OAK RIDGE National Laboratory

ADIOS2 with Kokkos backend

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What to expect for the next 20 minutes

- What is ADIOS2
- Kokkos within ADIOS2
  - Kokkos applications using ADIOS2
    - API for storing/streaming files
    - Streaming Kokkos::View **--DEMO--**
  - ADIOS2 using Kokkos
    - Some performance numbers
    - Querying on derived variables **-- DEMO --**
- Kokkos wish list

What is ADIOS2

ADIOS

- High performance I/O abstraction to allow for on-line/off-line memory/file data subscription service
  - Declarative, **publish/subscribe API** is separated from the I/O strategy
  - **I/O engines** provide different strategies for data movement
  - **Operators** can be added to data transfers
  - Metadata is computed for **queries** on the reader side

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

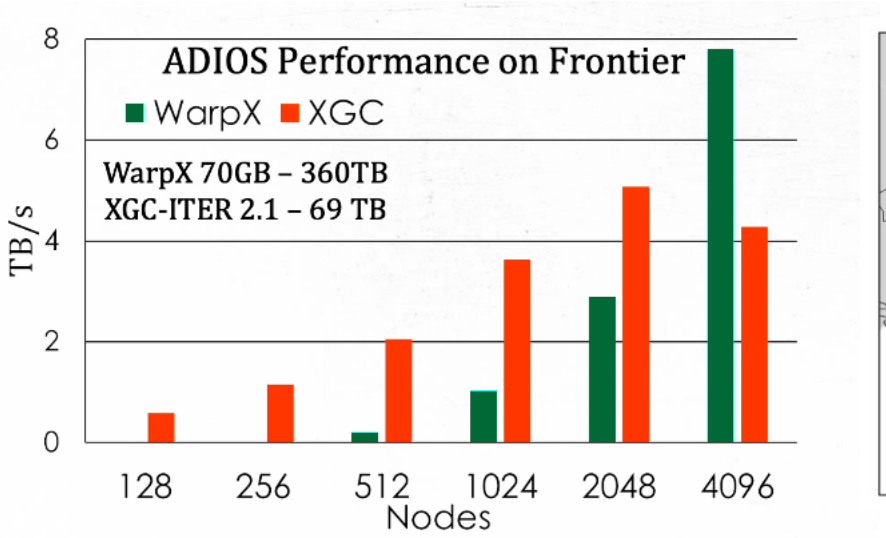
https://github.com/ornladios/ADIOS2

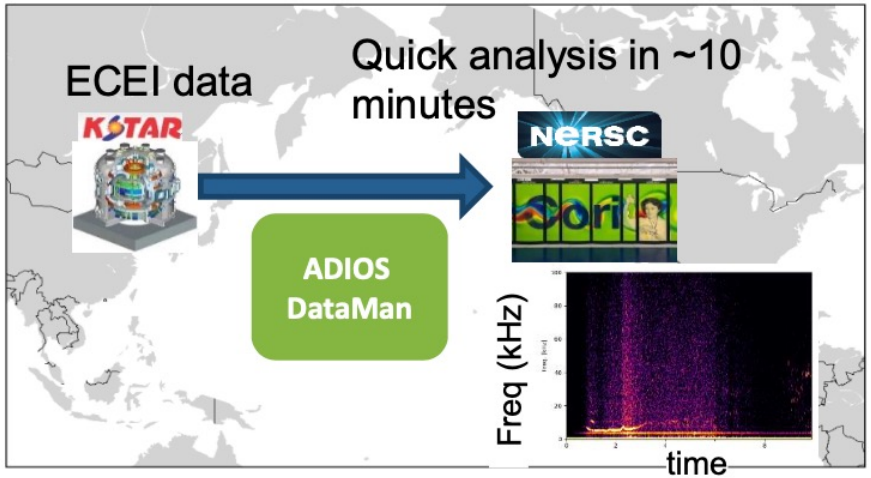
Contributors

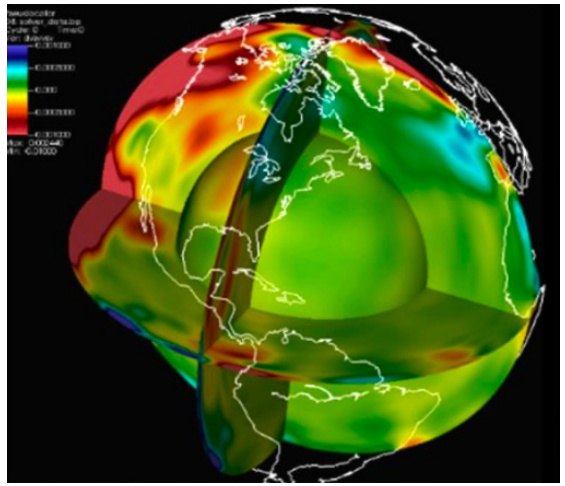
OAK RIDGE National Laboratory kitware BERKELEY LAB GEORGIA TECH RUTGERS

A few of our applications

- Wind Turbine (GE)
- Accelerator Physics (PIConGPU, WarpX)
- Fusion (GTC, XGC, GENE, KSTAR)
- Cancer research
- Combustion (S3D)
- Climate (E3SM)
- Radio astronomy (SKA)
- Seismic Tomography Workflow
- Molecular dynamic (DeepDriveMD)







A bit more on ADIOS2

- **Publish/subscribe API**
  - Define an ADIOS variable
    - With a certain global and local shape
  - Add an operator
  - Publish data
    - Aggregated in internal buffers
  - Subscribe to data

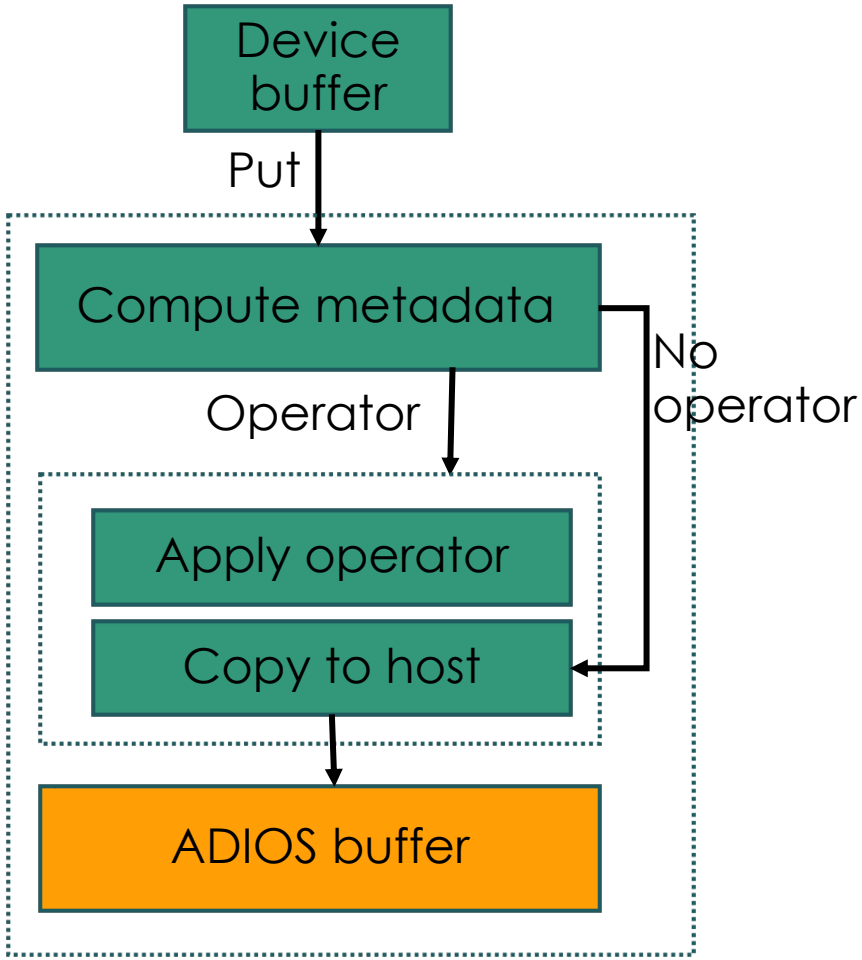
```
auto adiosVar = io.DefineVariable<float>(
                "var_name", shape, start, count);

adios2::Operator mgardOp =
      adios.DefineOperator("mgardCompressor",
adios2::ops::LossyMGARD);

adiosVar.AddOperation(mgardOp,
                {{adios2::ops::mgard::key::tolerance, tolerance}});


bpWriter.Put(adiosVar, userData);
```

- **I/O engines**
  - Keep the same code and switch the data management strategy

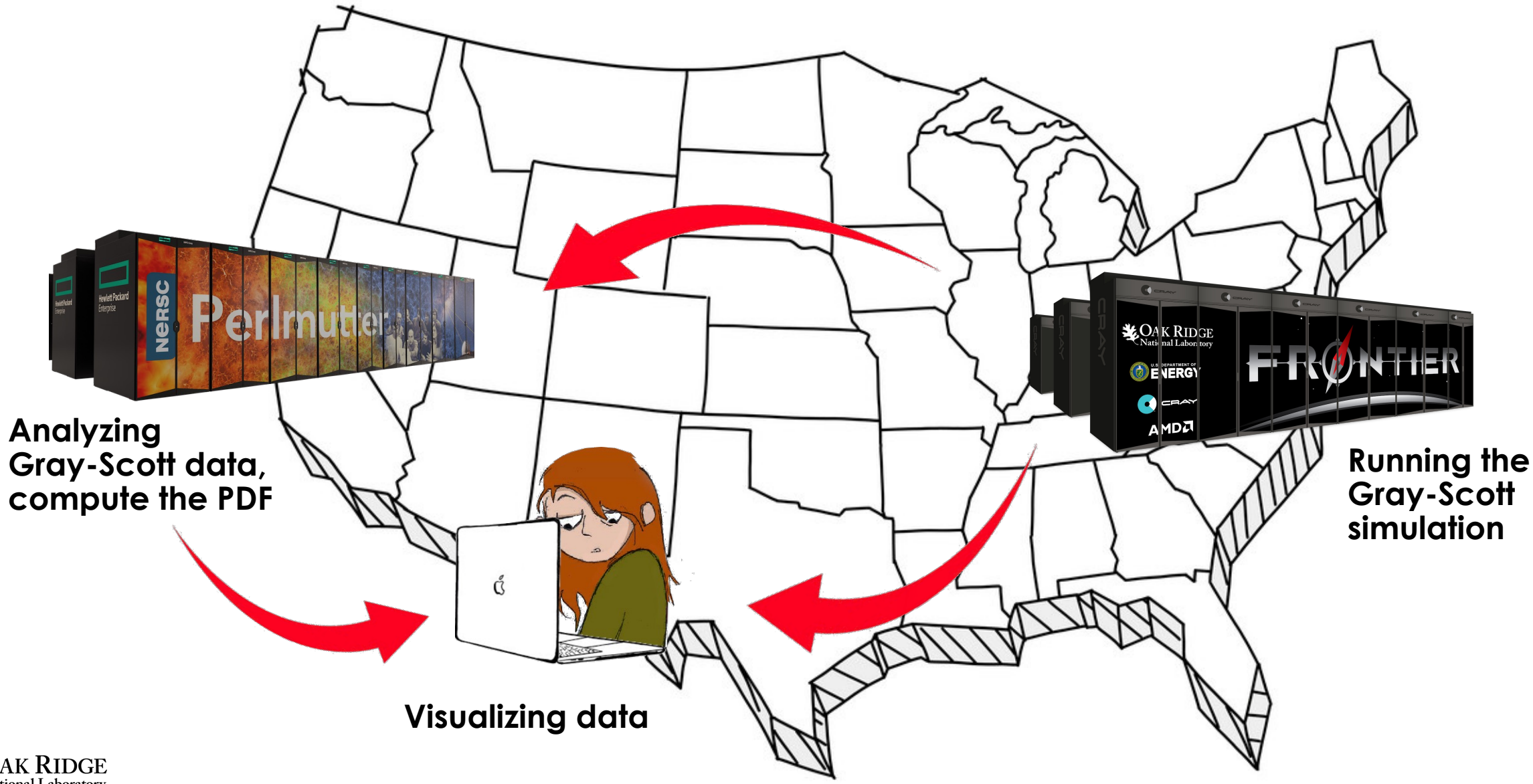
```
$ bpls gs.bp -l
  double   U     100*{64, 64, 64} = 0.0907619 / 1
  double   temp     100*{64} = 0 / 26.74846
  int32_t  step  100*scalar = 10 / 1000

$ bpls gs.bp -la
  double   temp_units                    attr   = "Celsius"
```

GPU-aware ADIOS2

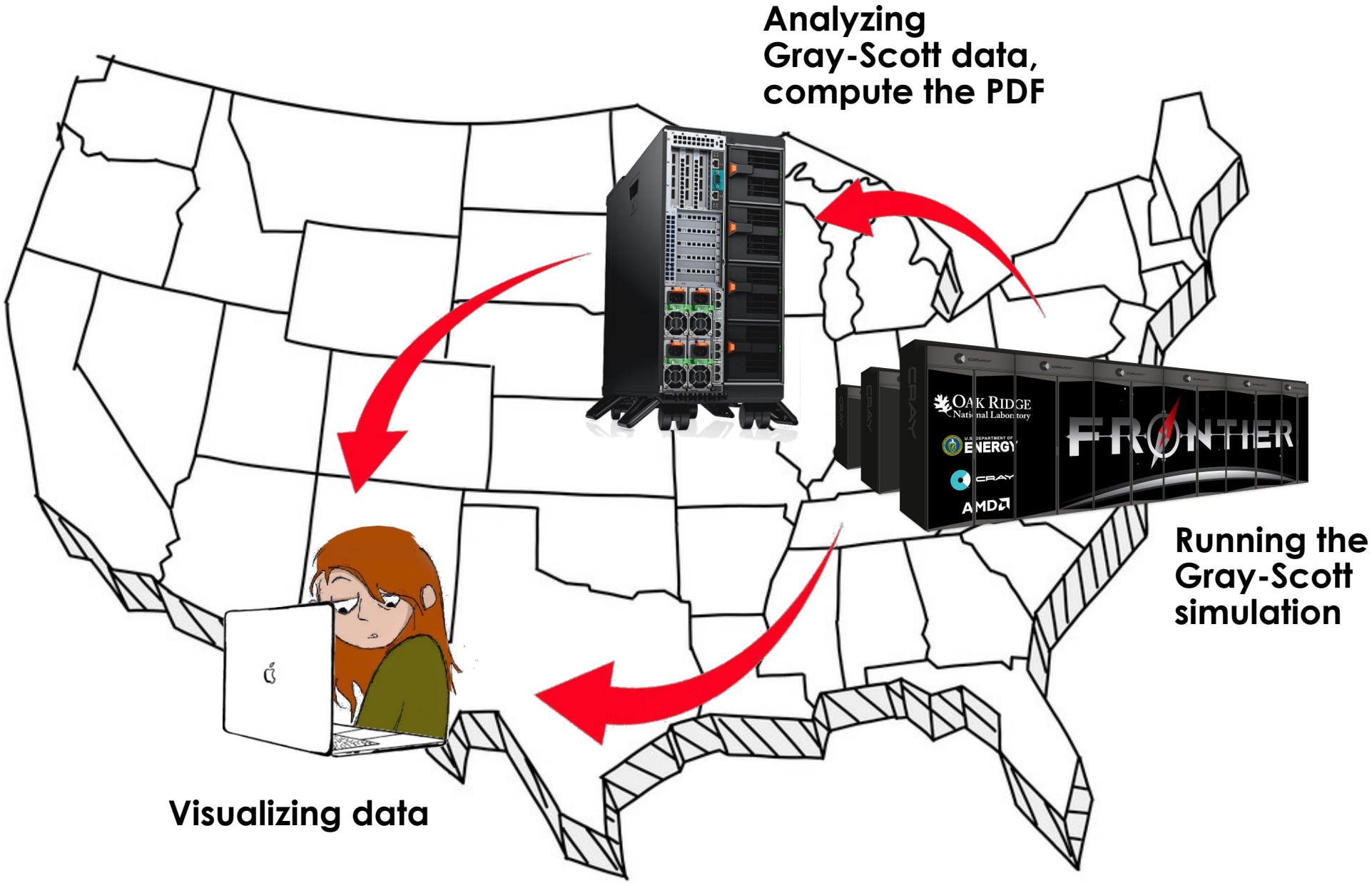
- Publish/subscribe directly GPU pointers
  - For Kokkos::View we extract the memory space and layout
- Internals
  - Copy the data to adios2 internal buffers
  - Compute metadata
    - Min/Max of blocks of data
  - Layout is handled by the adios2 variable dimensions



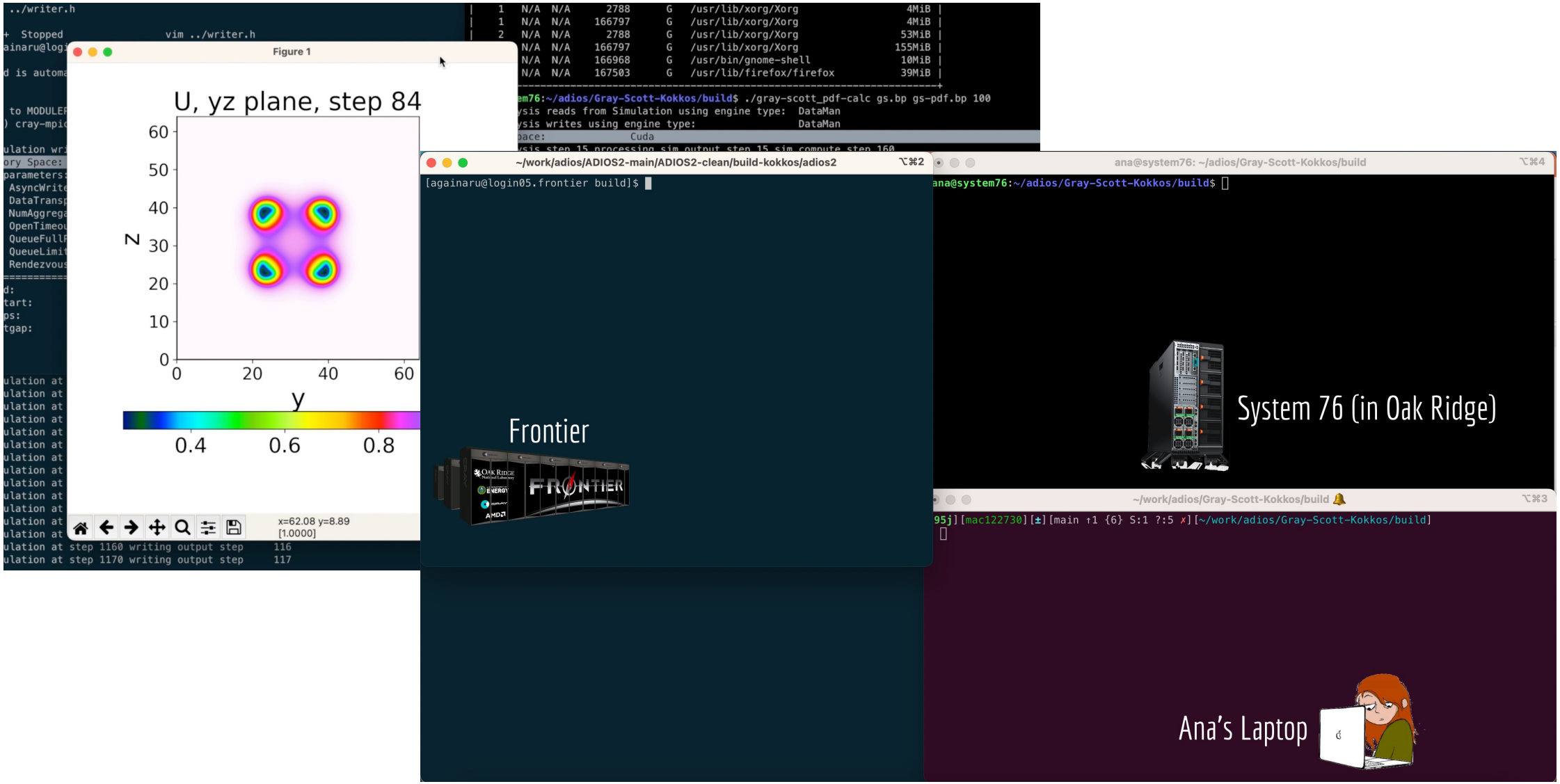
Demo remote access



Demo remote access



Demo 1



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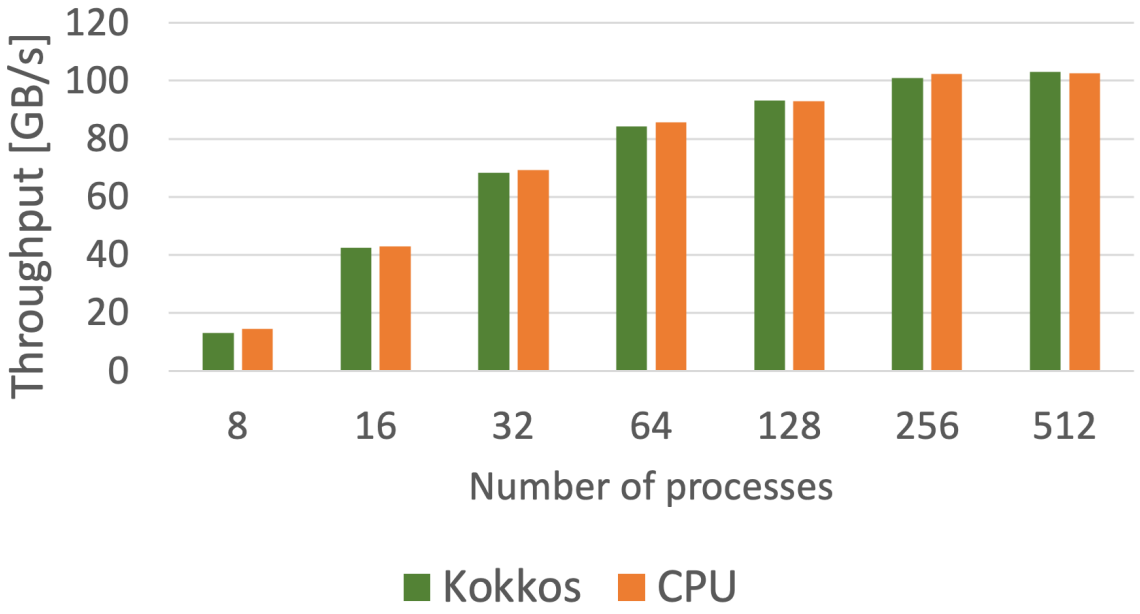
Performance

- When not collecting any metadata
  - Kokkos has the same performance as the CPU backend

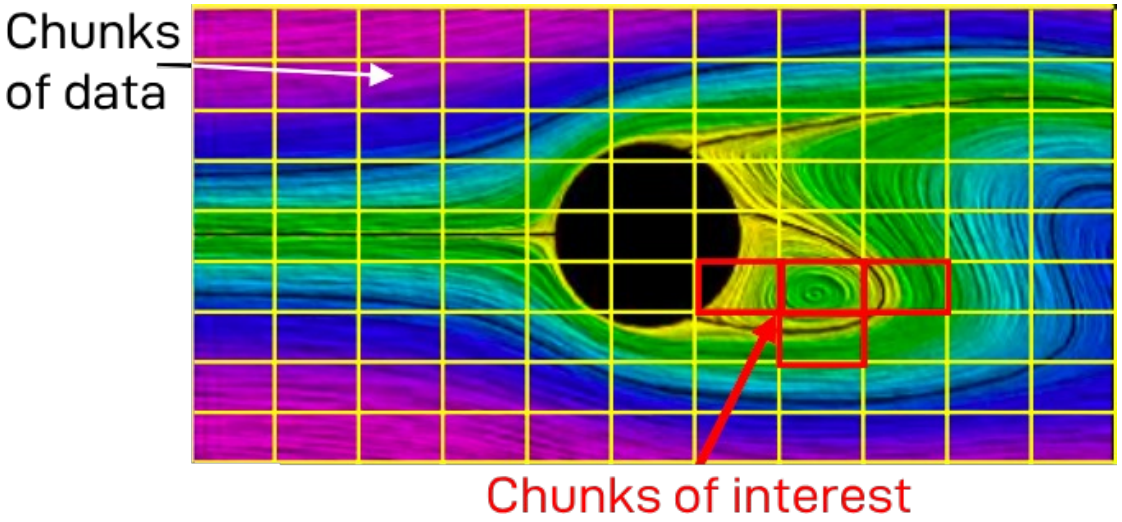


- Memory footprint
  - CPU backend
    - For chunks > 4MB
      - Move data directly from the user buffer
  - Kokkos backend
    - ADIOS2 always uses internal buffers to hold the GPU data
    - Currently we do not handle memory accessible from the Host

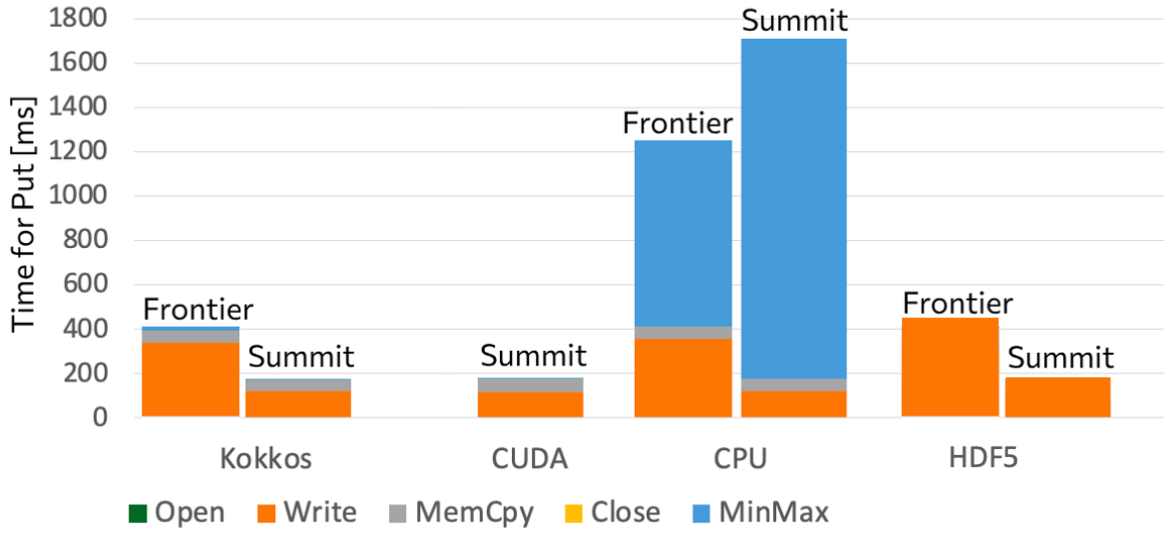
* Results for weak scaling on Summit, 64GB of data per node
* We measure the overall write throughput for all nodes.

Query

- Collecting min/max
  - Allows querying on the read side
  - Granularity of the chunk size affects how much more data we store
  - Trade-off with how much data is read



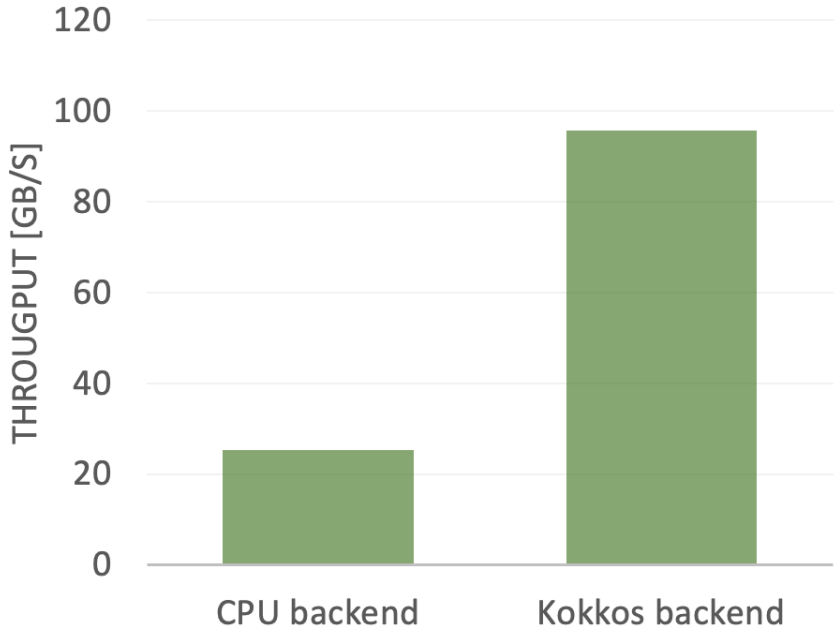
- Applications can define **Quantities of Interest**
  - E.g. curl, magnitude, derivative
  - ADIOS2 compute and stores metadata for derived variables

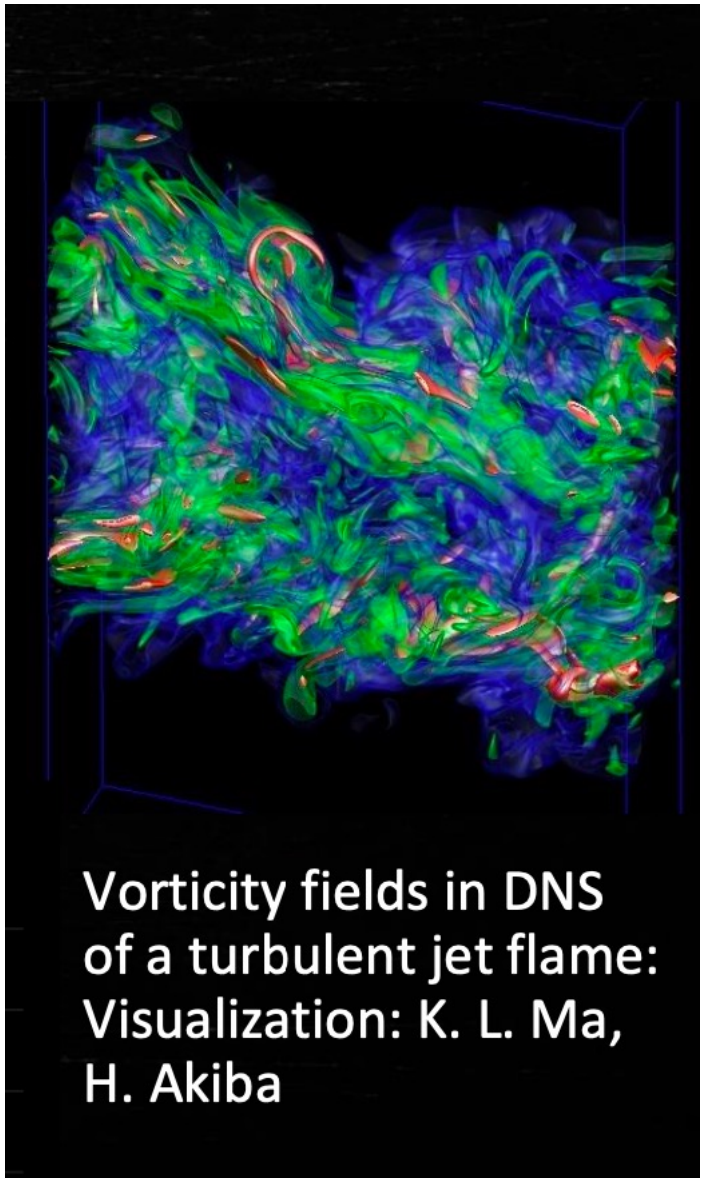


Performance

- Computing min/max and magnitude for S3D data
  - 229 nodes (7200 processes) on Frontier

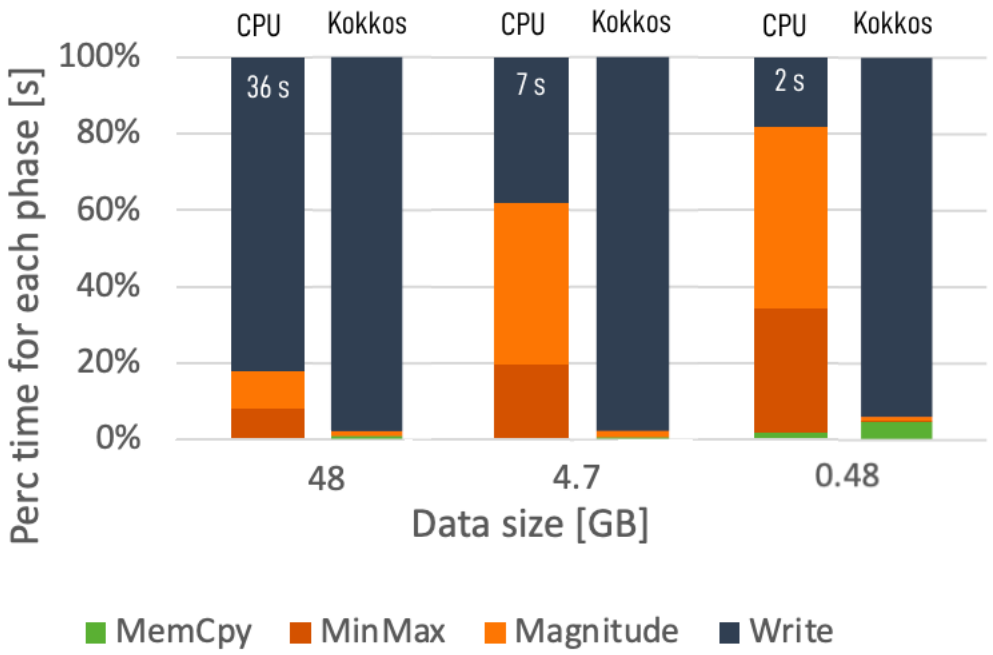
Total amount of data: 1.582 TB





Performance

- Profiling the CPU/Kokkos backends



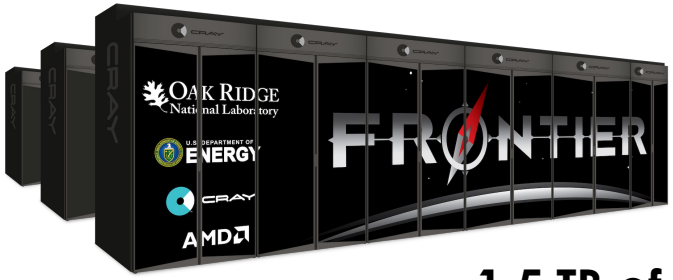

```
parallel_for("ADIOS::ComputePartialMagnitude",
        Kokkos::MDRangePolicy<Kokkos::Rank<2>> (
            {0, 0}, {dimensions, size}),
        KOKKOS_LAMBDA(int i, int j)
{
            auto val = data(i, j);
            Kokkos::atomic_add(&mag(j), val * val);
});

parallel_for("ADIOS::ApplySqrtToMagnitude",
        Kokkos::RangePolicy<>(0, size),
        KOKKOS_LAMBDA(int i)
{
            mag(i) = Kokkos::sqrt(mag(i));
});
```

- Memory footprint

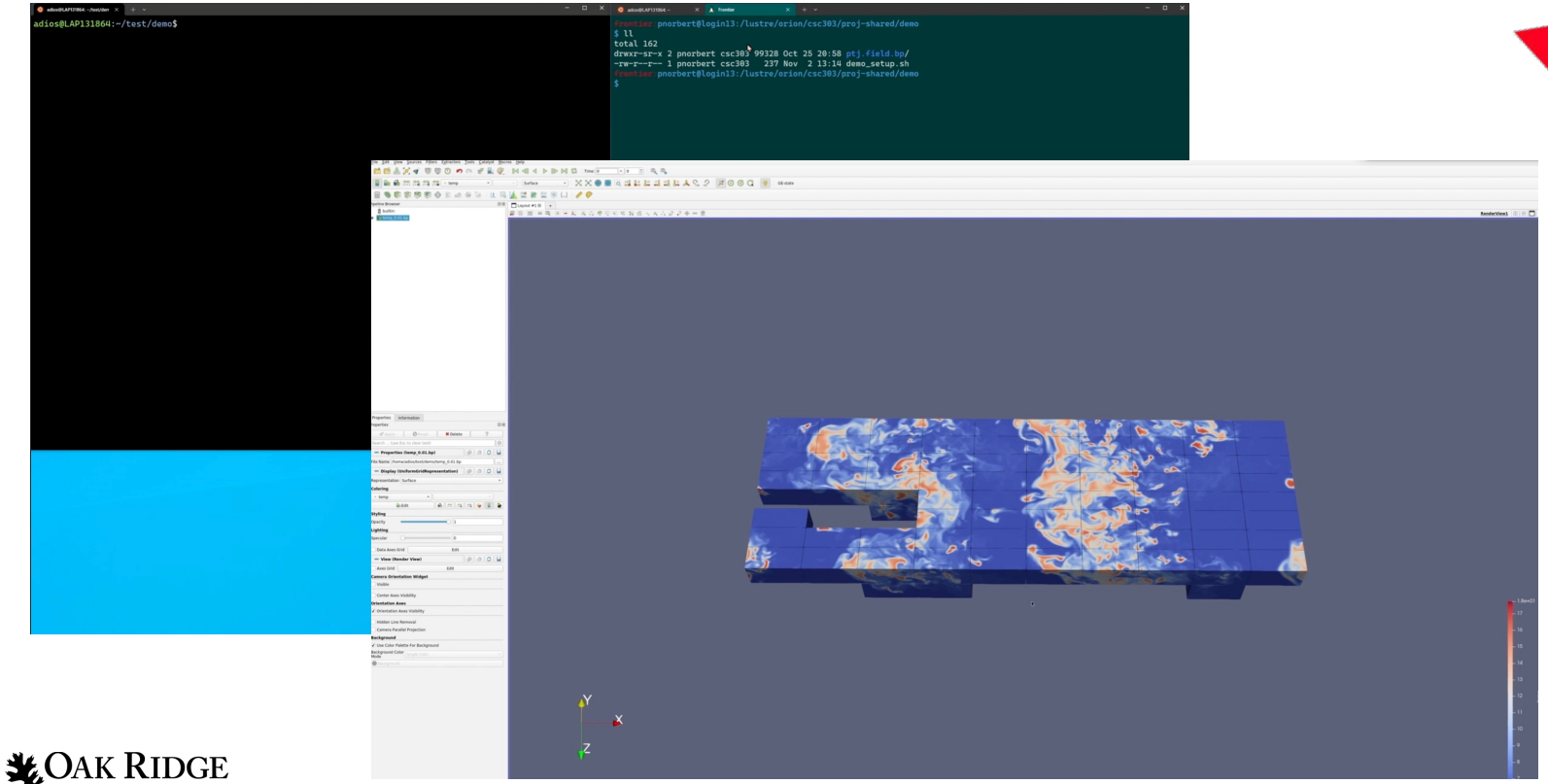
Size with magnitude	Size without magnitude
1.518 TB	1.582 TB

Demo query

Query and visualize data



1.5 TB of S3D data with derived metadata



Wish list from Kokkos

- Would be great
  - Get what device was set
  - Math functions

```
#ifdef ADIOS2_HAVE_KOKKOS_CUDA
  int device_id;
  cudaGetDevice(&device_id);
  settings.set_device_id(device_id);
#endif
```

- Not very probable
  - Detecting if a pointer was allocated on the device
  - I/O direct to storage
    - Only for CUDA

Thank you

ADIOS

- Tutorial
  https://users.nccs.gov/~pnorbert/ADIOS_tutorial_SC23.pdf

- https://adios-io.org/
- https://github.com/ornladios/ADIOS2

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Backup slides

Kokkos applications using ADIOS2

- Layout
  - ADIOS2 variables use by default LayoutRight (except for Fortran codes)
  - Based on the memory space
    - Internally we reverse the dimensions of the adios2 variable
    - Zero cost
    - Put/Get on different memory space might see transposed data
  - Write/read files, streaming

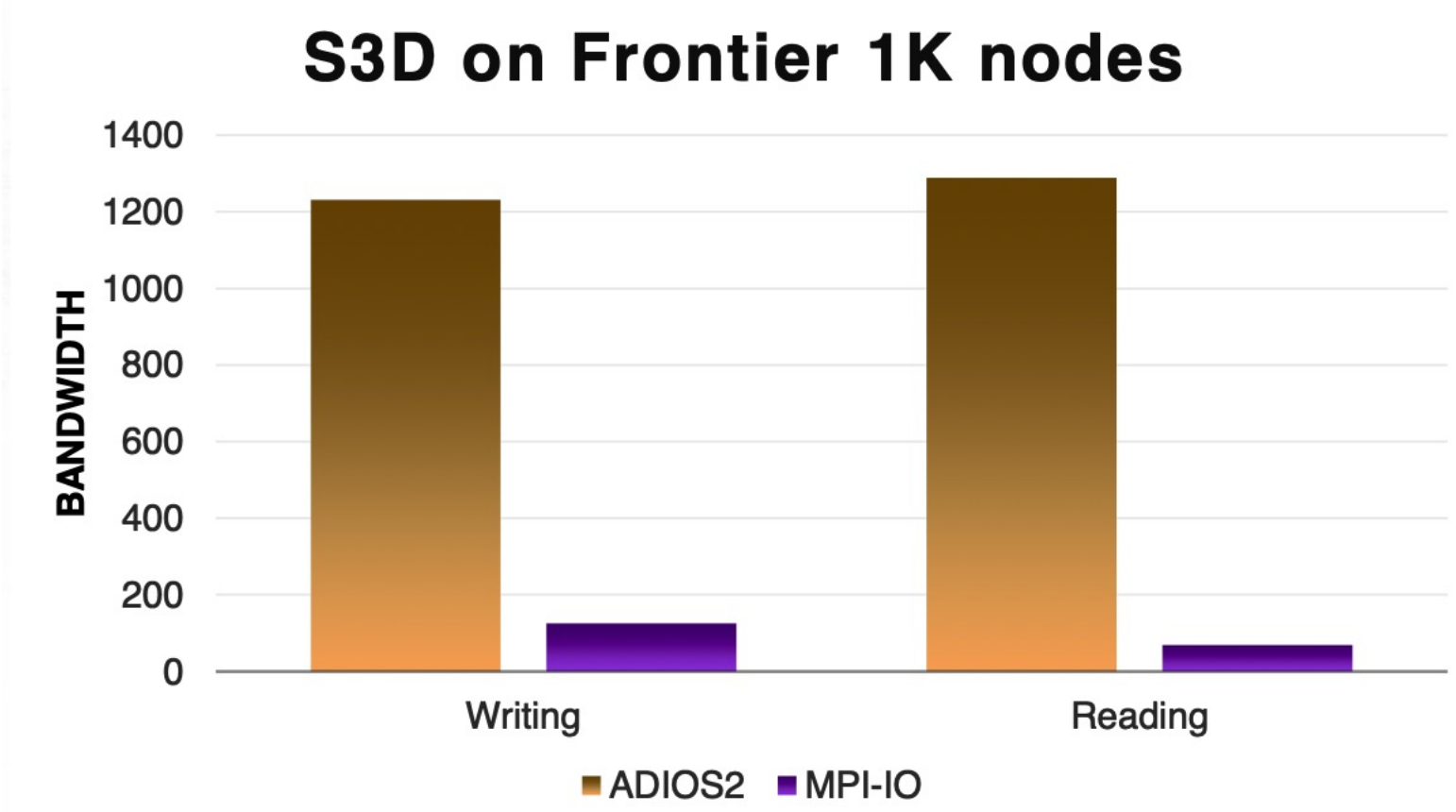
```
Kokkos::View<float **, MemSpace> data("data", Nx, Ny);

Kokkos::parallel_for("initializeData",
    Kokkos::MDRangePolicy< Kokkos::Rank<2>({0, 0}, {Nx, Ny}),
    KOKKOS_LAMBDA(int x, int y)
{
        data(x, y) = static_cast<float>(x);
 });
```

```
$ ./ReadKokkosView
Read on memory space: HIP
1 1 1 1
2 2 2 2
3 3 3 3
4 4 4 4
5 5 5 5
6 6 6 6
```

```
$ ./bin/bpls -l Kokkos.bp/ -d data -n 6
  float    data  {3, 6} = 1 / 6
    (0,0)    1 2 3 4 5 6
    (1,0)    1 2 3 4 5 6
    (2,0)    1 2 3 4 5 6
```

S3D Frontier results

1k nodes, 32 processes per node, ~6.5 GB/node



DataMan code

- ZeroMQ for data transfer
- Parameters
  - TransportMode: fast or reliable
  - MaxStepBufferSize: the default buffer size is 128 MB
  - Threading: true for reader, false for writer

```
adios2::ADIOS adios(MPI_COMM_WORLD);
adios2::IO dataManIO = adios.DeclareIO("WritePDF");
dataManIO.SetEngine("DataMan");
dataManIO.SetParameters({{"IPAddress", "127.0.0.1"},
                         {"Port", "12306"},
                         {"Timeout", "5"},
                         {"RendezvousReaderCount", "1"}});

dataManWriter.Put(adiosVar, KokkosData, adios2::Mode::Sync);
```