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Update on PIO: The Parallel I/O Library

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(telling you about work done by….)

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Motiviation: Trends in Climate Model Resolution

- High resolution configuration: 1/10th degree ocean/ice with 0.5 degree atmosphere.
  - Ocean: 3600 x 2400 x 42
  - Sea ice: 3600 x 2400 x 20
  - Atmosphere: 576 x 384 x 26
  - Land: 576 x 384 x 17
- Compared to CCSM3:
  - Ocean: 73x larger
  - Atmosphere: 7x larger

Trends in Climate Model Output

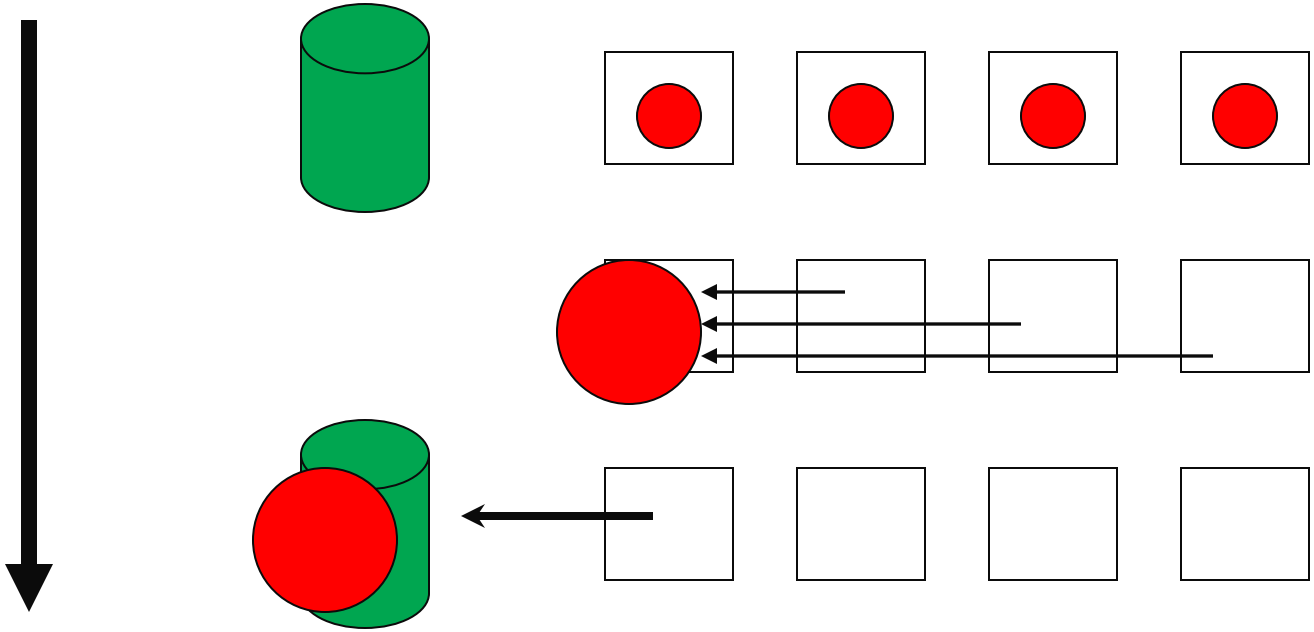
- History output sizes for high-resolution configuration *for one write of a single monthly average*
  - Atmosphere: 0.8 GB
  - Ocean: 24 GB (reduced; 100GB if full)
  - Sea Ice: 4 GB
  - Land: 0.3 GB

- Restart output:
  - Atmosphere: 0.9 GB
  - Ocean: 29 GB (96 GB with extra tracers)
  - Sea Ice: 5 GB
  - Land: 0.2 GB
  - Coupler: 6.5 GB

Versus: Trends in High Performance Computing systems

- Moore's Law is still increasing *transistor count* but now they are grouped in to **multiple cores**.
- Memory/core is nearly constant.
- Power/cooling constraints promote design for maximum flops/watt
  - BlueGene: low power nodes; **low memory**
    - *BG/L node: 2 440 Power PC, 0.7GHz;* ***512MB/node***
    - *BG/P node: 4 450 PowerPC, 0.85 GHz;* ***2GB/node***

Ye Olde Gather/Scatter with Serial Read/Write



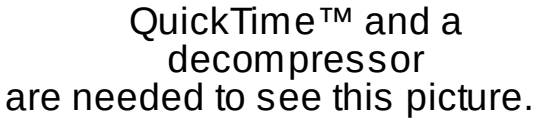
Example: gather and write

- As old as the first parallel program
- Still state-of-the-art

So..How does one gather 30GB of data on to a 2GB node for writing?

- Serialization: send one piece at a time and write it out. Slows down with more nodes or more data/node.
- Each node writes its own file: Then you have new post-processing headache of gathering up all the individual files into one file.
- Use nodes with more memory! Even large-memory nodes will be overrun by output from future models.

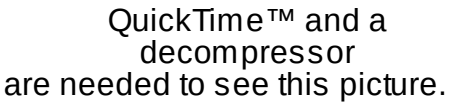
Solution: Parallel I/O!



(Figure and following general parallel I/O overview provided by **Rob Latham** (Argonne))

- Parallel I/O beings with hardware and **low-level** software forming a parallel file system
  - Many disks look like one big disk.
  - Examples: PVFS, Lustre, GPFS.

Software for Parallel I/O



- Applications require more software than just a parallel file system
- Support provided via multiple layers with distinct roles:
  - Parallel file system maintains logical space, provides efficient access to data (e.g. PVFS, GPFS, Lustre)
  - I/O Forwarding found on largest systems to assist with I/O scalability
  - Middleware layer deals with organizing access by many processes(e.g. MPI-IO, UPC-IO)
  - High level I/O library maps app. abstractions to a structured,portable file format (e.g. HDF5, Parallel netCDF)
- Goals: scalability, parallelism (high bandwidth), and usability

I/O presentation from Rob Latham (Argonne National Lab)

MPI-IO

- MPI-IO is an I/O interface specification for use in MPI apps
- Data model is same as POSIX
  - Stream of bytes in a file
- Features:
  - Collective I/O
  - Noncontiguous I/O with MPI datatypes and file views
  - Nonblocking I/O
  - Fortran bindings (and additional languages)
- Implementations available on most platforms

PNetCDF: NetCDF output with MPI-IO

- Based on NetCDF
  - Derived from their source code
  - API slightly modified
  - Final output is indistinguishable from serial NetCDF file
- Additional Features
  - Noncontiguous I/O in memory using MPI datatypes
  - Noncontiguous I/O in file using sub-arrays
  - Collective I/O
- Unrelated to netCDF-4 work

Goals for Parallel I/O in CCSM

- Provide a single interface to multiple I/O options: pnetcdf, binary with MPI-IO, “plain” netcdf.
- General enough to be used as I/O interface in all CCSM components.
- Simple interface for component developers to implement.
- Extensible for future I/O technology
- Preserve format of input/output files
- Supports 1D, 2D and 3D arrays

PIO Terms and Concepts:

- IO decomposition vs. physical model decomp
  - IO decomp == model decomp
    - *MPI-IO+ message aggregation*
  - IO decomp != model decomp
    - *Need to rearrange data from one decomposition to another.*

- No component specific info in library
  - Pair with existing communication technology
  - 1D arrays in library; component must flatten2D and 3D arrays

PIO Terms and Concepts:

- 3 modes of writing within PIO
  - PIO + MPI-IO: ("binary mode"). Call MPI-IO directly to write binary files
  - PIO + NetCDF ("netcdf mode" or "serial mode"). Gather pieces of data to node 0 (or other designated node) one piece at a time for writing netcdf files.
  - PIO + PNetCDF ("pnetcdf mode"). PIO calls PNetCDF directly to do parallel write of netcdf file.
- "degrees of freedom" or DOF = decomposition

PIO status at last workshop:

- PIO API defined
- API implemented in CAM (all dycores with input and output) on branch
- New serial netcdf mode avoids memory bottleneck through serializing the data gather.
- Early performance successes: I/O was faster as I/O processors were added
- Early feasibility success: Some high-res HOMME runs not possible without using PIO for reading input.
- Set up PIO Google group with publicly readable email list. Also set up repo at GoogleCode

Progress since last workshop:

- Pushing PNetCDF uncovered some memory leaks. Fixes released in PNetCDF 1.0.3 (December, 2008)

- Reorderd PIO file and directory structure so it can more easily build as both a component of CCSM or CAM and as a standalone library.

- PIO has made more progress in component models:
  - CAM: now a runtime option for history and restart on main versions of CAM (no longer just on a branch)
  - CPL7: PIO is default method for I/O.
  - CICE: implementation is nearly complete
  - POP and CLM: implementations using older versions of PIO need to be revisited or replaced.

Progress since last workshop:

- Flow control and throttling added to box-rearranger communication to improve performance and work around limitations in some MPI implementations.

- New I/O decomposition algorithm provides more optimal decomposition.

Major new feature: Comprehensive, extendable test suite

- Two methods for setting up a grid on which to test I/O:
  - Very flexible methods for setting a 3D rectangular grid of arbitrary size and regular decompositions of that grid in 1, 2 or 3 dimensions OR
  - Write out decomposition from real code (CAM, POP) and read it back in for testing (pio_writedof, pio_readdof)!

- Grid, decomposition and I/O method to test all specified in a namelist.

- Test program testpio.F90:
  - Reads namelist
  - Generates test data (integers, 4-byte reals and 8-byte reals)
  - Writes data with specified method (binary, netcdf, pnetcdf)
  - Reads data back and checks for correctness
  - Times reads and writes.

Major new feature: Comprehensive, extendable test suite

- Testpio directory already provides 47 namelists for testing various configurations.

- Namelist naming convention: testpio_in.nnXX
  - nn = “pn” = “pnetcdf with no rearrangement”
  - nn = “sb” = “serial netcdf with box rearrangement”
  - XX = 02 = “simple 2d xy decomp across all pes with all pes active in I/O”
  - XX = 04 = “simple 2d xy decomp with yxz ordering and stride=4 pes active in I/O

- Run scripts available for all CCSM target platforms (bluefire, jaguar, intrepid, franklin, kraken)

- Testpio used mostly for testing before checkins. Timings being done with CCSM and components.

PIO Recent Results:

- PIO is a success as an *enabling technology*: Allows simulations never before possible.
  - FV 0.25 degree with trop_mam3 chemistry on jaguar
  - FV 0.25 degree with trop_mozart chemistry and a total of 399 tracers on jaguar.
- PIO timings: continue to be mixed
  - PIO with MPI-IO is always fast. 1-2GB/s read/write obtained.
  - PIO with serial netcdf surprisingly good for some cases. Around Nov, 08, was always faster then pnetcdf.
  - PIO with pnetcdf has shown improvement in past month:
    - *FV 2-degree: pnetcdf now twice as fast as netcdf*
    - *HOMME on 512 BG/P nodes: pnetcdf now 100x faster than netcdf*
    - *FV 0.5 degree with trop-mozart: pio 2x faster than native.*

PIO Recent Results: Dealing with the zoo

- Example of odd timings:
  - 0.25 HOMME on Blackrose (intel linux cluster with inifinband and Lustre) using PIO+pnetcdf. Run on 128 cpus with different strides for I/O processors
    - *32: 21 MB/s*
    - *64: 102 MB/s*
    - *128: 32 MB/s*
- Strange animals and deep magic:
  - Lustre: PIO performance was improved when Lustre upgraded from 1.4 to 1.6 but reproducible performance still elusive.
  - BG: Need to add “bglockless:” to filename to avoid NFS-type file locking.
  - Bluefire: task binding degrades PIO performance. Use MP_TASK_AFFINITY=CORE instead.
  - MPI-IO hints: different hints needed for different hardware.

PIO and the broader community

- PIO currently developed within CCSM repository.

- Latest version of code **now available** at Google Code: parallelio.googlecode.com
  - Tags in CCSM repo are exported by PIO developers and then imported to Google Code.
  - Anonymous checkout allowed by anyone.
  - Checkin limited to “project members”. Membership can be extended to external users who would like to contribute.
  - Merging any contributed code back to CCSM repo up to CCSM PIO developers.

PIO future work

- Add more unit tests based on real decompositions
- Understanding performance across zoo of parallel I/O hardware/software. (John Dennis has two summer students who will be working on this.)
- Add to rest of CCSM
- Ask other application areas to try PIO and provide feedback.