1st exaFOAM Workshop
Parallel I/O

Exploitation of Exascale Systems for Open-Source Computational Fluid Dynamics by Mainstream Industry

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EuroHPC
Joint Undertaking

June 12th, 2023

Agenda

- Introduction to Parallel I/O
- OpenFOAM I/O Formats
- Towards Parallel I/O for OpenFOAM
- Conclusion

Introduction – Parallel File Systems

- Space and bandwidth scale with number of object storage hardware.

  → Up to O(TB/s).

- Storage metadata stored as **inode per file**.

  → minimize number of files.

- Lookup suffers contention if overutilized by many **requests**.

  → minimize I/O operations.

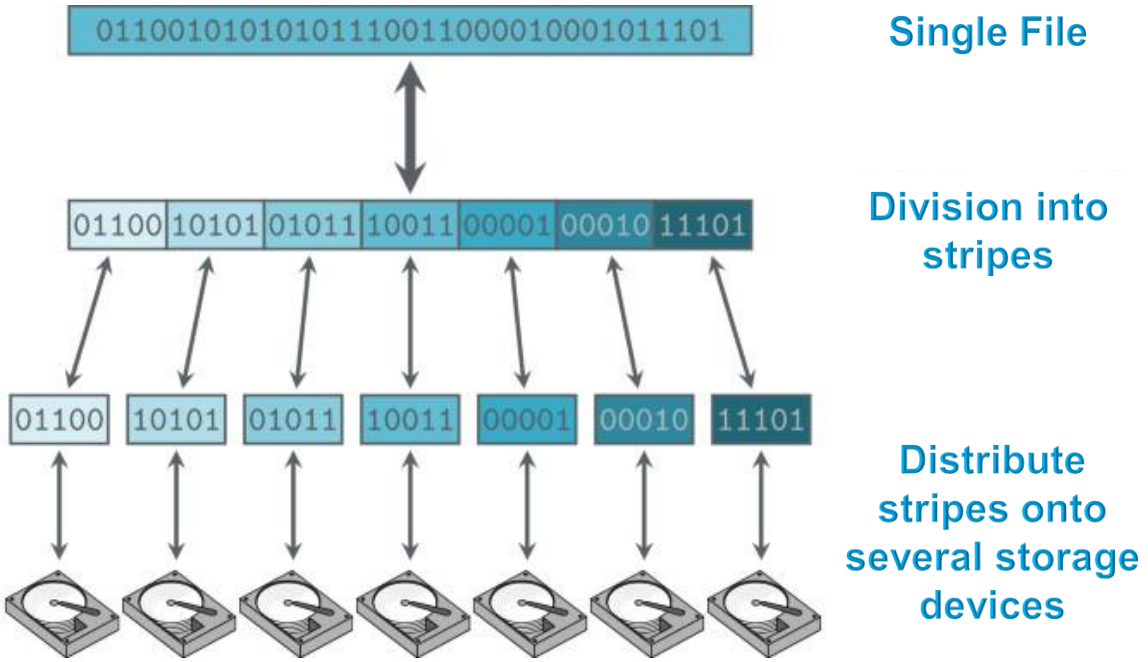

Figure modified and used under CC-BY 4.0 from [1]

Optimize number of files, I/O operations and access size.

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[1] M. Seiz et al. Lustre I/O Performance Investigations on Hazel Hen: Experiments and Heuristics. J. Supercomut 77, 12508-12536 (2021)

Introduction – Parallel File Systems

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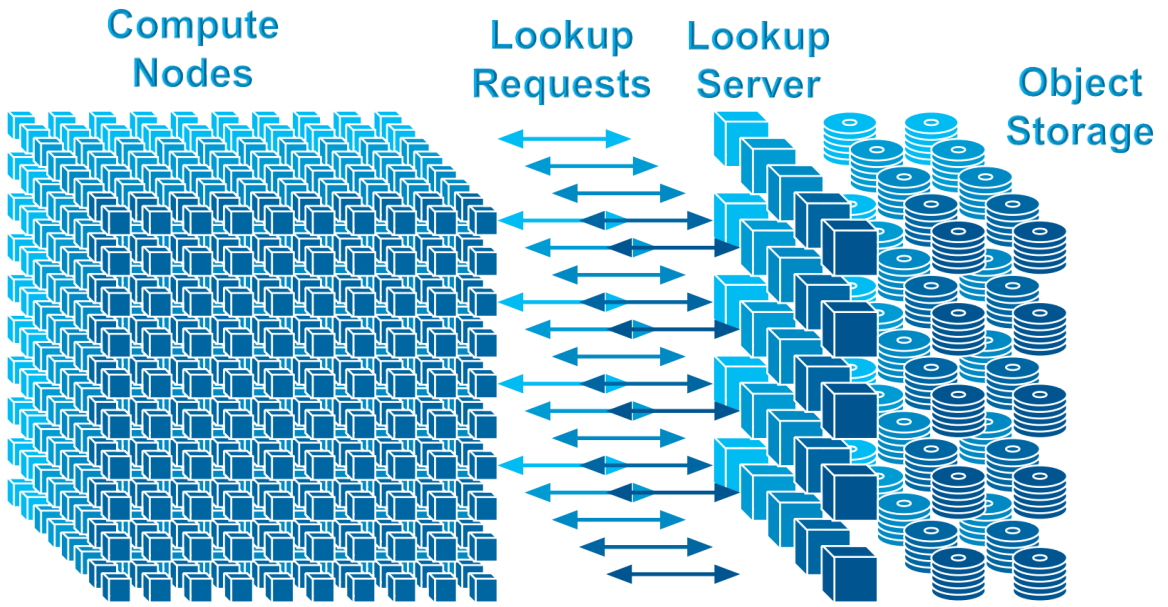

Figure modified from [2]

Optimize number of files, I/O operations and access size.

Introduction – Parallel I/O Libraries

MPI-IO

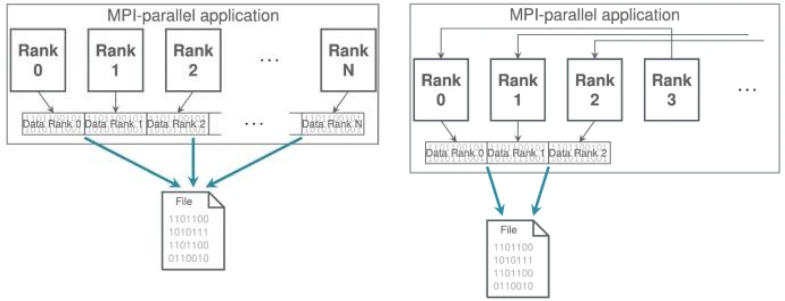

Figure modified and used under CC-BY 4.0 from [1]

- N:1 model or M:1 model.
- Plain binary data files.
- Flexible choice of # of writers at runtime.
- Can handle irregular access pattern.

ADIOS2

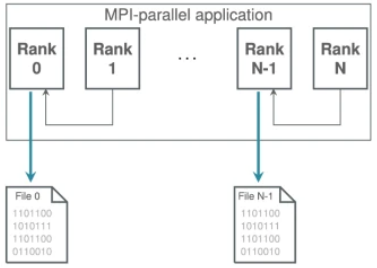

Figure modified and used under CC-BY 4.0 from [1]

```
.
`-- adios2.bp
    |-- data.0
    |-- data.1
    |-- data.*
    ...
    |-- md.0
    |-- md.idx
    |-- mmd.0
    `-- profiling.json
```

- N:M model.
- Structure of binary files by metadata.
- Flexible choice of # of files at runtime.
- Requires contiguous access pattern.

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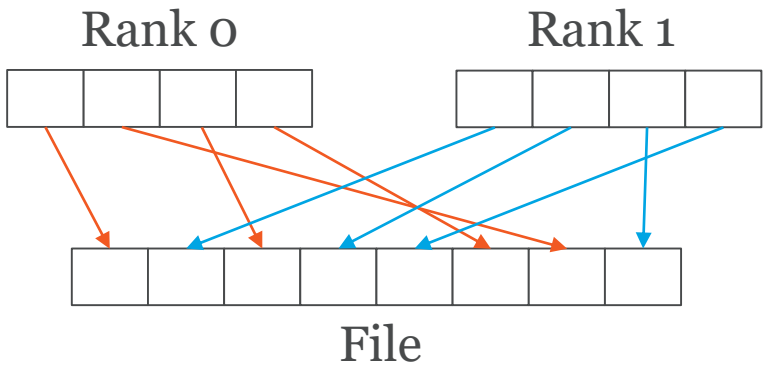
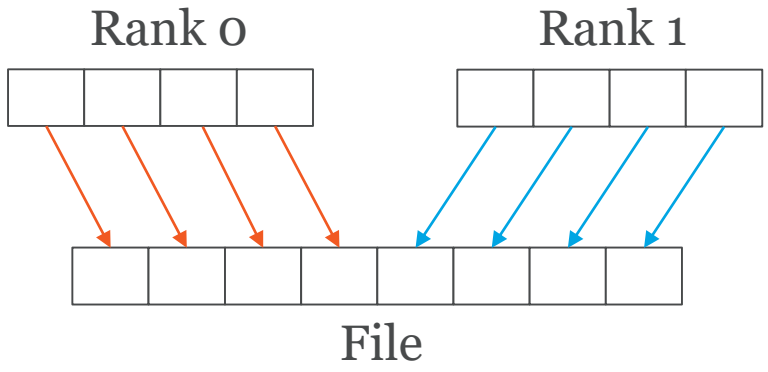
Introduction – I/O Access Patterns

Irregular Access Pattern



- Irregular mapping required.
- Assembly overhead during I/O.

Contiguous Access Pattern



- Start and size required.
- No reorganization.

Simple I/O access patterns optimize time spend in reorganization overheads.

OpenFOAM I/O Formats

OpenFOAM I/O Formats

Uncollated Format

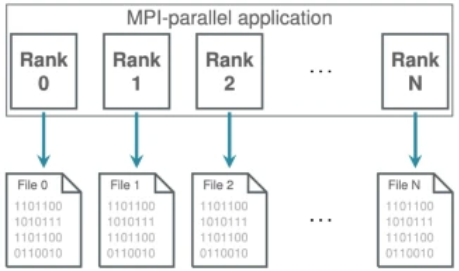


Figure modified and used under CC-BY 4.0 from [1]

- N:N model → # of inodes scales with # of processors
- Once the case is decomposed:
  - Only restarts on the same decomposition.
  - Modification in boundary conditions are tedious.
- Decomposition, reconstruction, and redistribution are costly for the time-to-solution.

Case structure parallel run

```
.
|-- processor0
|   |-- 0
|   |   |-- p
|   |   `-- U
|   `-- constant
|       `-- polyMesh
|           |-- boundary
|           |-- boundaryProcAddressing
|           |-- cellProcAddressing
|           |-- faceProcAddressing
|           |-- faces
|           |-- neighbour
|           |-- owner
|           |-- pointProcAddressing
|           `-- points
|-- processor1
|   |-- 0
|   |   |-- p
|   |   `-- U
```

Showstopper at scale.

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Collated Format

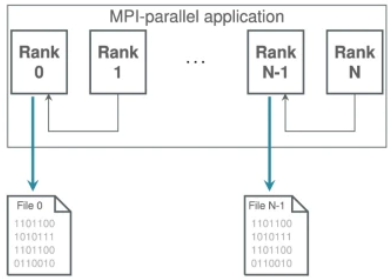
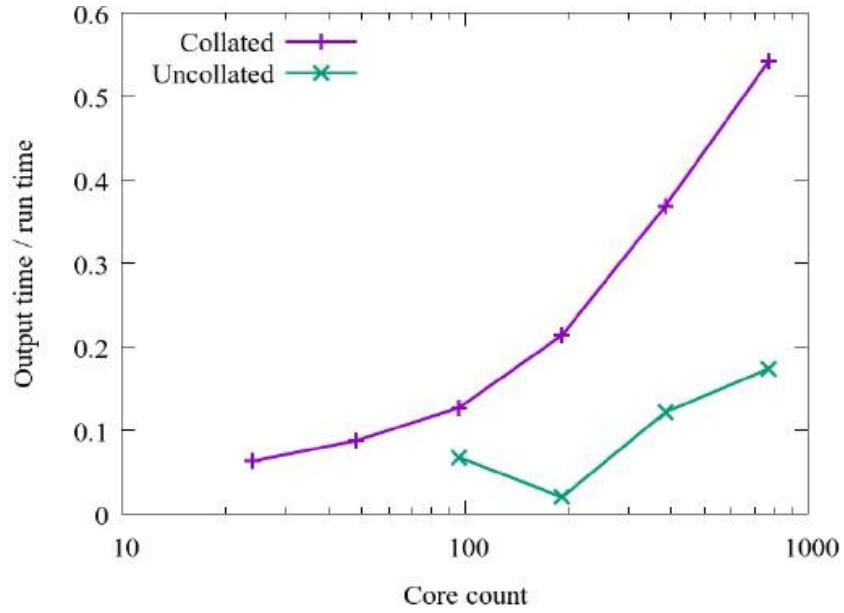


Figure modified and used under CC-BY 4.0 from [1]

- N:M model → Reduces the number of inodes.
- Once the case is decomposed:
  - Only restarts on the same decomposition.
- Adds considerable runtime overhead.
- Decomposition, reconstruction, and redistribution are costly for the time-to-solution.

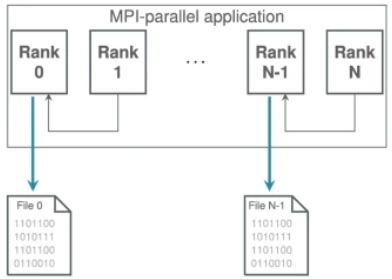
More than 50% of the runtime spend in I/O.

Figure modified from [3]



[1] M. Seiz et al. Lustre I/O Performance Investigations on Hazel Hen: Experiments and Heuristics. J. Supercomput 77, 12508-12536 (2021)
[3] https://www.archer2.ac.uk/training/courses/200624-openfoam-io/ - 14th Oct 2022 10AM

Collated Format



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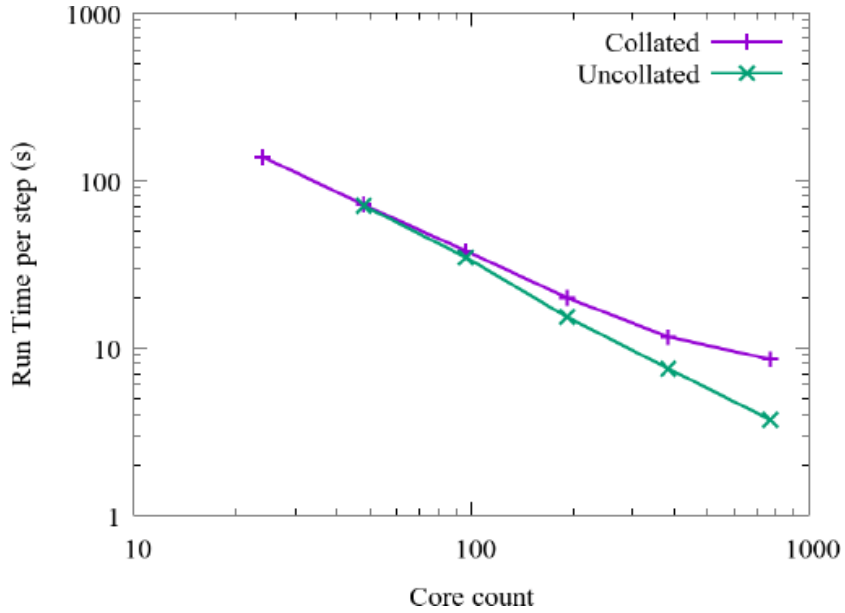
- N:M model → Reduces the number of inodes.
- Once the case is decomposed:
  - Only restarts on the same decomposition.
- Adds considerable runtime overhead.
- Decomposition, reconstruction, and redistribution are costly for the time-to-solution.

More than 100% increase in runtime.

Figure modified from [3]



Limited scalability.

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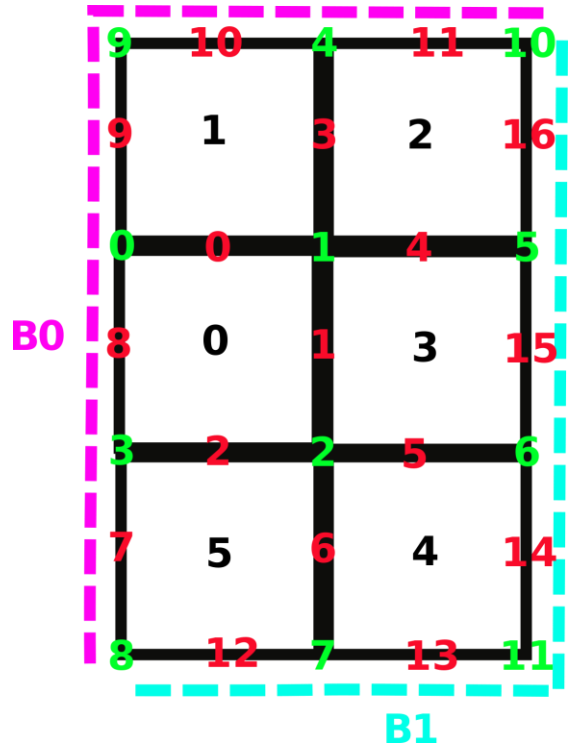
[3] https://www.archer2.ac.uk/training/courses/200624-openfoam-io/ - 14th Oct 2022 10AM

Data layout of OpenFOAM

- Storage of mesh connectivity by owner and neighbour cell IDs of faces.
- Boundary patch faces follow internal faces.
- Decomposition renumbers and fragments the mesh.
- Fragments would pose an irregular I/O access pattern.

Global			Partition 0			Partition 1		
face	owner	neighbour	face	owner	neighbour	face	owner	neighbour
0	0	1	0	0	1			
1	0	3	7	0		8	0	
2	0	5	8	0		9	2	
3	1	2	1	1	2			
4	2	3	9	2		7	0	
5	3	4				0	0	1
6	4	5				1	1	2
7	5					6	2	
8	0		2	0				
9	1		3	1				
10	1		4	1				
11	2		5	2				
12	5					5	2	
13	4					4	1	
14	4					3	1	
15	3					2	0	
16	2		6	2				



exaFOAM

HLRS

WIKKI

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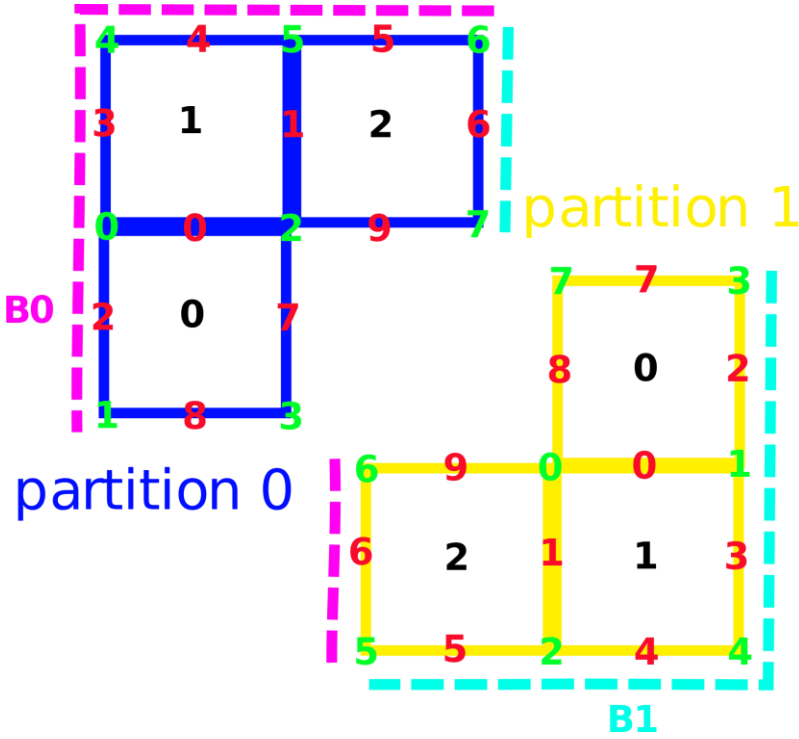
0	0	1	0	0	1			
1	0	3	7	0		8	0	
2	0	5	8	0		9	2	
3	1	2	1	1	2			
4	2	3	9	2		7	0	
5	3	4				0	0	1
6	4	5				1	1	2
7	5					6	2	
8	0		2	0				
9	1		3	1				
10	1		4	1				
11	2		5	2				
12	5					5	2	
13	4					4	1	
14	4					3	1	
15	3					2	0	
16	2		6	2				



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Towards Parallel I/O for OpenFOAM

Parallel I/O for exascale ready OpenFOAM.

Objectives

1. Reduce number of files and optimize I/O performance at scale. → Current showstopper for scalability.
2. Decrease time-to-solution by improved I/O access pattern. → “Performance optimization” sits here.

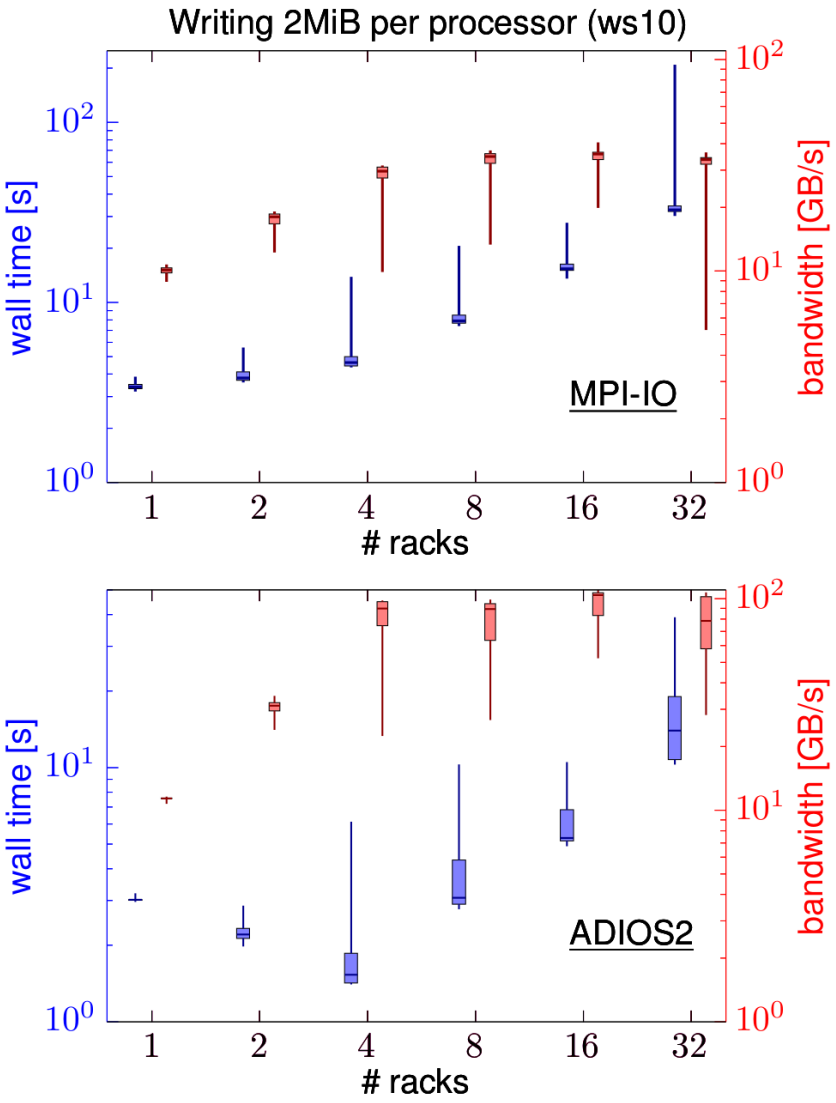
Approach

- Development of an I/O proxy application to compare I/O schemes and libraries.
- Design and implement contiguous I/O access pattern for FOAM-native parallel I/O.

I/O Proxy Application

- Simple heat transfer solver with contiguous data layout.
- Parallel I/O at scale with ADIOS2 and MPI-IO.
- Wall time of opening, writing, and closing.
- Weak scaling benchmark of writing 2MiB per processor.
- Blocking semantics in MPI-IO render ‘slower’ I/O ops.
- Non-blocking semantics of ADIOS2 facilitate ‘faster’ I/O ops.

32 racks are 524’288 cores and MPI ranks on the HAWK supercomputer at HLRS.



Reduced foam-extend 4.1 for design of parallel I/O

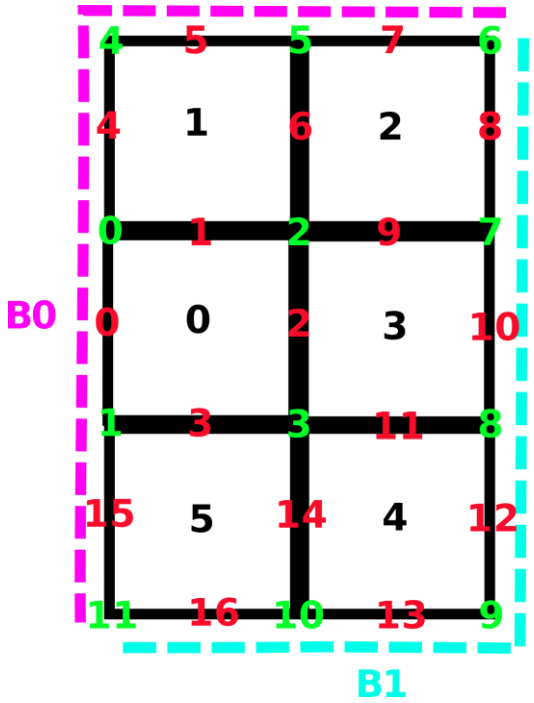
- Native implementation adds ADIOS2 in IOstream family of classes used by registered IOobjects.
- I/O serial in design of insertion (<<) and extraction (>>) operators.
  - Information for ADIOS2 is transferred and buffered during serial call tree of << and >>.
- Refactoring of I/O for polyMesh.
  - Coherent data layout in mesh I/O.
- Refactoring of I/O for GeometricField.
  - Adaptation of coherent data layout.
  - Different offsets of volume, surface, and point fields.

```
bool Foam::GeometricField::writeData(Ostream& os)
{
   os << *this;
   return os.good();
}


Foam::Ostream& Foam::operator<<
(
    Ostream& os,
    const GeometricField gf
)
{
    // Logic for serial uncollated I/O
    // Refactored for additions with parallel I/O
}

/* Somewhere in Ostream derived source */
…
    adiosStream.open(file);
    adiosStream.write(identifier, start, size, data);
    adiosStream.close();
…
```

ADIOS2 implementation in core (libfoam) library.

Coherent and sliceable data layout of the mesh.

- Upper triangular order/sorted by ownership incorporating boundary faces.
- Face-ordered ‘owner’ list → ‘ownerStart’ as cell-ordered list as entry point for coherence.
- Partitioning into slices of **cell-ordered lists**.
- Owners determine slices in **face-ordered lists**.
- Slices of **point-ordered lists** known by maximum ID in faces.



Decomposition		Ownership		Neighbourhood		Mesh Entities		
partition	partitionStart	cell	ownerStart	face	neighbour	faces	point	points
0	0	0	0	0	-1	(1 0)	0	(0.0 0.0)
1	3	1	4	1	1	(0 2)	1	(0.0 -0.1)
end	6	2	7	2	3	(2 3)	2	(0.1 0.0)
		3	10	3	5	(3 1)	3	(0.1 -0.1)
		4	12	4	-1	(0 4)	4	(0.0 0.1)
		5	15	5	-1	(4 5)	5	(0.1 0.1)
		end	17	6	2	(5 2)	6	(0.2 0.1)
				7	-1	(5 6)	7	(0.2 0.0)
				8	-2	(6 7)	8	(0.2 -0.1)
				9	3	(7 2)	9	(0.2 -0.2)
				10	-2	(7 8)	10	(0.1 -0.2)
				11	4	(8 3)	11	(0.0 -0.2)
				12	-2	(8 9)		
				13	-2	(9 10)		
				14	5	(10 3)		
				15	-1	(11 1)		
				16	-2	(10 11)		

max. ID

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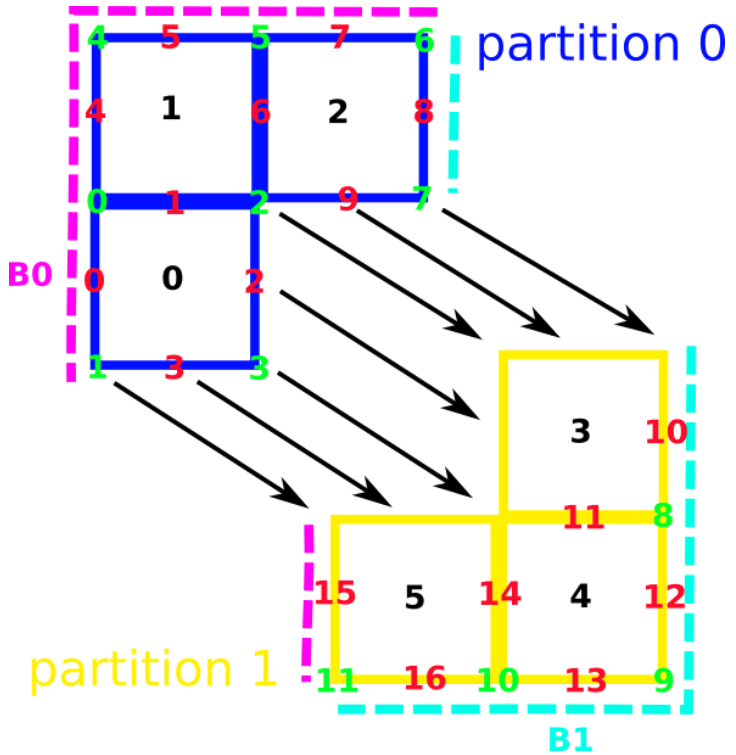

Decomposition		Ownership		Neighbourhood		Mesh Entities		
partition	partitionStart	cell	ownerStart	face	neighbour	faces	point	points
0	0	0	0	0	-1	(1 0)	0	(0.0 0.0)
1	3	1	4	1	1	(0 2)	1	(0.0 -0.1)
end	6	2	7	2	3	(2 3)	2	(0.1 0.0)
		3	10	3	5	(3 1)	3	(0.1 -0.1)
		4	12	4	-1	(0 4)	4	(0.0 0.1)
		5	15	5	-1	(4 5)	5	(0.1 0.1)
		end	17	6	2	(5 2)	6	(0.2 0.1)
				7	-1	(5 6)	7	(0.2 0.0)
				8	-2	(6 7)	8	(0.2 -0.1)
				9	3	(7 2)	9	(0.2 -0.2)
				10	-2	(7 8)	10	(0.1 -0.2)
				11	4	(8 3)	11	(0.0 -0.2)
				12	-2	(8 9)		
				13	-2	(9 10)		
				14	5	(10 3)		
				15	-1	(11 1)		
				16	-2	(10 11)		

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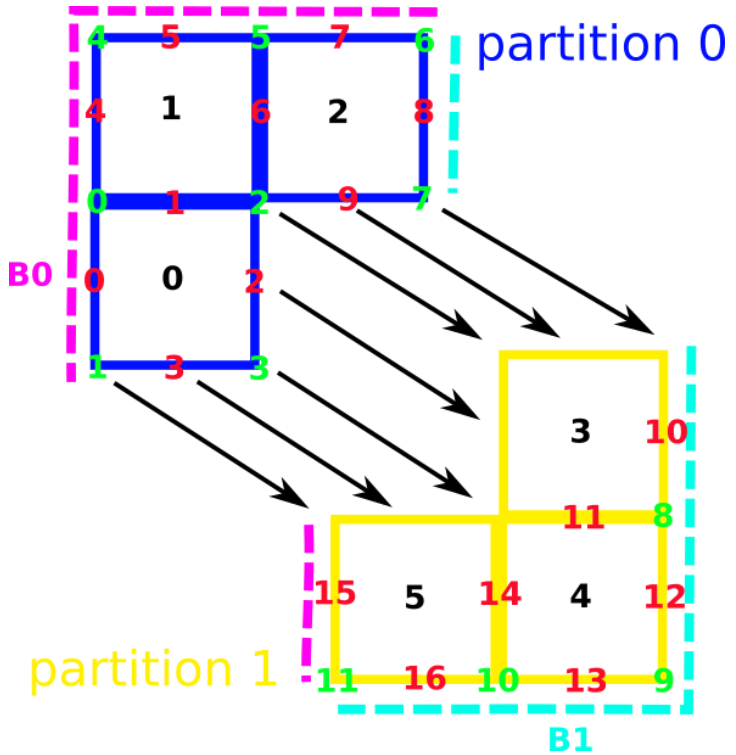

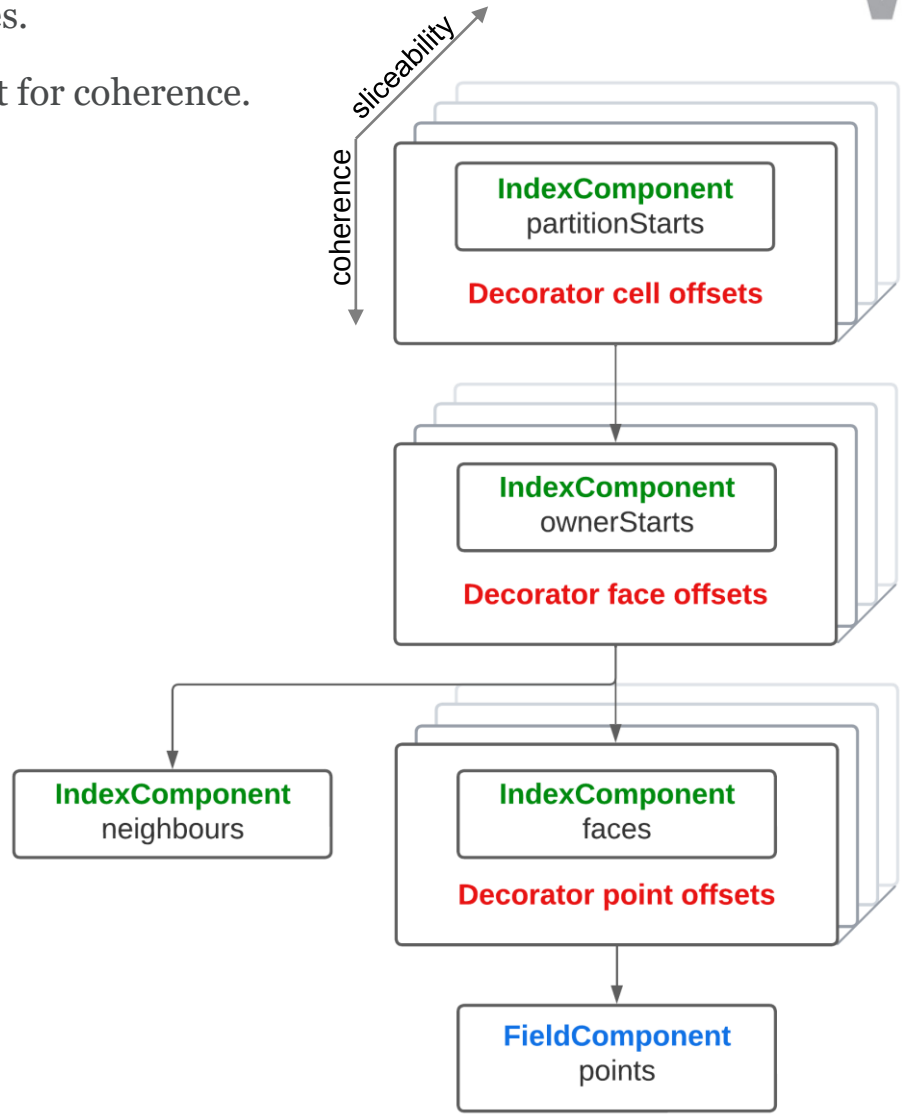

Coherent Data Layout for Field I/O

- Field data layout **adopts coherence** of mesh.
- Geometric fields consist of internal field and boundary patches.
  - Enables complex boundary fields.
  - Processor patches are either not present (volume fields) or integrated into the internal field (surface fields).
- **Plain time folders** for field I/O in serial and parallel runs (no processor folders)
  - Binary field data is stored in ADIOS2 files, i.e. data.bp
  - Field metadata stored in ASCII files, e.g. p, phi, U

Case structure serial/parallel run

```
.
|-- 0
|   |-- p
|   `-- U
|-- 0.05
|   |-- data.bp
|   |-- p
|   |-- phi
|   `-- U
|-- 0.1
|   |-- data.bp
|   |-- p
|   |-- phi
|   `-- U
|-- constant
|   |-- polyMesh.bp
|   `-- transportProperties
...
```

Significantly reduced time to solution.

Benefits

1. Reduction of inodes:
   - Exascale ready I/O strategy.
   - Flexible aggregation pattern at runtime.
2. Simplicity from coherent data layout:
   - Start a parallel run (without decomposition) on any number of cores.
   - No reconstruction for post-processing.
   - Edit ASCII metadata like boundary conditions in one place.

Work on your parallel case as if it was a serial case.

Demo.

Case structure serial/parallel run

```
.
|-- 0
|   |-- p
|   `-- U
|-- 0.05
|   |-- data.bp
|   |-- p
|   |-- phi
|   `-- U
|-- 0.1
|   |-- data.bp
|   |-- p
|   |-- phi
|   `-- U
|-- constant
|   |-- polyMesh.bp
|   `-- transportProperties
...
```

Conclusion

- Developed a new design for high performance parallel I/O.
- Implementation in the core (libfoam) of foam-extend 4.1.

1. Reduction of inodes.
    - Lower load on parallel file systems.
2. Coherent data layout simplifies pre- and post-processing of parallel cases.
    - Simplified user experience at all scales.
    - Significant reduction of time-to-solution.

Outlook

- Detailed benchmarks.
- Release into production code.

Thank you.

exafoam-project

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https://exafoam.eu/

Questions?

Presenter: R. Gregor Weiß
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EuroHPC Joint Undertaking

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