Challenges of mathematical and numerical modelling of the atmosphere dynamics

Prof. Dr. Pedro da Silva Peixoto

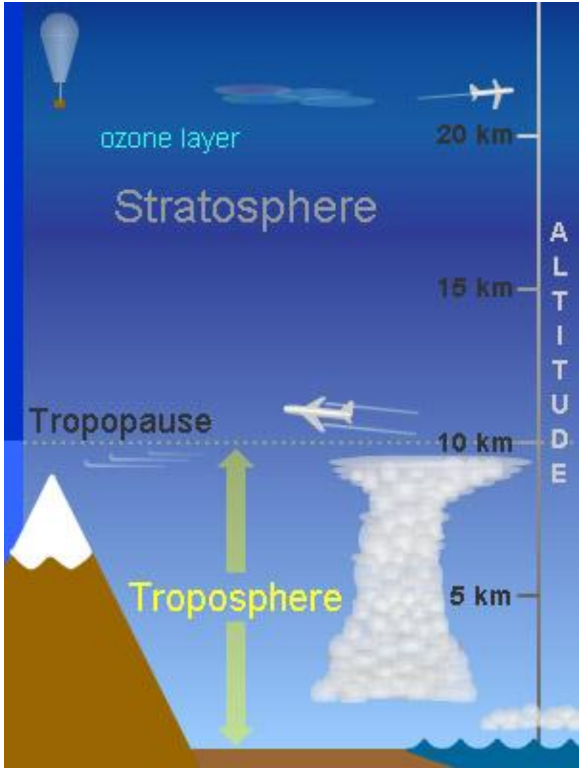
Applied Mathematics
Instituto de Matemática e Estatística
Universidade de São Paulo

This work was funded by FAPESP, being presented by Pedro Peixoto at the XII Summer Workshop in Mathematics UNB in 10-14 February 2020

February 2020

Atmosphere

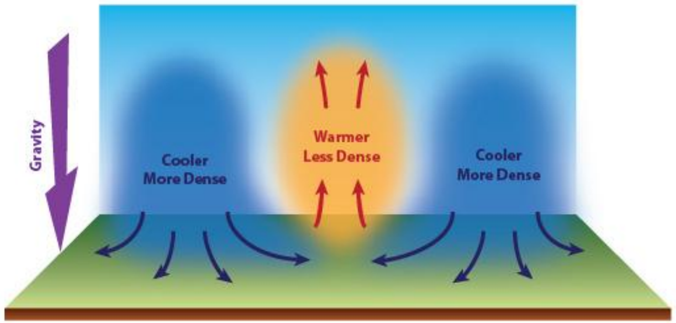
- The atmosphere is layered fluid (gas)



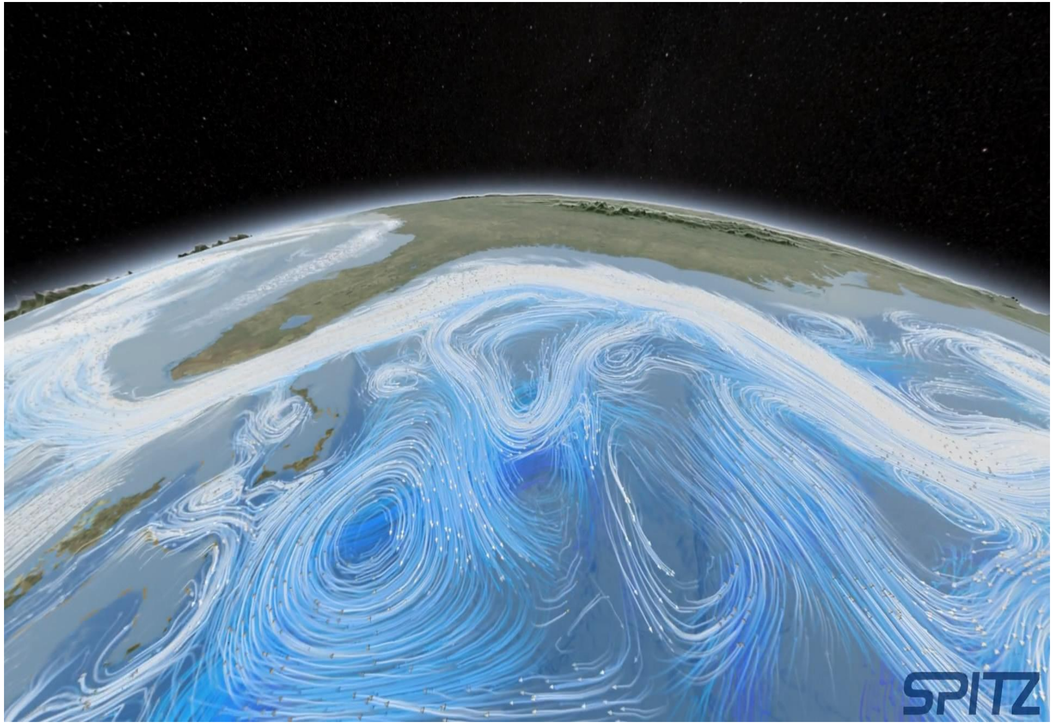
Images: < Nasa, ^ NCAR-UCAR

Atmosphere Dynamics

- Assume continuity
- Thermodynamics/Newton's law



- Waves
- Circulation
- Turbulence
- Convection
- Cyclones,...



Wallace, J.M. and Hobbs, P.V., 2006. *Atmospheric science: an introductory survey* (Vol. 92). Elsevier.

History

Vilhem Bjerknes (Norway 1862-1951)

- ~ 1890 Bjerknes's circulation theorem
- Kelvin's theorem applied to geophysical fluids (atmosphere and ocean)
- Conservation of vorticity along (homogeneous) barotropic ideal fluid flow
- Incompressible rotating fluid (angular velocity **Ω**)

$$\frac{D\Gamma}{Dt} = 0$$

$$\Gamma(t) = \oint_C (\boldsymbol{u} + \boldsymbol{\Omega} \times \boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{s}$$

$$= \int_A \boldsymbol{\nabla} \times (\boldsymbol{u} + \boldsymbol{\Omega} \times \boldsymbol{r}) \cdot \boldsymbol{n}\, \mathrm{d}S = \int_A (\boldsymbol{\nabla} \times \boldsymbol{u} + 2\boldsymbol{\Omega}) \cdot \boldsymbol{n}\, \mathrm{d}S$$

- Extensions to baroclinic fluids ($\nabla p \times \nabla \rho$ is not zero)
- Allows "predictability" of some simple atmosphere flows (ex: Cyclones)

Thorpe, A.J., Volkert, H. and Ziemiański, M.J., 2003. The Bjerknes' Circulation Theorem: A Historical Perspective.

Barotropic Vorticity Equation

Simple, but powerful model:

$$\frac{D\eta}{Dt} = 0$$

Material Derivative (along with flow)

$$\eta = \zeta + f$$

Absolute vorticity (Relative + Coriolis)

Single layer, non-divergent horizontal flow

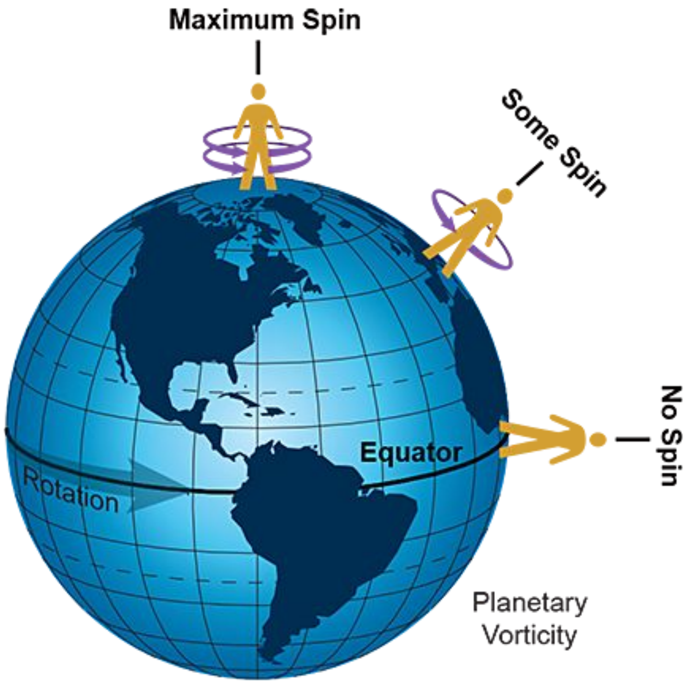
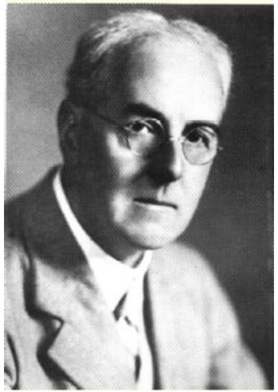


Image: NOAA (https://www.weather.gov/jetstream/climate_v_wx)

Pedro Peixoto (ppeixoto@usp.br)

History



Lewis Fry Richardson (UK 1881 -1953)

- Richardson, L.F., 1922. Weather prediction by numerical process. Cambridge university press.
- Primitive equations

Momentum Eq. (wind)

$$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = \vec{g} - \frac{1}{\rho} \nabla p - 2\vec{\Omega} \times \vec{v} - \vec{D}$$

Mass (density)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$$

Energy (temperature)

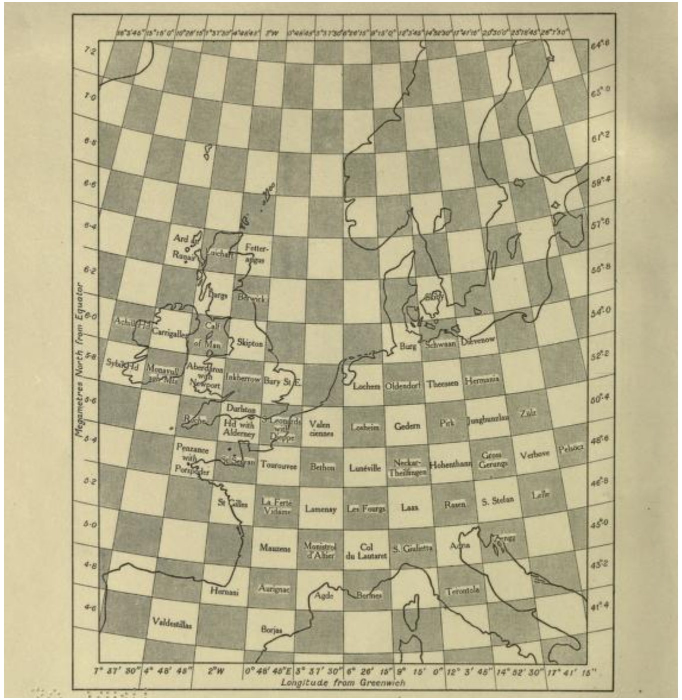
$$c_v \frac{dT}{dt} + p \frac{d\alpha}{dt} = q + f$$

State (pressure)

$$p = \rho R T$$

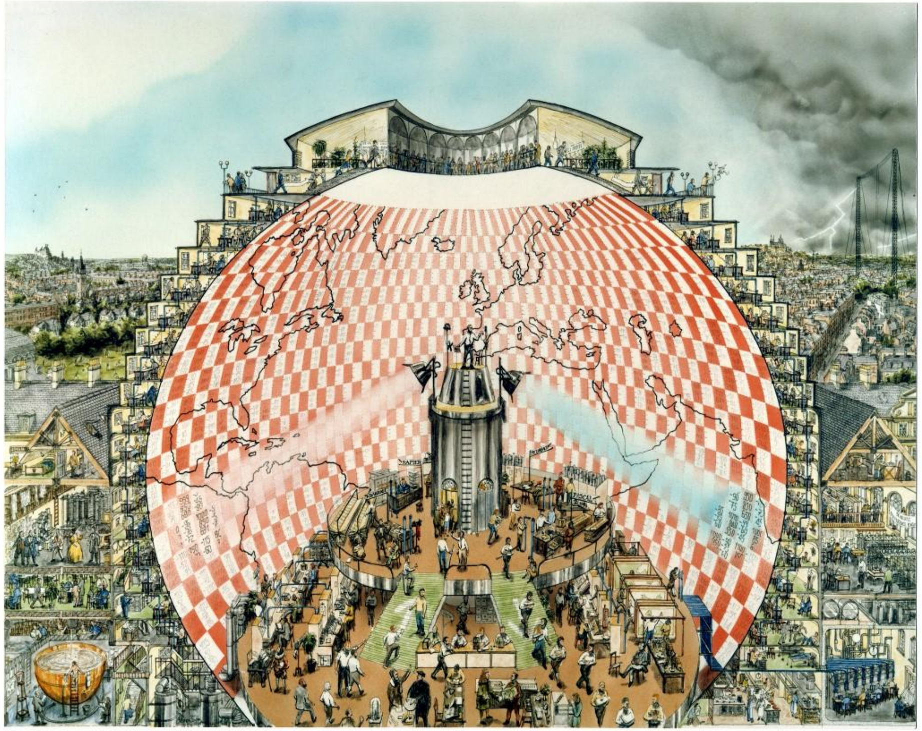
- Hydrostatic $\frac{\partial p}{\partial z} + \rho g = 0$

Weather prediction by numerical process



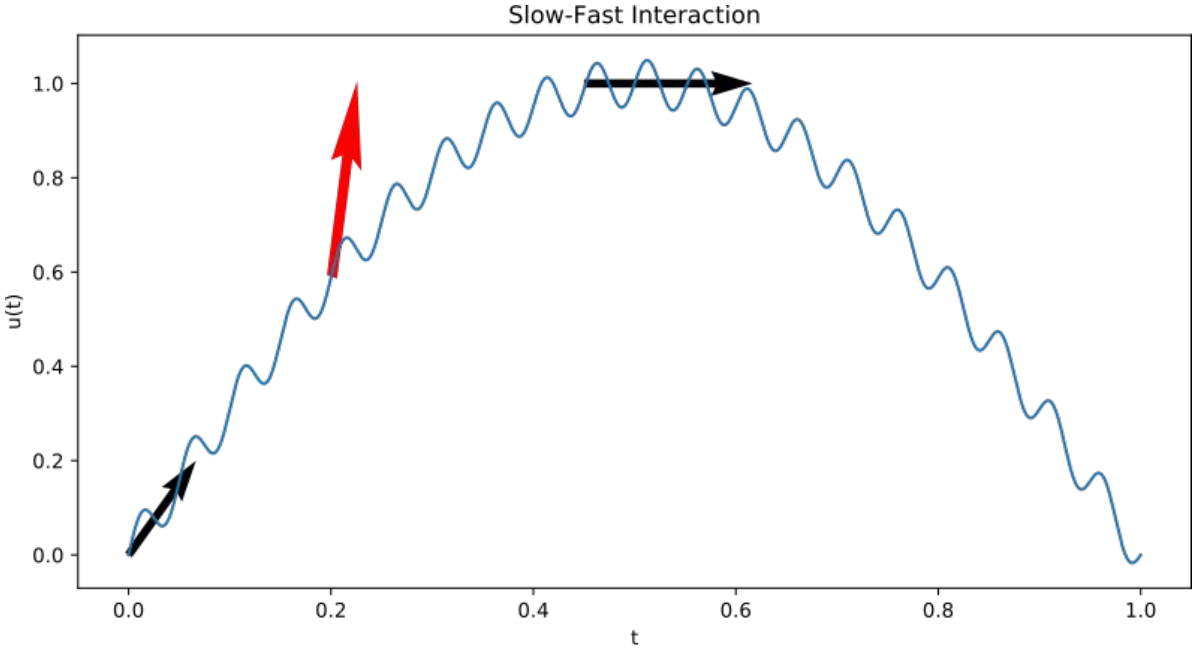
- Spherical coordinates
- Finite Differences (staggered E-grid)
- Resolution: aprox 200km

- Several months of hand calculation while in ambulance trips (driver) in WW-I



Richardson’s Results

- Predicted a 145mb change over 6 hours at a grid point
- Observations showed almost no pressure change



- **Great ideas, but the dynamics is multiscale!**
- **Model initialization issues**

Lynch, P., 1999. Richardson’s marvelous forecast. In The life cycles of extratropical cyclones. American Meteorological Society, Boston, MA.

Models for Atmosphere Dynamics

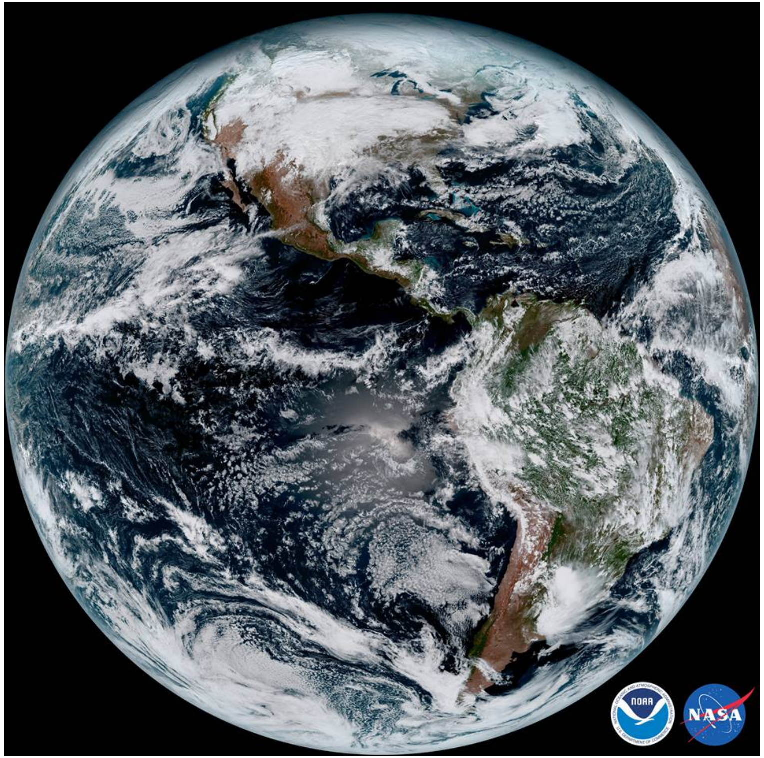


Image: GOES-16 Jan 2017

Three-dimensional Navier-Stokes equations

$\Downarrow$

Nonhydrostatic models

$\Downarrow$

Primitive equations
(hydrostatic equations)

} 3D

$\Downarrow$

Shallow water equations

$\Downarrow$

Quasi-geostrophic models

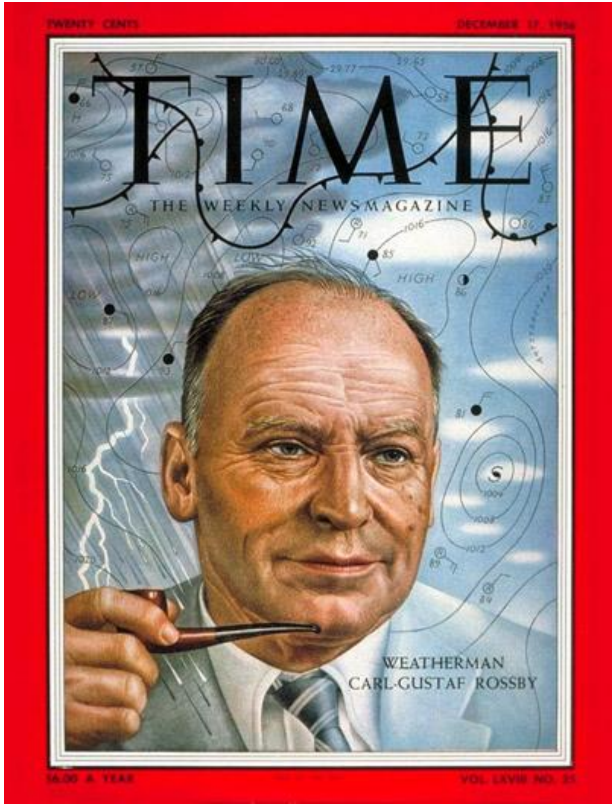
$\Downarrow$

Two-dimensional barotrophic equations.

} 2D

Temam, R. and Ziane, M., 2005. Some mathematical problems in geophysical fluid dynamics. In Handbook of mathematical fluid dynamics. North-Holland.

History



Carl-Gustaf Rossby (1898 -1957)

- Rossby, C.G., 1939. Planetary flow patterns in the atmosphere. Quart. J. Roy. Met. Soc, 66, p.68.
    - Large-scale motions of the atmosphere in terms of fluid mechanics, jet stream, long waves in the westerlies (Rossby waves).

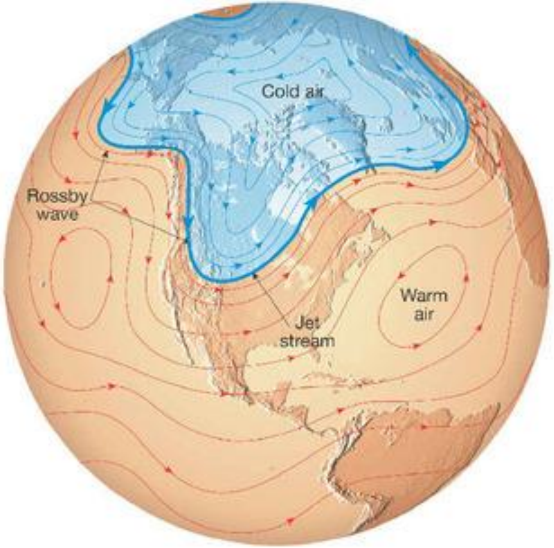
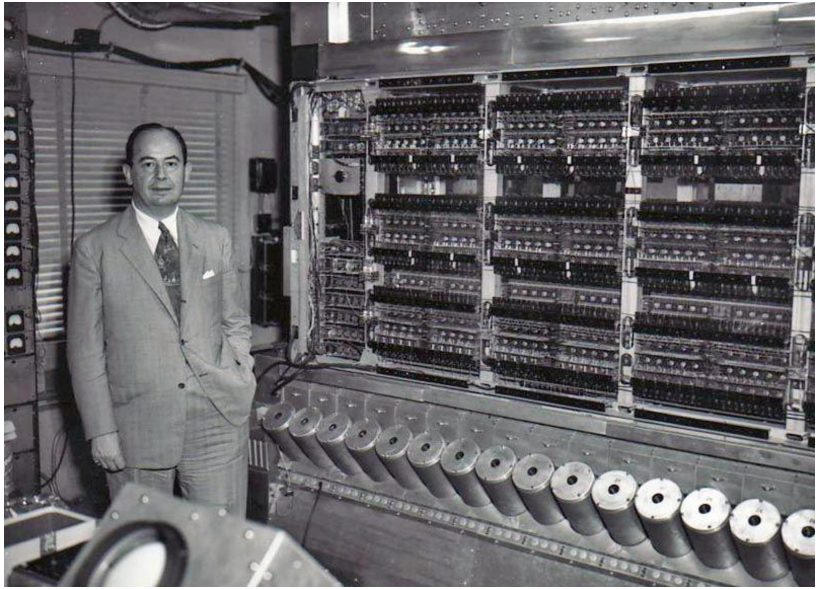


Image credit: stephenleahy.net

History



John von Neumann (1903 - 1957)

Meteorological Program, Princeton (1946):

- Jule Gregory Charney, Philip Thompson, Larry Gates, Ragnar Fjørtoft, Klara Dan von Neumann.
- ENIAC (Electronic Numerical Integrator and Computer) - 20,000 vacuum tubes - 100 kHz clock
- First successful numerical weather prediction

Thompson, P.D., 1983. A history of numerical weather prediction in the United States. *Bulletin of the American Meteorological Society*, *64*(7)

First Successful Weather Prediction

Charney, J.G., Fjörtoft, R. and Neumann, J., 1950. Numerical Integration of the Barotropic Vorticity Equation. Tellus Series A, 2, pp.237-254.

Barotropic vorticity equation:

$$\frac{D\eta}{Dt} = 0$$

Material Derivative (along with flow)

$$\eta = \zeta + f$$

Absolute vorticity (Relative + Coriolis)

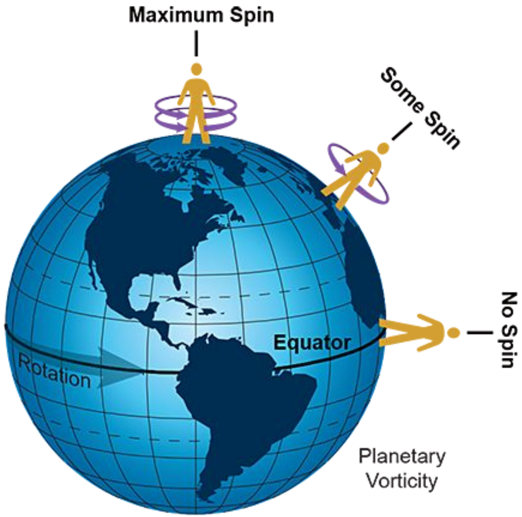


Image: NOAA (https://www.weather.gov/jetstream/climate_v_wx)

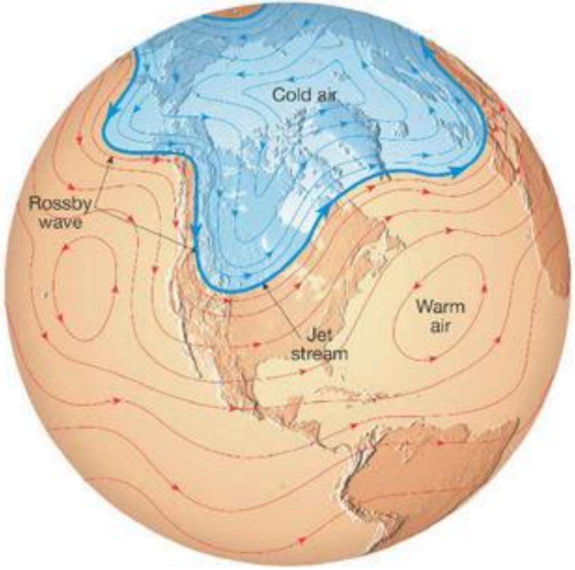
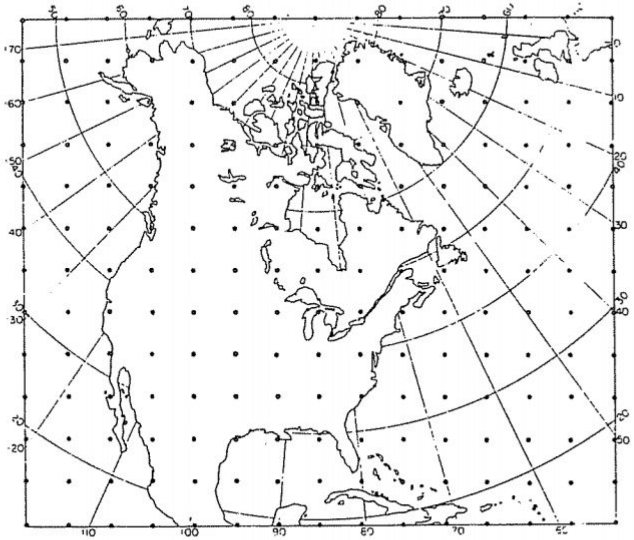
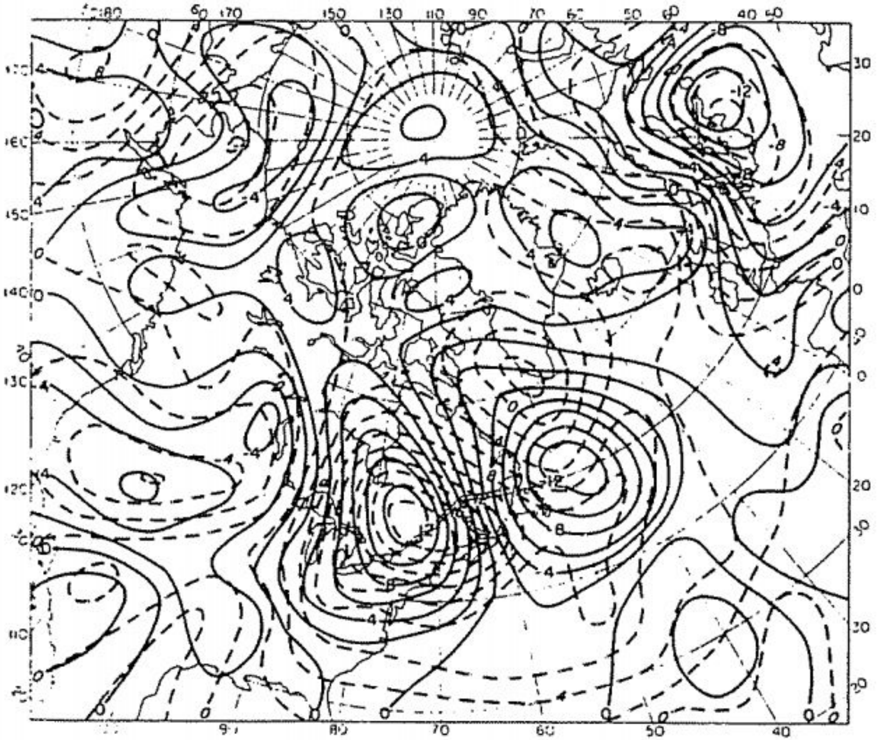


Image credit: stephenleahy.net

Numerical Integration of the Barotropic Vorticity

- Finite Differences
- Resolution ~740km
- 24hr computation for 24hr forecast (ENIAC)





Height change at 500mb after 24hrs Jan 30 1949 - Continuous line: Observation. Dashed: numerical

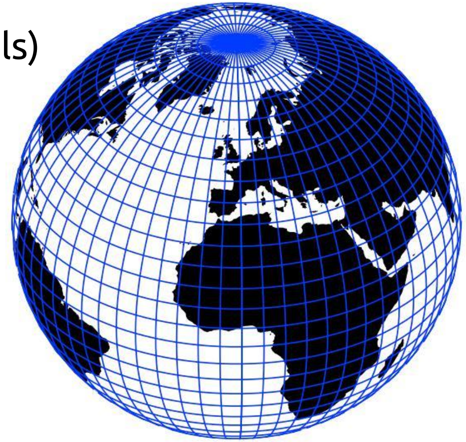
Charney, J.G., Fjörtoft, R. and Neumann, J., 1950. Numerical Integration of the Barotropic Vorticity Equation. Tellus Series A, 2, pp.237-254.

Early forecasts

- 1954: Rossby and team produced the first operational forecast in Sweden based on the barotropic equation.
- 1955-56: Charney, Thompson, Gates and team: Operational numerical weather prediction in the United States with layered barotropic models.
- 1959: Operational weather forecast in Japan

60's: **Primitive equations** are back (with improved initialization of the models)

(Climate change modelling started!)



New issues:

- Computacional instabilities (nonlinearities)
- Global model: Spherical geometries (pole problem?)
- Data assimilation
- ....

Randall, D.A., Bitz, C.M., Danabasoglu, G., Denning, A.S., Gent, P.R., Gettelman, A., Griffies, S.M., Lynch, P., Morrison, H., Pincus, R. and Thuburn, J., 2019. 100 Years of Earth System Model Development. *Meteorological Monographs*, *59*.

Latitude-Longitude Models

Traditional Eulerian Finite Differences:

- Stability usually requires $\Delta t \propto \Delta x$
- Pole requires Δt very small

Semi-Lagrangian semi-implicit

- Allows large Δt
- Solve a very large linear system at each time-step

Example of Operational Model:

- UKMetOffice: Endgame (SL-SI)
  Non Hydrostatic / Deep Atmosphere
  Resolution < 17km global (2014)

Wood, N., Staniforth, A., White, A., Allen, T., Diamantakis, M., Gross, M., Melvin, T., Smith, C., Vosper, S., Zerroukat, M. and Thuburn, J., 2014. An inherently mass-conserving semi-implicit semi-Lagrangian discretization of the deep-atmosphere global non-hydrostatic equations. *Quarterly Journal of the Royal Meteorological Society*, *140*(682), pp.1505-1520.

Spectral Models

Emerged around 1960-1970. Main concept: Derivatives are calculated in spectral space

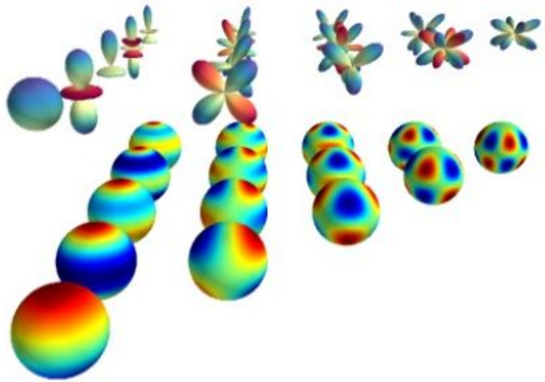
$$\Upsilon_n^m(\lambda,\theta) = e^{-im\lambda} P_n^m(\sin\theta)$$

1970s: Viability for Atmosphere shown by Eliasen et al (1970) & Orszag (1970) with nonlinear terms calculated “pseudo-spectrally” (products done in physical space)

$$P_n^m(\mu) = \frac{1}{\sqrt{2}} \frac{(1-\mu^2)^{|m|/2}}{2^n n!} \frac{d^{n+|m|}(1-\mu^2)}{d\mu^{n+|m|}}.$$

Spherical harmonics:

- Fourier expansion for each latitude circle
- Legendre polynomials on meridians



Barros, S.R.M., Dent, D., Isaksen, L., Robinson, G., Mozdzynski, G. and Wollenweber, F., 1995. The IFS model: A parallel production weather code. *Parallel Computing*, *21*(10), pp.1621-1638.

The state-of-the-art

Spherical harmonics with Fast Fourier Transform and “Fast” Legendre transforms global models

- Pseudo-spectral method
- Avoids the requirement of special treatment at the poles
- Semi-implicit is easier in spectral space
- With also Semi-Lagrangian : allows large Δt!
- Very accurate!

Operational Examples:

- IFS-ECMWF (European):
  <10km
- BAM-CPTEC-INPE (Brazil):
  ~20km
- GFS-NOAA (USA) - up to 2019:
  ~13km

♦ **Resolution increases of the deterministic 10-day medium-range Integrated Forecast System (IFS) over ~28 years at ECMWF:**

- ♦ **1983: T 63 (~316km)**
- ♦ **1987: T 106 (~188km)**
- ♦ **1991: T 213 (~95km)**
- ♦ **1998: T_L319 (~63km)**
- ♦ **2000: T_L511 (~39km)**
- ♦ **2006: T_L799 (~25km)**
- ♦ **2010: T_L1279 (~16km)**
- ♦ **2015: T_L2047 (~10km) Hydrostatic, parametrized convection**
- ♦ **2020-???: (~1-10km) Non-hydrostatic, explicit deep convection, different cloud-microphysics and turbulence parametrization, substantially different dynamics-physics interaction…**

The scalability problem

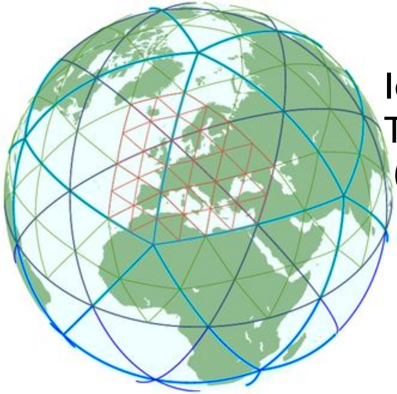
Weather forecasting needs to be done within a short time windows (1 or 2 hours wall clock time)

TUPÃ-CPTEC/INPE (~30k cores)

Massively Distributed Memory Parallel Machines

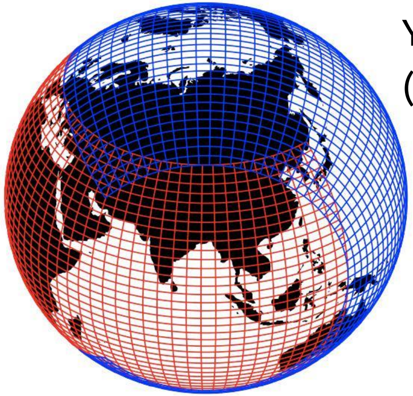
- Finite Differences: Pole communicates with many other computer nodes
- Semi-implicit: A lot of global communication required for the solution of the global linear system or spectral transforms
- Limited scalability on large supercomputers (cannot do the forecast within the time window for high resolutions)

Search for alternatives - more isotropic grids



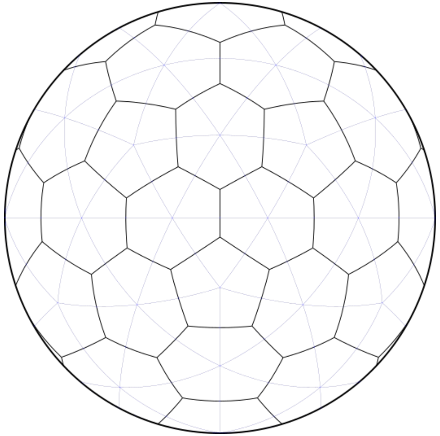
Icosahedral/
Triangular
(ICON-Germany)

Cubed Sphere (CAM-SE/FV3/NUMA-USA)

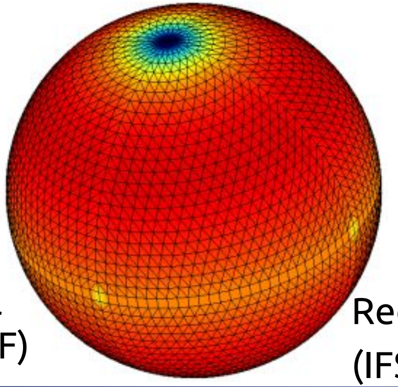


Yin-Yang
(GEM-Canada)

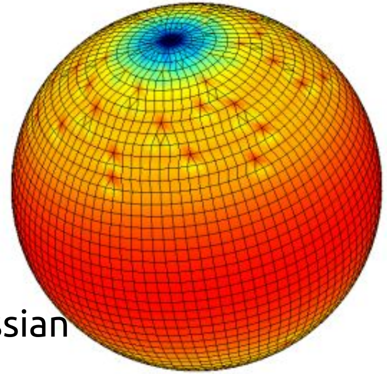
Voronoi
(MPAS/FIM/
OLAM-USA
NICAM-Japan)



Octahedral
(IFS-ECMWF)



Reduced Gaussian
(IFS-ECMWF)



Ultimate goal

Hydrostatic (primitive) equations: inadequate below ~20-10km horizontal resolution

To capture explicit convection (resolution << 10km):

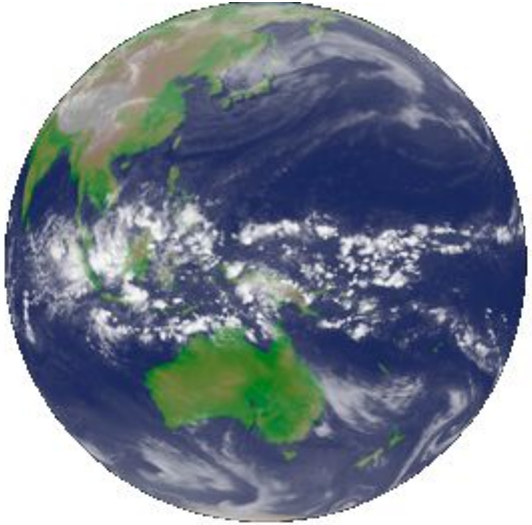


Image: NICAM Model (Japan)

Compressible Euler equations for atmosphere (ideal gas)

$$\frac{D\mathbf{u}}{Dt} = -2\boldsymbol{\Omega}\times\mathbf{u} - \frac{1}{\rho}\nabla p + \mathbf{g} + \mathbf{F}_r \text{ (Momentum)}$$

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\mathbf{u} \text{ (Continuity)}$$

$$c_v\frac{DT}{Dt} = -\frac{p}{\rho}\nabla\cdot\mathbf{u} \text{ (Thermodynamics)}$$

- $\mathbf{u} = (u, v, w)$: wind velocity
- p: pressure
- ρ: density
- T: temperature
- $D/Dt = \partial/\partial t + \mathbf{u}\cdot\nabla$: Material derivative

Intermediate step

3D Incompressibility (constant density):

$$\nabla \cdot \vec{v} = 0, \quad (\rho = \rho_0)$$

Hydrostatic balance:

$$\frac{\partial p}{\partial z} = -\rho_0 g,$$

Free surface $h_T(x, y, t)$ where $h_T = h_0 + h$, with $h_0(x, y)$ topography, $h(x, y, t)$ fluid depth.

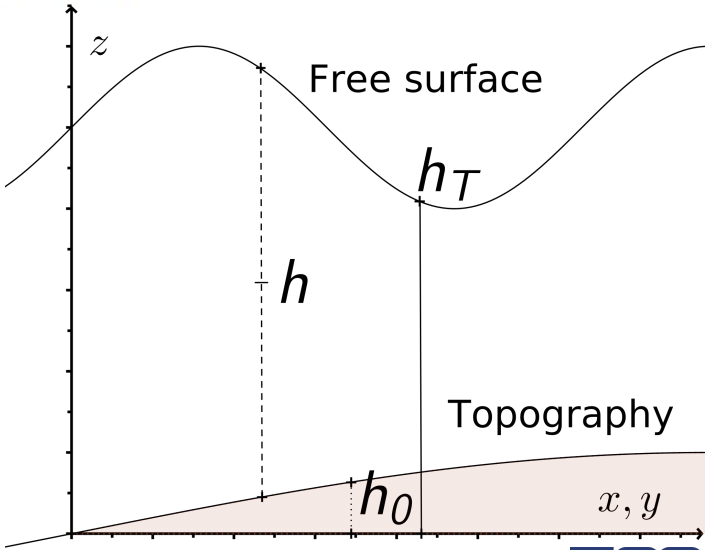
$$\int_z^{h_T} \frac{\partial p}{\partial z} dz = -\int_z^{h_T} \rho_0 g dz$$

$$p(z) = \rho_0 g(h_T - z) + \underbrace{p(h_T)}_{\text{Constant}}$$

Pressure gradient:

$$\nabla p = \rho_0 g \nabla h_T$$

Vertical Integration (Mean Flow)



Shallow Water Equations

Horizontal Momentum Equations ($\vec{v} = (u, v)$):

$$\frac{\partial \vec{v}}{\partial t} + \underbrace{(\vec{v} \cdot \nabla)\vec{v}}_{\text{nonlinear advection}} = \underbrace{-f\vec{k} \times \vec{v}}_{\text{Coriolis}} \underbrace{-g\nabla(h + h_0)}_{\text{Pressure}}$$

(f-plane approximation)

Shallow Water Equations

3D Incompressibility :

$$\nabla \cdot \vec{v} = \partial_x u + \partial_y v + \partial_z w = 0,$$

$$\partial_z w = -\partial_x u - \partial_y v$$

Free surfave must have w velocity:

$$\frac{Dh_T}{Dt} = w(x, y, h_T, t)$$

Topography height must have w_0 velocity:

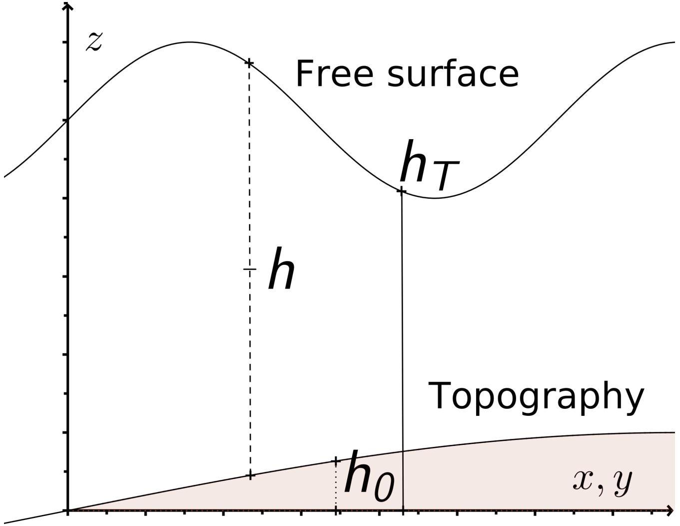
$$\frac{Dh_0}{Dt} = w(x, y, h_0, t) \Rightarrow w(x, y, h_0, t) = \vec{v} \cdot \nabla h_0$$

Integrate 3D incompressibility:

$$\int_{h_0}^{h} \partial_z w dz = -\int_{h_0}^{h} (\partial_x u + \partial_y v) dz$$

$$w_h - w_0 = -(h - h_0) \nabla \cdot \vec{v}$$

Vertical Integration (Mean Flow)



Shallow Water Equations

$$\vec{v}(x,y,t) = (u(x,y,t), v(x,y,t))$$

$$h(x,y,t) = h_T(x,y,t) - h_0(x,y)$$

2D Continuity equation:

$$\frac{\partial h}{\partial t} + \nabla \cdot (h\vec{v}) = 0$$

$$\frac{\partial h}{\partial t} + \underbrace{\vec{v} \cdot \nabla h}_{\text{transport}} = \underbrace{-h\nabla \cdot \vec{v}}_{\text{flow divergence}}$$

2D Horizontal Momentum Equations:

$$\frac{\partial \vec{v}}{\partial t} + \underbrace{(\vec{v} \cdot \nabla)\vec{v}}_{\text{nonlinear advection}} = \underbrace{-f\vec{k} \times \vec{v}}_{\text{Coriolis}} \underbrace{-g\nabla(h + h_0)}_{\text{Pressure}}$$

(f-plane approximation)

Shallow Water Equations on the Sphere

Vector invariant form:

$$\frac{\partial h}{\partial t} + \nabla \cdot (h\vec{v}) = 0$$

$$\frac{\partial \vec{v}}{\partial t} + \eta \vec{k} \times \vec{v} = -\nabla K - g\nabla(h + h_0)$$

- $\vec{v}$ is the 3D velocity vector tangent to the sphere
- $f = 2\Omega \sin(\theta)$
- ∇ gradient on tangent plane
- $\vec{k}$ unit vector point out of the sphere

$$(\vec{v} \cdot \nabla)\vec{v} = (\nabla \times \vec{v}) \times \vec{v} + \frac{1}{2}\nabla(\vec{v} \cdot \vec{v})$$

Many properties: Conserves mass, energy, enstrophy, Coriolis neutral in energy budget, normal modes - inertia-gravity waves, Rossby waves, etc...

Challenges

- Finite Differences and Spectral on unstructured grids?

  -> **Finite Volume** and Finite Element Schemes

- Example of desired properties for horizontal shallow water equations:
  - Accurate and stable
  - Scalable (Local operators - no global operations)
  - Mass and energy conservation
  - Accurate representation slow/fast waves (staggering)
  - Curl-free pressure gradient $\nabla \times \nabla \psi = 0$
  - Energy conservation of pressure terms $\vec{v} \cdot \nabla h + h \nabla \cdot \vec{v} = \nabla \cdot (h\vec{v})$
  - Energy conserving Coriolis term $\vec{v} \cdot \vec{v}^{\perp} = 0$

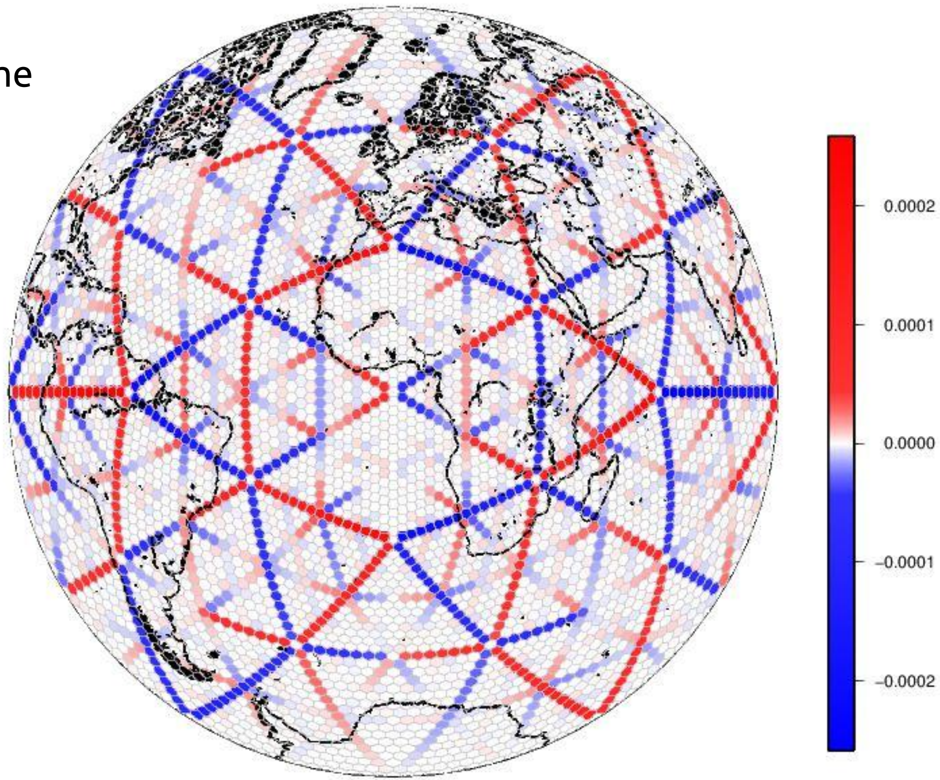
Solved for Finite Differences on Lat-Lon grids (apart from scalability!)
Open problem for Finite Volumes on arbitrary polygonal spherical grids

TRiSK Scheme: Ringler, T.D., Thuburn, J., Klemp, J.B. and Skamarock, W.C., 2010. A unified approach to energy conservation and potential vorticity dynamics for arbitrarily-structured C-grids. Journal of Computational Physics.

Grid Imprinting

- Grid influences numerical errors of Finite Volume

Classic Finite Volume Discretization error for 2D divergence of solid body rotation (should be zero everywhere!)

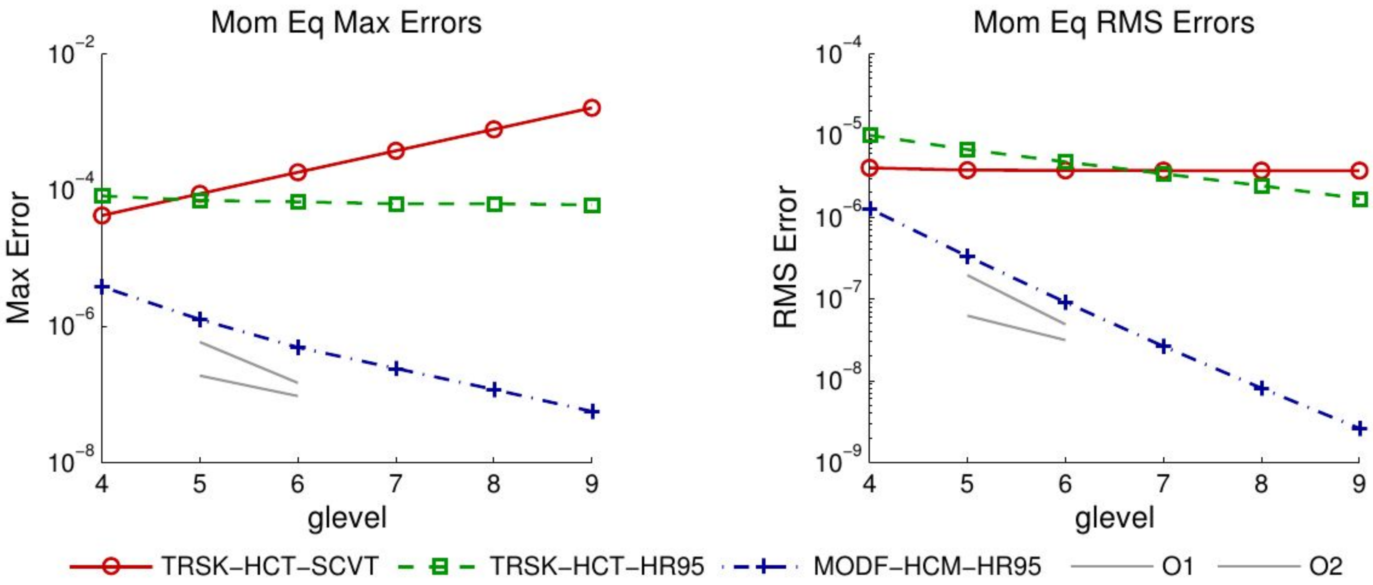


Peixoto, P.S. and Barros, S.R., 2013. Analysis of grid imprinting on geodesic spherical icosahedral grids. Journal of Computational Physics, 237, pp.61-78.

Accuracy

- Accurate and Stable Finite Volume Schemes

  ⇒ Finite Volume Schemes may loose consistency/convergence on irregular grids



Finite Volume scheme (TRiSK - used in MPAS model) truncation error for 2D Momentum Equation

Peixoto, P.S., 2016. Accuracy analysis of mimetic finite volume operators on geodesic grids and a consistent alternative. Journal of Computational Physics, 310, pp.127-160.

Numerical Stability

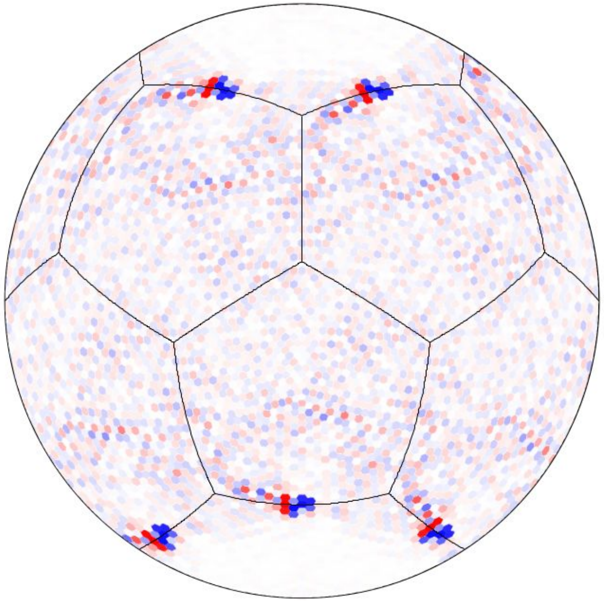
- Energy conserving schemes on polygonal grids use vector relation

$$\vec{v} \cdot \nabla \vec{v} = \nabla K + \zeta \vec{k} \times \vec{v}$$

Equivalently for 2D:

$$uu_x + vu_y = \left(\frac{u^2 + v^2}{2}\right)_x + (v_x - u_y)(-v)$$

$$uv_x + vv_y = \left(\frac{u^2 + v^2}{2}\right)_y + (v_x - u_y)(u)$$



Terms in red cancel analytically, but maybe not numerically...
Lack of numerical cancellation may lead to instability.

Peixoto, P.S., Thuburn, J. and Bell, M.J., 2018. Numerical instabilities of spherical shallow-water models considering small equivalent depths. *Quarterly Journal of the Royal Meteorological Society, 144(710), pp.156-171.*

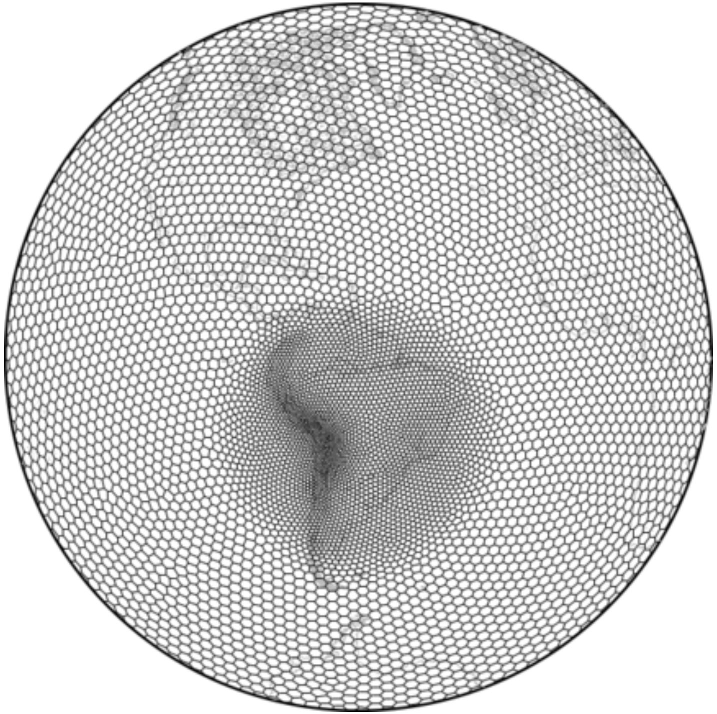
New generation of models

Characteristics

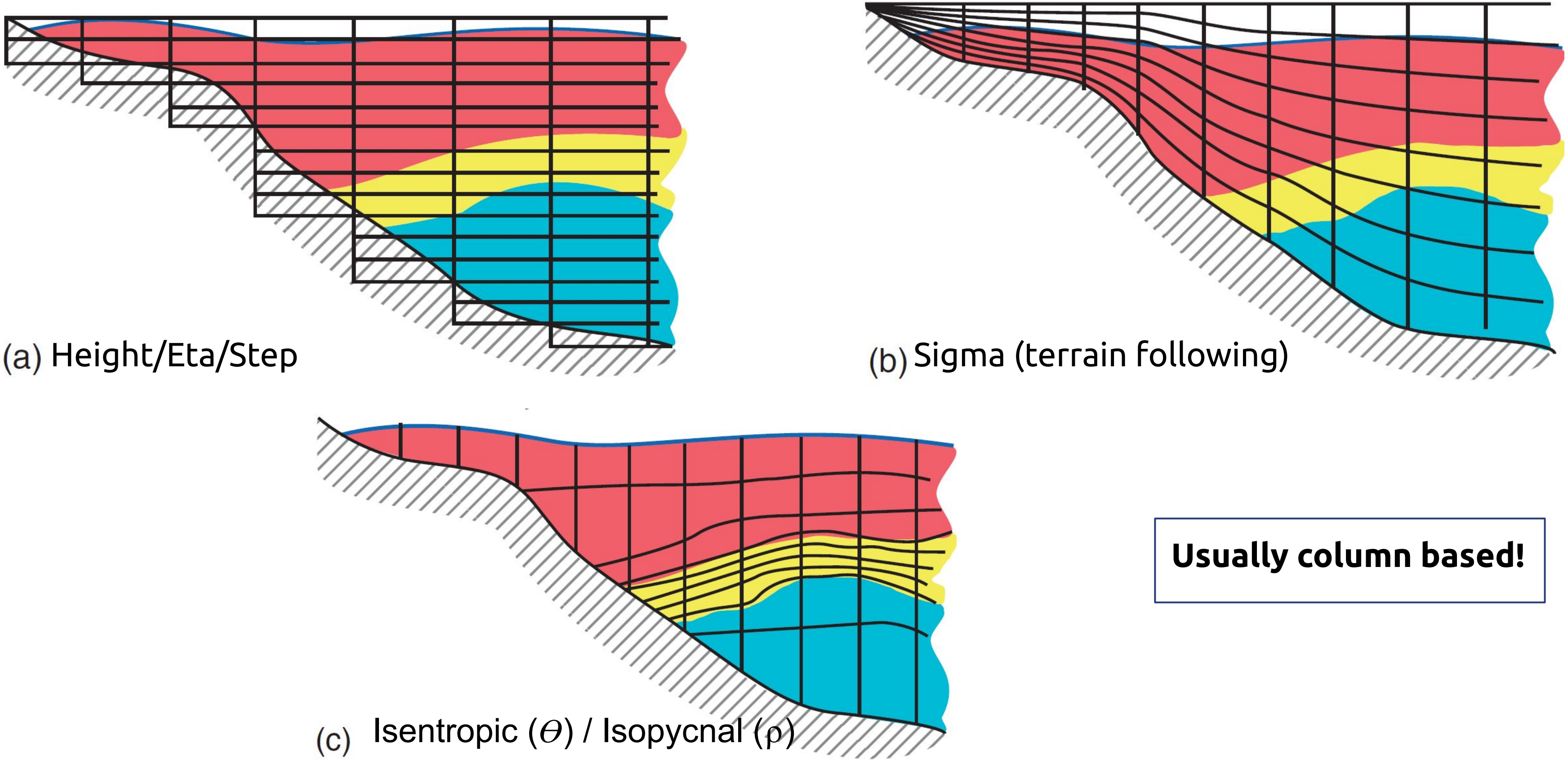
- Grids:
  - Cubed sphere - logically rectangular
  - Triangular/Voronoi - flexible for refinement

- Methods:
- Finite Volume
  - Low order/grid effects with good properties
  - Higher order with less mimetic properties
- Finite Element
  - Mixed finite elements: Mimetic properties
  - Spectral elements/DG: Accuracy, scalable

Several open problems!



Vertical Coordinates/Grid



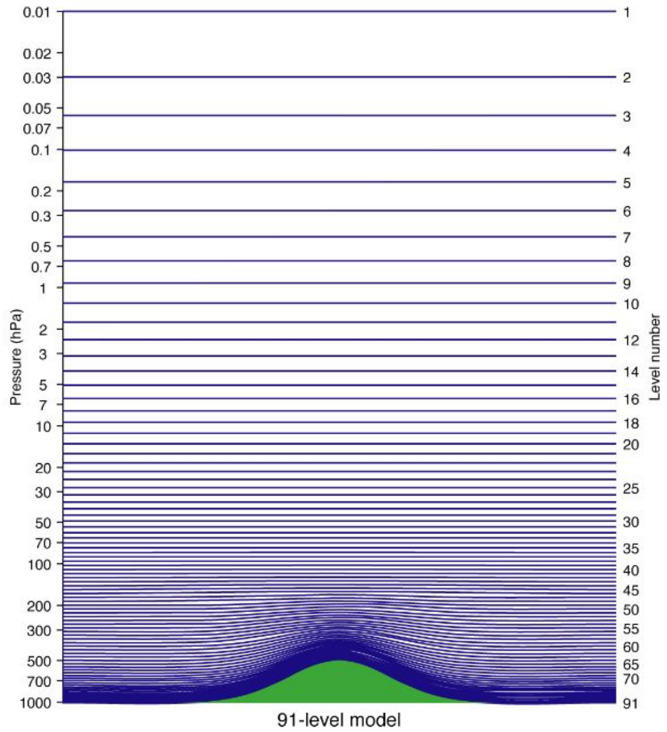
Usually column based!

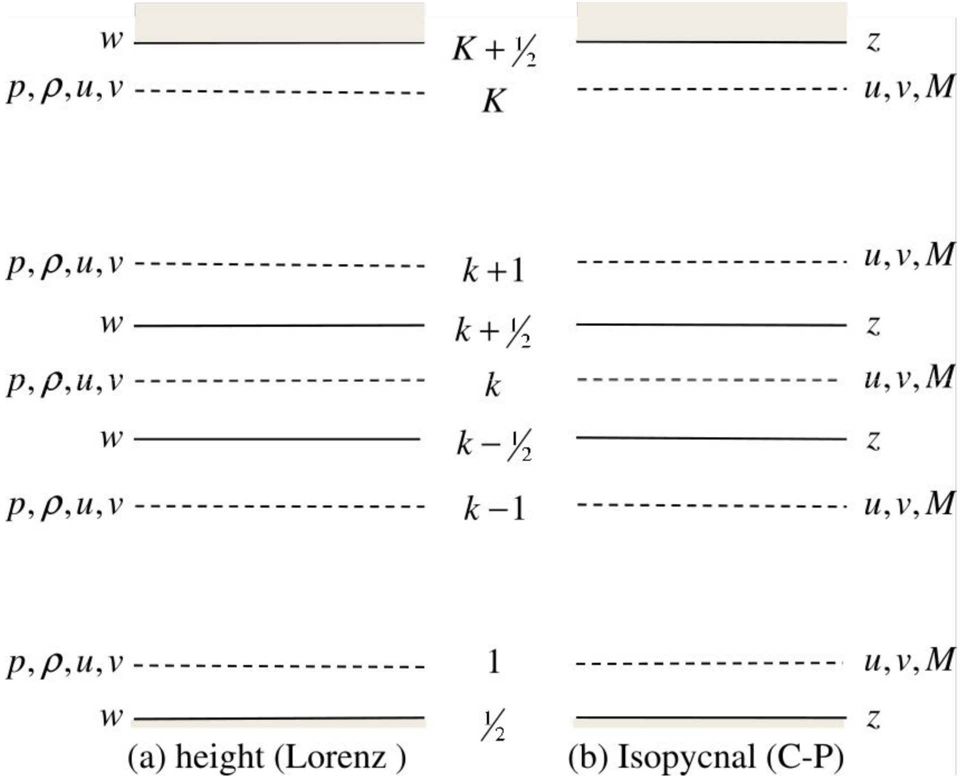
Hodges, B., 2009. Hydrodynamical Modeling.(EL Gene, Ed.) Encyclopedia of Inland Waters. *Academic Press-Elsevier. doi*, *10*, pp.B978-012370626.

Vertical

Ex: Hybrid sigma (terrain following)/pressure

Image: IFS-ECMWF documentation

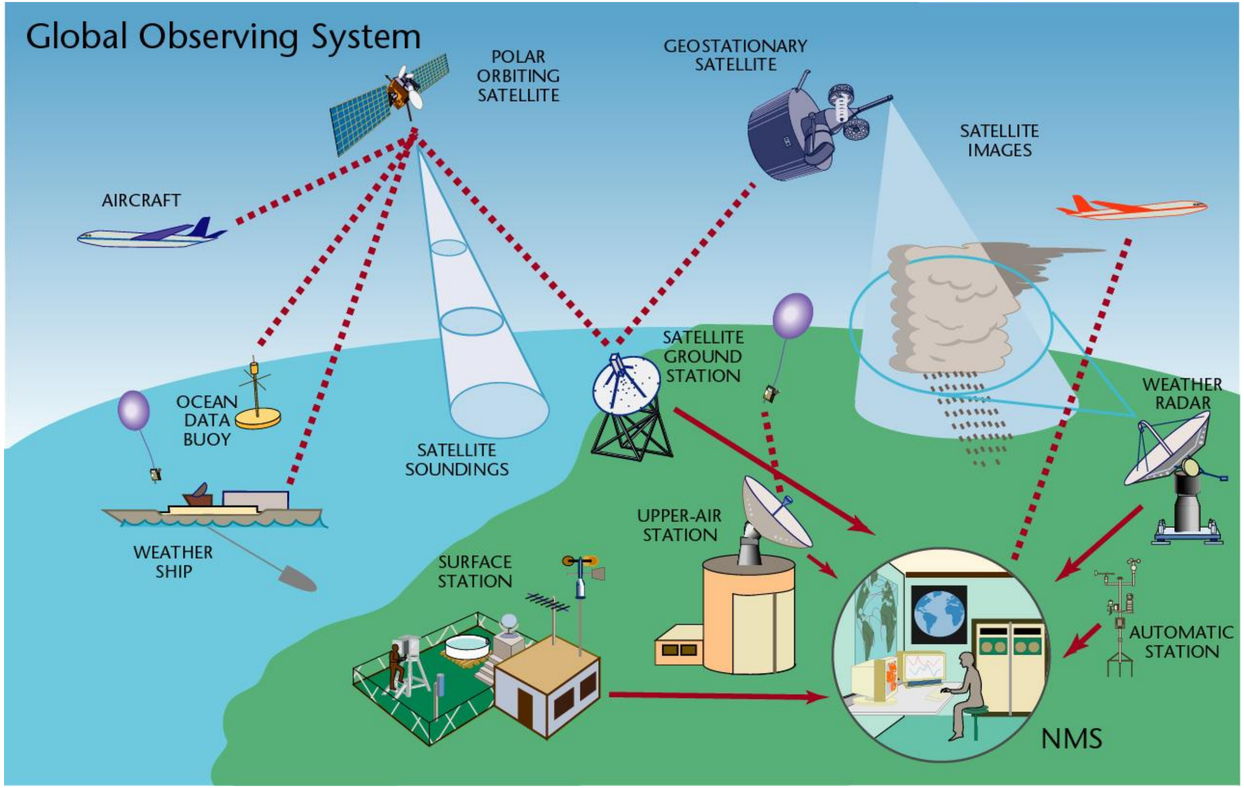




Bell, M.J., Peixoto, P.S. and Thuburn, J., 2017. Numerical instabilities of vector-invariant momentum equations on rectangular C-grids. *Quarterly Journal of the Royal Meteorological Society, 143*(702), pp.563-581.

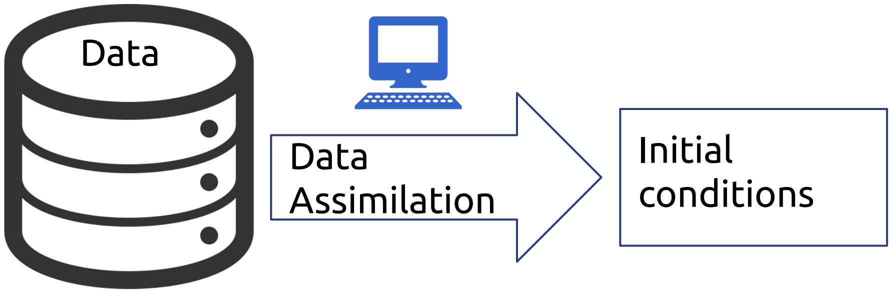
Operational Weather Forecasting

Data: Global Observing System



https://www.wmo.int/pages/prog/www/OSY/GOS.html

Data Assimilation



- Use previous model forecast for background state
- Inverse problem: Minimize distance between observations and background state
- Can be done in a time window (ex: 4DVAR, Kalman Filter)

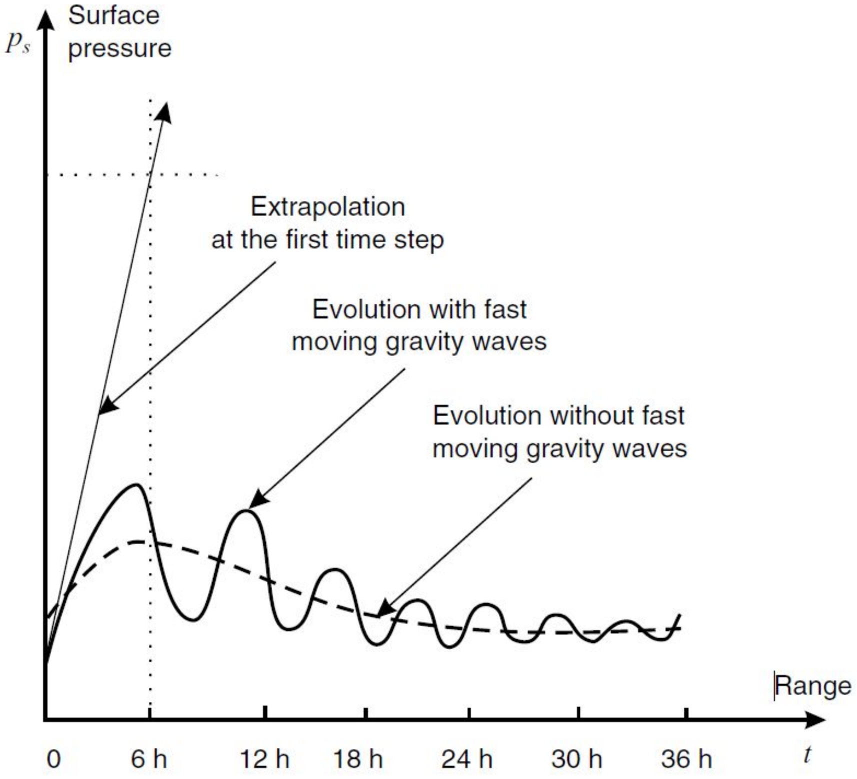
Coiffier, J., 2011. Fundamentals of numerical weather prediction. Cambridge University Press.

Model Initialization

Initial conditions

Normal mode initialization

Initial conditions:
- Remove noise/fast oscillations to keep only the "slow manifold"



Coiffier, J., 2011. Fundamentals of numerical weather prediction. Cambridge University Press.

Parameterised processes

Sub-grid scale physics:
- Moist/Clouds
- Radiation
- Boundary layer
- Land/Sea/Ice
- Turbulence

Chemistry:
- Aerosols
- Greenhouse Gases
- Reactive Gases

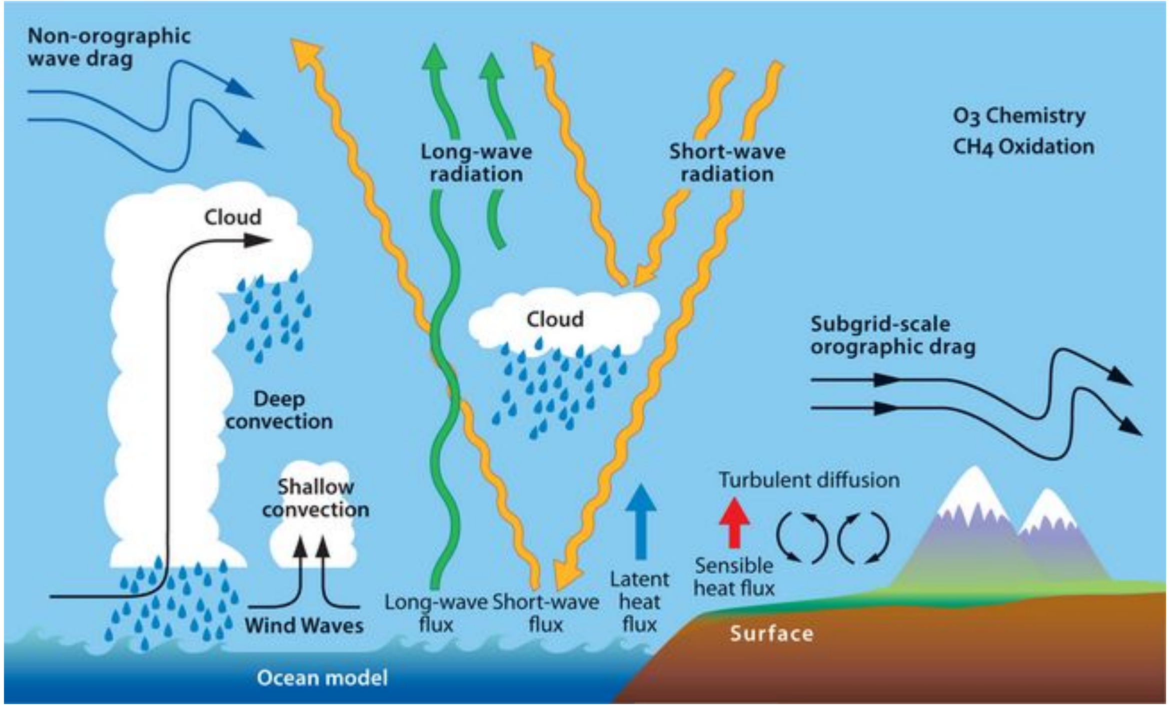
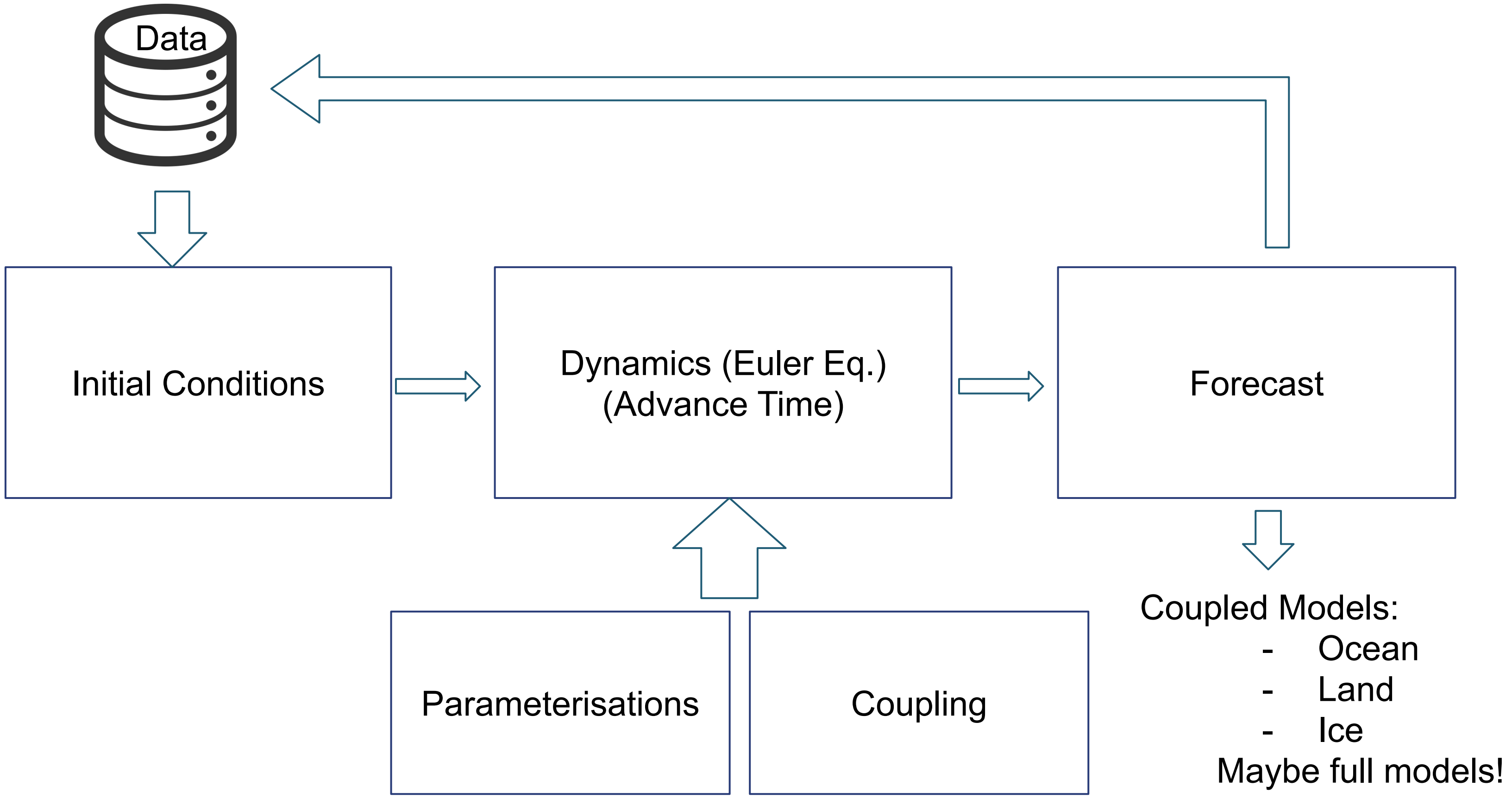


Image: ECMWF

Operational Weather Forecast



Conclusions

“All models are wrong but some are useful”

— George Box

Thanks!

More at: www.ime.usp.br/~pedrosp

Contact for collaboration/advisory: ppeixoto@usp.br

Acknowledgements:

- Many collaborators!
- FAPESP Jovem Pesquisador/BPE
- CNPq Universal/Produtividade
- CAPES Auxílios/Bolsas