Improving I/O Performance of the Weather Research and Forecast (WRF) Model

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Agenda

- **Numeric prediction models become increasingly complex as size and availability of HPC resources increase**
  - Forecast accuracy improves
  - Simulations at grid resolutions < 2km over entire globe can generate terabytes of weather information written frequently over forecast cycle
  - Increased demands on I/O subsystems creates performance bottlenecks
- **WRF offers a range of different I/O options**
  - How do we use the asynchronous and parallel I/O features of WRF to best take advantage of a Cray Lustre parallel file system and Cray MPI-IO?
- **Initial results using DataWarp**
- **Summary and Q&A**

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WRF Background (wrf-model.org)

- **Collaborative project by NCAR, NOAA, NCEP, Air Force Weather Agency, NRL, University of Oklahoma, and the FAA**
- **Regional to global scale numerical weather prediction model for both research and operational forecast systems**
- **Suitable for broad range of meteorological applications across scales from meters to thousands of kms**
- **Used by weather agencies all over the world, e.g., by NOAA for primary regional forecast model for 5 days ahead**
- **Open source, over 10,000 registered users**
- **Designed to perform well on massively parallel computers**
  - Uses MPI and OpenMP
  - Written in Fortran90
  - Components have been ported to GPUs and to Intel MIC

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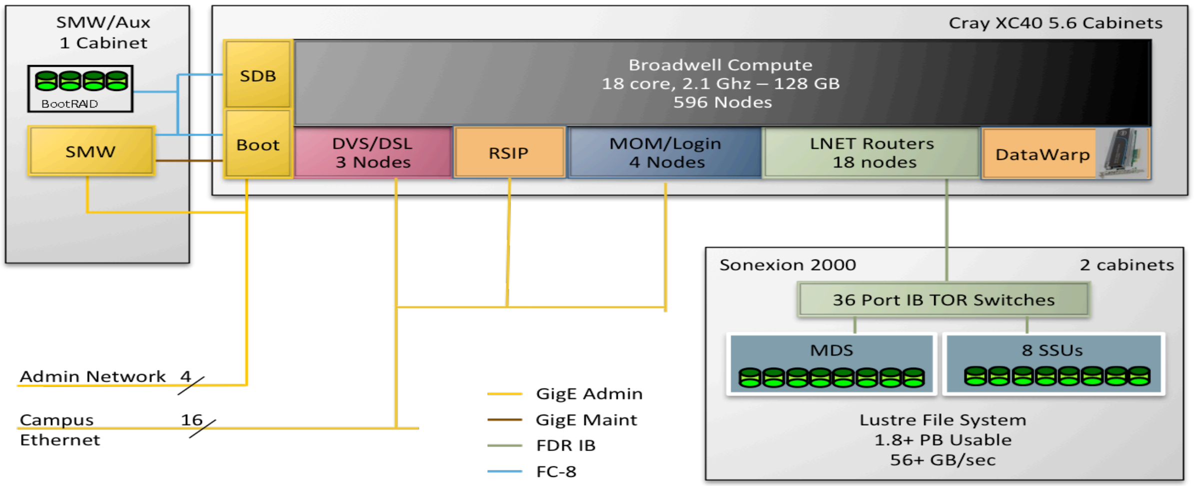
Benchmark System (Cray XC40)

- Intel Broadwell processors (18-core, 2.1ghz)
- 128GB DDR4 (2400mhz) memory per node
- Sonexion 2000 storage, 16 Lustre OSTs
- Also: Cray DataWarp storage (3 nodes)

See paper for more detail



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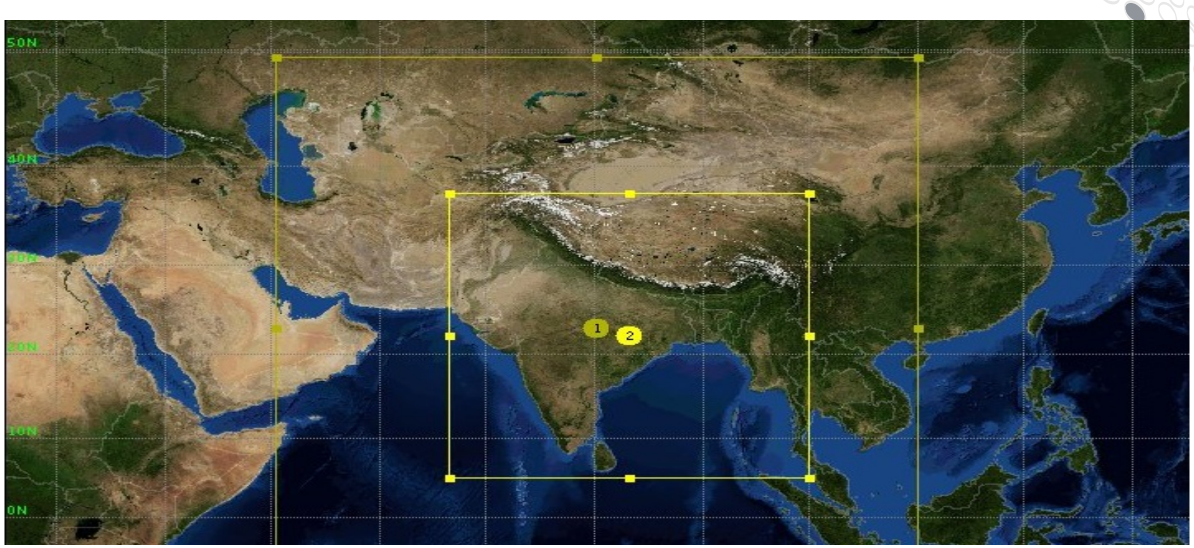
WRF Benchmark Configuration

Typical high-resolution configuration used by weather services

- Southeast Asia
- Two nested domains, 3km and 1km
  - Dom1: 1770x1986
  - Dom2: 2974x3118
- 28 vertical levels



- 30 minute simulation
- 5 second timestep
- History files written every 15 mins by each domain
  - Dom1: 19.8GB per output step
  - Dom2: 7.5GB per output step

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WRF I/O Implementations....

1. Serial NetCDF (default)

- Set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data
- Common data format used in environmental sciences
- Provided as part of Programming Environment on Cray XC

2. Parallel NetCDF

- Extension of NetCDF that supports parallel I/O
- Collaborative effort from Argonne and Northwestern University
- Implemented using Cray MPI-IO layer

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WRF I/O Implementations (cont.)

3. **Quilt Servers (output only)**
   - I/O servers increasingly common feature in weather/climate codes
   - Asynchronous I/O
   - Assign number of ranks for I/O only in groups
   - Serial NetCDF writes within server groups

4. **Quilt Servers with Parallel NetCDF (output only)**
   - As above but with parallel writes within groups
   - Implemented by Andrew Porter, STFC Daresbury Lab (cf. 2010 CUG paper)

Main focus on output I/O only in what follows....

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1. Serial NetCDF

- **Writing a file:**
  - All data gathered onto master MPI rank 0 using mpi_gatherv
  - Rank 0 reconstructs data array and writes to disk using serial NetCDF library
  - All other ranks block, stalling the computation, until write is complete
    - “Effective” write time as seen by compute ranks includes gather and formatting as well as actual disk write

- **Drawbacks:**
  - Easy to use, good for small rank counts, but....
  - Rank 0 requires lots memory (though can use MPMD to place it on its own node)
  - Overhead of mpi_gatherv rapidly becomes huge bottleneck at higher MPI rank counts
  - MPI/OpenMP hybrid mode can help, but eventually need another solution....

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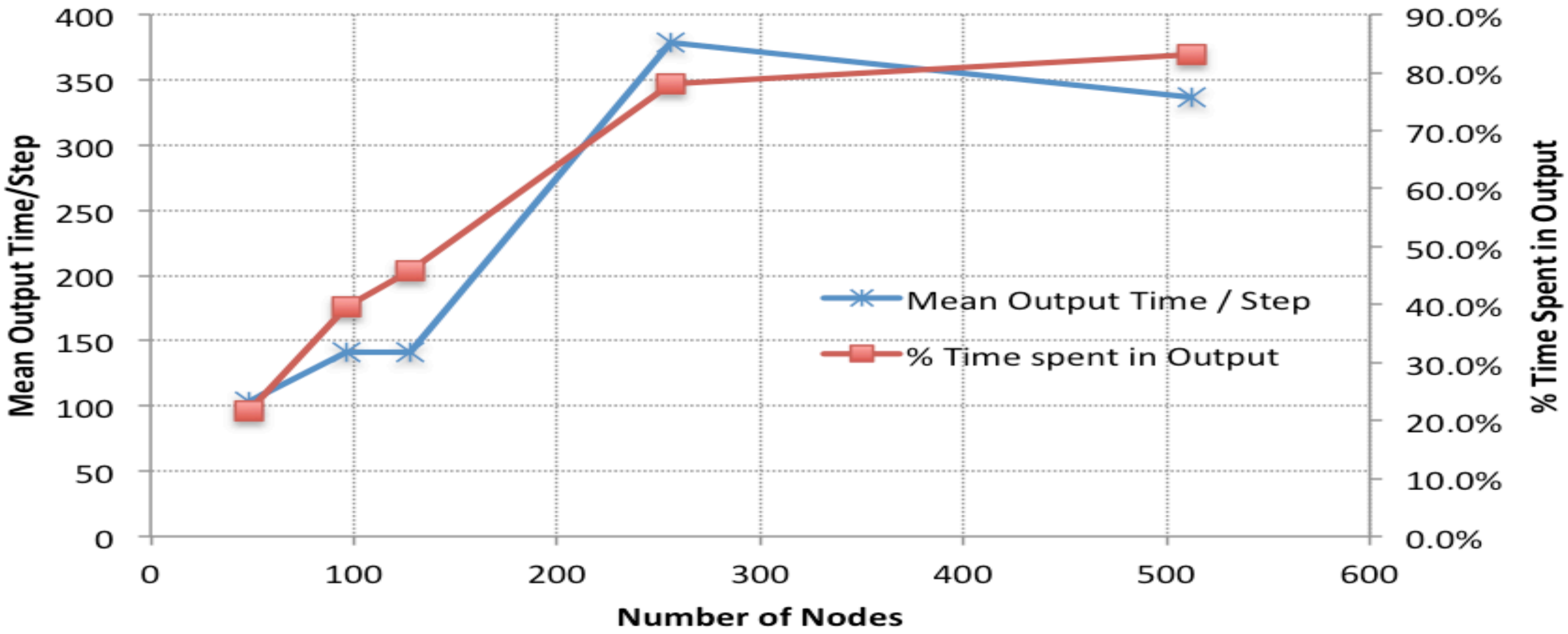
Serial NetCDF - overhead



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2. Parallel NetCDF

- **Compile with parallel NetCDF enabled and set in input namelist at runtime**
- **MPI ranks aggregated into groups**
  - Number of groups = Lustre stripe count of input/output file
  - Or can be set via MPI-IO hints. For example:
    - *export MPICH_MPIIO_HINTS= "wrfout*:striping_factor=16"*
  - One aggregator from each group writes to file
  - Reduces gather time and contention
    - Cray MPI-IO is optimized to align I/O with parallel file system striping
    - Cray MPI-IO collective buffering assigns one aggregator per OST and spreads aggregators out evenly across the nodes
    - More OSTs available = more parallelism possible
- **Cray MPI-IO layer on the XC provides useful environment variables to control diagnostics.....**

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MPICH_MPIIO_AGGREGATOR_PLACEMENT_DISPLAY=1

```
Aggregator Placement for wrfinput_d01
RankReorderMethod=3  AggPlacementStride=-1
 AGG    Rank       nid
 ----  ------  --------
    0       0  nid00016
    1     434  nid00041
    2     868  nid00125
    3    1302  nid00221
    4    1736  nid00245
    5    2170  nid00269
    6    2604  nid00293
    7    3038  nid00317
    8      18  nid00349
    9     452  nid00373
   10     886  nid00773
   11    1320  nid00797
   12    1754  nid00821
   13    2188  nid00845
   14    2622  nid00869
   15    3056  nid00893
```

Shows:

- How many aggregators have been assigned
- Whether rank reordering was used
- MPI rank numbers of assigned aggregators
- Node NID numbers of assigned aggregators

Note the spreading of aggregators among the MPI ranks and the nodes

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MPICH_MPIIO_HINTS_DISPLAY=1

```
PE 0: MPIIO hints for wrfoutput_d01:
cb_buffer_size                        = 16777216
romio_cb_read                         = automatic
romio_cb_write                        = automatic
cb_nodes                  = 16
cb_align                  = 2
romio_no_indep_rw         = false
romio_cb_pfr                          = disable
romio_cb_fr_types         = aa
romio_cb_fr_alignment     = 1
romio_cb_ds_threshold = 0
romio_cb_alltoall         = automatic
ind_rd_buffer_size        = 4194304
ind_wr_buffer_size        = 524288
romio_ds_read             = disable
romio_ds_write            = disable
striping_factor           = 16
striping_unit             = 1048576
romio_lustre_start_iodevice = 0
direct_io        = false
aggregator_placement_stride = -1
abort_on_rw_error         = disable
cb_config_list            = *:*
romio_filesystem_type     = CRAY ADIO:
```

Look out for the value of cb_nodes – if not equal to the expected number of aggregators (stripes), we have a problem!

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MPICH_MPIIO_STATS=1

```
+-----------------------------------+
| MPIIO read access patterns for
| wrfinput_d01
|   independent reads       = 1
|   collective reads        = 457452
|   independent readers     = 1
|   aggregators             = 16
|   stripe count            = 16
|   stripe size             = 1048576
|   system reads            = 7727
|   stripe sized reads      = 7512
|               total bytes for reads = 7964753971
|                                     = 7595 MiB = 7 GiB
|   ave system read size    = 1030769
|   number of read gaps     = 1
|   ave read gap size       = 1
| See "Optimizing MPI I/O on Cray XE
| Systems" S-0013-20 for explanations.
+-----------------------------------+
```

For best performance, we want many collective reads, few independent reads, and few gaps.

Try MPICH_MPIIO_STATS=2 for much more performance information including a timeline and data to generate bandwidth charts.

man intro_mpi

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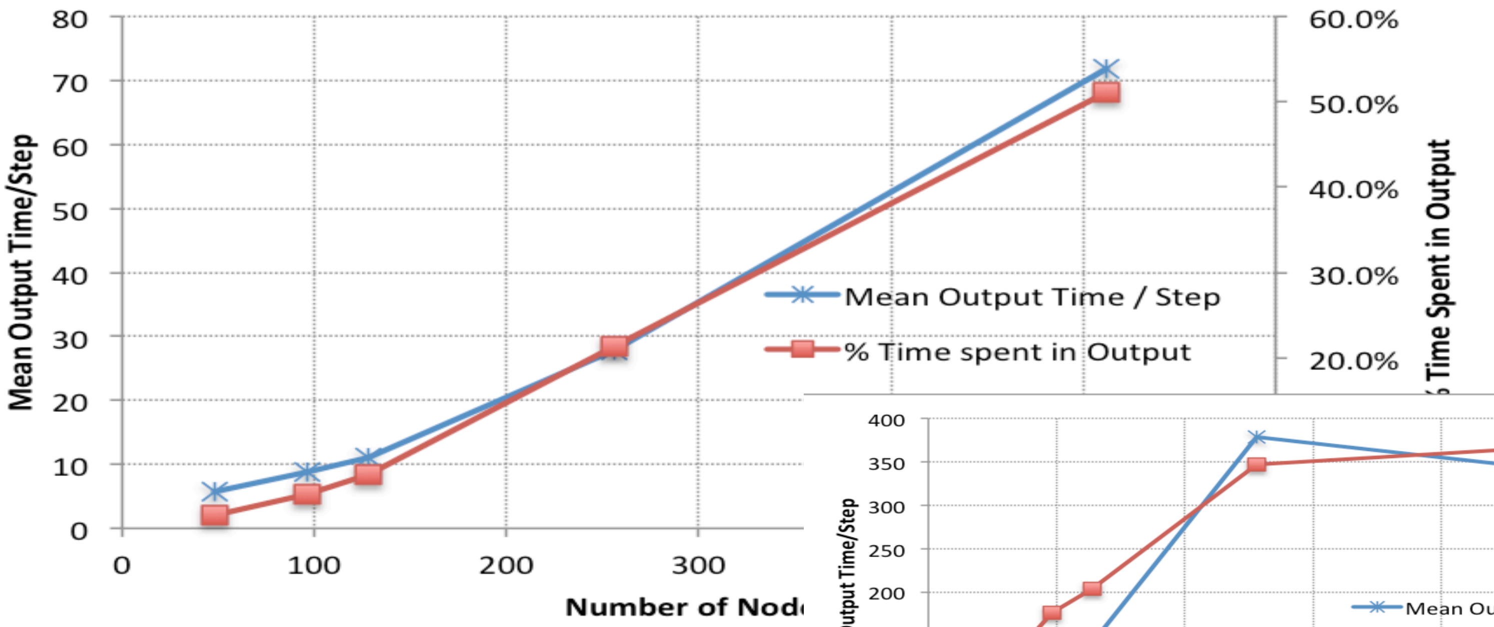
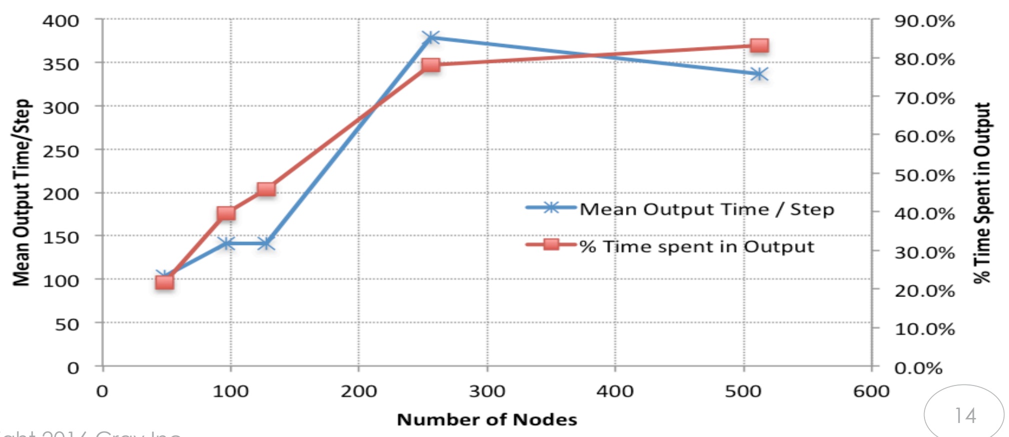
Back to WRF and Parallel NetCDF...





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3. Quilt Servers (asynchronous I/O)

- **Quilt servers deal exclusively with I/O**
  - Groups of compute ranks are mapped onto quilt servers as evenly as possible
    - Ideally have equal numbers of ranks per server [much more important in next method]
  - Send data to assigned I/O server then continue with integration while data is formatted and written to disk asynchronously
- **Select via input namelist nio_groups of I/O servers and nio_tasks_per_group servers per group**
  - One group can only work on one output frame at a time
  - Need more than one group if write more than one frame per step (e.g. multiple domains, restart + history, etc.)
  - Need more than one group if next output step is reached before previous write is finished otherwise all ranks have to wait
- **"Effective" write time seen by compute ranks is now minimal (<1s)**
- **Actual time to write to disk much higher as performed serially by each I/O group**

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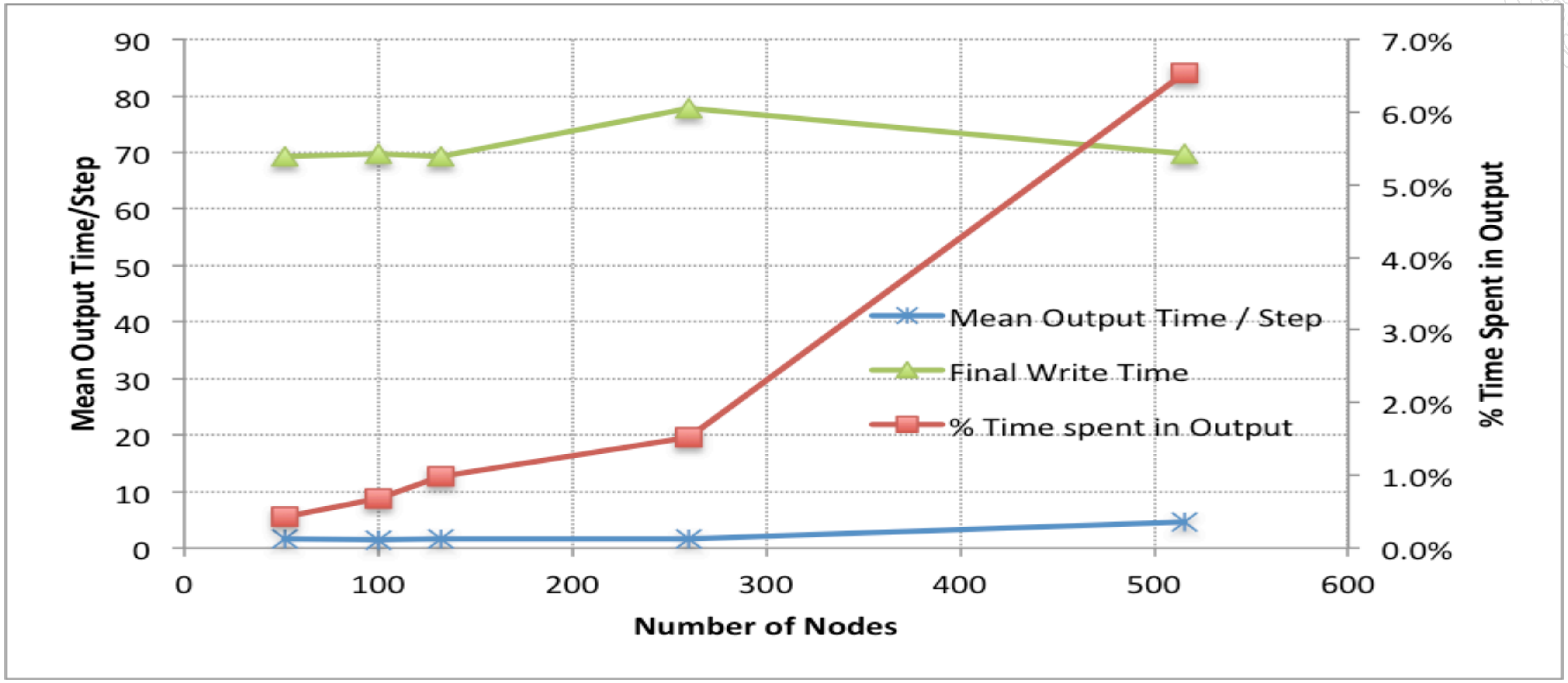
Quilt Servers – Output overhead



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Quilt Servers: Drawbacks

- **Final write step is slow as cannot be overlapped**
  - This might not matter for a long simulation, but can overwhelm shorter forecasts or benchmarks
  - Can affect ensemble runs
  - Effect worsens at higher total rank counts
- **I/O servers require much more memory than compute ranks and so can only assign a few per node**
  - Use ALPS MPMD to achieve this (see paper)
- **Need more and more I/O groups if time between output steps decreases, e.g.,**
  - More MPI ranks so faster compute times
  - Frequent output required (e.g. severe thunderstorm forecasting)
- **... So need to assign more and more nodes to I/O**
- **What if we could speed up the output within each quilt server group?**

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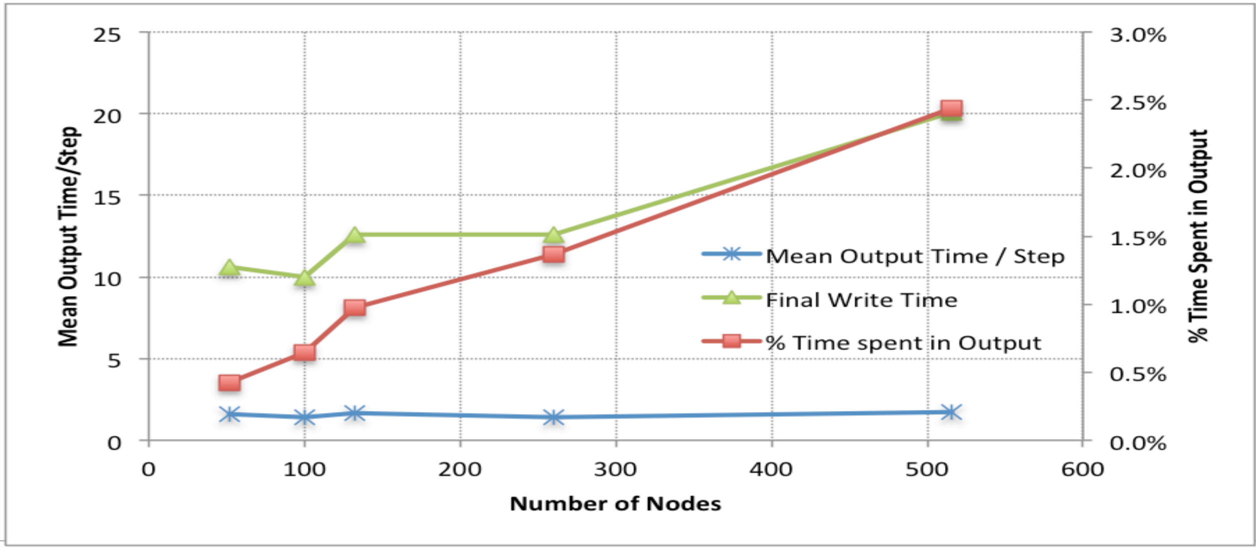
... We can! 4. Quilt Servers PLUS Parallel NetCDF

- **Percentage of time spent in output now below 3% AND final write time much lower than in previous case**
  - Wallclock time to complete forecast under half that of serial case
  - Allows more frequent output and higher scaling
  - Can handle short runs better



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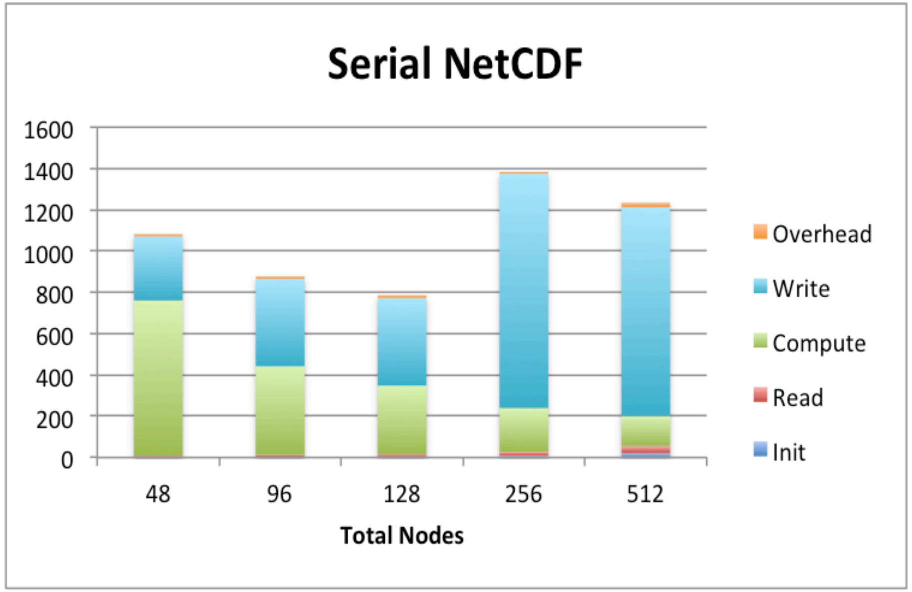
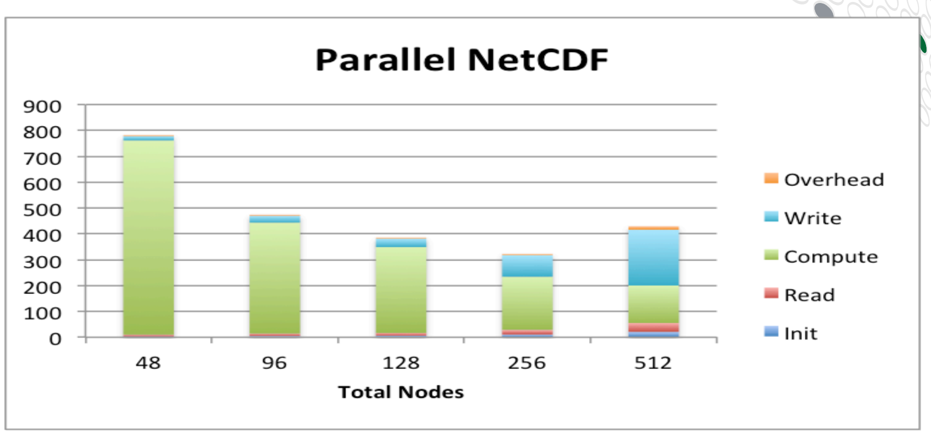
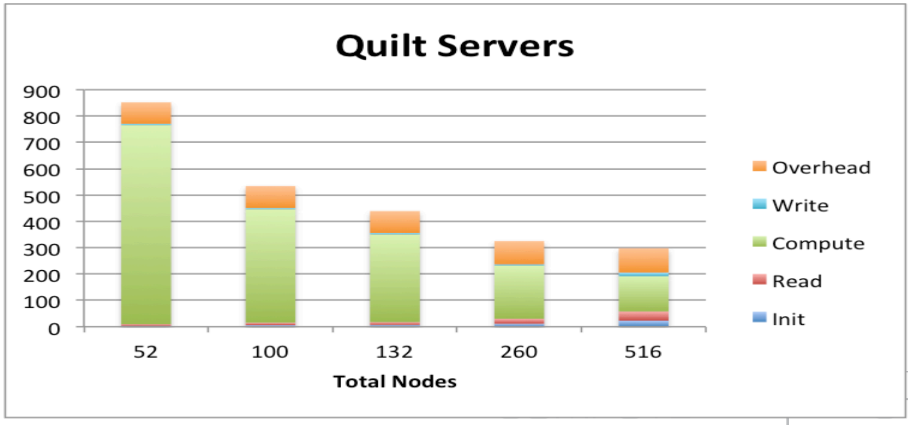
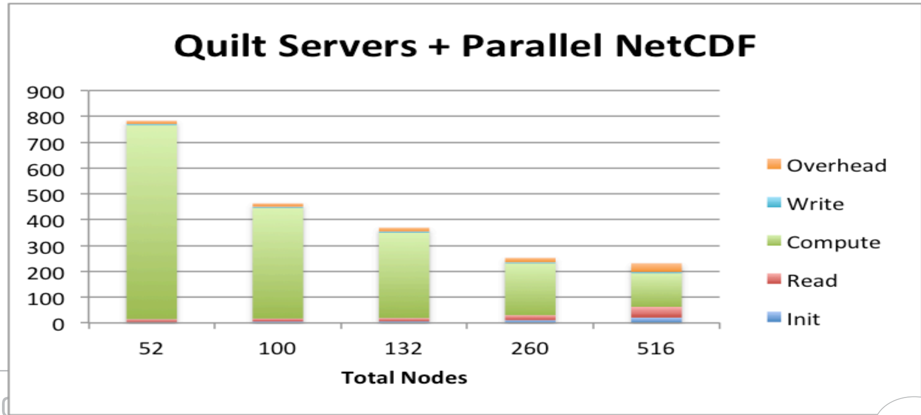
Final Comparison









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Initial observations on WRF with Cray DataWarp

- **SSD-based hardware (two Intel P3608 SSD per node)**
  - Lower cost than Lustre (comparing SSU to DW), higher reliability
- **Cray-developed software, integrated with SLURM and other WLMs**
- **Input file pre-staged to DataWarp and output history files staged to permanent Lustre storage at end of run**
  - Preprocessing output or periodic restart files could be kept in scratch and not staged in or out
- **Directives to stage files are parsed by WLM (see paper for more)**

  #DW jobdw type=scratch access_mode=striped capacity=1150GiB

  #DW stage_in type=file source=INPUT/wrfinput_d01 destination=$DW_JOB_STRIPED/wrfinput_d01

  #DW stage_out type=file destination=OUTPUT/wrfout_d01_2015-03-10_00_00_00 source=$DW_JOB_STRIPED/wrfout_d01_2015-03-10_00_00_00
- **Compared 3 DataWarp nodes against 3 and 16 Lustre OST stripes**
  - Ongoing studies at KAUST scaling up to 100 nodes and beyond

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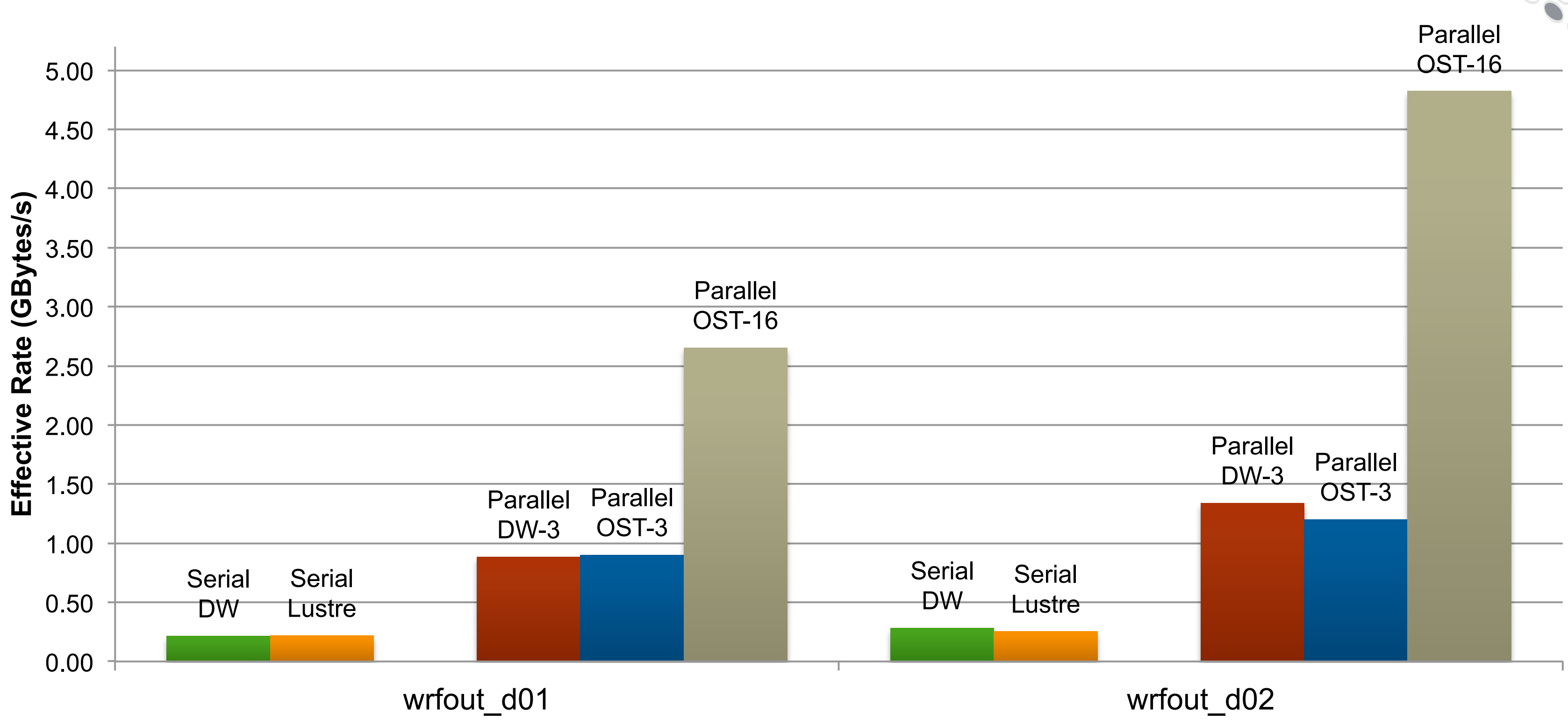
DataWarp/Lustre Comparison - Output



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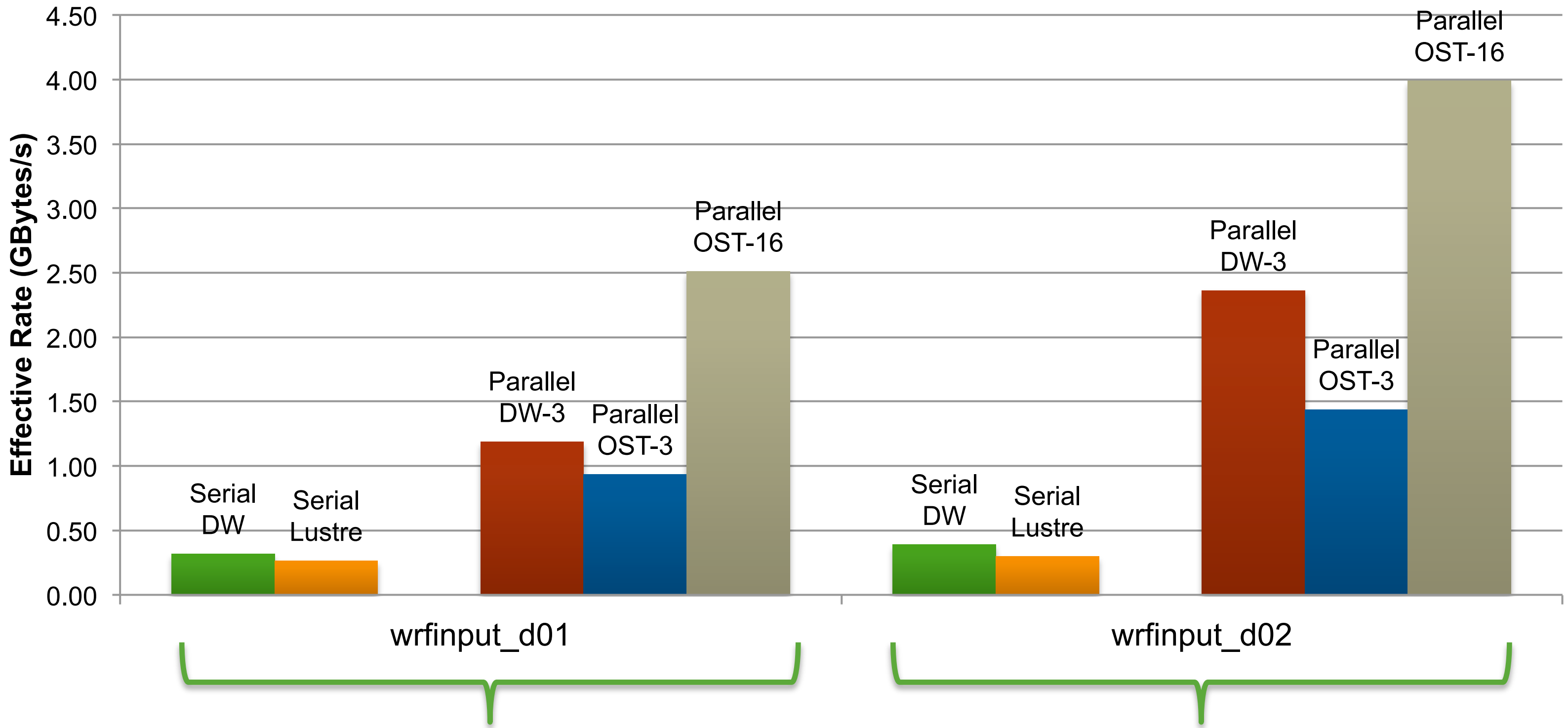
DataWarp/Lustre Comparison - Input



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Summary

- **I/O overhead can drastically limit scaling of WRF to higher core counts and higher output frequencies**
- **Existing methods, especially parallel NetCDF + quilts can effectively hide much of the I/O overhead and enable realistic scaling**
  - Cray MPI-IO layer a great advantage on XC
- **Use of Parallel NetCDF + quilts can improve time to forecast compared to serial NetCDF by over 2x**
  - Method should be more widely used! See paper for hints on usage.
- **Cray DataWarp could be a great option for WRF I/O**
  - Not only for forecast input and output, but as scratch storage during pre and post processing over an entire workflow

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Q&A

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