Managing Large-Scale Data Using ADIOS

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Knoxville, TN

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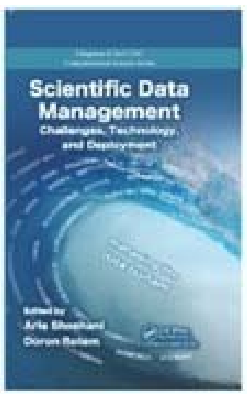
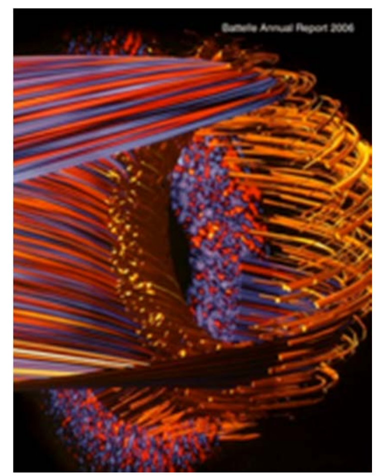




Outline

- ADIOS Introduction
- ADIOS Write API
- Hands-on 1, Write data with ADIOS
- Hands-on 1, Tools
- ADIOS Read API
- Hands-on 1, Read data with ADIOS
- Hands-on 1++, Spatial aggregation
- Hands-on 2, ADIOS Write API (Non-XML version)
- Hands-on 4, Multi-block writing with non-XML API
- Hands-on 3, Staging example
- Hands-on 4, Visualization of ADIOS data
- Hands-on 5, I/O skeleton generation with Skel
- ADIOS + Matlab
- Hands-on 8 Python
- Hands-on 9, Java
- Summary

ADIOS Participants

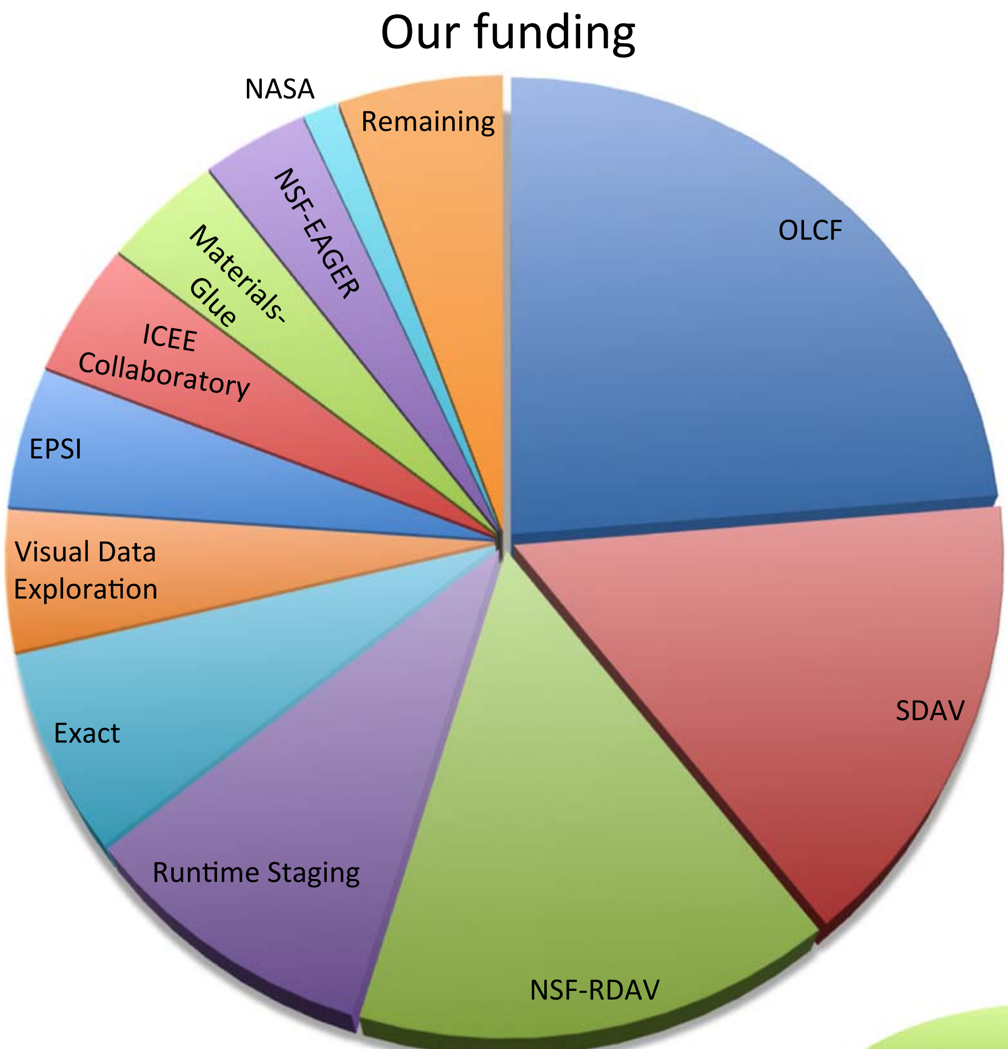
- ORNL: Hasan Abbasi, Jong Youl Choi , **Scott Klasky**, Qing Liu, Kimmy Mu, Norbert Podhorszki, Dave Pugmire, Roselyne Tchoua
- Georgia Tech: Greg Eisenhauer, Jay Lofstead, Karsten Schwan, Matt Wolf, Fang Zhang
- UTK: Jeremy Logan, Yuan Tian
- Rutgers: C. Docan, Tong Jin, Manish Parashar, Fan Zhang
- NCSU: Drew Boyuka, Z. Gong, Nagiza Samatova,
- LBNL: Arie Shoshani, John Wu
- Emory University: Tahsin Kurc, Joel Saltz
- Sandia: Jackie Chen, Todd Kordenbock, Ken Moreland
- NREL: Ray Grout
- PPPL: C. S. Chang, Stephane Ethier , Seung Hoe Ku, William Tang
- Caltech: Julian Cummings
- UCI: Zhihong Lin
- Tsinghua University (China): Wei Xue, Lizhi Wang

*Red marks major research/developer for the ADIOS project, Blue denotes student, Green denotes application scientists

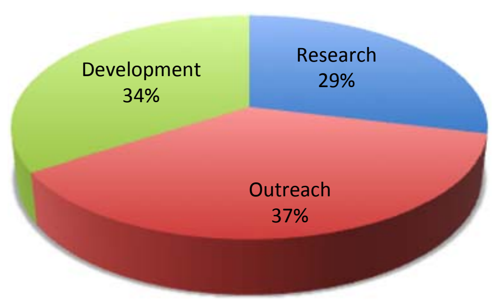
Thanks for our Current Funding ☺

1. OLCF: ADIOS, Barb Helland (Buddy Bland)
2. Runtime Staging, Exascale-SDM, ASCR: Lucy Nowell
3. Scalable Data Management, Analysis and Visualization Institute, ASCR: Lucy Nowell
4. ASCR, International Collaboration Framework for Extreme Scale Experiments (ICEE): Rich Carlson
5. NSF, An Application Driven I/O Optimization Approach for PetaScale Systems and Scientific Discoveries: Almadena Chtchelkanova
6. ASCR, SciDAC, Edge Physics Simulation (EPSI): Randall Laviolette, John Mandrekas
7. NSF, Remote Data Analysis and Visualization: Barry Schneider
8. NASA, An Elastic Parallel I/O Framework for Computational Climate Modeling: Tsengdar Lee
9. OFES, Center for Nonlinear Simulation of Energetic Particles in Burning Plasmas (CSEP), John Mandrekas
10. OFES, Energetic Particles, John Mandrekas
11. BES, Network for ab initio many-body methods: development, education and training, Hans M. Christen
12. NSF-NSFC, High Performance I/O Methods and infrastructure for large-scale geo-science applications on supercomputers., D. Katz

Application Partners



Over 158 Publications from 2006 - 2013



Application	Code	Contact
Astrophysics	Chimera	T. Mezzacappa
Combustion	S3D	J. Chen
AMR	Chombo	B. Van Straalen
CFD	Fine/Turbo	M. Gontier
Fusion-Edge	XGC1	C. S. Chang
Fusion-Edge	XGC0	S. H. Ku
Geoscience	AWP-ODC	Y. Cui
Materials	LAMMPS	A. Frachioni
Weather	GRAPES	W. Xue
Nuclear	HFODD	H. Nam
Relativity	Maya	P. Laguna
Sub surface		M. Wheeler
Materials		M. Parashar
Fusion	GTC-P	S. Ethier
Fusion	GTS	W. Wang
Fusion	M3D-C1	S. Jardin
Fusion	M3D-K	G. Y. Fu
Fusion	GTC	Z. Lin
Fusion	GEM	S. Parker
Quantum	QLG2Q	M. Soe
Image Analysis		T. Kurc
AMR	Boxlib	J. Bell
Relativity	Cactus	G. Allen
Weather	NASA	T. Clune
Materials	QMC	J. Kim
Climate		J. Fu
Climate	CAM	K. Evans

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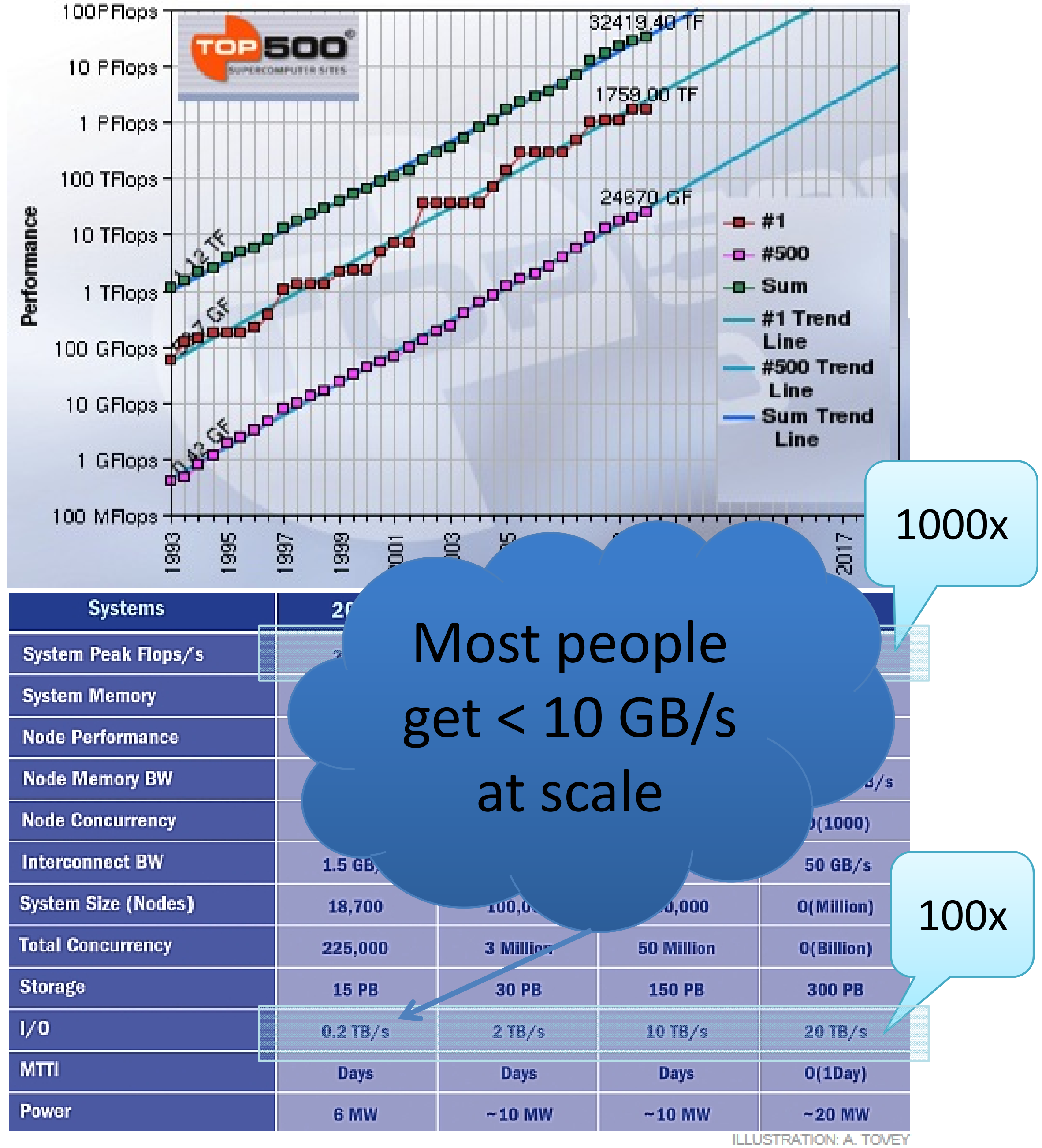
ADIOS

Extreme scale computing

- Trends
  - More FLOPS
  - Limited number of users at the extreme scale
- Problems
  - Performance
  - Resiliency
  - Debugging
  - Getting Science done
- Problems will get worse
  - Need a “revolutionary” way to store, access, debug to get the science done!



From J. Dongarra, “Impact of Architecture and Technology for Extreme Scale on Software and Algorithm Design,” Cross-cutting Technologies for Computing at the Exascale, February 2-5, 2010.

File Systems

File system	Hard links	Symbolic links	Block journaling	Metadata-only journaling	Case-sensitive	Case-preserving	File Change Log	Snapshot	XIP	Encryption	COW	integrated LVM	Data deduplication	Volumes are resizeable
CP/M file system	No	No	No	No	No	No	No	No	No	No	No	No	No	Unknown
DECtape	No	No	No	No	No	No	No	No	No	No	No	No	No	Unknown
Level-D	No	No	No	No	No	No	No	No	No	No	Unknown	Unknown	Unknown	Unknown
RT-11	No	No	No	No	No	No	No	No	No	No	No	No	No	Unknown
DOS (GEC)	No	No	No	No	No	No	No	No	No	No	No	No	No	Unknown
OS4000	No	Yes[71]	No	No	No	No	No	No	No	No	No	No	No	Unknown
V6FS	Yes	No	No	No	Yes	Yes	No	No	No	No	No	No	No	Unknown
V7FS	Yes	No[72]	No	No	Yes	Yes	No	No	No	No	No	No	No	Unknown
FAT12	No	No	No	No	No	Partial	No	No	No	No	No	No	No	Offline[73]
FAT16	No	No	No	No	No	Partial	No	No	No	No	No	No	No	Offline[73]
FAT32	No	No	No	No	No	Partial	No	No	No	No	No	No	No	Offline[73]
exFAT	No	No	Unknown	No	No	Yes	No	Unknown	Unknown	No	Unknown	Unknown	Unknown	Unknown
GFS	Yes	Yes[74]	Yes	Yes[75]	Yes	Yes	No	No	No	No	Unknown	Unknown	Unknown	Unknown
GPFS	Yes	Yes	Unknown	Unknown	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	No	Online
HPFS	No	No	No	No	No	Yes	No	Unknown	No	No	Unknown	Unknown	No	Unknown
NTFS	Yes	Yes[76]	No[77]	Yes[77]	Yes[78]	Yes	Yes	Partial[79]	Yes	Yes	Partial	Unknown	No	Online[80]
HFS	No	Yes[81]	No	No	No	Yes	No	No	No	No	No	No	No	Unknown
HFS Plus	Yes[82]	Yes	No	Yes[83]	Partial[84]	Yes	Yes[85]	No	No	No[86]	No	No	No	Offline
FFS	Yes	Yes	No	No[87]	Yes	Yes	No	No	No	No	No	No	No	Offline (cannot be shrunk)[88]
UFS1	Yes	Yes	No	No	Yes	Yes	No	No	No	No	No	No	No	Unknown
UFS2	Yes	Yes	No	No[89][90]	Yes	Yes	No	Yes	Unknown	No	No	No	No	Offline (cannot be shrunk)[91]
LFS	Yes	Yes	Yes[92]	No	Yes	Yes	No	Yes	No	No	Unknown	Unknown	Unknown	Unknown
ext2	Yes	Yes	No	No	Yes	Yes	No	No	Yes[93]	No	No	No	No	Online[94]
ext3	Yes	Yes	Yes[95]	Yes	Yes	Yes	No	No	Yes	No	No	No	No	Online[94]
ext4	Yes	Yes	Yes[95]	Yes	Yes	Yes	No	No	Yes	No	No	No	No	Online[94]
Lustre	Yes	Yes	Yes[95]	Yes	Yes	Yes	Yes in 2.0	No[58]	No	No[58]	No[58]	No[58]	No[58]	Online[96]
NILFS	Yes	Yes	Yes[92]	No	Yes	Yes	Yes	Yes	No	No	Yes	Unknown	Unknown	Unknown
ReiserFS	Yes	Yes	No[97]	Yes	Yes	Yes	No	No	No	No	No	No	No	Offline
Reiser4	Yes	Yes	Yes	No	Yes	Yes	No	Unknown	No	Yes[98]	Yes	No	Unknown	Online (can only be shrunk offline)
OCFS	No	Yes	No	No	Yes	Yes	No	No	No	No	Unknown	Unknown	Unknown	Unknown
OCFS2	Yes	Yes	Yes	Yes	Yes	Yes	No	Partial[99]	No	No	Unknown	No	No	Online for version 1.4 and higher
Reliance	No	No	No[100]	No	No	Yes	No	No	No	No	Yes	No	No	Unknown
Reliance Nitro	Yes	Yes	No[100]	No	Depends on OS	Yes	No	No	No	No	Yes	No	No	Unknown
XFS	Yes	Yes	Yes	Yes	Yes[101]	Yes	No	No	No	No	No	No	No	Online (cannot be shrunk)
JFS	Yes	Yes	No	Yes	Yes[102]	Yes	No	Yes	No	No	Yes	Unknown	Unknown	Online (cannot be shrunk)[103]
QFS	Yes	Yes	No	Yes	Yes	Yes	No	No	No	No	Unknown	Unknown	Unknown	Unknown
Be File System	Yes	Yes	No	Yes	Yes	Yes	Unknown	No	No	No	No	No	No	Unknown
NSS	Yes	Yes	Unknown	Yes	Yes[104]	Yes[104]	Yes[105]	Yes	No	Yes	Unknown	Unknown	Unknown	Unknown
NWFS	Yes[106]	Yes[106]	No	No	Yes[104]	Yes[104]	Yes[105]	Unknown	No	No	No	Yes[107]	Unknown	Unknown
ODS-2	Yes	Yes[108]	No	Yes	No	No	Yes	Yes	No	No	Unknown	Unknown	Unknown	Unknown
ODS-5	Yes	Yes[108]	No	Yes	No	Yes	Yes	Yes	Unknown	No	Unknown	Unknown	Unknown	Unknown
UDF	Yes	Yes	Yes[92]	Yes[92]	Yes	Yes	No	No	Yes	No	No	No	No	Unknown
VxFS	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes[109]	Unknown	No	Unknown	Unknown	Unknown	Unknown
Fossil	No	No	No	No	Yes	Yes	Yes	Yes	No	No	Unknown	No	Yes[110]	Unknown
ZFS	Yes	Yes	Yes[111]	No[111]	Yes	Yes	No	Yes	No	Yes	Yes	Yes	Yes	Online (cannot be shrunk)[112]
VMFS2	Yes	Yes	No	Yes	Yes	Yes	No	No	No	No	Unknown	Unknown	Unknown	Unknown
VMFS3	Yes	Yes	No	Yes	Yes	Yes	No	No	No	No	Unknown	Unknown	Unknown	Unknown
Btrfs	Yes	Yes	Unknown	Yes	Yes	Yes	Unknown	Yes	No	Planned[113]	Yes	Yes	Work-in-Progress	Online
File system	Hard links	Symbolic links	Block journaling	Metadata-only journaling	Case-sensitive	Case-preserving	File Change Log	Snapshotting	XIP	Encryption	COW	integrated LVM	Data deduplication	Volumes are resizeable

The SOA philosophy for HPC/ADIOS

- The overarching design philosophy of our framework is based on the Service-Oriented Architecture
  - Used to deal with system/application complexity, rapidly changing requirements, evolving target platforms, and diverse teams
- Applications constructed by assembling services based on a universal view of their functionality using a well-defined API
- Service implementations can be changed easily
- Integrated simulation can be assembled using these services
- Manage complexity while maintaining performance/scalability
  - Complexity from the problem (complex physics)
  - Complexity from the codes and how they are
  - Complexity of underlying disruptive infrastructure
  - Complexity from coordination across codes and research teams
  - Complexity of the end-to-end workflows

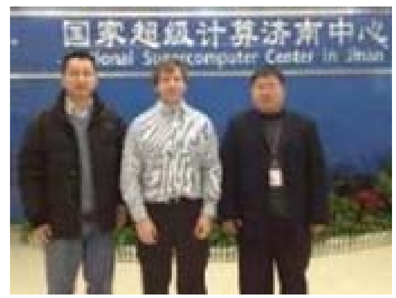
Our Goals for sustainable software development

- Ease of use

- High Performance

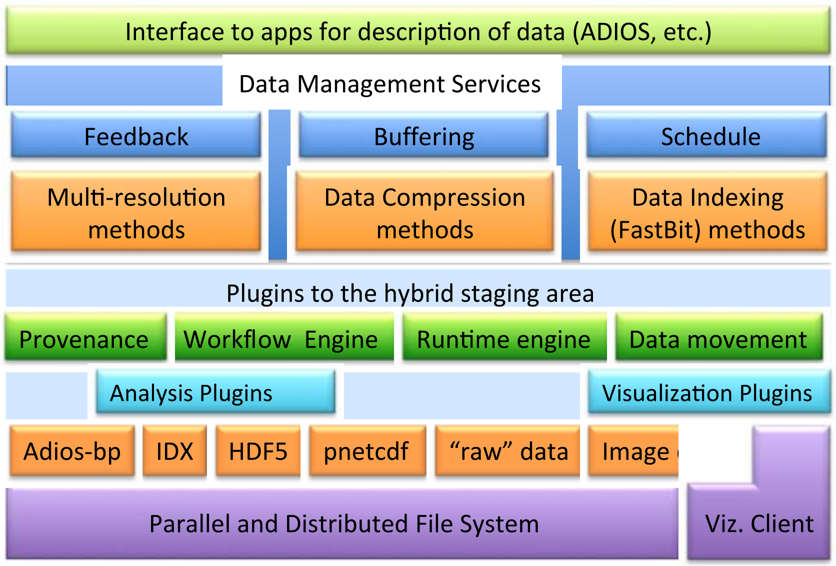
- Scalable

Portable

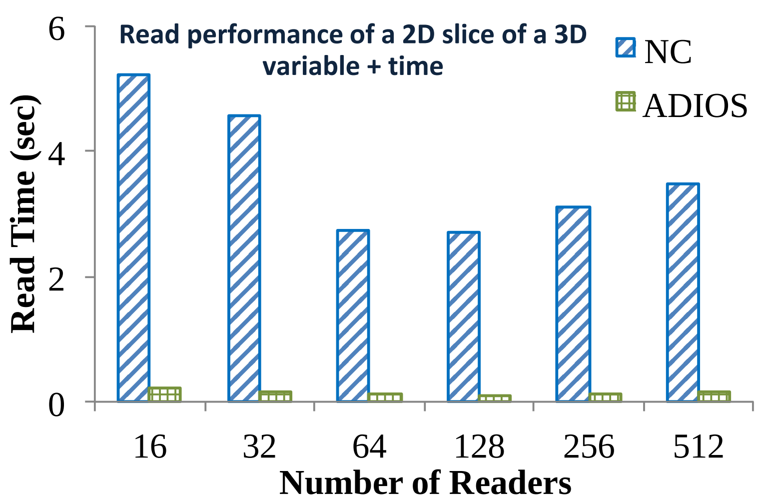


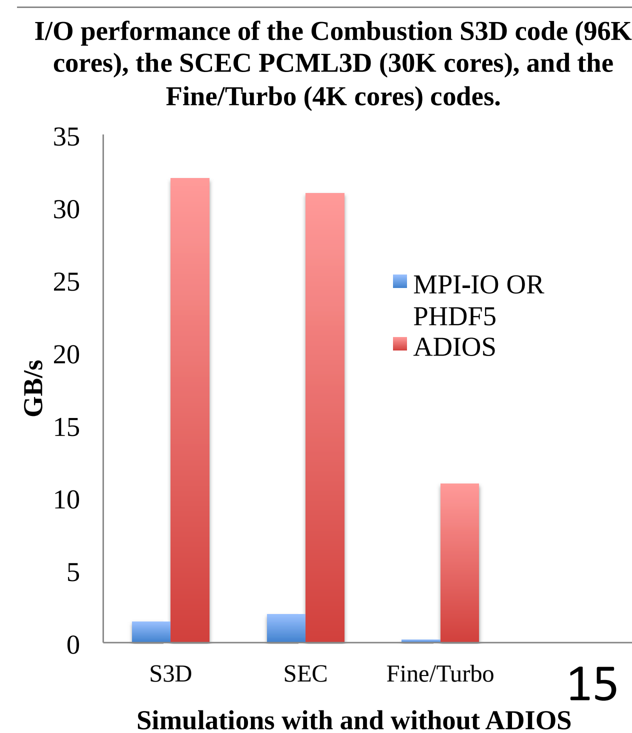
- Easy to master

ADIOS



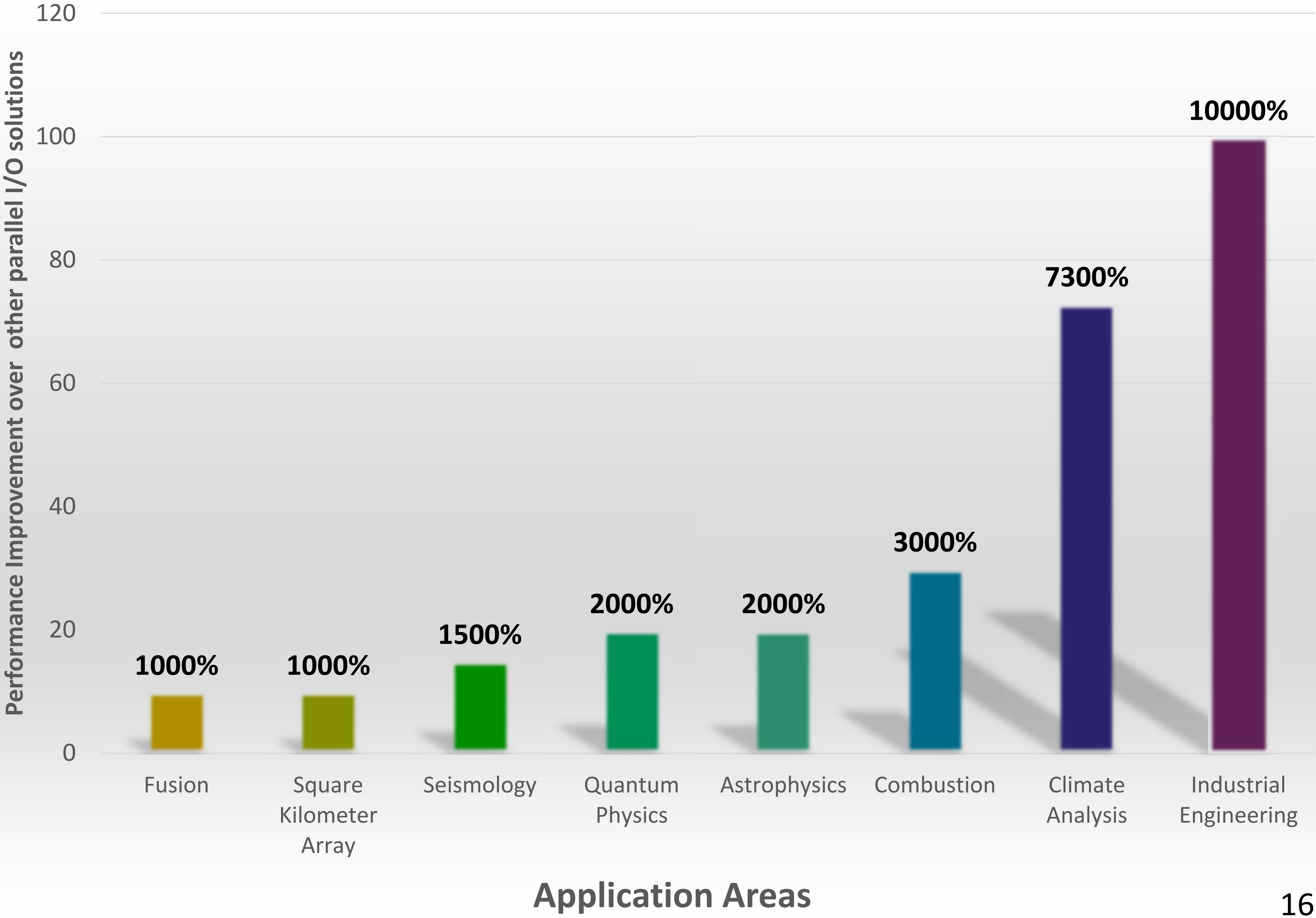
- An I/O abstraction framework
- Provides portable, fast, scalable, easy-to-use, metadata rich output
- Change I/O method on-the-fly
- Abstracts the API from the method http://www.nccs.gov/user-support/center-projects/adios/
- Typical 10X performance improvement for synchronous I/O over other solutions





Georgia Tech, Rutgers, NCSU, Emory, Auburn, Sandia, LBL, PPPL

ADIOS contributions in bridging the data gap for high fidelity science



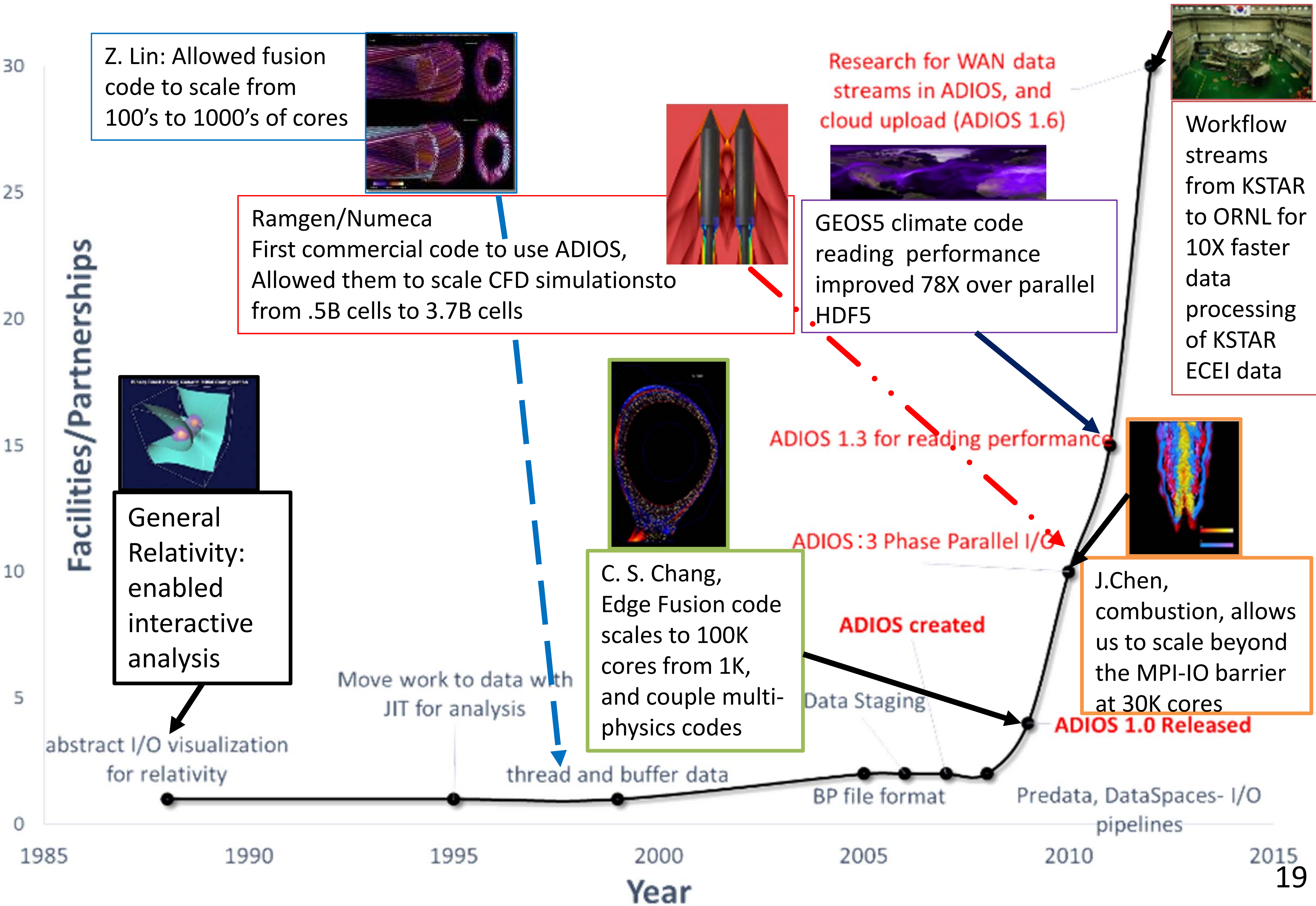
Most cited ADIOS-related publications

- 96 Flexible io and integration for scientific codes through the adaptable io system (adios)
- 81 Datastager: scalable data staging services for petascale applications
- 76 Adaptable, metadata rich IO methods for portable high performance IO
- 53 PreDatA preparatory data analytics on peta-scale machines
- 46 Managing variability in the IO performance of petascale storage systems
- 43 Grid-based parallel data streaming implemented for the gyrokinetic toroidal code
- 36 DataSpaces: An interaction and coordination framework for coupled simulation workflows
- 35 High performance threaded data streaming for large scale simulations
- 32 Workflow automation for processing plasma fusion simulation data
- 26 Plasma edge kinetic-MHD modeling in tokamaks using Kepler workflow for code coupling, data management and visualization
- 26 An autonomic service architecture for self-managing grid applications
- 23 Extending i/o through high performance data services
- 19 EDO: improving read performance for scientific applications through elastic data organization
- 19 Six degrees of scientific data: reading patterns for extreme scale science IO
- 19 Compressing the incompressible with ISABELA: In-situ reduction of spatio-temporal data

ADIOS information

- ADIOS is an I/O framework
  - Similar software philosophy as Linux: there is no single owner
  - Provides multiple methods to stage data to a staging area (on node, off node, off machine)
  - Data output can be anything one wants
    - Different methods allow for different types of data movement, aggregation, and arrangement to the storage system or to stream over the local-nodes, LAN, WAN
  - It contains our own file format if you choose to use it (ADIOS-BP)
  - In the next release, it will be able to compress/decompress data in parallel: plugged into the transform layer
  - In the next release: it will contain mechanisms to index and then query the data

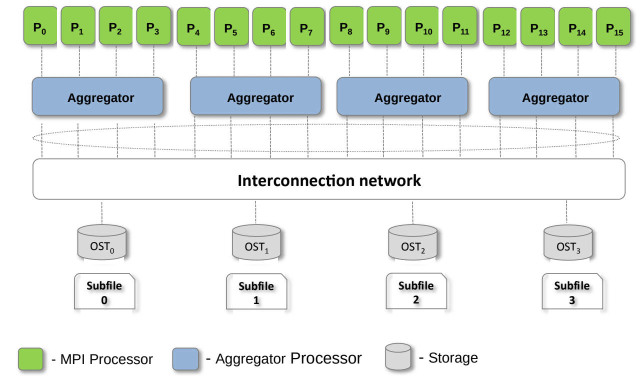
The History of ADIOS



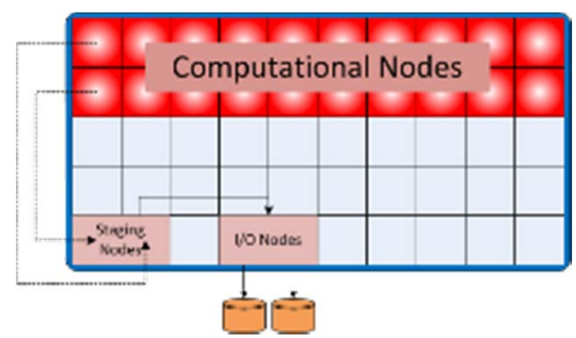
ADIOS latest Release

- **1.5.0 Release June 2013**
- http://www.olcf.ornl.gov/center-projects/adios/
- New staging methods:
  - DIMES
  - FLEXPATH
- CMAKE build files (besides Automake files)
- New write method VAR_MERGE for spatial aggregation of small per-process-output into larger chunks. It improves both write and read performance for applications
- Please give us suggestions for future releases after the next one at SC-2013.

- Aggregated file read method



- Staged write C code
  - Uses any staging or file method to read data, writes with any ADIOS method

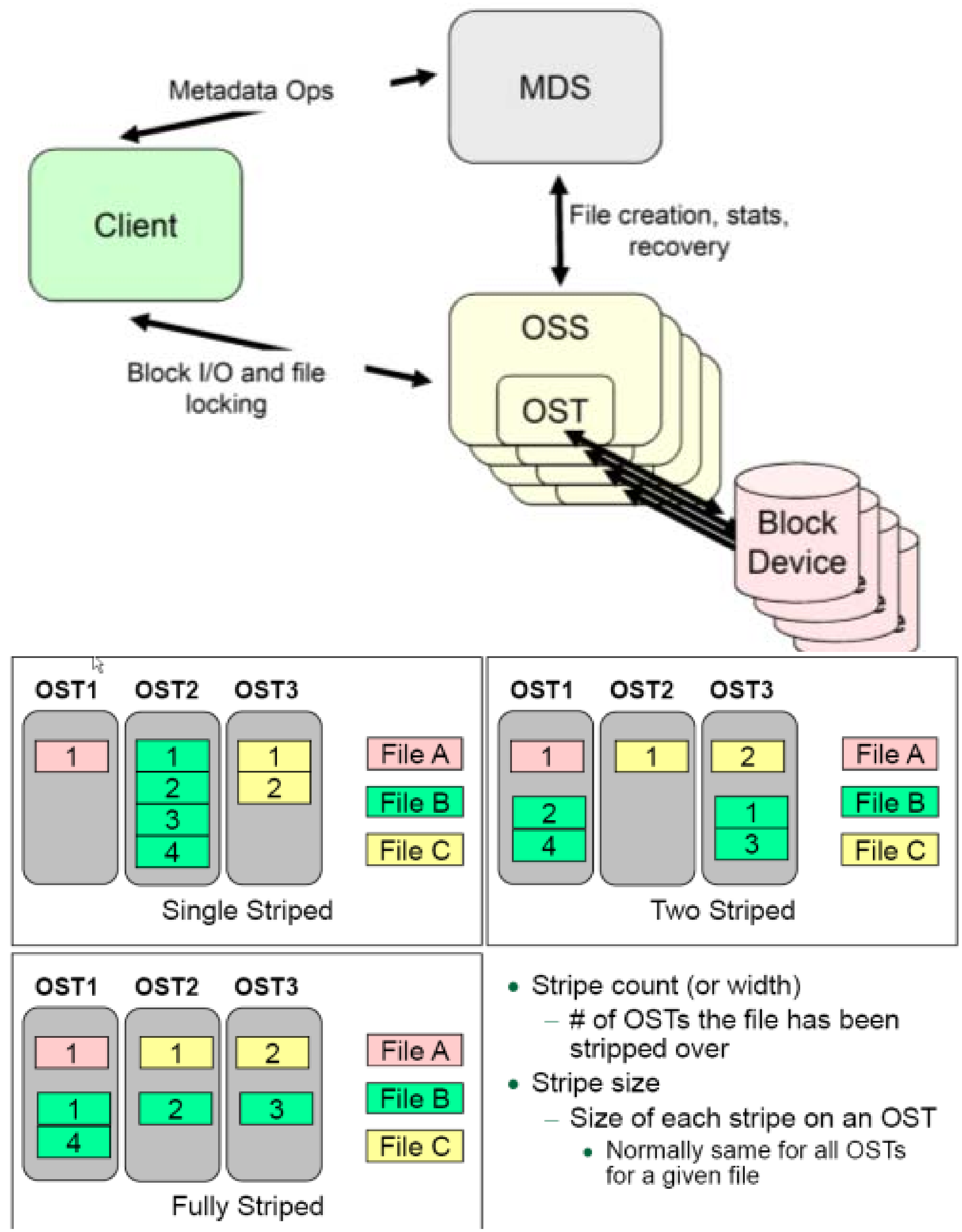


Favorite highlights

- "I appreciate the clean yet capable interface and that from my perspective, it just works," Grout.
- “ADIOS has allowed us to couple fusion codes to solve new physics problems”, Chang.
- “So far I have found that even using ADIOS in the way you said is bad and silly in every aspect, the I/O performance is still improved by about 10X”, J. Wang ICAR
- “… thanks to Dr. Podhorszki, the developers at Numeca have had excellent support in integrating ADIOS into FINE/Turbo. We have observed a 100x speedup of I/O, which is difficult to achieve in commercial codes on industrial applications”, Grosvenor.

LUSTRE

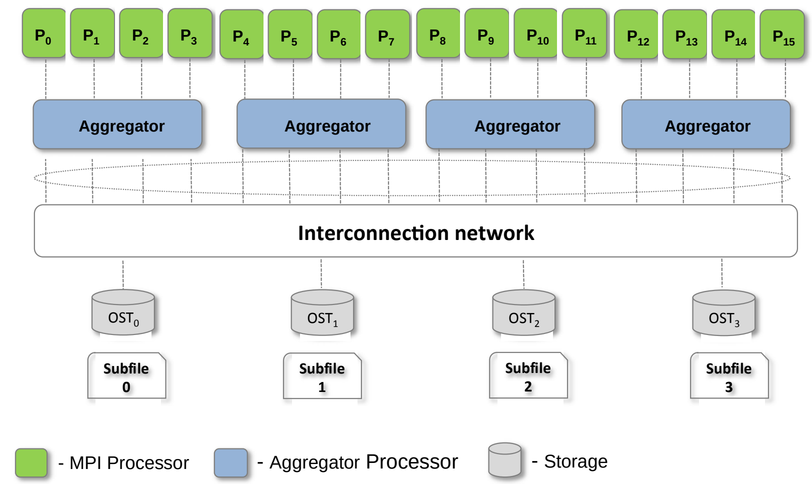
- Lustre consists of four major components
  - MetaData Server (MDS)
  - Object Storage Servers (OSSs)
  - Object Storage Targets (OSTs)
  - Clients
- Performance: Striping, alignment, placement
- GPFS is similar, but …

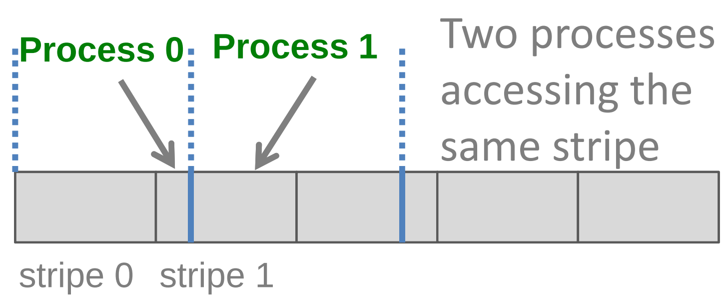


http://www.nas.nasa.gov/hecc/support/kb/Lustre-Best-Practices_226.html

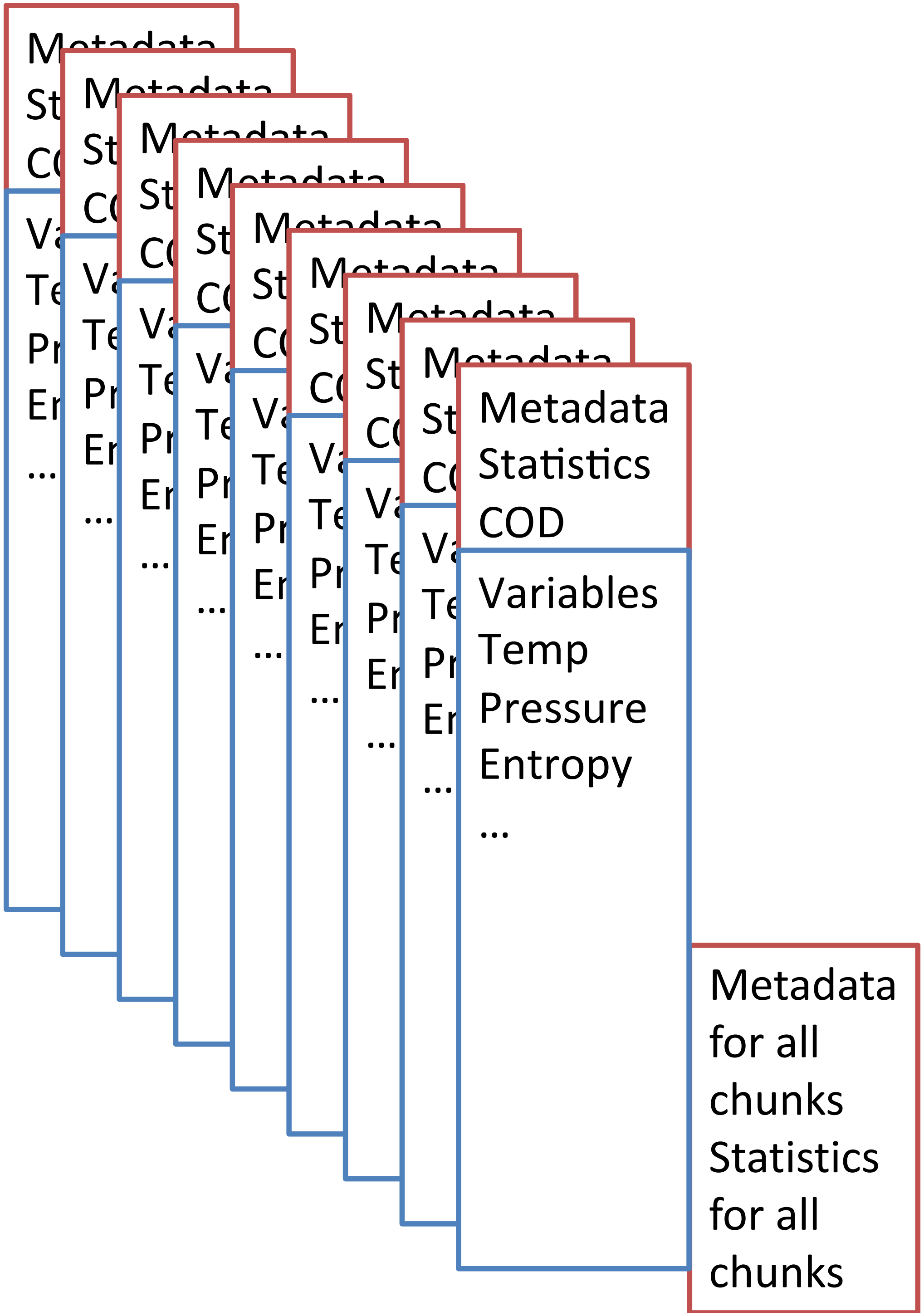
Writing to file system

- Avoid latency (of small writes)
  - Buffer data for large bursts
- Avoid accessing a file system target from many processes at once
  - Aggregate to a small number of actual writers
    - proportionate to the number of file system targets, not MPI tasks
- Avoid lock contention
  - by striping correctly
  - Our method writes to subfiles
- Avoid global communication during I/O
  - ADIOS-BP file format





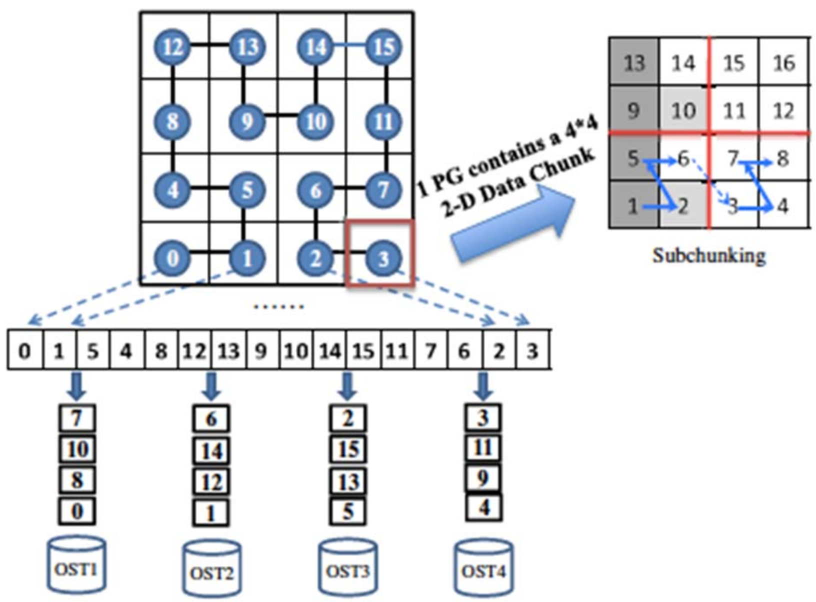
ADIOS Self-describing Format for Data Chunks/Streams



- All data chunks are from a single producer
  - MPI process
  - Single diagnostic
- Ability to create a separate metadata file when "sub-files" are generated
- Allow code to be integrated to streams
- Allows variables to be individually compressed
- Format is for "data-in-motion" and "data-at-rest"

Reading performance

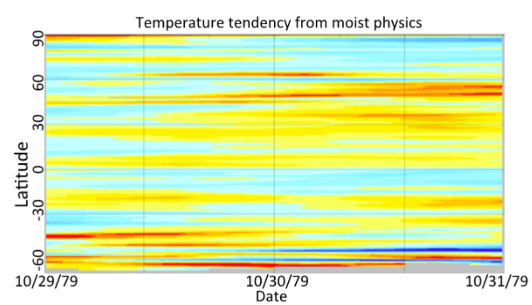
- Aggregate and place chunks on file system with an Elastic Data Organization
- Ability to optimize for common read patterns (e.g. 2D slice from 3D variable), space-time optimizations
- **Achieved a 73x speedup for read performance, and 11x speedup for write performance in mission critical climate simulation GEOS-5 (NASA), on Jaguar.**



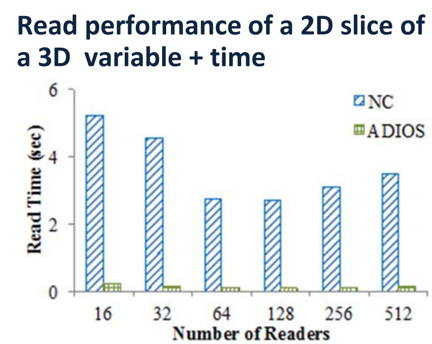
(b) SFC-based Placement with EDO

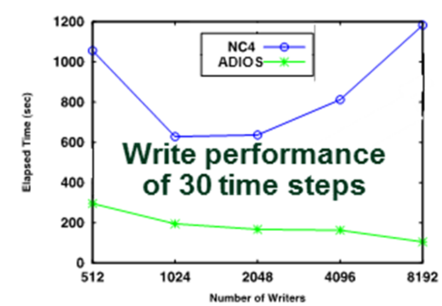
First place ACM student Research Competition 2012

- Common read patterns for GEOS-5 users are reduced from 10 – 0.1 seconds
- Allows interactive data exploration for mission critical visualizations



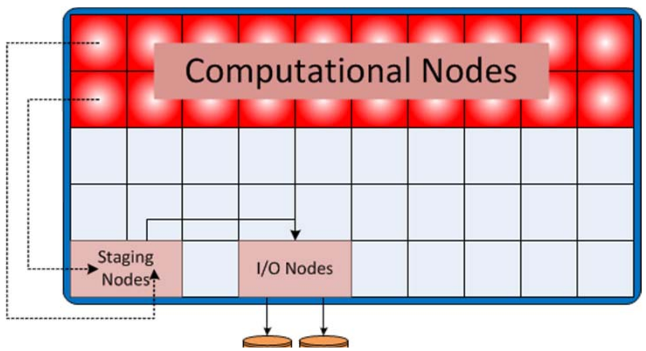
GEOS-5 Results

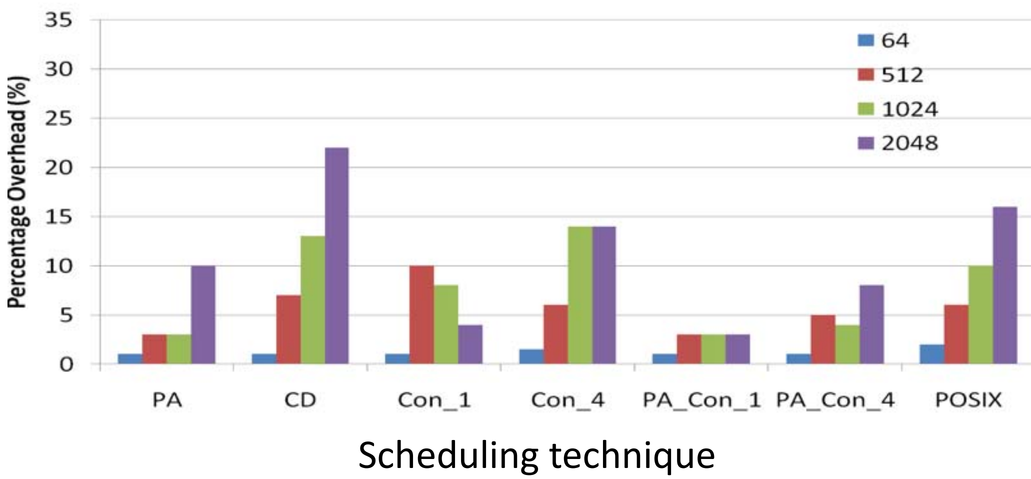




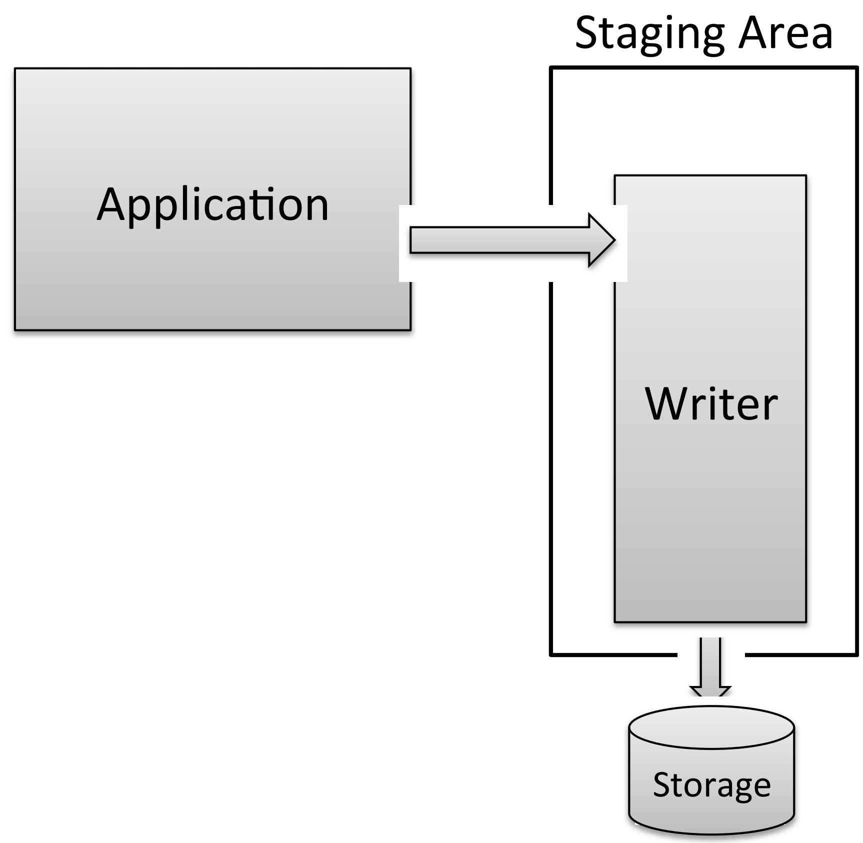
Introduction to Staging

- Initial development as a research effort to minimize I/O overhead
- Draws from past work on threaded I/O
- Exploits network hardware support for fast data transfer to remote memory





Using Staging as an I/O burst buffer

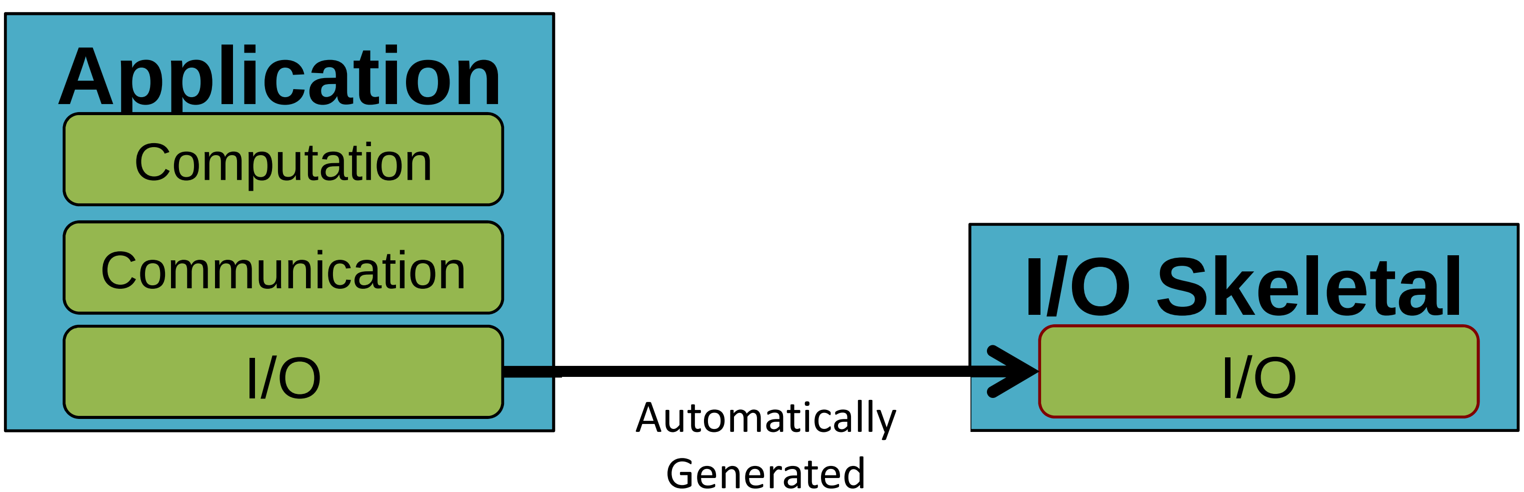


Hasan Abbasi, Matthew Wolf, Greg Eisenhauer, Scott Klasky, Karsten Schwan, Fang Zheng: DataStager: scalable data staging services for petascale applications. Cluster Computing 13(3): 277-290 (2010)

Ciprian Docan, Manish Parashar, Scott Klasky: DataSpaces: an interaction and coordination framework for coupled simulation workflows. Cluster Computing 15(2): 163-181 (2012)

Automatic Benchmark Generation

- **Skel** addresses various issues with I/O kernels
  - Automatic generation reduces development burden and enhances applicability
  - Skeletals are easily kept up to date with application changes
  - Skel provides a consistent user experience across all applications
    - No scientific libraries are needed
    - No input data is needed
    - Measurements output from skeletals are standard for all applications
- The correctness of Skel has been validated for several applications and three synchronous I/O methods



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Writing setup/cleanup API

- Initialize/cleanup
  - #include "adios.h"
  - adios_init ('config.xml', comm)
    - parse XML file on each process
    - setup transport methods
    - MPI_Comm
      - only one process reads the XML file
      - some staging methods can connect to staging server
  - adios_finalize (rank)
    - give each transport method opportunity to cleanup
    - particularly important for asynchronous methods to make sure they have completed before exiting
    - call just before MPI_Finalize()
  - adios_init_noxml (comm)
    - Use instead of adios_init() when there is no XML configuration file
    - Extra APIs allows for defining variables

Fortran

```
use adios_write_mod
call adios_init ("config.xml", comm, err)
call adios_finalize (rank, err)
call adios_init_noxml (comm, err)
```

API for writing 1/3

- Open for writing
  - adios_open (fh, *"group name"*, *"file name"*, mode, comm)
    - int64_t fh handle used for subsequent calls for write/close
    - *"group name"* matches an entry in the XML
      - identifies the set of variables and attributes that will be written
    - Mode is one of 'w' (write) or 'a' (append)
    - Communicator tells ADIOS what processes in the application will perform I/O on this file
- Close
  - adios_close (fh)
    - handle from open

Fortran

```
integer*8 :: fd
call adios_open (fd, group_name, filename,
                 mode, comm, err)
call adios_close (fd, err)
```

API for writing 2/3

- Write
  - adios_write (fh, *"varname"*, data)
    - fh is the handle from open
    - Name of variable in XML for this group
    - Data is the reference/pointer to the actual data
  - NOTE: with a XML configuration file, adios can build Fortran or C code that contains all of the write calls for all variables defined for a group
- Must specify one call per variable written

Fortran
call adios_write (fd, varname, data, err)

Important notes about the write calls

- adios_write()
  - usually does not write to the final target (e.g. file)
  - most of the time it only buffers data locally
  - when the call returns, the application can re-use the variable’s memory
- adios_close()
  - takes care of getting all data to the final target
  - usually the buffered data is written at this time

API for writing 3/3

One final piece required for buffer overflows

- adios_group_size (int64_t fh, uint64_t data_size, uint64_t &total_size)
  - called after adios_open(), before any adios_write()
  - fh is the handle returned from open
  - data_size is the size of the data in bytes to be written
    - by this particular process
    - i.e. the size of all writes between this particular open/close step
  - total_size is returned by the function
    - how many bytes will really be written (your data + all metadata) from this process
- gpp.py generates
  - the adios_group_size and all adios_write statements
  - 2 files per group (1 for read, 1 for write) in the language specified in the XML file (C style or Fortran style)
    - you need to include the appropriate file in your source after adios_open

Fortran
call adios_group_size (fd, data_size, total_size, err)

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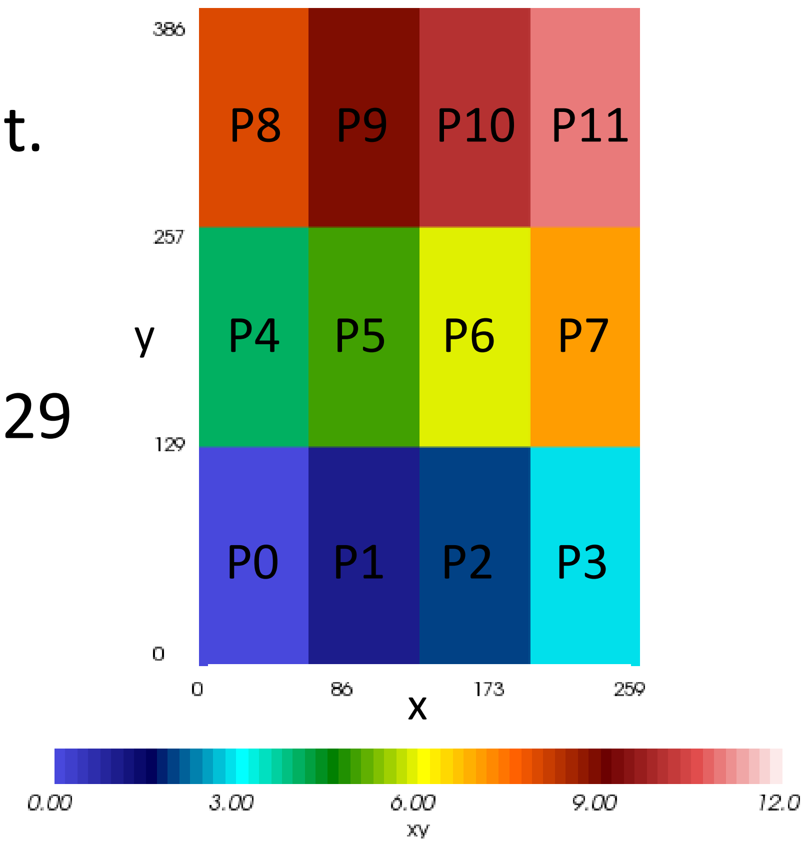
ADIOS Hands on demo -1

- Goals
  - Write an Fortran90/MPI code with ADIOS I/O
  - How to compile ADIOS codes.
  - How to run ADIOS codes.
  - How to create global arrays.

Write Example

- In this example we start with a 2D code which writes data of a 2D array, with a 2D domain decomposition, as shown in the figure.
  - `xy = 1.0*rank + 1.0*ts`
- We write out 2 time-steps, in separate files.
- For simplicity, we work on only 12 cores, arranged in a 4 x 3 arrangement.
- Each processor allocates a 65x129 array (xy).
- The total size of the array = 4*65, 3*129



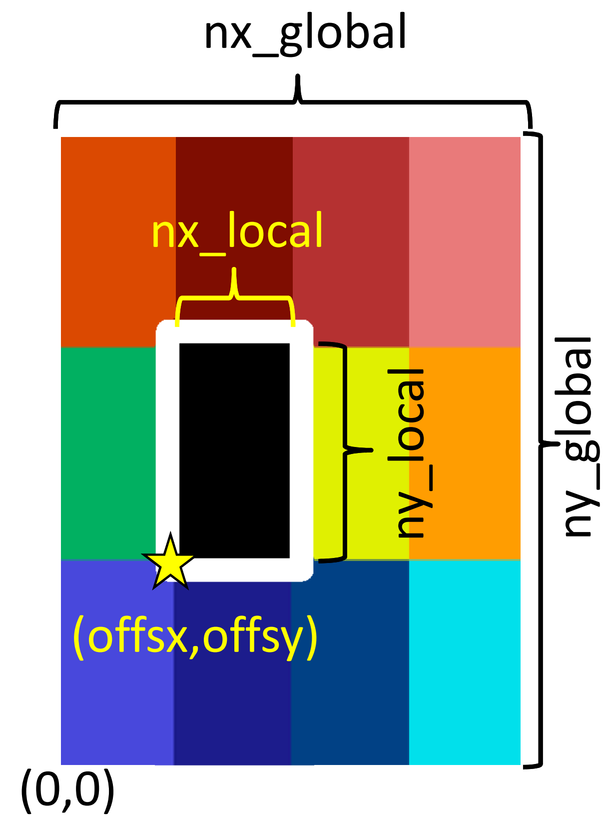
The ADIOS XML configuration file

- Describe each IO grouping.
- Maps a variable in the code, to a variable in a file.
- Map an IO grouping to transport method(s).
- Define buffering allowance
- “XML-free” API are also provided

XML Overview

- writer.xml describes the output variables in the code

```
<adios-group name="writer">
    <var name="nx_global" type="integer"/>
    <var name="ny_global" type="integer"/>
    <var name="nx_local"  type="integer"/>
    <var name="ny_local"  type="integer"/>
    <var name="offs_x"   type="integer"/>
    <var name="offs_y"   type="integer"/>
    <global-bounds dimensions="nx_global, ny_global"
                   offsets="offsx,offsy">
        <var name="xy" type="double"
             dimensions="nx_local,ny_local"/>
    </global-bounds>
</adios-group>
<transport group="writer" method="MPI"/>
```



XML overview (global array)

- We want to read in xy from an arbitrary number of processors, so we need to write this as a global array.
- Need 2 more variables, to define the offset in the global domain
  - <var name=“offs_x” type=“integer”/>
  - <var name=“offs_y” type=“integer”/>
- Need to define the xy variable as a global array
  - Place this around the lines defining xy in the XML file.
  - <global-bounds dimensions="nx_global,ny_global"
    offsets="offs_x,offs_y">
  - </global-bounds>

Calculating sizes and dimensions

posx = mod(rank, npx) ! 1st dim: 0, npx, 2npx... are in the same X position

posy = rank/npx ! 2nd dim: npx processes belong into one dim

offs_x = posx * ndx ! The processor offset in the x dimension for the global dimensions

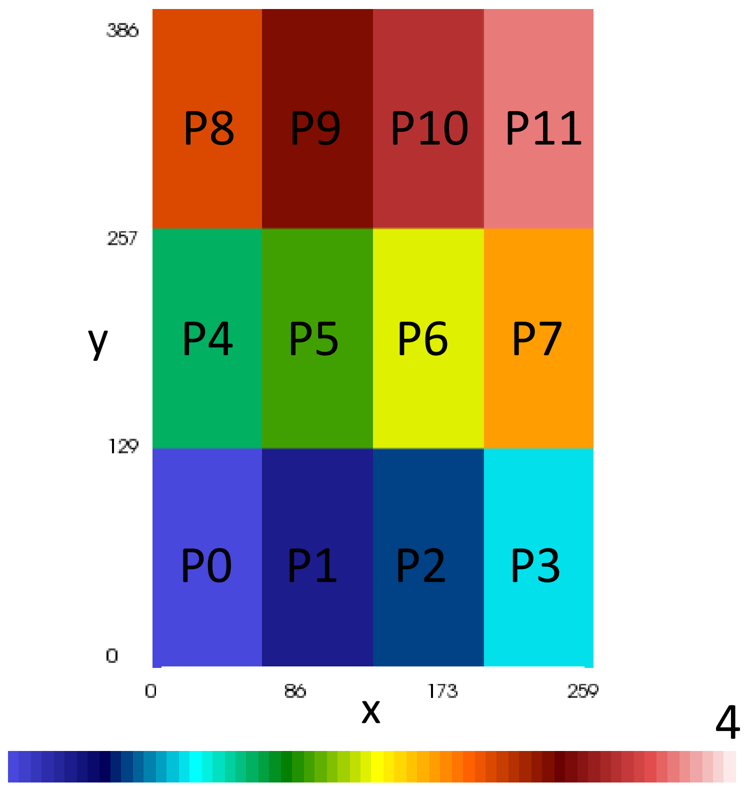
offs_y = posy * ndy ! The processor offset in the x dimension for the global dimensions

nx_local = ndx ! The size of data that the processor will write in the x dimension

ny_local = ndy ! The size of data that the processor will write in the y dimension

nx_global= npx * ndx ! The size of data in the x dimension for the global dimensions

ny_global= npy * ndy ! The size of data in the y dimension for the global dimensions



XML Overview

- Need to define the method, we will use MPI.
  - <transport group="writer" method="MPI"/>
- Need to define the buffer
  - <buffer size-MB="4" allocate-time="now"/>
  - Can use any size, but if the buffer > amount to write, the I/O to disk will be faster.
- Need to define the host language (C or Fortran ordering of arrays).
  - <adios-config host-language="Fortran">
- Set the XML version
  - <?xml version="1.0"?>
- And end the configuration file
  - </adios-config>

ADIOS

The final XML file

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

    <adios-group name=“writer”>
        <var name=“nx_global” type=“integer”/>
        <var name=“ny_global” type=“integer”/>

        <var name=“offs_x” type=“integer”/>
        <var name=“offs_y” type=“integer”/>
        <var name=“nx_local” type=“integer”/>
        <var name=“ny_local” type=“integer”/>

        <global-bounds dimensions="nx_global,ny_global" offsets="offs_x,offs_y">
            <var name=“xy” type=“real*8” dimensions=“nx_local,ny_local”/>
        </global-bounds>

    </adios-group>

    <transportgroup="writer" method="MPI"/>
    <buffer size-MB="4" allocate-time="now"/>

</adios-config>
```

gpp.py

- Converts the XML file into F90 (or C) code.
- > gpp.py writer.xml
- > cat gwrite_writer.fh

```
adios_groupsize = 4 &
 + 4 &
 + 4 &
 + 4 &
 + 4 &
 + 4 &
 + 8 * (nx_local) * (ny_local)
call adios_group_size (adios_handle, adios_groupsize, adios_totalsize, adios_err)
call adios_write (adios_handle, "nx_global", nx_global, adios_err)
call adios_write (adios_handle, "ny_global", ny_global, adios_err)
call adios_write (adios_handle, "offs_x", offs_x, adios_err)
call adios_write (adios_handle, "offs_y", offs_y, adios_err)
call adios_write (adios_handle, "nx_local", nx_local, adios_err)
call adios_write (adios_handle, "ny_local", ny_local, adios_err)
call adios_write (adios_handle, "xy", xy, adios_err)
```

Writing with ADIOS I/O (simplest form)

```
call adios_init ("writer.xml", group_comm, adios_err)
…
call adios_open (adios_handle, "writer", trim(filename),
                 "w", group_comm, adios_err)

#include "gwrite_writer.fh"

call adios_close (adios_handle, adios_err)
…
call adios_finalize (rank, adios_err)
```

Source file extension should be .F90 (instead of .f90) to enforce macro preprocessing at compile time

Compile ADIOS codes

- Makefile
  - use adios_config tool to get compile and link options

Chester

```
ADIOS_DIR = /sw/xk6/adios/1.5.0/cle4.0_pgi12.10.0
ADIOS_INC = $(shell ${ADIOS_DIR}/bin/adios_config -c -f)
ADIOS_FLIB = $(shell ${ADIOS_DIR}/bin/adios_config -l -f)
ADIOSREAD_FLIB := $(shell ${ADIOS_DIR}/bin/adios_config -l -f –r)
```

  - Codes that write and read

```
writer: writer.F90 gwrite_writer.fh
	${FC}   -g -c -o writer.o ${ADIOS_INC} writer.F90
	${LINKER}   -g -o writer writer.o ${ADIOS_FLIB}

gwrite_writer.fh: writer.xml
	${GPP} writer.xml
```

Compile and run the code

Chester

```
$ cd /tmp/work/<username>/adios-1.5.0-tutorial-chester
$ qsub -I -X -lwalltime=2:00:00,nodes=1
$ cd $PBS_O_WORKDIR
$ cd write_read
$ make
$ aprun -n 12 ./writer
 ts= 0
 ts= 1
$ ls -l *.bp
-rw-r--r-- 1 esimmon esimmon 815379 2013-06-12 09:44 writer00.bp
-rw-r--r-- 1 esimmon esimmon 815628 2013-06-12 09:44 writer01.bp
```

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ADIOS Hands on: Tools

- Goals
  - Learn how to look at an ADIOS-BP file
  - Learn how to convert the data to HDF5 and NetCDF-3 files

ADIOS Tools

- bpls
  - Similar to h5dump+h5ls and ncdump
  - Also shows array min/max values
  - Metadata performance independent of data size
- bp2h5, bp2ncd
  - Convert BP format into HDF5 or NetCDF

bpls

Chester

$ module load adios/1.5.0

$ bpls -lv writer00.bp

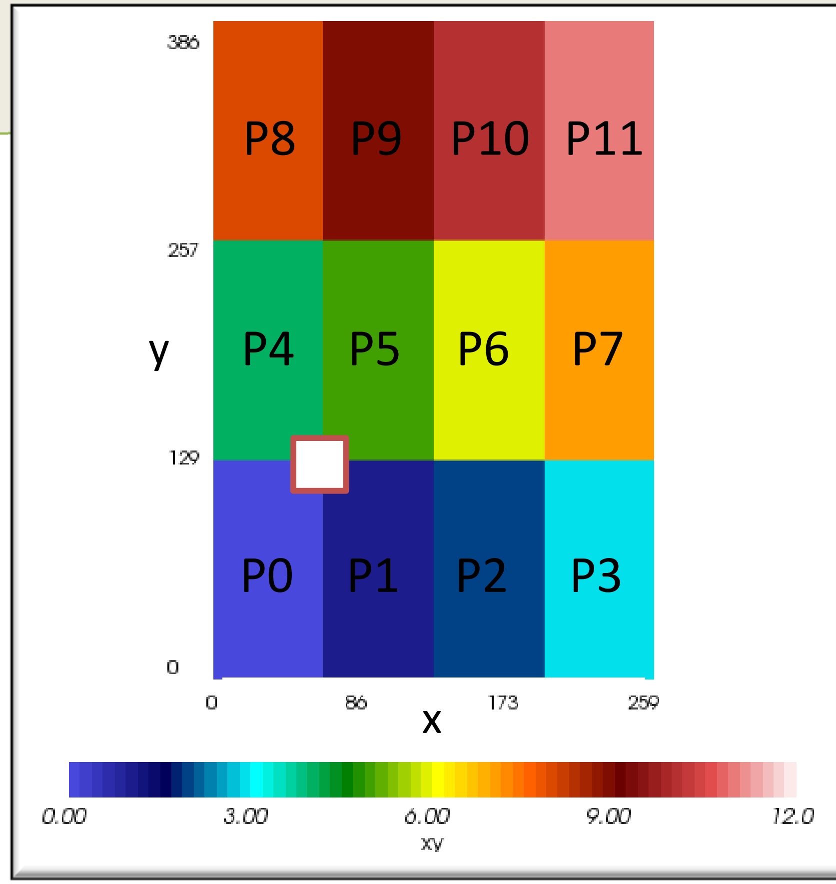
```
  File info:
      of groups:     1
      of variables:  7
      of attributes: 0
      time steps:    0 - 0
      file size:     796 KB
      bp version:    1
      endianness:    Little Endian
      statistics:    Min / Max / Avg / Std_dev

  Group writer:
      integer  /nx_global      scalar = 260
      integer  /ny_global      scalar = 387
      integer  /offs_x         scalar = 0
      integer  /offs_y         scalar = 0
      integer  /nx_local       scalar = 65
      integer  /ny_local       scalar = 129
      double   /xy            {387, 260} = 0 / 11 / 5.5 / 3.45205
```

bpls

- Use bpls to read in a 2D slice

```
$ bpls writer00.bp -d xy -s "128,64" -c "2,2" -n 2
double    /xy    {387, 260}
 slice (128:129, 64:65)
 (128,64)     0 1
 (129,64)     4 5
```



- -d var
  - dump var
- -s / -start
  - define beginning offset
- -c / -count
  - define size in each dimension
- -n 2
  - print 2 values per row

bp2h5, bp2ncd

```
$ bp2h5 writer00.bp writer00.h5
$ h5ls writer00.h5
    nx_global    Dataset {1}
    nx_local     Dataset {1}
    ny_global    Dataset {1}
    ny_local     Dataset {1}
    offs_x       Dataset {1}
    offs_y       Dataset {1}
    xy           Dataset {387, 260}
```

```
$ bp2ncd writer00.bp
$ ncdump -h  writer00.nc
    netcdf writer00 {
    dimensions:
        nx_global = 260 ;
        ny_global = 387 ;
        nx_local = 65 ;
        ny_local = 129 ;
        offs_x = 65 ;
        offs_y = 129 ;
    variables:
        double xy(nx_global, ny_global) ;
    }
```

Block layout of the example

- map.c
  - uses ADIOS API to inquire the local dimensions and offsets of each writer

```
$ ./map writer00.bp
 …
  double  /xy[387, 260]: min=0 max=11
    step   0:
      block   0: [   0:128,    0:  64]
      block   1: [   0:128,   65:129]
      block   2: [   0:128,  130:194]
      block   3: [   0:128,  195:259]
      block   4: [129:257,    0:  64]
      block   5: [129:257,   65:129]
      block   6: [129:257,  130:194]
      block   7: [129:257,  195:259]
      block   8: [258:386,    0:  64]
      block   9: [258:386,   65:129]
      block  10: [258:386,  130:194]
      block  11: [258:386,  195:259]
```

slow dimension, fast dimension
from:to, from:to

ADIOS Componentization

- ADIOS can allow many different I/O methods
  - POSIX
  - POSIX1
  - MPI_AGGREGATE: needs *num_ost*, and *num_aggregators*

    <transport group="writer" method="MPI_AGGREGATE">num_aggregators=4;num_ost=2</transport>
  - PHDF5:
    - Limited functionality in ADIOS 1.5, but will be improved in future releases.
    - Must remove attributes and PATHS for this to work
  - NC4: same expectations as PHDF5
- Rule of thumb:
  - Try Posix, then move to MPI, then MPI_AGGREGATE

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Read API basics

- Common API for reading files and streams (with staging)
  - In staging, one must process data step-by-step
  - Files allow for accessing all steps at once
- Schedule/perform reads in bulk, instead of single reads
  - Allows for optimizing multiple reads together
- Selections
  - bounding boxes, list of points, selected blocks and automatic
- Chunking (optional)
  - receive and process pieces of the requested data concurrently
  - staging delivers data from many producers to a reader over a certain amount of time, which can be used to process the first chunks

Read API basics

- Step
  - A dataset written within one adios_open/…/adios_close
- Stream
  - A file containing of, or a staged, series of steps of the same dataset
  - not a byte stream!
  - the step is quite a large unit
- Read API is designed to read data from one step at a time, then advance forward
  - alternative API allows for reading all steps at once from a file

Read API

- Initialization/Finalization
  - One call per each read method used in an application
  - Staging methods usually connect to a staging server / other application at init, and disconnect at finalize.

int **adios_read_init_method** (
    enum ADIOS_READ_METHOD method,
    MPI_Comm comm, const char * parameters)

int **adios_read_finalize_method**(enum ADIOS_READ_METHOD method)

Fortran
use adios_read_mod
call adios_read_init_method (method, comm, parameters, err)
call adios_finalize_method (method, err)

Read API

- Open as a stream or as a file
  - for step-by-step reading (both staged data and files)

```
ADIOS_FILE * adios_read_open (
    const char * fname,
    enum ADIOS_READ_METHOD method,
    MPI_Comm comm,
    enum ADIOS_LOCKMODE lock_mode
    float timeout_sec)
```

  - for seeing all timesteps at once (files only!)

```
ADIOS_FILE * adios_read_open_file (
    const char * fname,
    enum ADIOS_READ_METHOD method,
    MPI_Comm comm)
```

- Close

```
int adios_read_close (ADIOS_FILE *fp)
```

Fortran

```
use adios_read_mod
call adios_read_open (
    fp, fname, method, comm,
    lockmode, timeout_sec, err)
call adios_read_open_file (
    fp, fname, method, comm, err)
call adios_read_close (fp, err)
```

Locking options

- ALL
  - lock current and all future steps in staging
  - ensures that reader can read all data
  - reader’s priority, it can block the writer
- CURRENT
  - lock the current step only
  - future steps can disappear if writer pushes more newer steps and staging needs more space
  - writer’s priority
  - reader must handle skipped steps
- NONE
  - no assumptions, anything can disappear between two read operations
  - be ready to process errors

Locking modes

- Current (or None)
  - “next” := next available
- All
  - “next” := current+1

Advancing a stream

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

  int **adios_advance_step** (ADIOS_FILE *fp, int last, float timeout_sec)

  – last: advance to “next” or to latest available
    - “next” or “next available” depends on the locking mode
    - locking = all: go to the next step, return error if that does not exist anymore
    - locking = current or none: give the oldest, still available step after the current one

  – timeout_sec: block for this long if no new steps are available

- Release a step if not needed anymore
  – optimization to allow the staging method to deliver new steps if available

  int **adios_release_step** (ADIOS_FILE *fp)

Reading data

- Read is a scheduled request, …

```
int64_t adios_schedule_read (
            const ADIOS_FILE          * fp,
            const ADIOS_SELECTION     * selection,
            const char                * varname,
            int                         from_steps,
            int                         nsteps,
            void                      * data)
```

  – in streaming mode, only one step is available

- …executed later with other requests together

```
int adios_perform_reads (const ADIOS_FILE *fp, int blocking)
```

Fortran

```
call adios_schedule_read (
    fp, selection, varname,
    from_steps, nsteps, data, err)
call adios_perform_reads (
    fp, err)
```

Inquire about a variable (no extra I/O)

- ADIOS_VARINFO * **adios_inq_var** (ADIOS_GROUP *gp,
  const char * varname)
  - Inquiry about a variable in a group.
  - Value of a scalar variable can be retrieved with this function instead of reading.
  - This function does not read anything from file but processes info already in memory after open.
  - It allocates memory for the ADIOS_VARINFO struct and content, so you need to free resources later with adios_free_varinfo().
  - ADIOS_VARINFO variables
    - int ndim Number of dimensions
    - uint64_t *dims Size of each dimension
    - int nsteps Number of steps of the variable in file. Streams: always 1
    - void *value Value (for scalar variables only)
    - int nblocks Number of blocks that comprise this variable in a step
    - void *gmin, *gmax, gavg, gstd_devStatistical values of the global arrays
    - see adios_read_v1.h for more information
- int **adios_inq_var_stat** (ADIOS_FILE *fp, ADIOS_VARINFO * varinfo,
  int per_step_stat, int per_block_stat)
  - Get statistics about an array variable (min, max, avg, std_dev)
    - globally, per step, per written block
- int **adios_inq_var_blockinfo** (ADIOS_FILE *fp, ADIOS_VARINFO * varinfo)
  - Get writing layout of an array variable (bounding boxes of each writer)

Fortran
call adios_get_scalar (fp, varname, data, err)
call adios_inq_file (fp, vars_count, attrs_count, current_step, last_step, err)
call adios_inq_varnames (fp, vnamelist, err)
call adios_inq_var (fp, varname, vartype, nsteps, ndim, dims, err)

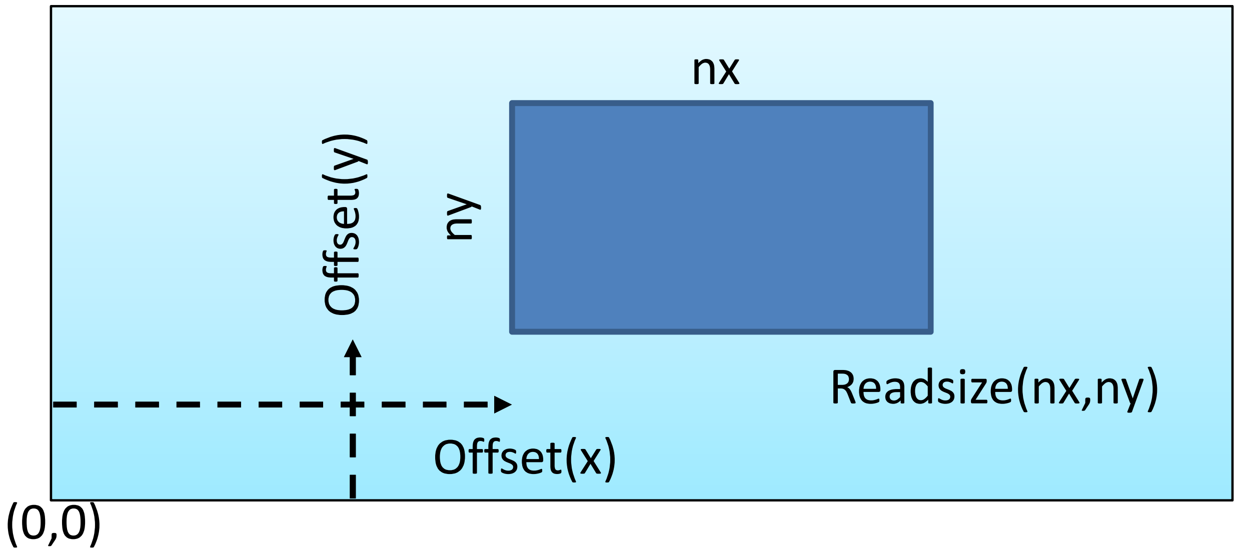
Read an attribute (no extra I/O)

- int **adios_get_attr** (ADIOS_FILE * fp,
  const char * attrname,
  enum ADIOS_DATATYPES * type,
  int * size,
  void ** data)
  - Attributes are stored in metadata, read in during open operation.
  - It allocates memory for the content, so you need to free it later with free().

Fortran
call adios_inq_attr (fp, attrname, attrtype, attrsize, err)

Select a bounding box

- In our example we need to define the selection area of what to read from an array.



- ADIOS_SELECTION * **adios_selection_boundingbox** (
 int ndim, uint64_t * offsets, uint64_t * readsize)

Fortran
call adios_selection_boundingbox (integer*8 sel,   -- return value
 integer ndim, integer*8 offsets(:), integer*8 readsize(:))

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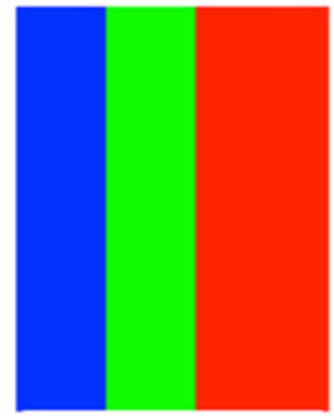
ADIOS Hands on: Read

- Goals
  - Learn how to read in data from an arbitrary number of processors.

Compile and run the read code

- We can read in data from 1 – 260 processors with a 1D domain decomposition



```
$ cd ../write_read
$ make
$ mpirun -n 1 ./reader
$ ls fort.*;tail -n 4 fort.100
    fort.100
     1 256 386 12.0
     1 257 386 12.0
     1 258 386 12.0
     1 259 386 12.0
```

Each line contains:
timestep x (global) y(global) xy

```
$ mpirun -n 7 ./reader
$ ls fort.*;tail -n 4 fort.100
    fort.100 fort.101 fort.102 fort.103 fort.104 fort.105 fort.106
     1 33 386 9.0
     1 34 386 9.0
     1 35 386 9.0
     1 36 386 9.0
```

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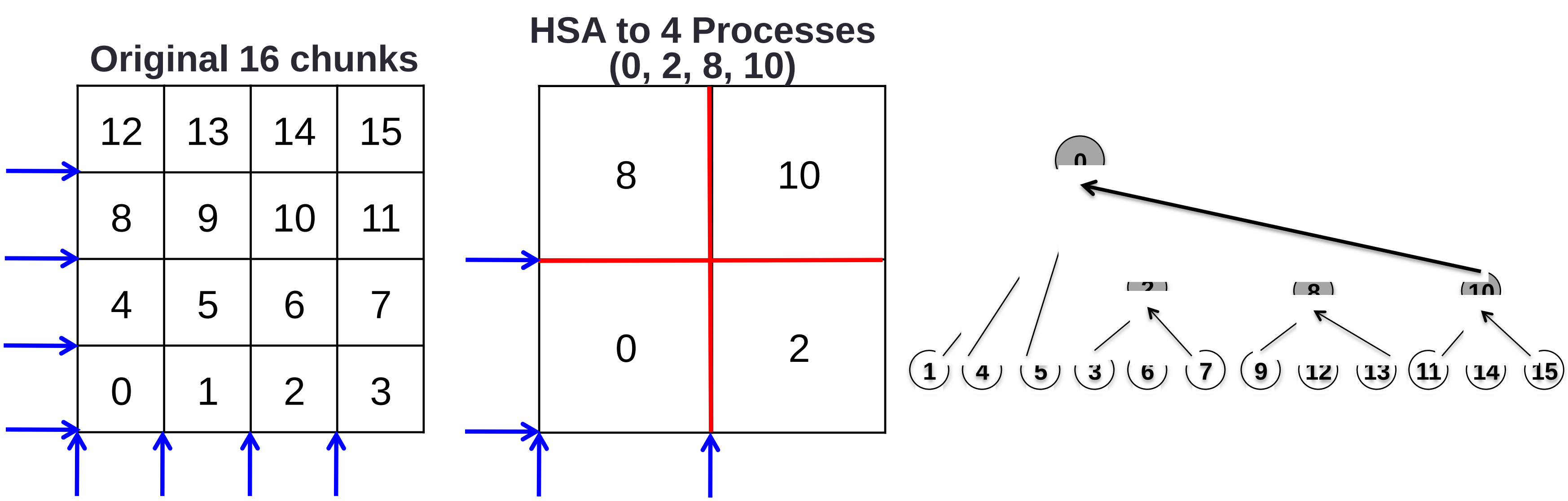
Hierarchical Spatial Aggregation

- Small chunks need to be consolidated to reduce seek overhead
- Simple concatenation doesn't change the number of seeks
- Spatial Aggregation with hierarchical topology merges spatially adjacent chunks into one
  - Spatial locality of every data point is reserved
  - Writing: less writers, less contention at storage during output
  - Reading: improve read performance for common spatial access patterns



VAR_MERGE transport method

- Applies Hierarchical Spatial Aggregation to consolidate small data variables
- It can/should be combined with other ADIOS methods
  - to achieve good I/O performance on a specific system
- Supports up to **three** dimensional variable with any kind of domain decomposition
- Currently supports up to 2 levels of aggregation
  - One level merges 2^n processes (for n-dimensional variables)
  - Merging 64 chunks into 1 for a 3-D variable with 3-D domain decomposition in two steps

How to use VAR_MERGE

```
<method group="genarray" method="VAR_MERGE">
      chunk_size=1048576;io_method=MPI_LUSTRE;
      io_parameters=stripe_count=4,stripe_size=1048576</method>
```

- chunk_size: the minimum of merged chunk size.
  - For example, for a 3-D variable with 3-D domain decomposition, spatial aggregation will be applied if the chunk_size=1MB, and each process has a chunk <128KB (1024KB/8).
  - Default chunk_size is 2MB.
- io-method: the underlying I/O transport method.
  - Default is ADIOS MPI method.
- io_parameters: the parameters required for using the specified "io_method"
  - Must be a comma-separated string of options, not a semicolon-separated one

VAR_MERGE on write_read example

- Only aggregator processes write the variable to file

<transport group="writer"
method="VAR_MERGE”>io_method=MPI
</transport>

```
$ cd ../write_read
$ vi writer.xml
$ mpirun -np 12 ./writer
$ ./map writer00.bp
 …
  double   /xy[387, 260]: min=0 max=11
    step    0:
      block    0: [   0:386,    0:259]
```

- 2 merges:
  - 12 → 4 then 4 → 1

<transport group="writer” method="VAR_MERGE”>
chunk_size=300000;io_method=MPI
</transport>

```
$ mpirun -np 12 ./writer
$ ./map writer00.bp
 …
  double   /xy[387, 260]: min=0 max=11
    step    0:
      block    0: [   0:257,    0:129]
      block    1: [   0:257, 130:259]
      block    2: [258:386,    0:129]
      block    3: [258:386, 130:259]
```

- 1 Level of merge
  - 12 → 4
  - Due to the limited buffer in the chunk_size

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ADIOS non-XML APIs

- Limitation of the XML approach
  - Must have all variables defined in advance
- Approach of non-XML APIs
  - Similar operations to what happens internally in adios_init
  - Define variables and attributes before opening a file for writing
  - The writing steps are the same as XML APIs
    - open file
    - set group size (size the given process will write)
    - write variables
    - close file

Non-XML API functions

- Initialization
  - init adios, allocate buffer, declare groups and select write methods for each group.

    adios_init_noxml ();

    adios_allocate_buffer (ADIOS_BUFFER_ALLOC_NOW, 10);

    - when and how much buffer to allocate (in MB)

    adios_declare_group (&group, "restart", "iter", adios_flag_yes);

    - group with name and optional timestep indicator (iter) and whether statistics should be generated and stored

    adios_select_method (group, "MPI", "", "");

    - with optional parameter list, and base path string for output files

Non-XML API functions

- Definition

  int64_t adios_define_var (group, “name”, “path”, type,
  “local_dims”, “global_dims”, “offsets”)

  – Similar to how we define a variable in the XML file
  – returns a handle to the specific definition

- Dimensions/offsets can be defined with
  – scalars (as in the XML version)
    - ```
      id = adios_define_var (g, "xy", "", adios_double,
                 "nx_global, ny_global",
                 "nx_local, ny_local",
                 "offs_x,offs_y")
      ```
    - need to define and write several scalars along with the array
  – actual numbers
    - ```
      id = adios_define_var (g, "xy", "", adios_double,
               "100,100", "20,20", "0,40")
      ```

Multiple blocks per process

- AMR codes and load balancing strategies may want to write multiple pieces of a global variable from a single process
- ADIOS allows one to do that but
  - one has to write the scalars defining the local dimensions and offsets for each block, and
  - group size should be calculated accordingly
  - This works with the XML API, too, but because of the group size issue, pre-generated write code cannot be used (should do the adios_write() calls manually)
  - Array definition with the actual sizes as numbers saves from writing a lot of scalars (and writing source code)

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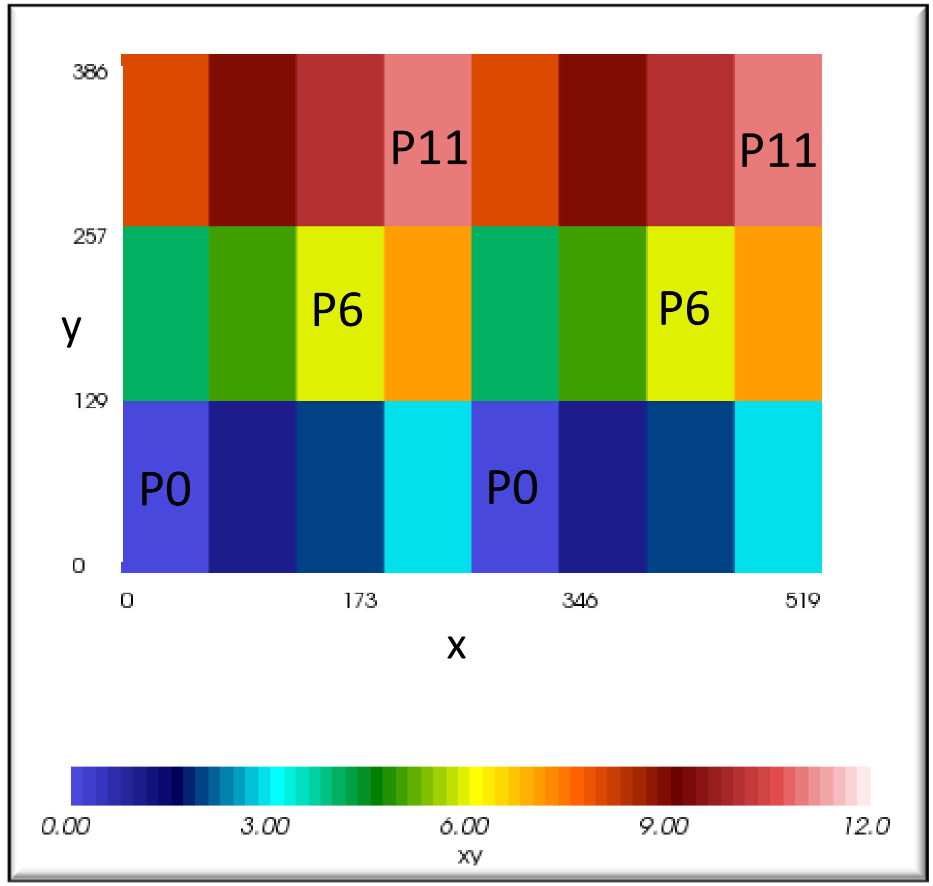
ADIOS Hands on Non-XML Write API

- Goals
  - Use Non-XML API of ADIOS
  - How to write multiple blocks of a variable from a process

Multi-block example (Fortran)

- Here we repeat the first tutorial example, except that each process writes 2 blocks (2^{nd} block shifted in the X offset).
  - 12 cores, arranged in a 4 x 3 arrangement.
  - 24 data blocks
- Each processor allocates an 65x129 array (xy)
  - we write the same array to two places in the output
- Total size of the array
  - 2*4*65 x 3*129
- Use the non-XML API
  - define and write xy array without scalars



noxml example

```
$ cd ../noxml_F90
$ make
$ mpirun -np 12 ./writer_noxml
 ts= 0
 ts= 1
$ ls -l *.bp
-rw-r--r-- 1 esimmon esimmon 1618482 2013-06-12 09:44 writer00.bp
-rw-r--r-- 1 esimmon esimmon 1618731 2013-06-12 09:44 writer01.bp
$ bpls -l writer00.bp
  double   /xy   {387, 520} = 0 / 11 / 5.5 / 3.45205
$ bpls -l writer01.bp
  double   /xy   {387, 520} = 1 / 12 / 6.5 / 3.45205
```

Block layout of the example

- map.c
  - uses ADIOS API to inquire the local dimensions and offsets of each writer

```
$ ../write_read/map
../write_read/writer00.bp
 …
  double  /xy[387, 260]: min=0 max=11
    step   0:
      block   0: [  0:128,   0: 64]
      block   1: [  0:128,  65:129]
      block   2: [  0:128, 130:194]
      block   3: [  0:128, 195:259]
      block   4: [129:257,   0: 64]
      block   5: [129:257,  65:129]
      block   6: [129:257, 130:194]
      block   7: [129:257, 195:259]
      block   8: [258:386,   0: 64]
      block   9: [258:386,  65:129]
      block  10: [258:386, 130:194]
      block  11: [258:386, 195:259]
```

```
$ ../write_read/map writer00.bp
  …
   double   /xy[387, 520]: min=0 max=11
      step   0:
         block   0: [  0:128,   0: 64]
         block   1: [  0:128, 260:324]
         block   2: [  0:128,  65:129]
         block   3: [  0:128, 325:389]
         block   4: [  0:128, 130:194]
         block   5: [  0:128, 390:454]
         block   6: [  0:128, 195:259]
         block   7: [  0:128, 455:519]
         block   8: [129:257,   0: 64]
         …
         block  16: [258:386,   0: 64]
         block  17: [258:386, 260:324]
         block  18: [258:386,  65:129]
         block  19: [258:386, 325:389]
         block  20: [258:386, 130:194]
         block  21: [258:386, 390:454]
         block  22: [258:386, 195:259]
         block  23: [258:386, 455:519]
```

noxml example

Quit the interactive job here. We will run the next example as a batch job.

```
$ exit
$ module load adios/1.5.0
```

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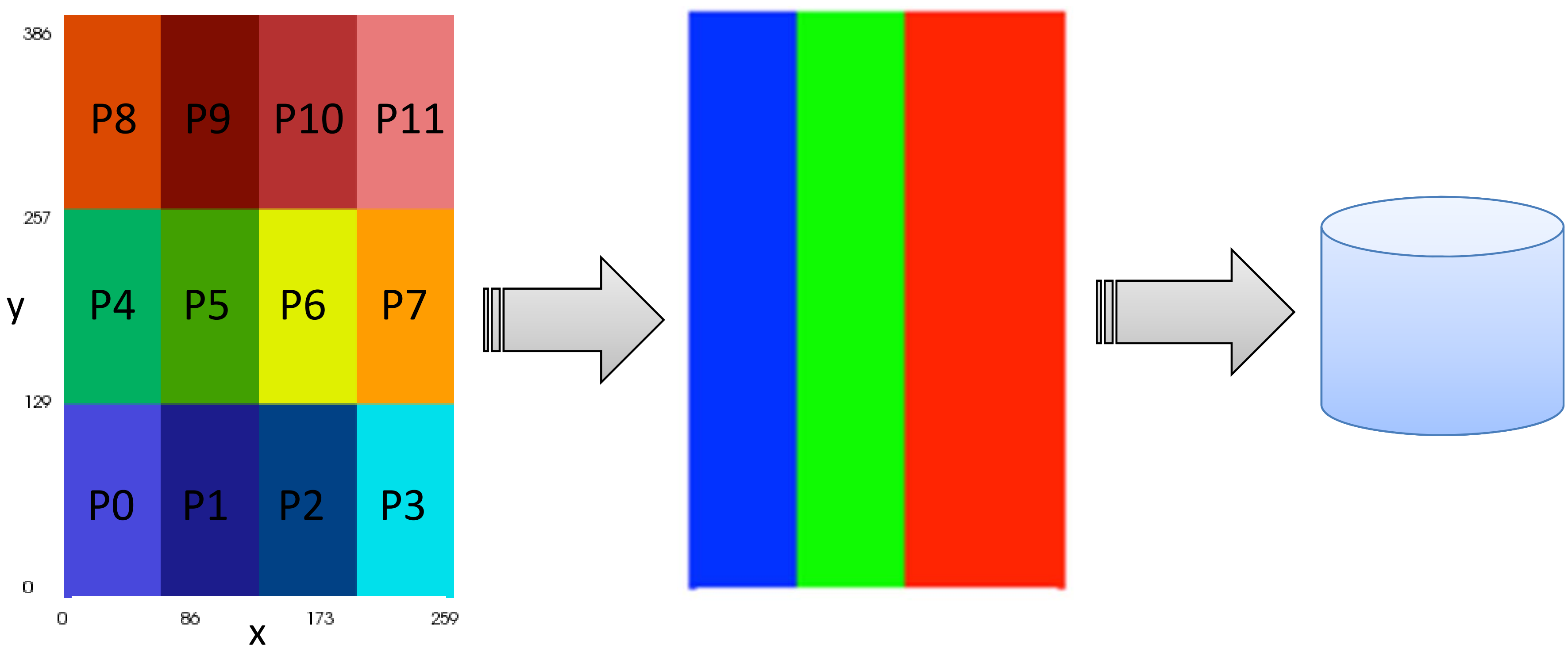
ADIOS Hands on

- Goals
  - Couple the write and read example with a staging method
  - How to write the streaming read code.
  - How to run a staging code.

Coupling Example

- The first write and read examples running together
  - We write out 5 time-steps, into the same file(name).
  - Write from 12 cores, arranged in a 4 x 3 arrangement.
  - Read from 3 cores, arranged as 1x3



coupling example

```
$ cd ../coupling
$ make
$ qsub job.chester
-- wait for who knows how long –
-- commands: showq, showstart, showbf
$ ls -l *.bp
-rw-r--r-- 1 pnorbert ccsstaff 1615244 Aug  4 09:56 reader_001.bp
-rw-r--r-- 1 pnorbert ccsstaff 1615493 Aug  4 09:56 reader_002.bp
-rw-r--r-- 1 pnorbert ccsstaff 1615742 Aug  4 09:56 reader_003.bp
-rw-r--r-- 1 pnorbert ccsstaff 1615991 Aug  4 09:56 reader_004.bp
-rw-r--r-- 1 pnorbert ccsstaff 1616240 Aug  4 09:56 reader_005.bp
$ bpls -l reader_001.bp
  integer  /info/rank  scalar = 0
  integer  /gdx        scalar = 260
  integer  /gdy        scalar = 387
  integer  /ldx        scalar = 86
  integer  /ldy        scalar = 387
  integer  /ox         scalar = 0
  integer  /oy         scalar = 0
  double   /xy         {387, 260} = 0 / 11 / 5.5 / 3.45205
  double   /xy2        {387, 260} = 0 / 2.55 / 1.28269 / 0.884548
```

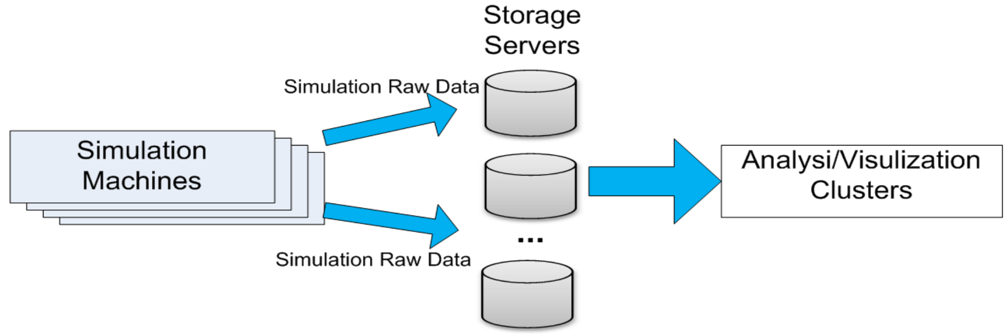
Previous Approaches for Sharing Data between Coupled Applications

Disk files

+ asynchronous communication

+ easy, commonly-used APIs

- affected by parallel IO performance



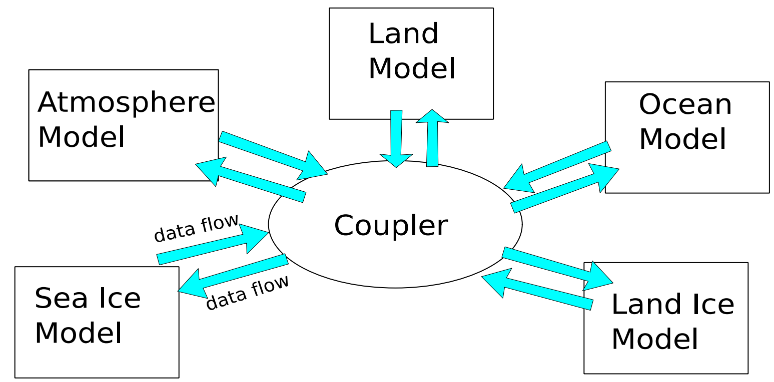
Simulation Data Analysis Pipeline Workflow (based on disk IO)

Coupler approach

+ asynchronous communication

+ data aggregation/transformation at the coupler

- centralized coupler(s) can become a bottleneck



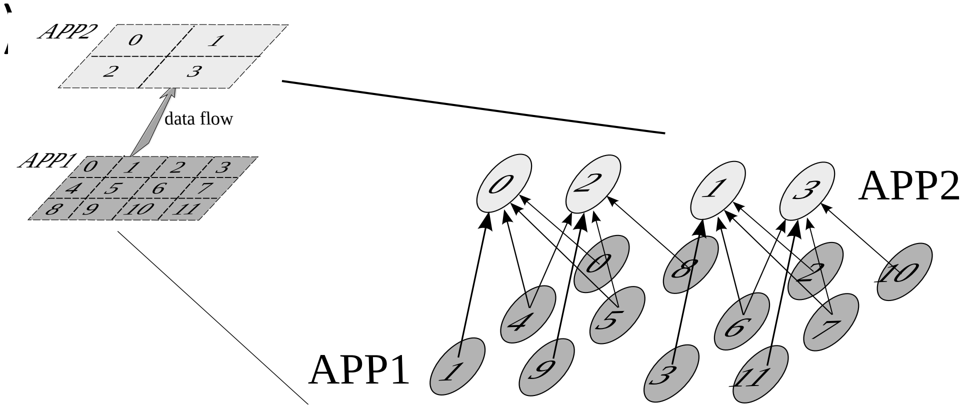
Integrated Climate Modeling Workflow (based on coupler)

Direct parallel data transfer (DIMES, FLEXPATH)

+ fast and scalable data movement

- programming complexity (hand coded)

- need for asynchronous interactions

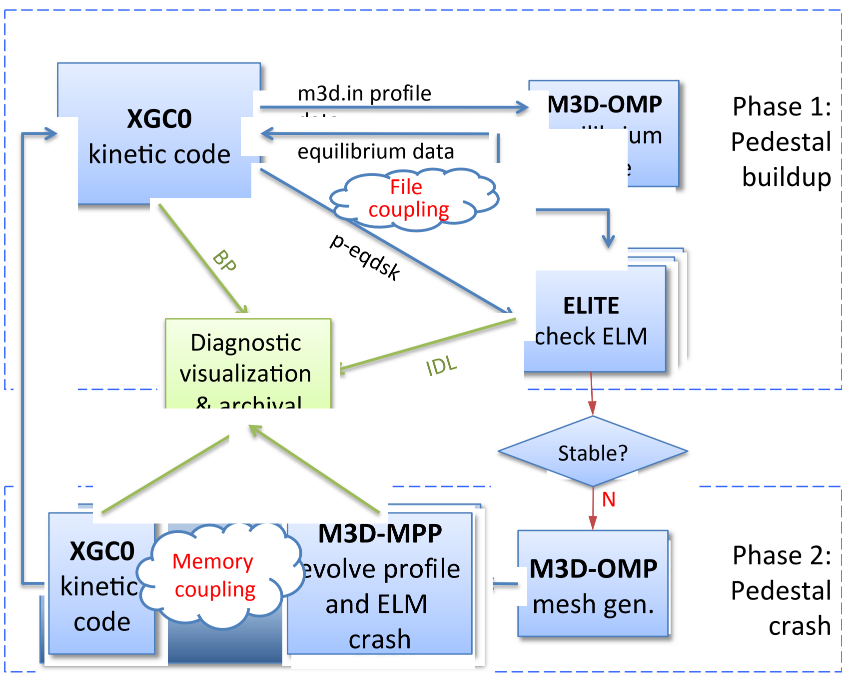


Tightly Coupled Two-Apps Workflow (based on direct parallel transfer)

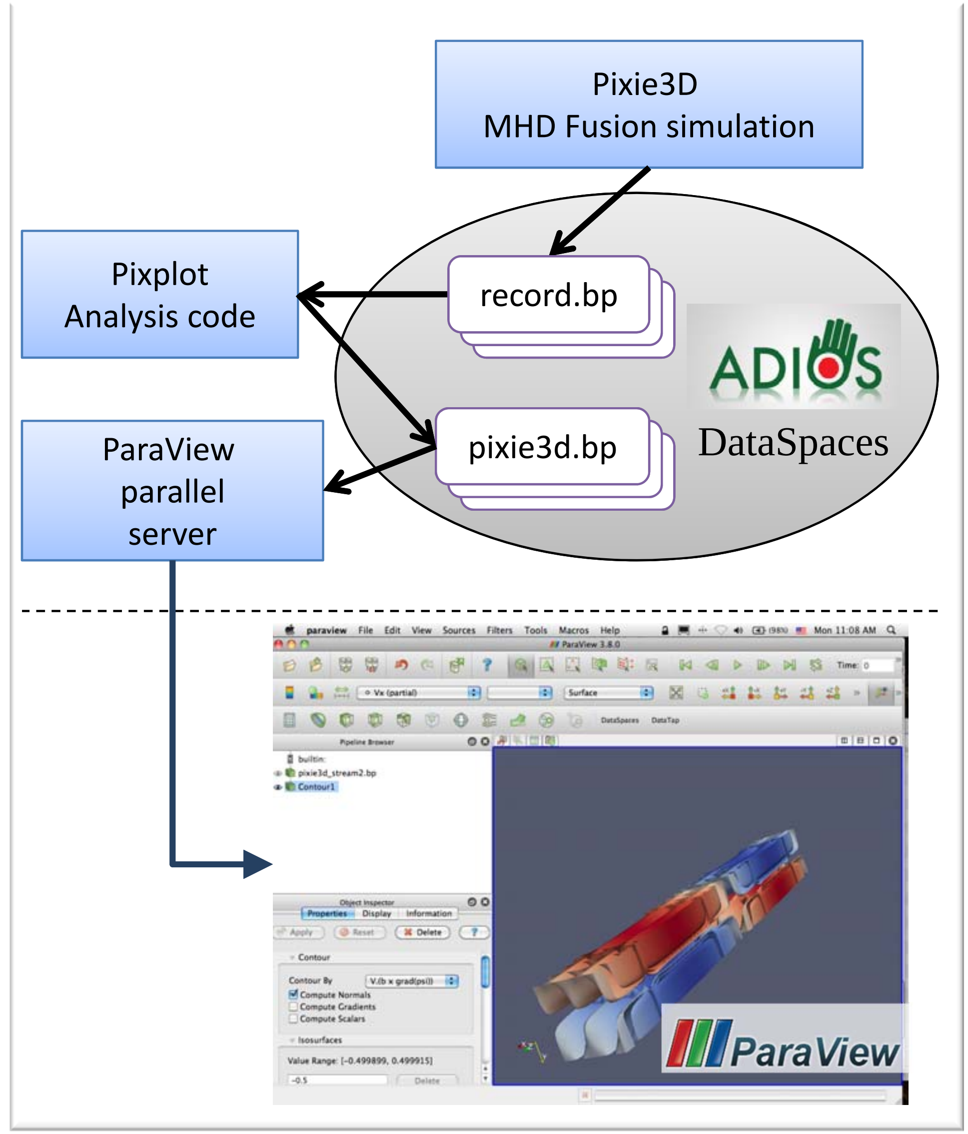
Coupling codes with ADIOS+staging method

ADIOS + DataSpaces/DIMES/FLEXPATH

+ asynchronous communication
+ easy, commonly-used APIs
+ fast and scalable data movement
+ not affected by parallel IO performance
- data aggregation/transformation at the coupler



Fusion code coupling (CPES project)



Interactive visualization pipeline of fusion simulation, analysis code and parallel viz. tool

ADIOS Read API for streams

Code which reads file data

```
call adios_read_init_method (ADIOS_READ_METHOD_BP, group_comm,“”,ierr);
call adios_read_open_stream (inh, infn, 0, group_comm,
                             ADIOS_LOCKMODE_CURRENT, 60.0, ierr)
do while (ierr != err_stream_terminated)
   call adios_selection_boundingbox (sel, 0, offset, readsize)
   call adios_schedule_read (inh, sel, "gdx", 1, 1, gdx, ierr)
   call adios_schedule_read (inh, sel, "gdy", 1, 1, gdy, ierr)
   call adios_perform_reads (inh, ierr)
   ! … calculate offsets and sizes of xy to read in…
   call adios_selection_boundingbox (sel, 2, offset, readsize)
   call adios_schedule_read (inh, sel, "xy", 1, 1, xy, ierr)
   call adios_perform_reads (inh, ierr)
   call adios_advance_step(inh, 0, 60.0, ierr)
enddo
call adios_read_close (inh, ierr)
```

ADIOS Read API for streams

Code which reads stream data

```
call adios_read_init_method (ADIOS_READ_METHOD_DATASPACES, group_comm,"",ierr);
call adios_read_open_stream (inh, infn, 0, group_comm,
                             ADIOS_LOCKMODE_CURRENT, 60.0, ierr)
do while (ierr != err_stream_terminated)
   call adios_selection_boundingbox (sel, 0, offset, readsize)
   call adios_schedule_read (inh, sel, "gdx", 1, 1, gdx, ierr)
   call adios_schedule_read (inh, sel, "gdy", 1, 1, gdy, ierr)
   call adios_perform_reads (inh, ierr)
   ! … calculate offsets and sizes of xy to read in…
   call adios_selection_boundingbox (sel, 2, offset, readsize)
   call adios_schedule_read (inh, sel, "xy", 1, 1, xy, ierr)
   call adios_perform_reads (inh, ierr)
   call adios_advance_step(inh, 0, 60.0, ierr)
enddo
call adios_read_close (inh, ierr)
```

Now we have memory to memory coupling

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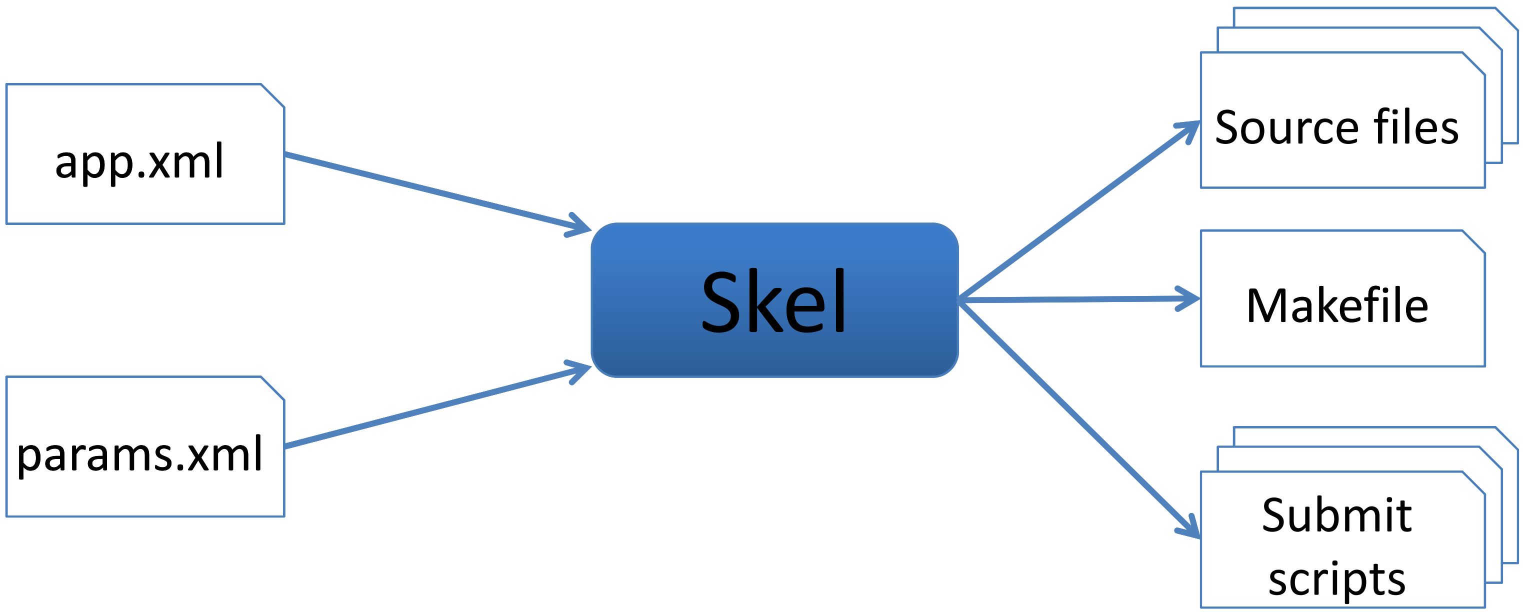
Skel: Automatic generation of I/O Skeletal Benchmarks

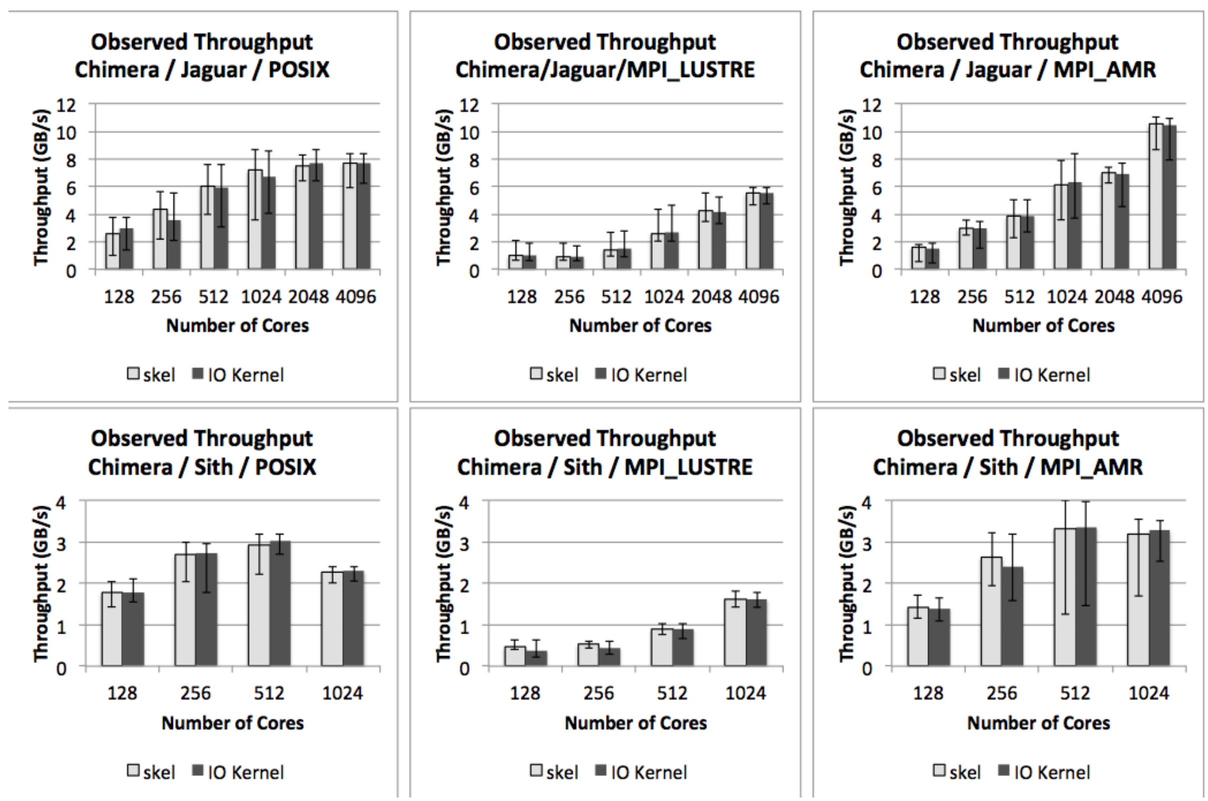


- Skeletal applications perform the same I/O operations as an application, but eliminate computation and communication
- Created from ADIOS XML file and a handful of additional parameters
- Easy to create, run, and update, compared to instrumented apps or I/O kernels

Skel: Users and Impact

- Extensible collection of relevant I/O benchmarks
- Focus less on measuring and more on improving I/O performance
- Create a comprehensive and relevant set of I/O benchmarks for new or existing hardware platforms
- Demonstrated to work well with these applications (so far):
  - S3D (Combustion)
  - GTS (Fusion)
  - CHIMERA (Astrophysics)
  - GRAPES (Weather)
  - GEOS-5 (Climate)

1 app,
2 machines,
3 methods



Skel Tutorial

```
# Begin with the XML file for the application
$ cd ../skel/
$ mkdir –p grapes
$ cd grapes
$ cp ../grapes.xml  .
$ ls
  grapes.xml

# First, generate the XML file for the skeletal app.
# just to filter out from xml file what would not work with skel
$ skel xml grapes
# skel sub_command project_name
$ ls
   grapes_skel.xml   grapes.xml
```

Skel Tutorial

\# Now create a default parameter file

```
$ skel params grapes
$ ls
    grapes_params.xml.default    grapes_skel.xml    grapes.xml
```

\# Copy the default parameters (this makes it more difficult to accidentally overwrite your settings)

```
$ cp grapes_params.xml.default grapes_params.xml
```

Skel Tutorial

Edit the parameters

$ vi grapes_params.xml

“target” defines the platform you are running on.

<scalars> are used to define array sizes

<arrays> can be initialized randomly or with specific

patterns (helpful for debugging)

<tests> allow multiple runs using different methods

or, just use a prepared run

$ cp ../grapes_params.xml .

Skel Tutorial

Generate the Makefile

$ skel makefile grapes

Generate the source file

$ skel source grapes

look at the generated code

$ vi grapes_skel_post_process_write.f90

Build the skeletal application

$ make

executable: grapes_skel_post_process_write

Skel Tutorial

And run it

```
$ mpirun -np 4 ./grapes_skel_post_process_write
 **************************
   Groupsize:              375892
   Open Time:   1.88302993774414063E-003
   Access Time:   8.32605361938476563E-003
   Close Time:   9.05203819274902344E-003
   Total Time:   1.54860019683837891E-002
 **************************
```

output file: out_post_process_write_1

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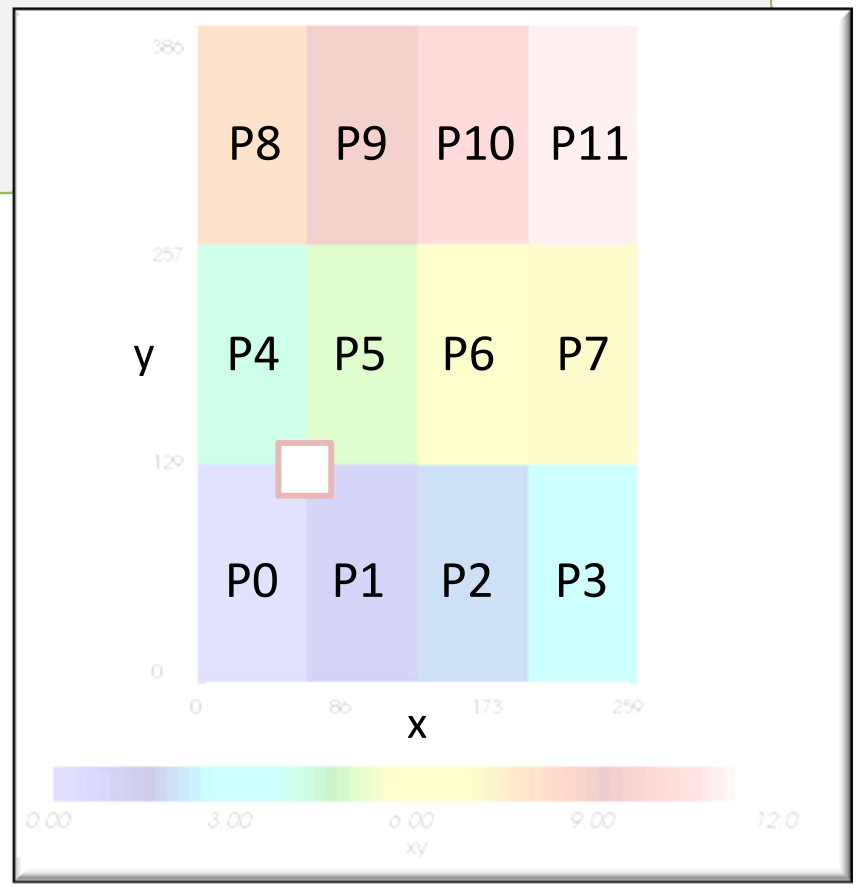
bpls

- Use bpls to read in a 2D slice

```
$ bpls writer00.bp -d xy -s "128,64" -c "2,2" -n 2
double   /xy   {387, 260}
 slice (128:129, 64:65)
 (128,64)     0 1
 (129,64)     4 5
```

- How do we the same in Matlab?



Matlab startup on Chester

```
$ module load matlab
$ matlab -nodesktop –nosplash

                          < M A T L A B (R) >
                Copyright 1984-2012 The MathWorks, Inc.
                  R2012b (8.0.0.783) 64-bit (glnxa64)
                            August 22, 2012


To get started, type one of these: helpwin, helpdesk, or demo.
For product information, visit www.mathworks.com.

>>
```

Matlab

```
>> data=adiosread('writer00.bp','xy','Slice',[65 2; 129 2])
data =
    0    4
    1    5
```

bpls result was

```
(128,64)    0 1
(129,64)    4 5
```

- Matlab is column-major, bpls (which is C) is row-major
  - 128, 64 → 64, 128
- Matlab array indices start from 1 (bpls/C starts from 0)
  - 64, 128 → 65, 129

```
>> f=adiosopen('writer00.bp');
>> data=adiosread(f.Groups,'/xy');
>> whos data
 Name       Size          Bytes   Class     Attributes

   data    260x387       804960   double
>> adiosclose(f);
```

Matlab API functions

- Open

  INFO = ADIOSOPEN (FILE);

  INFO = ADIOSOPEN (FILE, 'Verbose', LEVEL)

  - see definition in matlab: help adiosopen

- Close

  ADIOSCLOSE (STRUCT)

  - STRUCT is the return value of ADIOSOPEN

- Read from an opened file

  DATA = ADIOSREAD (STRUCT, VARPATH)

  - STRUCT is the return value of ADIOSOPEN

- Read from an unopened file

  DATA = ADIOSREAD (FILE, VARPATH)

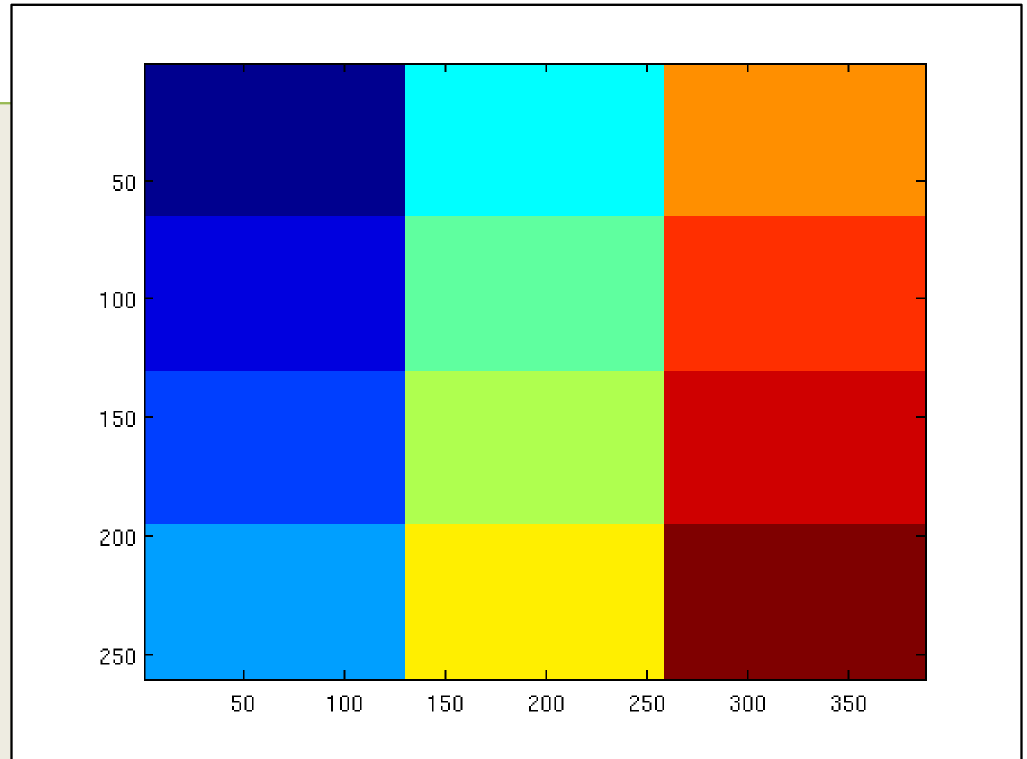
  - File is the path string here

Matlab reader.m for write_read example

```
function reader (file)

    % f=adiosopen(file);
    f=adiosopen(file, 'Verbose',0);

    % list metadata of all variables
    for i=1:length(f.Groups.Variables)
        f.Groups.Variables(i)
    end

    % read in the data of xy
    data=adiosread(f.Groups,'/xy');

    adiosclose(f)

    % export the last variable in the file as 'xy' in matlab
    assignin('base','xy',data);

    % check out the variable after the function returns
    %    whos('xy')
```

reader.m

```
>> reader('writer00.bp');
…
ans =
       Name: '/xy'
       Type: 'double'
       Dims: [260 387]
    Timedim: 0
  GlobalMin: 0
  GlobalMax: 11

>> whos
 Name      Size            Bytes  Class     Attributes
 xy      260x387           804960  double
>> imagesc(xy)
```



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ADIOS Python Wrapper Build

- Prerequisite modules and tools
  - NumPy: array and matrix representation
  - MPI4Py: MPI for Python
  - Cython: provide C/C++ interface to Python
  - Cmake: makefile generator
- Build
  - Run cmake which will detect python libraries and generate Makefile

    ```
    $ cmake /dir/to/adios-source/wrapper/numpy
    ```

  - Type make which will make adios.so

    ```
    $ make
    ```

  - Copy adios.so where python can access (E.g., ~/.local/lib/python2.6/site-packages)
- Use in Python

  ```
  >>> import adios
  ```

Writer Example

- Use the same Fortran example (01_write_read)
- Import necessary modules

```
import numpy as np
from mpi4py import MPI
import adios
```

- Use NUMPY for array/matrix

```
xy = np.zeros((ndx, ndy), dtype=np.float64)
```

- Call adios write functions

```
fd = adios.open("writer", filename, "w")
adios.set_group_size(fd, groupsize)
adios.write_int(fd, "nx_global", nx_global)
...
adios.write(fd, "xy", xy)
adios.close(fd)
```

Python Write API functions

- Init and finalize

  Init(CONFIG);

  finalize()

  - CONFIG is a filename for Adios XML config file
- Open & Close

  FOBJ = open(GRPNAME, FILENAME, MODE);

  close (FOBJ)

  - FOBJ is adios file object
- Write to an opened file

  write_int (FOBJ, VARNAME, VALUE)

  write (FOBJ, VARNAME, NUMPY_ARR)

  - NUMPY_ARR is a NumPy array/matrix object

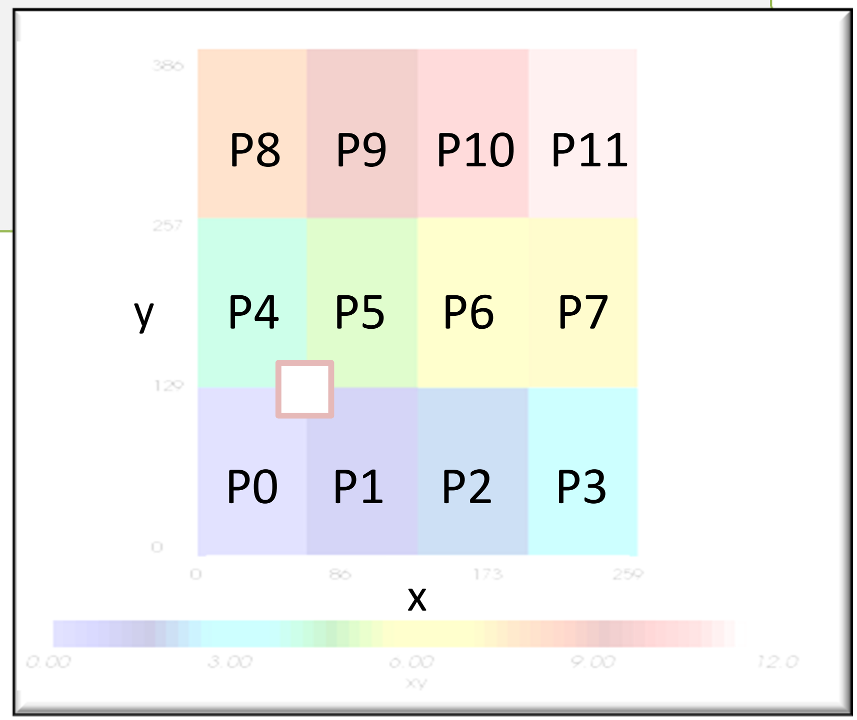
Writing

- We will get the same result with MPI

```
$ mpirun –np 12 ./writer.py
```

- Use bpls to read in a 2D slice

```
$ bpls writer00.bp -d xy -s "128,64" -c "2,2" -n 2
double    /xy    {387, 260}
 slice (128:129, 64:65)
 (128,64)     0 1
 (129,64)     4 5
```



Read Example

- Import necessary modules

```
import numpy as np
from mpi4py import MPI
import adios
```

- Call adios read functions

```
f = adios.AdiosFile(filename)
g = f.group["writer"]
## Scalar reading
nx_global = g.var["/nx_global"].read().item()
## Array/Matrix reading
xy = g.var["/xy"].read(offset, offset + count)
f.close()
```

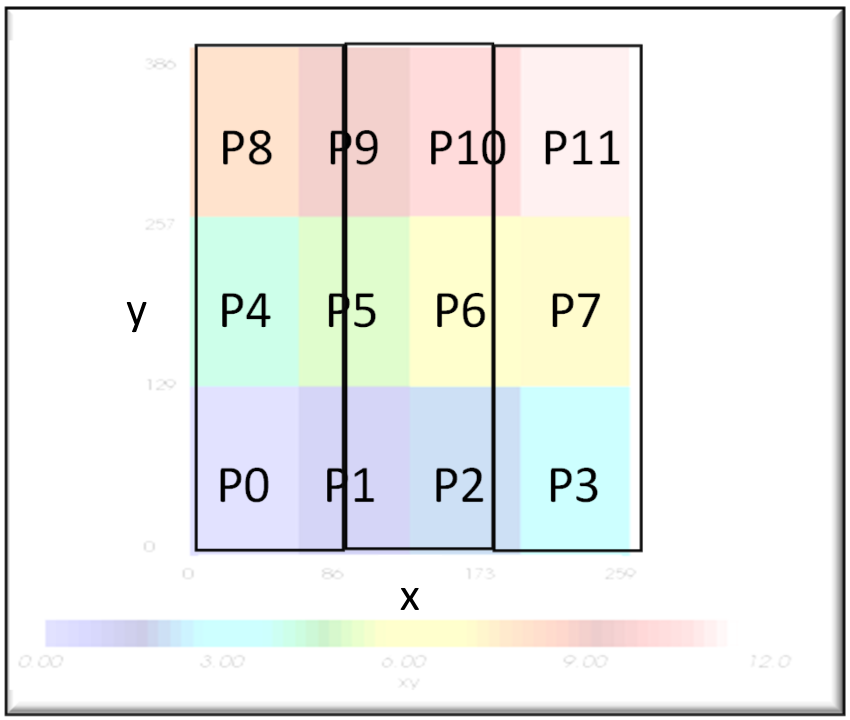
- read() will return NumPy object (array/matrix)

read

- Run with MPI

```
$ mpirun –np 3 ./reader.py
```

- Each process writes python.NNN (NNN is rank)
- Full matrix (387-by-260) will be decomposed by column-wise



Python Read API functions

- File Open & Close

  FOBJ = AdiosFile(FILENAME);

  FOBJ.close()

  - FOBJ is adios file object
- Group open

  GOBJ = FOBJ.group[GRPNAME]

  - GOBJ is adios group object
  - GRPNAME is a group name
- Read variables

  VOBJ = GOBJ.var [VARNAME]

  NUMPY_ARR = VOBJ.read()

  - VARNAME is a variable name
  - VOBJ is Adios variable object
  - NUMPY_ARR is a NumPy array/matrix object

Outline

- ADIOS Introduction
- ADIOS Write API
- Hands-on 1, Write data with ADIOS
- Hands-on 1, Tools
- ADIOS Read API
- Hands-on 1, Read data with ADIOS
- Hands-on 1++, Spatial aggregation
- Hands-on 2, ADIOS Write API (Non-XML version)
- Hands-on 2, Multi-block writing with non-XML API
- Hands-on 3, Staging example
- Hands-on 4, Visualization of ADIOS data
- Hands-on 5, I/O skeleton generation with Skel
- ADIOS + Matlab
- Hands-on 8 Python
- Hands-on 9, Java
- Summary

ADIOS Java Wrapper Build

- Prerequisite modules and tools
  - Java JDK: need Java Native Interface (JNI)
  - Cmake: makefile generator
- Build
  - Run cmake which will detect Java libraries and generate Makefile

    ```
    $ cmake /dir/to/adios-source/wrapper/java
    ```
  - Type make which will make libAdiosJava.so and AdiosJava.jar

    ```
    $ make
    ```
  - Copy libAdiosJava.so and AdiosJava.jar to a shared location (E.g., $ADIOS_DIR/lib)
- Use in Java

  ```
  import gov.ornl.ccs.Adios;      // For Writer
  import gov.ornl.ccs.AdiosFile; // For Reader
  import gov.ornl.ccs.AdiosGroup;
  import gov.ornl.ccs.AdiosVarinfo;
  ```

Java Write API functions

- MPI Init and finalize

  MPI_Init();

  MPI_Finalize()

  - Adios Java wrapper contains own MPI init and finalize routine
- Adios Init and finalize

  Init()

  Finalize(ID)

  - ID is a rank
- Open & Close

  H = open(GRPNAME, FILENAME, MODE);

  close (H)

  - H is adios file handler
- Write to an opened file

  Write (H, VARNAME, VAL)

  - Overloaded. VAL can be scalar or array (int, double, byte, ...)

Writer Example

- Same tasks with Fortran example (01_write_read)
- Import necessary class

```
import gov.ornl.ccs.Adios;
import gov.ornl.ccs.AdiosFile;
import gov.ornl.ccs.AdiosGroup;
import gov.ornl.ccs.AdiosVarinfo;
```

- Call adios write functions

```
long adios_handle = Adios.Open ("writer”,
            String.format("writer%02d.bp", ts), "w", comm);
Adios.SetGroupSize (adios_handle, groupsize);

Adios.Write (adios_handle, "nx_global", nx_global);
...
Adios.Write (adios_handle, "xy", xy);
Adios.Close (adios_handle);
```

mpiexec and bpls

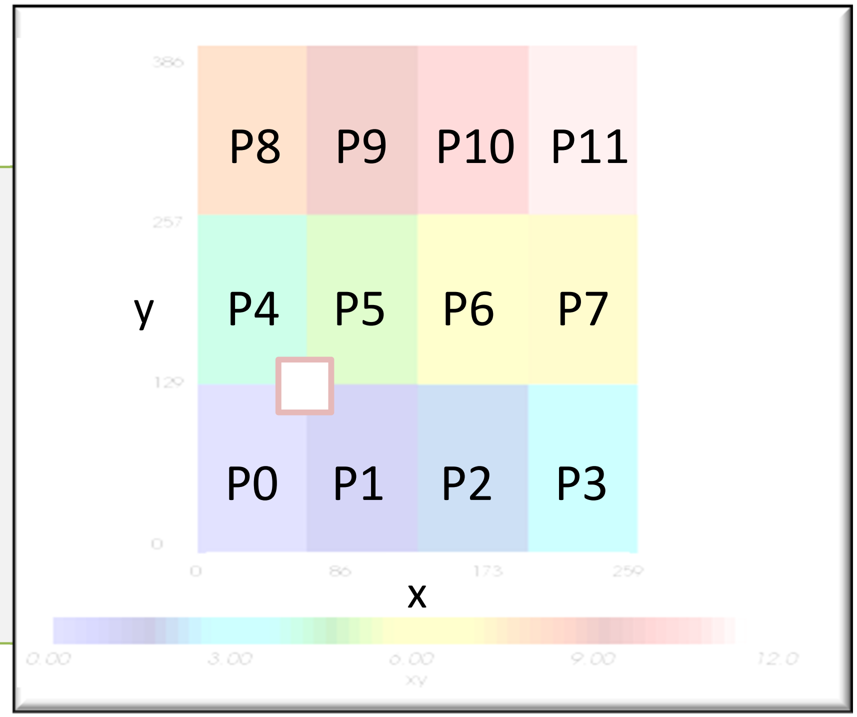
- We will get the same result with MPI

```
$ mpiexec -n 12 java -Djava.library.path=/opt/adios/1.5.0/lib -classpath /opt/adios/1.5.0/lib/AdiosJava.jar:. Writer
```

  - Add AdiosJava.jar in the classpath
  - Specify the directory contains libAdiosJava.so (shared lib) in java.library.path

- Use bpls to read in a 2D slice

```
$ bpls writer00.bp -d xy  \
  -s "128,64” -c "2,2" -n 2
double    /xy    {387, 260}
 slice (128:129, 64:65)
 (128,64)     0 1
 (129,64)     4 5
```



Java Read API functions

- File open & close

  ```
  AdiosFile FH = new AdiosFile();
  FH.open(FILENAME, COMM);
  FH.close()
  ```

  - H is adios file handler

- Group open & close

  ```
  AdiosGroup GH = new AdiosGroup(FH);
  GH.group(GRPNAME)
  ```

  - GH is adios group handler
  - GRPNAME is a group name

- Read variables

  ```
  AdiosVarinfo VH = new AdiosVarinfo(GH);
  VH.inq(VARNAME)
  VH.readIntValue()
  VH.read(OFFSET, COUNT, ARR)
  ```

  - VARNAME is a variable name
  - VH is Adios variable handler
  - After inq(), call readIntValue() for scalar or read() for array

Read Example

- Import necessary library

```
import gov.ornl.ccs.AdiosFile;
import gov.ornl.ccs.AdiosGroup;
import gov.ornl.ccs.AdiosVarinfo;
```

- Open file, group, and varinfo

```
AdiosFile file = new AdiosFile();
file.open(String.format("writer%02d.bp", ts), comm);
AdiosGroup group = new AdiosGroup(file);
group.open("writer");
AdiosVarinfo var1 = new AdiosVarinfo(group);
var1.inq("nx_global");
```

- Read scalar or array

```
int nx_global = var1.readIntValue();
double[] xy = new double[...];
var3.read(offset, readsize, xy);
```

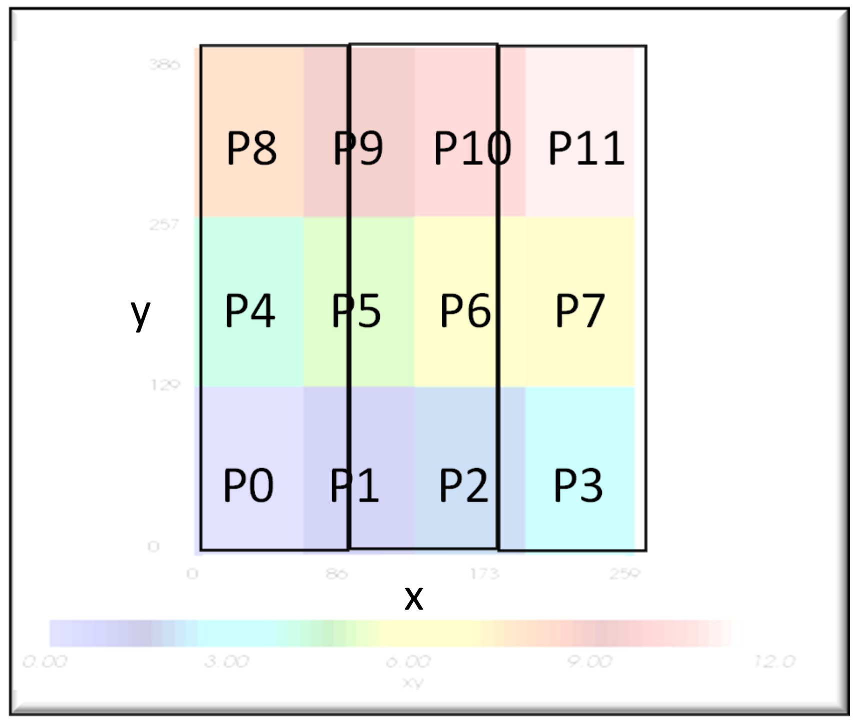
mpiexec and bpls

- Run with MPI

```
$ mpiexec -n 3 java -Djava.library.path=/opt/adios/1.5.0/lib -classpath /opt/adios/1.5.0/lib/AdiosJava.jar:. Reader
```

  - Add AdiosJava.jar in the classpath
  - Specify the directory contains libAdiosJava.so (shared lib) in java.library.path

- Each process writes java.NNN (NNN is rank)
- Full matrix (387-by-260) will be decomposed by column-wise



Summary

- ADIOS is an abstraction for data pipelines
  - Over 60 publications
- Typically the ADIOS team creates new I/O methods when applications require them
  - Fusion applications (Particle-in-cell, MHD)
  - Combustion (DNS, LES, AMR)
  - Astrophysics
  - Relativity
  - Climate
  - Weather
  - QCD
  - High Energy Physics
- ADIOS 1.5 includes staging services
  - I/O abstraction allows codes to be executed in staging area
- ADIOS 2.0 will be a new version of ADIOS using SOA methodologies