Parallel I/O for the CGNS system

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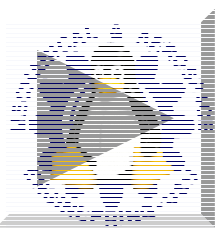
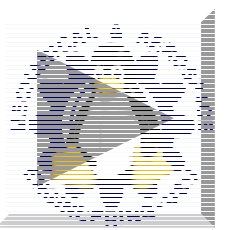


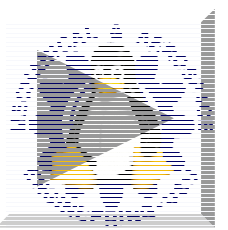
Outline

- Motivation
- Background of parallel I/O
- Overview of CGNS
  - Data formats
  - Parallel I/O strategies
- Parallel CGNS implementation
- Usage examples
  - Read
  - Writing ▪



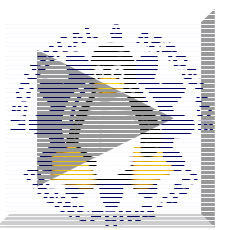
Why parallel I/O

- Supercomputer
  - A computer which turns a CPU-bound problem into an I/O-bound problem.
- As computers become faster and more parallel, the (often serialized) I/O bus can often become the bottleneck for large computations
  - Checkpoint/restart files
  - Plot files
  - Scratch files for out-of-core computation



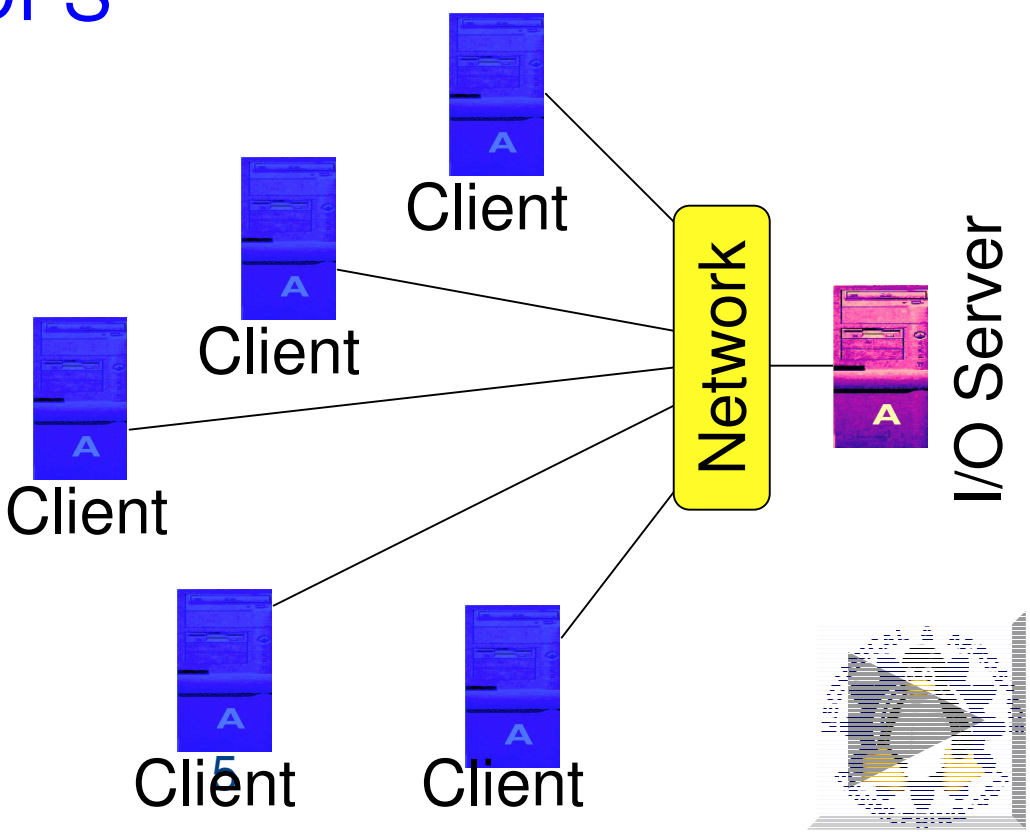
I/O Needs on Parallel Computers

- High Performance
  - Take advantage of parallel I/O paths (when available)
  - Support for application-level tuning parameters
- Data Integrity
  - Deal with hardware and power failures sanely
- Single System Image
  - All nodes "see" the same file systems
  - Equal access from anywhere on the machine
- Ease of Use
  - Accessible in exactly the same ways as a traditional UNIX-style file system



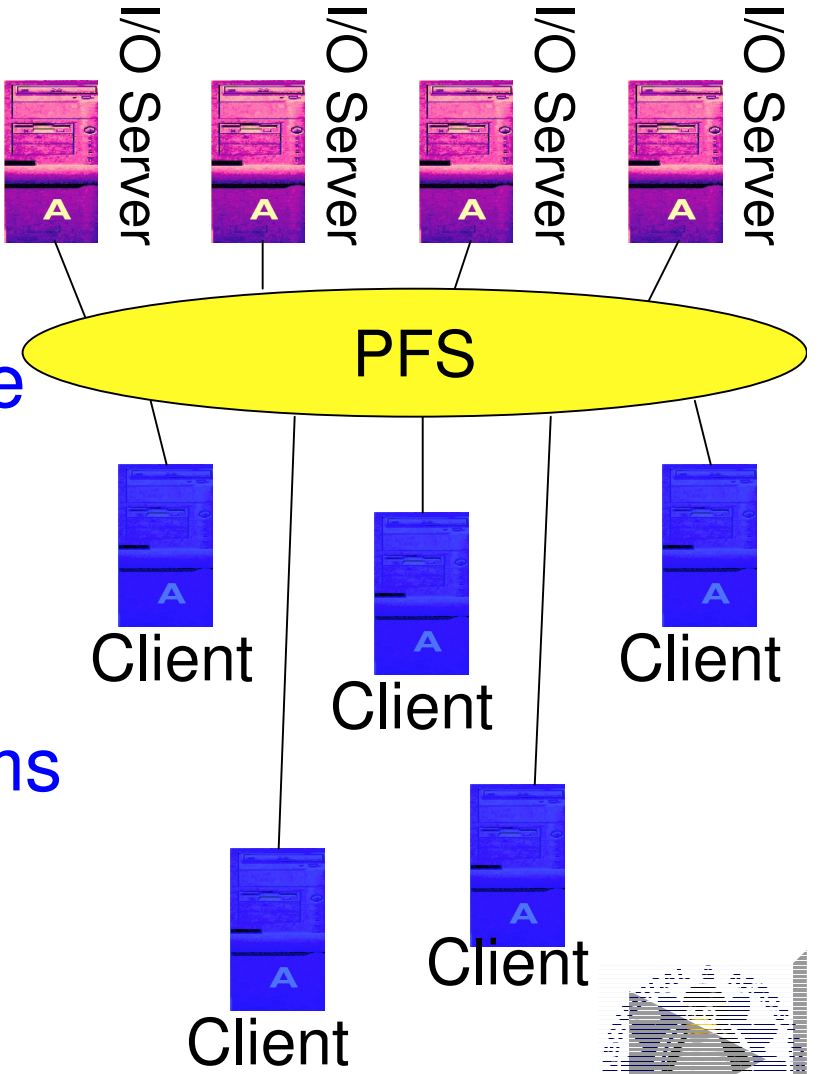
Distributed File Systems

- Distributed file system (DFS)
  - File system stored locally on one system (the server)
  - Accessible by processes on many systems (clients).
- Some examples of a DFS
  - NFS (Sun)
  - AFS (CMU)
- Parallel access
  - Possible
  - Limited by network
  - Locking problem



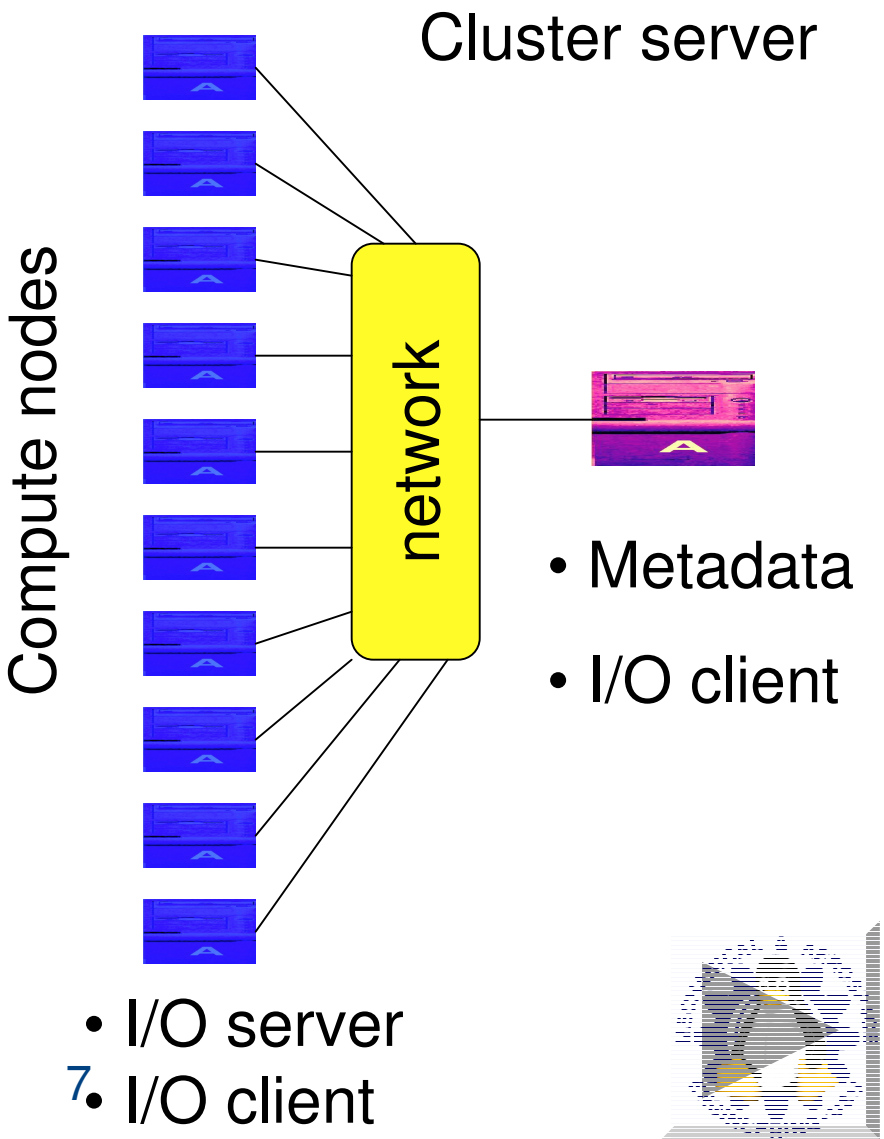
Parallel File Systems

- A parallel file system
  - multiple servers
  - multiple clients
- Optimized for high performance
  - Very large block sizes (=>64kB)
  - Slow metadata operations
  - Special APIs for direct access
- Examples of parallel file systems
  - GPFS (IBM)
  - PVFS2 (Clemson/ANL)



PVFS2 - Parallel Virtual File System

- Three-piece architecture
  - Single metadata server
  - Multiple data servers
  - Multiple clients
- Multiple APIs
  - PVFS library interface
  - UNIX file semantics using Linux kernel driver

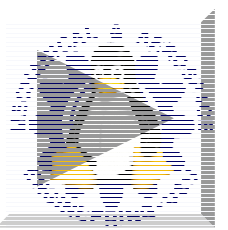


Simplistic parallel I/O

I/O in parallel programs without using a parallel I/O interface

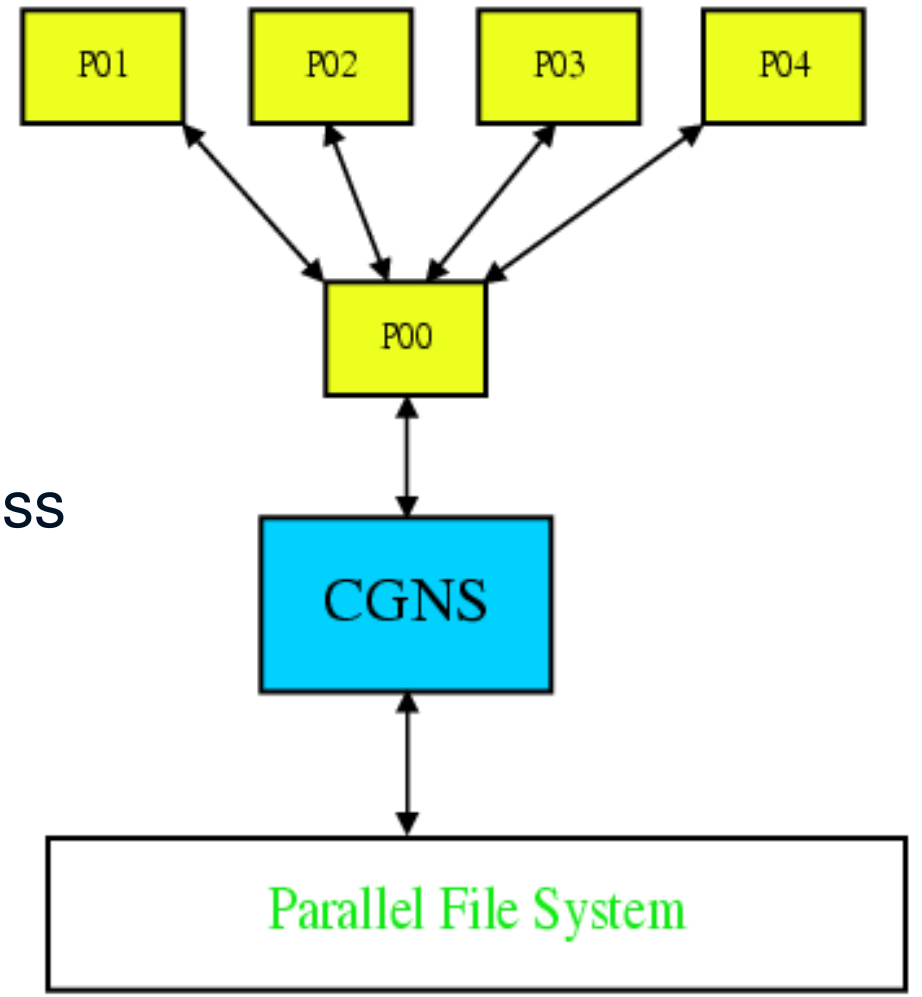
- Single I/O Process
- Post-Mortem Reassembly

Not scalable for large applications



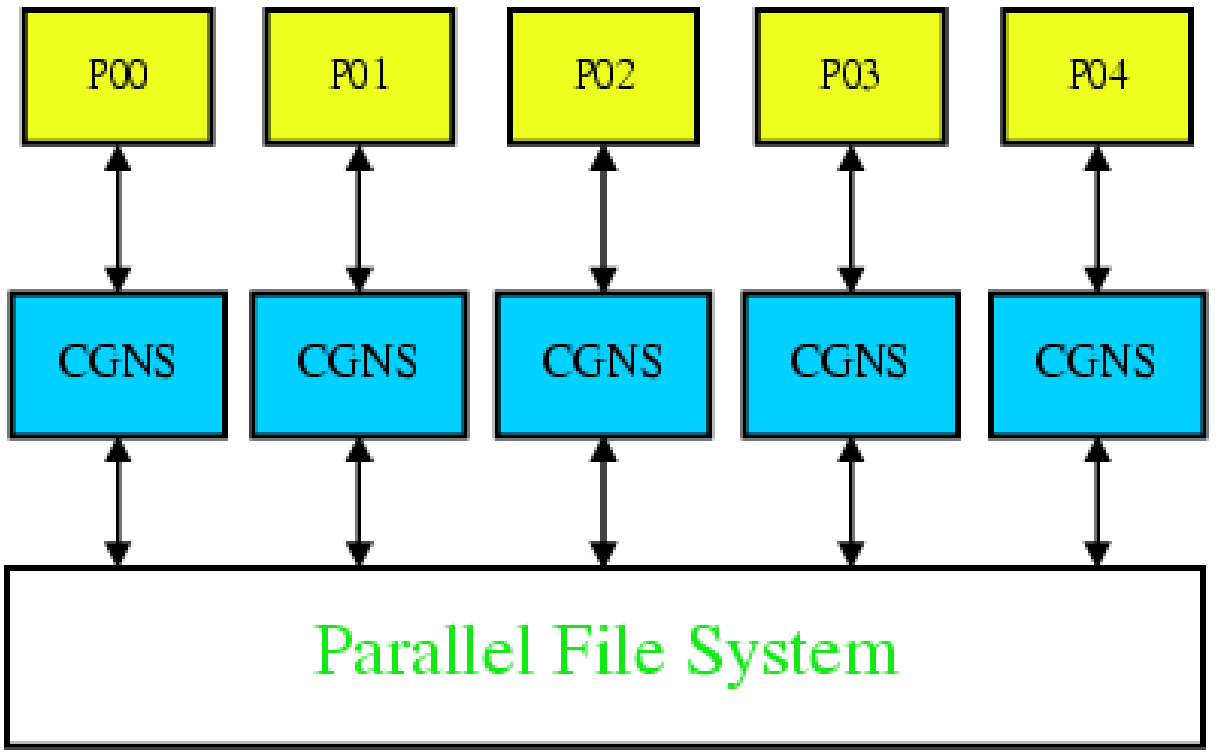
Single Process I/O

- Single process I/O.
  - Global data broadcasted
  - Local data distributed by message passing
- Scalability problems
  - I/O bandwidth = single process bandwidth
  - No parallelism in I/O
  - Consumes memory and bandwidth resources



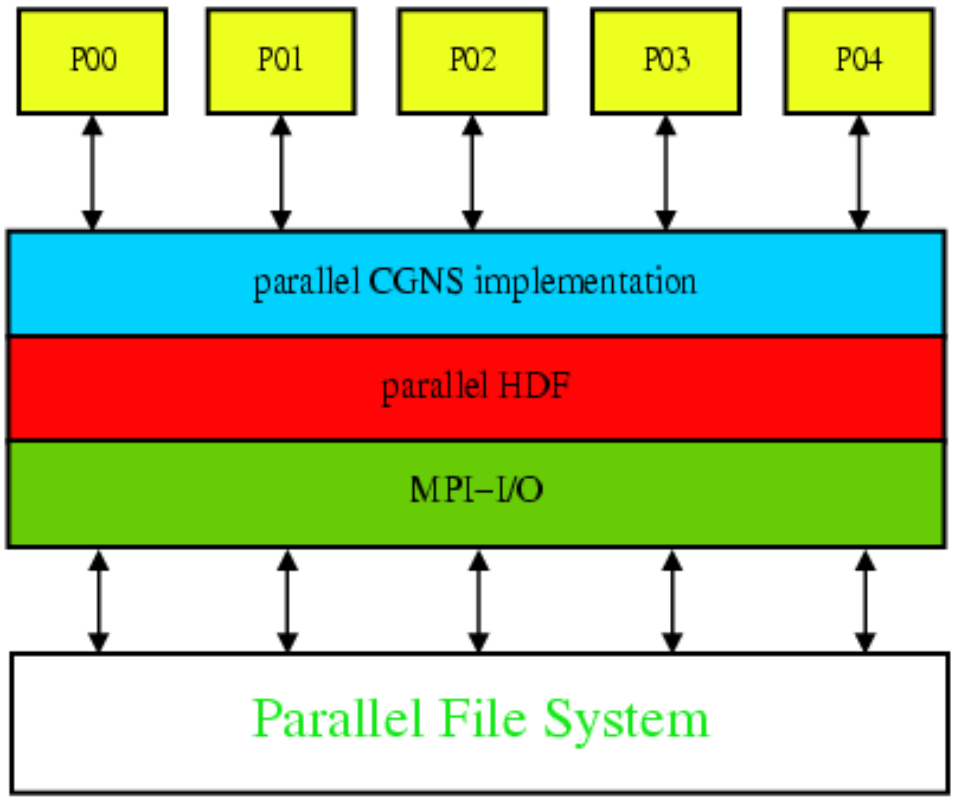
Post-Mortem Reassembly

- Each process does I/O into local files
- Reassembly necessary
- I/O scales
- Reassembly and splitting tool
  - Does not scale



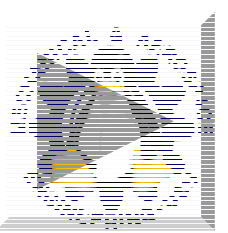
Parallel CGNS I/O

- New parallel interface
- Perform I/O cooperatively or collectively
- Potential I/O optimizations for better performance
- CGNS integration



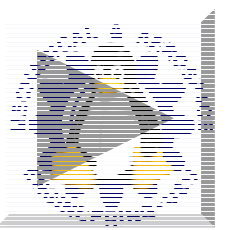
Parallel CGNS I/O API

- The same CGNS file format
  - Using the HDF5 implementation
- Maintains the look and feel of the serial midlevel API
  - Same syntax and semantics
    - Except: open and create
  - Distinguished by cgp_ prefix
- Parallel access through the parallel HDF5 interface
  - Benefits from MPI-I/O
  - MPI communicator added in open argument list
  - MPI info used for parallel I/O management and further optimization



MPI-IO File System Hints

- File system hints
  - Describe access pattern and preferences in MPI-2 to the underlying file system through
  - (keyword,value) pairs stored in an MPI_Info object.
- File system hints can include the following
  - File stripe size
  - Number of I/O nodes used
  - Planned access patterns
  - File system specific hints
- Hints not supported by the MPI implementation or the file system are ignored.
- Null info object (MPI_INFO_NULL) as default



Parallel I/O implementation

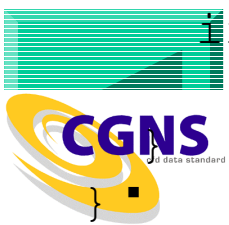
- Reading: no modification, except opening file
- Writing: Split into 2 phases
- Phase 1
  - Creation of a data set, e.g. coordinates, solution data
  - Collective operation
- Phase 2
  - Writing of data into previously created data set
  - Independent operation

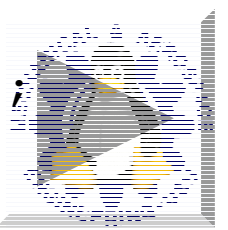
Examples

- Reading
  - Each process reads it's own zone
- Writing
  - Each process writes it's own zone
  - One zone is written by 4 processors
    - Creation of zone
    - Writing of subset into the zone

Example Reading

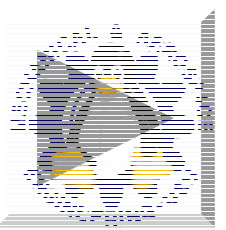
```
if (cgp_open(comm, info, fname, MODE_READ, &cgfile))
    cg_error_exit();
 if (cg_nbases(cgfile, &nbases)) cg_error_exit();
 cgbase = 1;
 if (cg_base_read(cgfile, cgbase, basename, &cdim, &pdim))
     cg_error_exit();
 if (cg_goto(cgfile, cgbase, "end")) cg_error_exit();
if (cg_units_read(&mu, &lu, &tu, &tempu, &au)) cg_error_exit();
if (cg_simulation_type_read(cgfile, cgbase, &simType))
    cg_error_exit();

if (cg_nzones(cgfile, cgbase, &nzones)) cg_error_exit();
nstart[0] = 1;  nstart[1] = 1;  nstart[2] = 1;
nend[0] = SIDES;  nend[1] = SIDES;  nend[2] = SIDES;
 for(nz=1; nz <= nzones; nz++) {
   if(cg_zone_read(cgfile, cgbase, nz, zname, zsize)) cg_error_ex
   if(mpi_rank == nz-1) {
   if (cg_ncoords(cgfile, cgbase, nz, &ngrids)) cg_error_exit();
      if (cg_coord_read(cgfile, cgbase, nz, "CoordinateX",
          RealDouble, nstart, nend, coord)) cg_error_exit();
 }
```





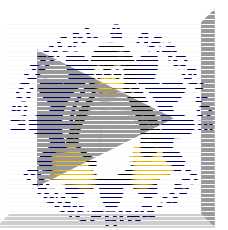
Each Process writes one Zone - 1

```
 if(cgp_open(comm, info, fname, MODE_WRITE, &cgfile) ||
     cg_base_write(cgfile, "Base", 3, 3, &cgbase) ||
     cg_goto(cgfile, cgbase, "end") ||
     cg_simulation_type_write(cgfile, cgbase,
NonTimeAccurate))
        cg_error_exit();
for(nz=0; nz < nzones; nz++) {
if(cg_zone_write(cgfile, cgbase, name, size, Structured,
    ▪ &cgzone[nz][0])) cg_error_exit();
    if (cgp_coord_create(cgfile, cgbase, cgzone[nz][0],
         RealDouble, "CoordinateX", &cgzone[nz][1]))
  cg_error_exit();
```



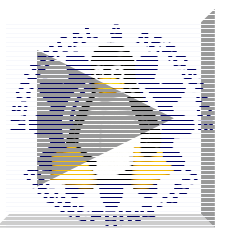
Each Process writes one Zone - 2

```
for(nz=0; nz < nzones; nz++)
 {
   if(mpi_rank == nz)
   {
     if(cgp_coord_write(cgfile, cgbase,
          cgzone[mpi_rank][0], cgzone[mpi_rank][1],
          coord) ||
      cgp_coord_write(cgfile, cgbase,
          cgzone[mpi_rank][0], cgzone[mpi_rank][2],
          coord) ||
      cgp_coord_write(cgfile, cgbase,
          cgzone[mpi_rank][0], cgzone[mpi_rank][3],
          coord))  cg_error_exit();
   }
 }
```



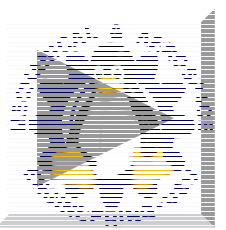
Writing One Zone

```
/* size is the total size of the zone */
if(cg_zone_write(cgfile, cgbase, name, size, Structured,
      &cgzone[nz][0])) cg_error_exit();
if (cgp_coord_create(cgfile, cgbase, cgzone[nz][0],
                     RealDouble, "CoordinateX",
                     &cgzone[nz][1]) ||
    cgp_coord_create(cgfile, cgbase, cgzone[nz][0],
                     RealDouble, "CoordinateY",
                     &cgzone[nz][2]) ||
    cgp_coord_create(cgfile, cgbase, cgzone[nz][0],
                     RealDouble, "CoordinateZ",
                     &cgzone[nz][3])) cg_error_exit();

if(cgp_coord_partial_write(cgfile, cgbase, cgzone,
                           cgcoord, rmin, rmax, coord))
   cg_error_exit;
```

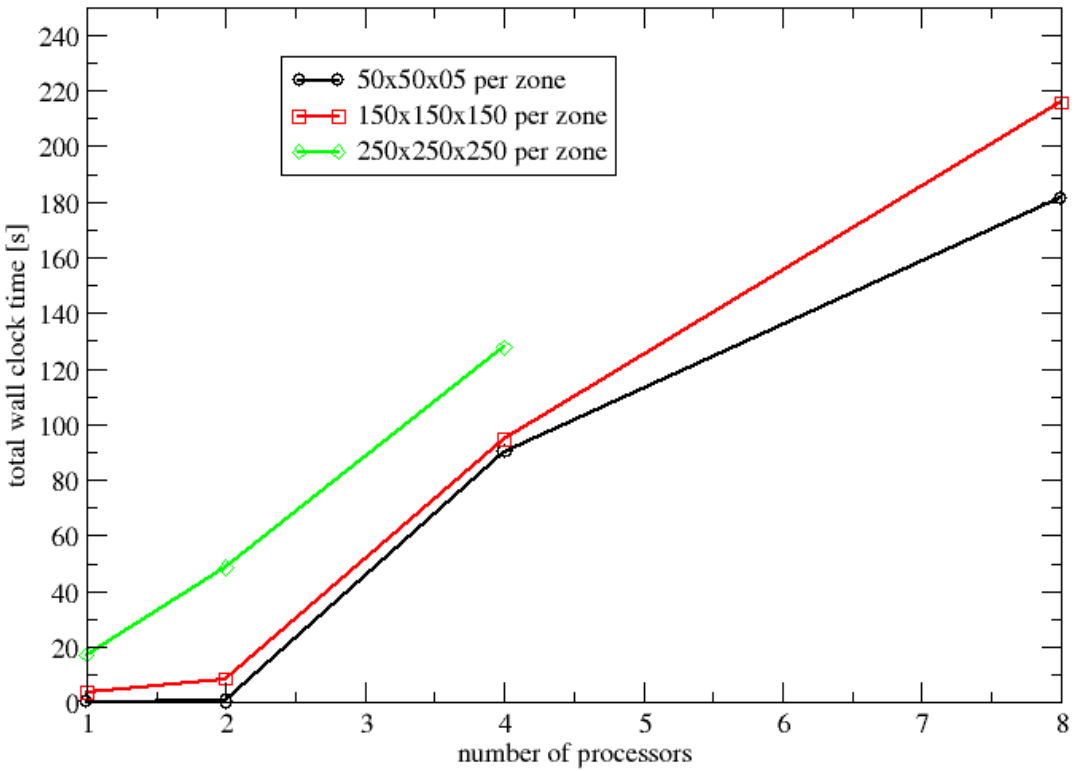


Write Performance

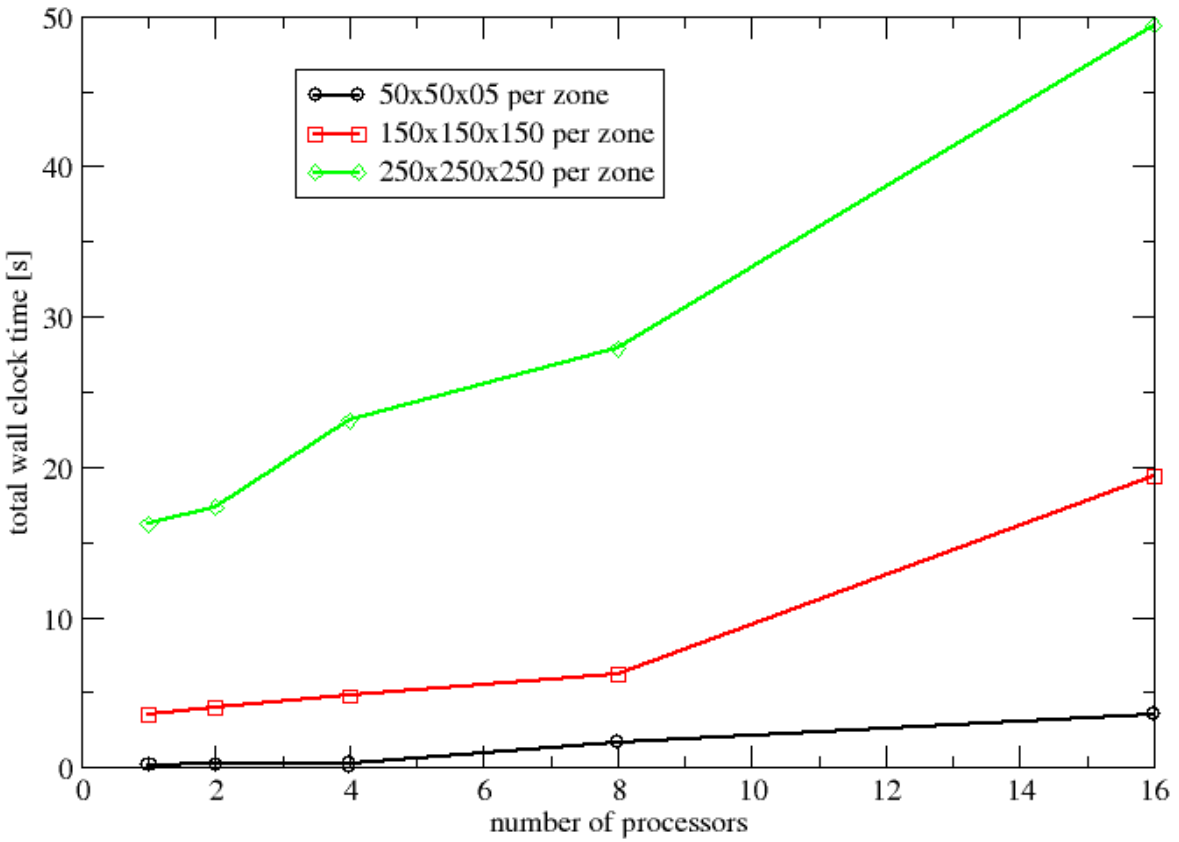
- 3 Cases
  - 50x50x50 points x number of processors
    - 23.0MB
  - 150x150x150 points x number of processors
    - 618 MB
  - 250x250x250 points x number of processors
    - 2.8GB
- Increasing the problem size with the number of processors



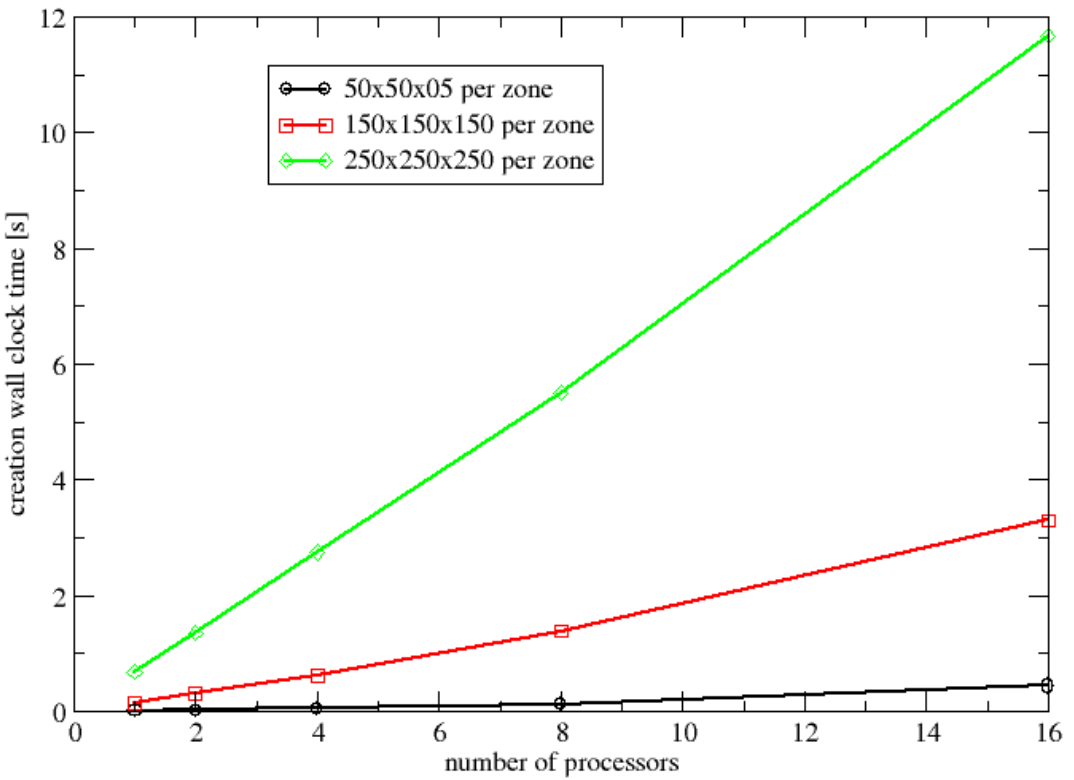
Total write time - NFS



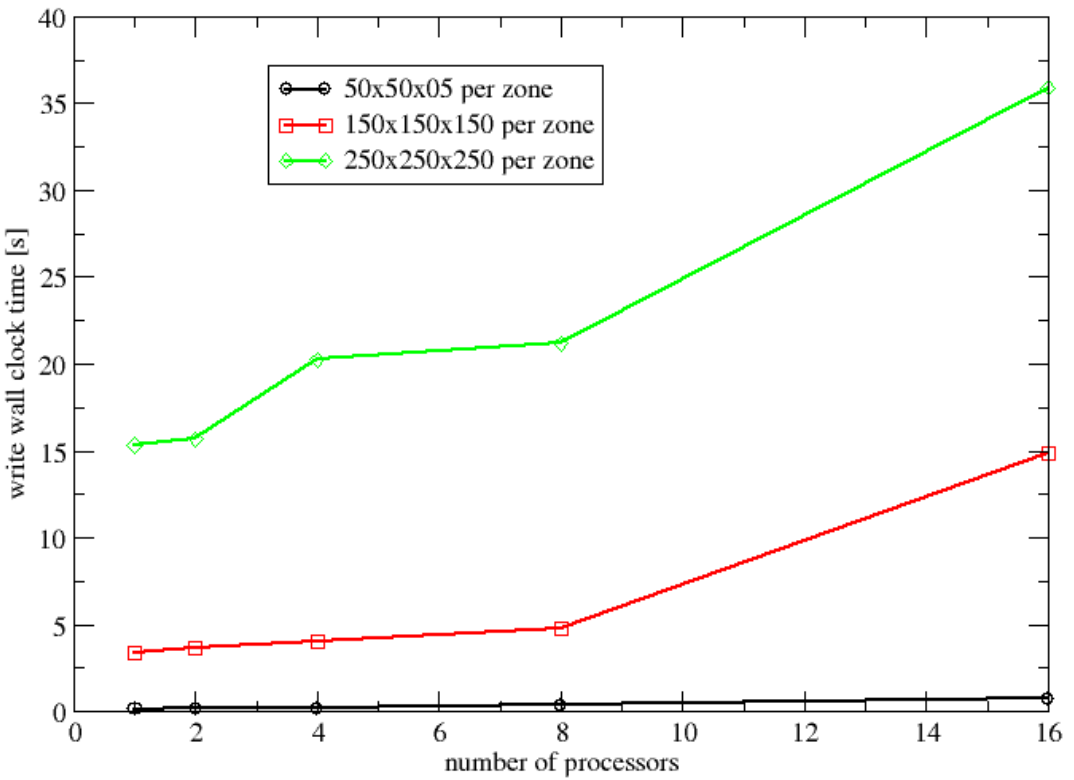
Total write time – PVFS2



Creation Time – PVFS2



Write Time – PVFS2



Conclusion

- Implemented a prototype of parallel I/O within the framework of CGNS
  - Built on top of existing HDF5 interface
  - Small addition to the midlevel library cgp_* functions
- High-performance I/O possible with few changes
- Splitting the I/O into two phases
  - Creation of data sets
  - Writing of data independently into the previously created data set
- Testing on more platforms