Building state-of-the-art Earth System Models

Presented by Matt Norman
(with contributions from others in the ESM theme)

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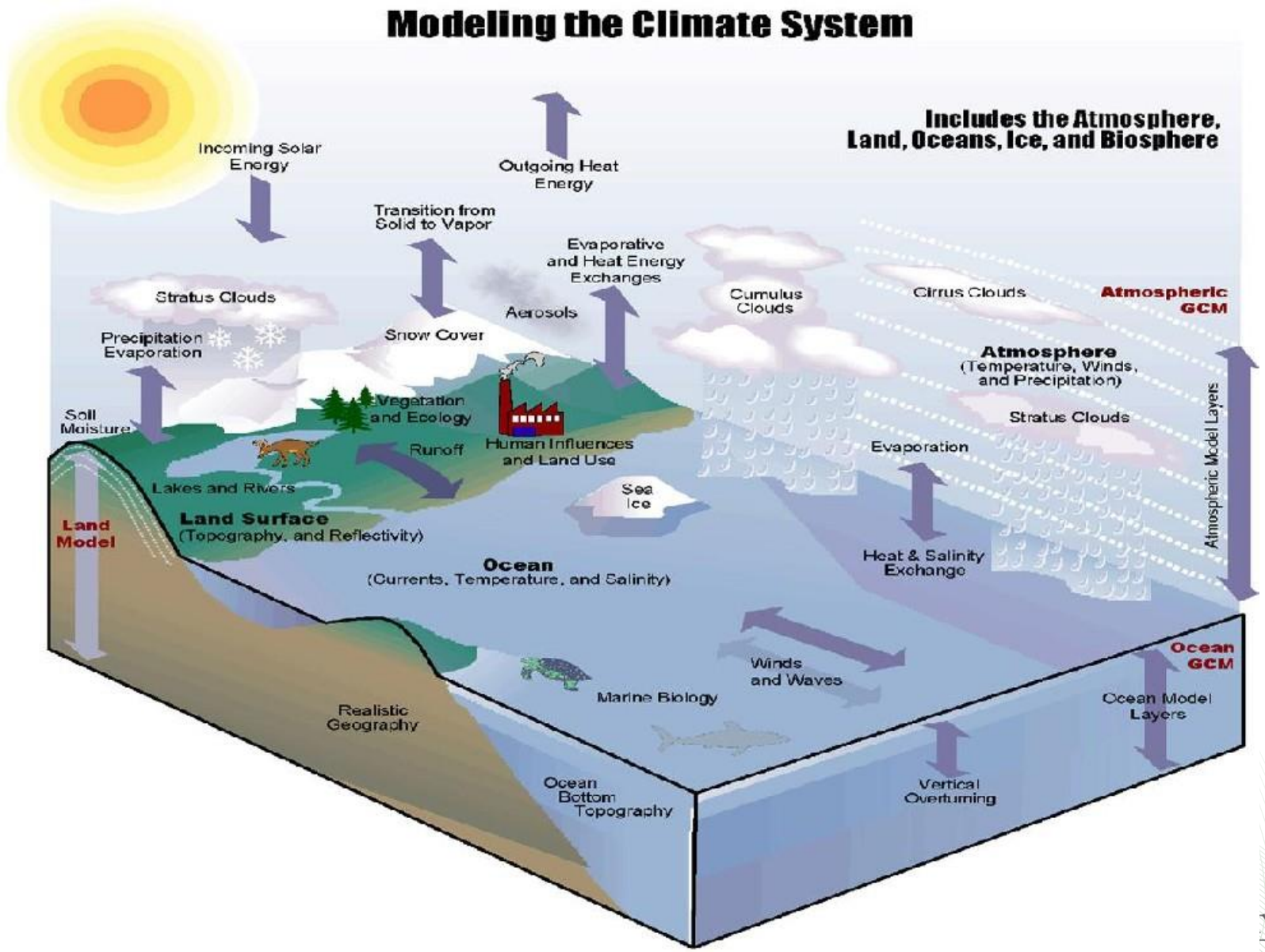
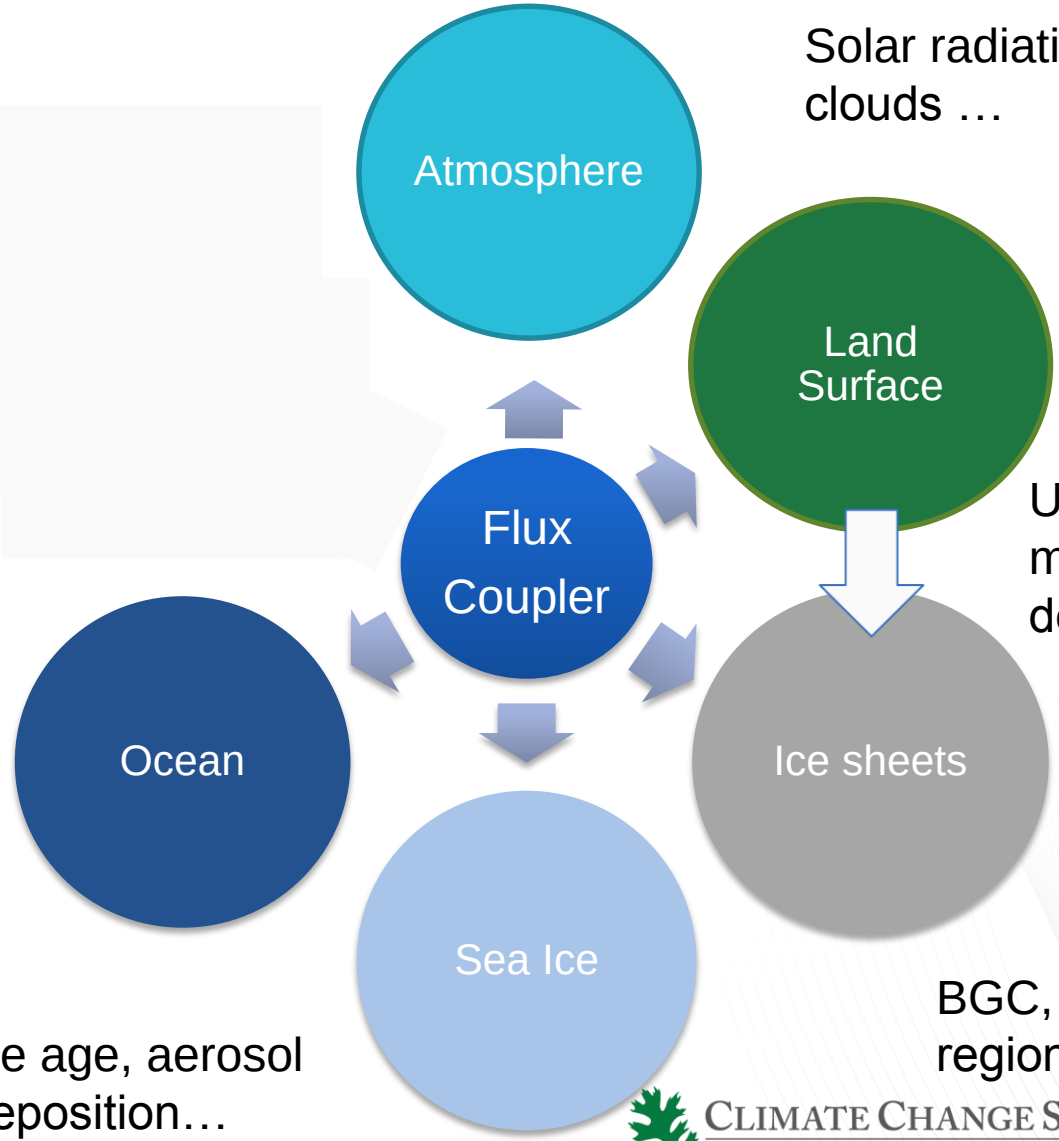
The Earth system is complicated.



Climate Models comprise a collection of components



Solar radiation, chemistry, clouds …

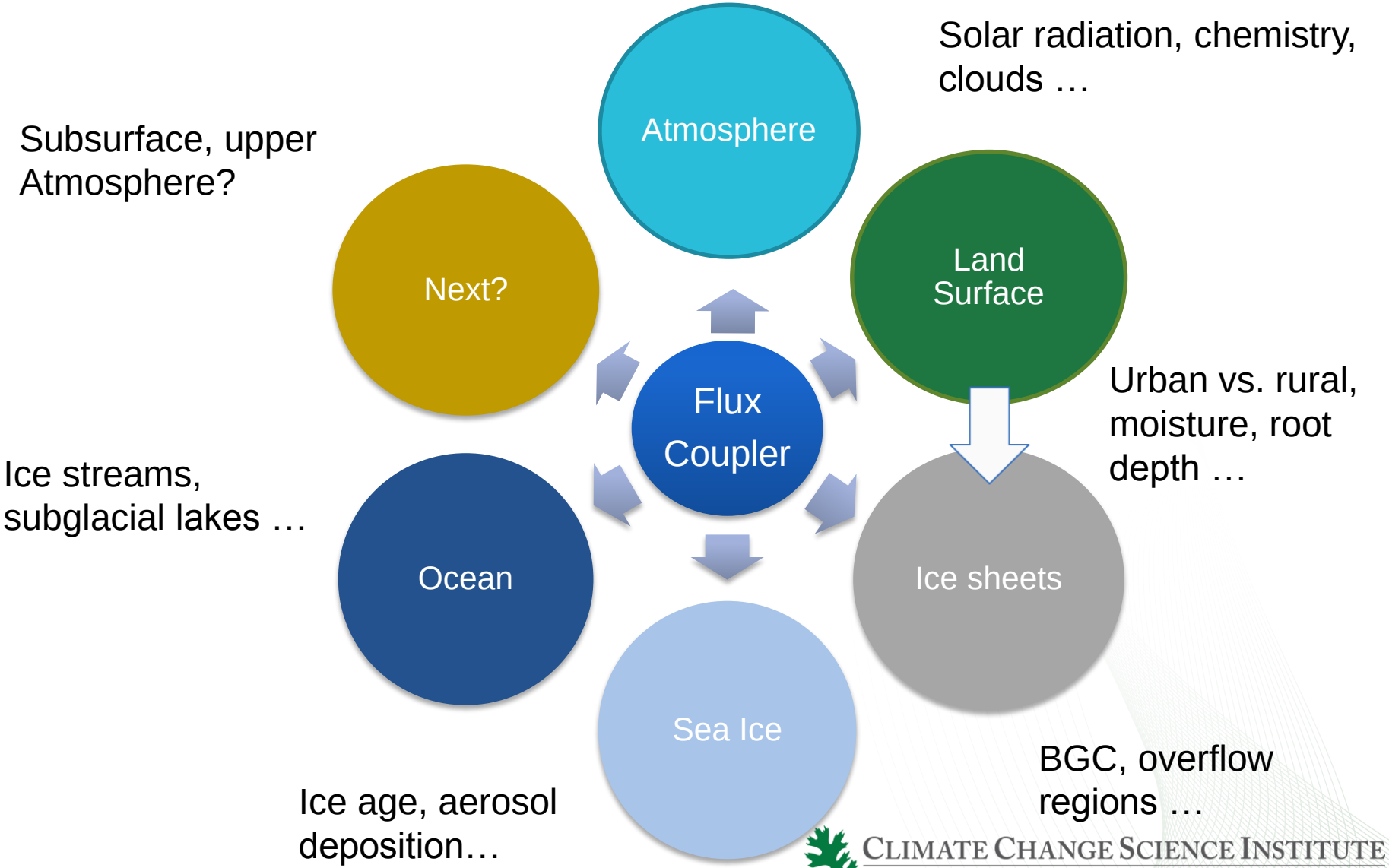
Urban vs. rural, moisture, root depth …

Ice streams, subglacial lakes …

BGC, overflow regions …

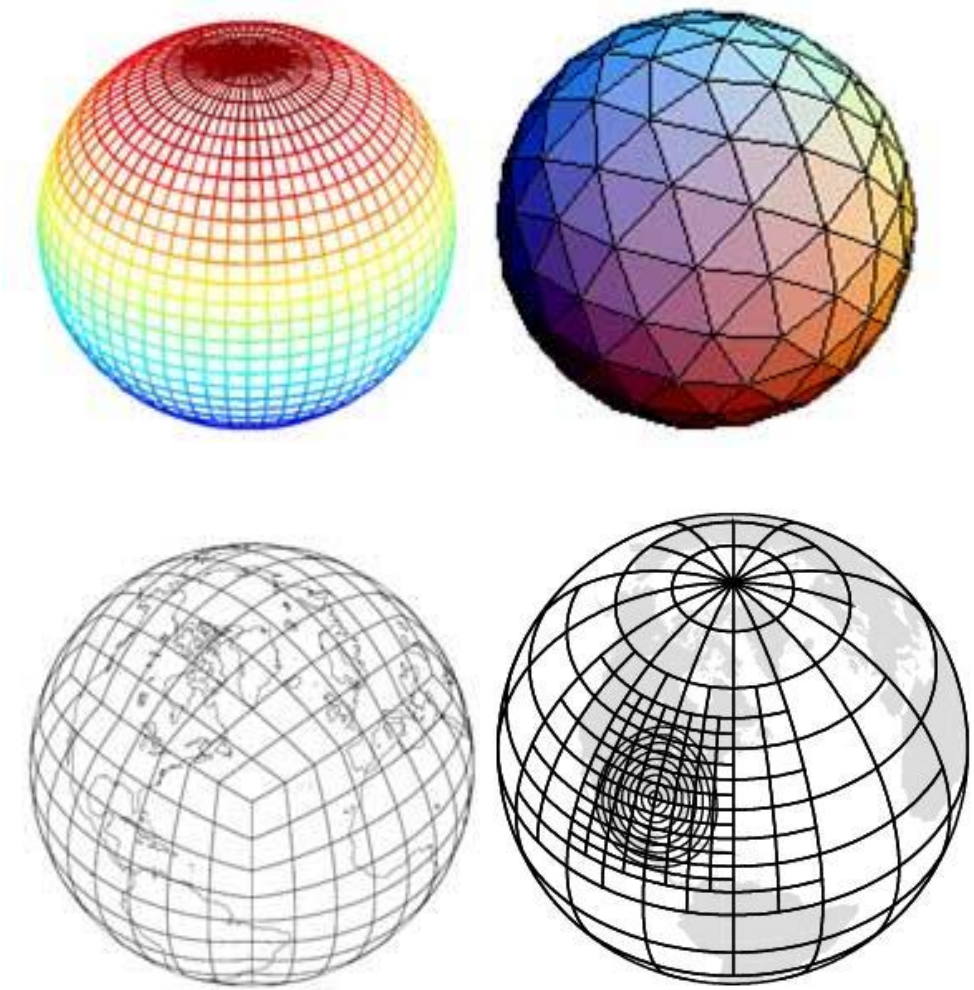
Ice age, aerosol deposition…

Climate Models comprise a collection of components



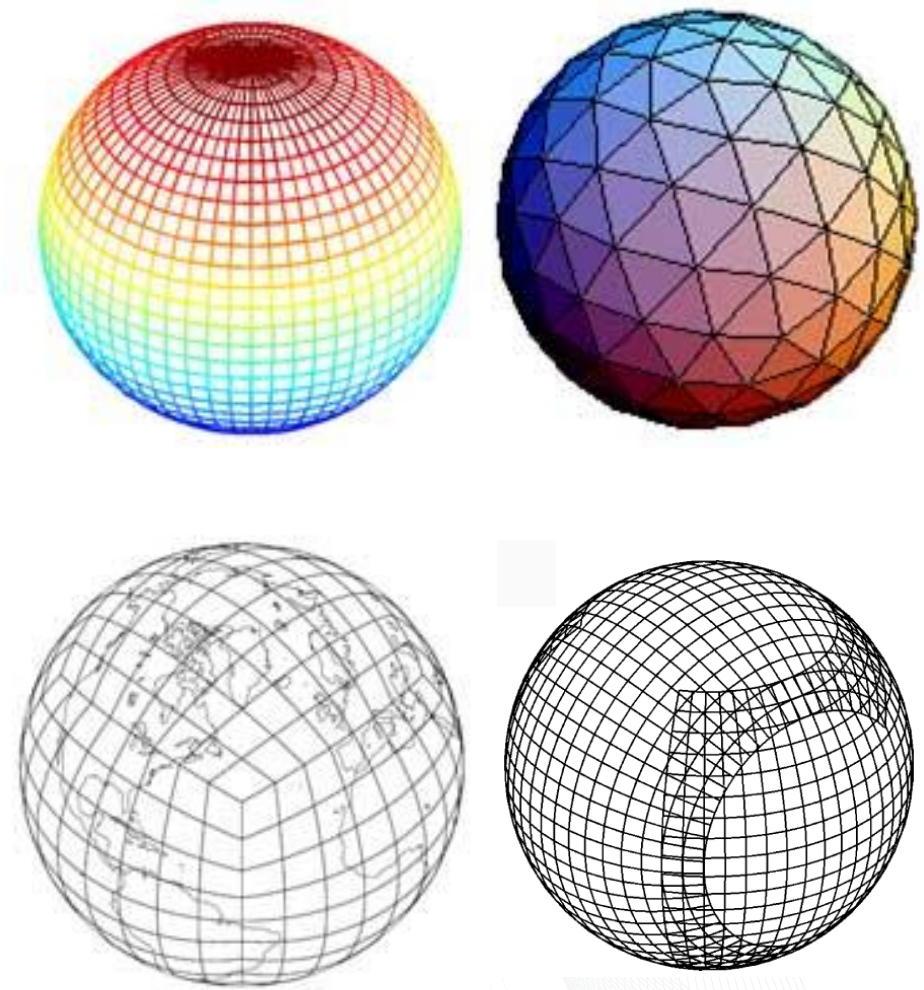
Global Atmospheric Climate Models:

- A variety of numerical methods have been tried and used to optimize accuracy and efficiency
- Other considerations: conservation, monotonicity, scalability and effective use of LCF
- Horizontal grid types: lat-lon, geodesic, cubed sphere, and locally refined (static or adaptive)



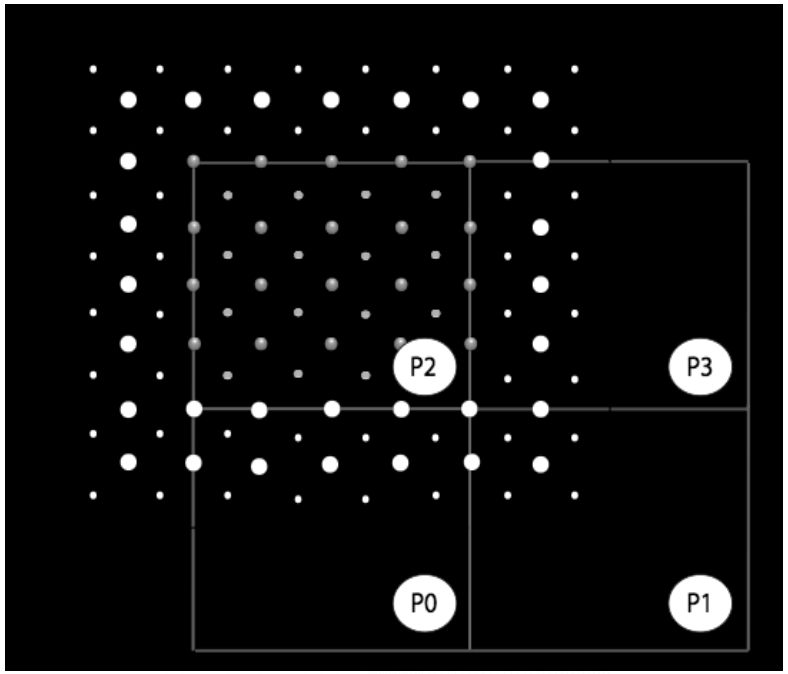
Global Atmospheric Climate Models: Grids

- Is there a singularity?
  - Lat-lon pole problems
  - Cubed-Sphere & Icosahedron have <u>weaker</u> singularities
- Is the grid spacing regular?
  - Lat-lon poles have much smaller grid spacing
  - Leads to time step restrictions
- Is the grid rectangular?
  - Lat-lon & cubed-sphere are, but icosahedron is not
- Is the grid orthogonal?
  - Lat-lon & "yin-yang" are, but cubed-sphere & icosahedron are not



Spatial Operators

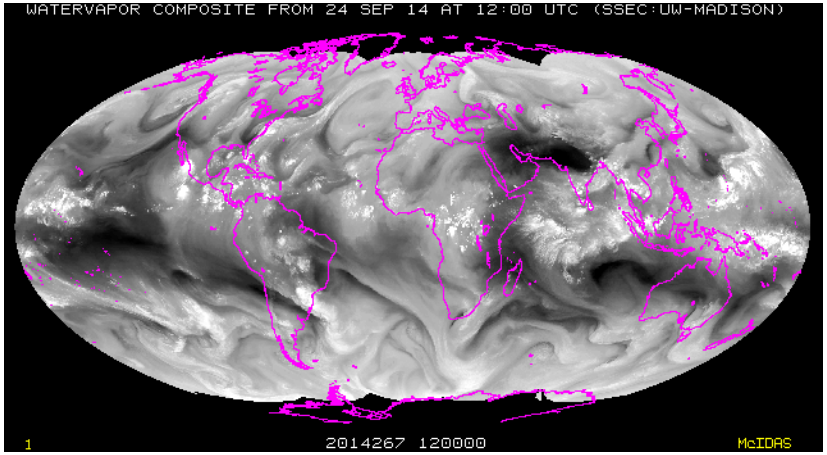
- Key Issues for Spatial Operators
  - How does the fluid vary <u>within</u> a grid cell / element?
  - "Reconstruction": Use several DOFs to create a spatial function of variation
  - Which / how many DOFs do I use to reconstruct?
  - Do I need my neighbor's information to reconstruct?
  - How easy is it to work in difficult geometries?
  - What kind of time step should I expect?
  - Can the method handle non-smooth data?



Layout of the finite difference grid for CISM1.0 including ghost cells for parallel communication

Spatial Operators: Full Spectral

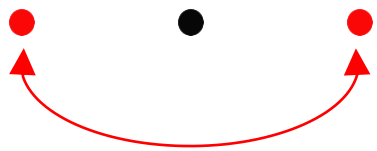
Snapshot of atmospheric column integrated water vapor: lots of waves



- Apply a transform (Legendre or Fourier) to the PDE
- Each grid point depends on <u>all</u> of the others
- Pros: accurate; Very large stable time step; cheap
- Cons: massive parallel communication; cannot handle non-smooth data; difficult for tough geometries; leaks mass

Spatial Operators: Finite-Differences

- Finite-Differences: $\frac{\partial q_i(x,t)}{\partial t} + \frac{\partial f_i(x,t)}{\partial x} = 0$

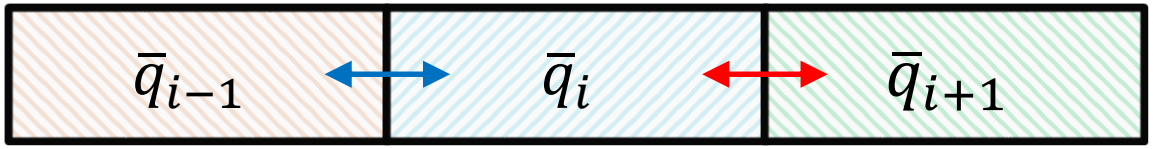


$$\left.\frac{\partial f}{\partial x}\right|_{x_i} = \frac{f_{i+1} - f_{i-1}}{\Delta x}$$

  - Do nothing to the PDE ("strong form"); solve PDE at <u>points</u> in space
  - Use neighboring points to reconstruct fluid variation at your point
  - Pros: Easy to implement and understand; Large time step
  - Cons: Leaks mass; <u>Dies when q is non-smooth</u>; Can't handle tough geometry; Needs neighboring information to reconstruct (parallel comm.)

Spatial Operators: Finite-Volumes

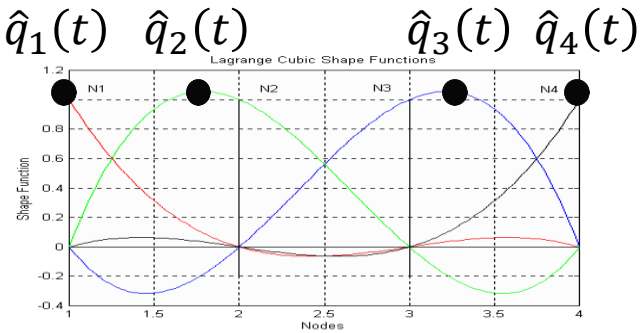
- Finite-Volumes: $\int_{x_L}^{x_R} \frac{\partial q_i(x,t)}{\partial t} \mathrm{d}x + [f_i(x_R,t) - f_i(x_L,t)] = 0$



  - Integrate in space ("weak form") <u>so that you don't need spatial derivatives</u> of q to update q; solve for cell <u>averages</u> instead of points
  - Cell average updated by "fluxes" at cell boundary (in versus out)
  - Use neighboring cell avgs to reconstruct fluid variation w/in cell
  - Pros: Easy to implement; Conserves mass; Large Time Step; <u>Handles non-smooth q</u>
  - Cons: Needs neighboring information to reconstruct (parallel comm.); Reconstruction uses information from farther away (accuracy); High-order not good for tough geometry

Spatial Operators: Finite-Elements

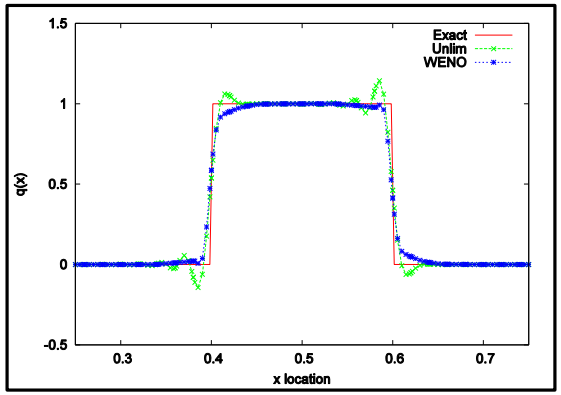
- Finite-Elements: $\frac{d\hat{\boldsymbol{q}}}{dt} = -M^{-1}S\hat{\boldsymbol{q}}\,(t)$



  - Multiply a smooth spatial-only "test function", which you will later use to "<u>take the derivative</u>" from q
  - Integrate in space over the element and apply integration by parts
  - Assume the solution itself is a weighted sum of those test functions
  - Sets up a linear system, which you solve to update fluid state
  - Pros: <u>Reconstructs without neighboring data (parallel comm.)</u>; Fits any geometry easily; Conserves Mass; Handles non-smooth data
  - Cons: Much smaller stable time step; Tough to understand conceptually; Tougher to limit

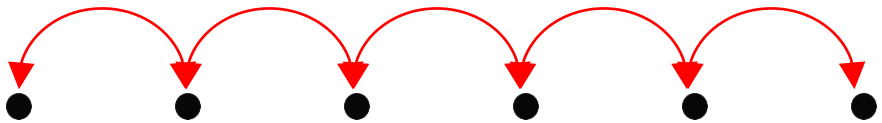
Spatial Operators: Limiting

- When data is non-smooth, “oscillations” appear in the solution



- Negative values occur, which are often non-physical
  - Flux-Corrected Transport (FCT) limits fluxes to avoid negatives
  - “Hole Fillers” fill in negatives, then take mass away from other cells
- Diffusion damps out oscillations
- Hyperiffusion selectively damps out smaller-scale oscillations
- Non-linear limiters use neighboring information to control noise more selectively

Time Stepping



- Key Issues
  - What does the next time step's data depend on?
  - What is the time step length for the method?
  - Does the method require me to store "stages" of data?
  - Does the method require me to store previous time steps' data?
  - Does the method keep new minima / maxima from occurring?
  - Can the method handle amplifying or decaying data without blowing up?

Time Stepping: Implicit versus Explicit

- "Time-Explicit": Next time step's data depends on this and previous time steps' data only
  - Pros: Very easy to implement, very low parallel communication
  - Cons: Maximum <u>stable</u> time step is quite small
- "Time-Implicit": Next time step's data also depends on <u>itself</u>
  - Sets up a global system that needs to be inverted
  - Pros: More accurate at same time step, much larger time step
  - Cons: Very complicated to implement, very high parallel communication

$$\frac{\mathbf{v}^{n+1}-\mathbf{v}^{n}}{\Delta t}+(\zeta^{n+1}+f)\mathbf{k}\times\mathbf{v}^{n+1}+\nabla\left(\frac{1}{2}\mathbf{v}^{n+1}\cdot\mathbf{v}^{n+1}+\Phi^{n+1}\right)=0$$

$$\frac{p^{p+1}-p^{n}}{\Delta t}+\nabla\cdot\left(p^{n+1}\mathbf{v}^{n+1}\right)=0$$

Time Stepping: Semi-Discrete Methods

- "Semi-Discrete": The most popular choice
  - Discretize in space only, and leave time dimension alone
  - Apply a well-known ODE integrator to the time dimension
  - Pros: Separates time & space; Easy to implement; Well known
  - Cons: Requires more memory & parallel comm. than other methods
- "Multi-Stage": Generate "stages" as point values in time, and then use those to reconstruct in time and integrate (e.g., Runge-Kutta)
- "Multi-Step": Use previous time steps' data as point values in time to reconstruct in time & extrapolate (e.g. Adams-Bashforth)

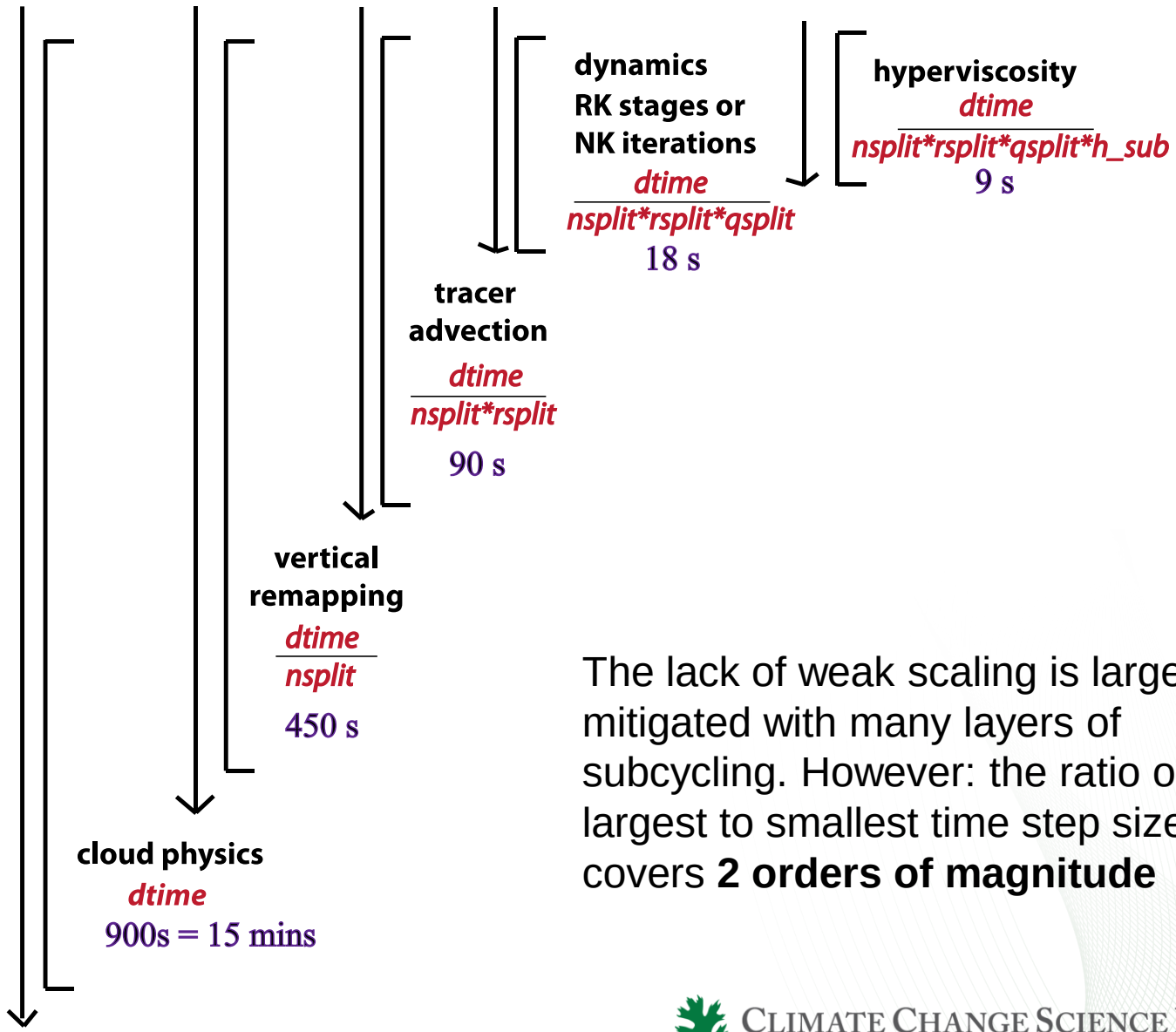
Time Stepping: Fully-Discrete Methods

- Semi-Lagrangian: Follow the fluid back in time using wind vectors.
  - The new fluid state is the previous fluid state at the departure point plus the forcing integrated along the way
  - Pros: Large Δt; Accurate; Low parallel comm.; Great for transport
  - Cons: Very tough to apply for full <u>non-linear</u> equations
- Iterated Time Information (e.g., ADER, Lax-Wendroff)
  - Use the PDE itself & spatial derivatives to <u>generate</u> time derivatives
  - Pros: Extremely accurate; Low parallel comm.; Large time step; Applies to full non-linear equations
  - Cons: Can become expensive at high-order

Time Stepping: Sub-Cycling

- Sub-cycling
  - Sometimes there is a clear scale separation between different dynamics
    - Sound waves 4x faster than wind in atm.; 50x faster in ocean
    - Typical transport speed much slower than jet streak speed
    - Model physics are expensive to run, and dynamics are cheap
  - Run different phenomena at <u>different time steps</u>
  - Pro: Allows more efficient overall simulation; easy to implement
  - Con: No interaction within subcycled scales; usually requires added damping to maintain stability

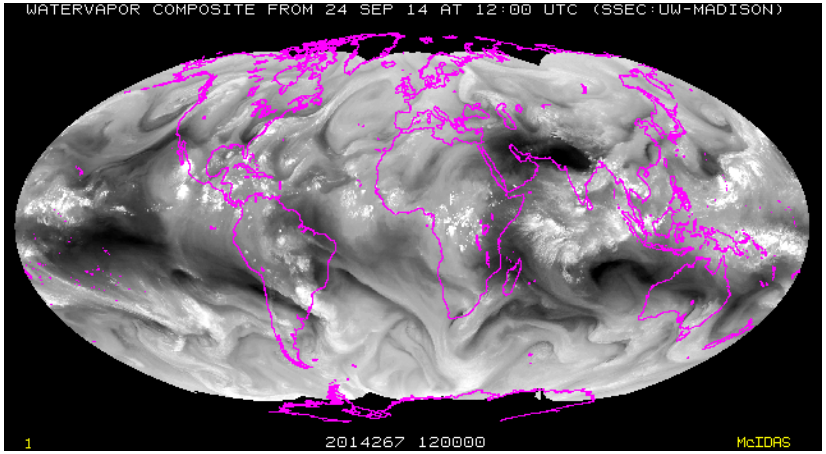
Anatomy of a Time Step: ¼° CAM-SE dycore



The lack of weak scaling is largely mitigated with many layers of subcycling. However: the ratio of the largest to smallest time step size covers **2 orders of magnitude**

Choices, Choices, Choices

Reasoning for Numerical Choices in CAM-SE



Snapshot of atmospheric column integrated water vapor: lots of waves

- Atmosphere dominated by moving waves (hyperbolic). Sound waves only 3x faster than max wind speed.
  - Time-explicit time stepping
- Plain Cubed-Sphere grid is regular, but irregular when spatially adapted
  - Finite-Elements
- Typically time step is very small
  - Very large-Δt Runge-Kutta
- Physics are very expensive; one hyperdiffusion isn't smooth enough
  - Sub-cycle them

Choices, Choices, Choices

Reasoning for Numerical Choices in MPAS-Ocean

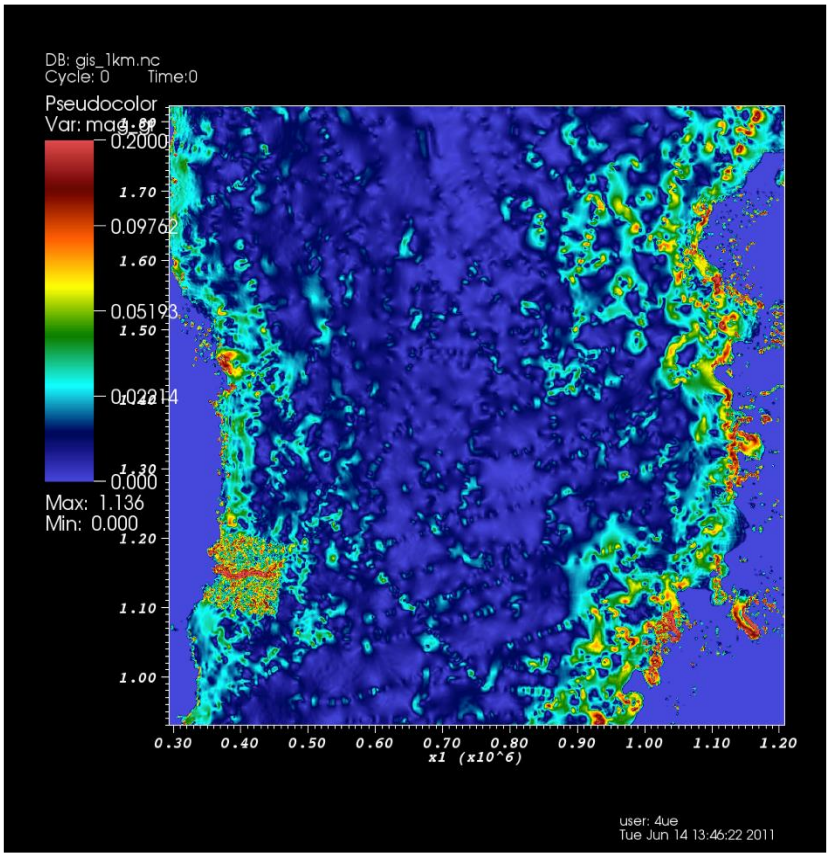
Kinetic Energy snapshot,
Global 30km resolution, courtesy Todd Ringler

- Ocean dominated by moving waves (hyperbolic). Sound waves 2 orders magnitude faster than currents.
  - Time-split into “barotropic” (fast) and “baroclinic” (slow) equations
  - Sub-cycle barotropic equations
  - Barotropic could go time-implicit, but that was judged too costly
- Irregular triangular grid
  - Very low-order finite-differences

Choices, Choices, Choices

Reasoning for Numerical Choices in CISM – Land Ice

1km Greenland Thickness Gradient



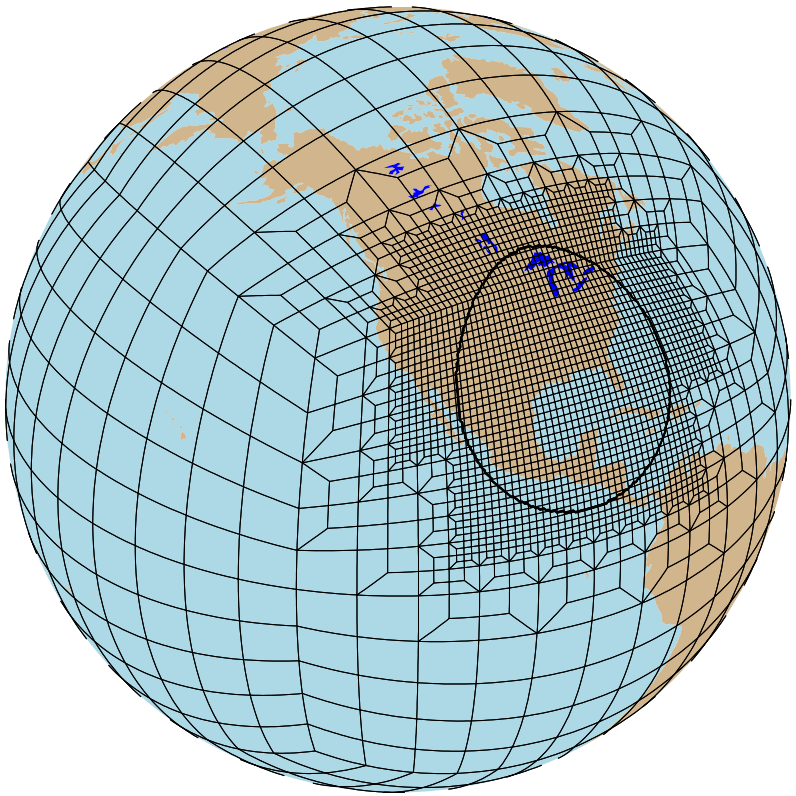
- Ice sheets dominated by diffusion (parabolic).
  - Time-explicit Δt <u>way</u> too small
  - Have to go time-implicit
- Small separate domains
  - Stereographic Cartesian structured grids
- Newer models choose to refine in active regions
  - Unstructured grid
  - Low-order finite-differences

Numerics Must Cooperate with Computers

- Modern computers: Nearly all cost attributed to data movement
  - You can only run as fast you can grab the data you need
  - Minimal data movement; Most efficient use of fetched data
- "Fat nodes" keep data "closer" together
  - OLCF's Summit computer is moving in the right direction
- "Flops are free"? Sure, but you can't do flops without data
- Algorithmic choices dominate amount data movement
  - High-order methods re-use data more efficiently
  - "Multi-Moment" methods require less data from others
  - Some algorithms have larger time steps than others
  - More expensive local physics improves fidelity & MPI scaling
  - JFNK implicit methods concentrate workload on local operations

Current ACME atmosphere model: CAM

Spectral Element, Continuous Galerkin



- Grid: cube mapped to the sphere "Cubed Sphere"
- Subcycled dynamics is 5-stage explicit runga-Kutta, has semi-implicit & fully implicit options
- GLL quadrature on each cube face
- Hydrostatic flow, hybrid finite difference vertical coordinates
- Scalability to 170K+ processors
- Regional refinement capability

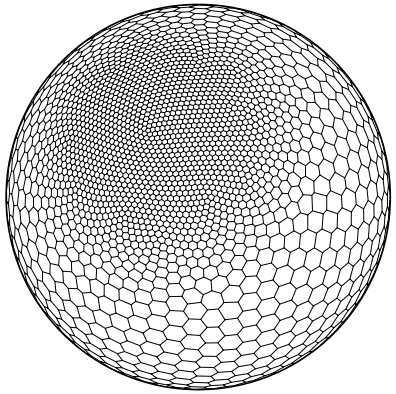
Also options for spectral, finite volume, SE with local refinement

MPAS-Ocean

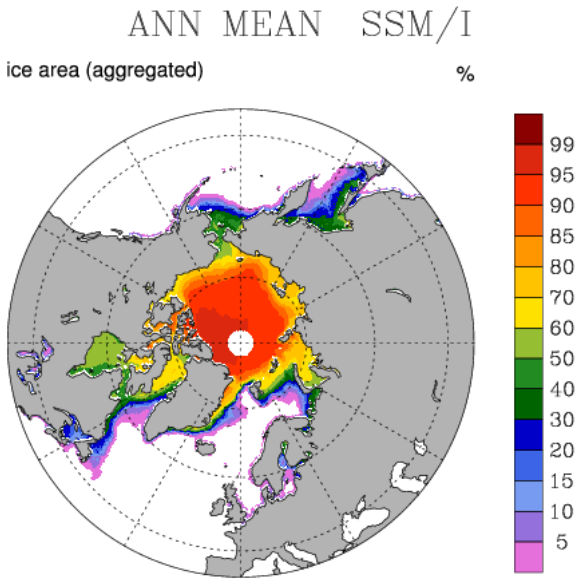
Kinetic Energy snapshot,
Global 30km resolution, courtesy Todd Ringler

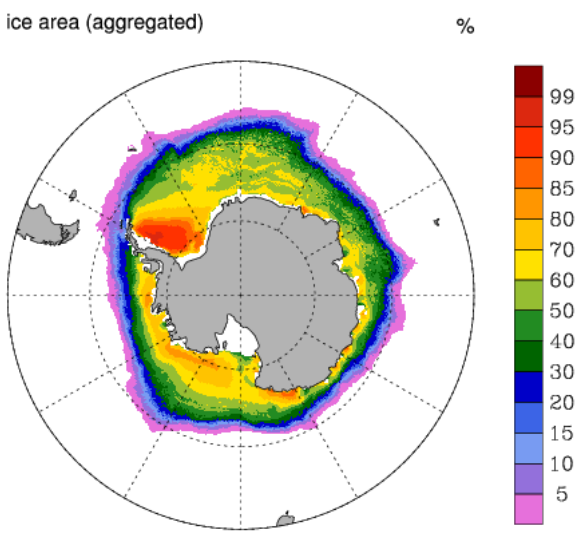
Unstructured SCVT Grid

- Isopycnal or z-level vertical grid
- Explicit 4th order Runga-Kutta, splitting coming
- Nominally 60km resolution or variable resolution using quads or Voronoi tessellations
- 3rd order hoz transport. 2nd order vertical transport



Community Ice CodE (CICE)





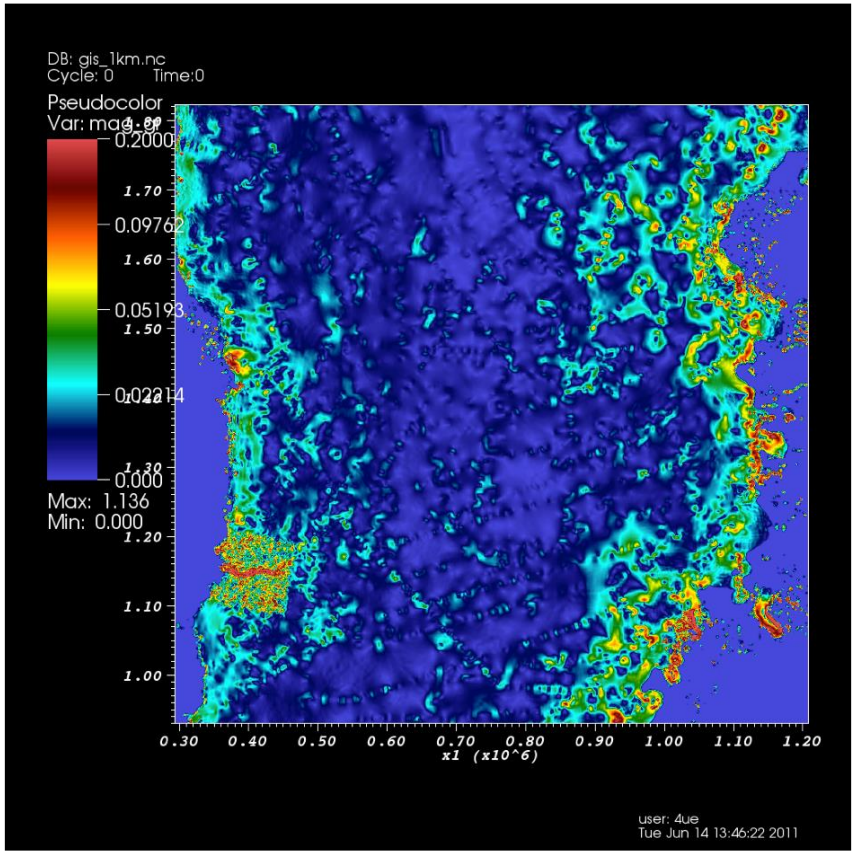
Courtesy Julie McClean, Scripps

- Fully explicit elastic, viscous, plastic (EVP) model (see Hunke and Zhang, 1999)
- Simulations at the typical 1 degree or 1/10 degree (right) resolutions on the same grid as the current ocean model, POP
- Several interacting components: thermodynamics (ice growth), dynamics (velocity), transport, ridging parameterization
- Subcycling of velocity within viscosity
- JFNK methods used to solve velocity in a testbed VP model showed increased efficiency (Lemieux et al (2010))

Community Ice Sheet Model

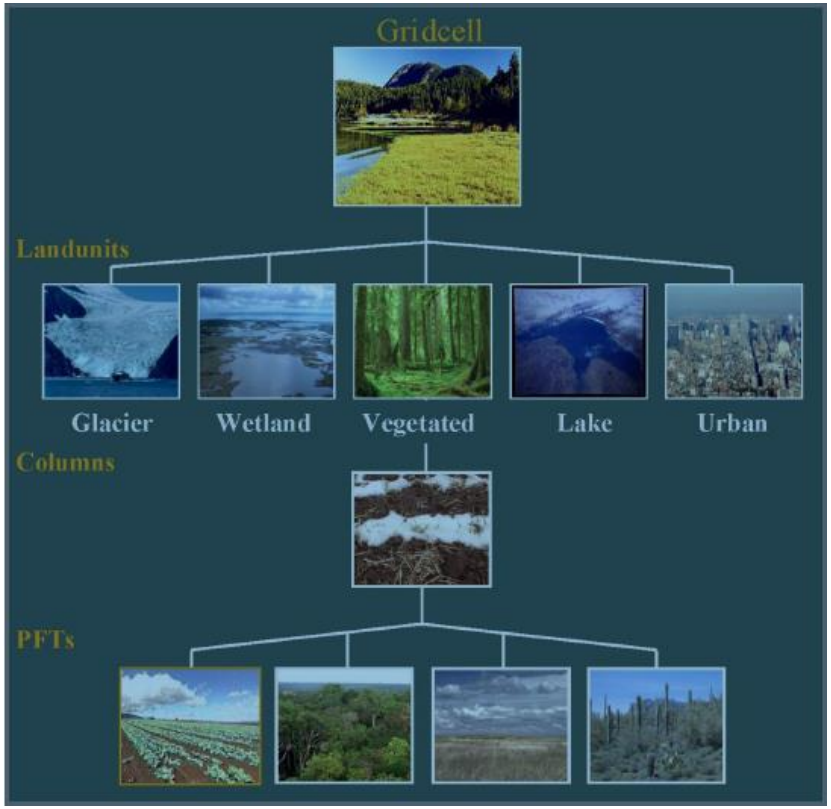
Newest Member of CESM in Jan 2011; version 2.0 going into ACME

1km Greenland Thickness Gradient



- Finite difference, regular grid
- Solves 1st order approx. velocity with Newton-Krylov
- Diagnostic T and CFL limited vertical remapping
- Nonlinear viscosity
- Finite Element, MPAS grid and Chombo based adaptive grid being developed as part of the PISCEES project

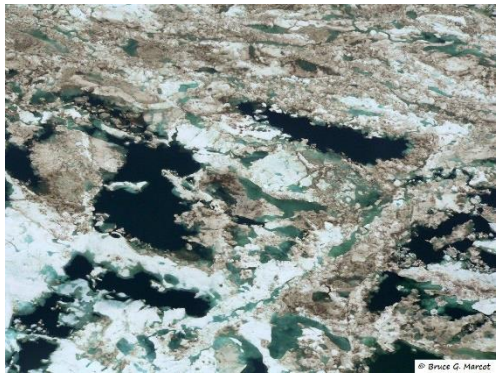
Community Land Model



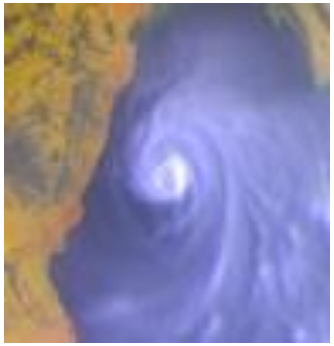
Unique structure of all the components

- Land cover is represented using a histogram of nested subgrid tiles
- Many simulated processes within a grid cell, then averaged to send to the atmosphere
- Tri-diagonal solves of temperature & moisture diffusion dominate cost

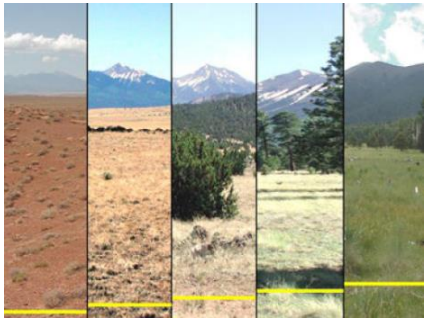
Driver/Flux coupler.



Ice - Atm



Atm - Ocean



Atm - Land

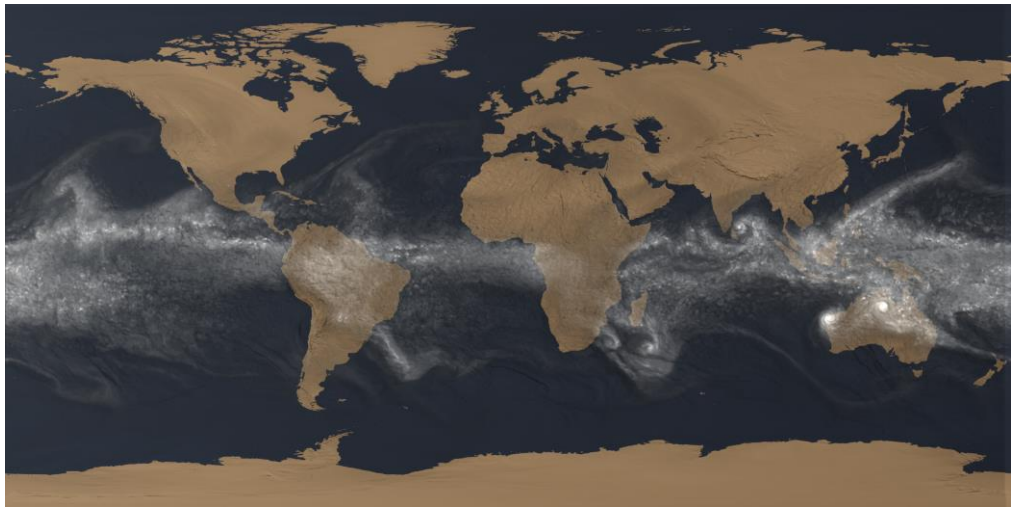
From Dennis et al (2011)

- Single executable for all components
- Components can run concurrently, sequentially, or a combination
- Performs mapping, merging, diagnostics …
- Physical coupling fields are passed through generic init, run, and finalize phases
- Frequency of communication can be altered through the namelist

Questions?

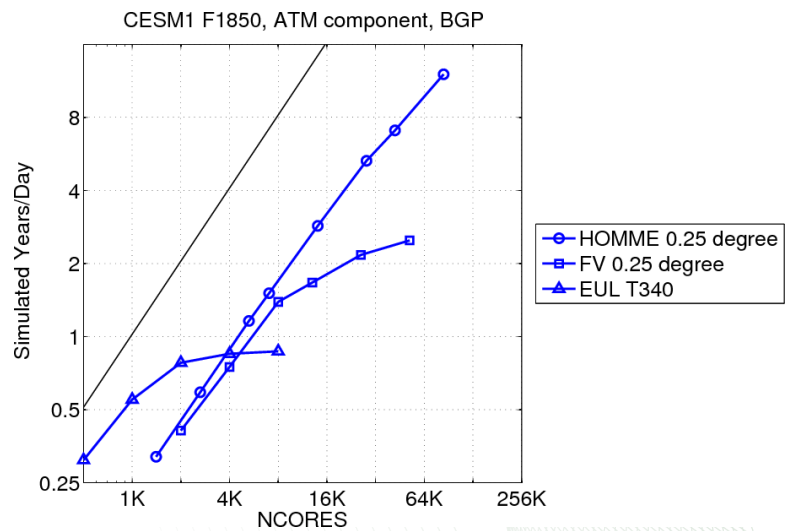
Fully coupled CESM, 1/4 resolution atmosphere, 1/10 degree ocean, 220K cores on Jaguar

Worley et al, 2011

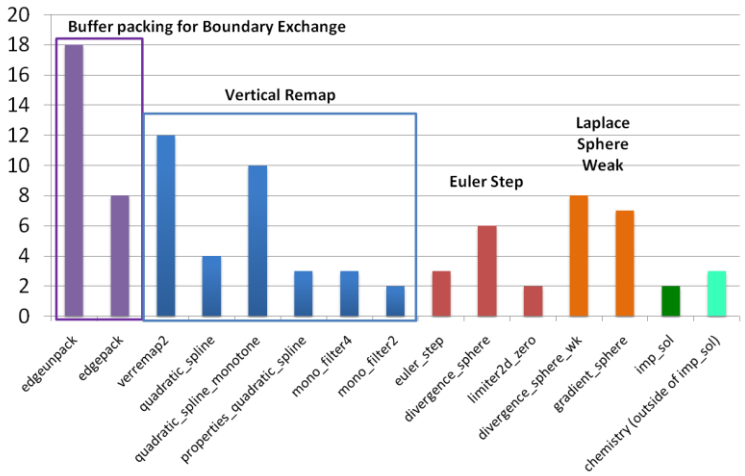


1/4 degree CAM-SE on ALCF's Intrepid

Dennis et al, 2011



Performance profile to target GPU



Carpenter et al, 2012

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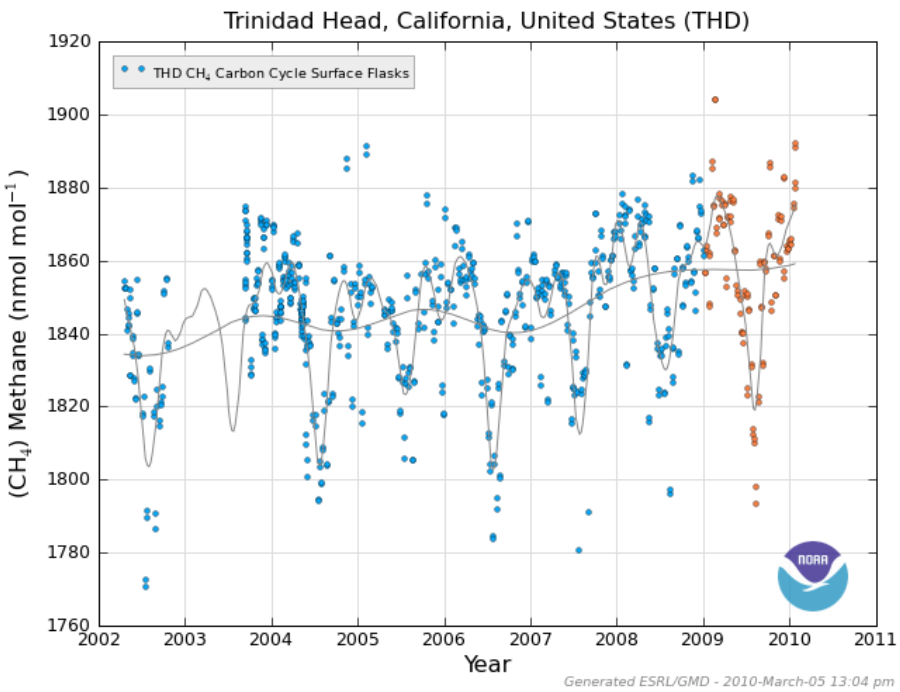
Community Atmosphere offline Models, e.g. Mozart Chemistry

Methane, measured at Trinidad Head, CA



- Chemistry: 100 tracers in full chemistry mode
- Global 3D offline transport model that can use analyzed dynamics or fully integrated dynamics calculations
- CAM: Troposphere and stratosphere, WACCM can use it for upper-troposphere through the mesosphere
- Solves fast chemistry implicitly and slow chemistry explicitly