Climate Computing: The State of Play AOS Student Seminar

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NOAA/GFDL and Princeton University

22 February 2016

Outline

- Marcoloft GFDL Strategic Plan: 2012-2016
- FMS and FRE
- 3 Scientific drivers: complexity, resolution, uncertainty
 - Atmospheric physics and chemistry
 - Marine and terrestrial biogeochemistry
 - Decadal predictability and prediction studies
- Towards exascale
- The Finite-Volume Cubed-Sphere Dynamical Core
 - Mosaic representation
 - Variable-resolution gridding within the cubed-sphere
 - Global cloud-resolving model
- 6 CM4 Development
- Comparing real performance across models and machines
- Summary

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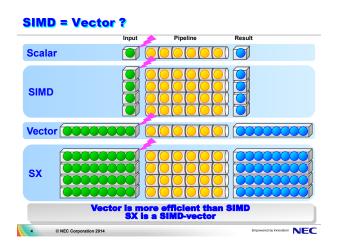
GFDL and Princeton University

"Milestones in Scientific Computing", from Nature (23 March 2006)



- 1946 "ENIAC, ... the first electronic digital computer"
- 1969 "results from first coupled ocean-atmosphere general circulation model are published by Syukuro Manabe and Kirk Bryan, paving the way for later climate simulations that become a powerful tool in research on global warming..."
- 1972 "... the first hand-held scientific calculator"
- 1989 "Tim Berners-Lee ... develops the World Wide Web"

Scalars, vectors, parallel, parallel vectors



Courtesy Rudi Fischer, NEC.

Commodity clusters: Beowulf



About	
Call For Papers	
Registration	
Program Committee	
Venue	
Hotel	
Directions	

About the Workshop

This workshop will mark the 20th anniversary of the introduction of commodity (AKA Beowulf) clusters, an architectural approach to creating parallel computers using mostly or entirely commodity components and open source system software. The initial target of the Beowulf cluster project was inexpensive, small to moderate parallel computing platforms; the Beowulf approach was extremely successful and adopted worldwise by teams ranging from high-school students to senior scientists. The Beowulf approach is now the basis of most of the world's most powerful computers as well.

The workshop will also celebrate the 65th birthday of Thomas Sterling, who has made major contributions over his career (so far), including playing a key role in conceiving and implementing commodity cluster computing (aka Beowulf), HPC architecture, run time systems, and exascale systems.

Dates

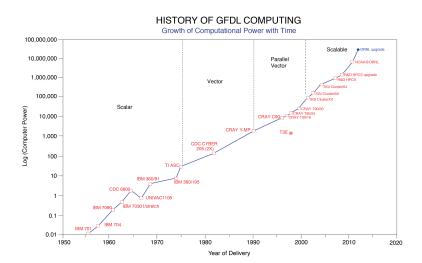
October 13-14, 2014

Agenda Oct



http://crest.iu.edu/beowulf14/

History of GFDL Computing



Courtesy Brian Gross, NOAA/GFDL.

GFDL Strategic Plan: 2012-2016

- Basic climate processes and their representations in models.
- Comprehensive modeling of climate system variability and change.
- Understanding, detection and attribution, and prediction of extreme events.
- Understanding, detection and attribution, and predictability of modes of climate variability.
- Cryospheric amplification of climate change and sea-level rise.
- Understanding the Earth system including biosphere and human activities.
- Climate science, impacts and services.

Google "GFDL Strategic Science Plan".

Current suite of GFDL models

- CM3: comprehensive tropospheric and stratospheric chemistry, aerosol-cloud feedbacks.
- ESM2M and ESM2G: free-running carbon cycle.
- DECP: decadal prediction models at various resolutions with advanced initialization (ECDA).
- C180, C360: atmospheric models with AM3 physics optimized for tropical storm "permitting" simulations (HiRAM).
- Cloud-resolving models (C2560) with bulk microphysics.
- Under development for CM4: unified ocean core MOM6, simplified aerosol chemistry.
- Performance guidelines for CMIP-class models: 4 models running at 100 years/month using half the available machine.
- Spinup and millennial control runs are capability runs. Note ESMs require very long spinup...

All models built on common framework and run within a single distributed workflow.

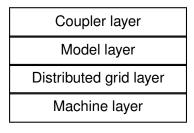
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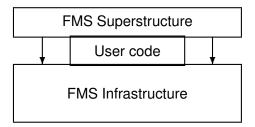
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FMS: Summary

- Scalable high-performance framework on up to $\mathcal{O}(10^5)$ processors.
- Good, stable, dedicated team in Modeling Services.
- Broad acceptance and widespread contributions to a working system: many useful contributions from external users.
- Impressive list of features: mosaics, parallel ensemble capability, experiment database. Equally impressive list of components and options.
- Component list:
 - atmosphere dycore: FV-CS, FV-LL, BGRID, SPECTRAL, ZETAC.
 - atmospheric physics and chemistry: AM2, AM2.1 (HiRAM), AM2.1 (Lin), AM3, simple, dry. Fast-Chem
 - ocean: MOM6, GOLD, MOM5, MOM4p1, MOM4p0, mixed-layer.
 - land: LAD/LM2, SHE/LM3v, LAD2/LM3, river.
 - ocean BGC: TOPAZ, COBALT, BLING.
 - ice: SIS, SIS2 with elements from LANL-CICE.

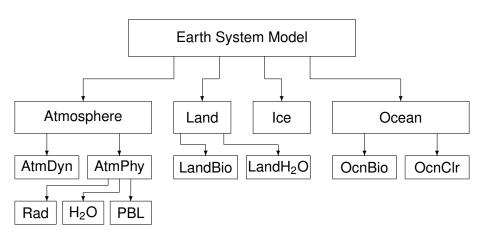
FMS is in its second decade of active use





- Flexible Modeling System effort began in 1998, when GFDL first moved on to distributed memory machines
- Provided simplified interface to parallelism and I/O: mpp. Abstract types for "distributed grid" and "fields".
- Diagnostic output, data override, time manager.
- Component-based design, abstract types for component state vectors, exchange grid.
- "Sandwich" model influential in community.

Earth System Model Architecture



Complexity implies many different instruction sequences; no hotspots.

FRE: the FMS Runtime Environment

- Operational since 2003, designed to provide an environment for integrated testing and production.
- Rigorous standardized test procedure for evaluating new code and new model assemblies and configurations.
- Integrated existing post-processing structure.
- Captures complete configuration from source assembly to compilation to running, post-processing and analysis.
- Simulation database provides retrieval of model output, model analysis, and now model state and configuration information.
- Again influential in community, with "curators" being prototyped at various sites.

The FMS user interface: FRE

Comprehensive website for all information and documentation: http://www.gfdl.noaa.gov/~fms

- Source code maintenance under cvs transitioning to git
- Model configuration, launching and regression testing encapsulated in XML;
- Relational database for archived model results;
- Standard and custom diagnostic suites;
- Regression Test Suite (RTS): ~100 model configurations continually tested for internal correctness, as well as with respect to reference run.

The FMS Runtime Environment (FRE) describes all the steps for configuring and running a model jobstream; archiving, postprocessing and analysis of model results.

fremake, frerun, frepp, frecheck, ...

Elements of FRE

```
fremake Checkout an appropriate subset of the FMS source code for an experiment and create an executable;
```

frerun run an experiment in multiple *segments*; resubmit if necessary;

frestatus check the status of an experiment that is underway;

frelist list available experiments;

frepriority switch a job sequence between queues;

frecheck run RTS checks for bitwise accuracy;

frepp FRE post-processing: create time series, time averages, and plots;

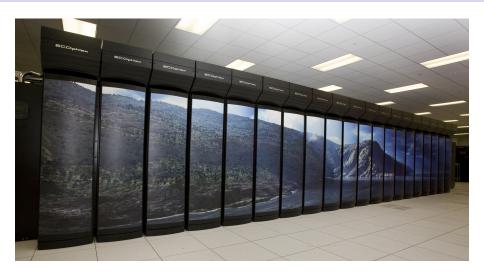
frescrub remove intermediate and redundant files;

freppcheck RTS checks on history and post-processing files.

fredb enter experiments into Curator DB.

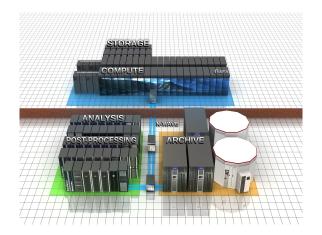
Project Chaco is rewriting the FRE infrastructure using Cylc.

Gaea



The NOAA Climate Modeling and Research System *Gaea*. Extended in 2013 to include GPU capabilities.

Gaea and GFDL

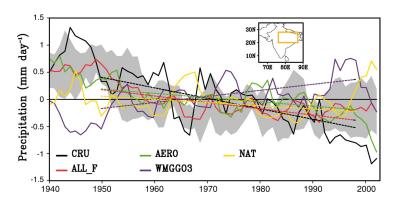


FRE and other elements in the GFDL modeling environment manage the complex scheduling of jobs across a distributed computing resource.

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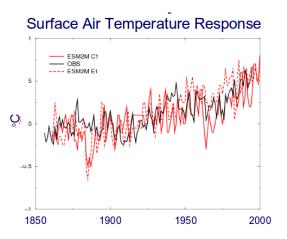
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Aerosol indirect effects weaken South Asian monsoon



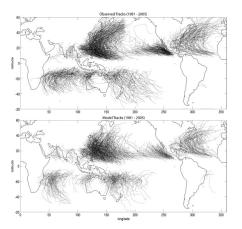
Cloud-aerosol feedbacks induce a weakening of the Indian monsoon (Figure courtesy Bollasina et al., **Science** 2011).

ESM2M: free-running carbon cycle



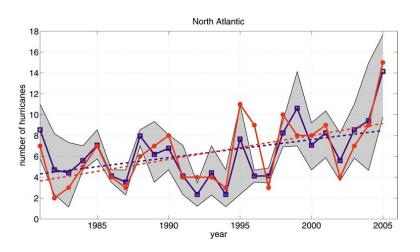
Free-running carbon cycle in ESM2M. Emissions-driven runs comparable to concentration driven runs (and to observations.) Figure courtesy Ron Stouffer, NOAA/GFDL.

Hurricane statistics from global high-resolution atmosphere models



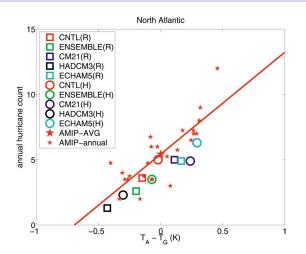
Observed and modeled hurricane tracks from 1981-2005 in a global 50 km (C180) atmospheric model forced by observed SSTs. (Figure 3 from Zhao and Held 2009).

Interannual variability of hurricane frequency



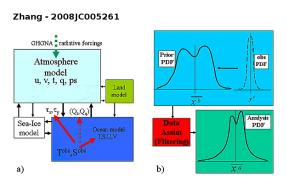
Interannual variability of W. Atlantic hurricane number from 1981-2005 in the C180 runs. (Figure 7 from Zhao and Held 2009).

A simple predictor of hurricane counts?



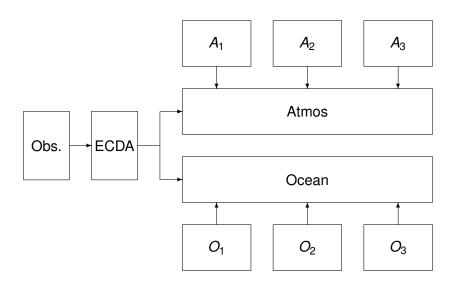
Difference between Atlantic surface temperature T_A and mid-tropospheric global temperature T_G dtermines hurricane generation rate. Figure 16 from Zhao et al (2009).

Data assimilation



Data assimilation uses ensembles to find likely model trajectory taking into account model error and observational error. (Figure courtesy Zhang et al 2008).

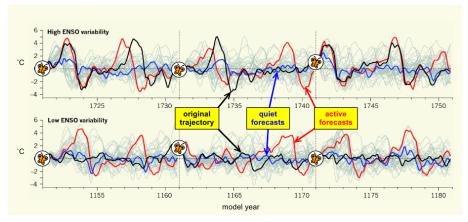
Ensemble Coupled Data Assimilation (ECDA)



Components ("instances") execute in parallel.

ENSO modulation: is it decadally predictable?

"Perfect-model" forecasts of NINO3 SSTA, for extreme-ENSO epochs simulated by CM2.1

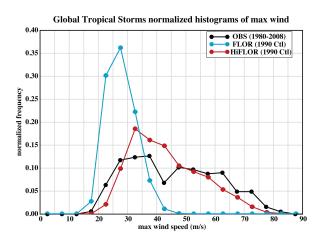


(External forcings held fixed at 1860 values.)

Wittenberg et al. (J. Climate, 2014)

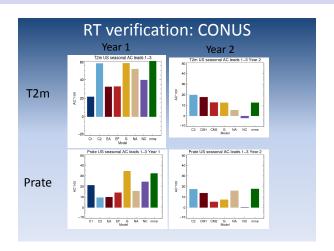
Effects of the proverbial "flap of a butterfly's wing"...

"TC-permitting" models get better with resolution



Intensity distribution improves with resolution. Figure courtesy Gabe Vecchi.

"TC-permitting" model FLOR is now used in the NMME



Seasonal forecasting product used in NMME and SPECS. Figure courtesy Gabe Vecchi.

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The hardware jungle

Upcoming hardware roadmap looks daunting! GPUs, MICs, DSPs, and many other TLAs...

- Intel straight line: IvyBridge/SandyBridge, Haswell/Broadwell: "traditional" systems with threading and vectors.
- Intel knight's move: Knights Corner, Knights Landing: MICs, thread/vector again, wider in thread space.
- Hosted dual-socket systems with GPUs: SIMD co-processors.
- BG/Q: CPU only with hardware threads, thread and vector instructions. No followon planned.
- ARM-based systems coming. (e.g with DSPs).
- FPGAs? some inroads in finance.
- Specialized processors: Anton for molecular dynamics, GRAPE for astrophysics.

The software zoo

Exascale using nanosecond clocks implies billion-way concurrency! It is unlikely that we will program codes with 10^6-10^9 MPI ranks: it will be MPI+X. Solve for X . . .

- CUDA and CUDA-Fortran: proprietary for NVIDIA GPUs. Invasive and pervasive.
- OpenCL: proposed standard, not much penetration.
- ACC from Portland Group, now a new standard OpenACC.
- Potential OpenMP/OpenACC merging...?
- PGAS languages: Co-Array Fortran, UPC, a host of proprietary languages.
- Code generation:
 - Domain-specific languages (DSLs): e.g STELLA.
 - Source-to-source translators.

GFDL between jungle and zoo

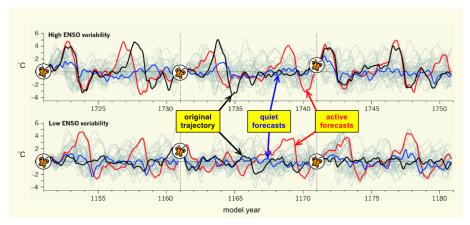
GFDL is taking a conservative approach:

- it looks like it will be a mix of MPI, threads, and vectors.
- Developing a three-level abstraction for parallelism: components, domains, blocks. Kernels work on blocks and must have vectorizing inner loops.
- Recommendation: sit tight, make sure MPI+OpenMP works well, write vector-friendly loops, reduce memory footprint, offload I/O.
- Other concerns:
 - Irreproducible computation
 - Tools for analyzing performance.
 - Debugging at scale.

Recent experience on Titan, Stampede and Mira reaffirm this approach.

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"Perfect-model" forecasts of NINO3 SSTA, for extreme-ENSO epochs simulated by CM2.1

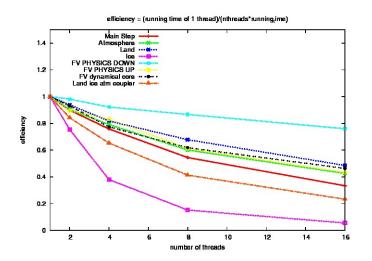


(External forcings held fixed at 1860 values.)

Wittenberg et al. (J. Climate, 2014)

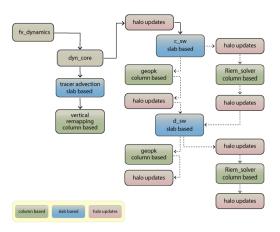
Effects of the proverbial "flap of a butterfly's wing"...

Most of FMS is now threaded



CM4 on up to 16 threads on gaea. (Figure courtesy Zhi Liang)

Analysis of dycore architecture for GPU/MIC



Study of code for MPI, threads, vectors. (Chris Kerr, Zhi, Kareem Sorathia (NASA), Duane Rosenberg (ORNL), Eric Dolven (Cray)...)

Blocking the dycore for GPU/MIC

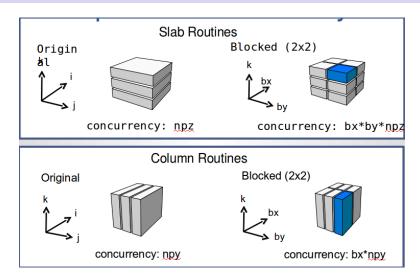


Figure courtesy Kareem Sorathia (NASA). Inner loops on i are retained for vectorization.

Performance summary: Xeon-SNB vs Xeon-Phi

Phi "speedup" over SNB:

- Overall: 0.73
- Communication: 0.34
- All Computation: 0.86
- Top 4: 0.996

Coding issues:

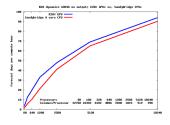
- Vector performance very hard to achieve, even with padding halos for alignment.
- Loop unrolling/stripmining/etc needs to be done by hand.
- Better performance analysis tools needed.

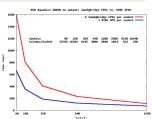
Courtesy Kareem Sorathia, NASA.

Results from NIM icosahedral dycore: SNB vs GPU

NIM Dynamics: GPU versus Intel-SB

- · Single source code optimized for CPU, MIC & GPU
 - OpenMP directives for CPU & MIC
 - OpenACC, F2C-ACC for NVIDIA GPU
- 15 KM model, 96 levels, single-precision
 - Strong scaling: 80 10240 GPUs
 - GPU 2-3x faster than CPU socket for 8192 columns





Courtesy Mark Govett, NOAA/ESRL.

OpenACC

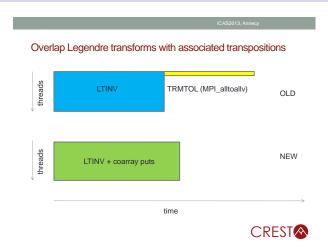
```
!$acc parallel num_gangs(ihe-ips+1) vector_length(64)
!$acc loop gang
   do ipn=ips,ihe
!$acc loop vector
   do k=1,nvl
      flxhi(k) = vnorm(k,edg,ipn)*dp_edg(k,edg,ipn)
```

Can merge gang and vector on same axis:

```
do k = kts,kte
!$acc loop gang vector
   do i = its,ite
      za(i,k) = 0.5*(zq(i,k)+zq(i,k+1))
```

Courtesy Mark Govett, NOAA/ESRL.

ECMWF uses PGAS (Co-Array Fortran)



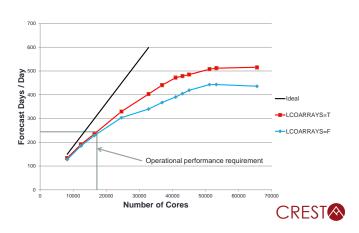
Co-array assignments become one-sided puts from within threaded regions.

Courtesy George Mozdzynski, ECMWF.

CAF results using Cray compiler CCE

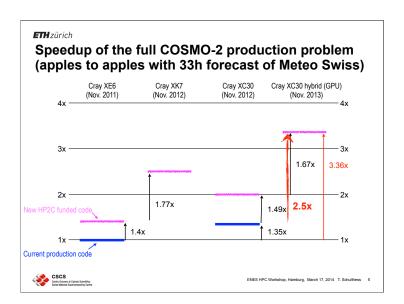
iCAS2013, Annecy

T2047L137 model performance on HECTOR (CRAY XE6) RAPS12 IFS (CY37R3), cce=8.0.6 -hflex_mp=intolerant

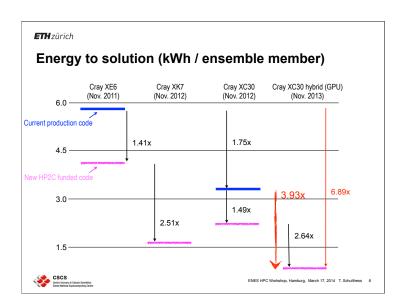


Courtesy George Mozdzynski, ECMWF.

COSMO: NWP production code using GPUs



COSMO: energy to solution



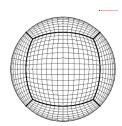
Summary of results in the jungle and zoo

- Billion-way concurrency still a daunting challenge for everyone: no magic bullets anywhere to be found. ECMWF's PGAS approach is unique and interesting, at least one production GPU model.
- GPU/MIC based systems show nominal \sim 10 increase in flops/socket, but actual performance about 1-2X (thus percent of peak drops from \sim 10% to \sim 1%)
- Software investment paid back in power savings (Schulthess).
- More threading needs to be found: to fit 10^{18} op/s within a 1 MW power budget, an operation should be 1 pJ: data movement is \sim 10 pJ to main memory; \sim 100 pJ on network!
- DARPA: commodity improvements will slow to a trickle within 10 years: go back to specialized computing?
- DOE: double investment in exascale.

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Cubed-sphere, Gnomonic Projection



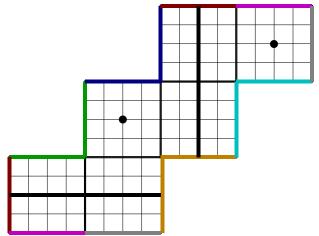
- True equal distance at the 12 edges of the cube
- All coordinate lines are great circles
- Coordinates are continuous at the edges; but derivatives are discontinuous



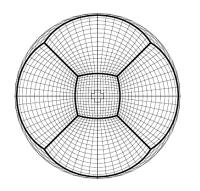
Putman and Lin, J. Comp. Phys. 2007.

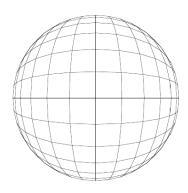
FMS index space representation of the cubed sphere

- Orientation changes (e.g $u \rightarrow -v, v \rightarrow u$)
- This is a C4 grid (C48 ~ 200 km resolution; C2880 ~ 3 km resolution)
- Typical pace of a coupled model: 10 y/d at C48; 3 y/d at C180.



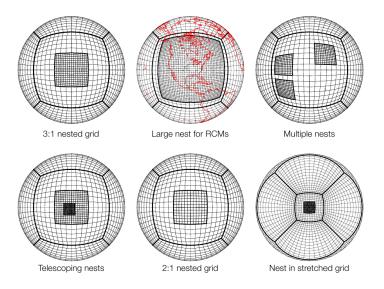
Stretched grids





- Opposing face gets very coarse
- Discontinuities in slope
- Scale-aware parameterizations required

Nested grids

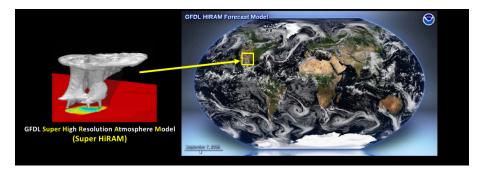


C2560: 3.5 km resolution global cloud-resolving model



Figure courtesy S-J Lin and Chris Kerr, NOAA/GFDL.

Towards global cloud-resolving models



Variable-resolution grid in the FV3 model, courtesy S-J Lin.

The NGGPS Effort

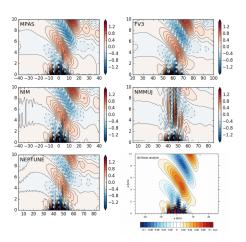
- NGGPS: Next-Generation Global Prediction System
- HIWPP: High-Intensity Weather Prediction Program

NGGPS and HIWPP launched a program to select a dynamical core for the next-generation forecast model (target: 3 km non-hydrostatic in 10 years). Selected dycores will undergo a substantial re-engineering effort for novel architectures.

- Scaling tests
- Idealized baroclinic wave test with embedded fronts (DCMIP 4.1)
- non-hydrostatic orographic mountain waves on reduced-radius sphere, no rotation
- idealized supercell thunderstorm on reduced-radius sphere, no rotation

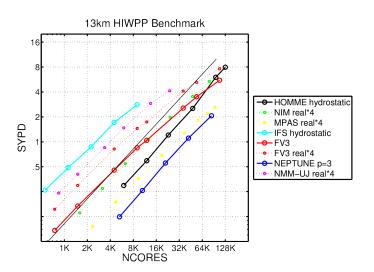
http://www.nws.noaa.gov/ost/nggps/dycoretesting.html

NGGPS Mountain Wave test case



http://www.nws.noaa.gov/ost/nggps/dycoretesting.html

NGGPS Scaling Study



http://www.nws.noaa.gov/ost/nggps/dycoretesting.html

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GFDL formed a new MDT for 2013-2016

In the 2013-2016 time frame, design and develop GFDL's best attempt at a climate model suitable for

- projection of climate change up to several hundred years into the future,
- attribution of climate change over the past century,
- prediction on seasonal to decadal time scales

keeping in mind the needs for improved regional climate information and assessments of diverse climate impacts.

The model will be capable of running from emissions in regard to both the carbon cycle and aerosols.

Courtesy Isaac Held, MDT Lead.

Target model configurations for CM4/ESM4

50 km atmosphere (C192) and 0.25° ocean (MOM6)

Determined by

- Lab experience regarding resources needed to develop and utilize a model for centennial-scale climate projections: at least 3-5 years/day throughput on no more than 1/8 of computational resource
- the GAEA computational resource

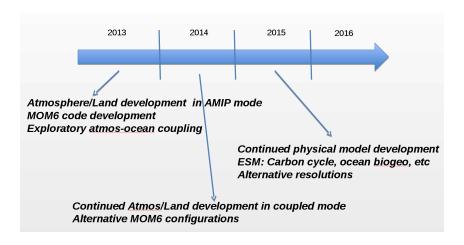
Increases in hardware resources and significant software development would allow us to redefine this trunk model towards higher resolution and/or greater comprehensiveness, e.g. full eddy-resolving ocean resolution; more complete stratosphere/troposphere chemistry module Courtesy Isaac Held.

Scientific and software challenges

- Oceanic mesoscale eddies Can we make a 0.25° degree model look like an eddy-resolving model?
- Aerosol/cloud interactions How do we best combine bottom-up (process-oriented) perspective and top-down constraints provided by 20th century observations?
- Atmospheric boundary layer/low cloud feedbacks Are we in a position to incorporate a dramatically new type of boundary layer/shallow convection module similar to CLUBB?
- Software Can we find more concurrency to improve wall clock performance so that we can increase complexity/resolution relevant to MDT goals

Courtesy Isaac Held.

CM4 Timeline

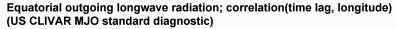


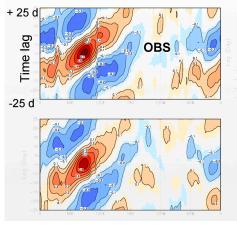
Courtesy Isaac Held.

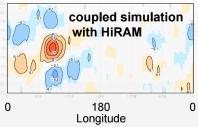
Current CM4 Status (June 2015)

- About 6 months behind timeline!
- Testing C96L48 (full-chem, ~100 species) and C192L32 (fast-chem, ~20 species) atmospheric models (also C96L32 for rapid test cycle
- boundary layer and convection schemes, gravity-wave drag, etc still under testing and tuning
- COBALT (~30 species) adds about 50% to the cost of the ocean model
- COBALT timestep decoupled from main loop (much faster!)
- alternate 1° version of MOM6 being developed for predictability research
- To run CMIP6 (DECK + endorsed MIPs: ~7500 years) on Gaea requires models costing about ~30,000 core-hours per simulated year (CHSY).

New metrics for evaluation of models: MJO







coupled simulation with alternative convection scheme (Ming Zhao)

New metrics for evaluation of models: TC climatology

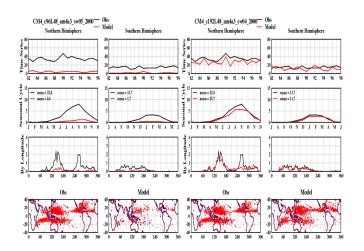
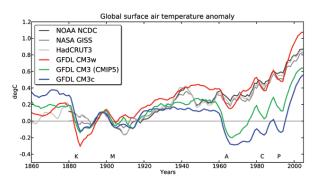


Figure courtesy John Dunne.

Model tuning: Process fidelity vs model bias

Tuning reduces model bias without violating process fidelity (but poses a problem for validation).



From Golaz et al 2012.

Outline

- GFDL Strategic Plan: 2012-2016
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Multi-model ensembles for climate projection

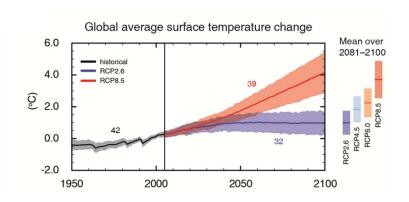
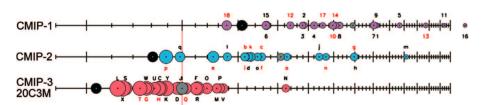


Figure SPM.7 from the IPCC AR5 Report. 20th century warming cannot be explained without greenhouse gas forcings.

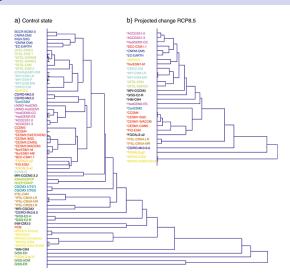
Multi-model ensembles to overcome "structural uncertainty"



Reichler and Kim (2008), Fig. 1: compare models' ability to simulate 20th century climate, over 3 generations of models.

- Models are getting better over time.
- The ensemble average is better than any individual model.
- Improvements in understanding percolate quickly across the community.

Genealogy of climate models



There is a close link between "genetic distance" and "phenotypic distance" across climate models (Fig. 1 from Knutti et al, GRL, 2013).

NRC Report on "Advancing Climate Modeling"

The 2012 NRC Report "A National Strategy for Advancing Climate Modeling" (Google for URL...) made several recommendations:

- Structural uncertainty: key issue to be addressed with common modeling experiments: maintain model diversity while using common infrastructure to narrow the points of difference.
- Global data infrastructure as critical infrastructure for climate science: data interoperability, common software requirements.
- "Nurture" at least one unified weather-climate effort: NWP methods to address climate model biases; climate runs to address drift and conservation in weather models.
- Forum to promote shared infrastructure: identify key scientific challenges, design common experiments, set standards for data interoperability and shared software.

Real model performance: some considerations

- Productions runs may be configured for capability (minimizing time to solution or SYPD) or capacity nn (minimizing allocation or CHSY).
- Computing resources can be applied to resolution or complexity: what is a good measure of model complexity?
- ESM architecture governs component concurrency: need to measure load balance and coupler cost.
- Codes are memory-bound: locate bloat (memory copies by user or compiler).
- Models configured for scientific analysis bear a significant I/O load (can interfere with optimization of computational kernels). Data intensity (GB/CH) is a useful measure for designing system architecture.
- Actual SYPD tells you if you need to devote resources to system and workflow issues rather than optimizing code.

Analysis of several GFDL models

- Measure overall computation cost for capability (Speed) or capacity (Throughput) configurations.
- Measure complexity as number of prognostic variables in the model. (There may be better measures based on cluster coefficients, etc.)
- Measure coupler cost and load imbalance separately.
- Measure memory bloat as actual memory (resident set size) compared to ideal memory (number of variables × data domain size).
- Measure I/O load by rerunning model with diagnostics off. (input files and restart files are considered an unavoidable cost and aren't counted here.)
- Measure actual SYPD for a complete run (from when you typed run to when the last history file was archived).

Analysis of GFDL models: results

Model	Resolution	Cmply	SYPD	CHSY	Coupler	Load Imb.	I/O	MBloat	ASYPD
Model		Cmplx.	5170	CHST	Coupler	Load IIIb.	1/0	MBIOAL	ASTPU
СМЗ Т	A2L48 O1L50 4.2E6	124	7.7	2.974	0.5%	41%	14.76%	3%	4.9
CM2.6 S	A0.5Ľ32 O0.1L50 4.9E8	18	2.2	212,465	5.71%	20%		12%	1.6
CM2.6 T	A0.5L32 O0.1L50 4.9E8 A0.5L32	18	1.1	177,793	1.29%	60%	24%	12%	0.4
CM2.5 T	A0.5L32 O0.25L50 8.3E7 A0.5L32	18	10.9	14,327	17%	0%			6.1
FLOR T	A0.5L32 O1L50 9.8E6 A2L24	18	17.9	5,844	0%	57%	5.1%	31%	12.8
ESM2G S	O1L50 3.9E6	63	36.5	279	8.91%	1%		34%	25.2
ESM2G T	A2L24 O1L50 3.9E6	63	26.4	235	2.63%	22%		34%	11.4

- More details in Curator database.
- Basis for CPMIP

Preliminary cross-model comparisons

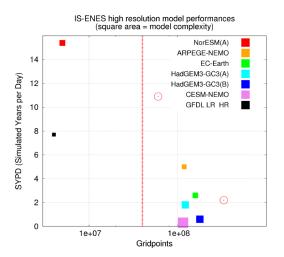


Figure courtesy Eric Maisonnave, Joachim Biercamp, Giovanni Aloisio and others on the ISENES2 team.

Preliminary cross-model comparisons: layout

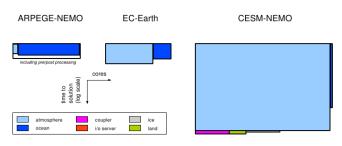
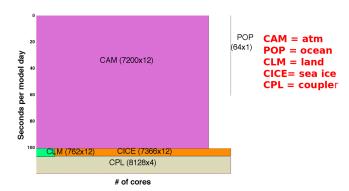


Figure 2: Parallelism and execution time (inverse of SYPD) for three of the participating ESMs

Figure courtesy Eric Maisonnave, Joachim Biercamp, Giovanni Aloisio and others on the ISENES2 team.

CESM component-wise layout and simulation rate on MIRA



Courtesy John Dennis and Rich Loft, NCAR. 0.25° atmosphere, 1° ocean on 32k cores of Mira at ~2 SYPD.

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Summary

- GFDL Strategic Plan: process studies; development of comprehensive models; climate extremes; experimental prediction; downstream science.
- Experimental seasonal to decadal prediction, including high-resolution fully coupled ensemble Kalman filter for data assimilation
- Continued development of extremely high-resolution atmosphere models using state of the art dynamical core
- Unification of ocean model development through MOM5 and MOM6 (incorporates capabilities from GOLD model into MOM, incorporates results of Climate Process Teams)
- Development of next generation climate model(s) CM4: convergence of multiple model branches into a few "trunk" models, through a Model Development Team led by Isaac Held.
- Increased integration of NOAA modeling across climate research and extended-range forecasting.