PIO: The Parallel I/O Library

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The 13th Annual CCSM Workshop, June 19, 2008

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 Resolution

- 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

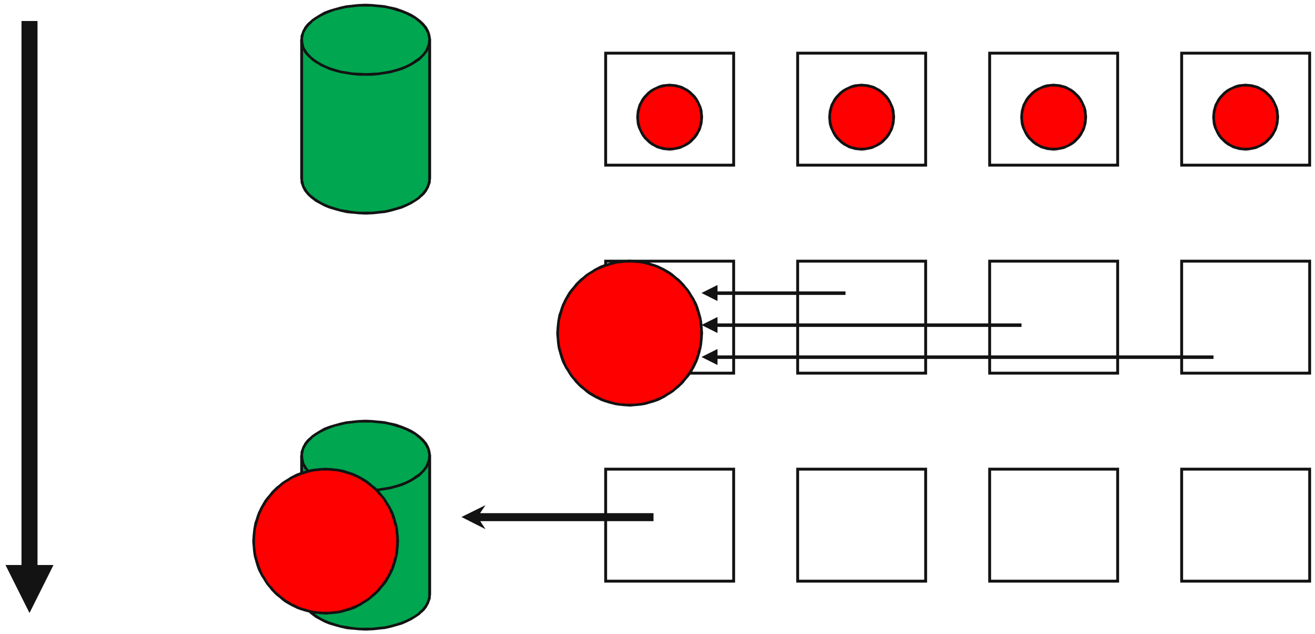
Trends in High Performance Computing systems

- 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 PowerPC, 0.7GHz; 512MB* ***(256MB/core)***
    - *BG/P node: 4 450 PowerPC, 0.85 GHz; 2GB* ***(512MB/core)***
  - SciCortex node: 6 MIPS64 cores, 0.5 GHz; (600 mW each!)

Ye Olde Gather/Scatter with Serial Read/Write



Example: gather and write

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

Solution: Parallel I/O!

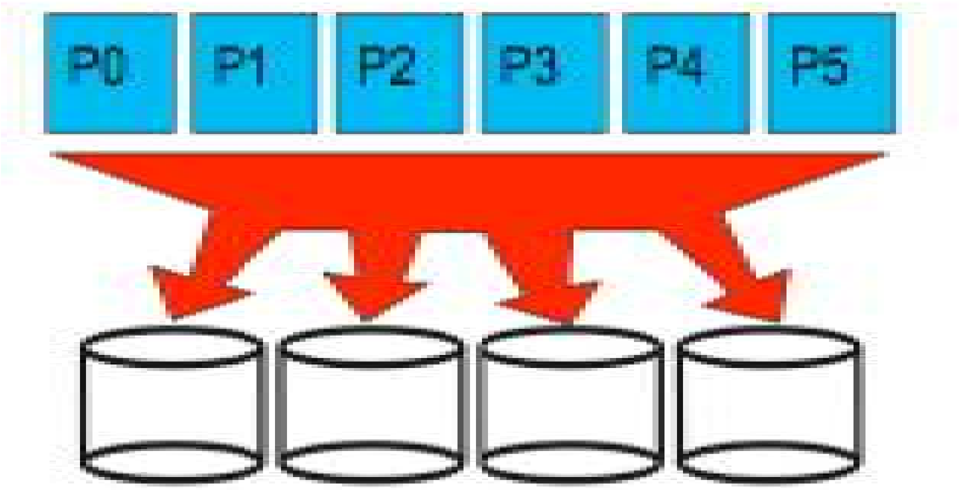


Figure and following general parallel I/O overview provided by **Rob Latham** (Argonne)

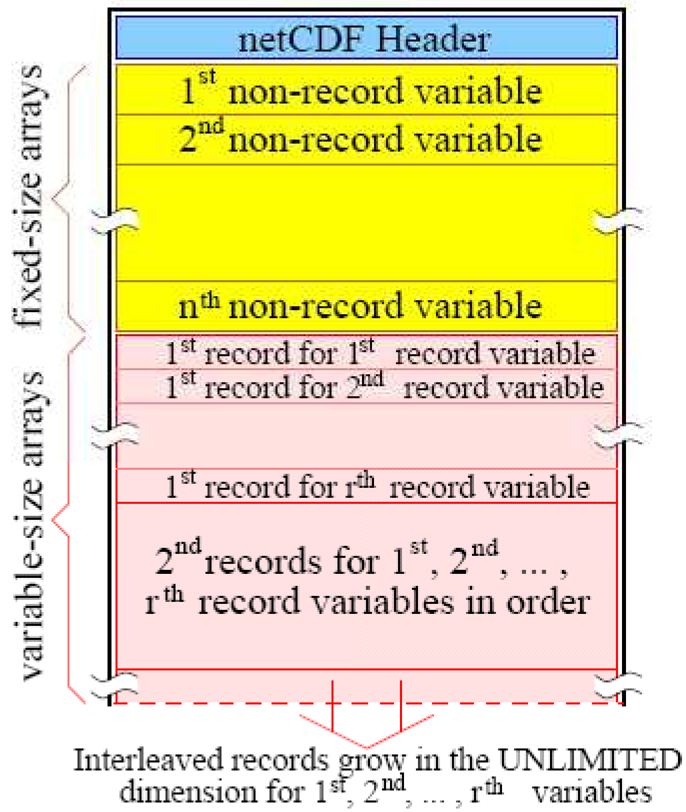
- Parallel I/O beings with hardware and **low-level** software forming a parallel file system
  - Many disks look like one big disk.
  - Related: old parallel I/O method of each processor writing its own file to local disk. Postprocessing needed to complete output.
  - Examples: PVFS, Lustre, GPFS.

MPI-IO

- The Message Passing Interface (MPI) is an interface standard for writing message passing programs
  - Most popular programming model on HPC systems
- 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

NetCDF: Standard file format used in climate modeling

- Data Model:
  - Collection of variables in single file
  - Typed, multidimensional array variables
  - Attributes on file and variables
- Features:
  - C and Fortran interfaces
  - Portable data format
- Data is always written in a big-endian format
- NetCDF files consist of three regions
  - Header
  - Non-record variables (all dimensions specified)
  - Record variables (ones with an unlimited dimension)



Parallel NetCDF: 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

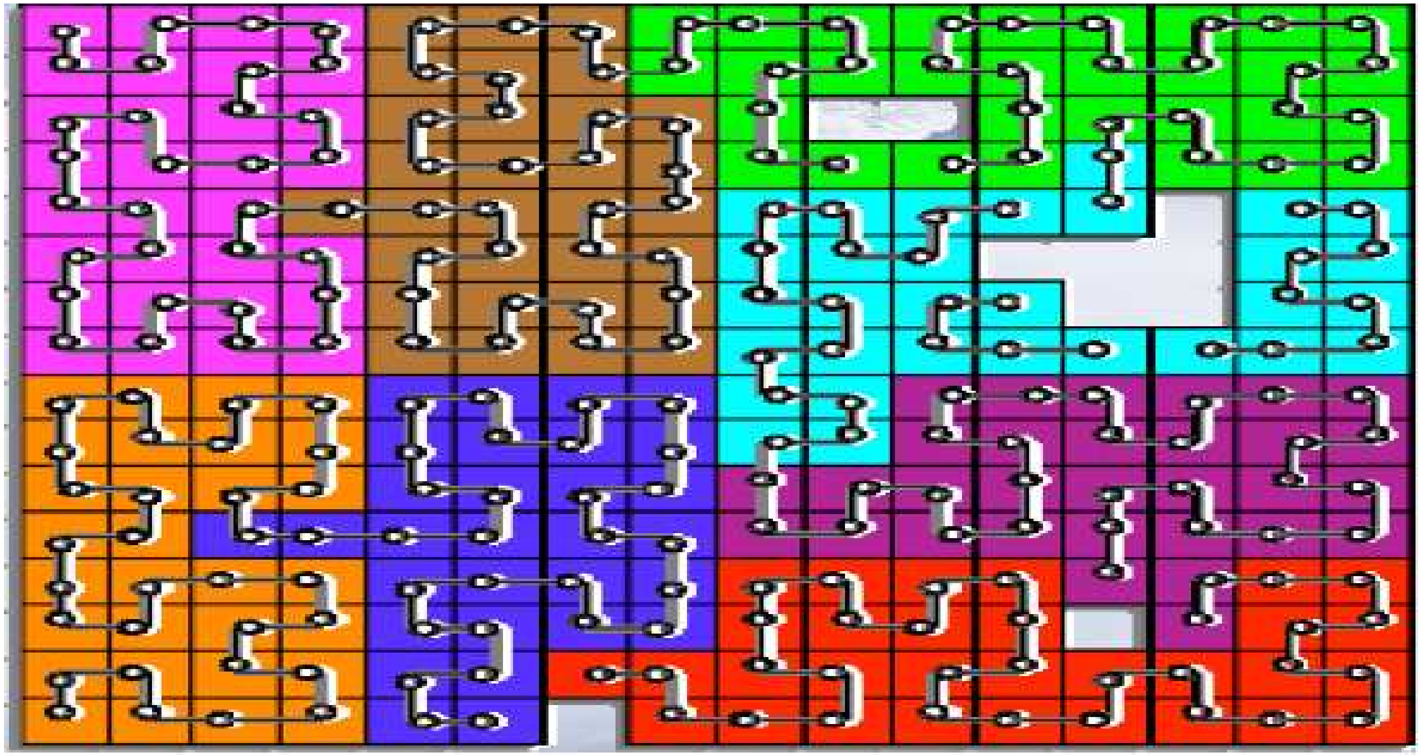
Goals for Parallel I/O in CCSM

- Provide parallel I/O for all component models
- Encapsulate complexity into library
- Simple interface for component developers to implement
- Extensible for future I/O technology

Goals for Parallel I/O in CCSM

- Backward compatible (node=0)
- Support for multiple formats
  - {sequential,direct} binary
  - netcdf
- Preserve format of input/output files
- Supports 1D, 2D and 3D arrays

Climate model decompositions can be complex



Ocean decomposition with space-filling curve

PIO Terms and Concepts:

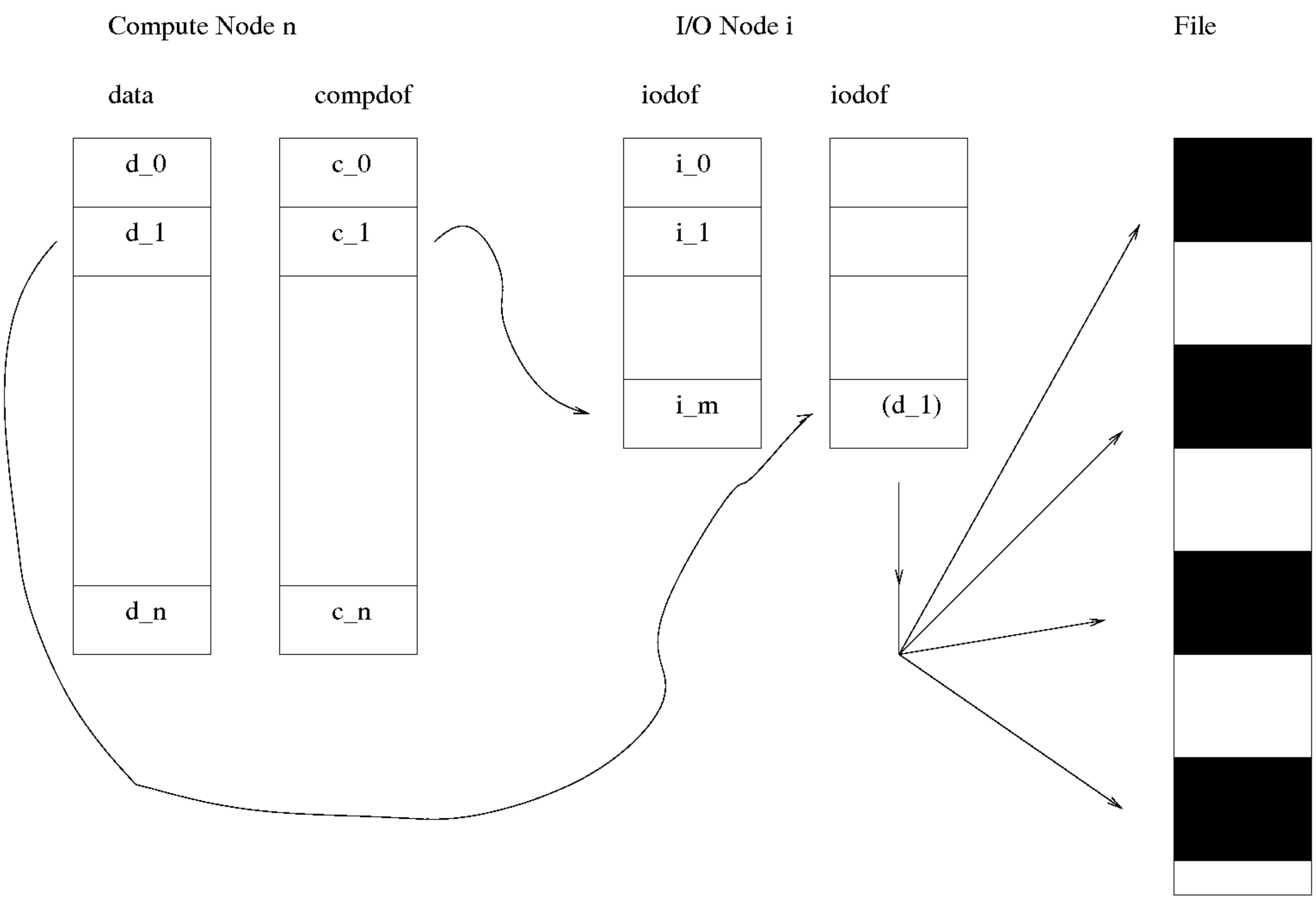
- I/O decomp vs. physical model decomp
  - I/O decomp == model decomp
    - *MPI-IO+ message aggregation*
  - I/O decomp != model decomp
    - *Need Rearranger: MCT, custom*

- No component-specific info in library
  - Pair with existing communication tech
  - 1-D arrays input to library; component must flatten 2-D and 3-D arrays

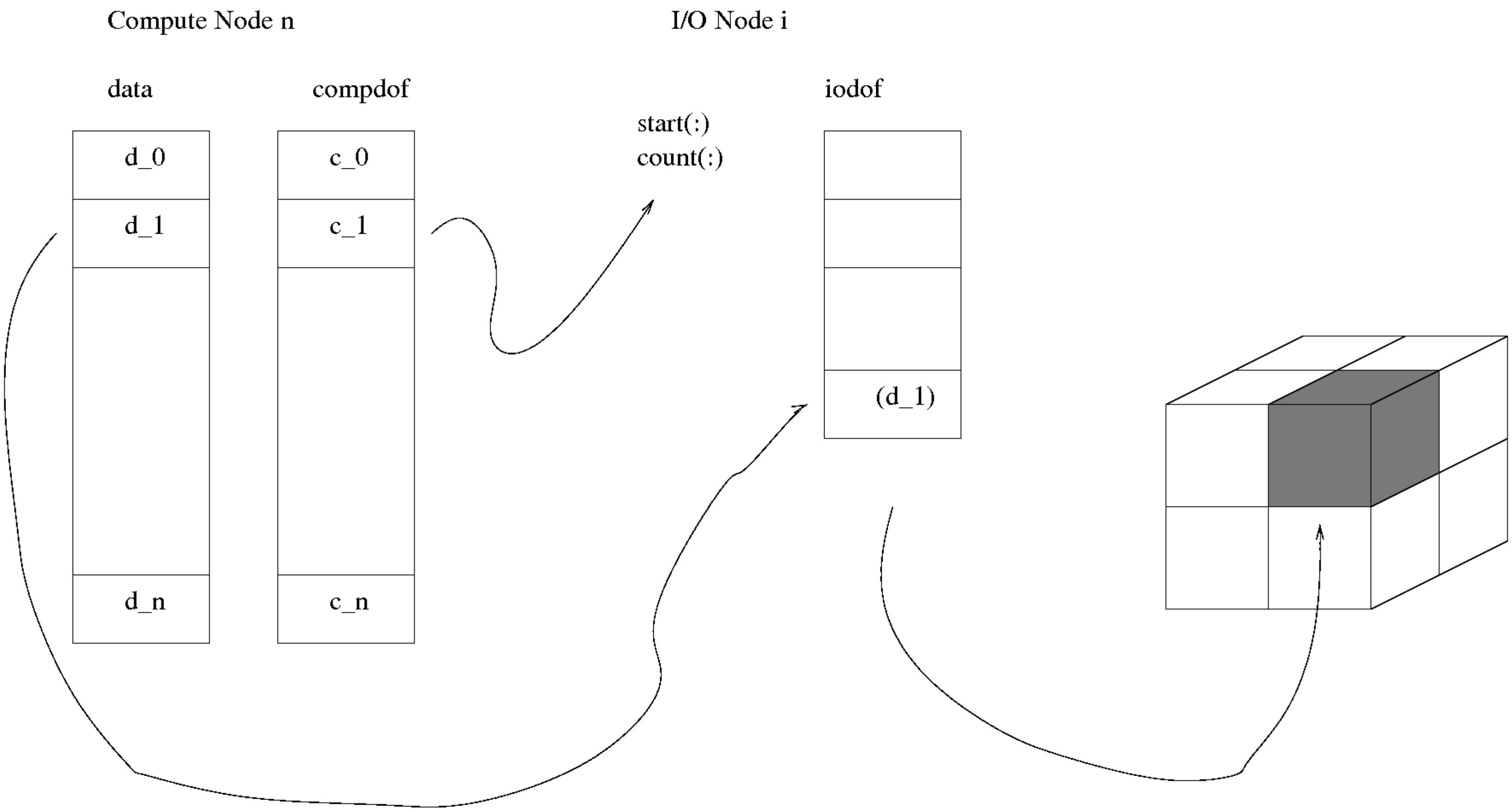
PIO Data Rearrangement

- Goal: redistribute data from computational layout of the model ("*compdof*") to a subset of processors designated for I/O ("*iodof*").
  - Provides direct control of number of procs reading/writing to maximize performance on a platform
  - This level of control not possible with pnetcdf API, also more portable than MPI-IO hints
  - I/O decomposition matched to actual read/write
- Initial method: MCT
  - Pro: MCT Rearranger is general, allows arbitrary pattern
  - Con: Setup is expensive (all-to-all matching); description of the decompositions can be large due to poor compression of small runs of indices
- Improved method: Box Rearranger
  - Netcdf/Pnetcdf reads/writes naturally operate on rectangular "box" subsets of output array variables

Data rearrangement



Box Rearranger



PIO Box Rearranger

- Mapping defined by extents of box for each I/O node
  – Extremely compact representation easily distributed
  – Reverse mapping computed at runtime
- Supports features needed for e.g. ocean vs. land
  – “holes” in computational decomposition
  – fill values for I/O dofs not covered
- Design evolved driven by performance of CAM integration
  – Initial design conserved space by creating send/receive types on-the-fly. *MPI too slow*.
  – Important to performance to cache MPI types and compute reverse mapping up-front during Rearranger creation

PIO API

```
subroutine PIO_init(comp_rank, comp_comm, num_iotasks, num_aggregator,
   stride, Rearranger, IOsystem, base)
      integer(i4), intent(in) :: comp_rank          ! (MPI rank)
      integer(i4), intent(in) :: comp_comm          ! (MPI communicator)
      integer(i4), intent(in) :: num_iotasks
      integer(i4), intent(in) :: num_aggregator
      integer(i4), intent(in) :: stride
      integer, intent(in) :: Rearranger  !defined in pio_types
    + PIO_rearr_none ! pio does no data rearrangment, data is assumed to be in it's final form when passed to pio
    + PIO_rearr_mct ! pio uses mct to rearrange the data from the computational layout to the io layout.
    + PIO_rearr_box ! pio uses an internal rearranger to rearrange the data from the computational layout to the io layout.
      type (IOsystem_desc_t), intent(out) :: IOsystem   ! Output
```

IOsystem stores the context

PIO API

subroutine **PIO_initDecomp**(Iosystem,baseTYPE,dims,compDOF,IOdesc)

```
type(IOSystem_desc_t), intent(in) :: IOsystem
integer(i4), intent(in) :: baseTYPE      ! type of array {int,real4,real8}
integer(i4), intent(in) :: dims(:)       ! global dimensions of array
integer (i4), intent(in) :: compDOF(:)   ! Global degrees of freedom for comp decomposition
type (IO_desc_t), pointer, intent(out) :: IOdesc
```

Automatically computes start(:) and cnt(:) to define the I/O mapping

PIO API

subroutine **PIO_initDecomp**(Iosystem,baseTYPE,dims,lenBLOCKS,compDOF, ioDOFR,ioDOFW,start,cnt,IOdesc)

```
type(IOSystem_desc_t), intent(in) :: IOsystem
integer(i4), intent(in) :: baseTYPE      ! type of array {int,real4,real8}
integer(i4), intent(in) :: dims(:)            ! global dimensions of array
integer (i4), intent(in) :: lenBLOCKS
integer (i4), intent(in) :: compDOF(:)   ! Global degrees of freedom for comp decomposition
integer (i4), intent(in) :: ioDofR(:)       ! Global degrees of freedom for I/O decomp (Read op)
integer (i4), intent(in) :: ioDofW(:)      ! Global degrees of freedom for IO decomp (Write op)
integer (PIO_OFFSET), intent(in) :: start(:), cnt(:) ! pNetCDF domain decomosition information
type (IO_desc_t), pointer, intent(out) :: IOdesc
```

start(:) and cnt(:) define the I/O mapping

PIO API

subroutine **PIO_write_darray**(data_file, varDesc, IOdesc, array, iostat, fillval)

```
type (File_desc_t), intent(inout) :: data_file          ! file information (netcdf or binary)
type (IOsystem_desc_t), intent(inout) :: iosystem ! io subsystem information
type (var_desc_t), intent(inout) :: varDesc           ! variable descriptor
type (io_desc_t), intent(inout) :: iodesc               ! io descriptor defined in initdecomp
intent(in) :: array ! array to be written (currently integer, real*4 and real8 types are supported, 1
                                                          dimension
integer, intent(out) :: iostat ! error return code
intent(in), optional :: fillvalue ! same type as array, a fillvalue for pio to use in the case of missing
                                                                      data
```

Cached I/O mapping and structures reusable for multiple writes/reads (via IOdesc)

PIO API

subroutine **PIO_read_darray**(data_file, varDesc, iodesc, array, iostat)

type (File_desc_t), intent(inout) :: data_file ! info about data file

type (var_desc_t), intent(inout) :: varDesc ! variable descriptor

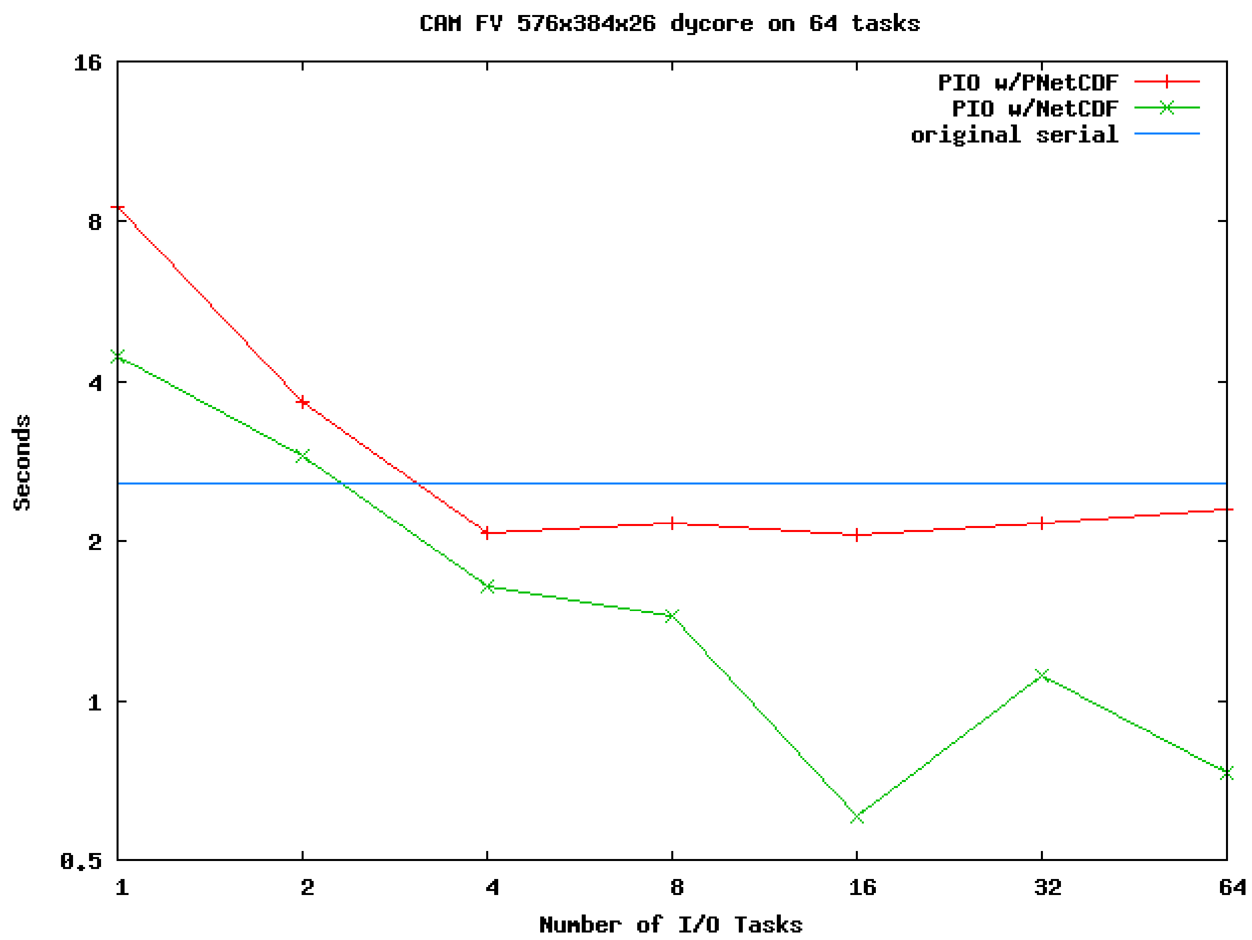
type (io_desc_t), intent(inout) :: iosystem

intent(in) :: array ! array to be read currently integer, real*4 and real8 types are supported, 1 dimension)

integer, intent(out) :: iostat ! error return code

No fillval needed in this direction (holes not modified)

PIO in CAM



CAM FV 576x384x26 dycore on 64 tasks
PIO w/PNetCDF
PIO w/NetCDF
original serial
Seconds
16
8
4
2
1
0.5
1
2
4
8
16
32
64
Number of I/O Tasks

PIO Success Stories

- PIO implementation in CCSM
  - Atmosphere: read and write history and restart; all dycores
  - Ocean: read and write history and restart
  - Land: write history
  - Sea Ice and Coupler: in progress

- PIO being used in high-resolution coupled model.

- Backwards-compatible NetCDF mode has value-added
  - Rearrangement to IO proc subset followed by gather/write one piece at a time.
  - Avoids overflowing memory of root processor

PIO success stories

- High resolution atmosphere model test cases with the HOMME dynamical core.

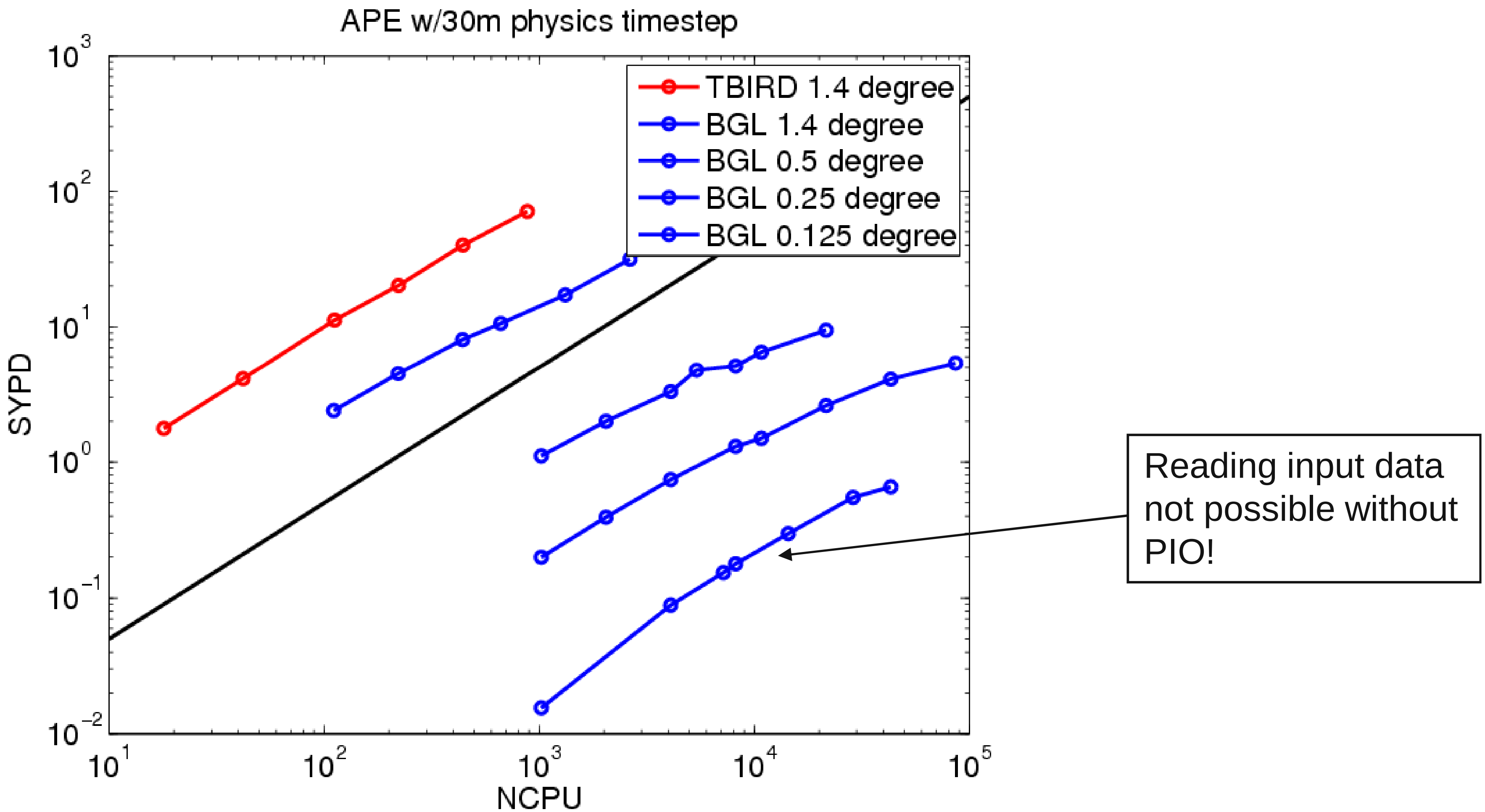


Figure provided by Mark Taylor, Sandia National Lab

CAM-HOMME on BG/P

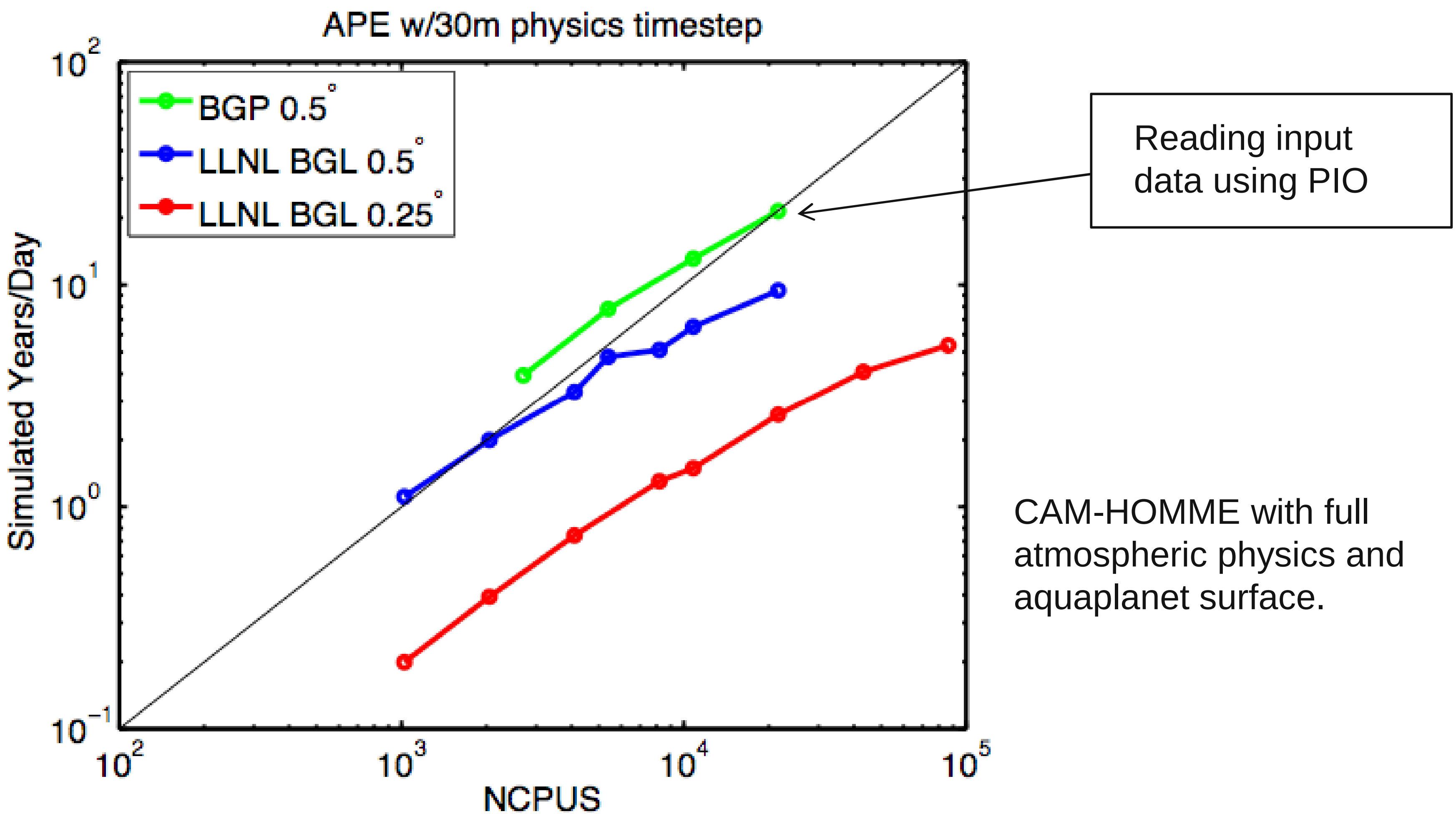


Figure provided by Mark Taylor, Sandia National Lab

CAM-HOMME with full atmospheric physics and aquaplanet surface.

PIO Deployment

- Developed configure system for portability across all CCSM platforms and sites.
  - Supports a large set of options (Enable/disable MCT,Parallel NetCDF,NetCDF,MPI-IO,serial compatibility,MPI-2,diagnostic modes,...)
- In current use on
  - Argonne BG/L, Intrepid (BG/P), Jazz (Intel,Linux)
  - Blueice (Power5+,AIX), Bangkok (Intel,Linux)
  - Jaguar (Opteron,XT4)
  - Sandia cluser (Intel+Infiniband)
- PIO currently developed within CCSM repository
  - Transitioning development to Google Code

Future work

- Clean up documentation
- More unit tests/ system tests
- Understanding performance across zoo of parallel I/O hardware/software
- Add to rest of CCSM
- You will soon be able to download, use and help develop PIO!
  - http://code.google.com/p/parallelio