

# ADIOS: Storage and in situ I/O:

## Accelerating Scientific Knowledge Discovery with the Adaptable Input Output System

**Presenter:** S. Klasky<sup>123</sup>,

**With contributions from:** N. Podhorszki<sup>1</sup>, A. Gainaru<sup>1</sup>, M. Wolf<sup>1</sup>, C. Atkins<sup>8</sup>, William Godoy<sup>1</sup>, Matthew Wolf<sup>1</sup>, Ruonan Wang<sup>1</sup>, Chuck Atkins<sup>8</sup>, Greg Eisenhauer<sup>3</sup>, Junmin Gu<sup>7</sup>, Philip Davis<sup>5</sup>, W. Godoy<sup>1</sup>, Jong Choi<sup>1</sup>, Kai Germaschewski<sup>10</sup>, Kevin Huck<sup>11</sup>, Axel Huebl<sup>7</sup>, Mark Kim<sup>1</sup>, James Kress<sup>1</sup>, Tahsin Kurc<sup>1</sup>, Jeremy Logan<sup>1</sup>, Kshitij Mehta<sup>1</sup>, Franz Poeschel<sup>8</sup>, Eric Suchyta<sup>1</sup>, Keichi Takahashi, Lipeng Wan<sup>1</sup>, Pradeep Subedi, Mark Ainsworth<sup>19</sup>, Berk Geveci<sup>8</sup>, Ben Whitney<sup>1</sup>

Science and Mathematics Division

<sup>2</sup> University of Tennessee, Knoxville, Department of Electrical Engineering and Computer Science

<sup>3</sup> Georgia Tech, School of Computer Science

<sup>4</sup> New Jersey Institute of Technology

<sup>5</sup> Rutgers University

<sup>6</sup> National Science Foundation, OAC

<sup>7</sup> Lawrence Berkeley National Laboratory

<sup>8</sup> Kitware

<sup>9</sup> Brown University

<sup>10</sup> University of New Hampshire

<sup>11</sup> University of Oregon

<sup>1</sup> Oak Ridge National Laboratory, Computer

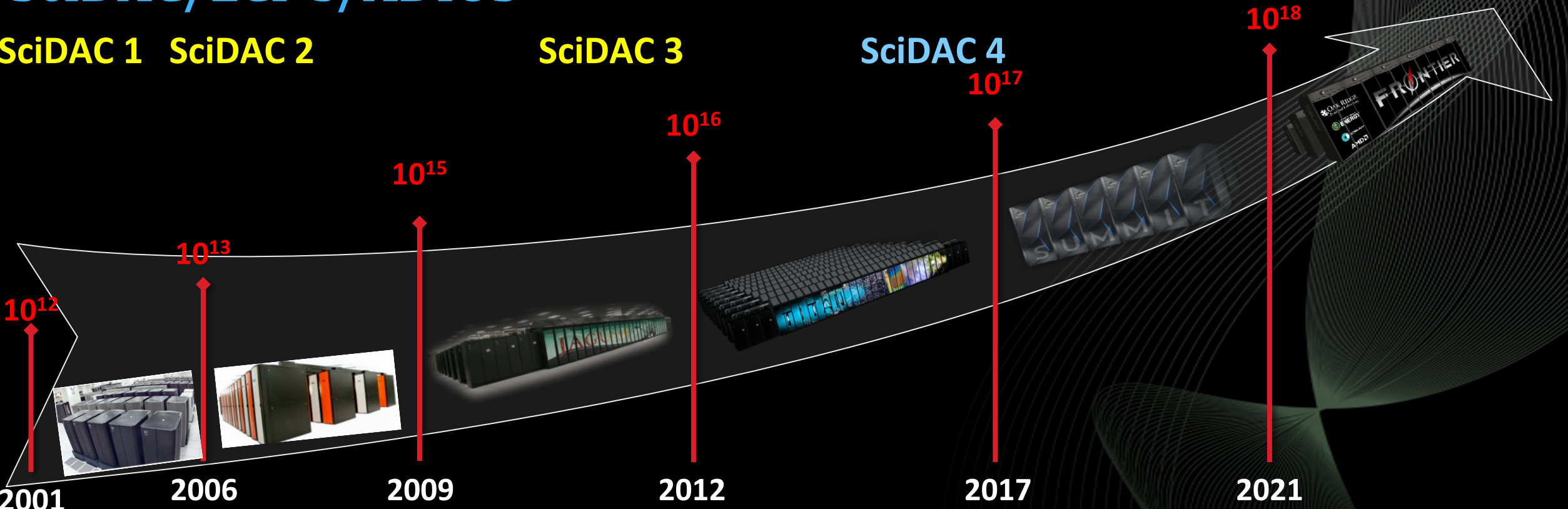
Community BOF, 3/30/2021

# SciDAC/LCF's/ADIOS

SciDAC 1   SciDAC 2

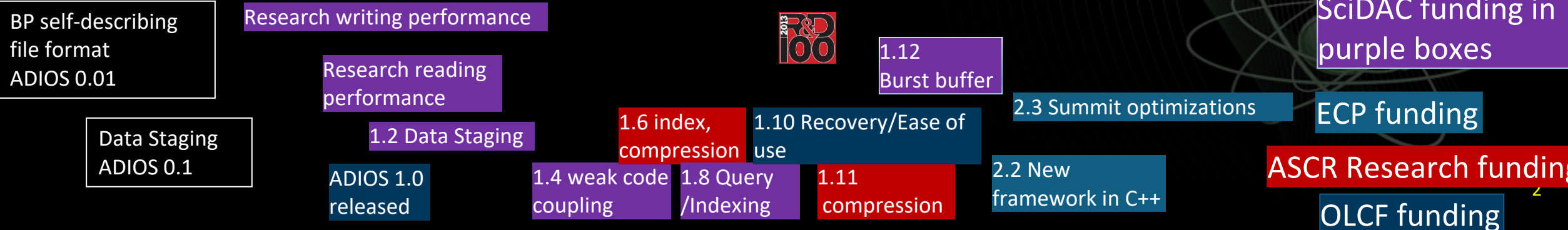
SciDAC 3

SciDAC 4



Seaborg: 20 TF   Jaguar: 25 TF   Jaguar 2: 2.3 PF   Titan: 27 PF   Summit: 200 PF   Frontier 1500 PF

## ADIOS timeline



SciDAC funding in purple boxes

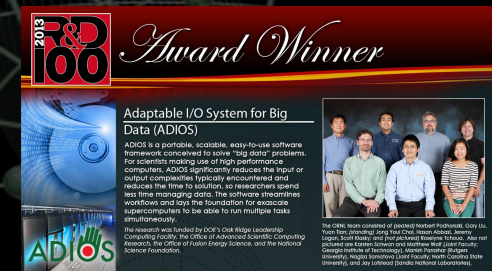
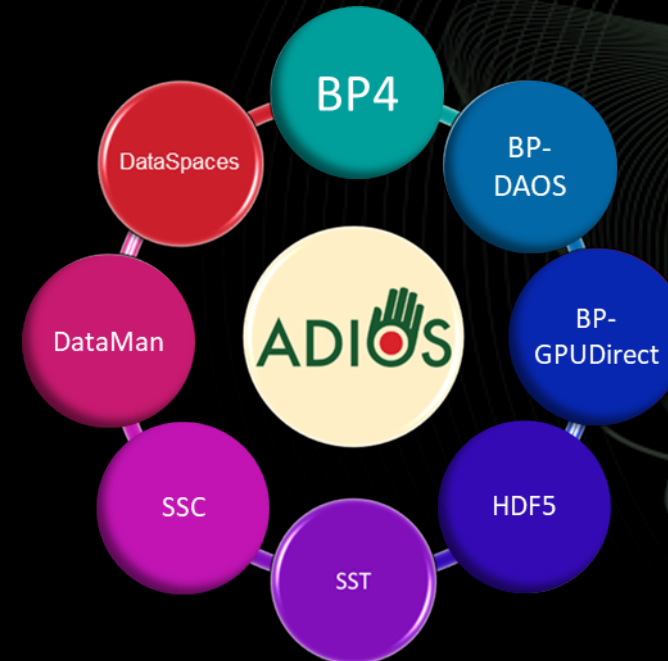
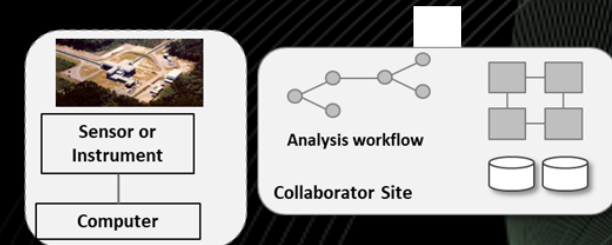
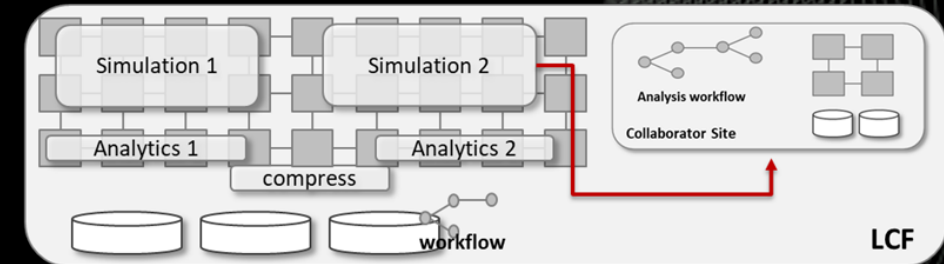
ECP funding

ASCR Research funding

OLCF funding

# ADIOS: High-Performance Publisher/Subscriber I/O framework

- An abstraction to allow for high-performance I/O to/from storage and for in situ processing
- Utilizes a publish/subscribe mechanism with self-describing data
- **Optimized I/O engines for C/R, strong/loose in situ coupling WAN data streaming, and in-memory object storage**
  - Fast Writing/Reading: BP4
  - DAOS optimizations: BP-DAOS
  - Write from GPU: BP-GPUDirect
  - Compatibility with HDF5: HDF5
  - Weak Code Coupling: SST
  - Tight Code Coupling: SSC
  - WAN streaming: DataMan
  - In memory object store: DataSpaces
  - Works with ECP reduction libs: MGARD, SZ, ZFP
- Typical for applications to achieve > 1 TB/s on Summit





# Sustainability: is a primary goal of the ADIOS project



- Nightly testing
  - Testing on many different platforms
- Continuous Integration
  - Only allow tested code to be merged
  - Almost 2,000 tests for each commit
- Static and dynamic analysis reports
  - Compile-time and run-time analysis
- Code coverage
  - Level of testing
- External testing
  - Allow feedback from user projects

Nightly testing on target HPC platforms

Nightly		Update	Configure		Build		Test		
Site ^	Build Name	Revision	Error	Warn	Error	Warn	Not Run	Fail	Pass
aaargh.kitware.com	Linux-EL7_GCC7	237f1b	0	0	0	0	0	0	95
aaargh.kitware.com	Linux-EL7_Intel17	237f1b	0	0	0	0	0	0	95
aaargh.kitware.com	Linux-EL7_Intel18	237f1b	0	0	0	0	0	0	95
aaargh.kitware.com	Linux-EL7_GCC7_MPICH	237f1b	0	0	0	0	1	0	203
aaargh.kitware.com	Linux-CrayCLE6-KNL_GCC_CrayMPICH	237f1b	0	0	0	0	1	0	203
cori.nersc.gov	Linux-CrayCLE6-KNL_Intel_CrayMPICH	237f1b	0	0	0	0	0	61	123
cori.nersc.gov	Linux-EL7-PPC64LE_GCC-7.1.0_NoMPI	237f1b	0	0	0	0	0	6	88
summitdev.ccs.ornl.gov			0	0	0	0	0		

coverage report

Coverage started on Friday, September 28 2018

Coverage Summary		Coverage Legend	
Total Coverage	72.75%	Satisfactory coverage	
Tested lines	10703	Unsatisfactory coverage	
Untested lines	4010	Dangerously low coverage	
Files Covered	166 of 166		
Files Satisfactorily Covered	122		
Files Unsatisfactorily Covered	44		

Show coverage over time

Directories (32) | No Executable Code (0) | Zero (11) | Low (11) | Medium (29) | Satisfactory (74) | Complete (41) | All (166) Show Filters

Show 25 entries

Directory	Status	Percentage	Lines not covered	Priority	Labels
source/adios2/toolkit/aggregator/mpl	Satisfactory	93.14%	12/175	None	
source/adios2/engine/institumpi	Satisfactory	93.08%	54/760	None	
source/adios2/engine/bp3	Satisfactory	91.45%	26/304	None	
source/adios2/toolkit/sst/dp	Satisfactory	87.86%	34/280	None	
source/adios2/toolkit/format/bp3	Satisfactory	85.29%	350/2380	None	
source/adios2/toolkit/sst/cp	Satisfactory	84.33%	376/2400	None	
source/adios2	Satisfactory	83.33%	6/36	None	
source/adios2/toolkit/format/dataman	Satisfactory	82.52%	50/286	None	
source/adios2/engine/dataman	Satisfactory	82.25%	41/231	None	
source/adios2/toolkit/transport/wan	Satisfactory	81.05%	29/153	None	
source/adios2/toolkit/transportman/dataman	Satisfactory	80.95%	24/126	None	
source/adios2/engine/sst	Satisfactory	80.71%	65/337	None	
bindings/CXX11/cxx11	Satisfactory	79.37%	26/126	None	
source/adios2/core	Satisfactory	74.46%	238/932	None	
source/adios2/toolkit/transportman	Satisfactory	74.03%	40/154	None	
source/adios2/engine/hdf5	Satisfactory	71.52%	47/165	None	
source/adios2/operator/calback	Satisfactory	71.43%	4/14	None	
bindings/Python	Satisfactory	70.83%	112/384	None	
source/adios2/toolkit/format	Satisfactory	70.00%	3/10	None	
source/adios2/toolkit/transport/file	Medium	63.10%	124/336	None	
bindings/fortran/f2c	Medium	62.60%	135/361	None	
source/adios2/helper	Medium	59.69%	472/1171	None	
source/adios2/bp2	Medium	58.01%	451/1074	None	
source/adios2/toolkit/transport	Medium	56.67%	26/60	None	
source/adios2/toolkit/interophdf5	Satisfactory	56.39%	297/681	None	

Showing 1 to 25 of 32 entries

First | Previous | 1 | 2 | Next | Last

Add more commits by pushing to the `sst-bp-compression-tests` branch on [JasonRuonanWang/ADIOS2](#).

**All checks have passed** [Hide all checks](#)  
13 successful checks

**Codacy/PR Quality Review** — Up to standards. A positive pull request. [Details](#)

**cdash** — Build and test results available on CDash [Required](#) [Details](#)

**ci/circleci: el7** — Your tests passed on CircleCI! [Required](#) [Details](#)

**ci/circleci: el7-gnu7** — Your tests passed on CircleCI! [Required](#) [Details](#)

**ci/circleci: el7-gnu7-openmpi** — Your tests passed on CircleCI! [Required](#) [Details](#)

**This branch has no conflicts with the base branch**  
Merging can be performed automatically.

[Merge pull request](#) or view [command line instructions](#).



# ADIOS Approach: “How”

- I/O calls are of **declarative** nature in ADIOS
  - which process writes what: add a local array into a global space (virtually)
  - `adios_close()` indicates that the user is done declaring all pieces that go into the particular dataset in that timestep
- 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

# Creating I/O abstractions to accelerate I/O to storage

- One change in the code or input file, to specify the engine

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

```
writer.BeginStep()
```

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

```
writer.EndStep()
```

```
writer.Close()
```

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

```
reader.BeginStep()
```

```
adios2::Variable<double> T =  
reader.InquireVariable("Temperature");
```

```
std::vector<double> t;
```

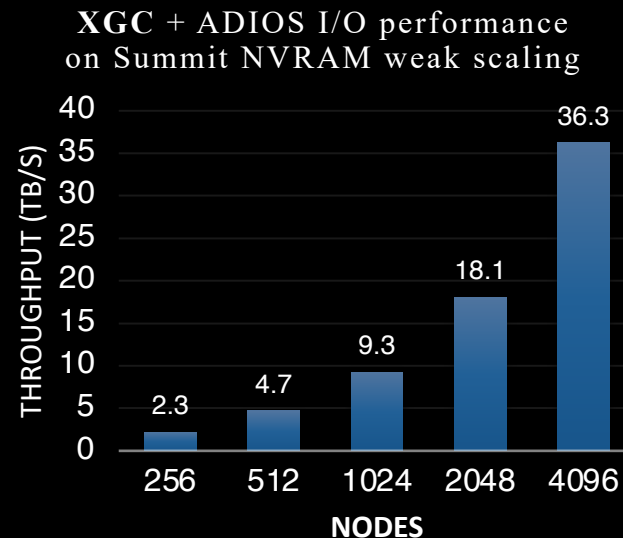
```
reader.Get(varT, t);
```

```
reader.EndStep()
```

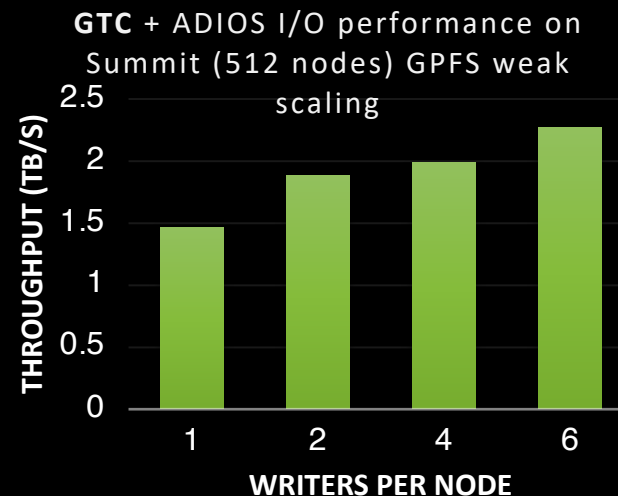
```
reader.Close()
```

The APIs are identical for code coupling

36.3 TB/s to NVRAM



2.3 TB/s to GPFS



# ADIOS performance results (measured by the app teams/not us)

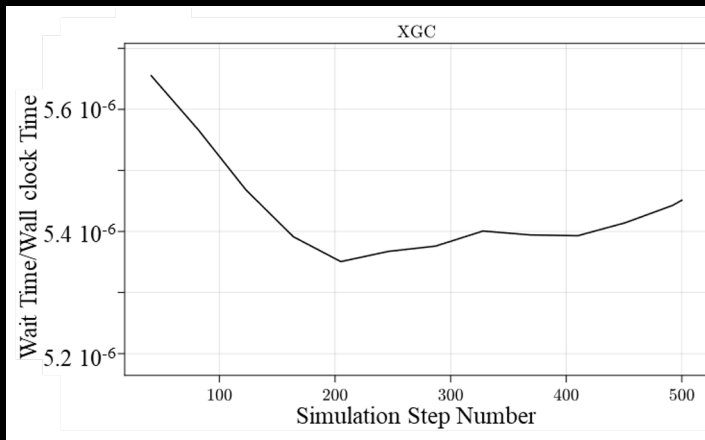
## WDMApp

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

From the WDMApp annual ECP review

XGC on 512 Summit nodes  
GENE on 6 Summit nodes  
 $N_m = 9,640,480$  vertices  
 $N_p = 8,922$  particles/vertex  
Timestep = 61.4 seconds.

XGC wait time during charge coupling



Contact: Amitava Bhattacharjee (PPPL)

## E3SM-MMF

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

ADIOS 2.x Port is integrated into master SCORPIO

SCREAM project evaluated it on their own and found 4-5x improvement in IO using ADIOS for TBs of data

New I-Case stresses IO

I-Case benchmark on Summit



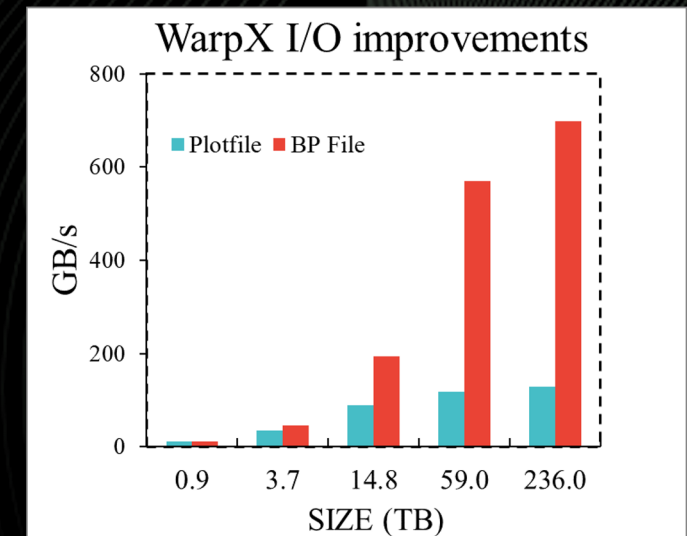
Simulating 1 day, 5 days and 10 days  
Writing data every simulated hour  
Run on Summit, 1344 MPI processes

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

## WarpX

BP4 improved append performance for ADIOS and now applications can see the benefits of that

WarpX and in general, OpenPMD users can get high throughput



WarpX on Summit, weak scaling  
6 GPUs, up to 256 nodes  
ADIOS vs original AMReX Plot files

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

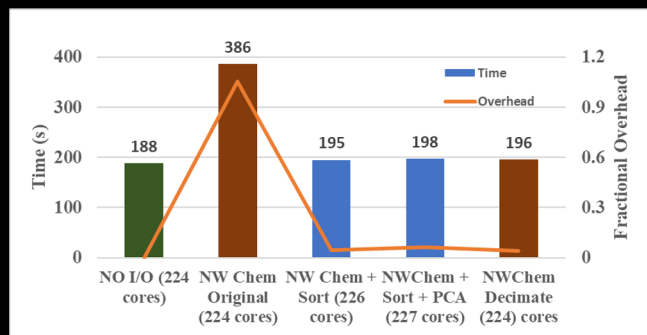
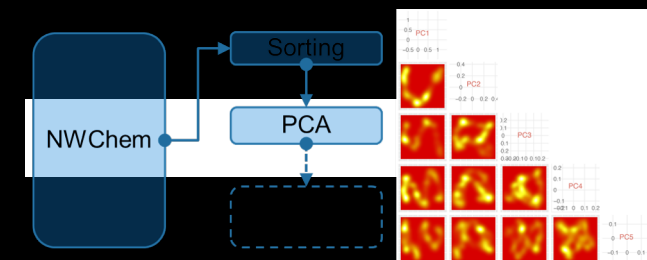


# ADIOS performance results (measured by the app teams/not us)

## NWChem

In situ sorting of atom trajectories can save 50% of runtime

Motion correction with PCA analysis (pbdR script) in situ



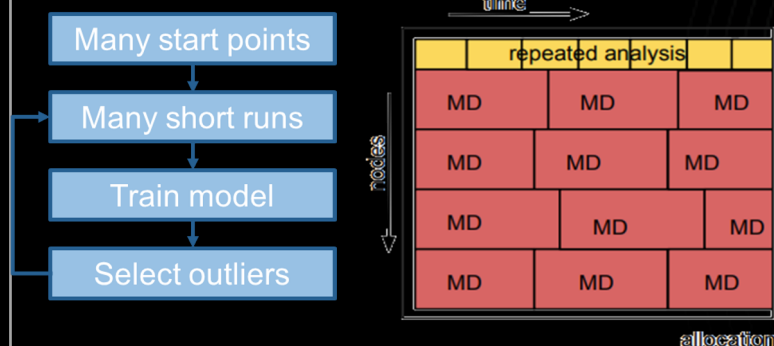
Contact: Tjerk Straatsma (ORNL)

## CANDLE/DeepDriveMD

CODAR collaboration for accelerating sampling of macromolecule potential energy surface via online coupling

Many concurrent MD runs + online training + inference (outlier search)

ADIOS for async collection of MD results to training allows for continuous simulation running and training



Contact: Arvind Ramanathan,  
Igor Yakushin (ANL)

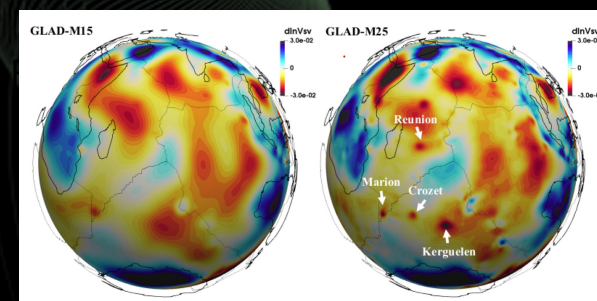
## Specfem3D\_globe

The Adaptable Seismic Data Format (ASDF) was developed that leverages the Adaptable I/O System (ADIOS) parallel library.

It allows for recording, reproducing, and analyzing data on large-scale supercomputers

1.5 PB of data is produced in every workflow step, which is fully processed later in adjoint simulation

<https://www.olcf.ornl.gov/2019/07/05/tromp-titan/>



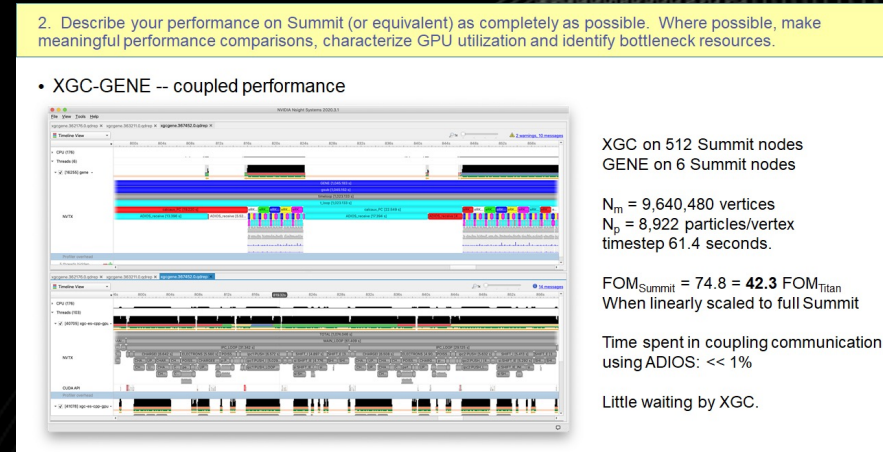
Global adjoint tomography—model GLAD-M25, Geophysical Journal International, Volume 223, Issue 1, October 2020, Pages 1–21, <https://doi.org/10.1093/gji/ggaa253>

Contact: Jeroen Tromp, Princeton University

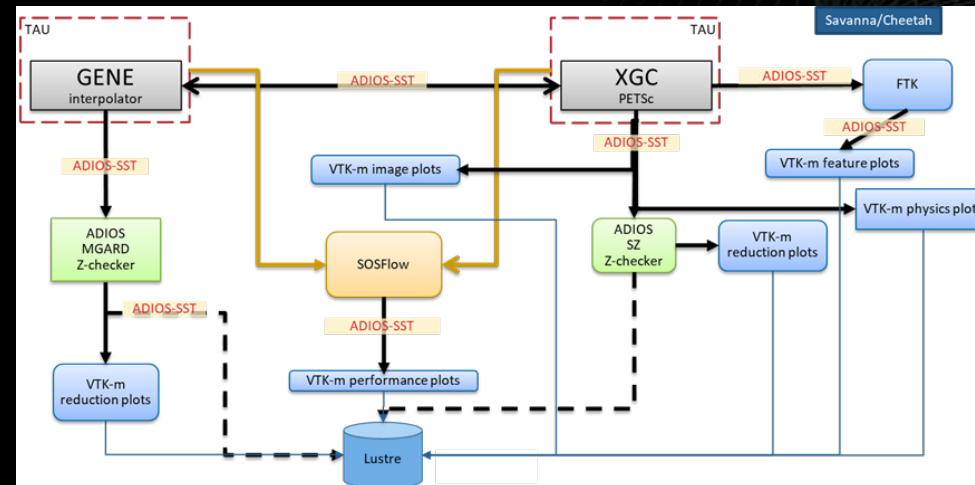
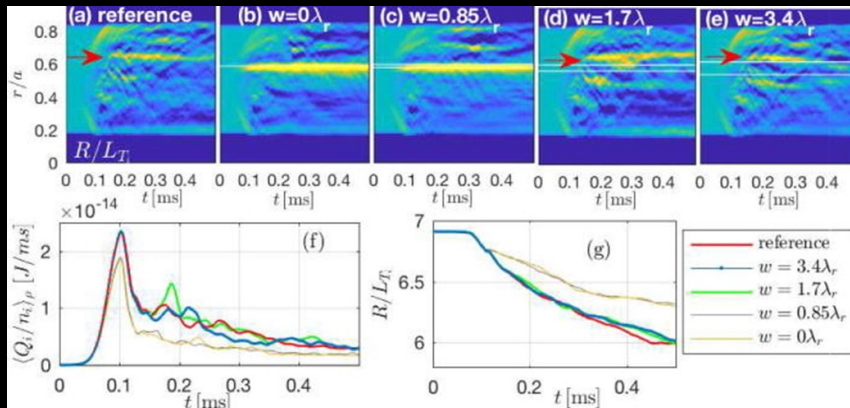
## 2.2.2.05 ADSE12-WDMApp: High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas

PI: Amitava Bhattacharjee, PPPL,  
C. S. Chang, PPPL

- Different physics solved in different physical regions of detector (spatial coupling)
- Core simulation: **GENE**  
Edge simulation: **XGC**  
Separate teams, **separate codes**
- Recently demonstrated first-ever successful kinetic coupling of this kind
- Data Generated by one coupled simulation is predicted to be > 10 PB/day on Summit



From FY21 WDMApp Review



Dominski, J., et al. "Spatial coupling of gyrokinetic simulations, a generalized scheme based on first-principles." *Physics of Plasmas* 28.2 (2021): 022301.

Merlo, G., et al. "First coupled GENE-XGC microturbulence simulations." *Physics of Plasmas* 28.1 (2021): 012303.

Cheng, Junyi, et al. "Spatial core-edge coupling of the particle-in-cell gyrokinetic codes GEM and XGC." *Physics of Plasmas* 27.12 (2020): 122510.



# Results: Seismic Tomography Workflow (PBs of data/run)

PI: Jeroen Tromp, Princeton

## Scientific Achievement

- Most detailed **3-D model of Earth's** interior showing the entire globe from the surface to the core–mantle boundary, a depth of 1,800 miles

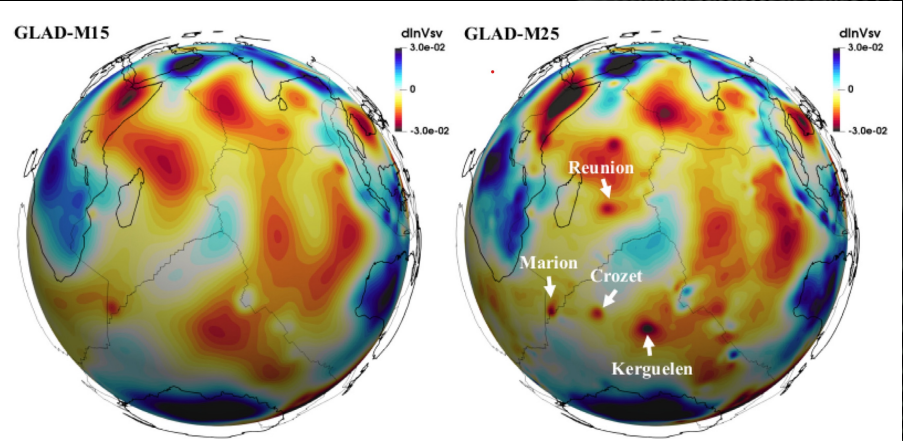
## Significance and Impact

- Updated (transversely isotropic) global seismic model GLAD-M25 where no approximations were used to simulate how seismic waves travel through the Earth. The data sizes required for processing 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.

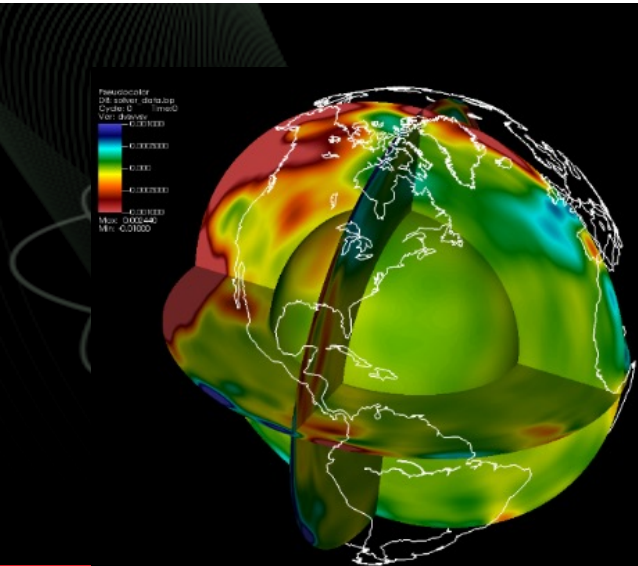
## Improvement by appending steps

- 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



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.



Wenjie Lei, Youyi Ruan, Ebru Bozdağ, Daniel Peter, Matthieu Lefebvre, Dimitri Komatitsch, Jeroen Tromp, Judith Hill, Norbert Podhorszki, David Pugmire **Global adjoint tomography—model GLAD-M25**, Geophysical Journal International, Volume 223, Issue 1, October 2020, Pages 1–21, <https://doi.org/10.1093/gji/ggaa253>



## **FES Highlight:** Established capability for near-real time networked analysis of big KSTAR data at NERSC (PPPL, ORNL, ESnet, NERSC, KSTAR, KISTI)

### Objectives

- 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

### Impact

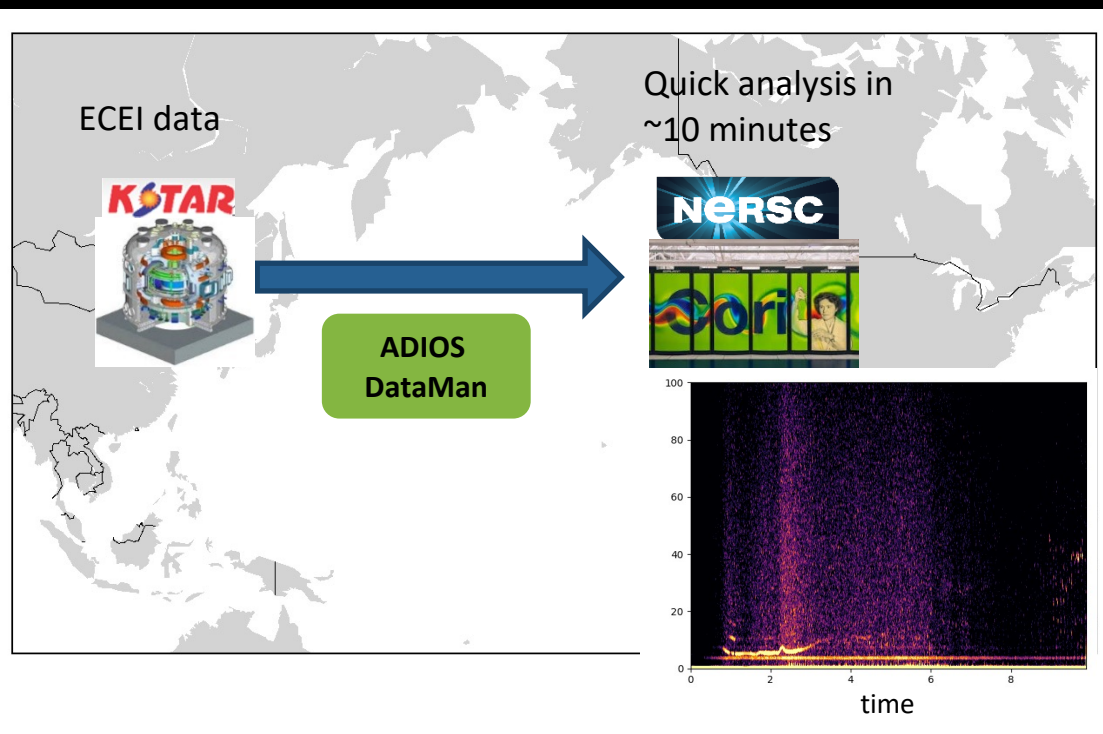
- Created a framework to enable US fusion researchers to have broader and faster access to the KSTAR data, enabling
  - Faster analysis of data
  - Faster and autonomous utilization of ML/AI algorithms for incoming data
  - More informed steering of experiment
  - Quicker utilization of US HPC for KSTAR collaboration

### Accomplishments


- Created end-to-end Python framework DELTA, streams data using ADIOS DataMan over WAN (at rates > 4 Gbps), asynchronously processes on multiple workers with MPI multi-threading
- Applied to KSTAR streaming data to NERSC Cori. Reduces time for an ECEi analysis from 12 hours on single-process to 10 minutes on 6 Cori nodes.
- Implemented deep convolutional neural networks for working with multi-scale fusion data, e.g. ECEi, for recognizing events of interest.<sup>2</sup>
- On-going: improve “adaptive” nature of data stream: adaptive compression at KSTAR source

Churchill RM, Klasky et al. A Framework for International Collaboration on ITER Using Large-Scale Data Transfer to Enable Near-Real-Time Analysis. Fusion Science and Technology. 2021 Feb 17;77(2):98-108

<sup>2</sup>R.M. Churchill, NeurIPS 2019







**Energy Exascale  
Earth System Model**

Select Language

[GitHub](#)
[ESGF](#)

ABOUT
RESEARCH
MODEL
DATA
PUBLICATIONS
RESOURCES

## ABOUT

**Vision and Mission**  
Long Term Roadmap  
Science Drivers

**Organization**  
The Leadership Team  
NGD Sub-Projects  
NGD Atmospheric Physics  
NGD Land and Energy  
NGD Nonhydrostatic Atmosphere  
NGD Software and Algorithms  
NGD BISICLES  
NGD Coastal Waves

**Events**  
E3SM Conferences  
2019 E3SM Spring Meeting  
E3SM Tutorials  
All-Hands Presentations

**Collaboration**  
Collaboration Request  
Ecosystem Projects  
Closely Related Projects

**News**

Home > About > News > PIO2 + ADIOS = Performance Improvement

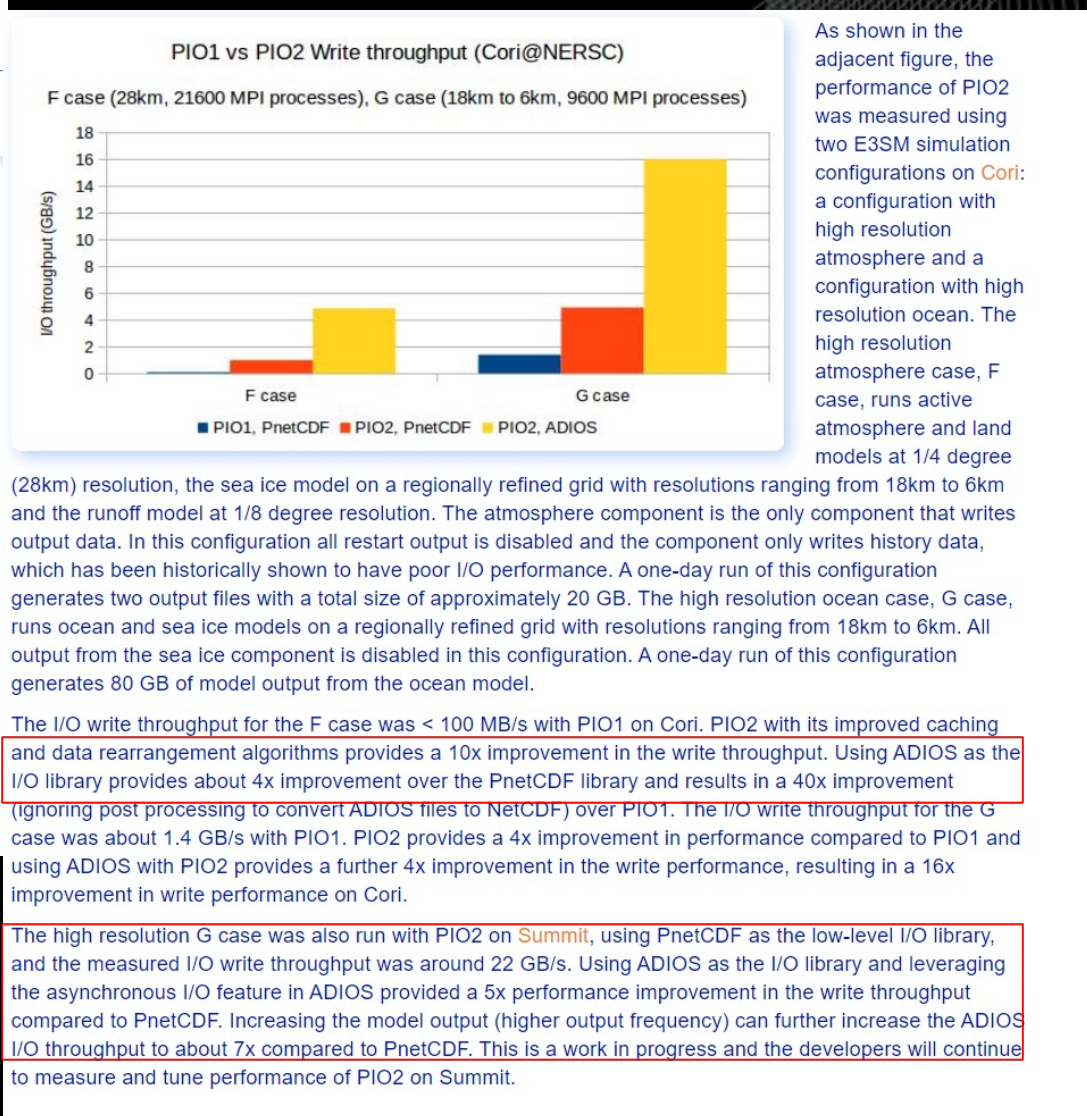
## PIO2 + ADIOS = PERFORMANCE IMPROVEMENT

August 8, 2019

Releases

The **Parallel Input/Output (I/O) library (PIO)** is used by all the model components in E3SM for reading input and writing model output. The library supports reading and writing data using low-level I/O libraries like PnetCDF and NetCDF. The user data in E3SM is not typically decomposed across the compute processes in an "I/O friendly" way and this requires some data rearrangement, supported by PIO, before using these low-level I/O libraries to write the model data. PIO2 is the latest version of the PIO library that includes a complete rewrite of the original Fortran PIO (PIO1) library into C/C++. PIO2 also supports advanced caching and data rearrangement algorithms and includes support for more low-level I/O libraries.

In recent months developers added support in PIO to read and write data using the The Adaptable I/O System (ADIOS) library. The ADIOS library provides a flexible way to describe scientific data that may be read, written or processed outside a simulation. The library supports MPI individual I/O, MPI collective I/O, POSIX I/O, asynchronous I/O and a visualization engine to process scientific data. The library also supports a NULL output option to disable all model output. The data is written out in the ADIOS file format (which uses the .bp extension) and can be converted to the NetCDF format using a post processing tool included with PIO. Since the user data is decomposed across multiple compute processes it typically requires some data rearrangement in PIO or the low level I/O libraries to write the data efficiently in contiguous chunks, as required by the NetCDF format. Since ADIOS writes data out in multiple files and does not require data to be written out in contiguous chunks, it saves time by partially rearranging data and reducing contention in the file system.



<https://e3sm.org/pio2-adios-performance-improvement/>



## WORLD'S FASTEST SUPERCOMPUTER PROCESSES HUGE DATA RATES IN PREPARATION FOR MEGA-TELESCOPE PROJECT

Wang, Ruonan, et al. "Processing full-scale square kilometre array data on the summit supercomputer." *2020 SC20: International Conference for High Performance Computing, Networking, Storage and Analysis (SC)*. IEEE Computer Society, 2020.

HOME / WORLD'S FASTEST SUPERCOMPUTER PROCESSES HUGE DATA RATES IN PREPARATION FOR MEGA-TELESCOPE PROJECT

SHARE ARTICLE: [TWITTER](#) [FACEBOOK](#)

TAGS

BIG DATA

OAK RIDGE NATIONAL LABORATORY

SHANGHAI ASTRONOMICAL OBSERVATORY

SHAO

SKA-LOW

SQUARE KILOMETRE ARRAY

SUMMIT

SUPERCOMPUTING

October 22, 2019

Scientists have processed 400 gigabytes of data a second as they tested data pipelines for the Square Kilometre Array (SKA) telescope.

Researchers from ICRAR in Perth, Oak Ridge National Laboratory in the US and Shanghai Astronomical Observatory in China used the world's most powerful supercomputer—Summit—to process simulated observations of the early Universe ahead of the radio telescope being built in Western Australia and South Africa.

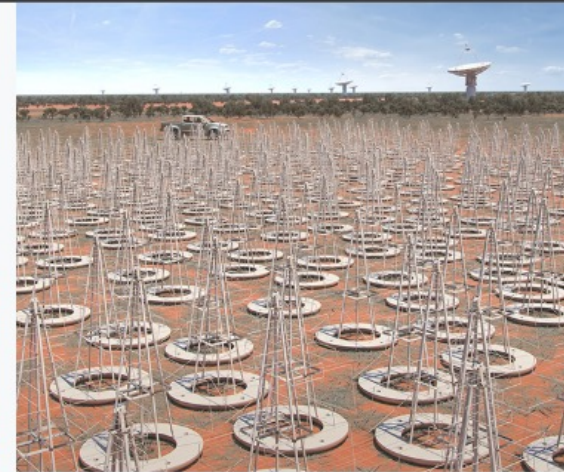


Summit — Oak Ridge National Laboratory's 200 petaflop supercomputer. Credit: Oak Ridge National Laboratory.

The data rate achieved was the equivalent of more than 1600 hours of standard definition YouTube videos every second.

Professor Andreas Wicenec, the director of Data Intensive Astronomy at the International Centre for Radio Astronomy Research (ICRAR), said it was the first time radio astronomy data has been processed on this scale.

"Until now, we had no idea if we could take an algorithm designed for processing data coming from today's radio telescopes and apply it to something a thousand times bigger," he said.



Computer generated image of what the SKA-low antennas will look like in Western Australia. Credit: SKA Project Office.

The billion-dollar SKA is one of the world's largest science projects, with the low frequency part of the telescope set to have more than 130,000 antennas in the project's initial phase, generating around 550 gigabytes of data every second.

Summit is located at the US Department of Energy's Oak Ridge National Laboratory in Tennessee.

It is the world's most powerful scientific supercomputer, with a peak performance of 200,000 trillion calculations per second.

Oak Ridge National Laboratory software engineer and researcher Dr Ruonan Wang, a former ICRAR PhD student, said the huge volume of data used for the SKA test run meant the data had to be generated on the machine itself.

"We used a sophisticated software simulator written by scientists at the University of Oxford, and gave it a cosmological model and the array configuration of the telescope so it could generate data as it would come from the telescope observing the sky," he said.

"Usually this simulator runs on just a single computer, generating only a small fraction of what the SKA would produce.

"So we used another piece of software written by ICRAR, called the Data Activated Flow Graph Engine (DALiUGe), to distribute one of these simulators to each of the 27,648 graphics processing units that make up Summit.

"We also used the Adaptable IO System (ADIOS), developed at the Oak Ridge National Laboratory, to resolve a bottleneck caused by trying to process so much data at the same time."

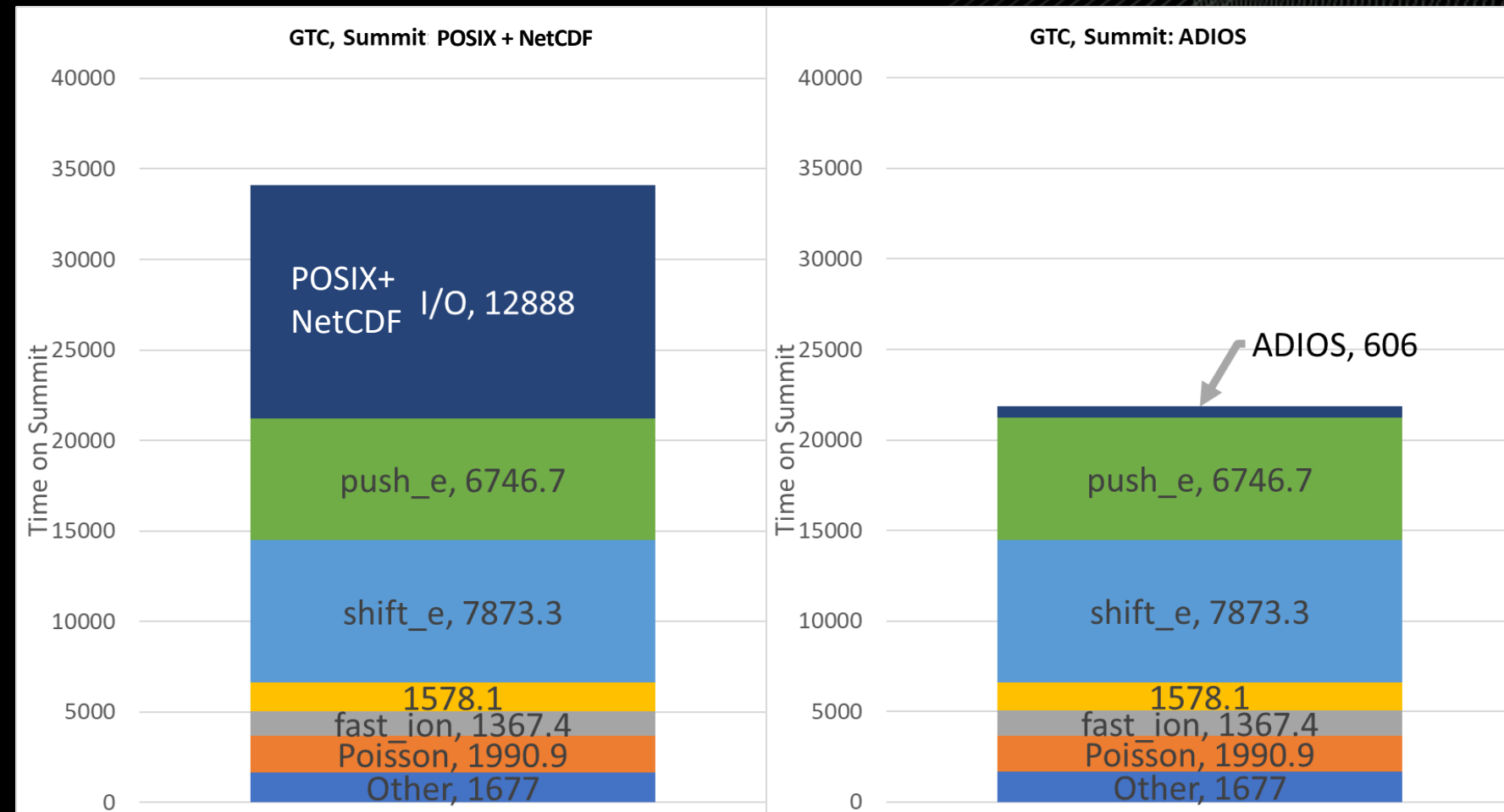
The test run used a cosmological simulation of the early Universe at a time

ANDREAS  
WICENEC,  
ICRAR, PI

2020 Gordon Bell  
Nominee



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



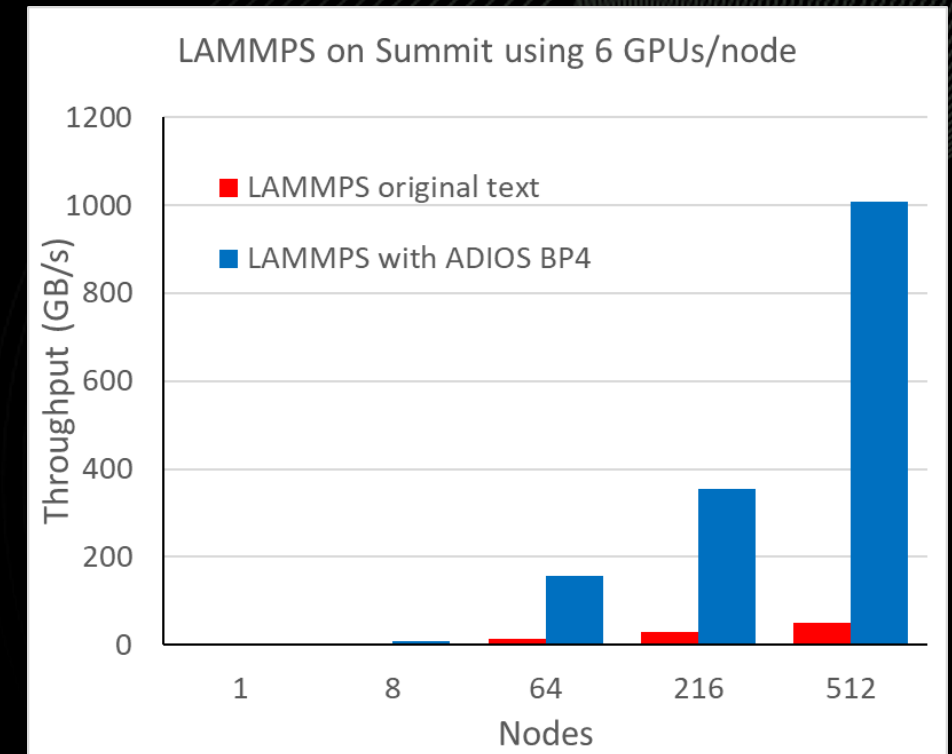
# Results: LAMMPS

PI: Steve Plimpton, Sandia

<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
- Concurrent reading is enabled

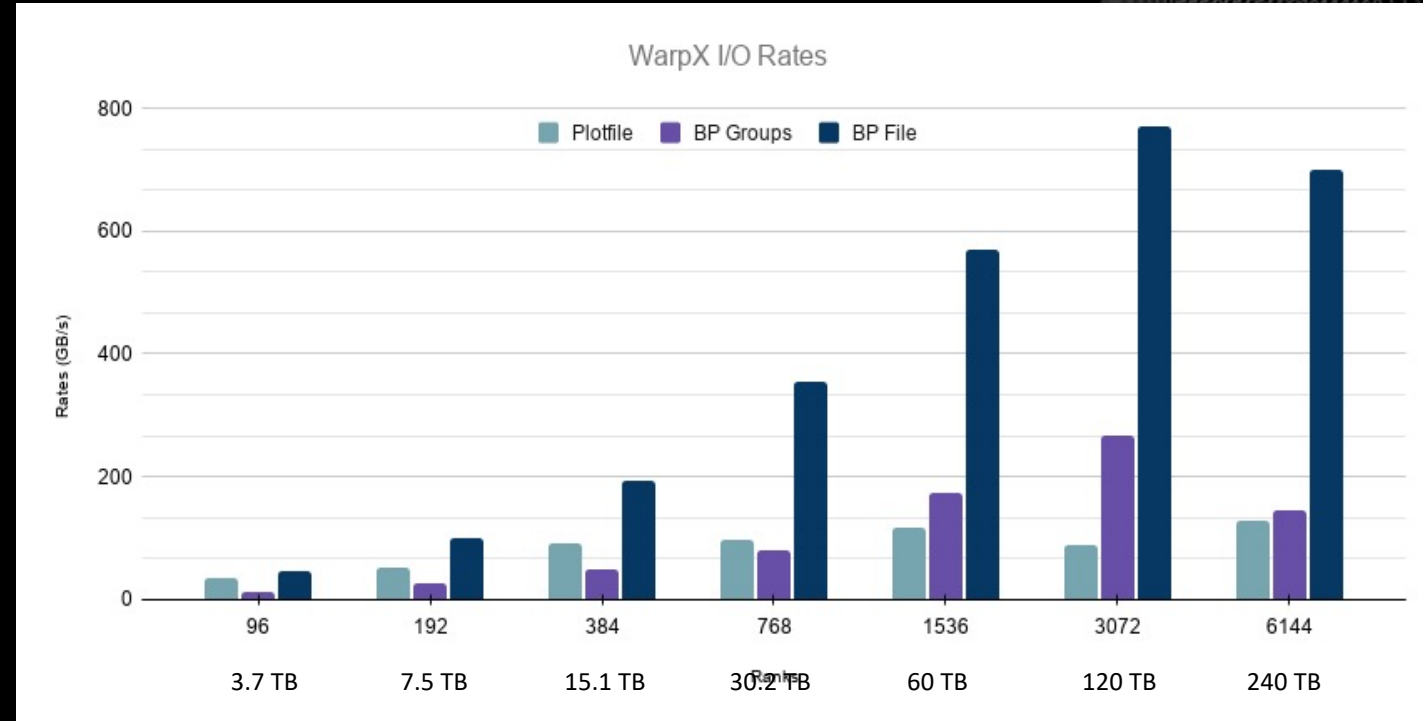
Results from ECP EXAALT Q4/FY19  
milestone report (for 2.2.1.04 EXAALT  
ADSE04-54)  
Summit 512 nodes  
12B atoms, 5 TB



# Results: WarpX

PI: Jan-Luc Vay, LBNL

- BPFile:
  - BP4: Use one file for all outputs.
- BPGroups:
  - BP3: Use one file / timestep
- Plot:
  - The AMReX plot file.
- One way to improve the I/O performance, is to use one ADIOS file for all time steps



Summit, 6 GPUs, 6 cores per node, up to 1024 nodes



# Writing performance is great but what about reading?

- Codes such as the WarpX code, which uses AMReX can take advantage of ADIOS-BP4 for “fast” writing
- The challenge is reading
- Development of a clustering algorithm for WarpX/AMReX data for fast writing/reading performance

