Argonne NATIONAL LABORATORY

parVis

U.S. DEPARTMENT OF ENERGY | Office of Science

Update on progress
(since Sept 30, 2011)

ParVis team

4th ParVis All-Hands meeting

March 22-23, 2012

Argonne National Laboratory

NCAR NATIONAL CENTER FOR ATMOSPHERIC RESEARCH | Sandia National Laboratories | Pacific Northwest NATIONAL LABORATORY | UCDAVIS UNIVERSITY OF CALIFORNIA | U.S. DEPARTMENT OF ENERGY

Progress made in all ParVis areas:

- Developing new Parallel Climate Analysis Library (**ParCAL**) and developing a parallel version of NCL (**ParNCL**) with it for DAV of ultra-large climate data sets.
  - Using DOE ASCR software such as MOAB (for grids) and Intrepid (for gradient operations) and PNetCDF (for parallel I/O).

- Speeding up current diagnostic workflows with Swift-based task parallelism.

- Taking advantage of hardware opportunities (GPU's, clouds) and avoiding limitations (disk space).

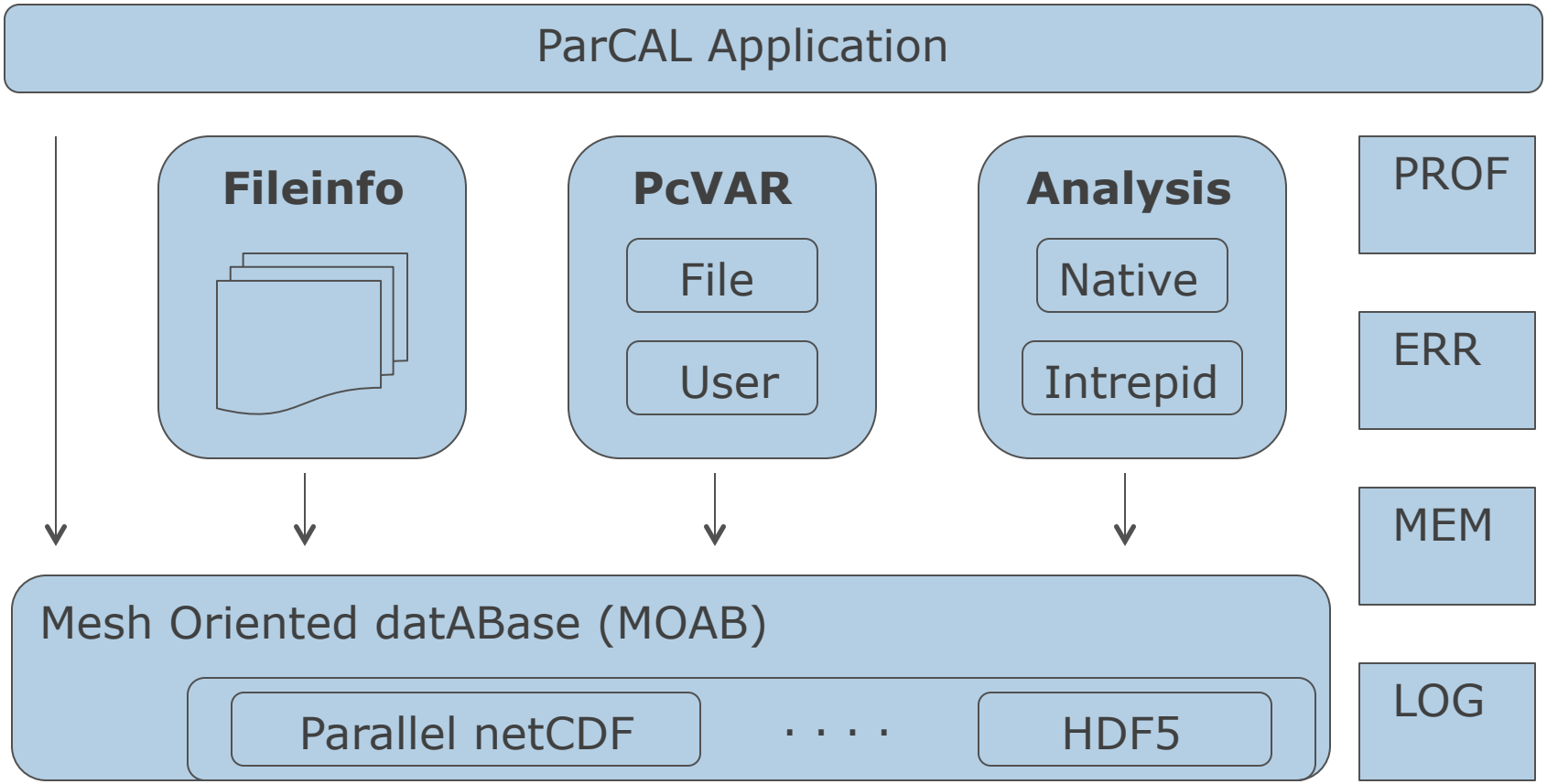
ParCAL: Parallel Climate Analysis Library

- Being built using PnetCDF, MOAB and Intrepid
  - MOAB and Intrepid have already solved the hard problem of how to represent and operate on structured and unstructured grids distributed over processors.

- Provides data-parallel core to perform typical climate post-processing currently done by either NCL or NCO.

- **Will be able to handle unstructured (CAM-SE (HOMME) and semi-structured grids in all operations (e.g. "zonal average") by building ParCAL on MOAB and Intrepid. Will support parallel I/O by using PnetCDF.**

ParCAL Architecture



Development with Intrepid (a component of ParCAL)

- Divergence and vorticity
  - developed parallel versions using Epetra package from Trilinos
  - will update current ParCAL implementation with new tag_reduce functionality from MOAB
- Streamfunction and velocity potential
  - implemented with Intrepid for global velocity fields
  - investigating approach for limited domains
  - will incorporate into ParCAL
- Irrotational and non-divergent velocity components
  - implementation underway

Calculating Streamfunction and Velocity Potential with Intrepid

- The finite element method is used to solve the following weak equations for streamfunction and velocity potential using Intrepid

$$\int \nabla\psi \cdot \nabla\varphi \, d\Omega = \int \mathbf{v} \cdot (\mathbf{k} \times \nabla\varphi) d\Omega$$

$$\int \nabla\chi \cdot \nabla\varphi \, d\Omega = \int \mathbf{v} \cdot \nabla\varphi d\Omega$$

- Periodic boundary conditions along the latitudinal boundary and Neumann boundary conditions at the poles are used

$$\int_\Gamma \left(\frac{\partial\chi}{\partial n} - \mathbf{v} \cdot \mathbf{n} \right) d\Gamma = 0 \qquad \int_\Gamma \left(\frac{\partial\psi}{\partial n} - \mathbf{v} \cdot \mathbf{t} \right) d\Gamma = 0$$

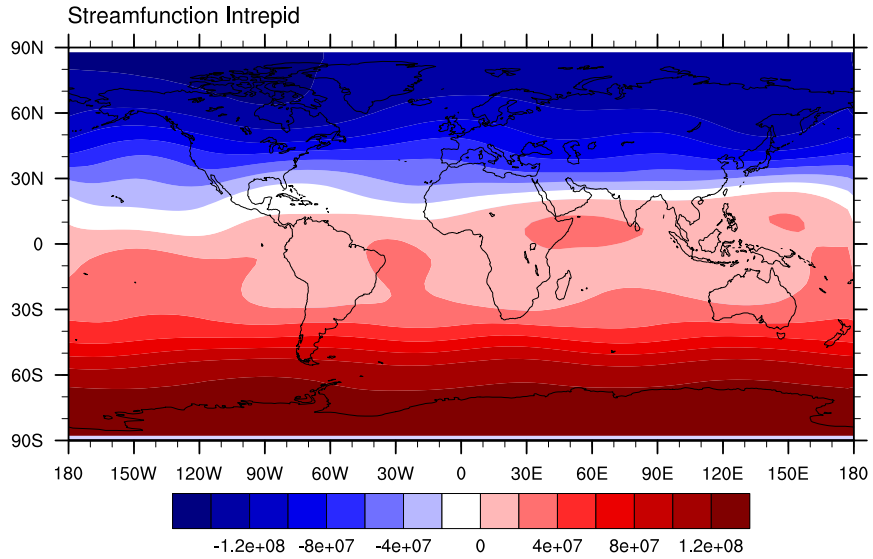
- The weak equations hold on arbitrary subdomains thereby enabling calculations from regional velocity data

- Intrepid can support solution of these equations on triangles and quads and eventually on polygons.

Calculating Streamfunction with Intrepid

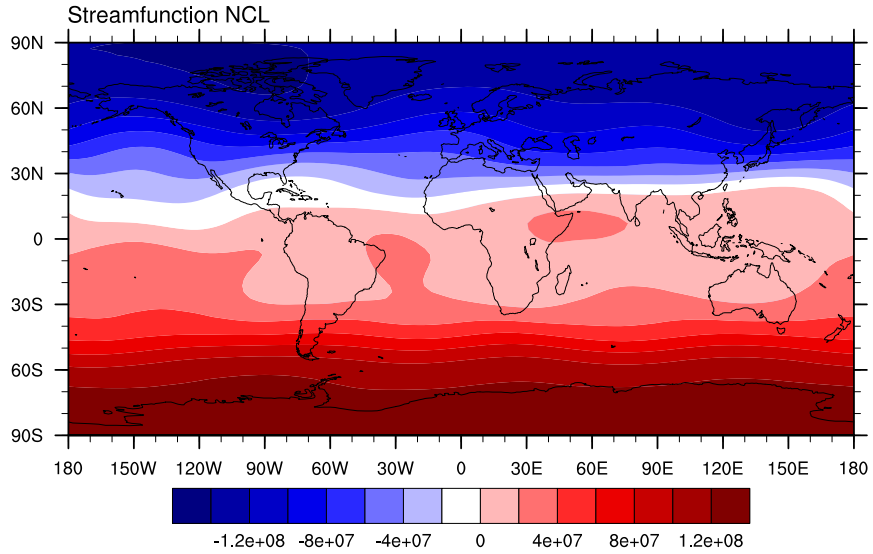
Intrepid

finite element method



NCL (uv2sfvpG)

spherical harmonics



$$\nabla^2 \psi = \nabla \times \mathbf{v}$$

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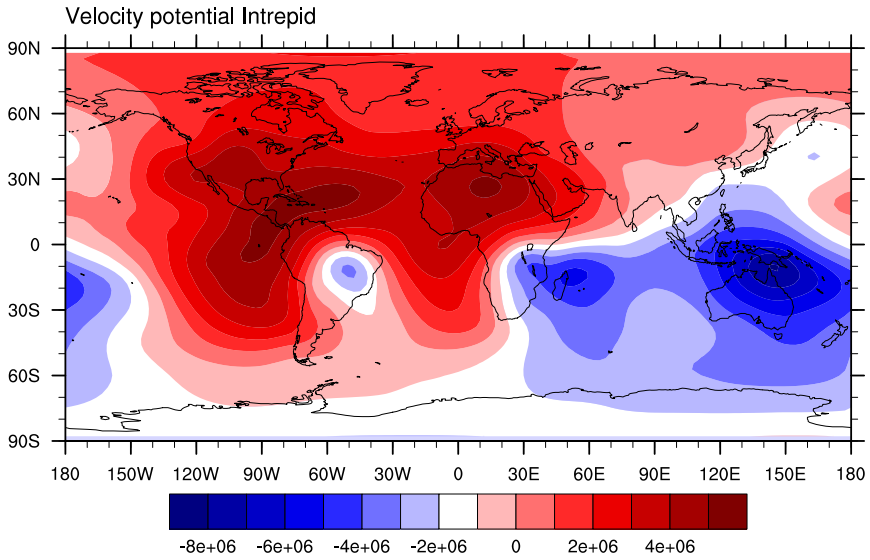
Calculating Velocity Potential with Intrepid

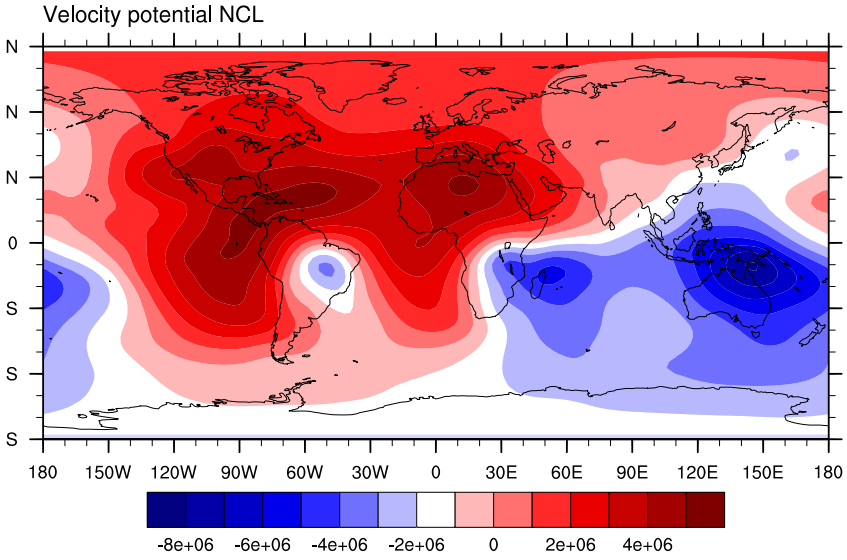
Intrepid

finite element method



NCL (uv2sfvpG)

spherical harmonics



$$\nabla^2 \chi = \nabla \cdot \mathbf{v}$$

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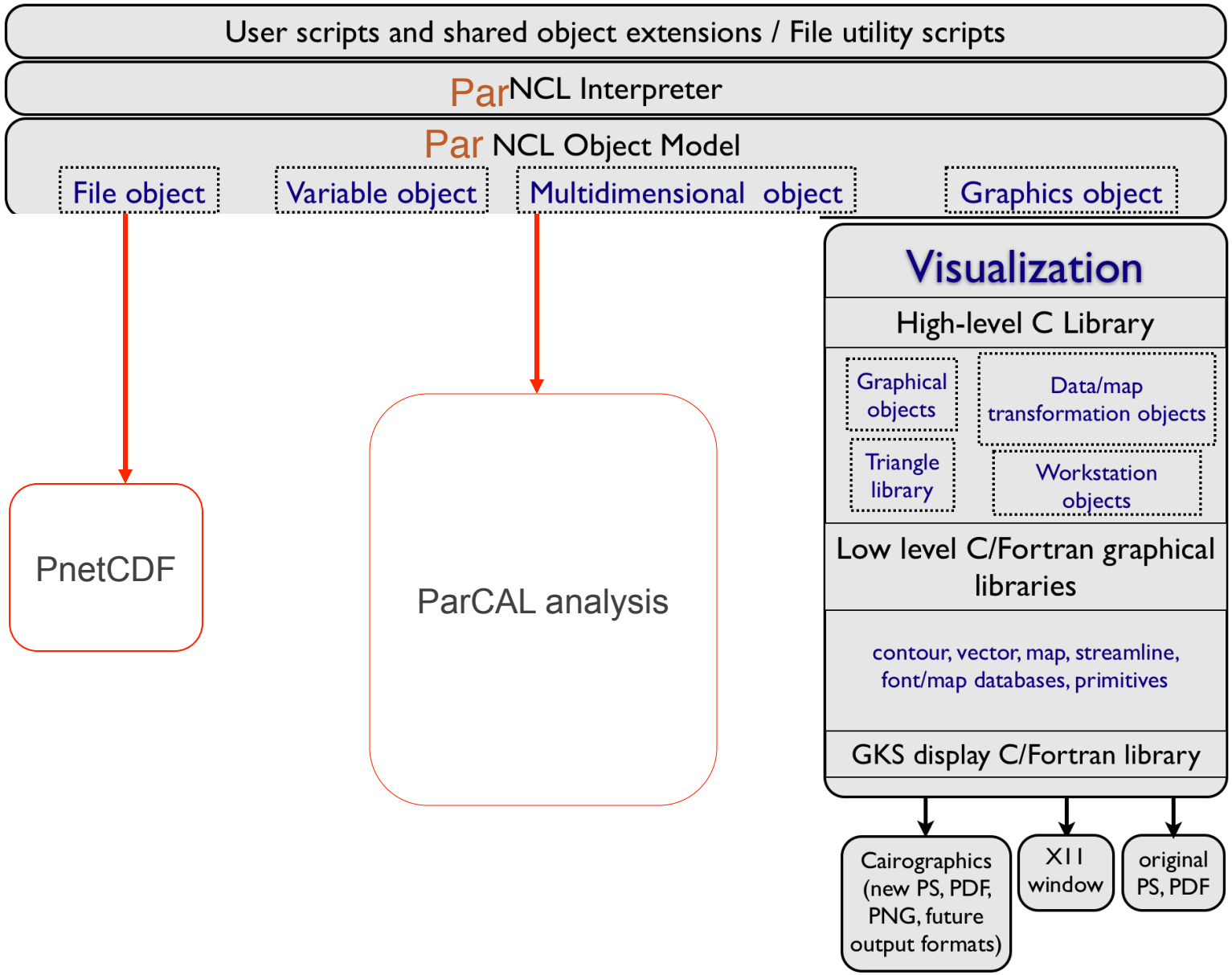
ParCAL Development

- Integrated Intrepid-based algorithms into ParCAL
  - divergence, vorticity
- Updated algorithms to use MOAB partition method (SQIJ)
  - Gather (internal to ParCAL), NCL functions dim_avg_n, max, min
- Implemented new NCL algorithms
  - dim_max_n
  - dim_min_n
  - dim_median_n
- Miscellaneous items
  - Added tests of different dimensions (time, lev, lat, lon) for all *_n algorithms
  - Added more test configurations to nightly build/test system
  - Added support within MOAB and ParCAL to read global and variable attributes
  - Updated installation documentation and README
  - Removed all of the warnings generated by GNU g++ compiler

ParCAL Function Table

NCL function Group	NCL Functions	ParCAL Function
File IO	addfile, addfiles	fileinfo, pcvar
Spherical Harmonic Routines	dv2uv* (4 funcs)	divergence
Meteorology	uv2dv_cfd	divergence
Spherical Harmonic Routines	uv2dv* (4 funcs)	divergence
Meteorology	uv2vr_cfd	vorticity
Spherical Harmonic Routines	uv2vr* (4 funcs)	vorticity
Spherical Harmonic Routines	uv2vrdv* (4 funcs)	vorticity, divergence
General Applied Math	dim_avg, dim_avg_n	dim_avg_n
General Applied Math	dim_max, dim_max_n	dim_max_n
General Applied Math	dim_min, dim_min_n	dim_min_n
General Applied Math	dim_median, dim_median_n	dim_median_n
General Applied Math	max	max
General Applied Math	min	min
Variable Manipulators	delete	pcvar
		gather

ParNCL architecture



ParNCL (Progress update)

- ParNCL supports addfiles(), NCL's multi-format file reader
  - Time slices of the variable read from file works
  - Need to test all corner cases
  - Only reads NetCDF for now (using PNetCDF).
- ParNCL supports calculating vorticity
  - Based on the current implementation in ParCAL
  - Specifically, duplicating function of uv2vrG_Wrap()
  - Adding support for other variations should be trivial from ParNCL perspective
- Simple math operations on distributed multidimensional variables work
  - abs, cos, asin, atan*, cos, exp, fabs, floor, log
  - Need to test more cases

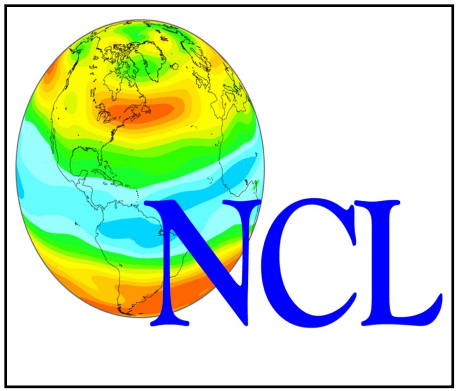
ParNCL (Progress update)

- Addition, subtraction of distributed multidimensional data works
- Scaling a distributed multidimensional array by a scalar works
- Build changes
  - Can build serial and parallel versions separately
  - Can disable profiling layer at build time and runtime
  - ParNCL executable is now named “parncl”

NCL Version 6.1.0-beta update

Scheduled mid-to-late April 2012

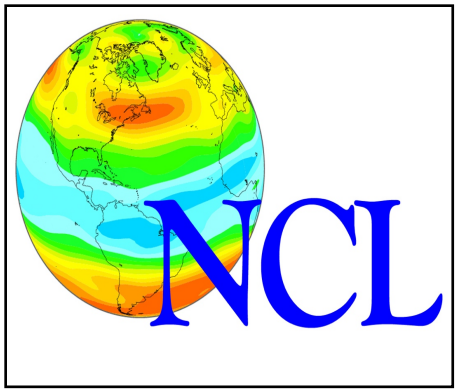
- Main features:
  - Overhaul of display model to allow for 32-bit color (RGBA versus RGB), transparency, > 256 color maps
  - Significant improvements made to raster-drawing algorithm
  - Interface to Earth System Modeling Framework (ESMF) regridding capabilities will be included



New raster drawing features

- Rewrite of NCL raster plotting that promises a significant speed up (more than a factor of 40 in preliminary tests using simplified scenario).
- Direct plotting of data cells – quadrilaterals only at first, but hexagonal and triangular cells are in the planning stages.
- Continuous zooming from many data cells per pixel to many pixels per data cell.
- Each data cell independently rendered – **parallel support considered in design**.
- Intend to provide visualization capabilities suitable for data of interest to the ParVis project

- Preliminary version by 6.1.0 beta (hopefully)



Progress in Task-parallel diagnostics: Swift and AMWG

- **Swift-based AMWG diagnostics released to community!**
  - Officially part of version 5.3 of AMWG released in Feb, 2012.
  - Used daily at NCAR
  - Installed on Lens, the DAV cluster at OLCF.
  - Initial tests of using Pagoda (parallel) in place of NCO (serial)

- Swift package recent developments
  - Working on parallel invocation of multiple MPI and OpenMP applications (for using Pagoda in AMWG)
  - Solved problems with scheduling on Eureka (the DAV cluster at ALCF. Improved scheduling on BG/P and Cray.

Swift version of OMWG diagnostics

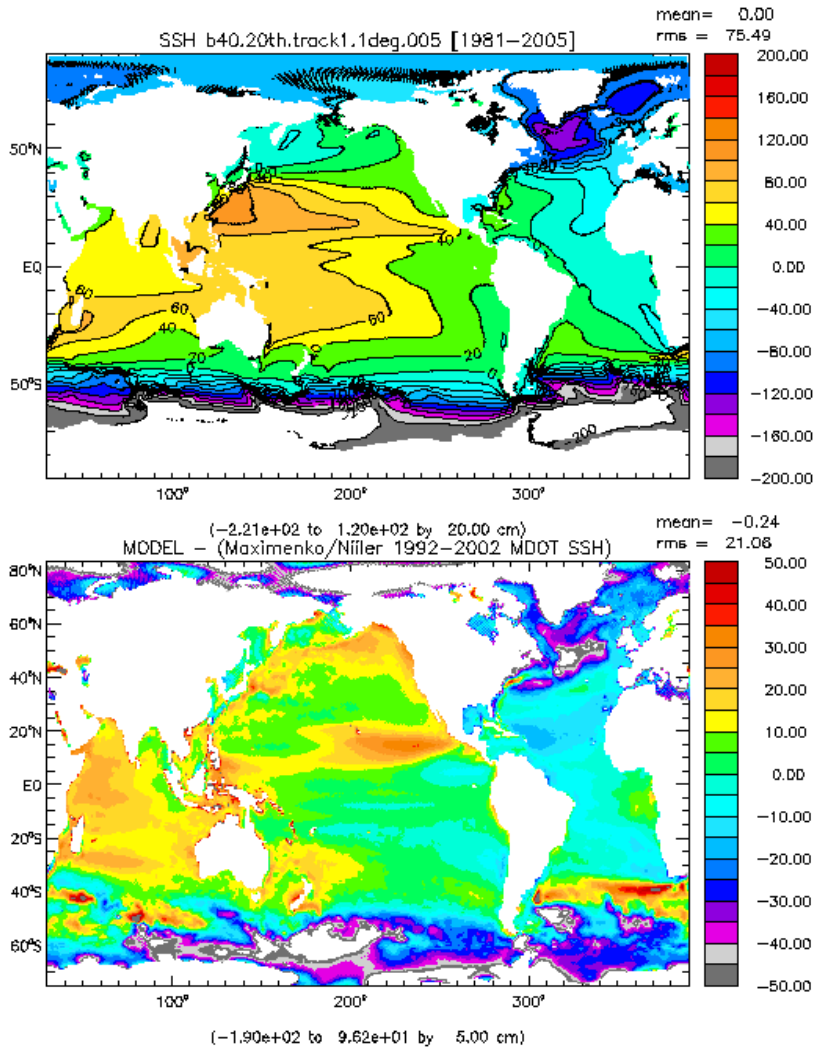
- Current OMWG diagnostics use non-free software.

- While building Swift version, convert to OMWG diags to all-NCL
  - 87 scripts converted from IDL to NCL
  - All three top-level OMWG control scripts modified to run NCL-based scripts exclusively
  - Graphics appear very similar with identical color table and level spacing to IDL graphics
  - Annotations are at least as original
  - Numerical output matches the original in all important respects
  - 2 routines written as Fortran shared objects for speed
  - Final testing and cleanup by end of April
  - For comparison, see NCL version at: http://www.ncl.ucar.edu/Applications/popdiag/pd.1981_2005/popdiag.html

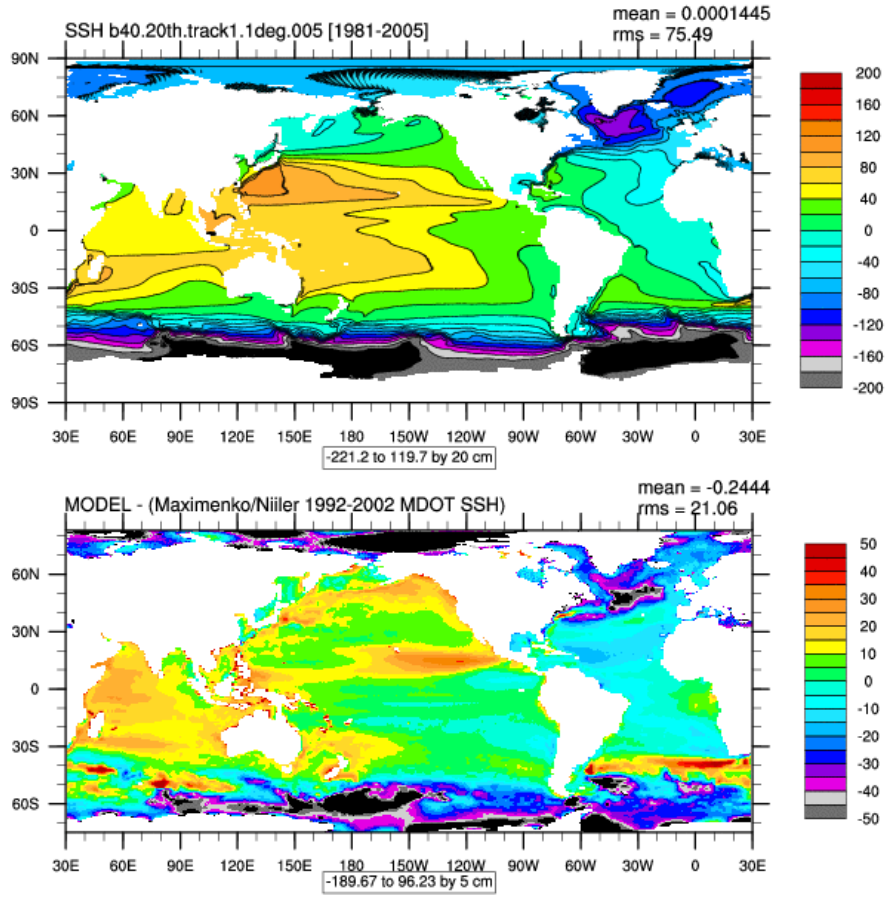
    vs. original version at http://www.cesm.ucar.edu/experiments/cesm1.0/diagnostics/b40.20th.track1.1deg.005/ocn_1981-2005-obs/popdiag.html
- Swift version being tested for many different file control options.
  - Already calling NCL scripts and can easily update to final versions.

OMWG diagnostics: Sea Surface Height

Original



NCL



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Cloud Computing paradigms: MapReduce

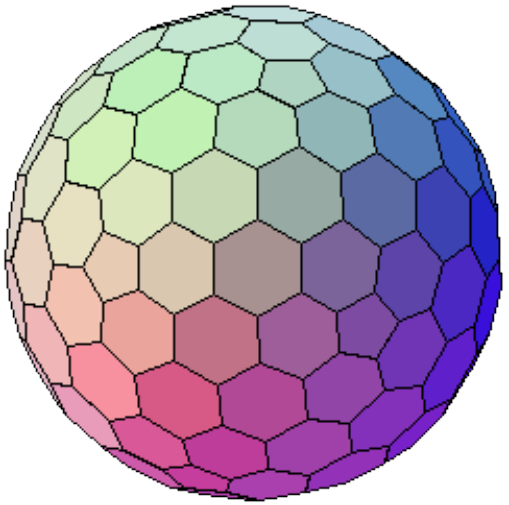
- Beginning of FY12: Working "Streaming Hadoop" prototype kernels for averaging
  - Testbed kernel for probability density function (PDF) estimation implemented; applied to problem of time-evolving PDF f(X,t) estimation
    - Publication: "Visualizing climate variability with time-evolving probability density functions, detecting it with information theory," to appear Workshop on Data Mining in Earth System Science, ICCS 2012
- FutureGrid (cloud computing resource) project granted, awaiting allocation to commence scalability tests and performance studies
- Paper "Mapping Climate Data Analysis onto the Map Reduce Programming Pattern" in preparation.

Using GPUs: Interactive Visualization of Large Geodesic Grid Data

Kwan-Liu Ma, UC Davis

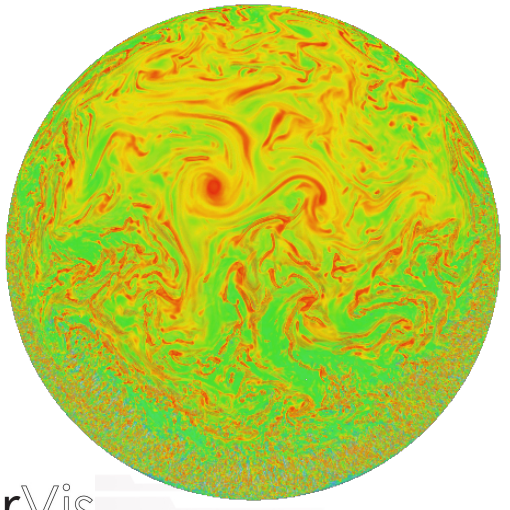
Existing 3D visualization solutions:

- Require a pre-partitioning of each hexagonal cell into multiple tetrahedral cells.
- Do not take advantage of latest GPU features
- Do not offer high-quality rendering



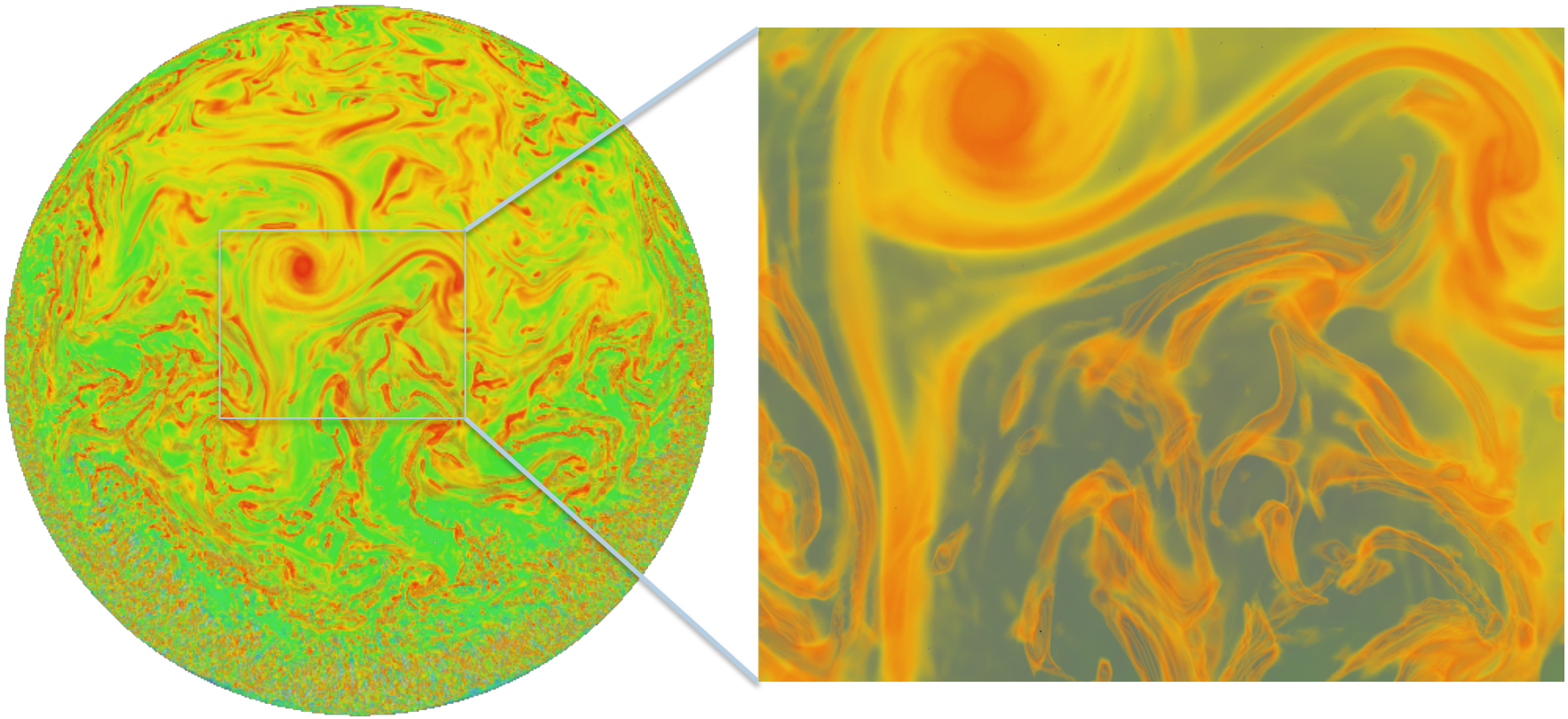
The UC Davis team seeks to provide:

- Advanced visualization of hexagonal grid data
- High quality 3D rendering
- GPU acceleration and parallelization to support Interactive interrogation



Interactive Visualization of Large Geodesic Grid Data

Kwan-Liu Ma, UC Davis



Data: CSU GCRM

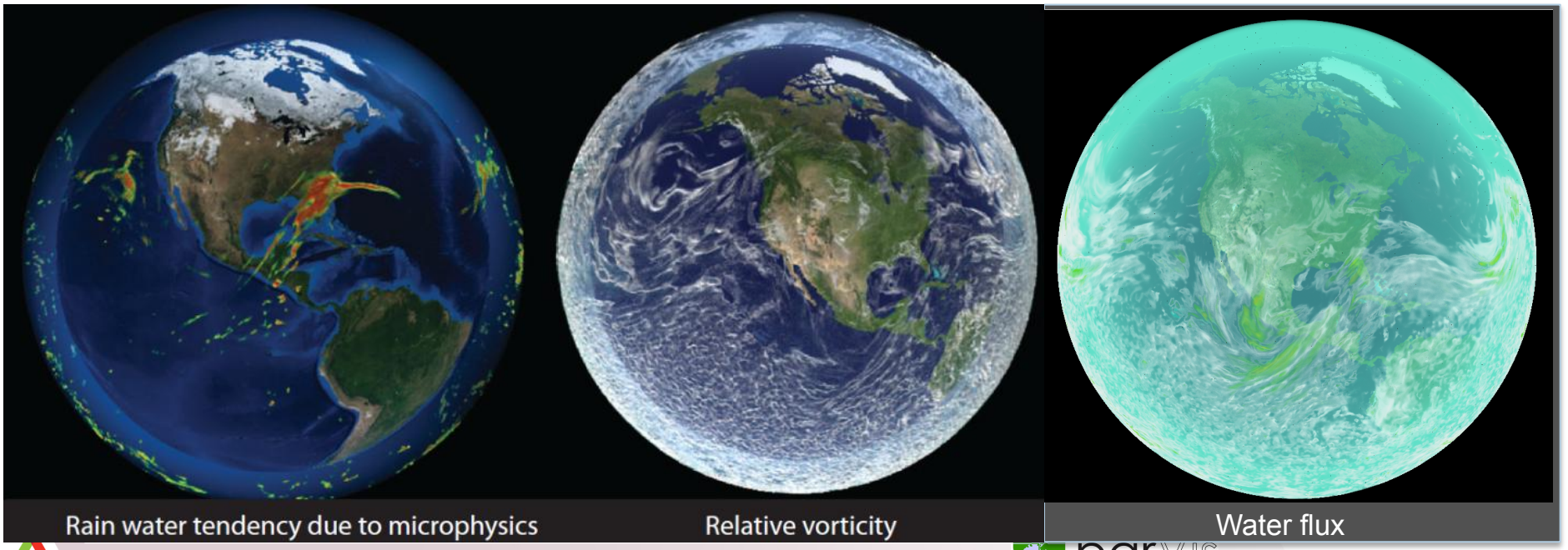
Interactive Visualization of Large Geodesic Grid Data

Kwan-Liu Ma, UC Davis

Further Work:

- Further optimizing performance
- Interactive interrogation
- Rendering on a GPU cluster
- Time-varying data visualization
- Working directly with the GCRM team
- In situ visualization

Data: CSU GCRM



Disk Space: Progress in Compression schemes

- Tested several compression schemes for climate data in first year.
- Need for compression is here now: Long run of 0.10 POP at NCAR has to output less data because can't fit on disk.
- Improve end-to-end performance of working with compressed data.
  - Reduce disk overhead
  - Reduce communication overhead
  - Offset computation overhead of compression
- Keeping compression easy to use
  - Application transparent if possible
  - Minimize software layers to be changed

Compression: File System Based Approach

- Change the file systems to return decompressed data
  - Caching to reduce computation overhead
  - Pipelining and Prefetching to reduce latency
- Advantage
  - Application transparent
- Disadvantage
  - Does not reduce communication cost
  - Need to change file systems

PnetCDF Based Approach

- Fetch compressed data through MPI-IO
- Advantages
  - Reduce disk overhead
  - Reduce communication overhead
- Disadvantage
  - Challenging when PnetCDF accesses and data compression are not aligned
  - Pipelining is difficult
- Implemented a proof of concept prototype and performed some preliminary measurements
  - Read a 2.7 gb netcdf file with uncomopressed data, 39.454 seconds, with compressed data, 27.429 second

Outreach to community

- Convened a session at Fall 2011 AGU with other Viz PI's (Williams, Bethel) "Challenges in Analysis and Visualization of Large Earth Science Data Sets"
  - Oral presentation on ParCAL/ParNCL
  - Poster on Swift AMWG

- Presented ParVis and ParCAL at UCAR Software Engineering Assembly, February, 2012

- Continue to update website and parvis-ann mailing list.

ParVis Near-term plans

- ParCAL/ParNCL
  - Continue implementing more NCL functions
  - Put priority on functions in new NCL analysis routines written by CSSEF Atmosphere Team
  - Read in and operate on CAM-SE unstructured grids.
  - Define unstructured grid functions for common atmospheric analysis such as “zonal average”

- Task-parallel diags
  - Finish OWMG diags and release in time for CESM Tutorial
  - Begin parallelization of LMWG diags to support CSSEF land modeling

- Outreach:
  - Poster accepted to EGU (April).
  - DOE Computer Graphics Forum (April)
  - Present at CESM Workshop (June) and CESM Tutorial
  - Submit paper to **IEEE Symposium on Large-Scale Data Analysis and Visualization** (Oct, 2012)

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http://trac.mcs.anl.gov/projects/parvis