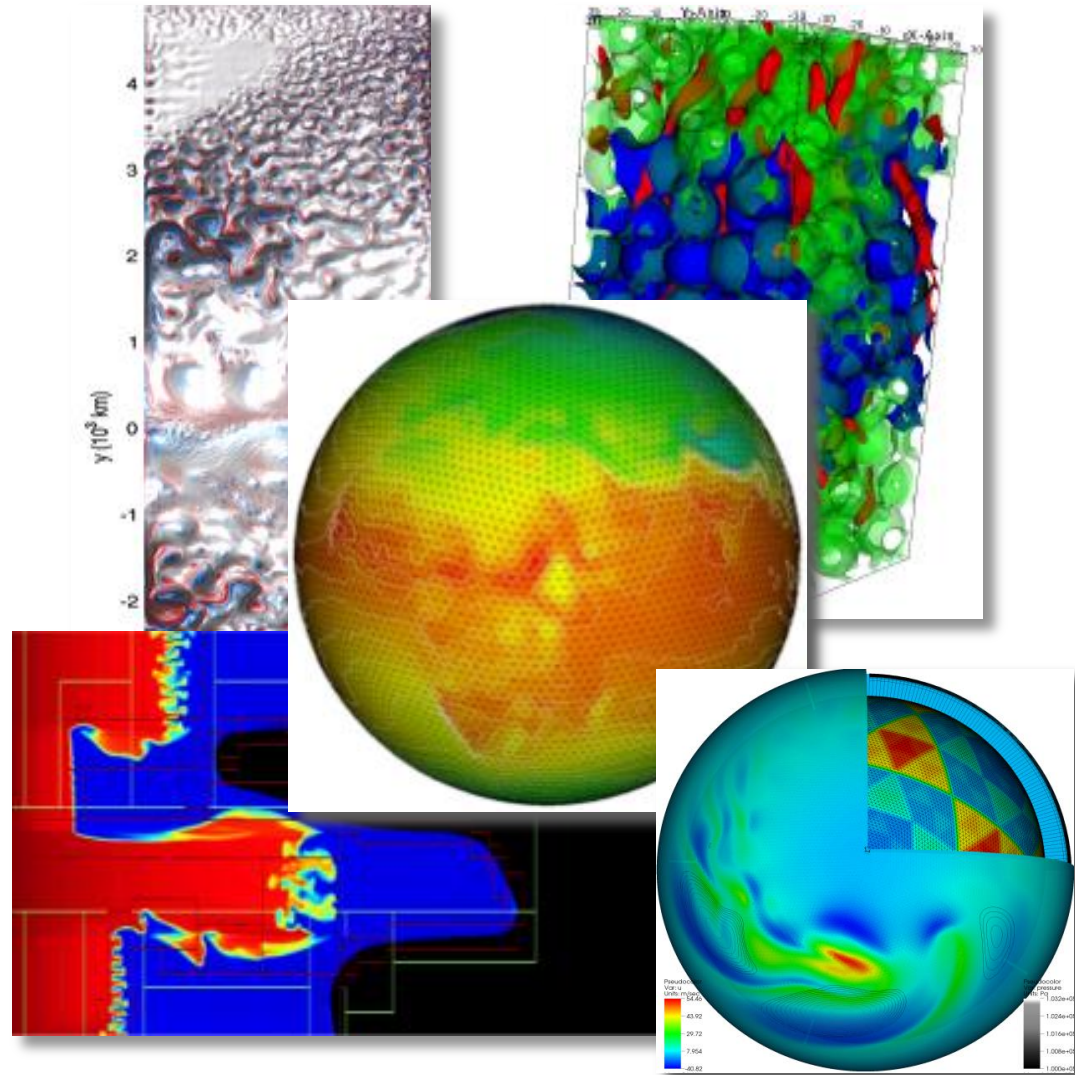# Scientific I/O: more than hard drives and file systems

- **Scientists think about data in terms of their science problem: molecules, atoms, grid cells, particles**

- **Ultimately, physical disks store bytes of data**

- **Layers in between, the application and physical disks are at various levels of sophistication**

Images from David Randall, Paola Cessi, John Bell, T Scheibe

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Example: FLASH Astrophysics

- FLASH is an astrophysics code for studying events such as supernovae
  - Adaptive-mesh hydrodynamics
  - Scales to 1000s of processors
  - MPI for communication
- Frequently checkpoints:
  - Large blocks of typed variables from all processes
  - Portable format
  - Canonical ordering (different than in memory)
  - Skipping ghost cells

Vars 0, 1, 2, 3, … 23

■ Ghost cell
■ Stored element
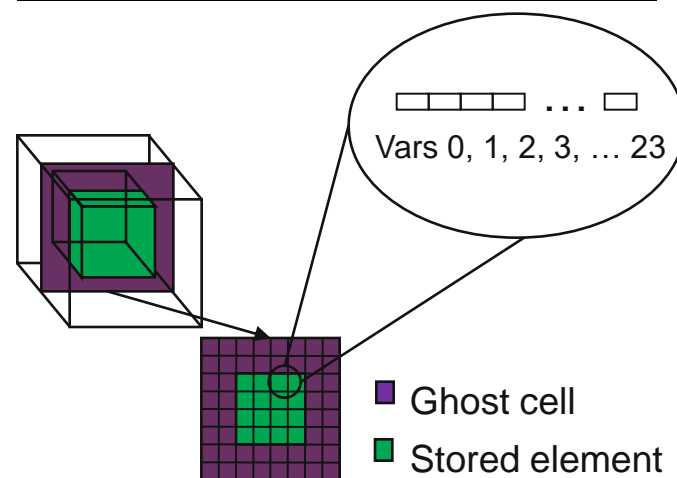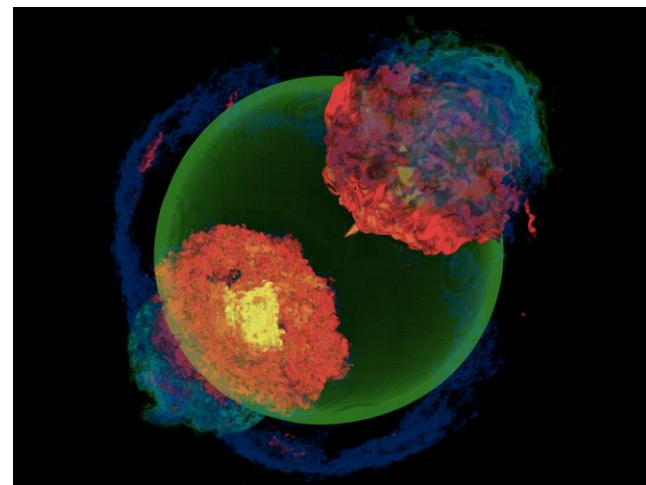
Example: FLASH's HDF5 requirements

- FLASH AMR structures do not map directly to HDF5 multidimensional arrays
- Must create mapping of the in-memory FLASH data structures into a representation in HDF5 multidimensional arrays
- Chose to
  - Place all checkpoint data in a single file
  - Impose a linear ordering on the AMR blocks
    - Use 4D variables
  - Store each FLASH variable in its own HDF5 variable
    - Skip ghost cells
  - Record attributes describing run time, total blocks, etc.

FLASH HDF5 Usage

- **Annotations describing data, experiment**

```
attribute_id = H5Acreate(group_id,
    "iteration",H5T_NATIVE_INT, dataspace_id, H5P_DEFAULT);
status = H5Awrite(attribute_id, H5T_NATIVE_INT, temp);
```

- **HDF5 variables for each FLASH variable**

```
ierr = H5Sselect_hyperslab(dataspace, H5S_SELECT_SET,
    start_4d, stride_4d, count_4d, NULL);
status = H5Dwrite(dataset, H5T_NATIVE_DOUBLE, memspace,
    dataspace, dxfer_template, unknowns);
```

HACC: understanding cosmos via simulation

- ■ "Cosmology = Physics + Simulation" (Salman Habib)
- ■ Sky surveys collecting massive amounts of data
  - – (~100 PB)
- ■ Understanding of these massive datasets rests on modeling distribution of cosmic entities
- ■ Seed simulations with initial conditions
- ■ Run for 13 billion (simulated) years
- ■ Comparison with observed data validates physics model.
- ■ I/O challenges:
  - – Checkpointing
  - – analysis

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