Software Engineering and the Parallel Climate Analysis Library (ParCAL)

Robert Jacob and Xiabing Xu
Mathematics and Computer Science Division
Argonne National Laboratory

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(Parallel Analysis Tools and New Visualization Techniques for Ultra-Large Climate Data Sets)

Motivation:
Ability to gain insight from current and future climate data sets

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Capability of current tools
Climate models are now running on 100K cores...

From Mark Taylor, SNL
...and they are outputting lots of data.

- CAM-SE at 0.125 degrees
  - Single 3D variable: 616 MB
  - Single 2D variable: 25 MB
  - Single history file: 24 GB
  - 1 year of monthly output: 288 GB
  - 100 years of monthly: 28.8 TB

- CSU GCRM 4km horizontal, 100 levels
  - Single 3D variable (cell center): 16 GB
  - Single 3D variable (cell edge): 50.3 GB
  - Single history file: 571 GB
  - 1 year of monthly output: 6 TB
  - 100 years of monthly: 0.6 PB
and the data is coming out on new, unstructured or semi-structured grids.

All current climate DAV tools require lat-lon grids for their internal analysis functions.
Existing Data Analysis and Visualization (DAV) tools have not kept up with growth in data sizes and grid types.

- NCAR Command Language (NCL)
- Climate Data Analysis Tools (CDAT)
- Grid Analysis and Display System (GrADS)
- Ferret

No parallelism
ParVis philosophy: Insight about climate comes mostly from computationally undemanding (to plot) 2D and 1D figures.

Why? The atmosphere and ocean have a small aspect ratio; 10,000 km vs. 10 km.
The climate viz problem for ultra-large data is mostly in post-processing the data for the figures. (data used does not come out directly from the models)

- *Post-processing* is an inextricable part of *visualization* of climate model output.

- It is the post-processing where the introduction of parallelism could have to largest impact on climate science using current visualization practice.
Two-pronged approach:

- Provide immediate help by speeding up current workflows with Task-parallelism

- Build a new data-parallel library for performing climate analysis on both structured AND unstructured grids.
Parvis Hardware Model

- Data Analysis Center’s (connected to large compute centers) will be a main venue for performing climate-model post-processing.
  - Eureka connected to Intrepid at ALCF (Argonne National Lab)
  - Lens connected to JaguarPF at NCCS (Oak Ridge National Lab)
  - DAV system connected to Yellowstone at NWSC (NCAR)

- Your desktop.
  - No longer any such thing as a single-processor workstation
  - Your desktop/laptop has 4, 8, 16 or more cores. Will increase. Your DAV tools likely not taking advantage of extra cores.
Argonne Leadership Computing Facility
Hardware Layout

**Intrepid**
- 40 racks/160k cores
- 556 TF

**Eureka (Viz)**
- 100 nodes/800 cores
- 200 GPUs
- 100 TF

**Networks**
(ESnet, internet2, UltraScienceNet,...)

**Tape Library**
- 5PB
- 6500 LT04 @ 800GB each
- 24 drives @ 120 MB/s each

**Switch Complex**
- (16) DDN 9900
  - 128 file servers
  - /intrepid-fs0 (GPFS)
  - 4.5PB
  - Rate: 60+ GB/s
  - /intrepid-fs1 (PVFS)
  - 0.5PB
  - Rate: 8+ GB/s

- (4) DDN 9550
  - 16 file servers
  - /gpfs/home 100TB

- (1) DDN 9900
  - 8 file servers
  - Tape Library 5PB
  - 6500 LT04 @ 800GB each
  - 24 drives @ 120 MB/s each
Parvis will provide immediate help with task-parallel versions of diagnostic scripts using **Swift**

- **Swift is a parallel scripting system for Grids and clusters**
  - for loosely-coupled applications - application and utility programs linked by exchanging files
- **Swift is easy to write**: simple high-level C-like functional language
  - *Small Swift scripts can do large-scale work*
- **Swift is easy to run**: a Java application. Just need a Java interpreter installed. Can use multiple cores on your desktop/laptop.
- Have rewritten CESM Atmospheric Model Working Group diagnostics with Swift
  - “The AMWG diagnostics package produces over 600 postscript plots and tables in a variety of formats from CESM (CAM) monthly netcdf files.”
- Timings with 10 years of 0.5 degree CAM data comparing with observations:
  - Original csh version on one core: 71 minutes
  - Swift and 16 cores: 22 minutes
ParCAL - Parallel Climate Analysis Library

- The main features
  - Data parallel C++ Library
  - Typical climate analysis functionality (such as found in NCL)
  - Structured and unstructured numerical grids

- Built upon existing Libraries
  - MOAB
  - Intrepid
  - PnetCDF
  - MPI

- Will provide data-parallel core to perform typical climate post-processing functions.

- Will be able to handle unstructured and semi-structured grids in all operations by building on MOAB and Intrepid. Will support parallel I/O by using PnetCDF.
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
Mesh-Oriented datABase (MOAB)

- MOAB is a library for representing structured, unstructured, and polyhedral meshes, and field data on those meshes
- Uses array-based storage, for memory efficiency
- Supports MPI-based parallel model
  - HDF5-based parallel read/write on (so far) up to 16k processors (IBM BG/P)
- Interfaces with other important services
  - Visualization: ParaView, VisIt
  - Discretization: Intrepid (Trilinos package)
  - Partitioning / load balancing: Zoltan
Intrepid (software, not to be confused with the BlueGene/P at ALCF)

**In**teroperable **T**ools for **R**apid **d**evelop**M**ent of compat**I**ble Discretizations

A Trilinos package for compatible discretizations:

- An extensible library for computing operators on discretized fields
- Will compute div, grad, curl on structured or unstructured grids maintained by MOAB!

When fully deployed (~2012) will provide

- support for more discretizations (FEM, FV and FD)
- optimized multi-core kernels
- optimized assembly (R. Kirby)

Developers: P. Bochev, D. Ridzal, K. Peterson, R. Kirby

http://trilinos.sandia.gov/packages/intrepid/
Software Engineering Practices in developing ParCAL (starting almost from scratch)

- Version Control System
  - Subversion (SVN)
- Automatic Documentation System
  - Doxygen
- Automatic Configuration
  - Autotools (Autoconf, Automake, libtool)
- Unit Tests
  - Boost Unit Testing Framework
- Automatic Nightly Tests
  - Buildbot System
- Project Management, Issue and Bug Tracking
  - Trac-based system
Common Tools

Version Control with svn

- `svn co https://svn.mcs.anl.gov/repos/parvis/parcal/trunk`
- Repository Layout (directories)
  - Branches: for different branch development
  - Tags: for different release versions
  - Trunk: main development repository
- Our sysadmins (at MCS) make it easy to set up an svn repo.

Doxygen In-Source Documentation System

- Support various programming languages (C, Java, Python, Fortran etc.)
- Automatic generation of on-line webpages and off-line reference manual
- Can be configured to document code structure (class, subclass)
Unit Test

Boost Test Library - Unit Test Framework
C++ framework for unit test implementation and organization
Very widely used. www.boost.org

Features:
- Simplify writing test cases by providing various testing tools
- Organize test cases into a test tree
- Relieve users from messy error detection, reporting duties and framework runtime parameters processing
Boost Test Tools:
You write a test program and call Boost functions

- Test Organization
  - BOOST_AUTO_TEST_SUITE (test_name)
  - BOOST_AUTO_TEST_CASE (test1)
  - BOOST_AUTO_TEST_CASE (test2)
  - BOOST_AUTO_TEST_SUITE_END ()

- Predefined Macros
  - BOOST_WARN(), BOOST_CHECK(), BOOST_REQUIRE()

- Pattern Matching
  - Compare against a golden log file

- Floating Point comparison
  - BOOST_CHECK_CLOSE_FRACTION (left-value, right-value, tolerance-limit)

- Runtime Parameter Options (handled by the Boost main() )
  - --log_level : specify the log verbosity
  - --run_test : specify test suites and test cases to run by names
Buildbot System

Goal:
- Automate the compile/test cycle to validate code changes
- trac.buildbot.net

Features:
- Run builds on a variety of platforms
- Arbitrary build process: handles projects using C, C++, Python etc.
- Status delivery through web pages, email etc.
- Track builds in progress, provide estimated completion time
- Specify the dependency of different test configurations
- Flexible configuration to test on a nightly basis or on every code changes
- Debug tools to force a new build
Nightly Build

Nine different configurations:
mpich, openmpi, gcc, intel, warning test, document generation etc.

Nightly build homepage

Doxygen API:

Doxygen PDF

Nightly build from trunk
Nightly Test Screenshot
Project Management with Trac

Web-based software project management system. Like svn, easy setup provided by MCS sysadmins

http://trac.edgewall.org/

- Built-in Wiki System
- Connects with svn repo
  - Browsing source code
  - Viewing changes to source code
  - Viewing change history log
- Ticket Subsystem
  - Using tickets for project tasks, feature requests, bug reports etc.

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

ParCAL Application

Fileinfo

PcVAR
- File
- User

Analysis
- Native
- Intrepid

Mesh Oriented datABase (MOAB)
- Parallel netCDF
- HDF5

PROF
ERR
MEM
LOG
ParCAL Architecture - contd

- Fileinfo
  - Abstraction of multiple files

- PcVAR
  - File Variables
  - User Variables
  - Read/write data through MOAB

- Analysis
  - Native: dim_avg_n, max, min (already implemented)
  - Intrepid

- MOAB
  - Parallel IO/Storage

- Misc utilities
  - MEM, ERR, LOG, PROF
ParCAL test of dim_avg_n

- **Input**
  - 0.1 degree Atmosphere (1800x3600x26) up-sampled from a $\frac{1}{4}$ degree CAM-SE cubed sphere simulation

- **Environment**: Argonne “Fusion” cluster
  - OS: Red Hat Enterprise Linux 5.4
  - Compiler: Intel-11.1.064
  - Optimization Level: -O2
  - MPI: Mvapich2 1.4.1
ParCAL dim_avg_n Performance
ParCAL and ParNCL

- ParCAL is a library.

- ParNCL is an application written using that library. A parallel version of NCL (which also allows computations on unstructured grids).
# NCAR Command Language (NCL)

*An scripting language tailored for the analysis and visualization of geoscientific data*

<table>
<thead>
<tr>
<th>Feature</th>
<th>Description</th>
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<tr>
<td>1. Simple, robust file input and output</td>
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<td>2. Hundreds of analysis (computational) functions</td>
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<td>3. Visualizations (2D) are publication quality and highly customizable</td>
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- Community-based tool
- Widely used by CESM developers/users
- UNIX binaries & source available, free
- Extensive website, [regular workshops](http://www.ncl.ucar.edu/)
Summary

- ParCAL and ParNCL beta versions exist. A few functions implemented.
  - Working on improving coverage, testing
  - Prioritizing NCL built in functions (300+) to implement

- Swift version of Atmospheric Model Working Group diagnostics released to user community.

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