New developments in modeling at GFDL

Second ISENES Workshop on HPC for Climate Models
Toulouse FRANCE

V. Balaji

NOAA/GFDL and Princeton University

31 January 2013

Outline

Outline

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.

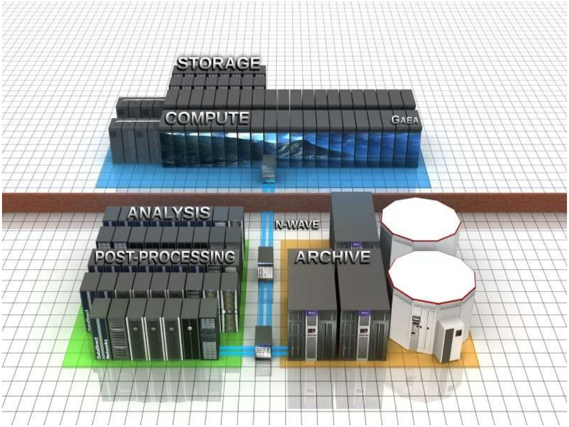
FMS: Summary

- 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. Simple-Chem
  - ocean: MOM6, GOLD, MOM5, MOM4p1, MOM4p0, mixed-layer.
  - land: LAD/LM2, SHE/LM3v, LAD2/LM3, river.
  - ocean BGC: TOPAZ, COBALT, BLING.
  - ice: SIS, CICE.

Gaea

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

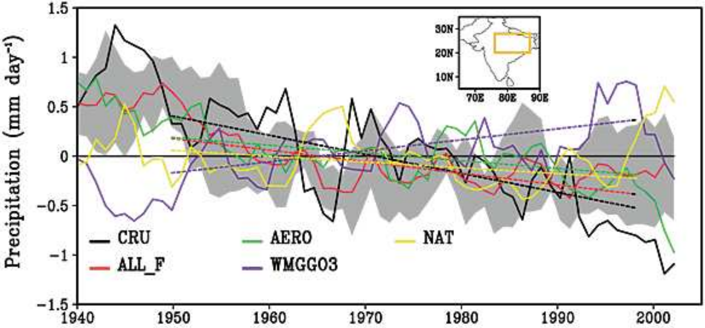
Gaea and GFDL



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

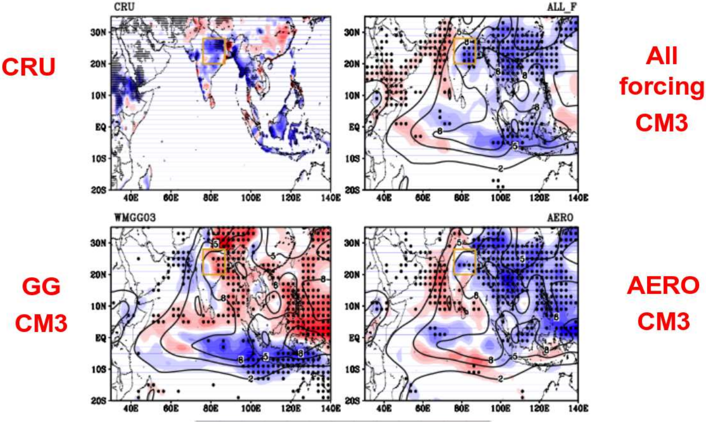
Outline

Aerosol indirect effects weaken South Asian monsoon



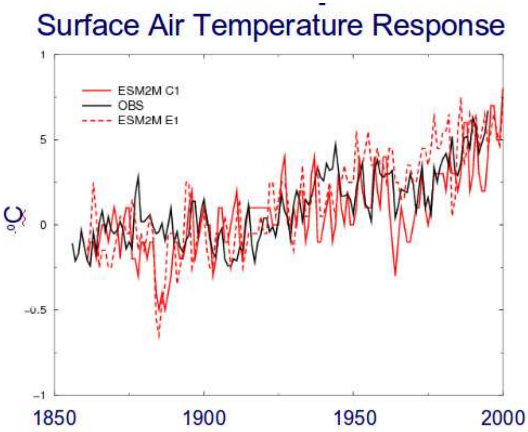
Cloud-aerosol feedbacks induce a weakening of the Indian monsoon (Figure courtesy Bollasina et al., **Science** 2011).

Aerosol indirect effects weaken South Asian monsoon: summer monsoon spatial pattern



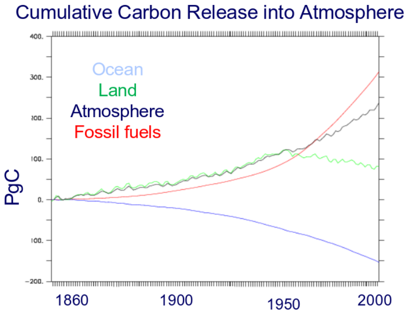
Cloud-aerosol feedbacks induce a weakening of the Indian monsoon (Figure courtesy Bollasina et al., **Science** 2011).

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; pre-publication.

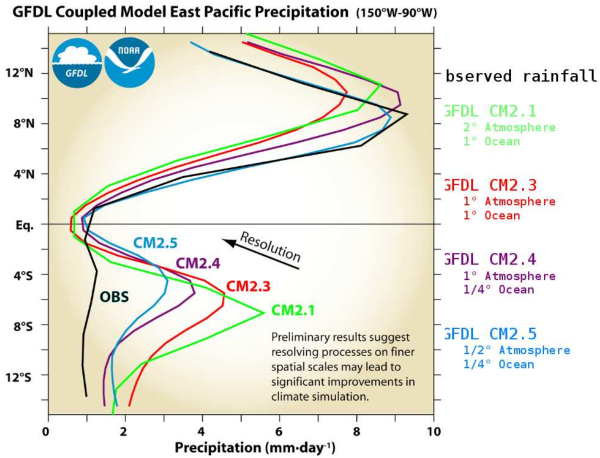
Carbon sources and sinks



- Land carbon fluxes dominant before 1960; then trend changes sign.
- Fossil fuels dominant contemporary source.
- Ocean uptake scales with pCO_2.

Figure courtesy Ron Stouffer, NOAA/GFDL; pre-publication.

Resolution as a cure for key model biases



The "double-ITCZ problem" appears to be improved by adding resolution (Figure courtesy Gabe Vecchi, NOAA/GFDL).

Annual mean SST bias in CM2.5 control

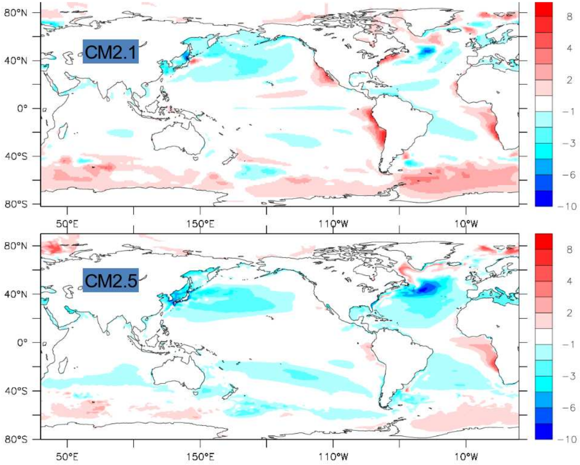
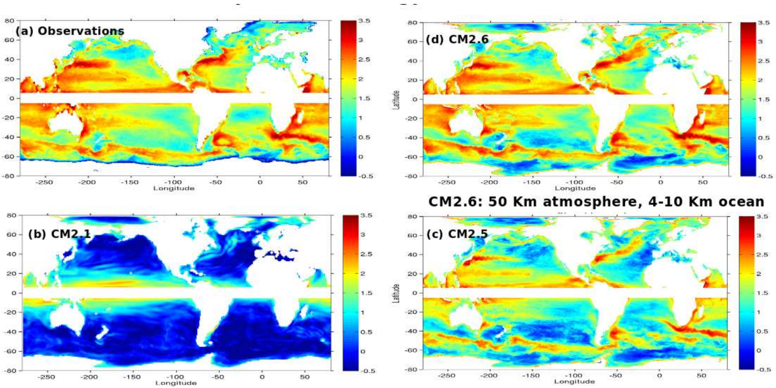


Figure courtesy Delworth et al (2012).

Ocean Eddy Kinetic Energy in CM2.5 and CM2.6



CM2.6: 50 Km atmosphere, 4-10 Km ocean

CM2.1: 200 Km atmosphere, 100 Km ocean

CM2.5: 50 Km atmosphere, 10-25 Km ocean

EKE patterns show marked improvement in the progression toward “eddy-permitting” and “eddy-resolving” ocean models. (Delworth et al 2012).

Subsurface temperature drift corrected by eddy dynamics

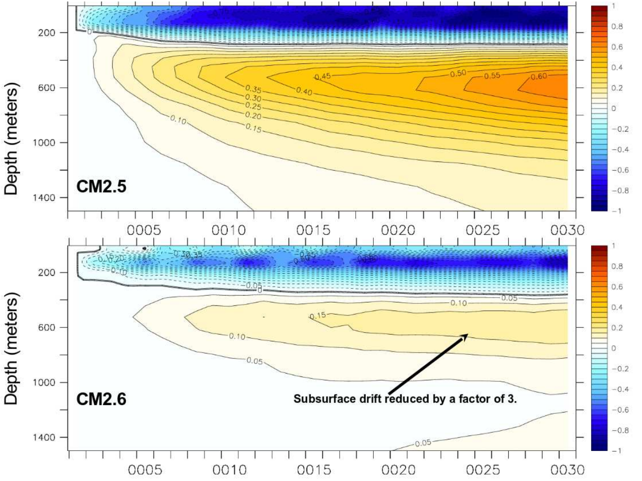
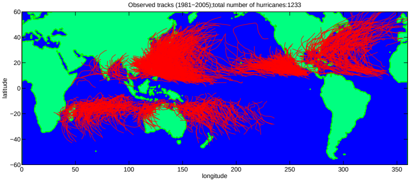
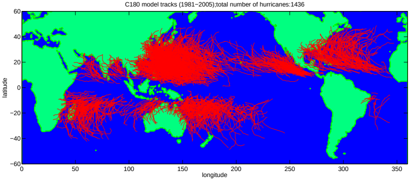


Figure courtesy Delworth et al (2012).

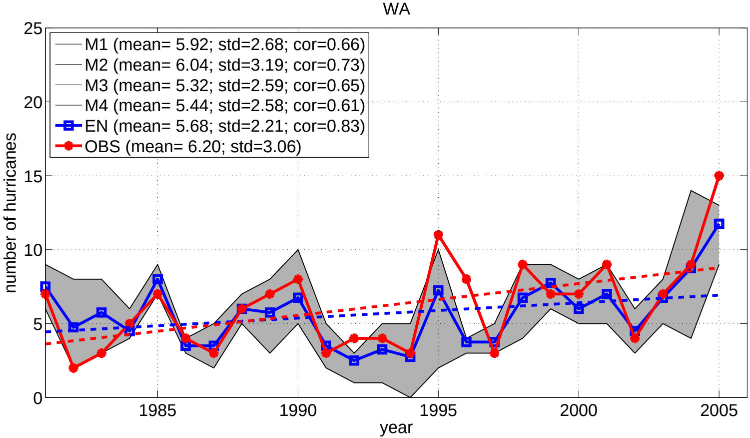
Hurricane statistics from global high-resolution atmosphere models





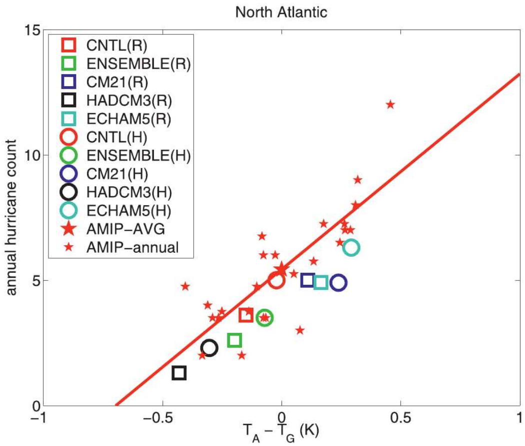
Observed and modeled hurricane tracks from 1981-2005 in a global 50 km (C180) atmospheric model forced by observed SSTs. (Figure courtesy Ming Zhao and Isaac Held, NOAA/GFDL).

Interannual variability of hurricane frequency



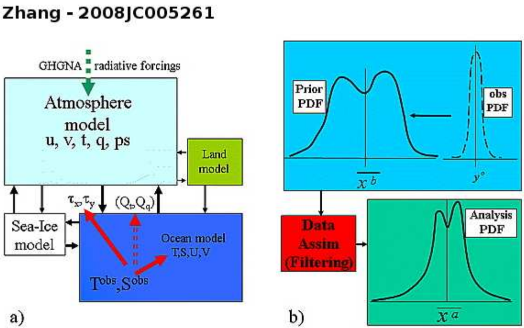
Interannual variability of W. Atlantic hurricane number from 1981-2005 in the C180 runs. (Figure courtesy Ming Zhao and Isaac Held, NOAA/GFDL).

A simple predictor of hurricane counts?



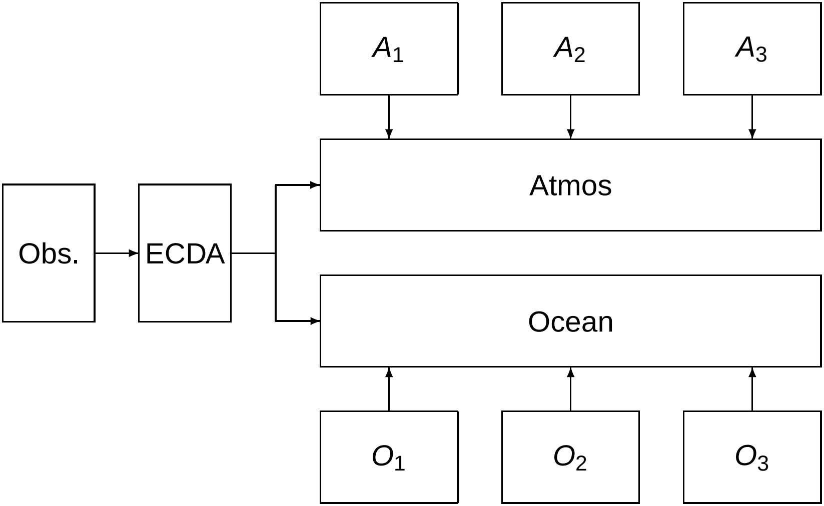
Difference between Atlantic surface temperature T_A and mid-tropospheric global temperature T_G dtermines hurricane generation rate. From Zhao et al (2009).

Data assimilation

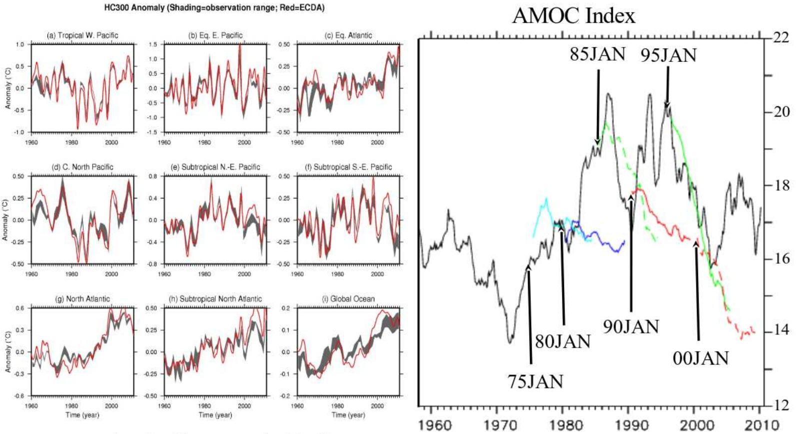


Data assimilation uses ensembles to find likely model trajectory taking into account model error and observational error. (Figure courtesy Zhang et al 2008).

Ensemble Coupled Data Assimilation (ECDA)



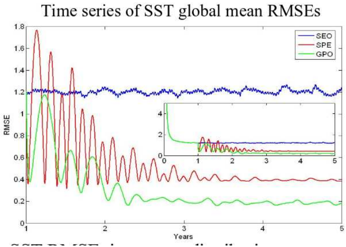
Model drift in decadal prediction

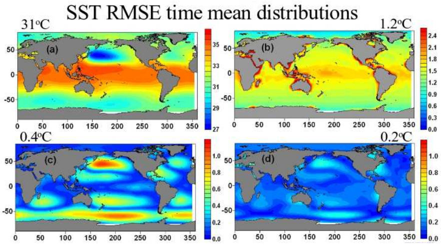


(Y.-S. Chang et al. 2012)

Figure courtesy Shaoqing Zhang and You-Soon Chang, NOAA/GFDL.

Adapting ECDA for parameter estimation





- Intermediate coupled model with 10 free parameters, all biased.
- SEO: State Estimation Only.
- SPE: Single Parameter Estimation, single-valued.
- GPO: Single Parameter Estimation, geographically dependent parameter optimization.
- Does not deconvolve structural uncertainty from parameter uncertainty.
- Can also be used for multi-parameter optimization (see Wu et al 2012a, 2012b).

Outline

The hardware jungle

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

- Intel/AMD x86 host coupled to NVIDIA GPU device: host launches many (32, 64, …) parallel threads on device.
- AMD Opteron/Firestream + AMD GPU: similar in structure to above, 64-bit FP registers.
- Firestream + AMD APU: integrated on-chip co-processor. Physical memory shared between host and device.
- Intel core + integrated Intel GPU (Ivy Bridge):.Intel version of above.
- Intel core + Intel MIC: still a host/device model but threads can be programmed in OpenMP.

The hardware jungle

More far-fetched stuff . . .

- NVIDIA Denver: ARM processor (low-power) + NVIDIA GPU: shared-memory.
- Texas Instruments! ARM + DSPs
- Convey: x86 + FPGAs. shared virtual memory, permits RMA.
- Tilera, FeiTeng: stream accelerators.
- BG/Q: CPU only, with OpenMP and vector instructions. Reportedly 8x faster than P. Memory/core is relatively small.

Some material above adapted from Wolfe (2012), in HPCWire.

The software zoo

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 for MICs that can also be implemented for GPUs.
- ACC from Portland Group: accelerator directives that will be treated as comments on non-compliant hardware. Now being proposed as a new standard OpenACC.
- PGAS languages: Co-Array Fortran, UPC, a host of proprietary languages.

The software 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, offload I/O.
- Other concerns:
  - Irreproducible computation
  - Tools for analyzing performance.
  - Debugging at scale.

Can frameworks hold the details of parallelism?

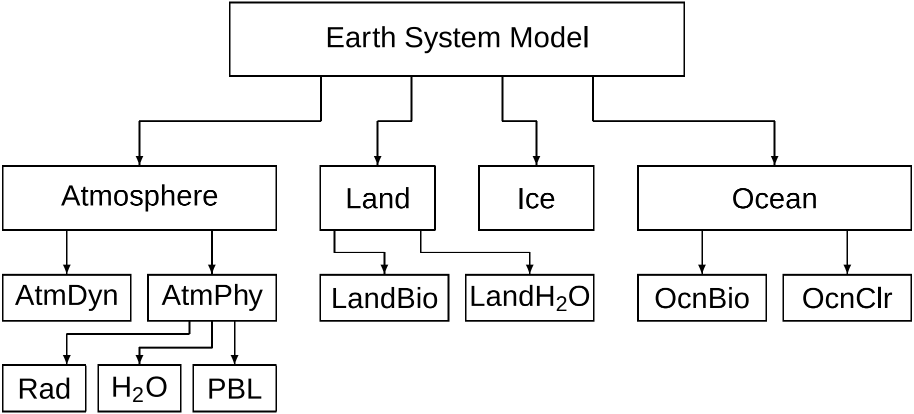
Existing and emerging modeling frameworks already implement distributed data objects.

Distributed array An `ESMF_Field` holds its distributed contents in an `ESMF_Array`, which already contains metadata describing distribution information (`DataMap`, `Layout`, `VM`). The actual (“naked”) local array can be attached and detached with no data copies.

```
type(ESMF_Field) ::  field
real ::  a(:,:,:)
a(:,:,:)  => ESMF_FieldGetDataPointer(field)
call ESMF_FieldHalo(field)
...  = a(i+1,j+1,k) + ...
```
(1)

Some current programming models (e.g CUDA for GPUs) are not amenable to a driver-kernel programming model.

ESM Architecture



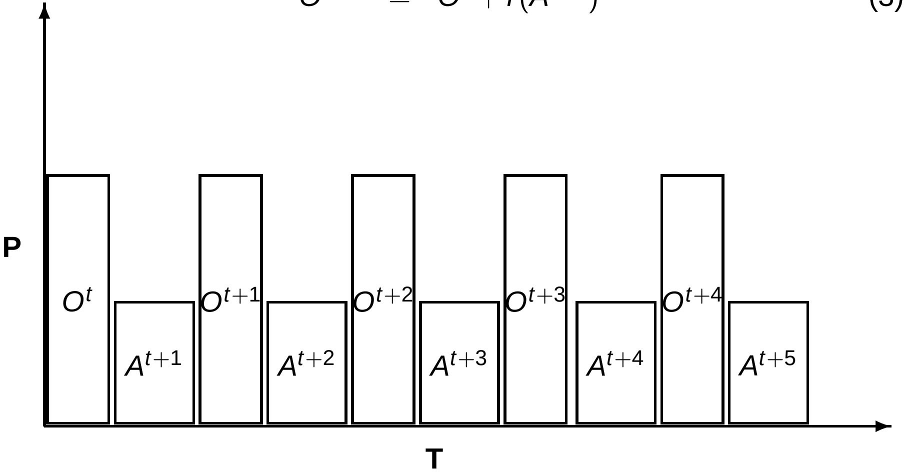
Extending component parallelism to $\mathcal{O}(10)$ requires a different physical architecture!

Serial coupling

Uses a forward-backward timestep for coupling.

$$A^{t+1} = A^t + f(O^t) \tag{2}$$

$$O^{t+1} = O^t + f(A^{t+1}) \tag{3}$$

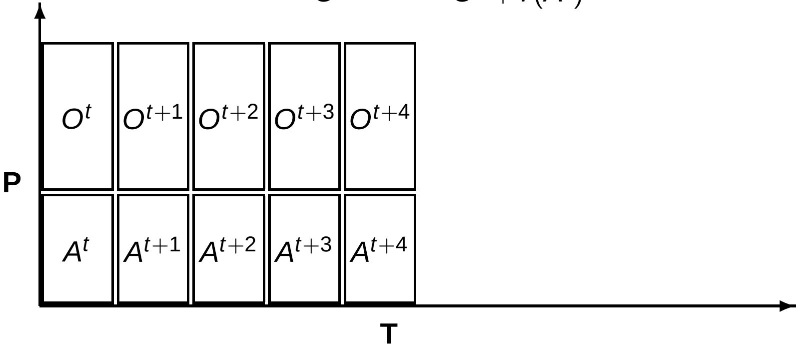


Concurrent coupling

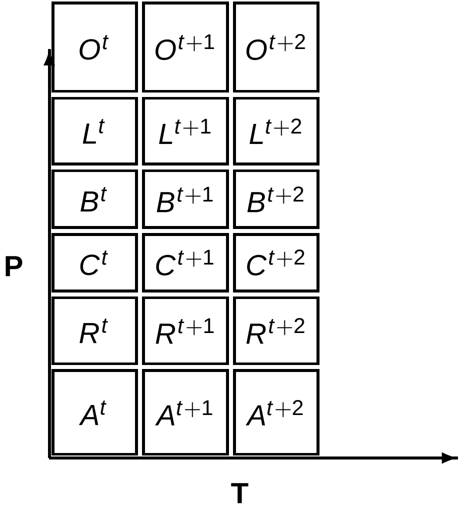
This uses a forward-only timestep for coupling. While formally this is unconditionally unstable, the system is strongly damped*. Answers vary with respect to serial coupling, as the ocean is now forced by atmospheric state from Δt ago.

$$A^{t+1} = A^t + f(O^t) \quad (4)$$

$$O^{t+1} = O^t + f(A^t) \quad (5)$$

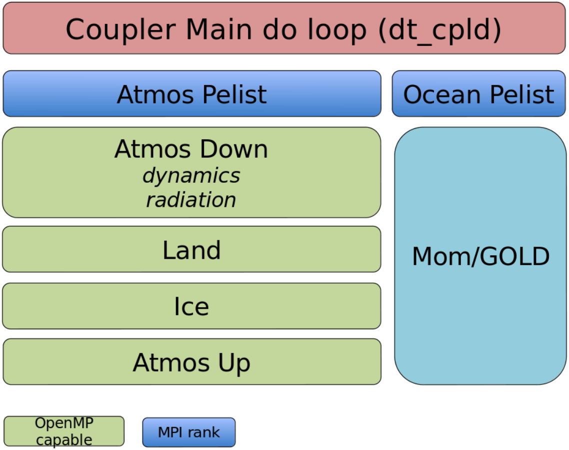


Massively concurrent coupling



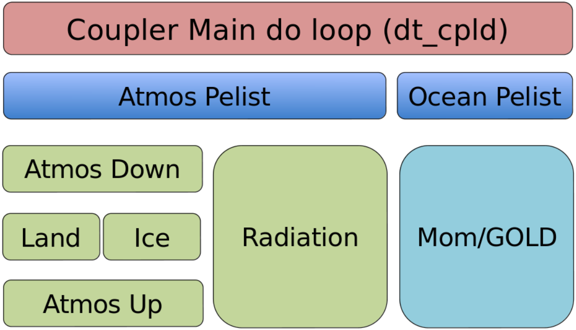
Components such as radiation, PBL, ocean barotropic solver, each could run with its own grid, timestep, decomposition, even hardware. Coupler mediates state exchange.

Traditional coupling sequence



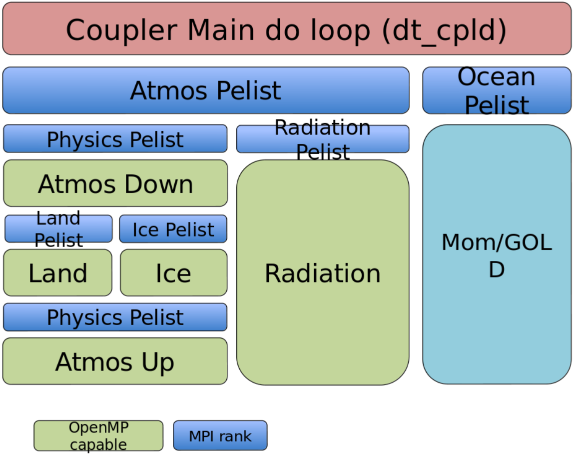
Radiation timestep much longer than physics timestep.
(Figure courtesy Rusty Benson, NOAA/GFDL).

Proposed coupling sequence



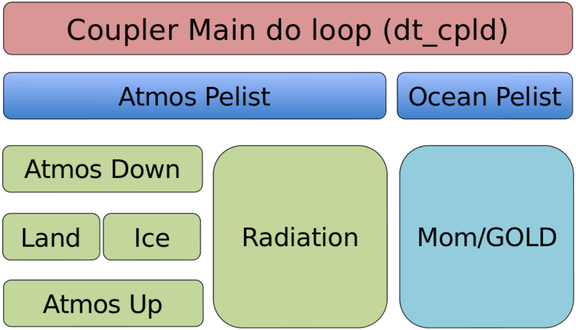
Radiation executes on physics timestep from lagged state.
(Figure courtesy Rusty Benson, NOAA/GFDL).

Proposed coupling sequence using pelists



Requires MPI communication between physics and radiation.
(Figure courtesy Rusty Benson, NOAA/GFDL).

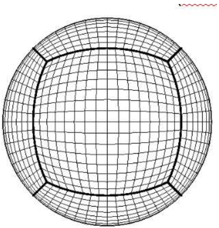
Proposed coupling sequence: hybrid approach



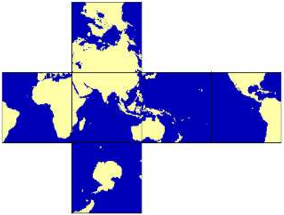
Physics and radiation share memory.
(Figure courtesy Rusty Benson, NOAA/GFDL).

Outline

Gnomonic Projection



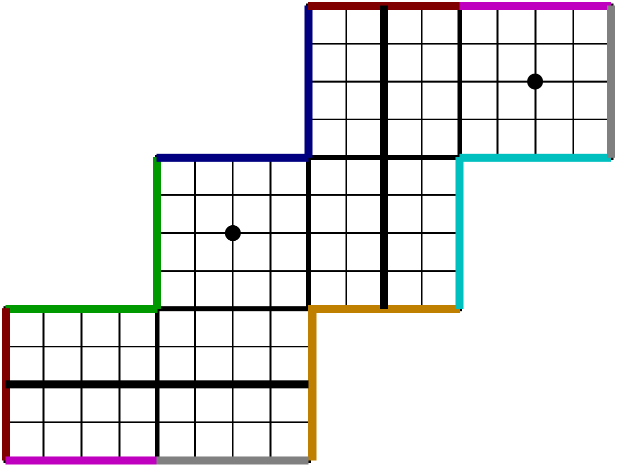
- True equal distance at the 12 edges of the cube
- All coordinate lines are great circles
- Coordinates are continuous at the edges; but derivatives are discontinuous



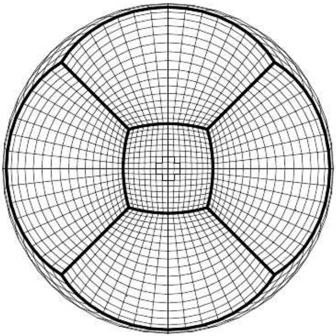
Putman and Lin, *J. Comp. Phys.* 2007.

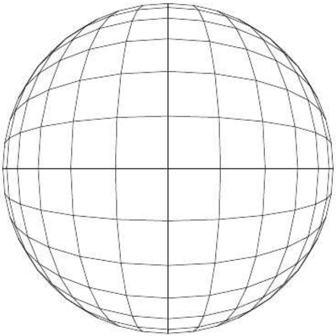
FMS index space representation of the cubed sphere

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



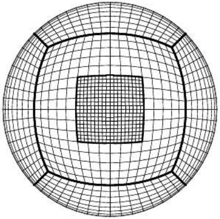
Stretched grids



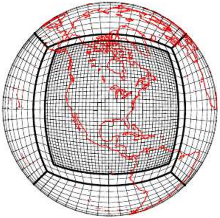


- Opposing face gets very coarse
- Discontinuities in slope
- Scale-aware parameterizations required

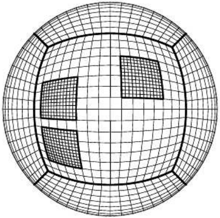
Nested grids



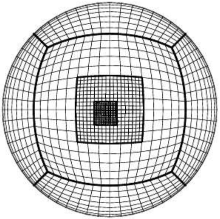
3:1 nested grid



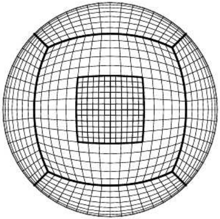
Large nest for RCMs



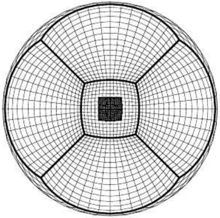
Multiple nests



Telescoping nests



2:1 nested grid



Nest in stretched grid

Lee vortices off Hawaii under two-way nesting

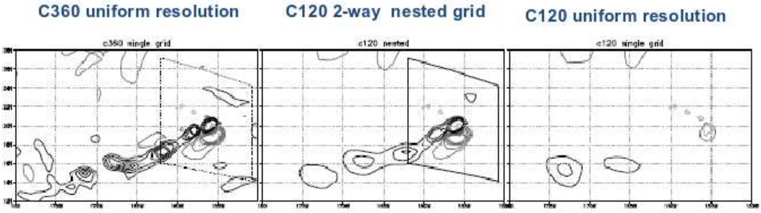
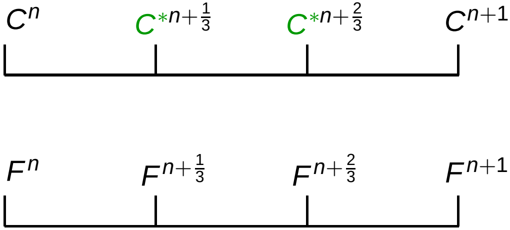


FIG. 15. Surface vorticity (contour interval 10^{-5} s^{-1}, negative values in gray, values above 5×10^{-5} s^{-1} not plotted) at $t = 72$ h in simulations initialized at 0000 UTC on 1 August 2010. Hawaii is at center-right in each panel. Dotted line in left-most panel shows where the nest would be in the nested-grid c120 simulation.

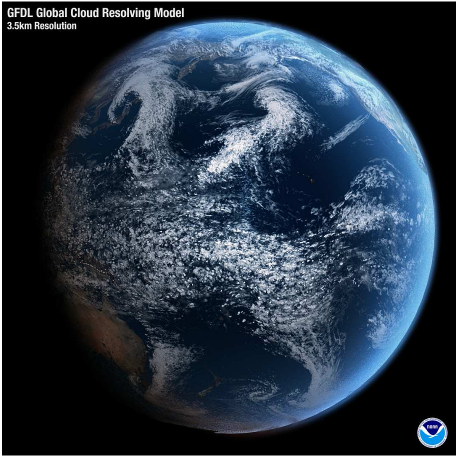
Figure courtesy Harris and Lin 2011, submitted to *Mon. Wea. Rev.*

Typical nesting protocols force serialization between fine and coarse grid timestepping, since the C^* are estimated by interpolating between C^n and C^{n+1}.



We enable concurrency by instead estimating the C^* by extrapolation from C^{n-1} and C^n, with an overhead of less than 10%. (See Harris and Lin 2012 for details.)

C2560: 3.5 km resolution global cloud-resolving model



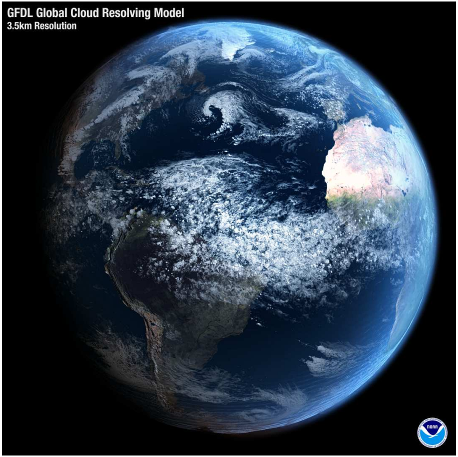


Figure courtesy S-J Lin and Chris Kerr, NOAA/GFDL.

Outline

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.

Challenges for the next generation of models

- Can we have high-level programming models or frameworks to take advantages of new approaches to parallelism? What are the right abstractions?
- Can component-level parallelism via framework superstructure be pushed to $\mathcal{O}(10)$?
- Can we approach models as experimental biological systems? (single organism or “cell line” not exactly reproducible; only the ensemble is.)
- How do we analyze and understand performance on a “sea of functional units” (Kathy Yelick’s phrase)?