# A tutorial on coupled modeling

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NCWCP
College Park MD

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NOAA/GFDL and Princeton University

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# Outline

1. The scientific basis for building coupled Earth system models
   - Atmospheres, oceans, clouds, ecosystems, photons, ...
   - Time and space scales
   - Dynamics and physics
2. The structure of a coupled Earth System Model
   - Components and grids
   - Conservation and accuracy
   - Timestepping and stability
   - The Exchange Grid
3. Coarse-grain concurrency
   - Concurrent physics example: radiation
   - Concurrent nesting
   - Ice-ocean boundary
   - Chemistry, dust, ...
4. Future approaches to coupling
   - Models as task graphs
5. Recap and bibliography

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# Atmospheric general circulation

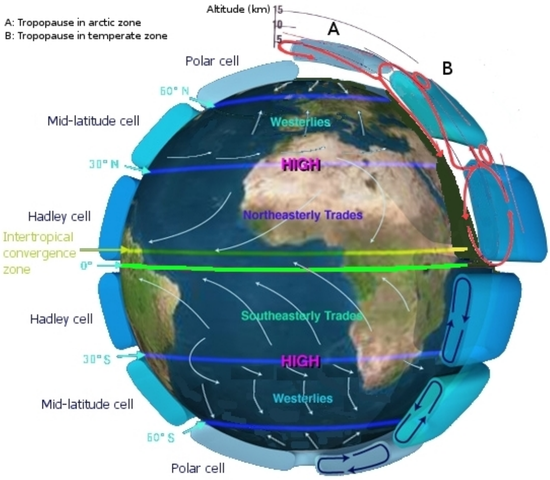



Figure courtesy NASA. Circulations driven by unequal heating on a rotating sphere.

# Ocean general circulation

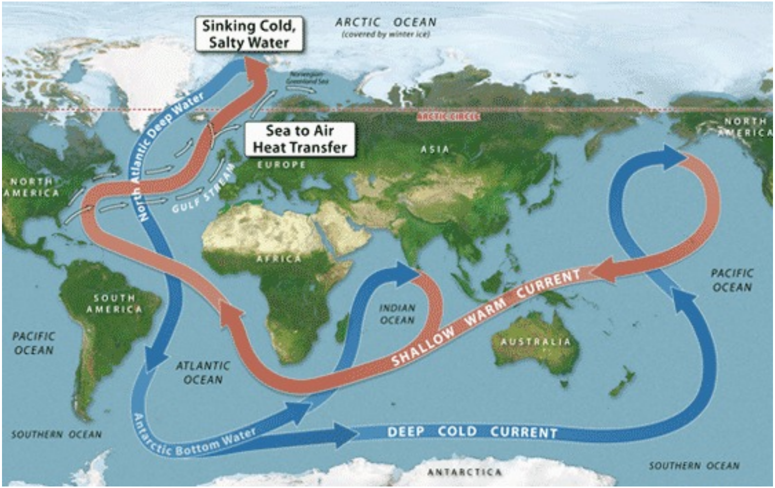



Figure courtesy Smithsonian Institution. Wind and radiation driven circulation of fluid with complex boundaries and terrain.

# Ecosystem interactions and the carbon cycle

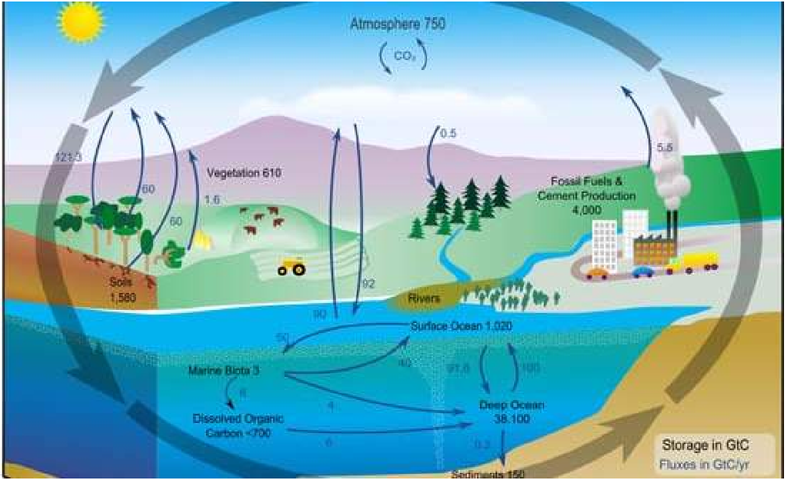



Figure courtesy NASA. Cycles exchange small amounts between large reservoirs.

# The global cloud field: a multiscale system

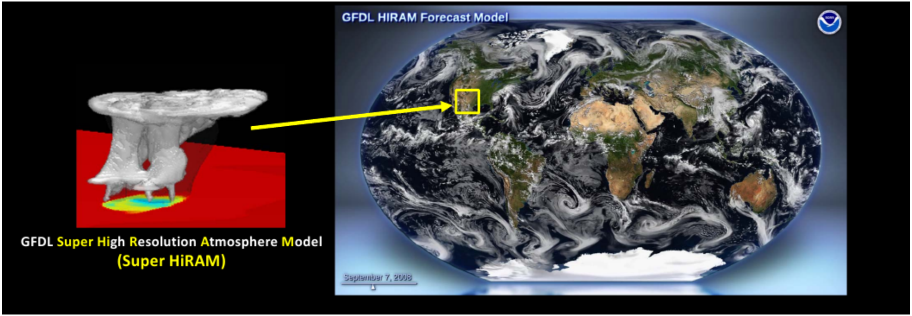



Figure courtesy S.-J. Lin and the FV3 team, NOAA/GFDL. Structure from metres to planetary scale. Does this image pass a climate Turing test?

# Earth Radiation budget

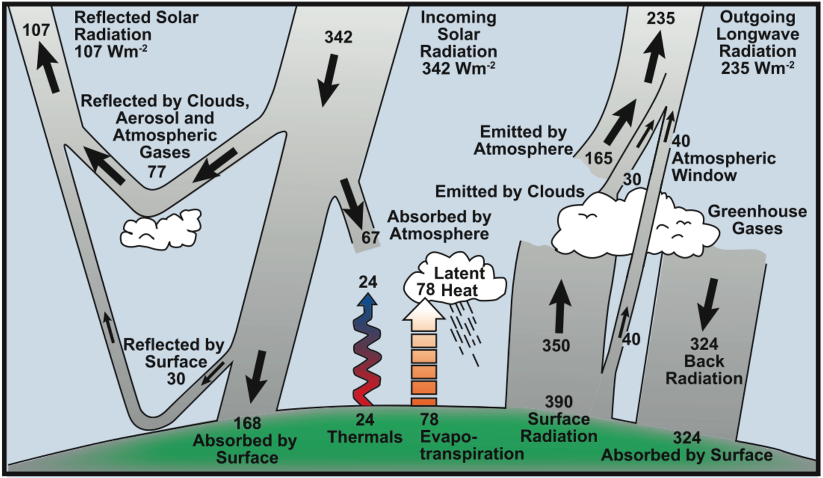



Figure courtesy IPCC FAQ. Warming results from a small net imbalance in the sum of many components and feedbacks.

# Atmospheric process scales

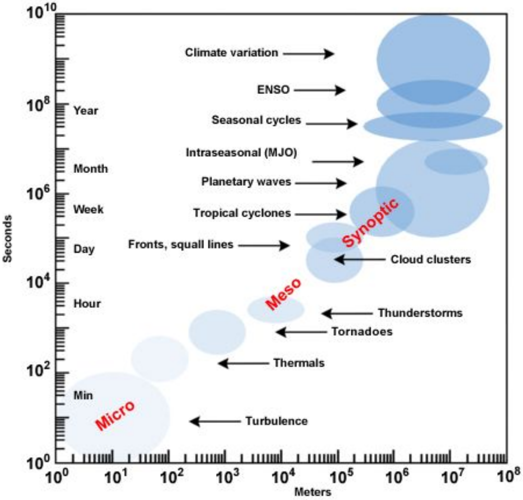



Figure courtesy UCAR.

# Oceanic process scales

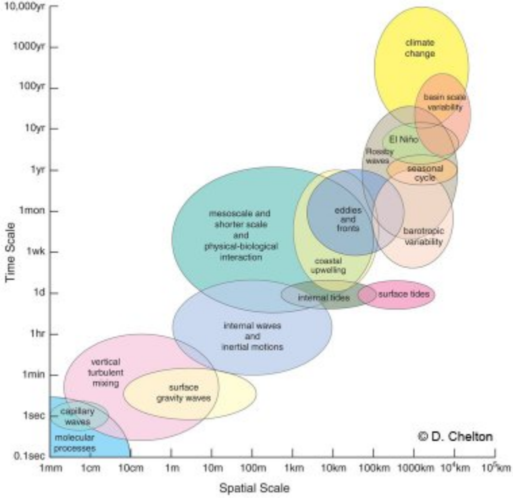
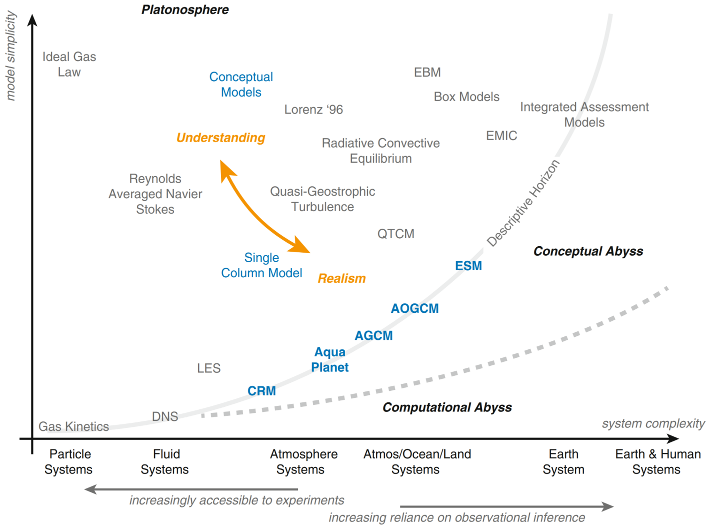


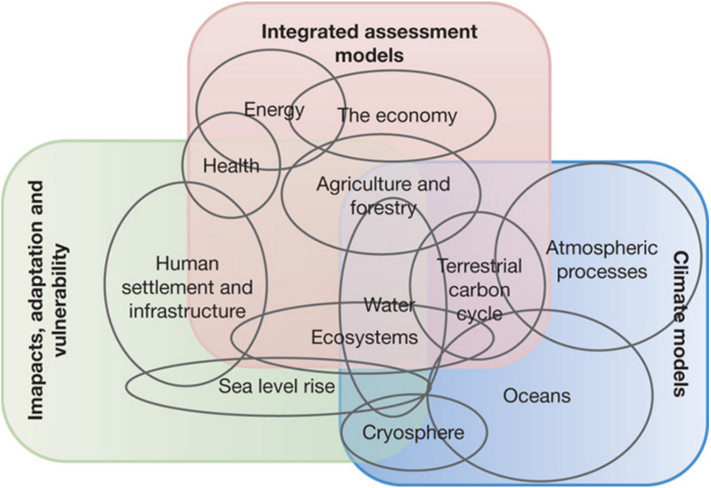

Figure courtesy Oregon State University.

# The model zoo



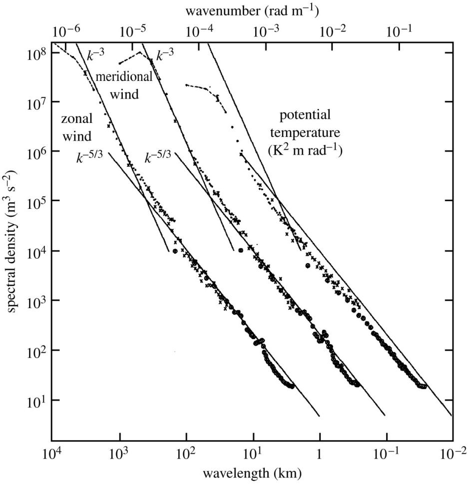

From Bony et al (2013).

# The brittleness of coupled systems




From Moss et al 2010. Coupling across this model chain is a social, scientific, semantic, and software challenge.

# No separation of "large" and "small" scales




Nastrom and Gage (1985). We arbitrarily truncate resolution at some point to separate “dynamics” from “physics”.

# Coupling terminology review

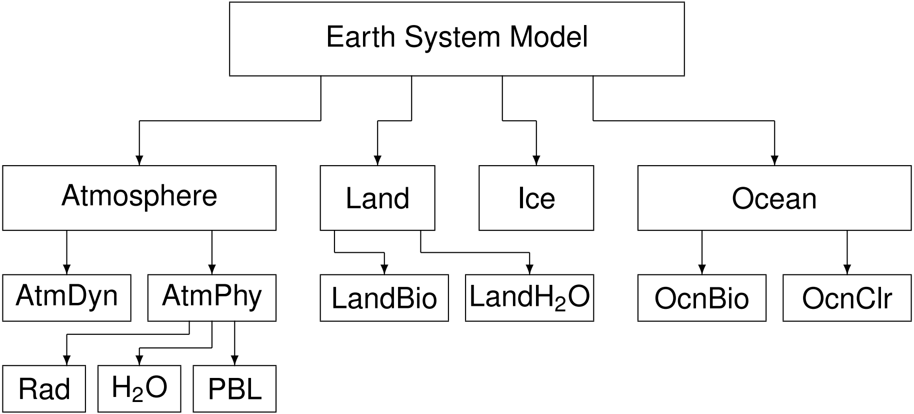
- Coupling: between different climate subsystems with feedbacks and fluxes in both directions.
- Nesting: a component of finer resolution coupled within the same component at coarser resolution.
  - One-way nesting: No feedback from fine-scale model to coarse-scale model (see also dynamical downscaling, regional or limited-area modeling).
  - Two-way nesting: fine-scale features feed back to modify coarse grid state.
- Chaining: models of different subsystems without feedback, e.g health, agriculture, human systems models.
- Dynamics and physics: resolved and unresolved scales of motion.

# Outline

# Earth system model evolution

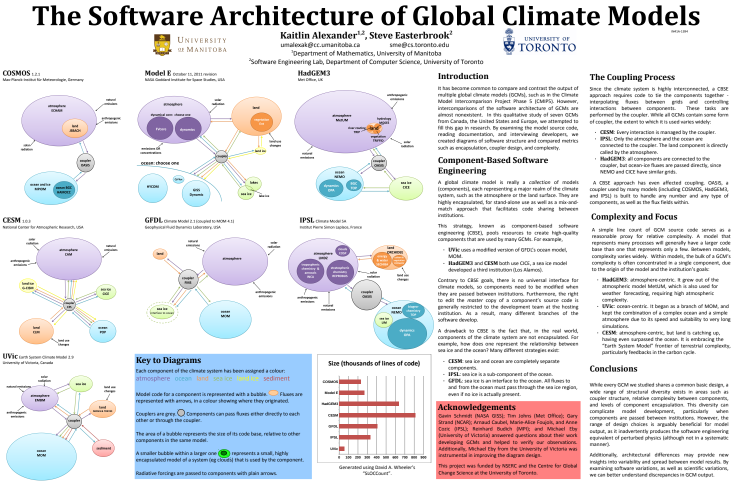

Figure courtesy IPCC.

# Notional Earth System Model Architecture




Component specialists must be free to choose algorithms, grids, discretizations, timestepping, ...

# Diversity of coupling architectures



# The Software Architecture of Global Climate Models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University of Toronto


IN41A-1394

**COSMOS** 1.2.1
Max-Planck-Institut für Meteorologie, Germany

**Model E** October 11, 2011 revision
NASA Goddard Institute for Space Studies, USA

**HadGEM3**
Met Office, UK

**CESM** 1.0.3
National Center for Atmospheric Research, USA

**GFDL** Climate Model 2.1 (coupled to MOM 4.1)
Geophysical Fluid Dynamics Laboratory, USA

**IPSL** Climate Model 5A
Institut Pierre Simon Laplace, France

**UVic** Earth System Climate Model 2.9
University of Victoria, Canada

## Key to Diagrams

Each component of the climate system has been assigned a colour:
atmosphere ocean land sea ice land ice sediment

Model code for a component is represented with a bubble. Fluxes are represented with arrows, in a colour showing where they originated.

Couplers are grey. Components can pass fluxes either directly to each other or through the coupler.

The area of a bubble represents the size of its code base, relative to other components in the same model.

A smaller bubble within a larger one represents a small, highly encapsulated model of a system (eg clouds) that is used by the component.

Radiative forcings are passed to components with plain arrows.

**Size (thousands of lines of code)**

COSMOS, Model E, HadGEM3, CESM, GFDL, IPSL, UVic

0 100 200 300 400 500 600 700 800 900

Generated using David A. Wheeler's "SLOCCount".

## Introduction

It has become common to compare and contrast the output of multiple global climate models (GCMs), such as in the Climate Model Intercomparison Project Phase 5 (CMIP5). However, intercomparisons of the software architecture of GCMs are almost nonexistent. In this qualitative study of seven GCMs from Canada, the United States and Europe, we attempted to fill this gap in research. By examining the model source code, reading documentation, and interviewing developers, we created diagrams of software structure and compared metrics such as encapsulation, coupler design, and complexity.

## Component-Based Software Engineering

A global climate model is really a *collection* of models (components), each representing a major realm of the climate system, such as the atmosphere or the land surface. They are highly encapsulated, for stand-alone use as well as a mix-and-match approach that facilitates code sharing between institutions.

This strategy, known as component-based software engineering (CBSE), pools resources to create high-quality components that are used by many GCMs. For example,

- **UVic** uses a modified version of GFDL's ocean model, MOM.
- **HadGEM3** and **CESM** both use CICE, a sea ice model developed a third institution (Los Alamos).

Contrary to CBSE goals, there is no universal interface for climate models, so components need to be modified when they are passed between institutions. Furthermore, the right to edit the *master* copy of a component's source code is generally restricted to the development team at the hosting institution. As a result, many different branches of the software develop.

A drawback to CBSE is the fact that, in the real world, components of the climate system are not encapsulated. For example, how does one represent the relationship between sea ice and the ocean? Many different strategies exist:

- **CESM**: sea ice and ocean are completely separate components.
- **IPSL**: sea ice is a sub-component of the ocean.
- **GFDL**: sea ice is an interface to the ocean. All fluxes to and from the ocean must pass through the sea ice region, even if no ice is actually present.


## Acknowledgements

Gavin Schmidt (NASA GISS); Tim Johns (Met Office); Gary Strand (NCAR); Arnaud Caubel, Marie-Alice Foujols, and Anne Cozic (IPSL); Reinhard Budich (MPI); and Michael Eby (University of Victoria) answered questions about their work developing GCMs and helped to verify our observations. Additionally, Michael Eby from the University of Victoria was instrumental in improving the diagram design.

This project was funded by NSERC and the Centre for Global Change Science at the University of Toronto.


## The Coupling Process

Since the climate system is highly interconnected, a CBSE approach requires code to tie the components together - interpolating fluxes between grids and controlling interactions between components. These tasks are performed by the coupler. While all GCMs contain some form of coupler, the extent to which it is used varies widely:

- **CESM**: Every interaction is managed by the coupler.
- **IPSL**: Only the atmosphere and the ocean are connected to the coupler. The land component is directly called by the atmosphere.
- **HadGEM3**: all components are connected to the coupler, but ocean-ice fluxes are passed directly, since NEMO and CICE have similar grids.

A CBSE approach has even affected coupling. OASIS, a coupler used by many models (including COSMOS, HadGEM3, and IPSL) is built to handle any number and any type of components, as well as the flux fields within.

## Complexity and Focus

A simple line count of GCM source code serves as a reasonable proxy for relative complexity. A model that represents many processes will generally have a larger code base than one that represents only a few. Between models, complexity varies widely. Within models, the bulk of a GCM's complexity is often concentrated in a single component, due to the origin of the model and the institution's goals:

- **HadGEM3**: atmosphere-centric. It grew out of the atmospheric model MetUM, which is also used for weather forecasting, requiring high atmospheric complexity.
- **UVic**: ocean-centric. It began as a branch of MOM, and kept the combination of a complex ocean and a simple atmosphere due to its speed and suitability to very long simulations.
- **CESM**: atmosphere-centric, but land is catching up, having even surpassed the ocean. It is embracing the "Earth System Model" frontier of terrestrial complexity, particularly feedbacks in the carbon cycle.

## Conclusions

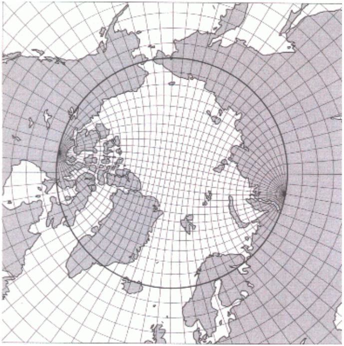
While every GCM we studied shares a common basic design, a wide range of structural diversity exists in areas such as coupler structure, relative complexity between components, and levels of component encapsulation. This diversity can complicate model development, particularly when components are passed between institutions. However, the range of design choices is arguably beneficial for model output, as it inadvertently produces the software engineering equivalent of perturbed physics (although not in a systematic manner).

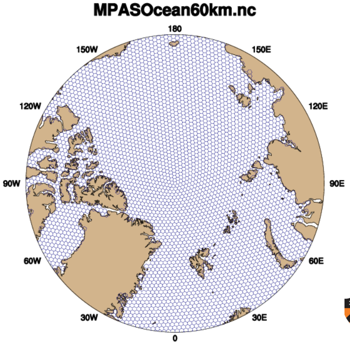
Additionally, architectural differences may provide new insights into variability and spread between model results. By examining software variations, as well as scientific variations, we can better understand discrepancies in GCM output.

Alexander and Easterbrook, AGU 2011.

# Diversity across model components

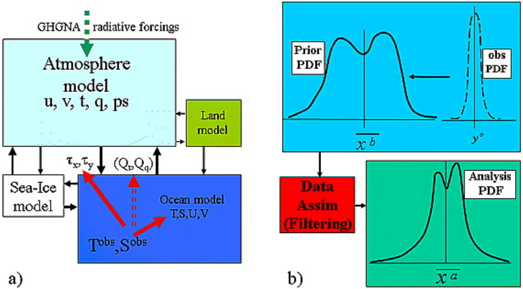
- Dycores: few key variables representing mass, momentum, energy but strong cross-cell dependencies. Wide range of numerics: FD, FV, FE methods all in active use.
- Land: no data dependencies across cells, but highly multivariate representations of ecosystem dynamics inside a cell.
- Numerical issues associated with poles and singularities.





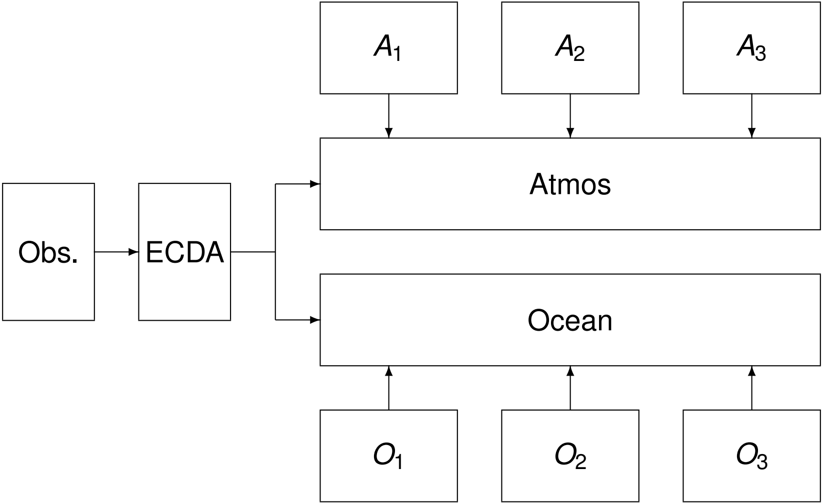
# Data assimilation

Zhang - 2008JC005261




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)



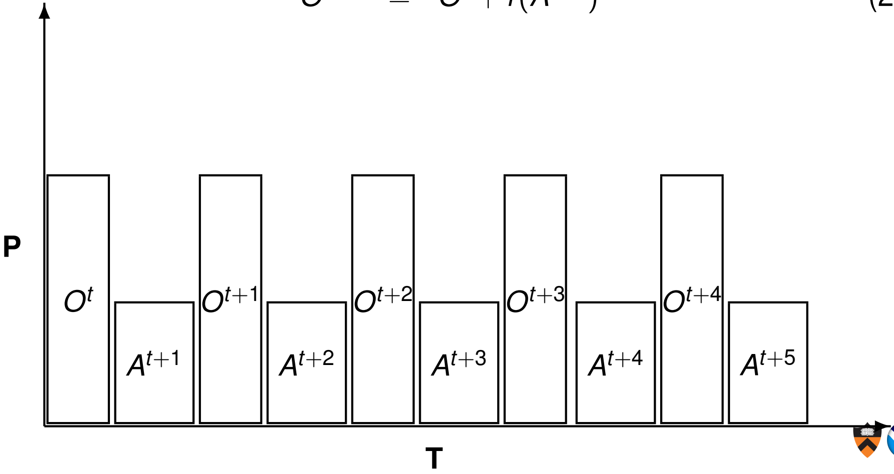

Components ("instances") execute in parallel.

# Serial coupling

Uses a forward-backward timestep for coupling.

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

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

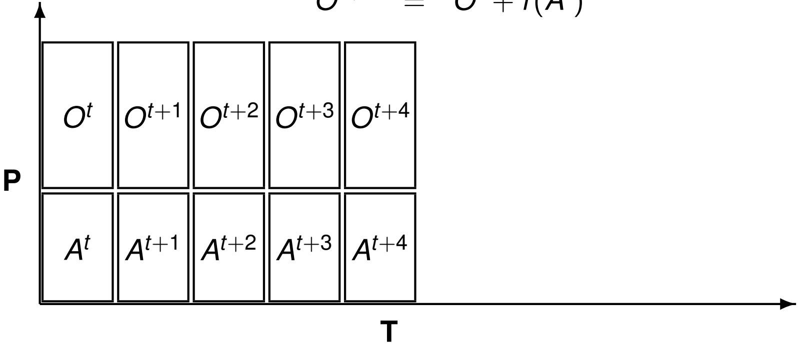


# Concurrent coupling

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 $\Delta t$ ago.

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

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



# Implicit coupling and the exchange grid

Fluxes at the surface often need to be treated using an implicit timestep. (e.g temperature flux in near-surface layers that can have vanishingly small heat capacity.)

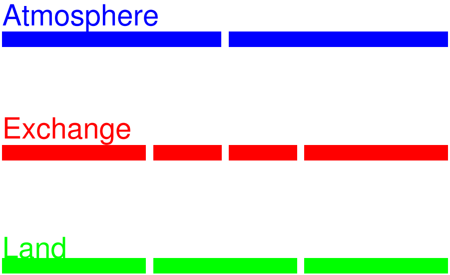
$$\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial z^2} \tag{5}$$

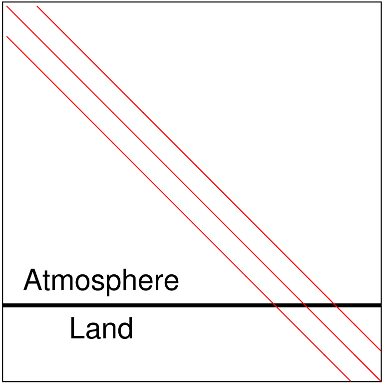
$$\frac{T_k^{n+1} - T_k^n}{\Delta t} = K\frac{T_{k+1}^{n+1} + T_{k-1}^{n+1} - 2T_k^{n+1}}{\Delta z^2} \tag{6}$$

$$\mathbf{A}\mathbf{T}^{n+1} = \mathbf{T}^n \tag{7}$$

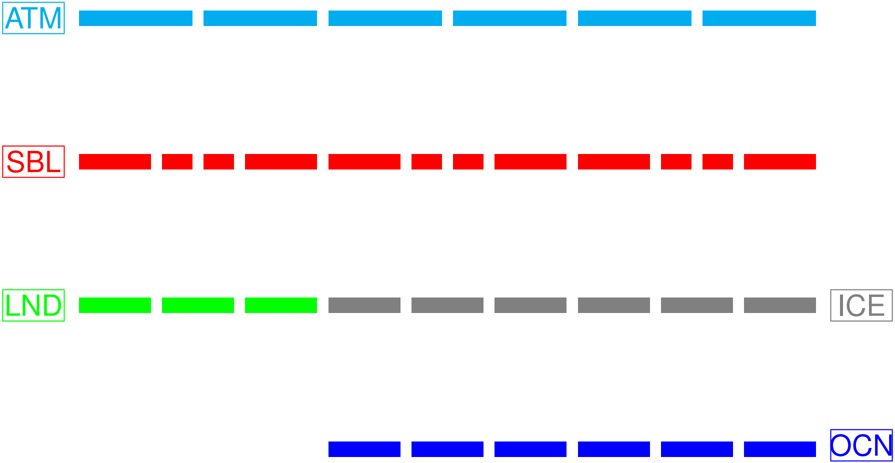
# Implicit coupling and the exchange grid

Tridiagonal solver in Eq. 7 across multiple components and grids.



# Coupled architecture with SBL on exchange grid



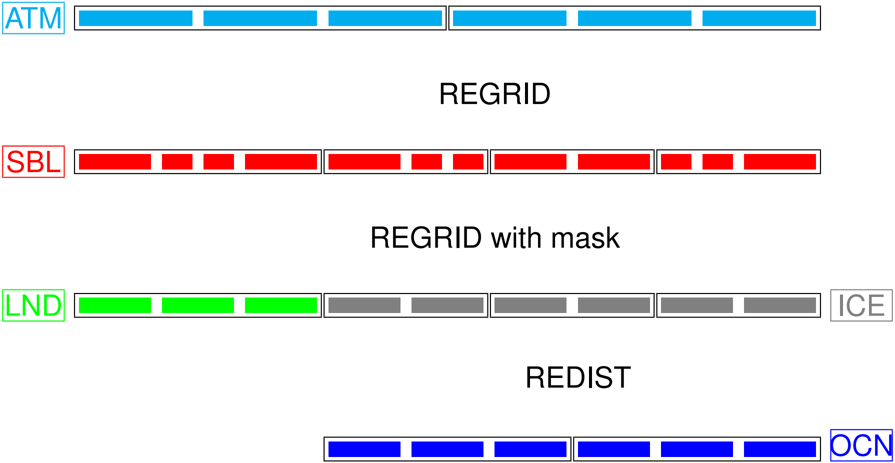
# Flux exchange

Three types of flux exchange are permitted: **REGRID**, **REDIST** and **DIRECT**.

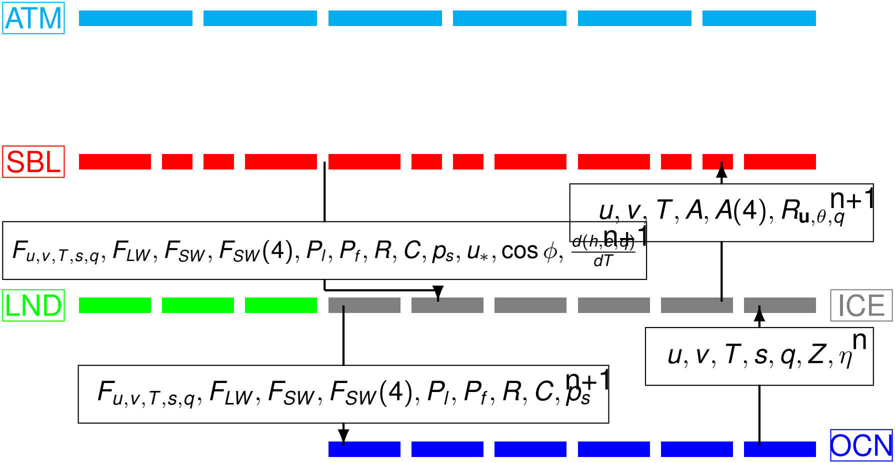
- REGRID: physically distinct grids, requires exchange grid.
- REDIST: identical global grid, different domain decomposition.
- DIRECT: identical grid and decomposition.

Current use: **REGRID** between **atmos**$\Longleftrightarrow$**ice**, **atmos**$\Longleftrightarrow$**land**, **land**$\Longleftrightarrow$**ice**, **REDIST** between **ocean**$\Longleftrightarrow$**ice**.

# Parallelism in the FMS coupler



# FMS coupled architecture: ice-ocean coupling



# Exchange grid: features

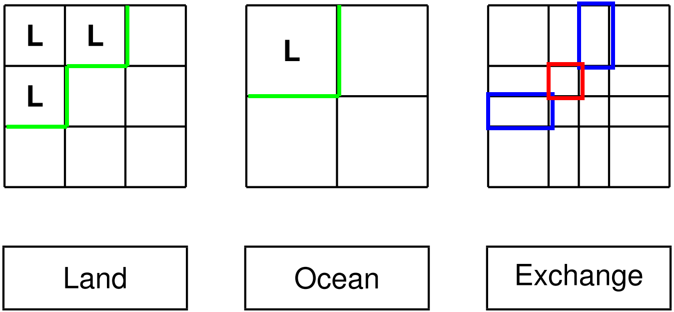
- Each cell on exchange grid "belongs" to one cell on each parent grid;
- Conservative interpolation up to second order; monotonicity can be imposed (required for positive-definite quantities).
- All calls exchange local data; data-sharing among processors is internal to the exchange software, and non-blocking.
- Physically identical grids (e.g ocean and sea ice) exchange data without interpolation.
- Exchange grid is computed and stored offline following a gridspec netCDF "standard".

# Exchange grid size

| Atmosphere | Ocean | Xgrid | Density | Scalability |
|---|---|---|---|---|
| 144×90 | 360×200 | 79644 | $8.5 \times 10^{-5}$ | 0.29 |
| 288×180 | 1080×840 | 895390 | $1.9 \times 10^{-5}$ | 0.56 |

Exchange grid sizes for typical climate model grids. The first column shows the horizontal discretization of an atmospheric model at “typical” climate resolutions of 2°and 1°respectively. The **`ocean`** column shows the same for an ocean model, at 1°and $\frac{1}{3}^{\circ}$. The **`Xgrid`** column shows the number of points in the computed exchange grid, and the density relates that to the theoretical maximum number of exchange grid cells. The **`scalability`** column shows the load imbalance of the exchange grid relative to the overall model when it inherits its parallel decomposition from one of the parent grids.

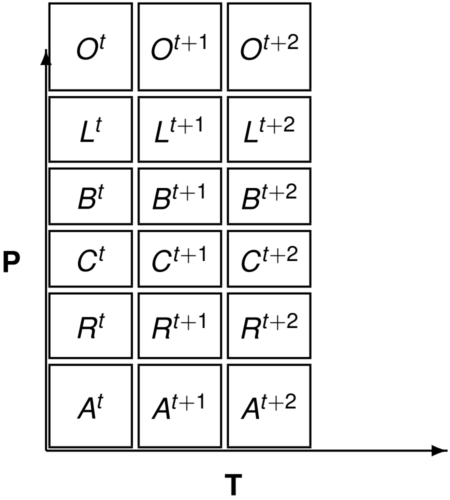
# The mask problem




An issue arises when grids of two independent components (e.g land and sea) share a boundary. The boundary is defined by a **mask** (e.g land-sea mask) but the mask is discretized independently on the two grids. However, exchange grid cells need to be uniquely assigned to a single component. This means that some cells get **clipped** on one or the other grid. In FMS, by convention, we choose to clip the land grid.

# Outline

# Massively concurrent coupling




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

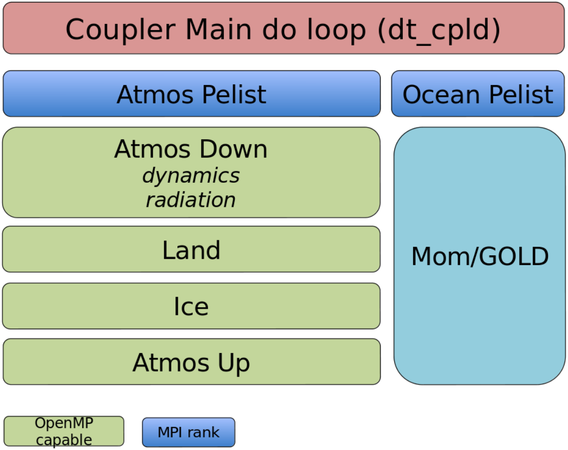
# The radiation component

The atmospheric radiation component computes radiative transfer of incoming shortwave solar fluxes and outgoing longwave radiation as a function of all radiatively active species in the atmosphere (greenhouse gases, aerosols, particulates, clouds, ...).

- The physics of radiative transfer is relatively well-known, but a full Mie-scattering solution is computationally out of reach.
- Approximate methods (sampling the “line-by-line” calculation into “bands”) have been in use for decades, and “standard” packages like RRTM are available.
- They are still very expensive: typically $\Delta t_{rad} > \Delta t_{phy}$ (in the GFDL models typically 9X). The model is sensitive to this ratio.
- Other methods: stochastic sampling of bands (Pincus and Stevens 2013), neural nets (Krasnopolsky et al 2005)

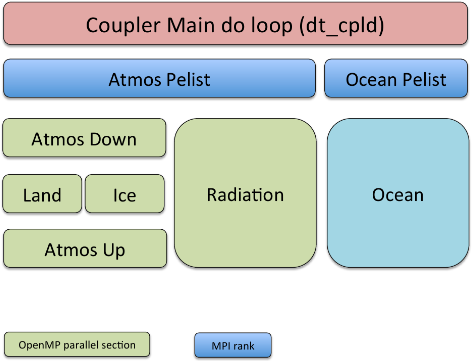
Challenge: can we exploit “cheap flops” to set $\Delta t_{rad} = \Delta t_{phy}$?

# Traditional coupling sequence



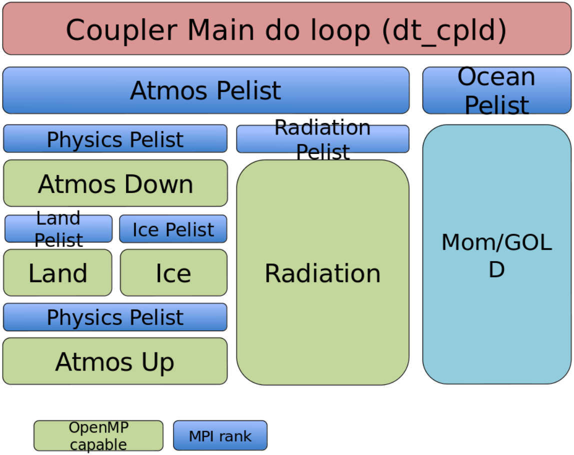

Radiation timestep much longer than physics timestep.
(Figure courtesy Rusty Benson, NOAA/GFDL).

# Concurrent coupling sequence



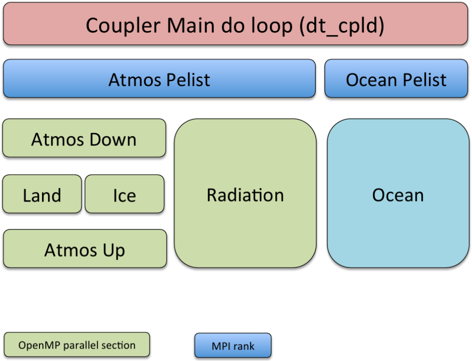

Radiation executes on physics timestep from lagged state.
(Figure courtesy Rusty Benson, NOAA/GFDL).

# Concurrent coupling sequence using pelists




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

# Concurrent coupling sequence: hybrid approach




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

# Results from climate run

20 year AMIP/SST climate runs have completed on Gaea (Cray XE6).

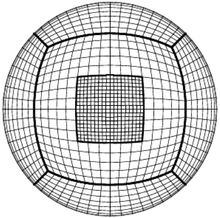
- Control: 9.25 sypd
  - $\Delta t_{rad} = 9\Delta t_{phy}$
  - 864 MPI-ranks / 2 OpenMP threads
- Serial Radiation: 5.28 sypd
  - $\Delta t_{rad} = \Delta t_{phy}$
  - 864 MPI-ranks / 2 OpenMP threads
- Concurrent Radiation: 5.90 sypd
  - $\Delta t_{rad} = \Delta t_{phy}$
  - 432 MPI-ranks / 4 OpenMP threads (2 atmos + 2 radiation)
  - Can get back to 9 sypd at about $\sim$2700 cores (roughly 1.6X).

Comparison of Concurrent Radiation to Control

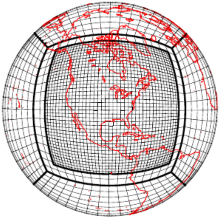
- climate is similar
- TOA balance is off by $\sim 4W/m^2$, mostly in the short wave, but easily retuned when ready to deploy

See Balaji et al (2016).

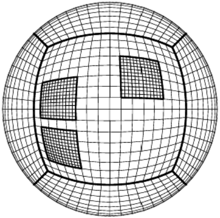
# Cubed-sphere grid with nests



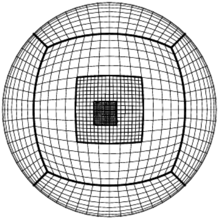
3:1 nested grid



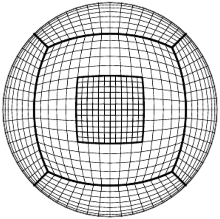
Large nest for RCMs



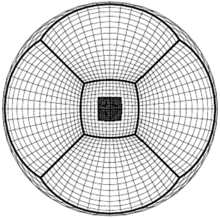
Multiple nests



Telescoping nests



2:1 nested grid

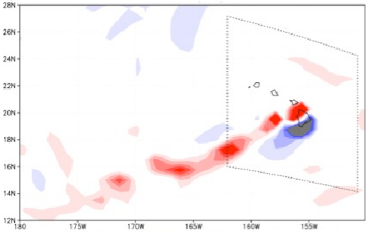


Nest in stretched grid

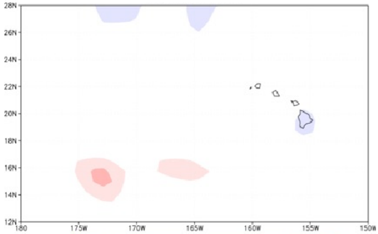
# Lee vortices off Hawaii under two-way nesting

- 72 hr forecast from 1 Aug 2010 00Z with real topography
- Showing Vorticity × $10^5$


c360 single grid




c120 single grid




c120 nested grid

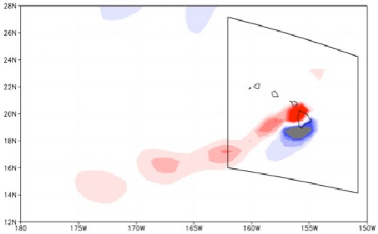
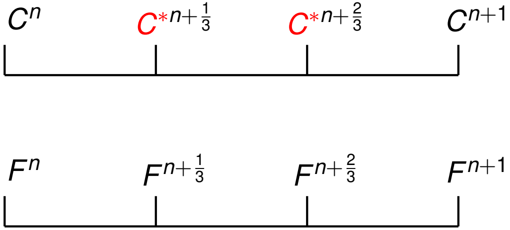



Figure courtesy Lucas Harris and S-J Lin, NOAA/GFDL.

# Concurrent two-way nesting

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.)

# Concurrent coupling: possible stability issues

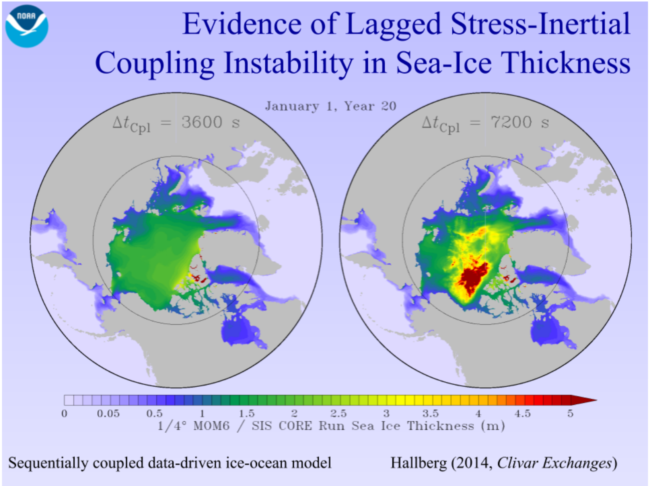



Figure courtesy Bob Hallberg (GFDL).

# Concurrent coupling: possible stability issues

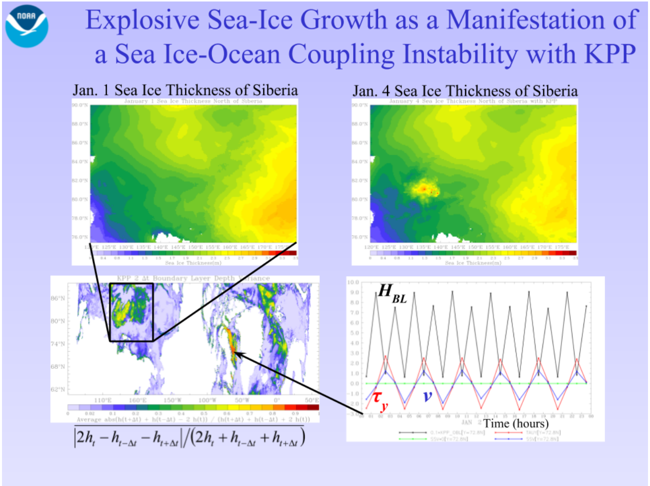



Figure courtesy Bob Hallberg (GFDL).

## Sequential coupling

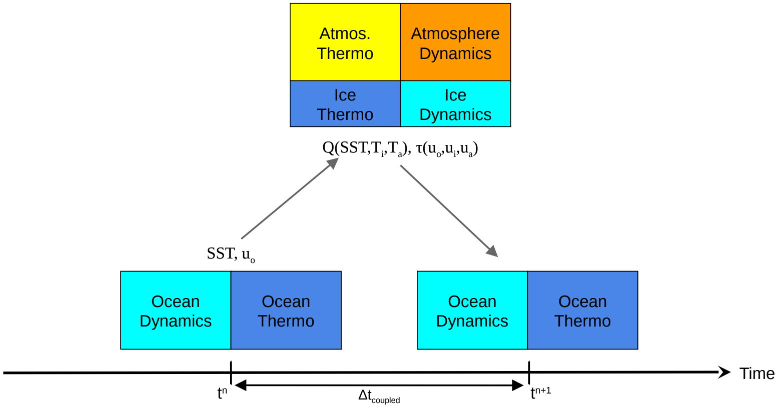



Figure courtesy Alistair Adcroft, Princeton and GFDL.

## Concurrent coupling

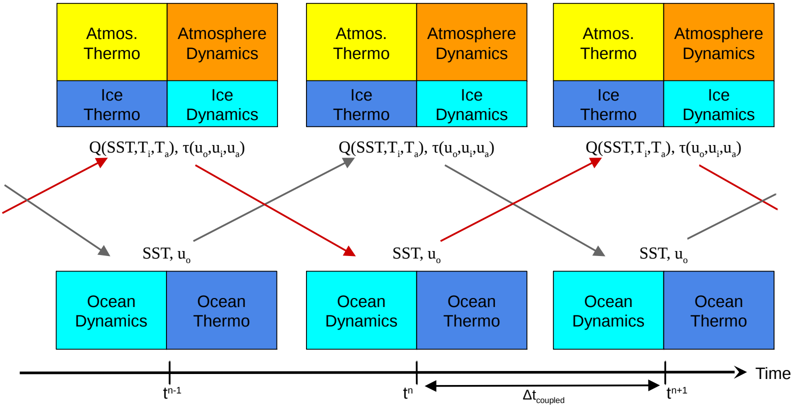



Figure courtesy Alistair Adcroft, Princeton and GFDL.

# Ice-ocean boundary

## Embedding SIS2

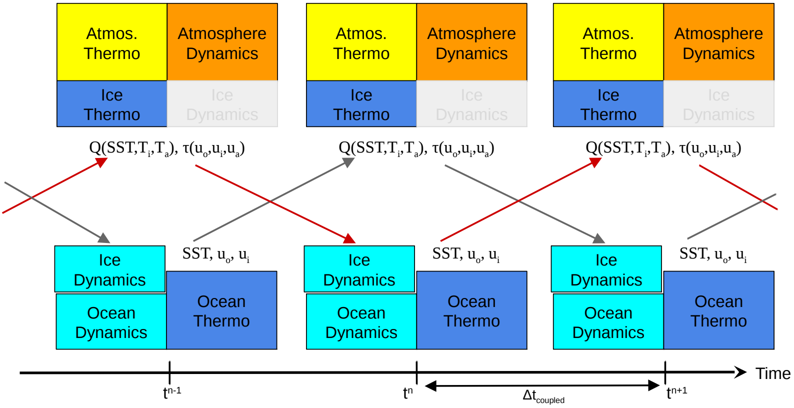



Figure courtesy Alistair Adcroft, Princeton and GFDL.

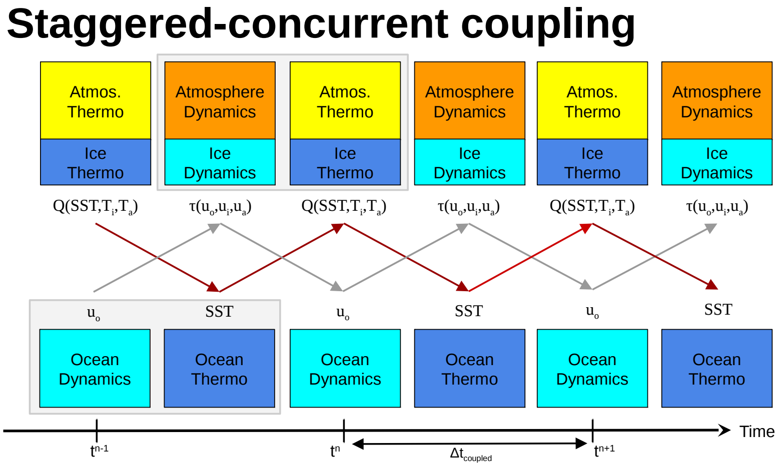



Figure courtesy Alistair Adcroft, Princeton and GFDL.

# Sequential coupling + Adams-Bashforth

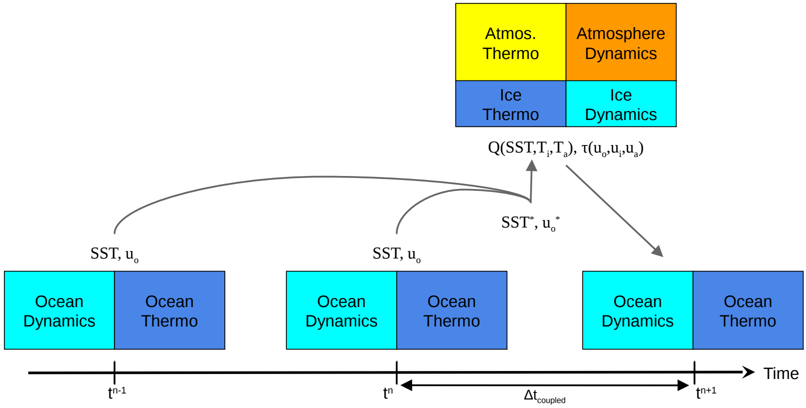



Figure courtesy Alistair Adcroft, Princeton and GFDL.

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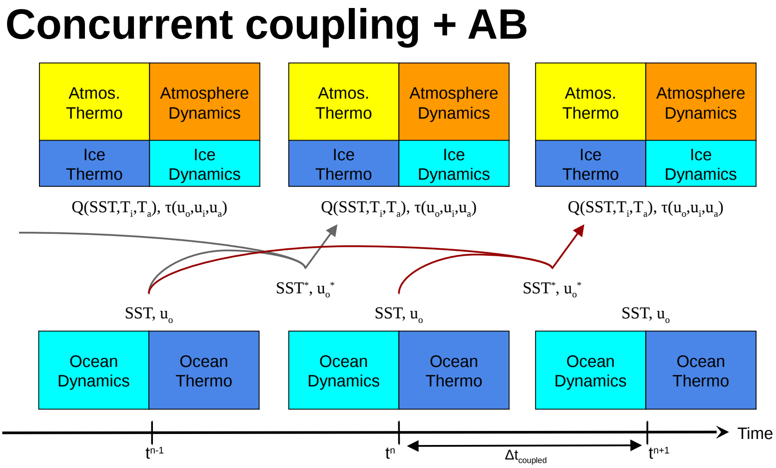



Figure courtesy Alistair Adcroft, Princeton and GFDL.

# Ice-ocean boundary

## Staggered-concurrent coupling + AB

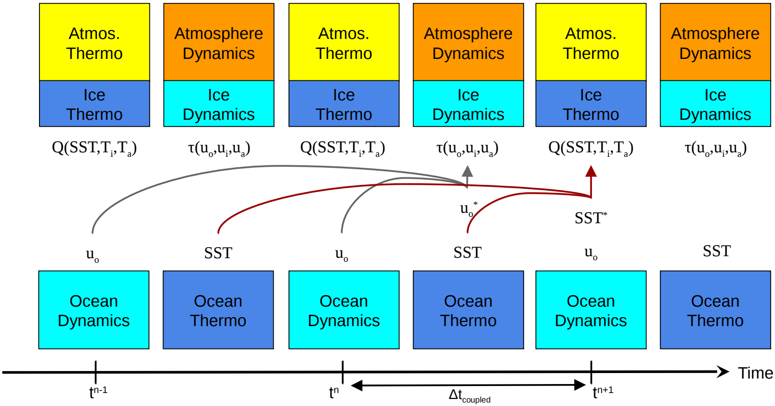



Figure courtesy Alistair Adcroft, Princeton and GFDL.

# Concurrent chemistry

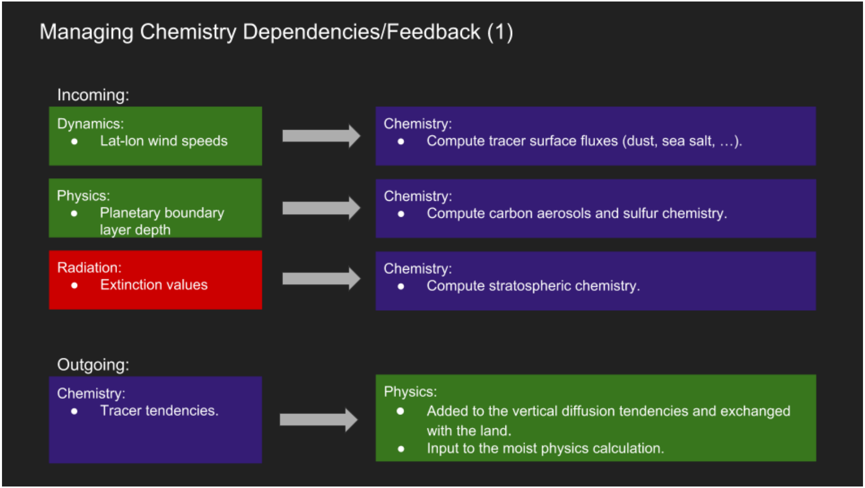
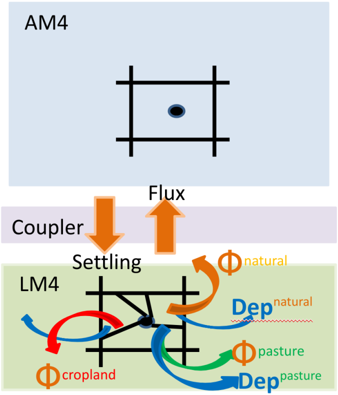



Figure courtesy Ray Menzel, Engility and GFDL.

# Dust in the the FMS Coupler




- Dust exchange calculated within vegetation canopy
- cells partitioned in tiles
- “settling” and “turbulent fluxes” between atmosphere and canopy,
- emission parameters tuned to match present day observations
- wet and dry deposition
- Same design serves for nitrogen coupling

- GFDL Exchange Grid continually evolves as science evolves
- GFDL/OAR implementing exchange grid in community coupler

Courtesy Paul Ginoux, Elena Shevliakova, Niki Zadeh, NOAA/GFDL

# Outline

# Examples of DAG parallelism

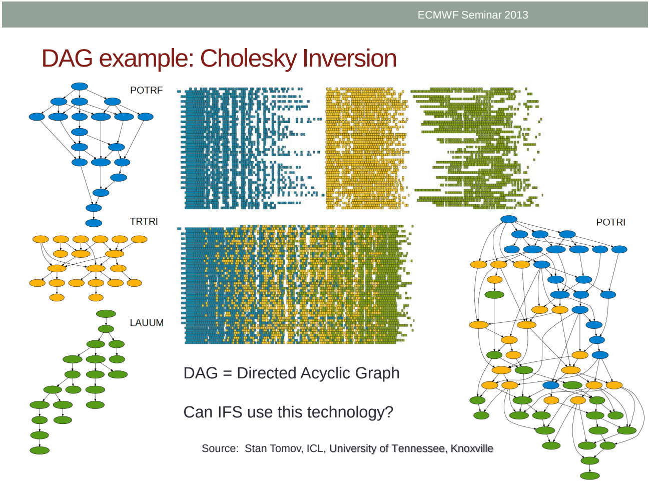
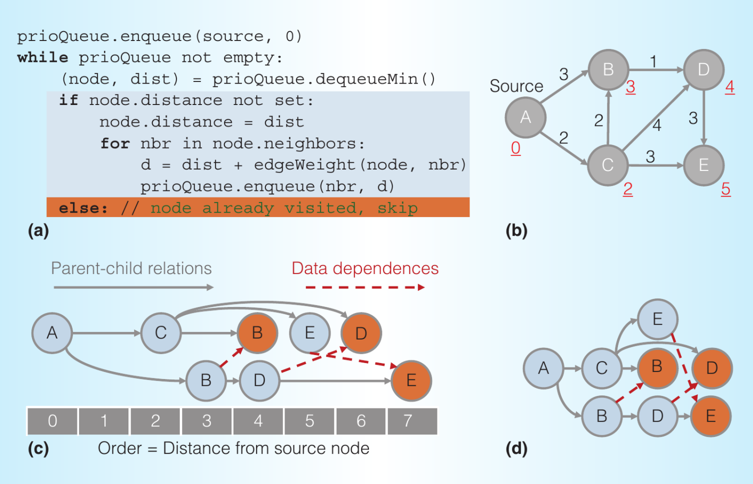



Figure courtesy George Mozdzynski, ECMWF.

# SWARM for DAGs




Jeffrey et al, *IEEE Micro* 2016.

# Outline

1. The scientific basis for building coupled Earth system models
   - Atmospheres, oceans, clouds, ecosystems, photons, ...
   - Time and space scales
   - Dynamics and physics
2. The structure of a coupled Earth System Model
   - Components and grids
   - Conservation and accuracy
   - Timestepping and stability
   - The Exchange Grid
3. Coarse-grain concurrency
   - Concurrent physics example: radiation
   - Concurrent nesting
   - Ice-ocean boundary
   - Chemistry, dust, ...
4. Future approaches to coupling
   - Models as task graphs
5. Recap and bibliography

# Recap

- Coupling, nesting, chaining
- "Chained" models that become coupled
- "Small differences between large quantities"
- Implicit vs explicit coupling
- Exchange grid
- Land-sea mask
- Use of couplers in data assimilation
- Coarse-grained concurrency

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# Bibliography


- "The Exchange Grid: A mechanism for data exchange between Earth System components on independent grids". Balaji et al (2005).
- Springer Monograph "Coupling Software and Strategies" Valcke et al (2012): covers multiple coupler implementations: ESMF, FMS, MCT, Oasis, TDT, ...
- "Climate Computing: The State of Play" Balaji 2015.
- "Coarse-grained component concurrency in Earth system modeling". Balaji et al (2016).
- Workshop series on "Coupling Technologies for Earth System Models: most recent (4th) workshop was CW2017.