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U.S. DEPARTMENT OF ENERGY

Collective I/O Optimizations for Adaptive Mesh Refinement Data Writes on Lustre File System

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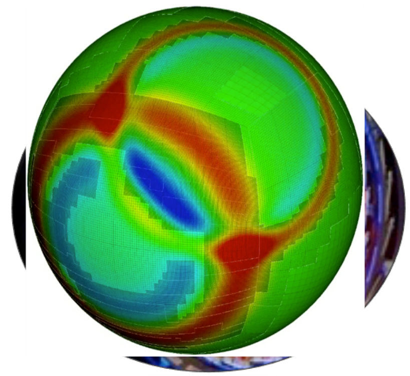
Overview

- Complex I/O patterns result in poor performance
- Adaptive Mesh Refinement (AMR) I/O is complex
- Poor I/O stalls AMR simulations
- Contributions of this paper
  - Identification of AMR I/O bottleneck in the Chombo library
  - Collective buffering optimizations
    - MPI-IO Collective buffering
    - Novel Aggregated Collective Buffering (ACB) strategy
  - I/O performance improvement with ACB

Data-driven science

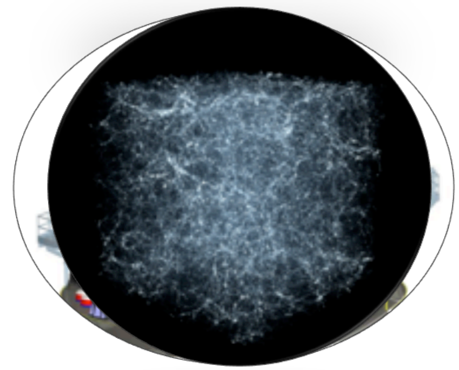
- **Simulations**
  - Multi-physics (FLASH) – 10 PB
  - Cosmology (NyX) – 10 PB
  - Plasma physics (VPIC) – 1 PB
- **Experimental and Observational data**
  - High energy physics (LHC) – 100 PB
  - Cosmology (LSST) – 60 PB
  - Genomics – 100 TB to 1 PB
- **Scientific applications rely on efficient access to data**



Climate

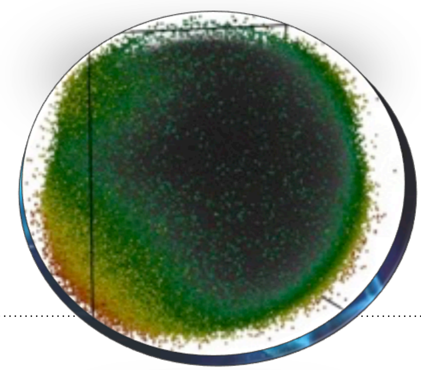
LHC

Dycore



NyX

LSST



VPIC

Genomics

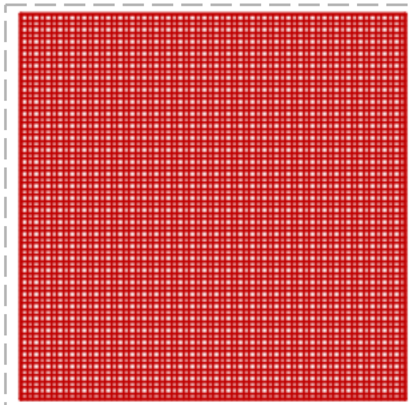
Background – Adaptive Mesh Refinement (AMR)

Dynamically adapts the spatial resolution of geometric meshes

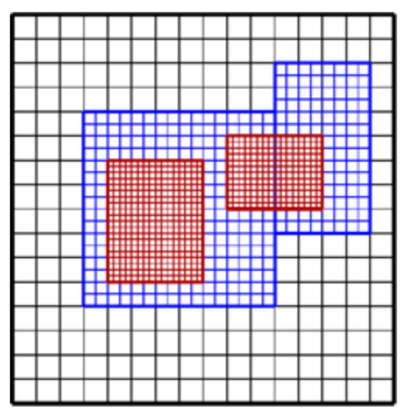
- Improved efficiency of computational resources while meeting desirable error levels

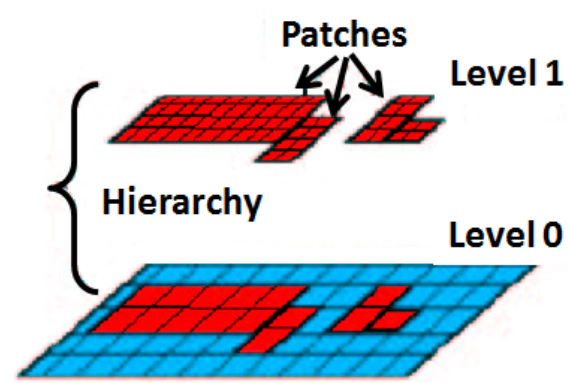
Block-structured AMR

- A hierarchy of levels of resolutions
- Boxes/Patches: non-overlapping, logically-rectangular regions



10^{15} cells
vs.
130,000 cells



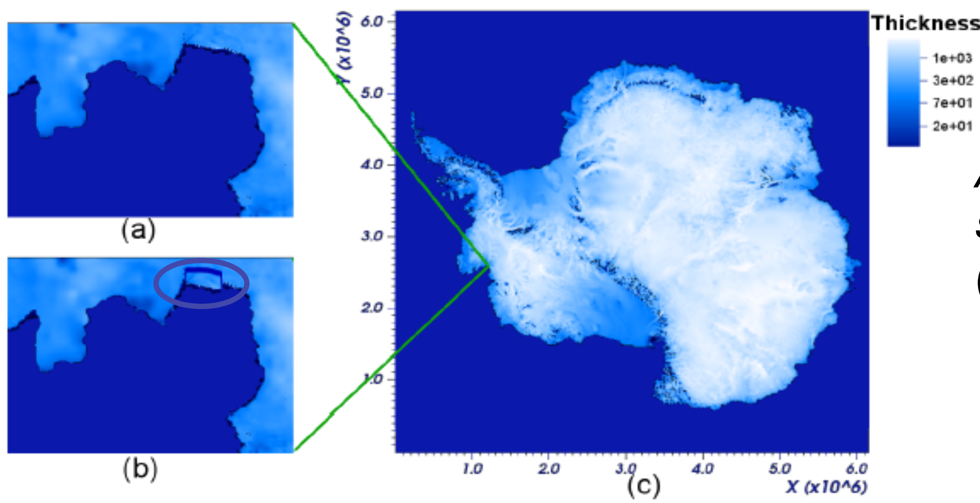


Sample AMR data structure

AMR use cases – Ice sheet simulations

- **BISICLES** is an AMR ice sheet model aimed at large (continental)-scale ice sheets, and is built on the Chombo framework
- Projections of future sea level rise resulting from impacts of climate change on large ice sheets

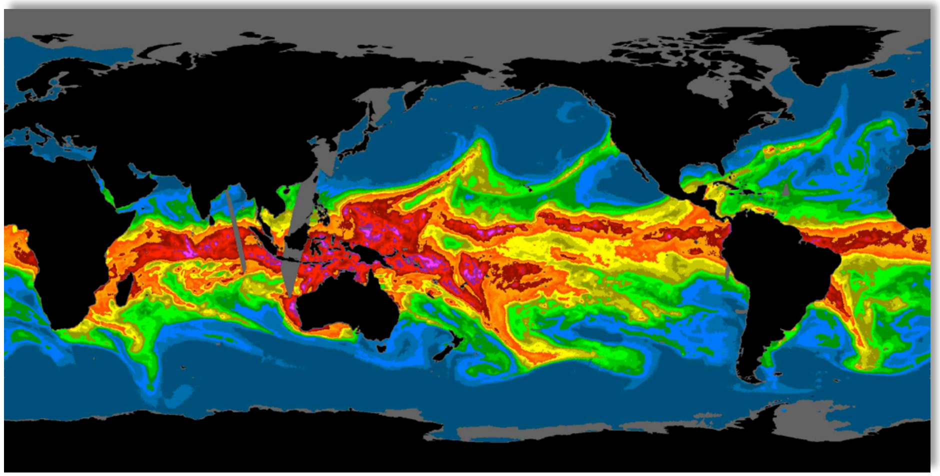
A rectangular region of ice (~30km x 26km in real size) detaches from the main shelf

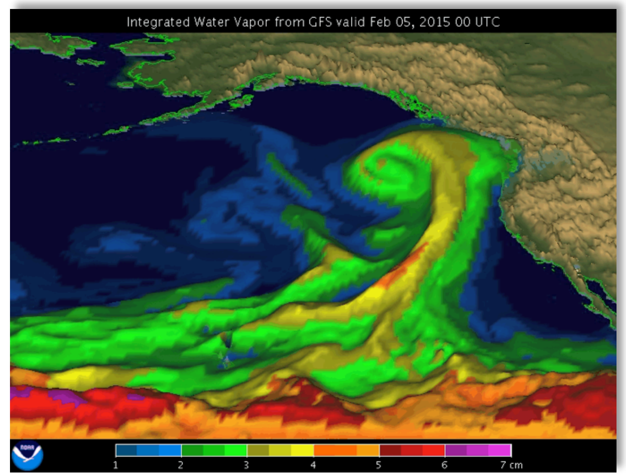


Antarctica glacier, surrounded by ocean (dark blue).

AMR use cases – Climate simulations

- The **AMR Dycore** is a high-accuracy AMR climate model “dynamical core” based on Chombo
- **<u>Significance</u>**: Identify atmospheric features (tropical cyclones, atmospheric rivers, etc.), and track them in time and at high resolution





Atmospheric River, fig from ESRL

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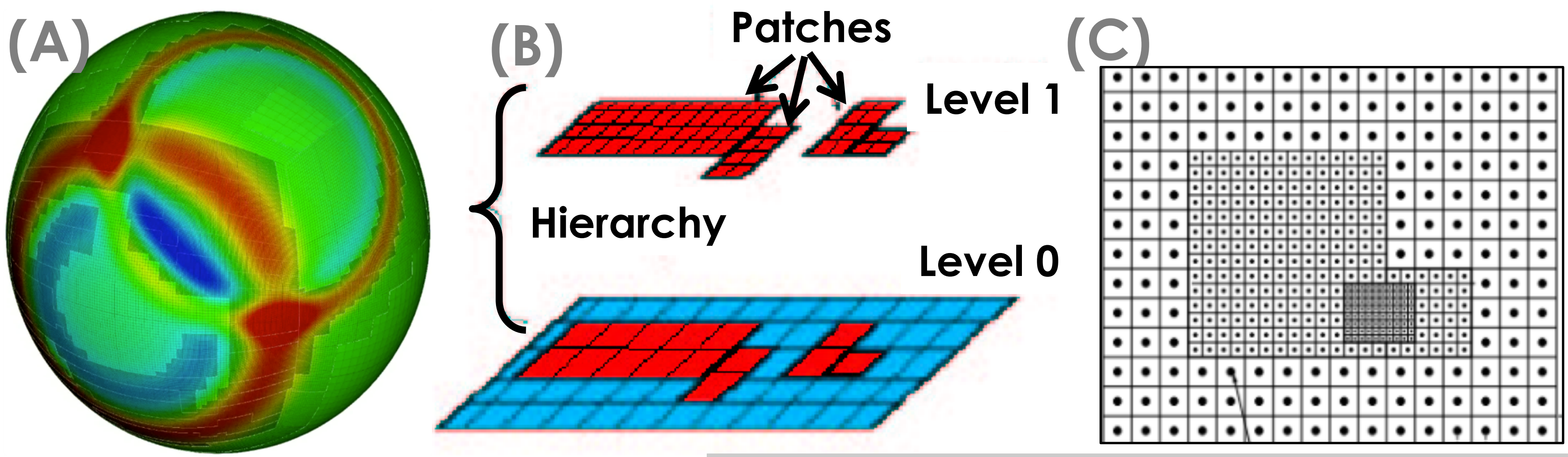
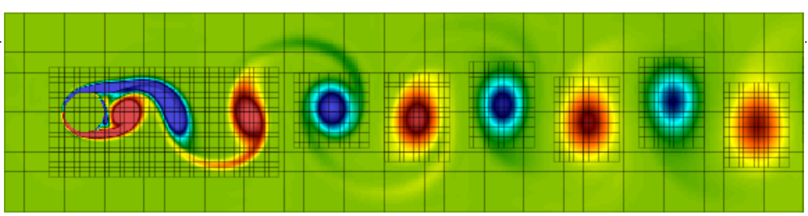
A brief intro to Chombo

- Software package for solving PDE-based physics models on AMR grids at large scales
- Utilities for simulating in domains with complex geometries, or on mapped grids

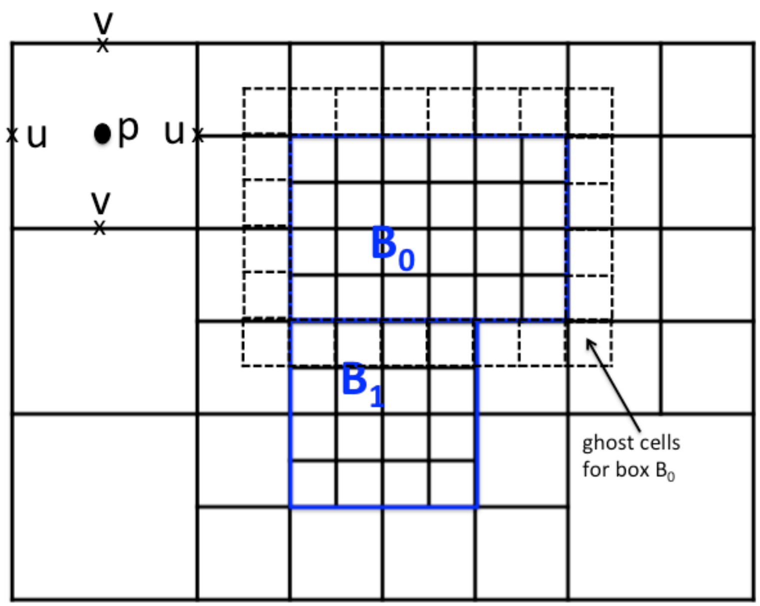




*(A) An example of a space-time adaptive mesh refinement calculation in a cubed sphere geometry, for Climate applications. (B) The **hierarchical levels of mesh refinement** are used to capture moving features (e.g., multiple overlapping pressure waves). (C) Each **level of refinement** consists of a **group of patches**, each contains multiple data points, and each point belongs to a single patch. Tracked features can span patches or multiple levels as they evolve in time.*

A brief intro to Chombo, cont.

- Implements block-structured AMR
  - Consists of hierarchy of uniform meshes, with resolution of 2 consecutive levels related by the refinement ratio
  - Each grid level divided into rectangular “boxes”



3 level AMR grid with 3 variables (u, v, p). The refinement ratio is 2 in each direction

Distribution of data in Chombo applications

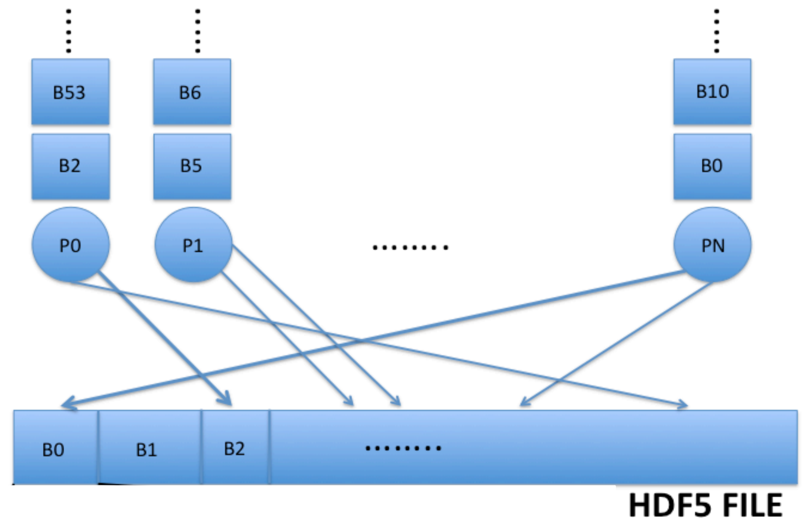
- Boxes distributed across MPI processes to balance loads across processes as much as possible
  - Load for box is usually proportional to number of points in a box

- Typical load balancing procedure:
  - Sort by Morton ordering (lists spatially adjacent boxes together)
  - Apply Kernighan-Lim algorithm to distribute boxes
    - Resulting distribution of boxes may appear random

Chombo's I/O pattern

- Boxes arranged in lexicographic order in file
  - Lexicographic order: Box B0 <= Box B1 if lower left corner of B0 <= lower left corner of B1 in grid
- Processes write independently to non-contiguous regions in the file
- Separate write for each box
- Results in several small independent write calls

Boxes distributed across MPI processes to balance loads



Boxes in lexicographic order in file

Performance bottleneck with current implementation

- Separate write for each box results in several write calls overall
  - Large scale Chombo simulations can have ~10^5 boxes
  - Large overhead for processing many write calls

- Each call only writes small amount of data (~1-4 MB per box)

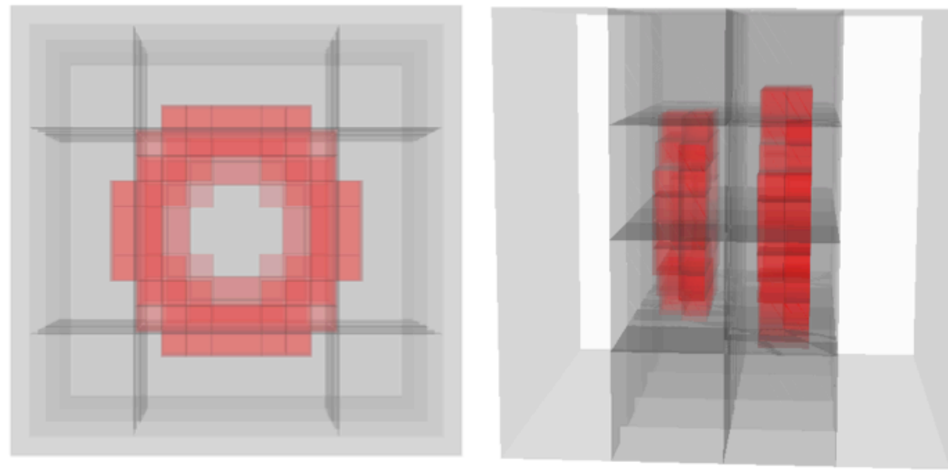
- Each call performs new seek to find file location for writing

Experimental Evaluation – Systems

- **NERSC Edison**
  - Cray XC30 supercomputer with Lustre file system
  - The *scratch2* file system has 96 OSTs with 72 GB/s peak I/O bandwidth
    - 4 OSTs per I/O server (OSS)
- **NERSC Cori (Phase 1)**
  - Cray XC40 supercomputer with Lustre file system
  - 248 OSTs with 744 GB/s peak I/O bandwidth
    - 1 OST per I/O server (OSS)

Experimental Evaluation– Chombo I/O Benchmark

- Isolates Chombo's write functionality
- Provides control over amount of data written through a replication factor parameter.
  - Parameter indicates number of times to replicate unit grid in each direction
  - In the experiments, we set this replication factor to write out 61 GB, 494 GB, and 987 GB data files



2 views (front and side) of one unit of AMR grid used in experiments. Grid has 3 levels. Refinement factor between levels is 4 (in each direction).

Darshan stats for existing I/O pattern

Darshan Counter	Independent I/O
Number of MPI-IO writes	115268
Number of POSIX writes	115628
Most common access size	4 M
Count of most common access size	115201
2nd most common access size	272 bytes
Count of 2nd most common access size	15

Number and size of writes determined by number and size of boxes (total number of boxes = 115628, each box ~ 4 MB)

Stats for run on Edison with 2304 processes (96 nodes).
File striped across 96 OSTs with stripe size of 8 MB. 494 GB was written.

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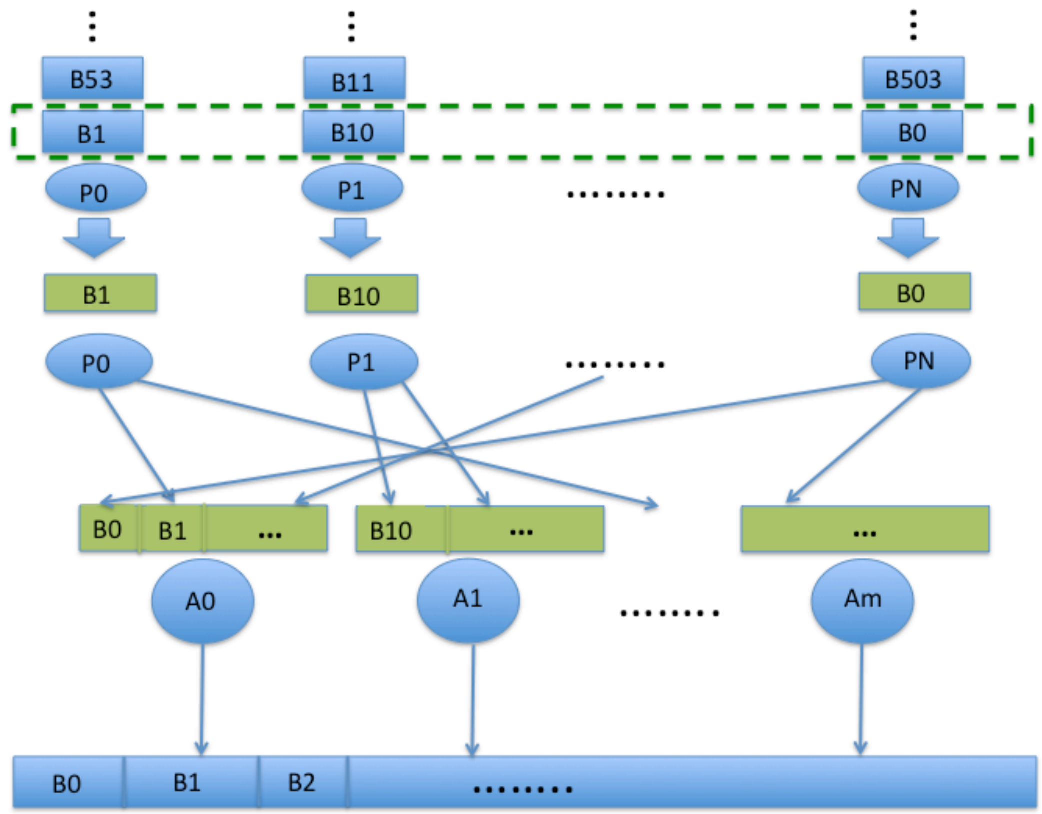
Aggregation with MPI-IO collective buffering

- Idea: aggregate contiguous data into buffers to reduce number of write calls
- Subset of MPI processes assigned to perform the aggregation
- CB2 mode of MPI-IO collective buffering optimizes for the Lustre file system

Collective buffering I/O pattern

- Aggregators (A0,…) collect boxes and reshuffle them into buffers
- Each process only sends a single box in each collective call
  - Each process can contain several boxes, resulting in many collective write calls



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Darshan stats for MPI-IO Collective buffering

Darshan Counter	Independent I/O	Collective buffering
Number of MPI-IO writes	115268	119808
Number of POSIX writes	115628	164270
Most common access size	4 M	4 M
Count of most common access size	115201	42689
2nd most common access size	272 bytes	8 M
Count of 2nd most common access size	15	4830

Get some larger writes with collective buffering

Number of CB aggregators = number of OSTs = 96

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Darshan stats for MPI-IO Collective buffering

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Count of 2nd most common access size	15	4830

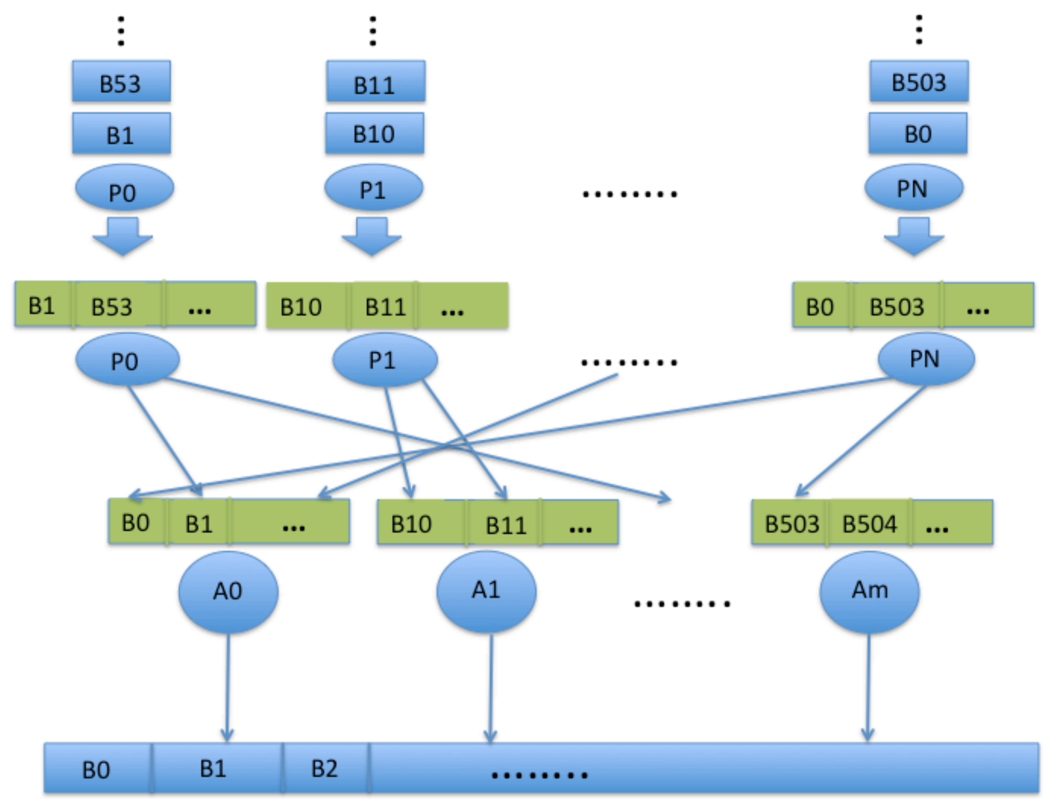
Still have many small writes

Get some larger writes with collective buffering

Number of CB aggregators = number of OSTs = 96

Aggregated Collective Buffering (ACB)

- Aggregate all boxes into one buffer on each process
  - Number of boxes copied into ACB buffer is a parameter, which can be tuned to balance performance and memory usage (future direction)
- MPI-IO aggregators reshuffle boxes for large contiguous writes



Darshan stats for ACB

Darshan Counter	Independent I/O	Collective buffering	ACB
Number of MPI-IO writes	115268	119808	6912
Number of POSIX writes	115628	164270	63241
Most common access size	4 M	4 M	8 M
Count of most common access size	115201	42689	63177
2^{nd} most common access size	272 bytes	8 M	272 bytes
Count of 2^{nd} most common access size	15	4830	16

ACB significantly reduces number of POSIX writes

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Darshan stats for ACB

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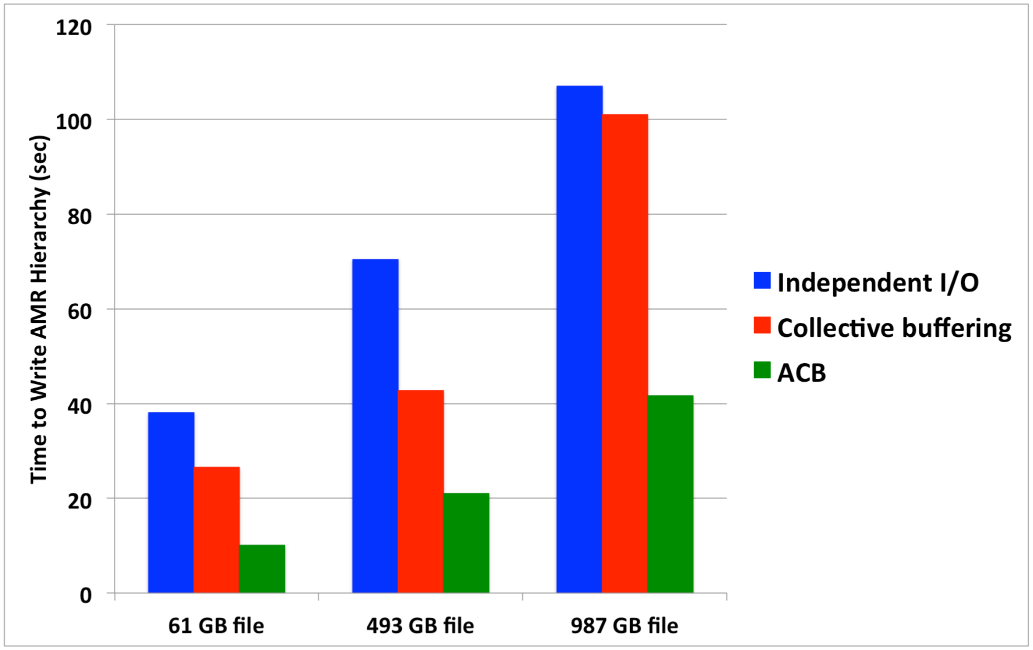
ACB significantly reduces number of POSIX writes

Most writes are relatively large

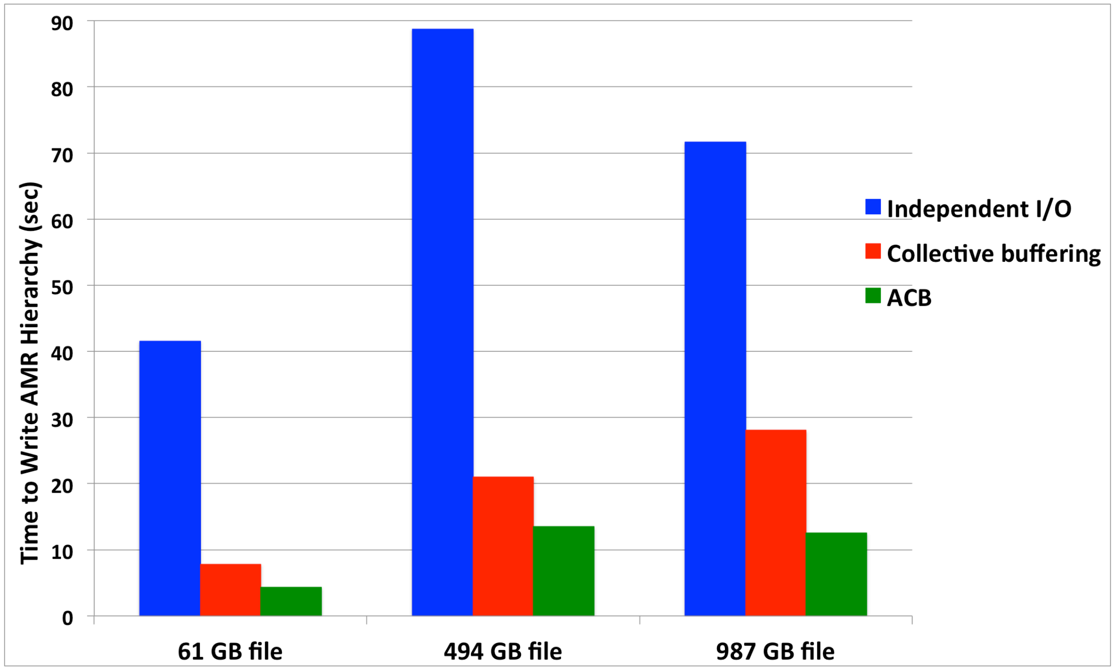
Performance on Edison



- 61 GB test: 576 procs (24 nodes), striped across 24 OSTs with 4 MB stripe size
- 494 GB test: 2304 procs (96 nodes), striped across 96 OSTs with 8 MB stripe size
- 987 GB test: 5760 procs (240 nodes), stripes across 96 OSTs with 16 MB stripe size

- ACB is 2.6x to 3.8x faster than independent I/O
- ACB is 2x to 2.6x faster than collective buffering
- Striping affects performance of collective buffering on 987 GB test case

Performance on Cori



- ACB is 5.7x to 9.6x faster than independent I/O
- ACB is 1.6x to 1.8x faster than collective buffering

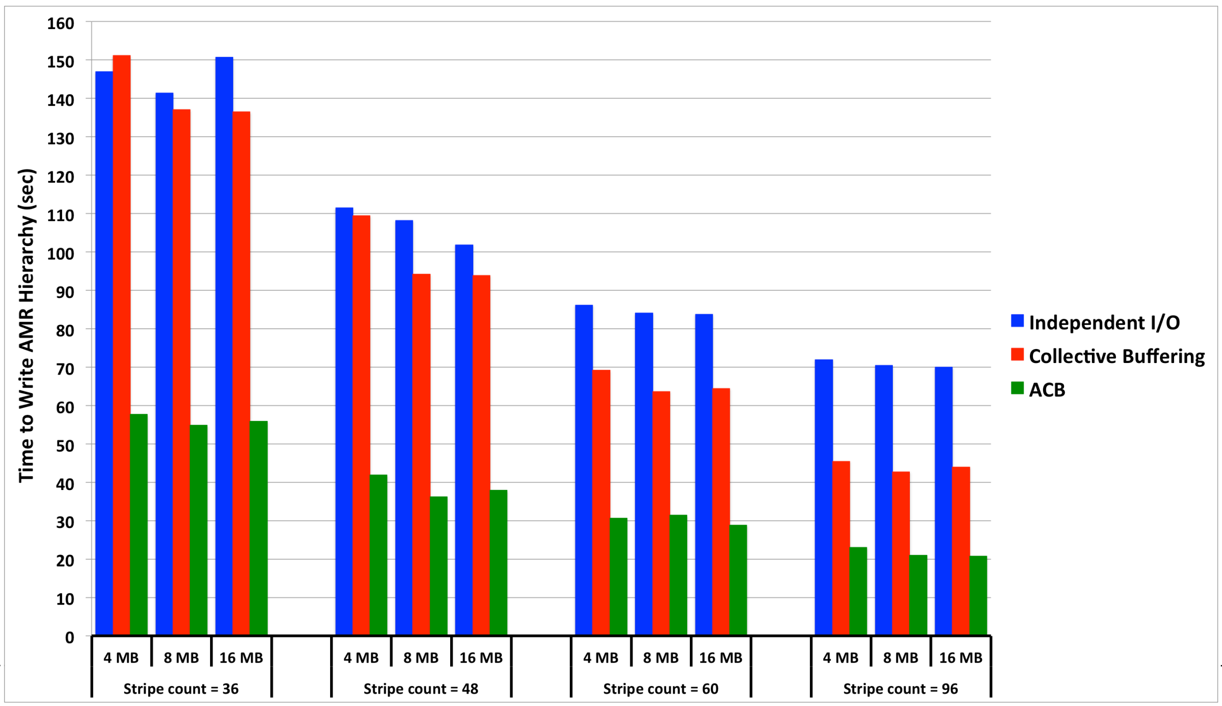
- 61 GB test: 576 procs (24 nodes), striped across 24 OSTs with 4 MB stripe size
- 494 GB test: 3072 procs (96 nodes), striped across 96 OSTs with 8 MB stripe size
- 987 GB test: 5856 procs (244 nodes), stripes across 244 OSTs with 16 MB stripe size

Evaluation with Lustre striping - Edison

Experiment specifics:

- 2304 procs (96 nodes)
- 494 GB file
- Striped across 96 OSTs
- Stripe size = 8 MB

ACB is 2x to 3.4x faster than independent I/O, and 2x to 2.6x faster than collective buffering



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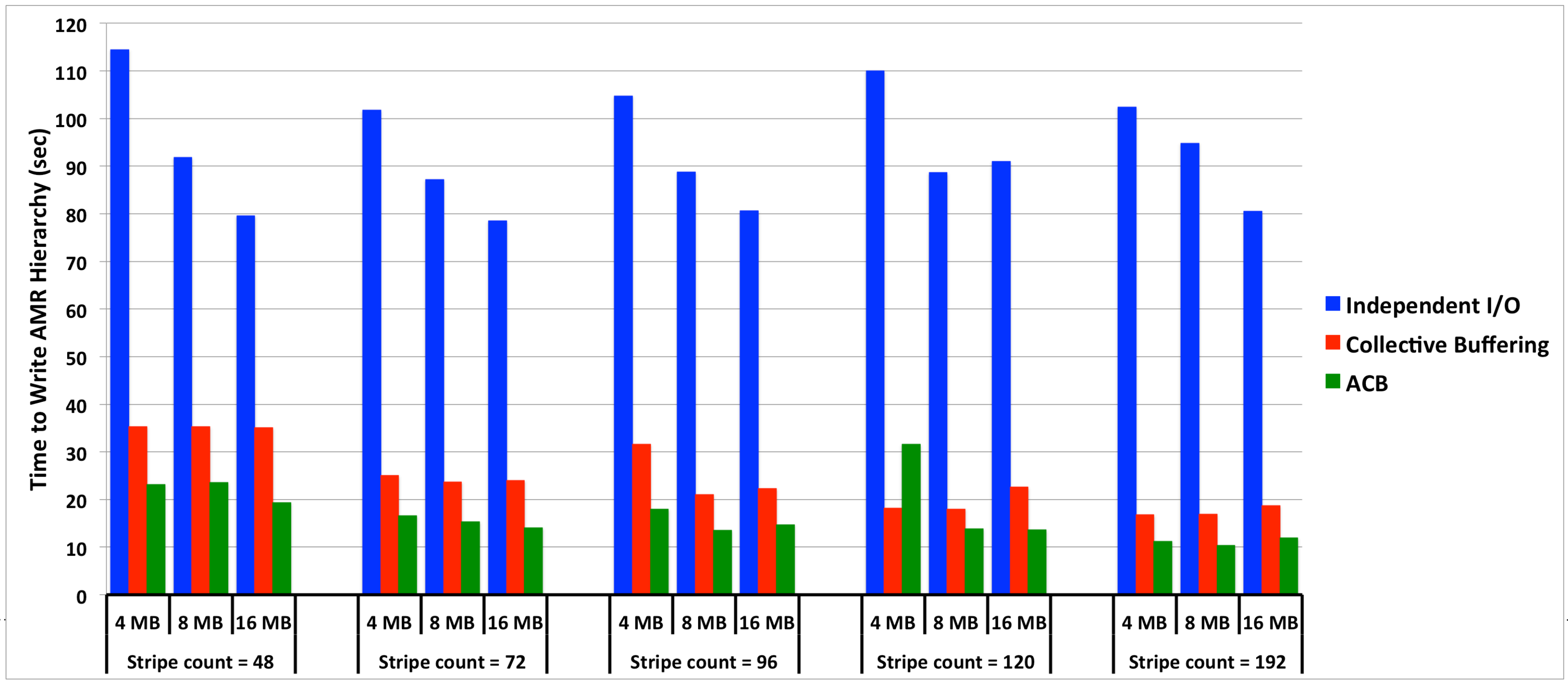
Evaluation with Lustre striping - Cori

Experiment specifics:
- 3072 procs (96 nodes)
- 494 GB file
- Striped across 96 OSTs
- Stripe size = 8 MB

ACB is 3.9x to 9.1x faster than independent I/O, and 1.5x to 1.8x faster than collective buffering



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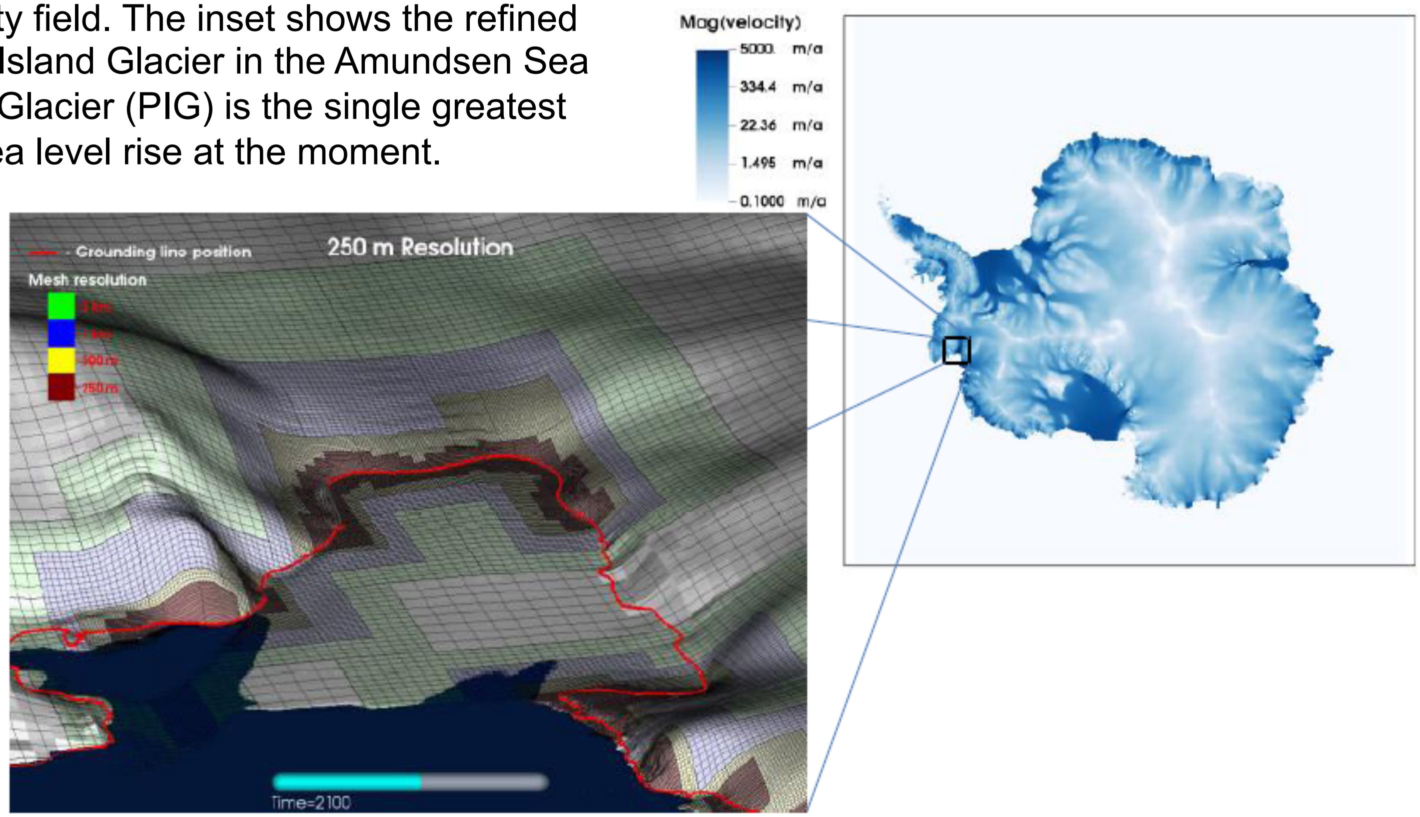
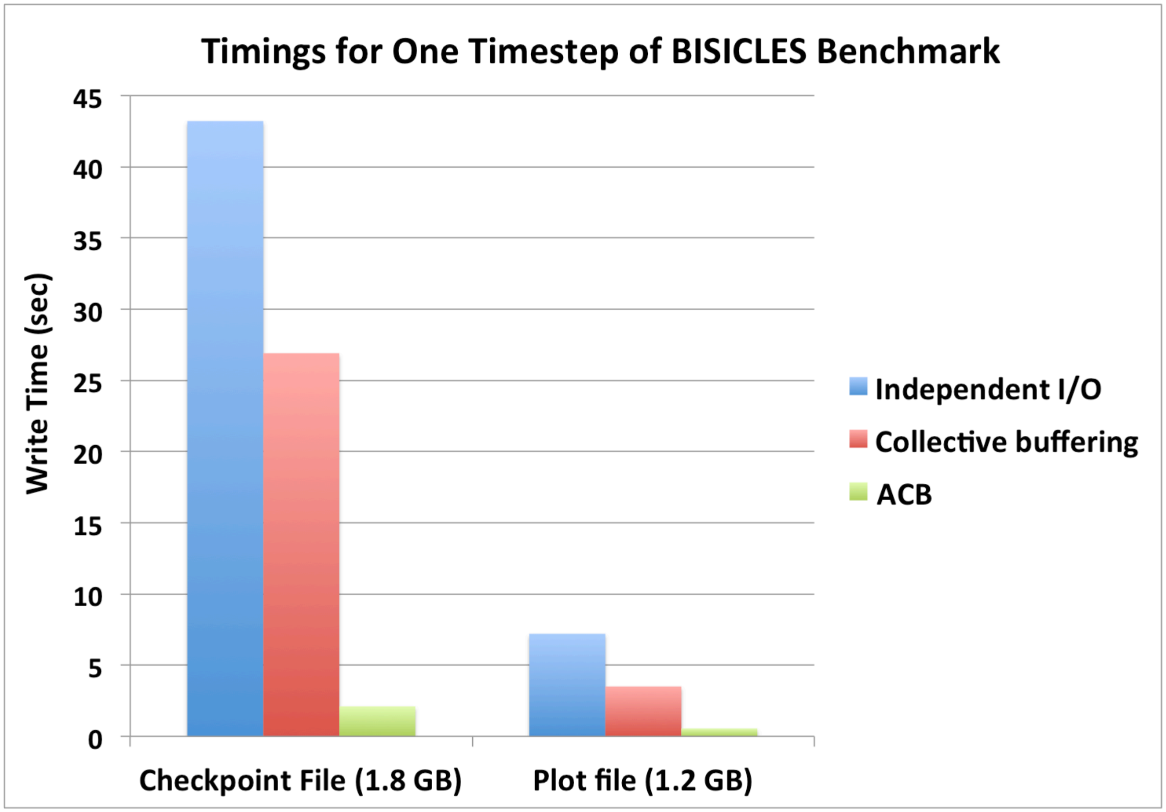
Performance of BISICLES w/ ACB

- Simulates evolution of Antarctic ice sheet over time
  - Solves nonlinear equation for ice velocity and advects the ice
  - Results in many boxes of varying sizes
    - Finest level contains 896 boxes; number of cells in a box ranges between 256 and 4096 cells; each process has at least one box; maximum number of boxes on a process is 6; average number of boxes is 1.5

Antarctic ice-sheet velocity field. The inset shows the refined meshes around the Pine Island Glacier in the Amundsen Sea Embayment. Pine Island Glacier (PIG) is the single greatest Antarctic contributor to sea level rise at the moment.



Performance of BISICLES w/ ACB, cont



Run on 576 procs (24 nodes) on Edison. Files striped across 24 OSTs with stripe size of 4 MB.

- For checkpoint files, ACB is **20X faster** than independent I/O, and **13X faster** than collective buffering
- For plot files, ACB is **13X faster** than independent I/O, and **6.4x faster** than collective buffering

Darshan analysis of BISICLES I/O w/ ACB

- Independent I/O and collective I/O perform several small writes, especially for checkpoint files
- ACB writes out large chunks of data

Top four write sizes (ACCESS SIZE) and corresponding counts from Darshan logs

	Ind I/O	Coll I/O	ACB
ACCESS SIZE 1	8736	5408	4 M
COUNT 1	4085	3182	477
ACCESS SIZE 2	5408	17920	272
COUNT 2	3229	3059	69
ACCESS SIZE 3	7680	19488	3848
COUNT 3	3080	2646	51
ACCESS SIZE 4	17920	7680	13160
COUNT 4	1333	1281	40

Checkpoint file statistics

	Ind I/O	Coll I/O	ACB
ACCESS SIZE 1	73440	73440	4 M
COUNT 1	1429	1529	322
ACCESS SIZE 2	204000	38880	272
COUNT 2	1378	1422	23
ACCESS SIZE 3	38880	204000	544
COUNT 3	1372	1298	13
ACCESS SIZE 4	300000	396000	40
COUNT 4	709	604	9

Plot file statistics

Conclusions and Future Work

- ACB issues fewer write calls than collective buffering and independent I/O
  - Each ACB write call sends relatively large chunks of data
- ACB speeds up independent I/O implementation by 2x to 9.1x, and collective buffering by 1.5x to 2.6x
- Apply and analyze ACB performance on EBChombo and cubed sphere climate application (CAMR)
- Eliminate extra buffer copy in ACB, and use unions of hyperslabs to specify locations of boxes in memory
- Explore ACB performance on burst buffers

Thanks!

Contact:

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Nagiza Samatova [nagiza.samatova@gmail.com]

Projects: **In situ AMR Indexing and Querying**
ExaHDF5

Thanks to DOE ASCR Program Manager Dr. Lucy Nowell

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