender driven workflow
  - Senders are configured to send data to pre-defined receivers.
- Query
  - Receiver driven workflow
  - Receivers are configured to query particular data (particular subsets of particular variables) from senders.
- Subscribe
  - Ad-hoc workflow
  - Free combination of senders (publishers) and receivers (subscribers).
  - Senders and receivers can be launched in any order, and they can be attached and detached freely without affecting other senders or receivers.

Inline engine: in-process in situ visualization

- An ADIOS 2 engine providing in-process communication between the writer and reader
- Features
  - Consumer has zero-copy access to the local data block of the producer's data in memory
  - Synchronous execution of consumer code, during producer's EndStep() call
- Target Applications
  - Traditional in situ visualization routines that scale well with the producer's size
- Caveat: Writer and reader must be created in the same IO object
  - Can't easily swap in at runtime as with other ADIOS engines

ParaView In Situ Engine plugin

- ADIOS plugin that uses the inline engine internally, along with the Catalyst API to enable in situ visualization with ParaView

- Features
  - This plugin sets up the inline writer and reader on the same IO object for you
  - No code changes are now necessary to use the inline engine
  - The engine is instrumented with the Catalyst API calls – no need to add this to your application directly

Fides and ParaView Catalyst

- Need to set 3 environment variables:
  - ADIOS2_PLUGIN_PATH: set this to point to the directory containing libParaViewADIOSInSituEngine.so
  - CATALYST_IMPLEMENTATION_NAME=paraview
  - CATALYST_IMPLEMENTATION_PATHS: set this to point to the directory containing the ParaView Catalyst build. Most likely something like: /path-to-paraview-build/lib/catalyst
- Setting the Catalyst environment variables will swap in the ParaView Catalyst implementation at runtime so you can use the full

Configuring the in situ engine plugin

- Set engine type to plugin
- PluginName is a name given to it for ADIOS to keep track of it
- PluginLibrary is the name of the shared lib for the plugin
- DataModel is a JSON file describing the mesh/fields
- Script is a ParaView Catalyst script

```
<io name="SimulationOutput">
    <engine type="plugin">
        <!-- general plugin engine parameters -->
        <parameter key="PluginName" value="fides"/>
        <parameter key="PluginLibrary" value="ParaViewADIOSInSituEngine"/>
        <!-- ParaViewFides engine parameters -->
        <parameter key="DataModel" value="catalyst/gs-fides.json"/>
        <parameter key="Script" value="catalyst/gs-pipeline.py"/>
    </engine>
</io>
```

Application: Which staging method to use?

- System considerations
  - Staging between machines/over a WAN? **DataMan**
  - Co-located execution? **SST**
  - Availability of RDMA high-speed network? **SST** optimized for this case.
- Coupling considerations
  - Highly synchronized writer/reader? **SSC**
  - 1 writer, many readers streaming? **SST** optimized for this use case.
  - 1 reader, many small producers (e.g. AI training)? **SST**
- Performance considerations
  - Often application-specific, and not always obvious.
  - Here's where it helps to have a flexible I/O framework…

Staging I/O

- Processing data on the fly by

  1. Reading from file concurrently, or

  2. Moving data without using the file system

Design choices for reading API

- One output step at a time
  - **One step is seen at once after writer completes a whole output step**
  - streaming is not byte streaming here
  - reader has access to all data in one output step
  - as long as the reader does not release the step, it can read it
    - potentially blocking the writer
- Advancing in the stream means
  - get access to another output step of the writer,
  - while losing the access to the current step forever.

ADIOS concepts for the read API (get)

- Step
  - A dataset written within one adios_begin_step/…/adios_end_step
- Stream
  - A file containing of series of steps of the same dataset
- Open for reading as a stream
  - for step-by-step reading (both staged data and files)

```
adios2::Engine reader = io.Open(filename, adios2::Mode::Read, comm);
```

- Close once at the very end of streaming

```
reader.Close();
```

Advancing a stream

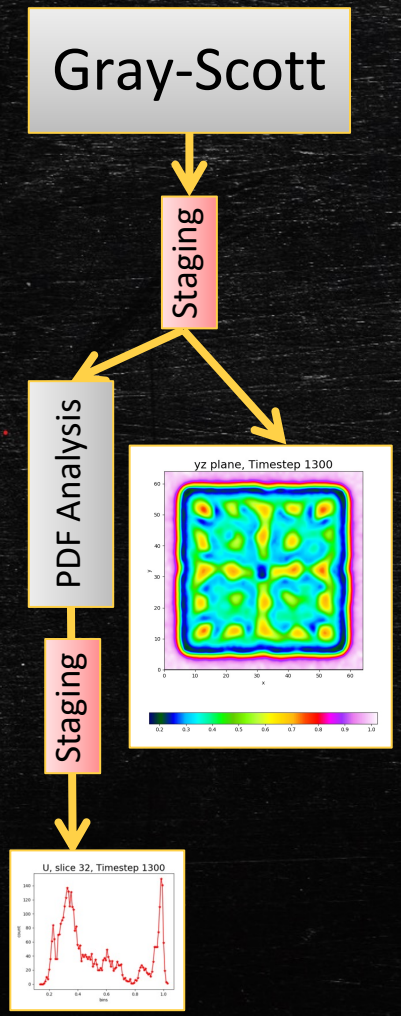
- One step is accessible in streams, advancing is only forward

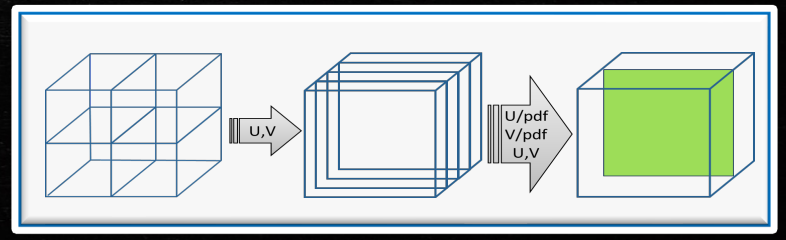
```
adios2::StepStatus read_status =
        reader.BeginStep(adios2::StepMode::Read, timeout);
if (read_status != adios2::StepStatus::OK) {
    break;
}
```

  - float timeout: wait for this long for a new step to arrive
- Release a step if not needed anymore
  - optimization to allow the staging method to deliver new steps if available

```
reader.EndStep();
```

Gray-Scott example with staging





Run the code

```
$ source ~/adios2-tutorial-source/adios2-tutorial-env.sh
$ cd ~/adios2-tutorial-source/ADIOS2-Examples/build/install/share/adios2-examples/gray-scott
$ ./cleanup.sh data
$ ls -l *.bp
ls: cannot access *.bp: No such file or directory
```

The runtime config file: adios2.xml

adios2.xml

```
<?xml version="1.0"?>
<adios-config>

  <!--====================================
      Configuration for for Gray-Scott and GS Plot
    ====================================-->
  <io name="SimulationOutput">
    <engine type="SST">

    </engine>
  </io>

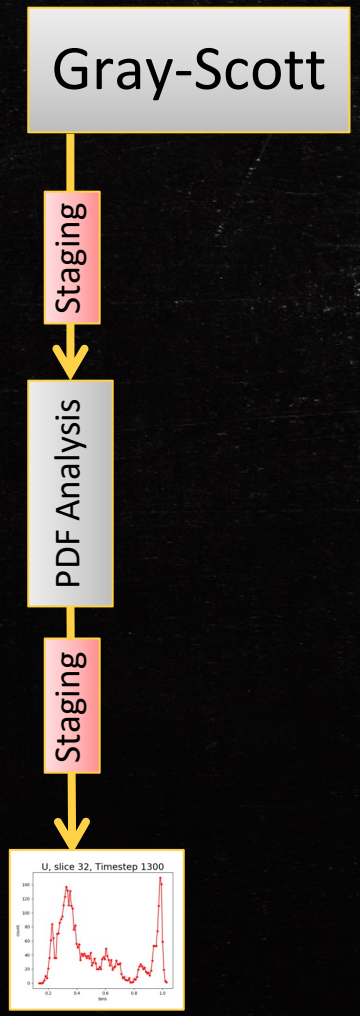
  <io name="PDFAnalysisOutput">
    <engine type="SST">
    </engine>
  </io>
```

Engine types
BP5
HDF5
FileStream
SST
SSC
DataMan

SST runtime parameters

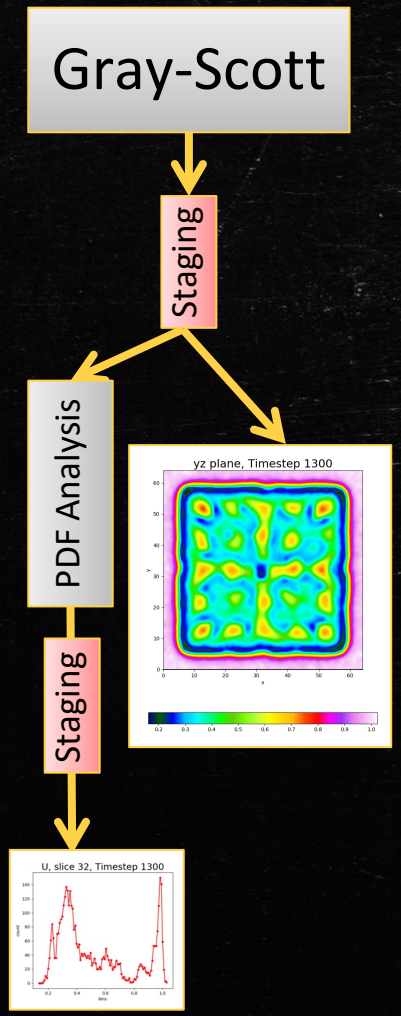
RendezvousReaderCount = 0 [1, 2, etc]
Block Producer to wait for N Consumers at Open()
QueueLimit = 1 [2, 3, etc]
Buffer K steps in Producer's memory for slow consumers
QueueFullPolicy = Disard or Block
What to do when Producer is faster than Consumer(s)
DataTransport = MPI, WAN, RDMA
Data is moved by MPI or TCP or libfabric (RDMA)
TCP is always available, MPI for MPICH 4.x, libfabric on systems that support it

Run the code




```
$ mpirun -n 4 ../../../bin/adios2-gray-scott settings-files.json : -n 1
../../../bin/adios2-pdf-calc gs.bp pdf.bp 100 : -n 1 python3 pdfplot.py -i pdf.bp
PDF analysis reads from Simulation using engine type:  SST
PDF analysis writes using engine type:                 SST
Simulation writes data using engine type:              SST
…
Simulation at step 10 writing output step     1
Simulation at step 20 writing output step     2
Simulation at step 30 writing output step     3
Simulation at step 40 writing output step     4
Simulation at step 50 writing output step     5
PDF Analysis step 0 processing sim output step 3 sim compute step 40
PDF Plot step 0 processing analysis step 0 simulation step 40
Simulation at step 60 writing output step     6
PDF Analysis step 1 processing sim output step 5 sim compute step 60
Simulation at step 70 writing output step     7
PDF Analysis step 2 processing sim output step 6 sim compute step 70
Simulation at step 80 writing output step     8
…
PDF Plot step 1 processing analysis step 1 simulation step 60
```

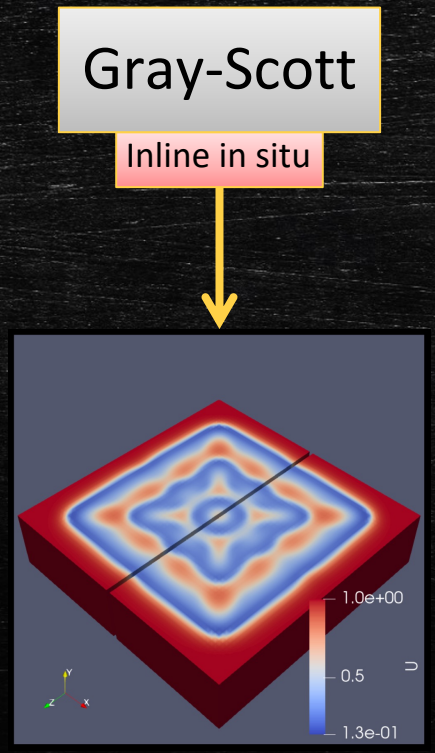
Run the code

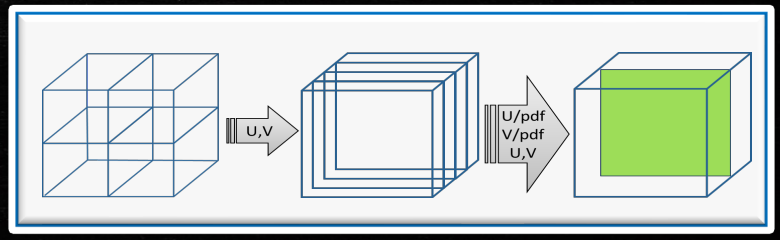



```
$ mpirun -n 4 ../../../bin/adios2-gray-scott settings-files.json : -n 1
../../../bin/adios2-pdf-calc gs.bp pdf.bp 100 : -n 1 python3 pdfplot.py -i pdf.bp :
-n 1 python3 gsplot.py -i gs.bp
```

Gray-Scott example

with inline in situ

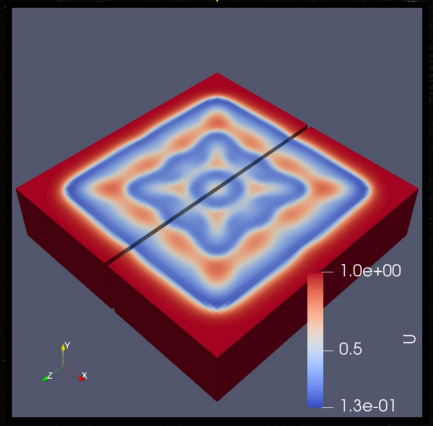




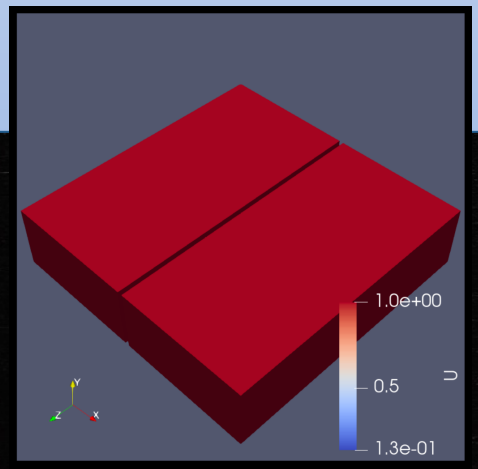
Run the code

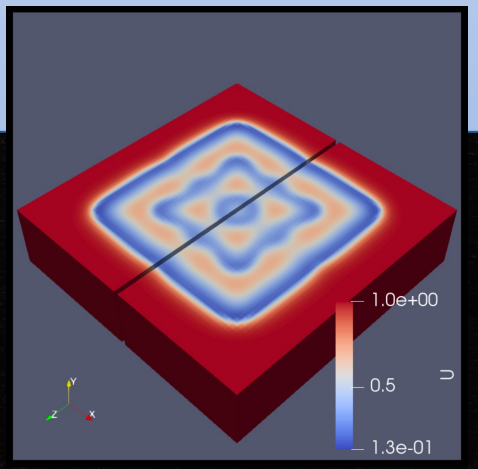
Gray-Scott

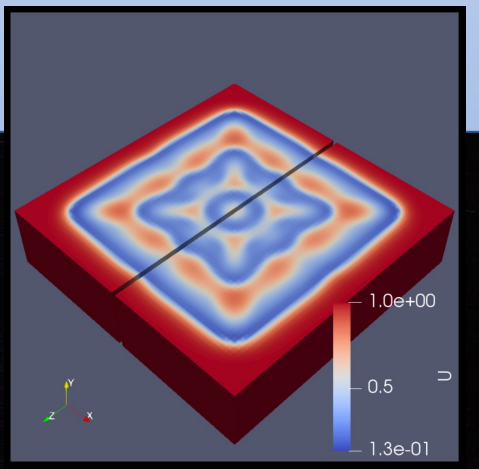
Inline in situ




```
$ ./cleanup.sh data
$ mpirun -n 4 ../../../bin/adios2-gray-scott settings-inline.json
       Catalyst Library Version: 2.0
       Catalyst ABI Version: 2
       Implementation: paraview
Simulation writes data using engine type:              plugin
…
Simulation at step 100 writing output step     1
(   1.781s) [pvbatch.0       ]         gs-pipeline.py:10    INFO| begin
'gs-pipeline'
(   2.418s) [pvbatch.0       ]         gs-pipeline.py:65    INFO| end
'gs-pipeline'
(   2.418s) [pvbatch.0       ]         gs-pipeline.py:52    INFO| in
'gs-pipeline::catalyst_execute'
$ eog . &
```

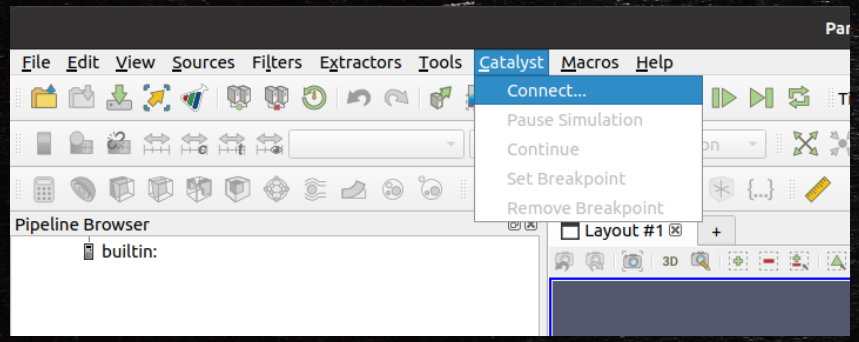




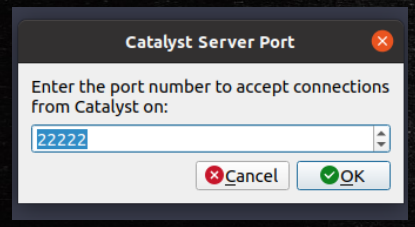


Setting up Catalyst Live in ParaView

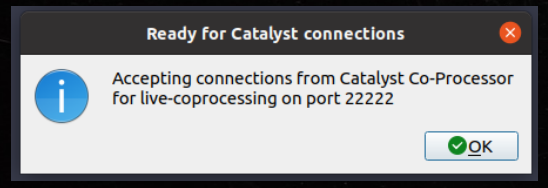
1. Connect to Catalyst



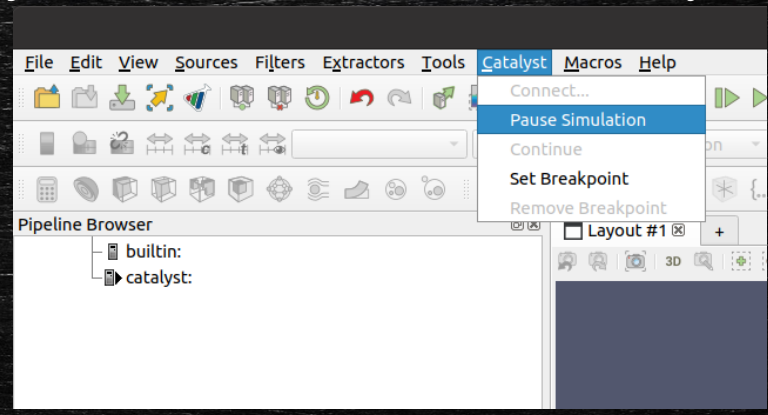
2. Enter the Port number.
We'll stick with the default 22222



3. Hit Okay. Catalyst Live is ready to connect to the simulation now.



4. Pause the simulation. This will ensure the simulation stops on the first step, so we can adjust the visualization if necessary

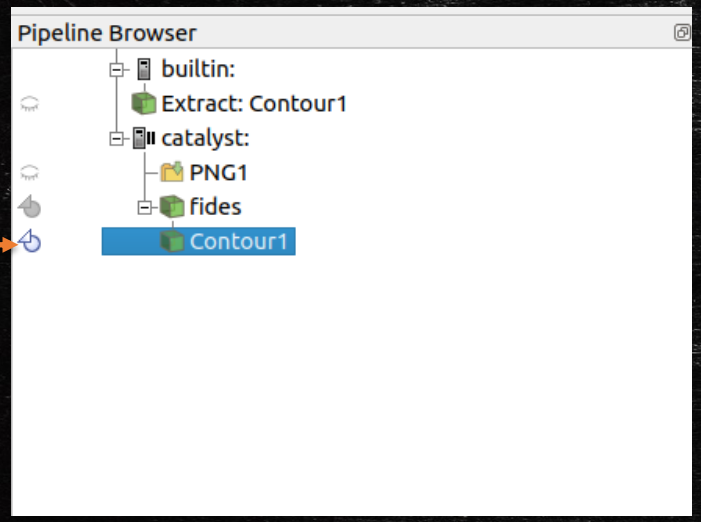


5. Run the simulation as before:

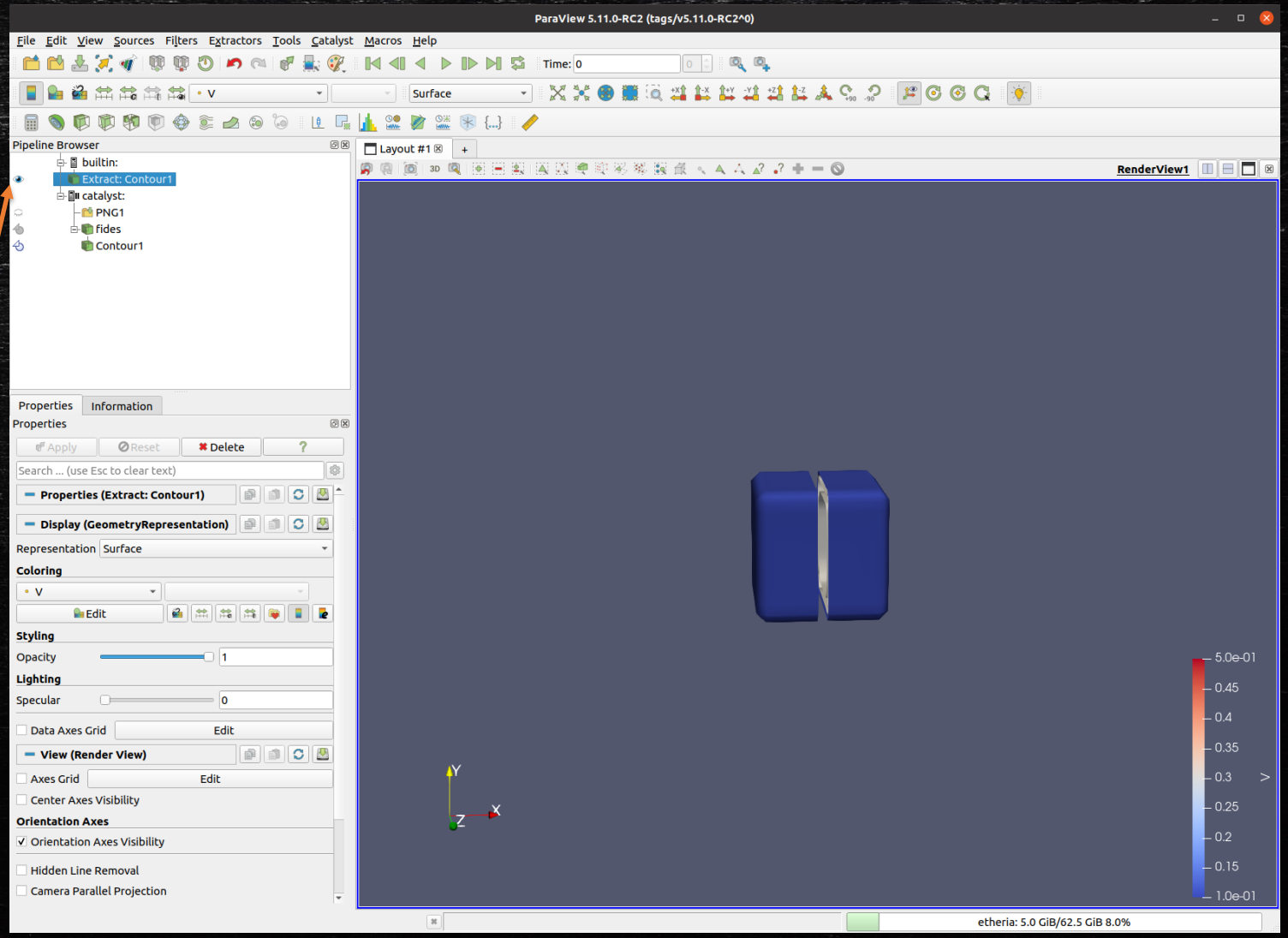
```
$ mpirun -n 4 ../../../bin/adios2-gray-scott settings-inline.json
```

Catalyst Live

6. Select an Extract

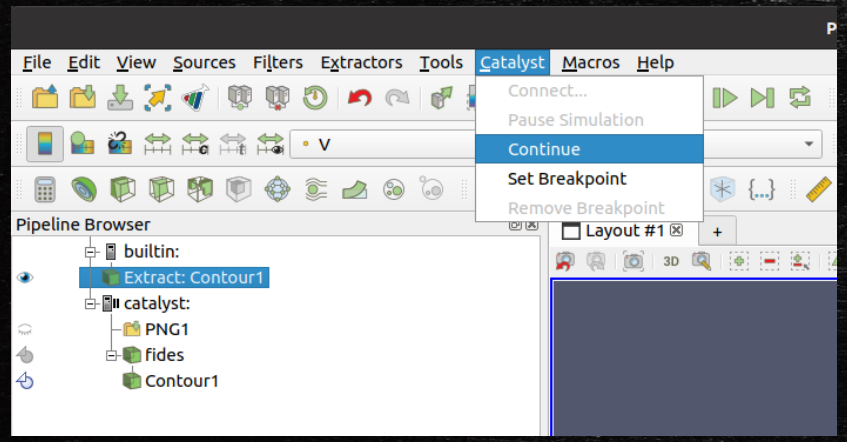


7. Toggle the visibility of the extract (”eye” button)

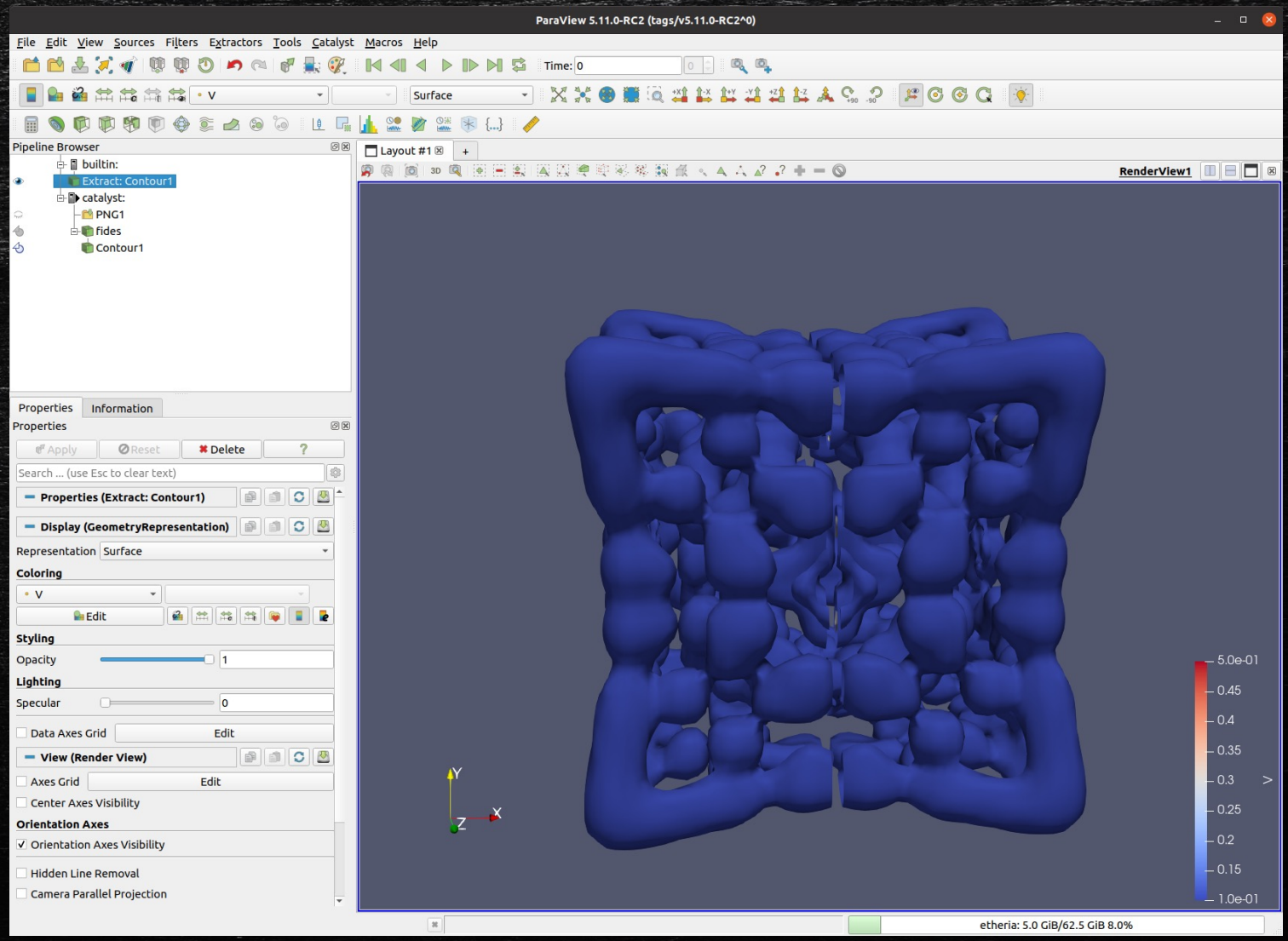


Catalyst Live

8. Continue the simulation from the Catalyst menu



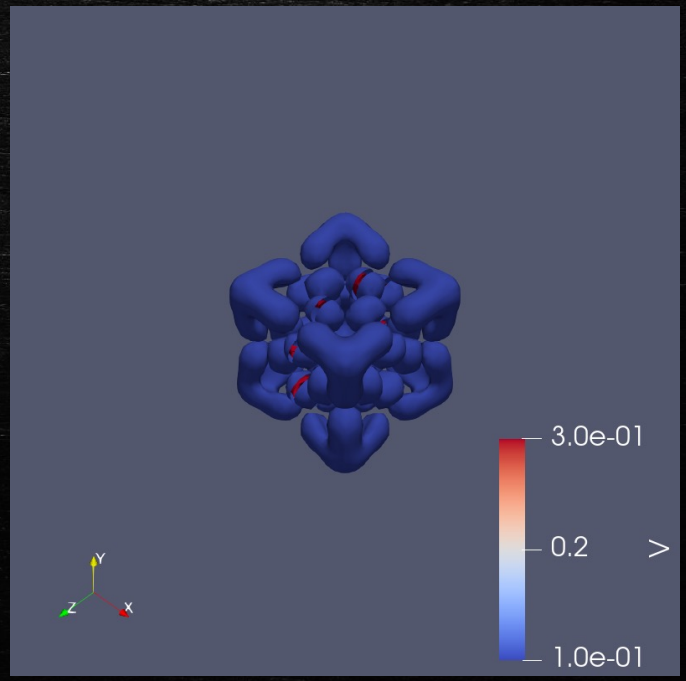
- Visualization will update as the simulation progresses.
- Can Pause/Continue as desired.
- Can add more filters to your pipeline



Hands-on Demo: Batch Visualization with ParaView and SST engine

- Batch visualization with a Python script (not using the GUI)
- Update settings-staging.json to use the adios2-fides-staging.xml
- Run from two terminals:
  $ mpirun -n 4 ../../../bin/adios2-gray-scott settings-files.json
  $ mpirun -n 2 pvbatch --force-offscreen-rendering catalyst/gs-pipeline.py –j catalyst/gs-fides.json –b gs.bp --staging

```
at 11:27:45 with caitlin.ross in share/adios2-examples/gray-scott took 22s
→ ls
adios2-fides-staging.xml  output-00014.png  output-00038.png  output-00062.png  output-00086.png
adios2-inline-plugin.xml  output-00015.png  output-00039.png  output-00063.png  output-00087.png
adios2.xml                output-00016.png  output-00040.png  output-00064.png  output-00088.png
catalyst                  output-00017.png  output-00041.png  output-00065.png  output-00089.png
ckpt.bp                   output-00018.png  output-00042.png  output-00066.png  output-00090.png
cleanup.sh                output-00019.png  output-00043.png  output-00067.png  output-00091.png
datasets                  output-00020.png  output-00044.png  output-00068.png  output-00092.png
decomp.py                 output-00021.png  output-00045.png  output-00069.png  output-00093.png
gs.bp                     output-00022.png  output-00046.png  output-00070.png  output-00094.png
gsplot.py                 output-00023.png  output-00047.png  output-00071.png  output-00095.png
output-00000.png          output-00024.png  output-00048.png  output-00072.png  output-00096.png
output-00001.png          output-00025.png  output-00049.png  output-00073.png  output-00097.png
output-00002.png          output-00026.png  output-00050.png  output-00074.png  output-00098.png
output-00003.png          output-00027.png  output-00051.png  output-00075.png  output-00099.png
output-00004.png          output-00028.png  output-00052.png  output-00076.png  pdfplot.py
output-00005.png          output-00029.png  output-00053.png  output-00077.png  README.md
output-00006.png          output-00030.png  output-00054.png  output-00078.png  settings-files.json
output-00007.png          output-00031.png  output-00055.png  output-00079.png  settings-inline.json
output-00008.png          output-00032.png  output-00056.png  output-00080.png  settings-staging.json
output-00009.png          output-00033.png  output-00057.png  output-00081.png  visit-bp4.session
output-00010.png          output-00034.png  output-00058.png  output-00082.png  visit-bp4.session.gui
output-00011.png          output-00035.png  output-00059.png  output-00083.png  visit-sst.session
output-00012.png          output-00036.png  output-00060.png  output-00084.png  visit-sst.session.gui
output-00013.png          output-00037.png  output-00061.png  output-00085.png
```



Summary

ADIOS brings a programming interface and a framework of many solutions to the generic problem of producing and consuming data

- The interface frees scientists from the limited scope of file-based data processing
  - Being fully applicable to file-based data processing
- Offering a bridge from their scientific workflows that work now to the future, where they will extend their workflows with
  - More efficient data processing
  - Interactive visualization
  - Code coupling
  - On-the-fly AI training
  - Combining experimental data with simulation data
- ADIOS + TAU gives scientists a way to monitor ADIOS performance along with writing ADIOS files and streams for on-line, off-line analytics of performance data
- ADIOS + Paraview gives scientists more advanced ways to investigate their data for on-line, off-line analytics