

Challenges of numerical modelling of the atmosphere dynamics on spherical polygonal grids

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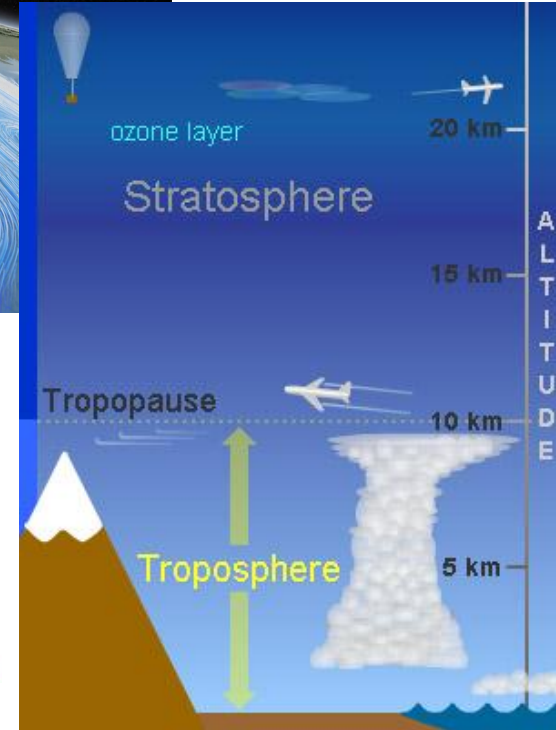
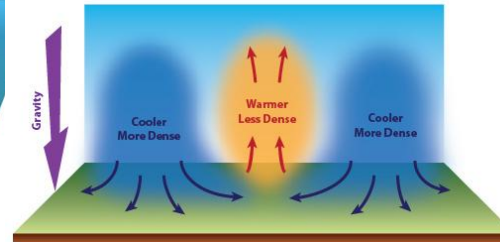
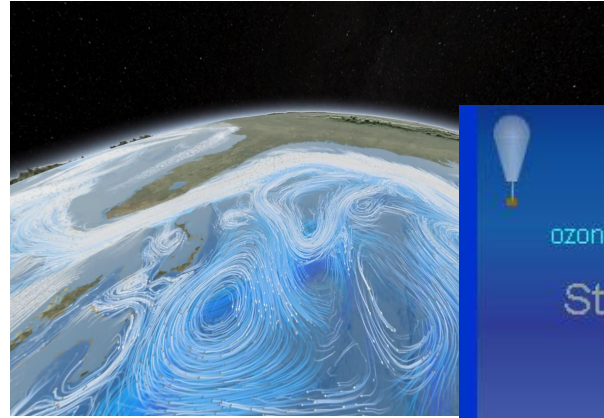
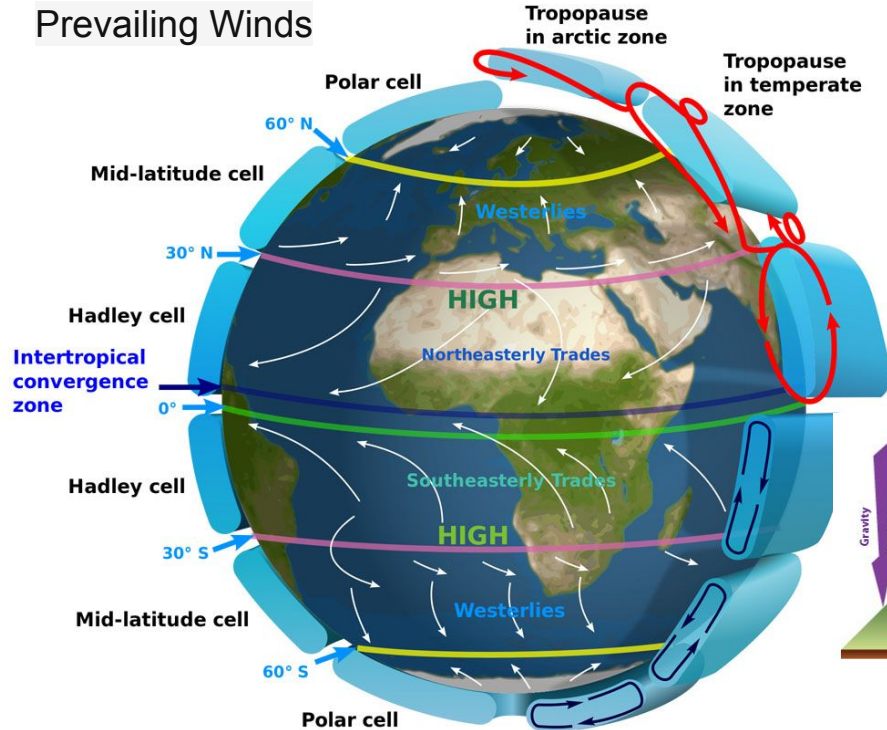
feb 2026

Centrepiece of study: Atmosphere

The atmosphere is a layered fluid (gas)

Remark: Many topics discussed in this talk are also valid for **ocean** models.

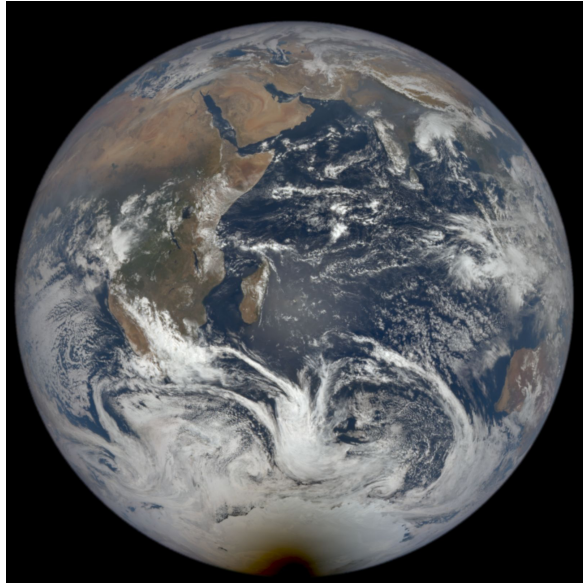
Prevailing Winds



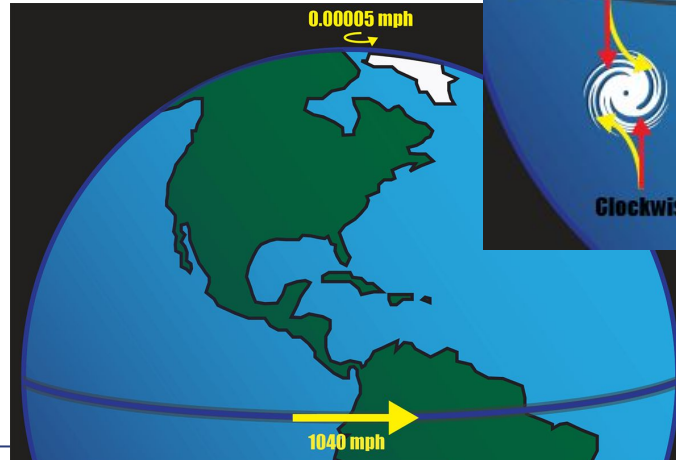
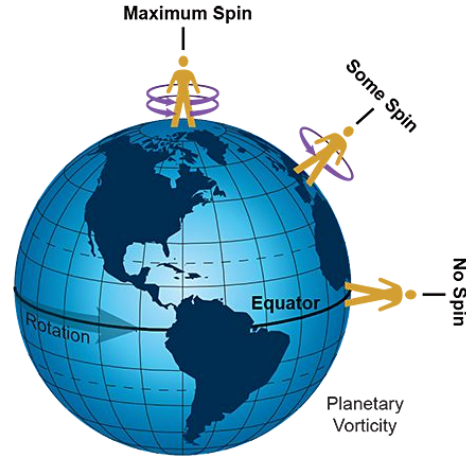
Images: < Nasa, ^ NCAR-UCAR

Images: Nat. Geo. / Wikimedia/Nasa ^

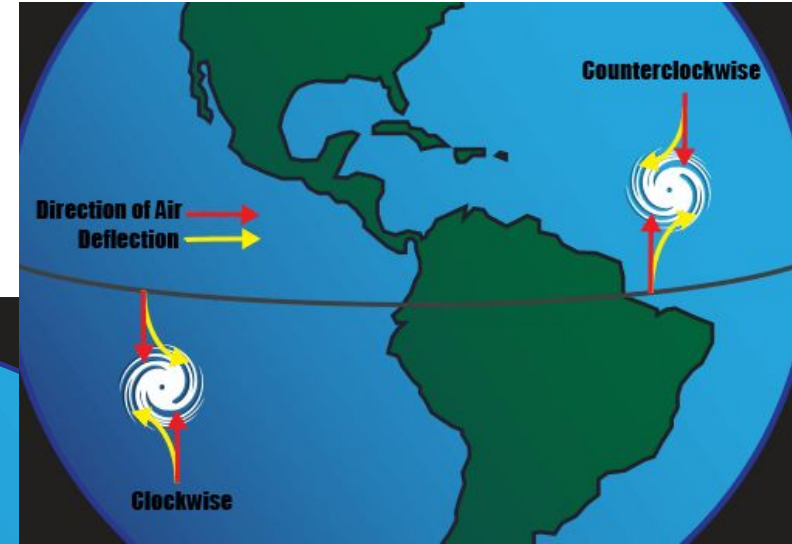
Earth: A rotating “sphere”



Images: NASA
<https://www.nasa.gov/image-feature/eclipse-over-antarctica>

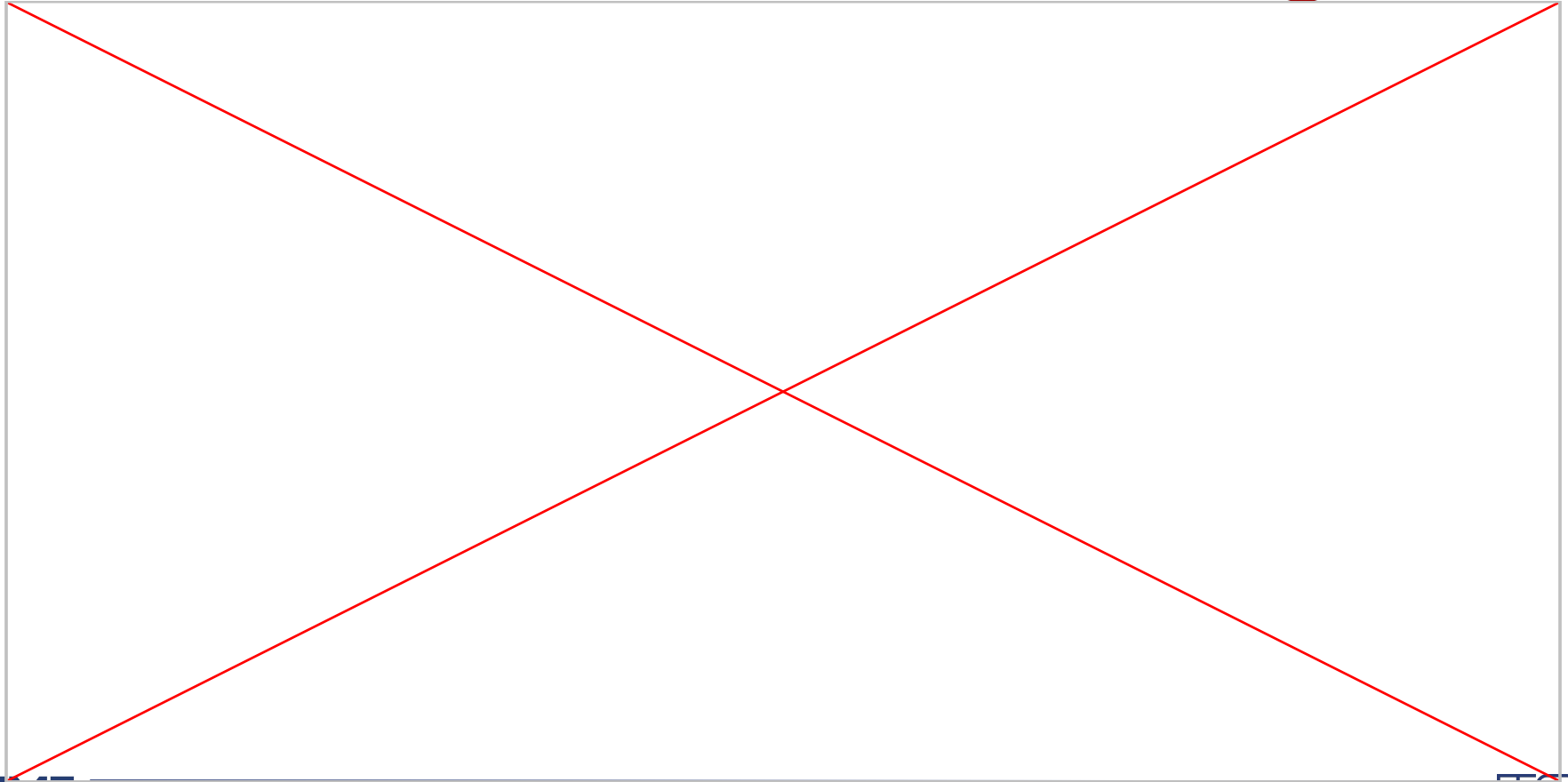


Coriolis Effect



Images: NOAA <https://scijinks.gov/coriolis/>

What are we trying to model?



History



Lewis Fry Richardson (UK 1881 -1953)

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

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

These equations are essentially derived from the balances of forces in the atmosphere.

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)

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

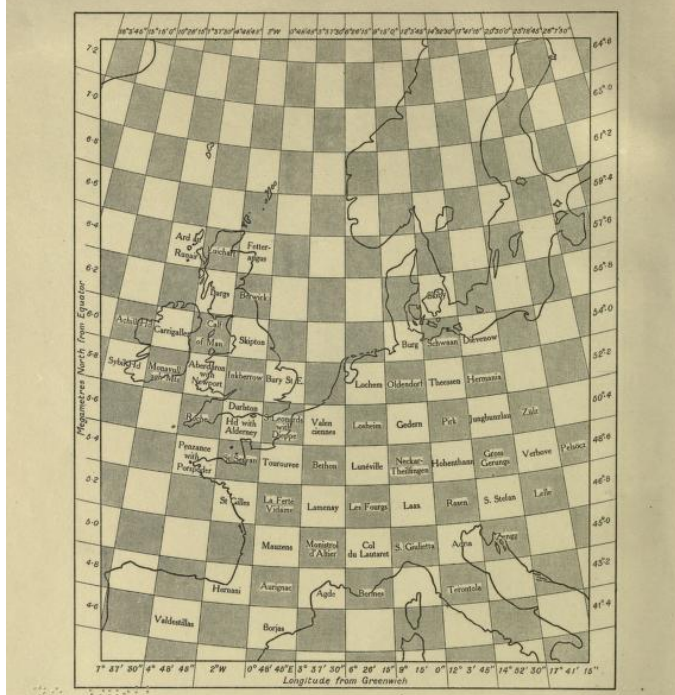
Energy (temperature)

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

State (pressure)

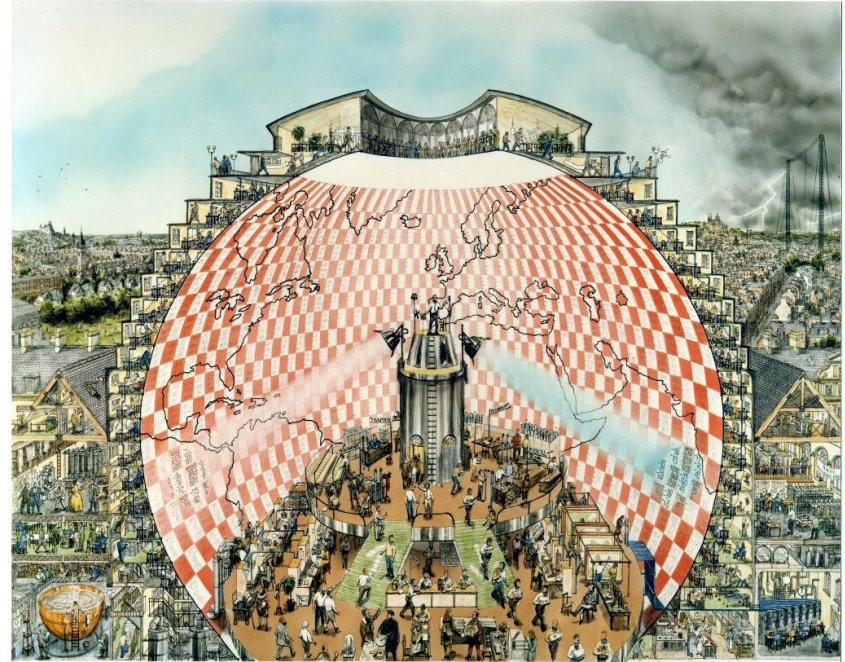
$$p = \rho R T$$

Weather prediction by numerical process



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

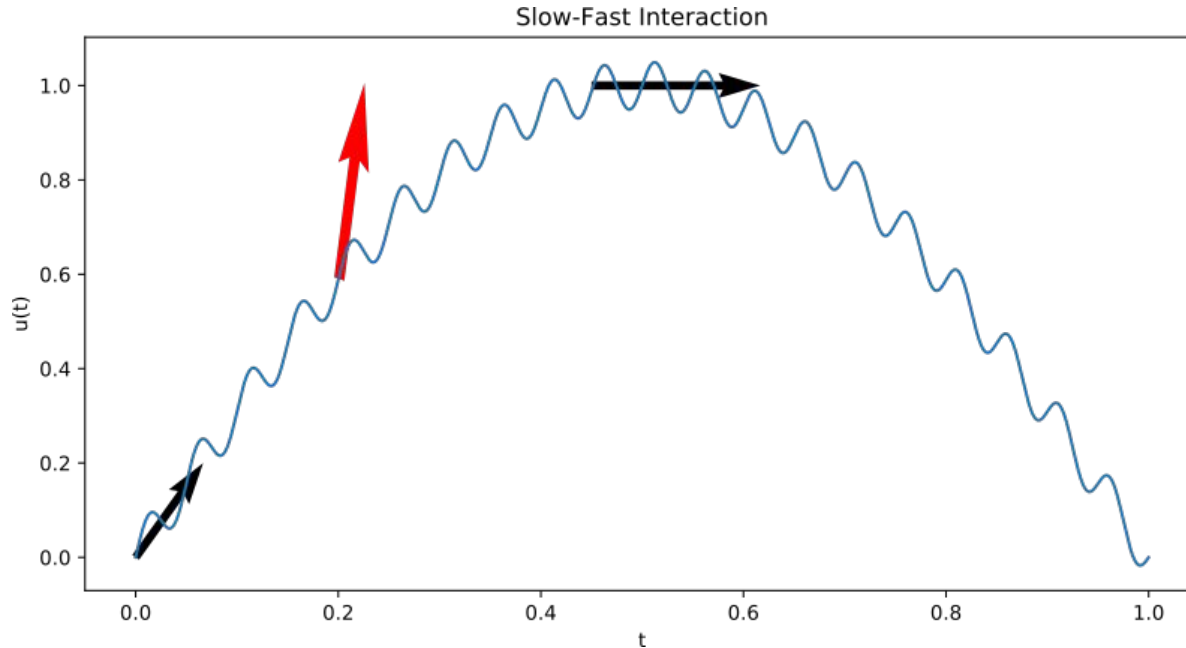
- Weeks of hand calculation while in ambulance trips (driver) in WW-I



"Weather Forecasting Factory" by Stephen Conlin, 1986.

Richardson's Results

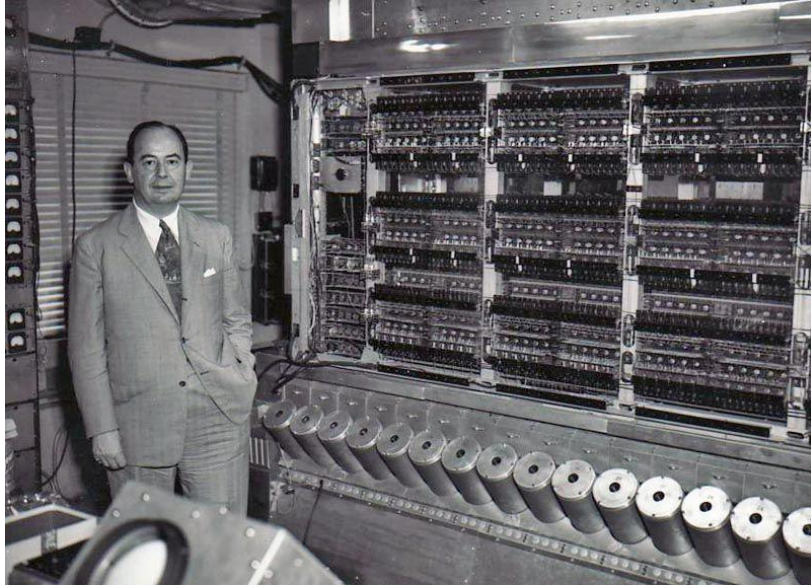
- Predicted a 145mb change over 6 hours at a grid point
- Observations showed almost no pressure change



- **Great ideas, but the dynamics is multiscale!**
- **Model initialization issues (initial imbalance between pressure and wind)**

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

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 Numerical 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)

Remark:

No gravity waves, so initialization is “easier”

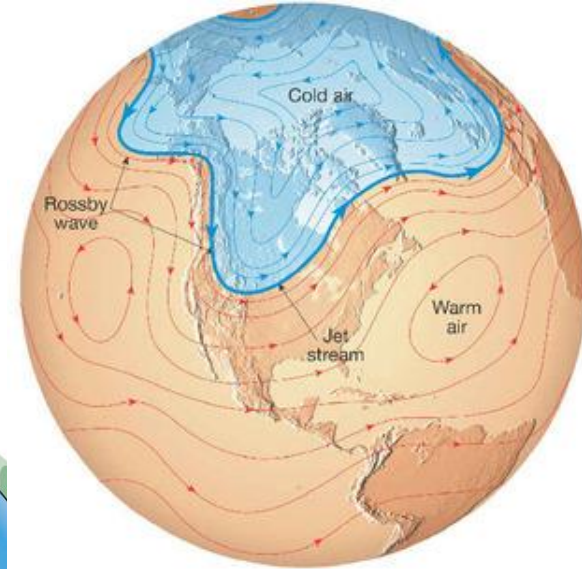
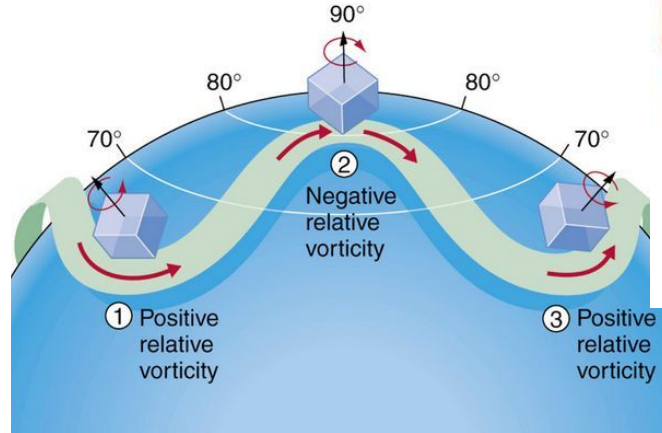
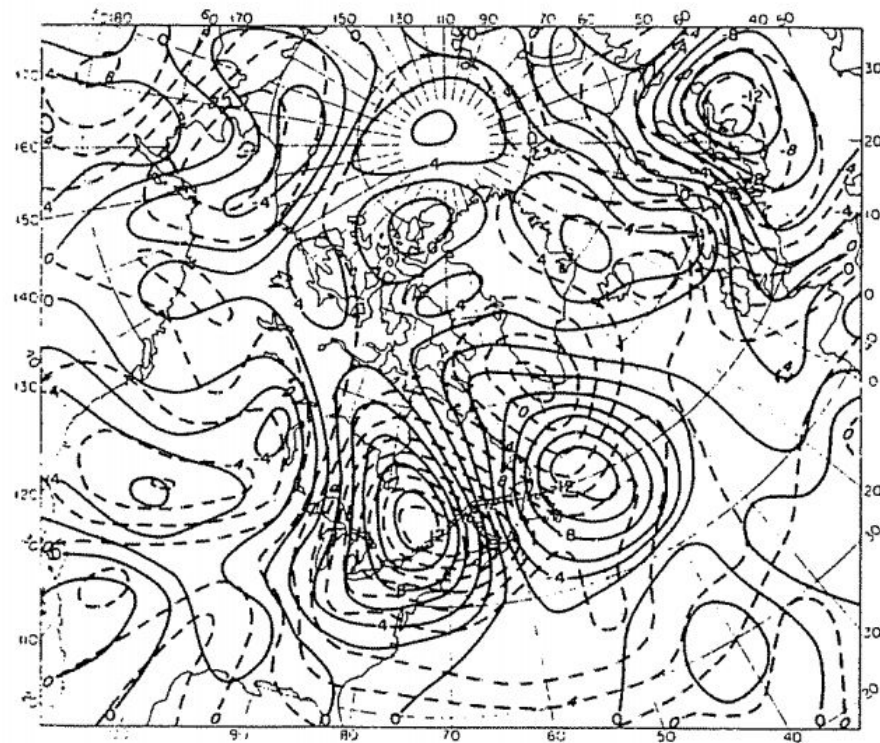
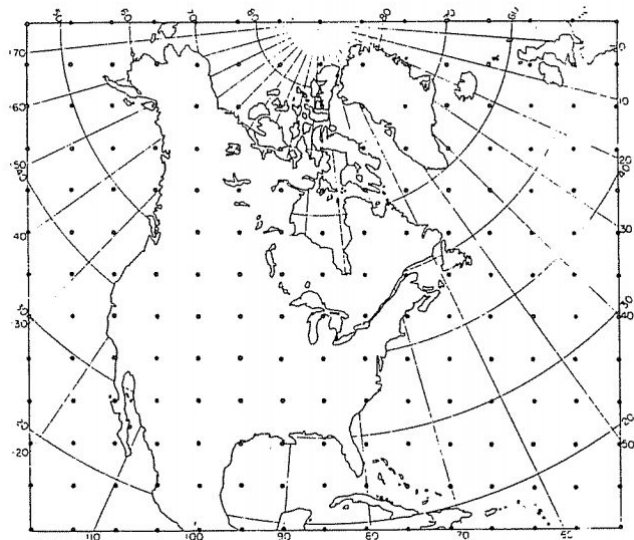


Image credit: stephenleahy.net ^
<<http://homework.uoregon.edu/pub/class/atm/ross1.html>>

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!



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.

Models for Atmosphere Dynamics

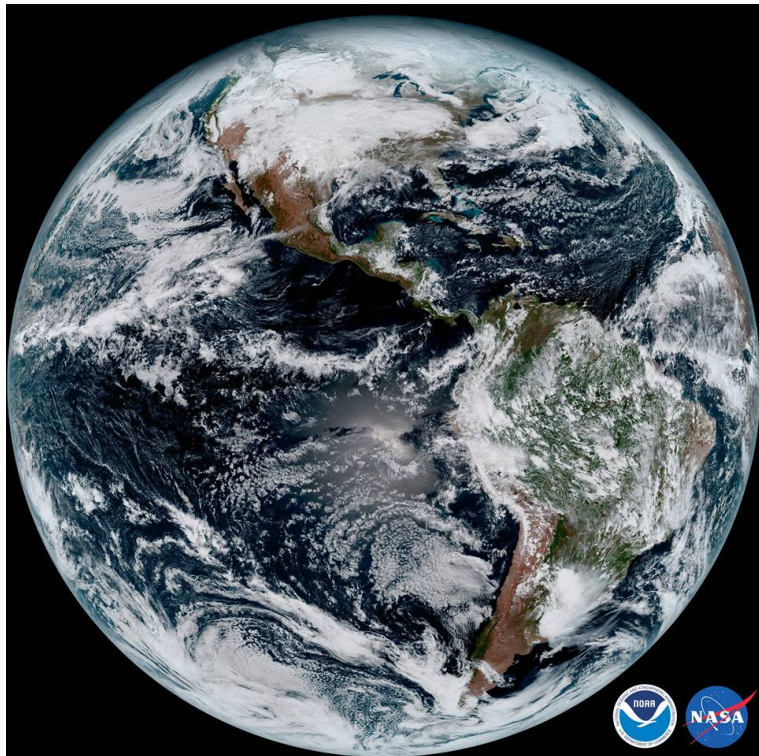


Image: GOES-16 Jan 2017

Three-dimensional Navier-Stokes equations



Nonhydrostatic models



Primitive equations
(hydrostatic equations)



Shallow water equations



Quasi-geostrophic models



Two-dimensional barotropic equations.

3D

2D

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

Ultimate goal

Hydrostatic (primitive) equations: maybe **inadequate** below ~10km horizontal resolution ?

To capture explicit convection (resolution $\ll 10\text{km}$):

Compressible Euler equations for atmosphere (ideal gas)

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

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

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

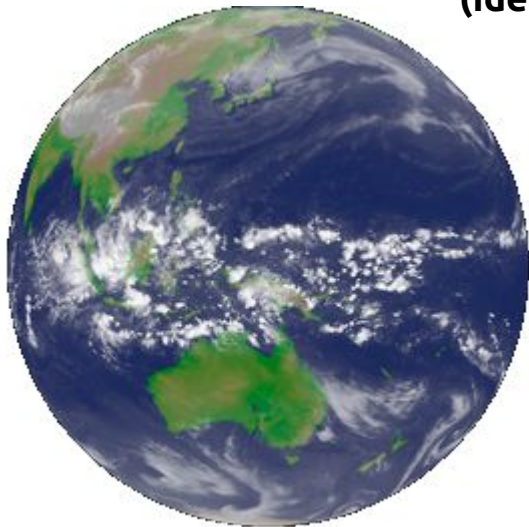


Image: NICAM Model (Japan)

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

Non-hydrostatic!

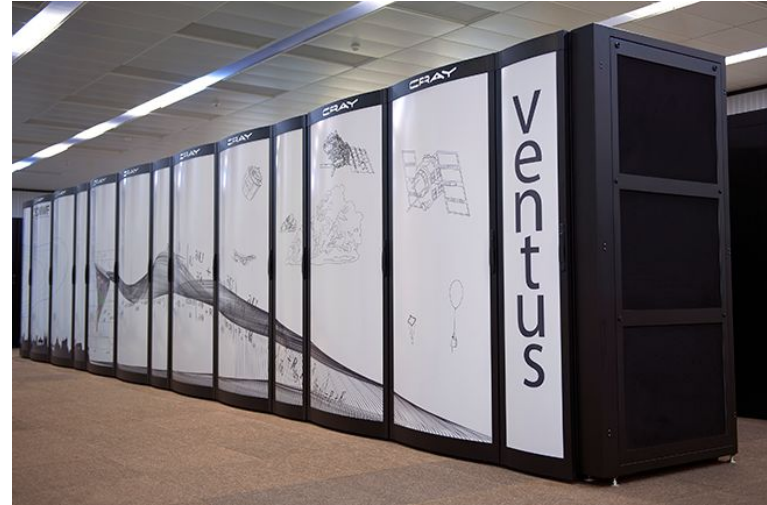
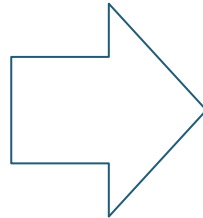
The underlying numerics...

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

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

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

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



<https://www.ecmwf.int/en/about/media-centre/news/2017/shaping-future-supercomputing-numerical-weather-prediction>

Finite Differences

2D on the sphere $(\lambda, \theta) = (\text{longitude}, \text{latitude})$

$$\left(\frac{\partial P}{\partial x}\right)_{ij} = \left(\frac{P_{i+1,j} - P_{i-1,j}}{2a \cos \phi_j \Delta \lambda}\right), \quad \left(\frac{\partial P}{\partial y}\right)_{ij} = \left(\frac{P_{i,j+1} - P_{i,j-1}}{2a \Delta \phi}\right),$$

What happens near/at the pole?

Explicit in time:

Stability constraints usually require $\Delta t \propto \Delta x$
>The CFL stability condition



Computationally not feasible in practice...

Latitude-Longitude Models

Semi-implicit time integration

- Future time depends implicitly on future time for linear waves
- Solve a very large linear system at each time-step
- Allows large Δt for waves

Semi-Lagrangian integration

- Transport of mass and momentum follow particle trajectories for each timestep
- Allows large Δt for advection/transport

Semi-Lagrangian Fully-implicit integration:

- UKMetOffice: Endgame
Resolution < 17km global, non-hydrostatic (2014)
Iterative implicit solver per timestep



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.



Latitude-Longitude Models

Models:

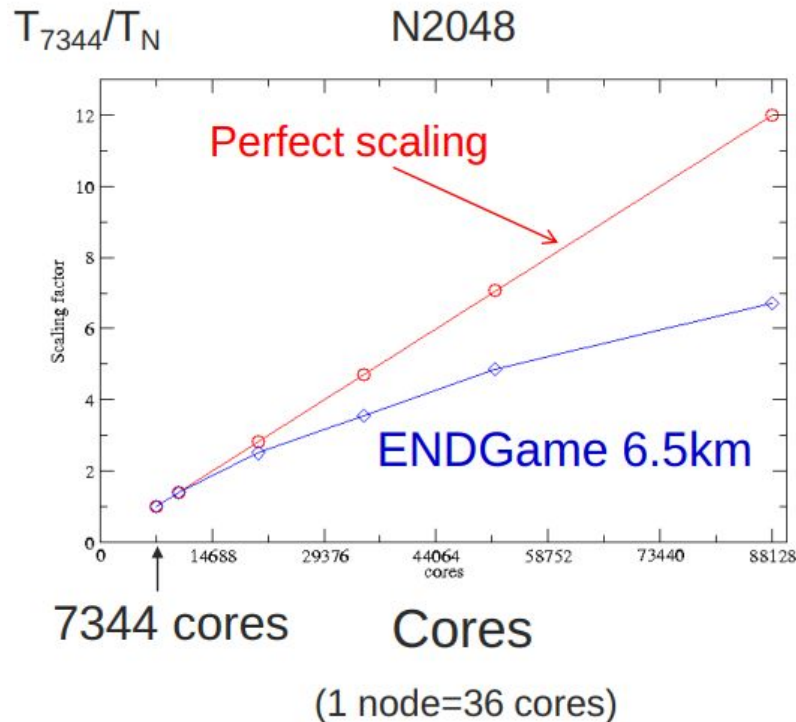
- UKMetOffice: Endgame - Semi-Lag/Implicit (2014)
- Russian: SL-AV20 - Semi-Lag/Semi-Implicit (2016)
Resolution ~20km, hydrostatic

Issues:

- Require significant data communication among the grid points clustered around the two poles. (Impacts SL)
- Reduced scalability (increasing the number of processors does not reduce the computational runtime proportionally).

UKMetOffice: GungHo! (Globally Uniform, Next Generation, Highly Optimised)

- Tolstykh, M., Shashkin, V., Fadeev, R. and Goyman, G., 2017. Vorticity-divergence semi-Lagrangian global atmospheric model SL-AV20: dynamical core. Geoscientific Model Development...
- Staniforth, A., Melvin, T., & Wood, N. (2013). Gungho! a new dynamical core for the unified model. In Proceed. of the ECMWF.
- https://wgne.net/wp-content/uploads/2019/10/WED_Wedi_WGNE34_scalabilitymixed.pdf



Spectral Models

Main idea:

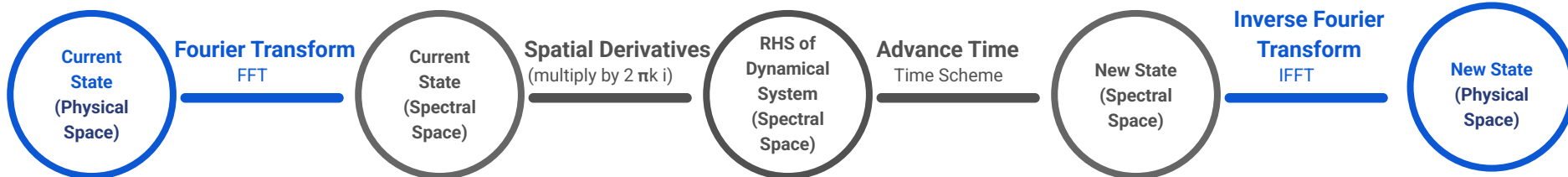
- Expand unknown functions as series of “simpler” basis functions (e.g. Fourier Series/transform)

$$q(x) = \sum_k \hat{q}_k e^{2\pi i k x}$$

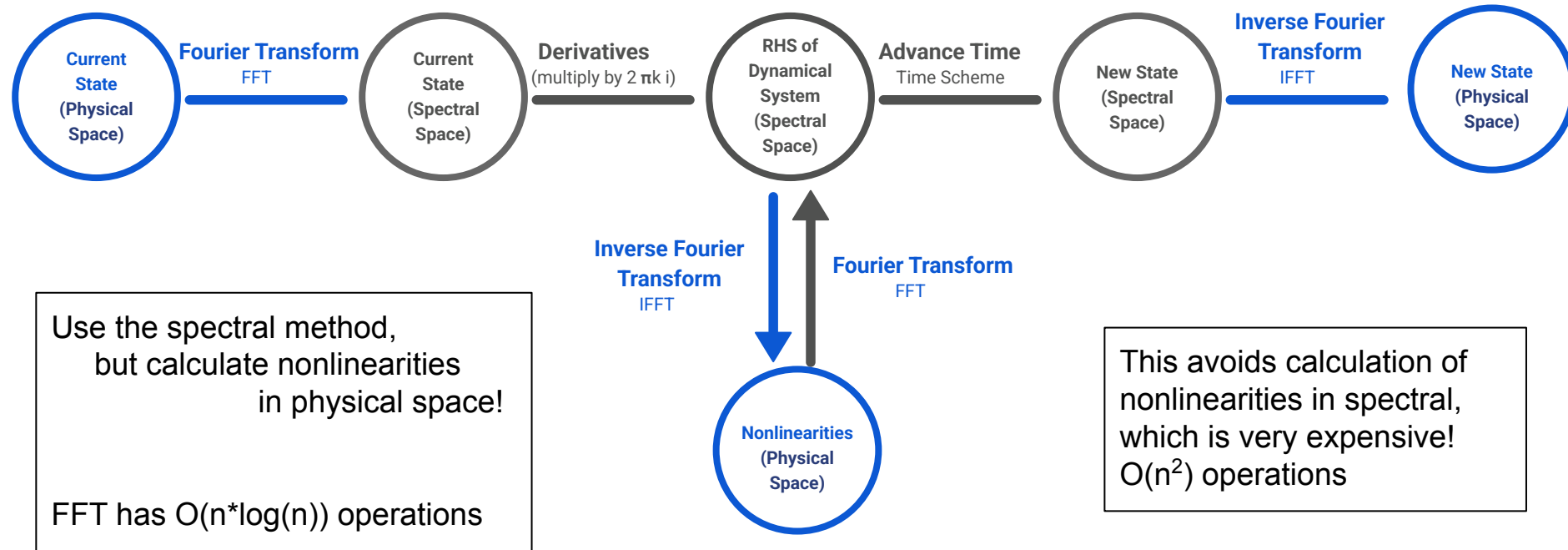
- Calculate derivatives in “spectral space” : derivatives are transformed into multiplications by $2\pi i k$.
- Calculate inverse transform to recover an algebraic equation with respect to spatial derivatives.
- Advance in time (pick your favourite time integrator)
- Use inverse transform to recover new state in physical space

Very accurate and fast
for linear equations!

Very expensive for
nonlinear equations!



Pseudo-Spectral Models



- Eliassen, E., Machenhauer, B. and Rasmussen, E., 1970. On a numerical method for integration of the hydrodynamical equations with a spectral representation of the horizontal fields ..
- Orszag, S.A., 1970. Transform method for the calculation of vector-coupled sums: Application to the spectral form of the vorticity equation. Journal of Atmospheric Sciences, 27(6)..

Spectral Models on the Sphere

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

Spherical harmonics basis:

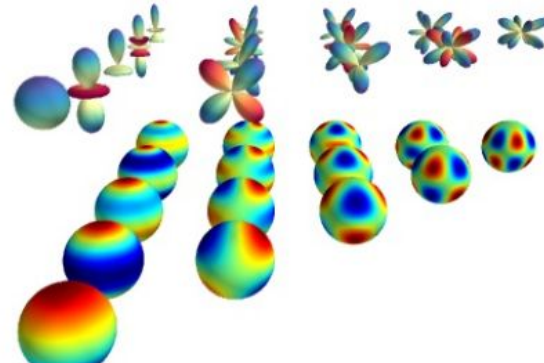
- Fourier expansion for each latitude circle
- Legendre polynomials on meridians

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

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

Characteristics:

- Use pseudo-spectral for nonlinearities
- Usually built as Semi-Lagrangian Semi-Implicit
- Easy Semi-Implicit problem (linear system is diagonal)
- Accurate (spectral order)
- Stable (avoids strong CFL restriction at poles)



- Eliassen, E., Machenhauer, B. and Rasmussen, E., 1970. On a numerical method for integration of the hydrodynamical equations with a spectral representation of the horizontal ...
- Orszag, S.A., 1970. Transform method for the calculation of vector-coupled sums: Application to the spectral form of the vorticity equation. Journal of Atmospheric Sciences...
- Barros, S.R.M., Dent, D., Isaksen, I., Robinson, G., Mozdzyński, 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!

♦ 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...

Operational Examples:

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

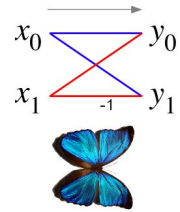
IFS Cycle 48r1 - June 2023

	Component	Horizontal resolution		Vertical resolution [levels]
Atmosphere	HRES	O1280	~9 km	137
	ENS	O1280	~9 km	137
	ENS extended	O320	~36 km	137
Wave	HRES-WAM	0.125°	~14 km	-
	ENS-WAM	0.125°	~14 km	-
	ENS-WAM extended	0.5°	~55 km	-
Ocean	NEMO 3.4	0.25°	~28 km	75

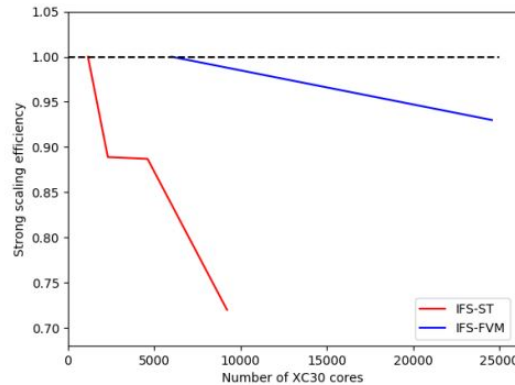
<https://confluence.ecmwf.int/display/FCST/Implementation+of+IFS+Cycle+48r1>

Scalability

Drawbacks:



- Legendre Transform is $O(N^2)$ operations
→ use “fast” Legendre transforms (Butterfly Algorithm)
- Spectral transforms require global communication
→ reduces scalability (parallelism has communication bottlenecks)

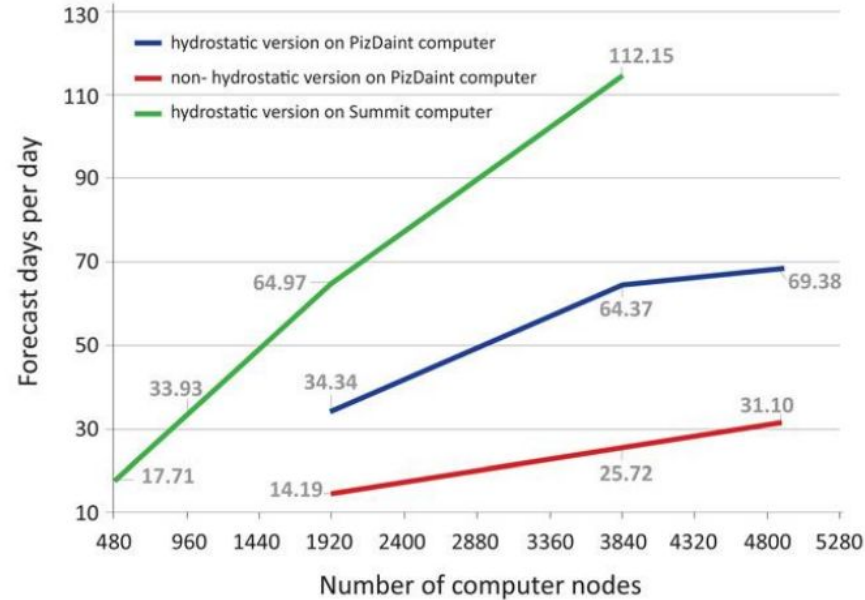


Strong scaling

IFS-ECMWF Example:

Time-to-solution

Speed comparison using: high-resolution ECMWF IFS
1.25 km, 62-vertical levels (TCO7999)



The scalability problem

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



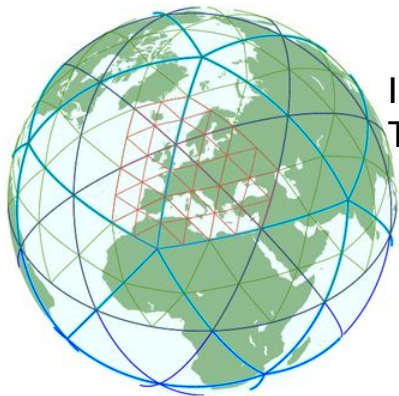
TUPA-CPTEC/INPE (~30k cores)

Massively Distributed Memory Parallel Machines

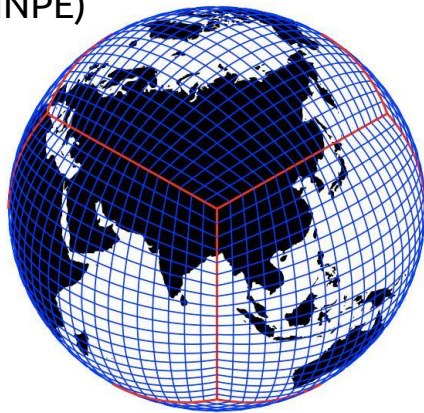
- Finite Differences: Pole communicates with many other computer nodes
- Semi-implicit: A lot of global communication required for the solution of the global linear system or spectral transforms
- Limited scalability on large supercomputers (cannot do the forecast within the time window for high resolutions)

Search for alternatives - more isotropic grids

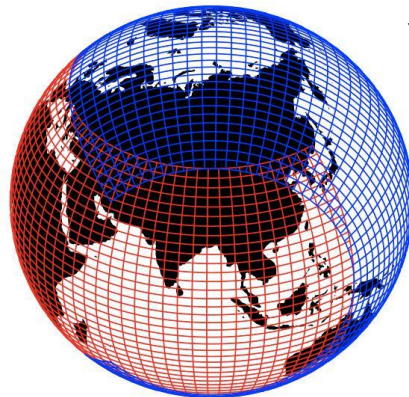
Cubed Sphere (CAM-SE/FV3/NUMA-USA,
GEF-INPE)



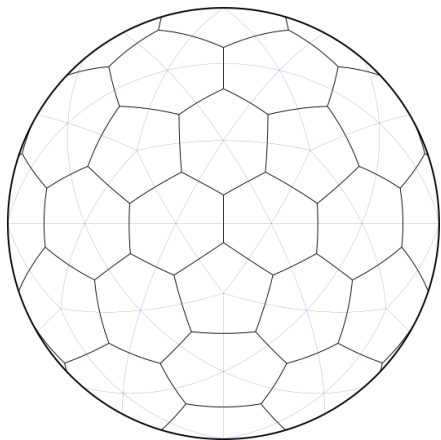
Icosahedral/
Triangular
(ICON-Germany)



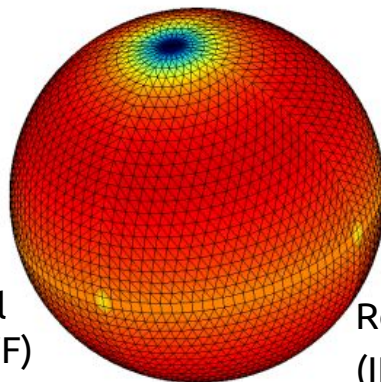
Yin-Yang
(GEM-Canada)



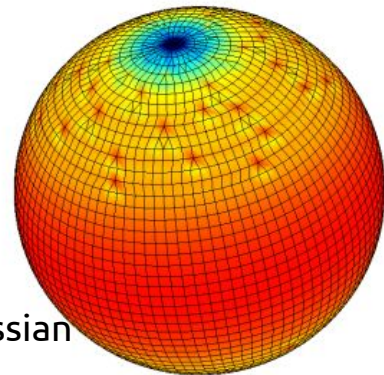
Voronoi
(MPAS/FIM/
OLAM-USA
NICAM-Japan)



Octahedral
(IFS-ECMWF)

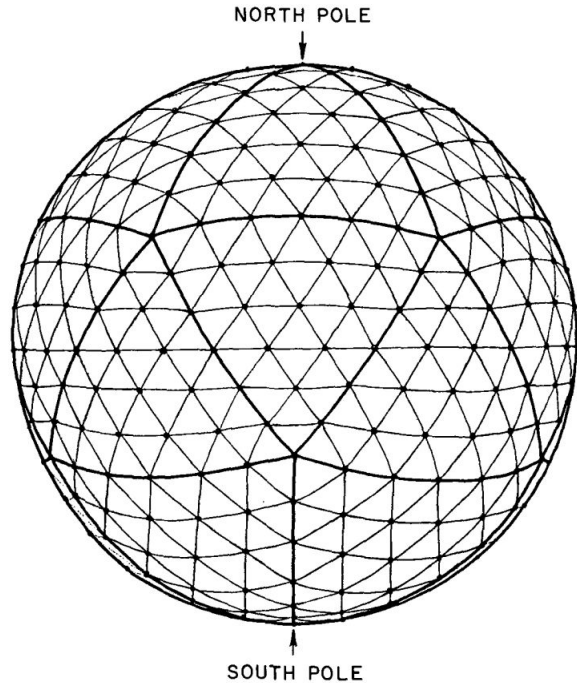


Reduced Gaussian
(IFS-ECMWF)

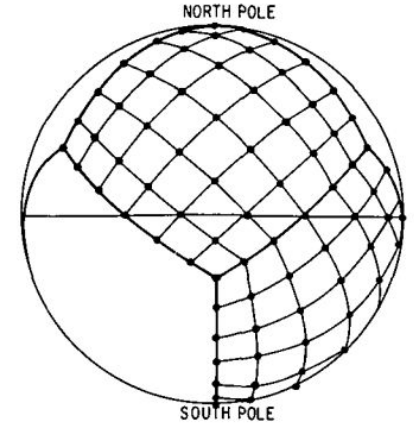
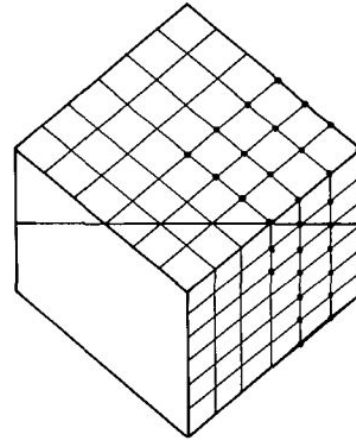


First Ideas

Sadourny, Arakawa, Mintz 1968



Sadourny 1972



Not competitive with latitude-longitude grids based methods at the time....

-Sadourny, R., Arakawa, A. and Mintz, Y., 1968. Integration of the nondivergent barotropic vorticity equation with an icosahedral-hexagonal grid for the sphere. Monthly Weather Review, 96(6), pp.351-356.

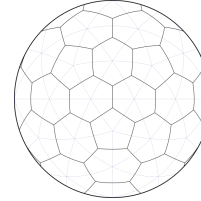
-Sadourny, R., 1972. Conservative finite-difference approximations of the primitive equations on quasi-uniform spherical grids. Monthly Weather Review, 100(2), pp.136-144.

New generation of models

From ~2000 onwards

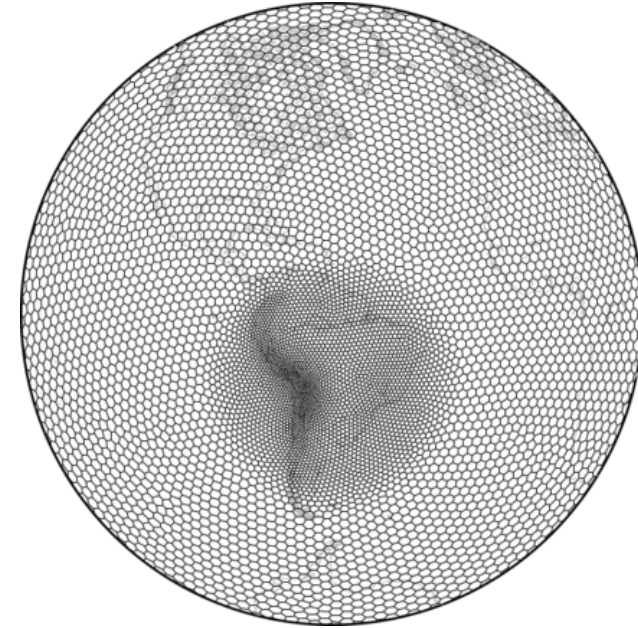
■ Grids:

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



■ Methods:

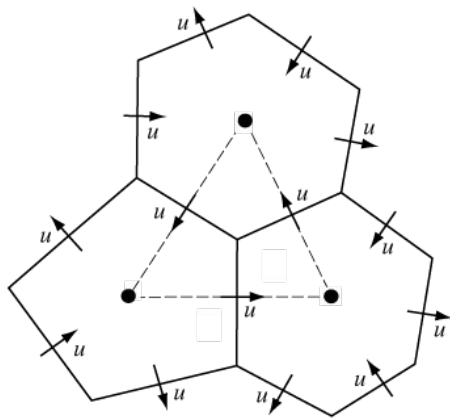
- Finite Volume
 - Low order/grid effects with good properties
 - Higher order with less mimetic properties
- Finite Element
 - Mixed finite elements: Mimetic properties
 - Spectral elements/DG: Accuracy, scalable



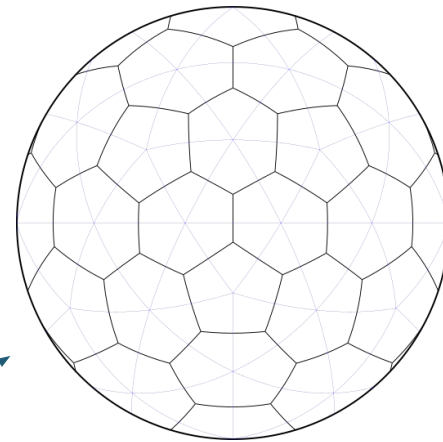
Several open problems!

Santos, L.F. and Peixoto, P.S., 2021. Topography based local spherical Voronoi grid refinement on classical and moist shallow-water finite volume models. *Geoscientific Model Development Discussions*, pp.1-31.

Model for Prediction Across Scales Dynamics

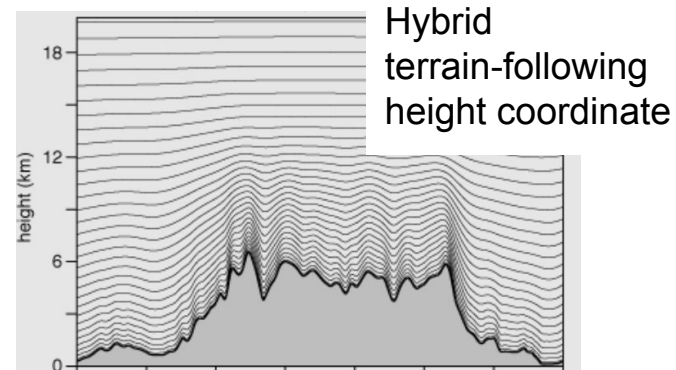


NCAR and Los Alamos Nat Lab



Compressible nonhydrostatic equations

C-grid staggered variables on the horizontal Voronoi mesh. Normal velocities are defined on the cell faces and all other scalar variables are defined at the cell centers. Vertical vorticity is defined at the cell vertices. (from: <https://mpas-dev.github.io/>)



- Skamarock, W.C., Klemp, J.B., Duda, M.G., Fowler, L.D., Park, S.H. and Ringler, T.D., 2012. A multiscale nonhydrostatic atmospheric model using centroidal Voronoi tessellations and C-grid staggering. Monthly Weather Review, 140(9)

MONAN

MONAN – Model for Ocean-land-Atmosphere prediction

“Produce the best weather, climate, and environmental forecasting available worldwide for the South American region and adjacent oceans.”

Computational grids

- a) Non-structured with the possibility of variable refinement or grid nesting;
- b) Global or limited area configuration (open borders);
- c) Finite volumes.

Dynamical core

- a) Locally conservative in mass;
- b) Non-hydrostatic and hydrostatic;
- c) Fully compressible;
- d) Transport with preservation of monotonicity and low numerical diffusivity;
- e) Suitable for 'deep' atmosphere (top space applications);
- f) \geq 2nd order of global and effective accuracy.



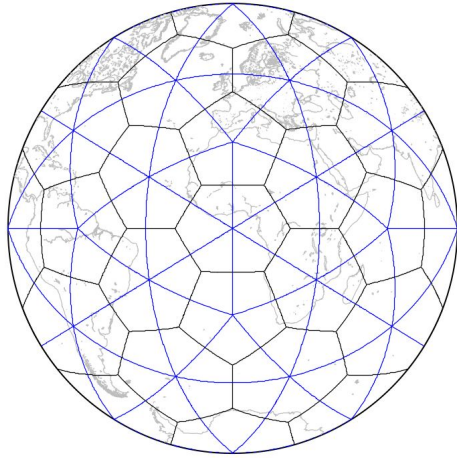
Based on:



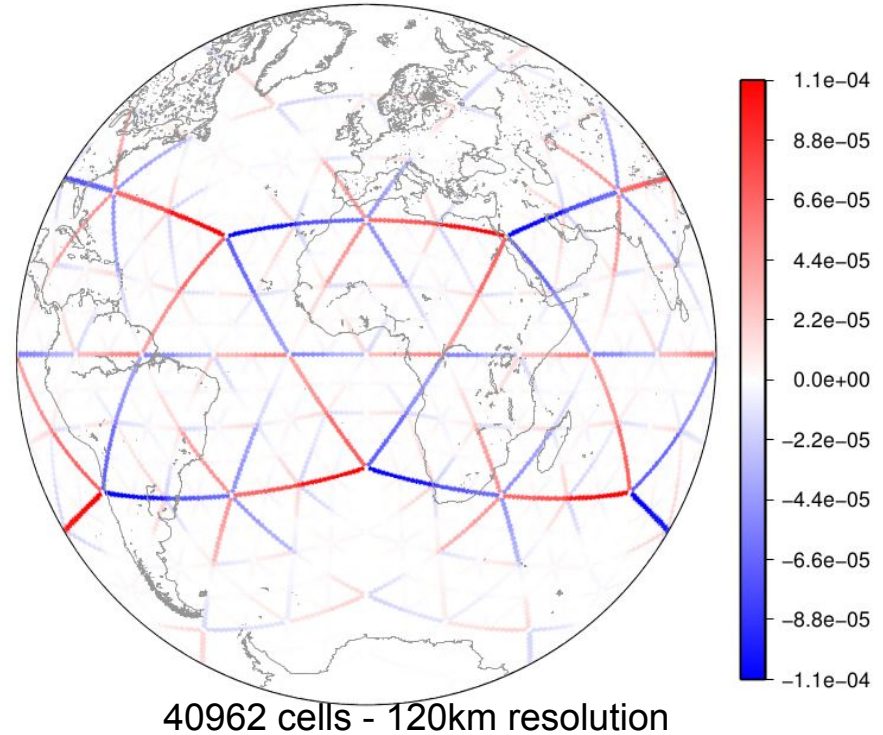
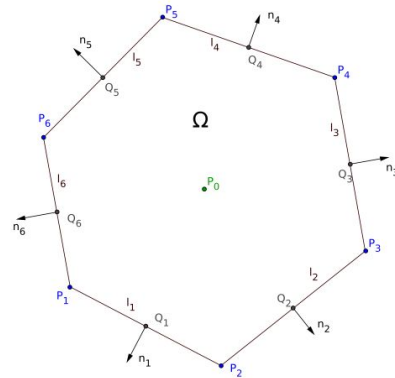
Grid Imprinting

- Grid influences numerical errors of Finite Volume

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



$$\text{div}(\vec{v})(P_0) \approx \frac{1}{|\Omega|} \sum_{i=1}^n \vec{v}(Q_i) \cdot \vec{n}_i l_i.$$

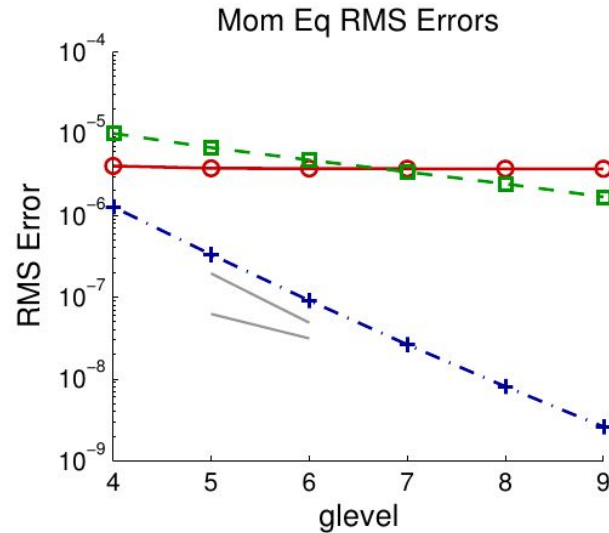
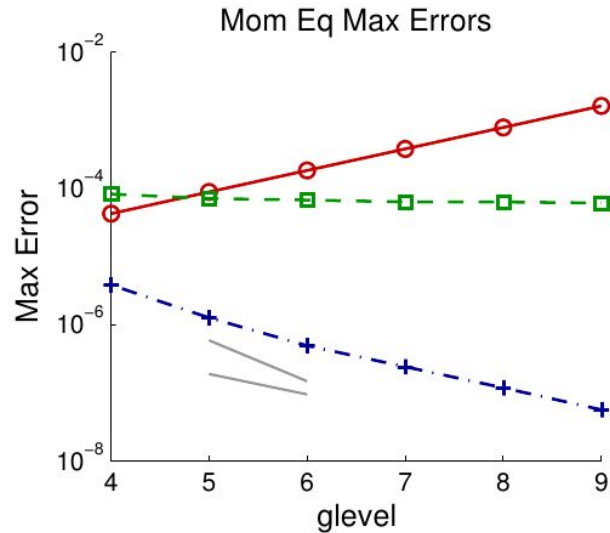


Peixoto, P.S. and Barros, S.R., 2013. Analysis of grid imprinting on geodesic spherical icosahedral grids. Journal of Computational Physics, 237, pp.61-78.

Accuracy

■ Accurate and Stable Finite Volume Schemes

➡ Finite Volume Schemes may lose consistency/convergence on irregular grids

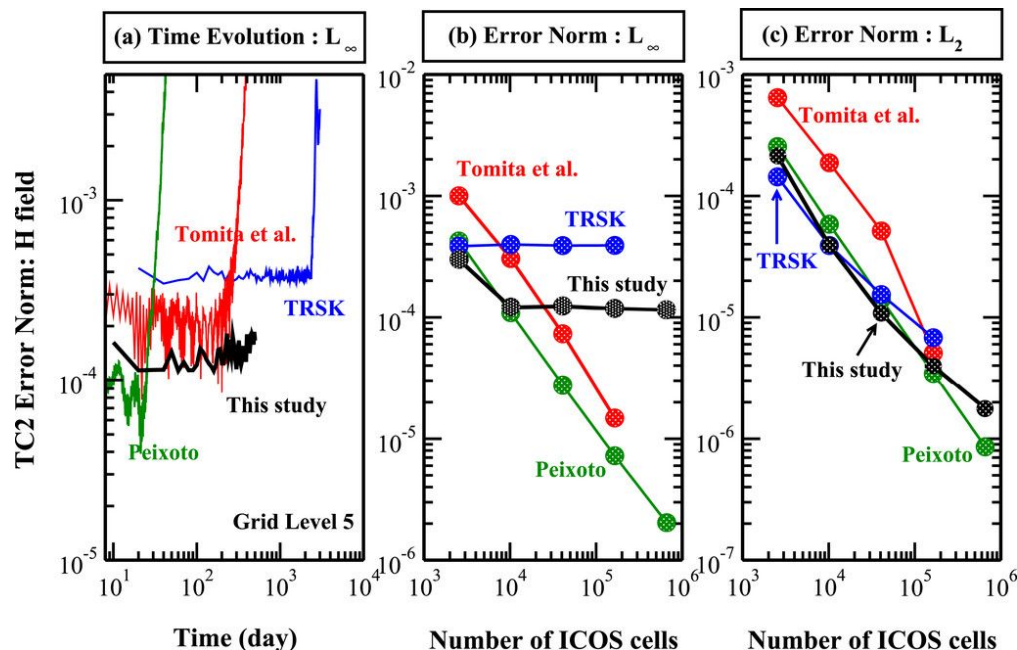


Finite Volume scheme (TRiSK - used in MPAS model) truncation error for 2D Momentum Equation

—○— TRSK-HCT-SCVT —■— TRSK-HCT-HR95 —+— MODF-HCM-HR95 — O1 — O2

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.

Accuracy vs stability issue



- 1) Mimetic, stable, but (very) low order
- 2) More accurate (convergent), but less stable

Yonggang Yu; Ning Wang; Jacques Middlecoff; Pedro Peixoto; Mark Govett, 2020: Comparing Numerical Accuracy of Icosahedral A-grid and C-grid Schemes in Solving the Shallow-Water Model (Monthly Weather Review)

Numerical Stability

- Energy conserving schemes on polygonal grids use vector relation

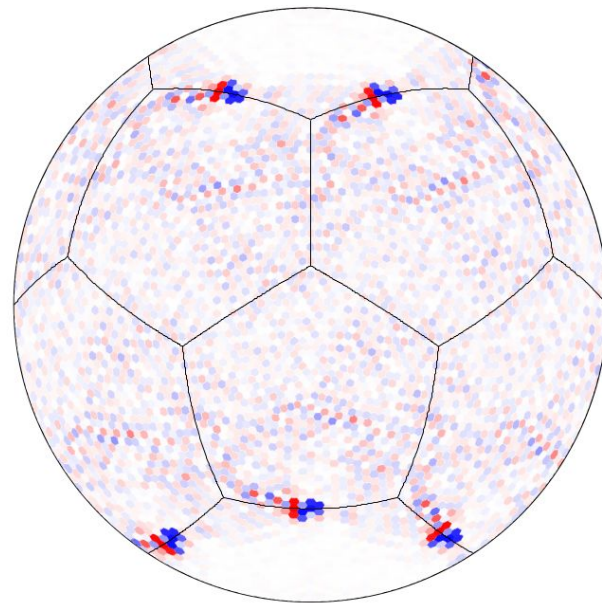
Equivalently for 2D:

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

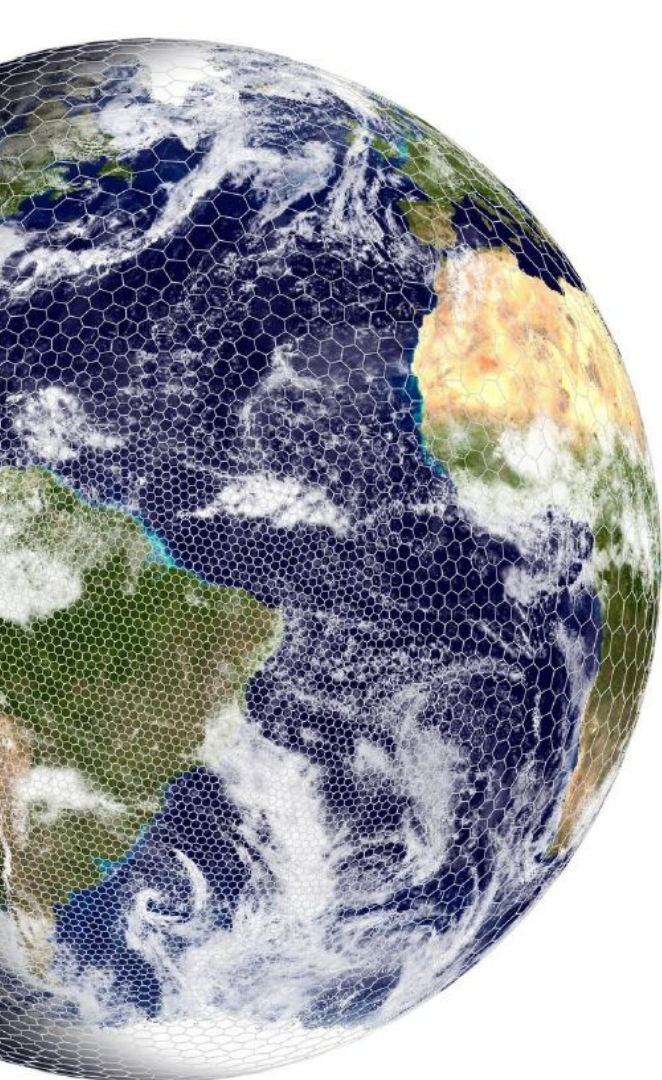
$$uu_x + vu_y = \left(\frac{u^2 + v^2}{2} \right)_x + (v_x - u_y)(-v)$$

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

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.



Key Problem

Development of robust methods for polygonal grids on the sphere for geophysical fluid dynamics (atmosphere, ocean, climate)

Finite Volume: High order may increase the stencil range (less parallelism potential), are usually more sensitive to grid deformations, and may show instabilities :-)

PolyDG: Highly parallel and robust to grid deformation :-)



FAPESP project for Sabbatical at MOX (1year)



Rotating Shallow Water Equations

Vertical
Integration
(Mean Flow)

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

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

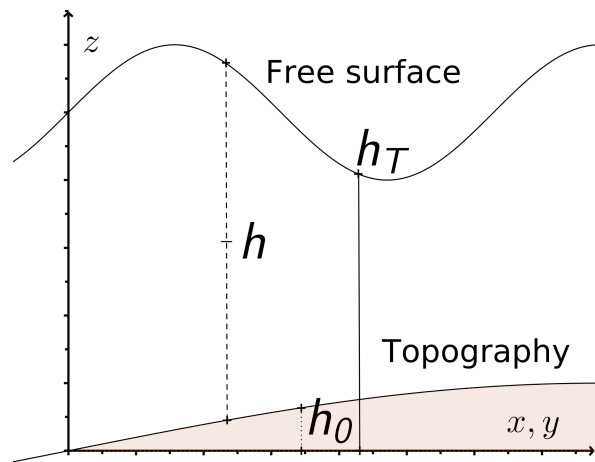
2D Continuity equation:

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

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

2D Horizontal Momentum Equations:

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

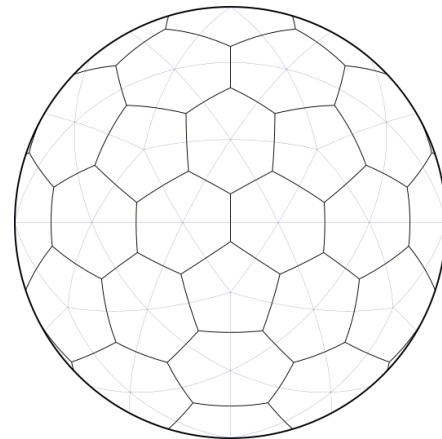


Biperiodic plane \rightarrow Sphere

(f -plane approximation)

Challenges

- Avoid Finite Differences and Spectral on unstructured grids.
-> **Finite Volume**, Finite Element Schemes, **DG**
- 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 problems for Finite Volumes on arbitrary polygonal spherical grids

Many open
problems for
PolyDG

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.

PolyDG

Many flavours



Vulpes

- **Vulpes/Lymph:** PolyDG with Symmetric Interior Penalty? LocalDG?
- **Vulpes/VEM++:** Virtual elements? (Connections with Mimetic FD could help on properties)



- **HARDCORE:** Hybrid High Order
(Good properties, more complexity?)



NEMESIS

New generation
methods for numerical
simulations



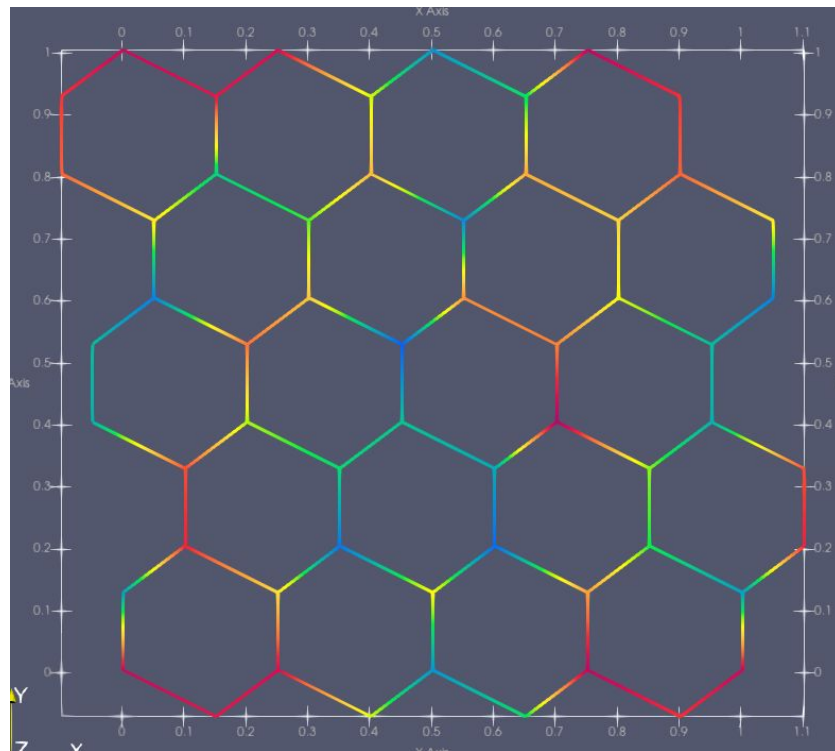
Workplan/Results

Starting point



Vulpes

- Periodic polygonal meshes functionalities: **already added to Vulpes!!!**
- Generalize current physics to periodic grids:
 - Laplacian/Poisson: **just finished!**
 - Heat: **almost ready**
- Add advection (linear/nonlinear) to Vulpes
- Add Rotating Shallow Water Equations on the f-plane

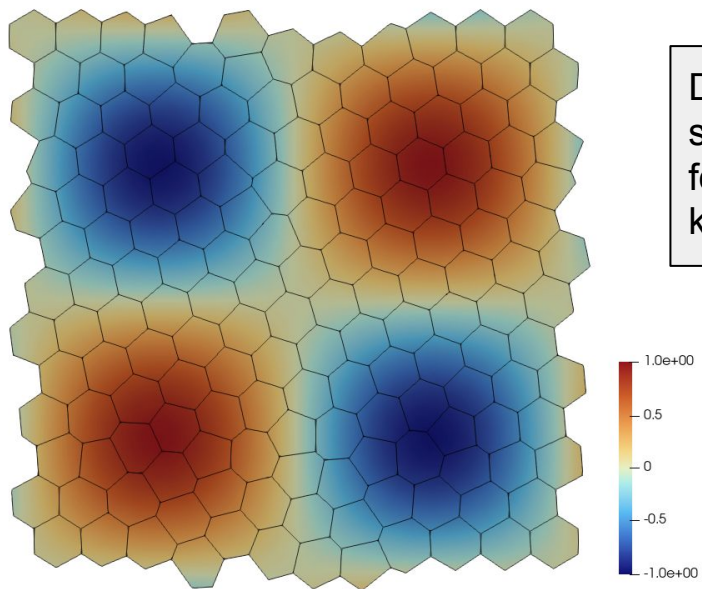


Long term: Spherical grids

Vulpes Poisson on bi-periodic plane

$$\begin{cases} -\Delta u = f & \text{in } \Omega = [0, 1]^2 \\ u(\mathbf{x} + \mathbf{L}) = u(\mathbf{x}) & \mathbf{L} \in \mathbb{Z}^2 \text{ (periodic BCs)} \end{cases}$$

$$f(x, y) = 8\pi^2 \sin(2\pi x) \sin(2\pi y)$$

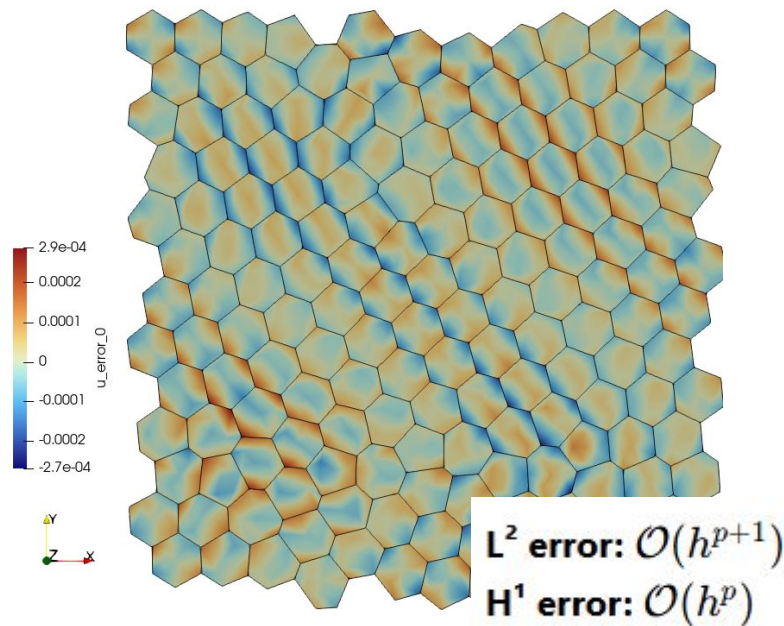


Dof pinning
strategy used
for non trivial
kernel!!!

PolyDg with Symmetric Interior Penalty

Penalty parameter: $\sigma = 10p^2$

Error for $p=3$ rd order modal ($\sim 1e-4$)



Thanks!

Please contact me for
collaborations!

I am here until Dec 2026

Other interests in Numerical Seismic Modelling
(FWI) and Biomathematics

Acknowledgements:



- Paola Antonietti (for hosting me at MOX!)
- Many collaborators, post-docs, students!
- FAPESP Jovem Pesquisador I e II/BPE
- CNPq Universal/Produtividade
- CAPES Auxílios/Bolsas

More info at: <http://pedrosp.ime.usp.br>

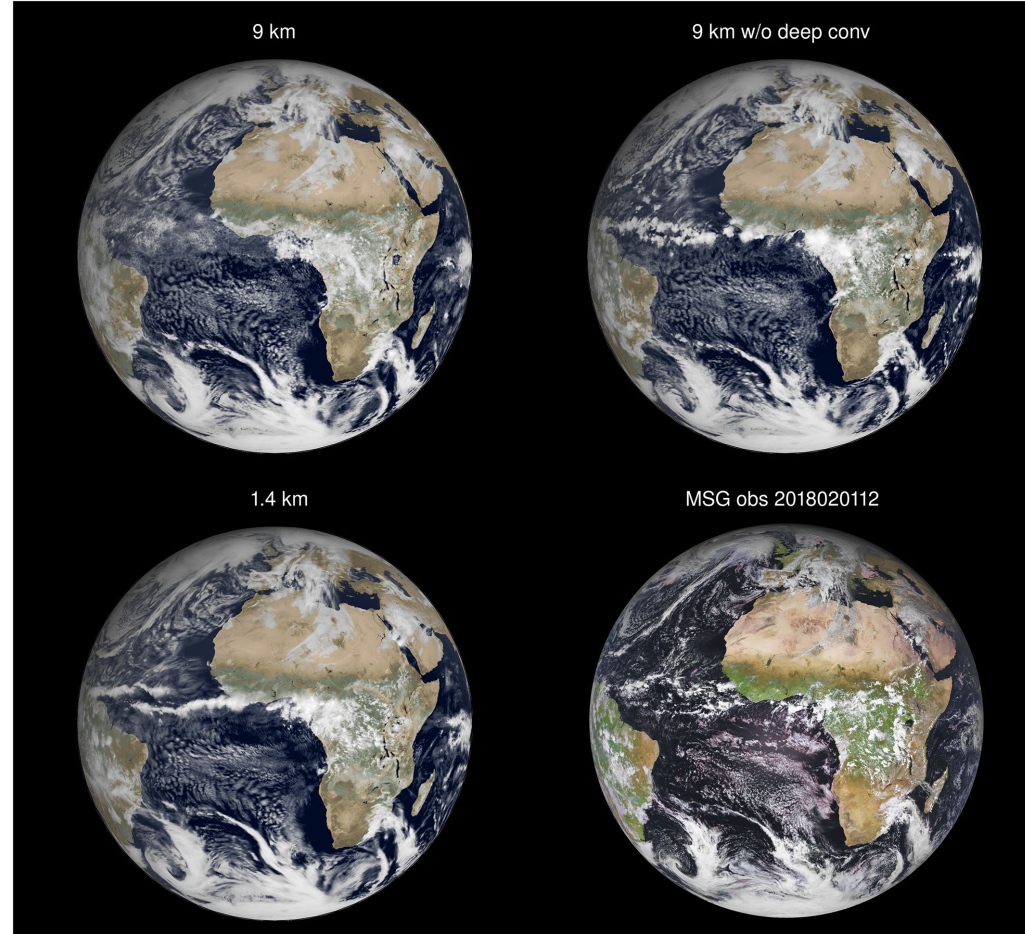


Hard goal...

ECMWF IFS Model

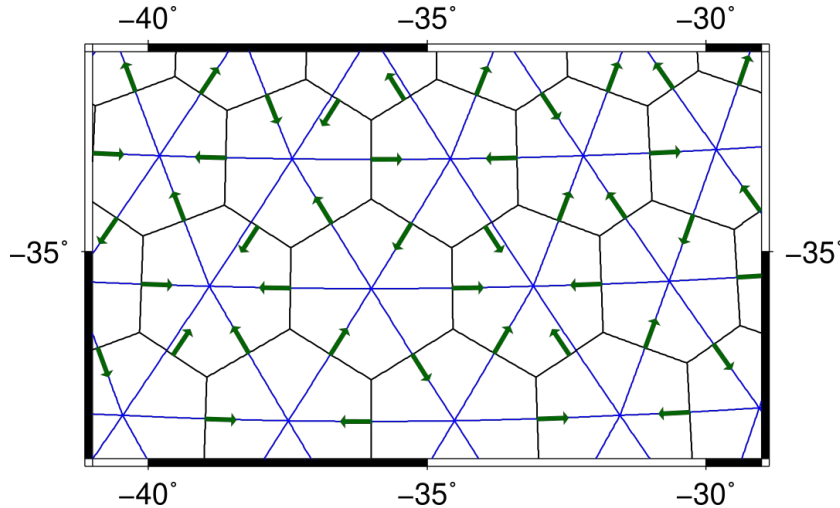
Global atmospheric model (Hydrostatic)

- Simulations with explicit or parameterized deep convection on different resolutions
- Visible Meteosat Second Generation satellite image is also shown at the same verifying time.
- Simulations are based on 3-hourly accumulated shortwave radiation fluxes compared to the instantaneous satellite image.



Wedi, N.P., Polichtchouk, I., Dueben, P., Anantharaj, V.G., Bauer, P., Boussetta, S., Browne, P., Deconinck, W., Gaudin, W., Hadade, I. and Hatfield, S., 2020. A baseline for global weather and climate simulations at 1 km resolution. *Journal of Advances in Modeling Earth Systems*, 12(11), p.e2020MS002192.

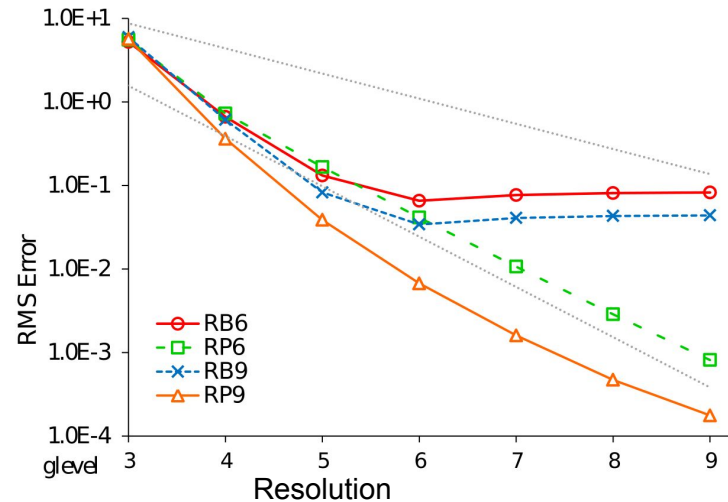
Staggered Grids -> Vector reconstruction



- Currently MPAS uses Radial Basis Functions
- May have difficulties in representing simple wind fields
- Several alternatives exists

Peixoto, P.S. and Barros, S.R., 2014. On vector field reconstructions for semi-Lagrangian transport methods on geodesic staggered grids. *Journal of Computational Physics*, 273,

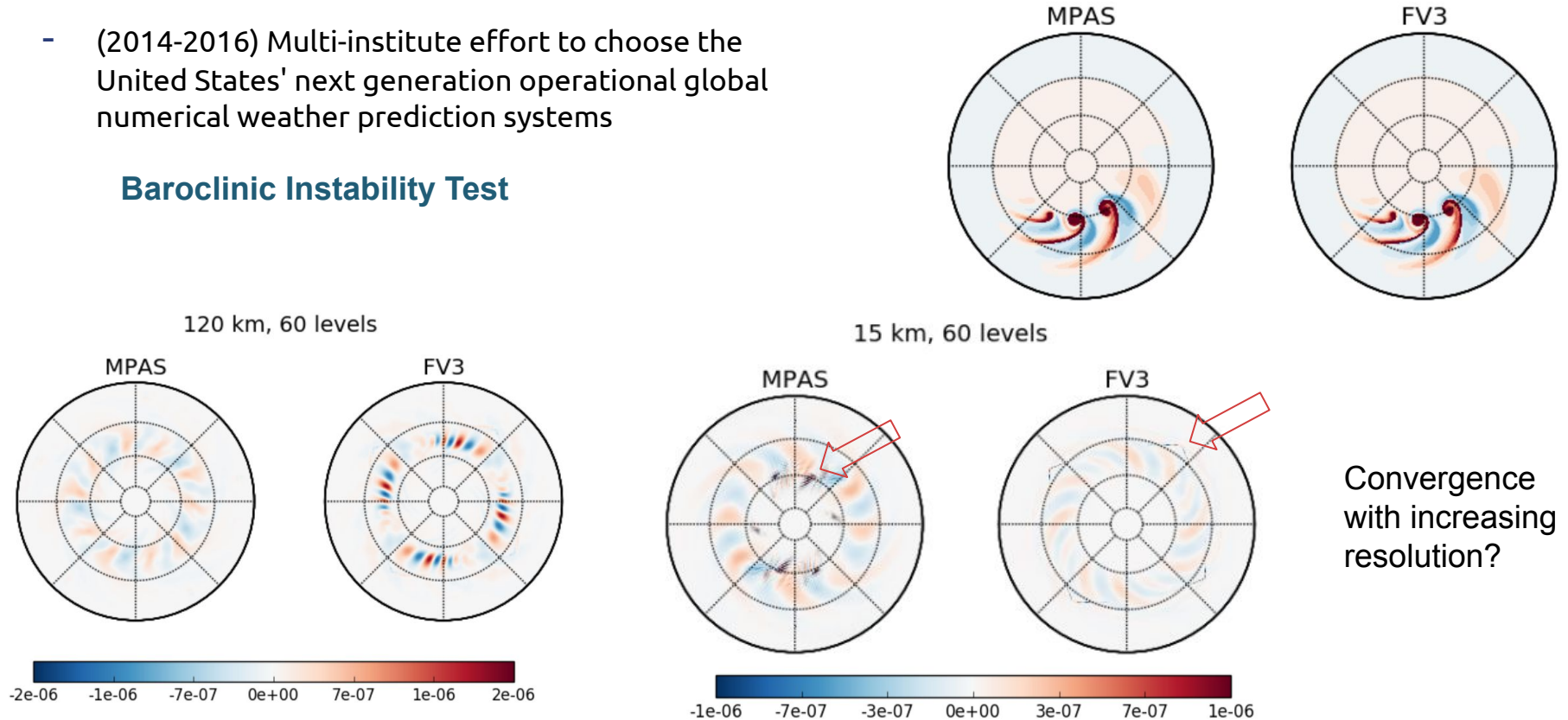
- No complete wind information is known within dynamical core integration.
- Wind needs to be reconstructed from partial information (normal velocities)



High Impact Weather Prediction Project

- (2014-2016) Multi-institute effort to choose the United States' next generation operational global numerical weather prediction systems

Baroclinic Instability Test



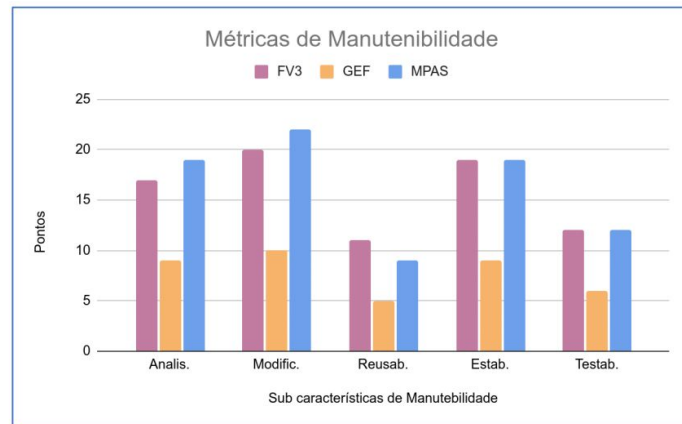
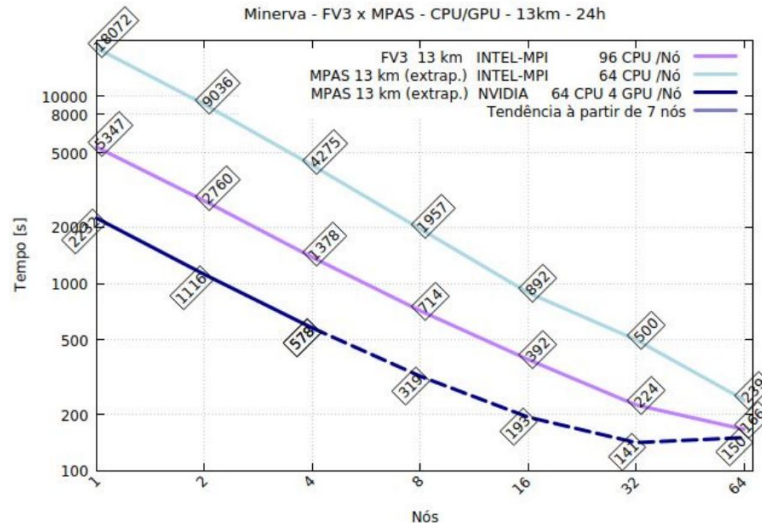
HIWPP Non-hydrostatic dynamical core tests - https://www.weather.gov/media/sti/nggps/HiWPP_idealized_tests-v8%20revised%2005212015.pdf
HIWPP Project Plan for Public Law - <http://www.cmалibrary.cn/ztwxk/zvyjiq/201803/P020180313393622242811.pdf>

9a reunião do Comitê Científico do MONAN (03/08/2023):

- Proposição do MPAS como base da estrutura de dados e dinâmica do componente atmosférico do MONAN.
- Relatórios de desempenho do MPAS FV3/Shield e GEF pelo GCC e GAM da DIMNT/INPE.
- Por unanimidade dos presentes, o CC referendou a recomendação feita pela DIMNT/INPE e, assim, oficialmente o MPAS será adotado como a versão inicial do MONAN-ATM.

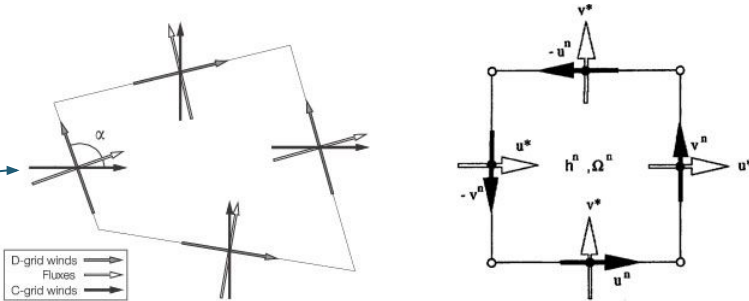
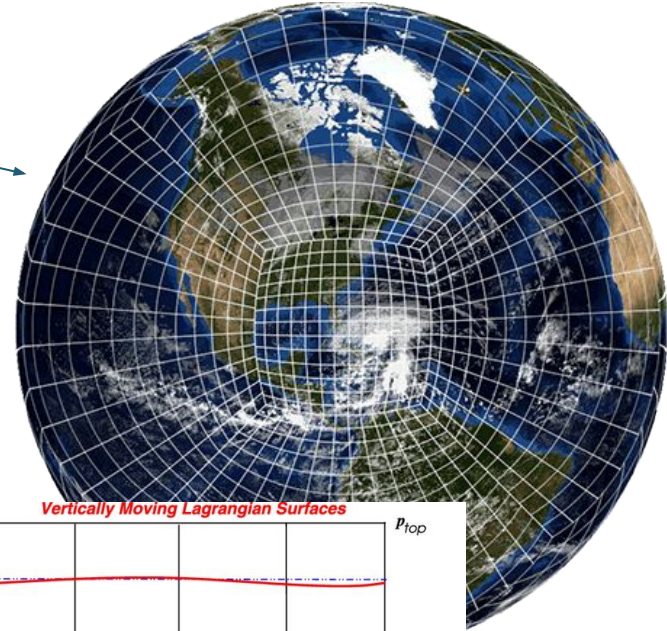


Performance Comparada

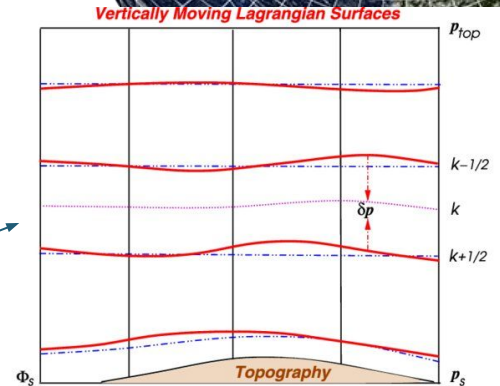


Finite Volume Cubed Sphere - FV3

- Geophysical Fluid Dynamics Laboratory-NOAA
- Gnomonic Cubed - non orthogonal
- Finite Volume
- D-grid, with C-grid winds used to compute fluxes
- Vertical mass based Lagrangian
- Refinement: stretching and two-way nested grid



Lagrangian vertical coordinate associated with a terrain-following pressure coordinate



References: <https://www.gfdl.noaa.gov/fv3/>

Figure Ref: Nair, Choi, Tufo (2009).
Computers & Fluids, 38(2), 309-319.

Latitude-Longitude Models

Traditional Eulerian Finite Differences:

- Use Finite-Differences in time and space
- Time discretization is **explicit**:
 - > Future times depends only on past times.
- **Stability** constraints usually require $\Delta t \propto \Delta x$
 - >The CFL stability condition
- Since at the **pole** Δx is **very small**,
this method requires **Δt to be very small**

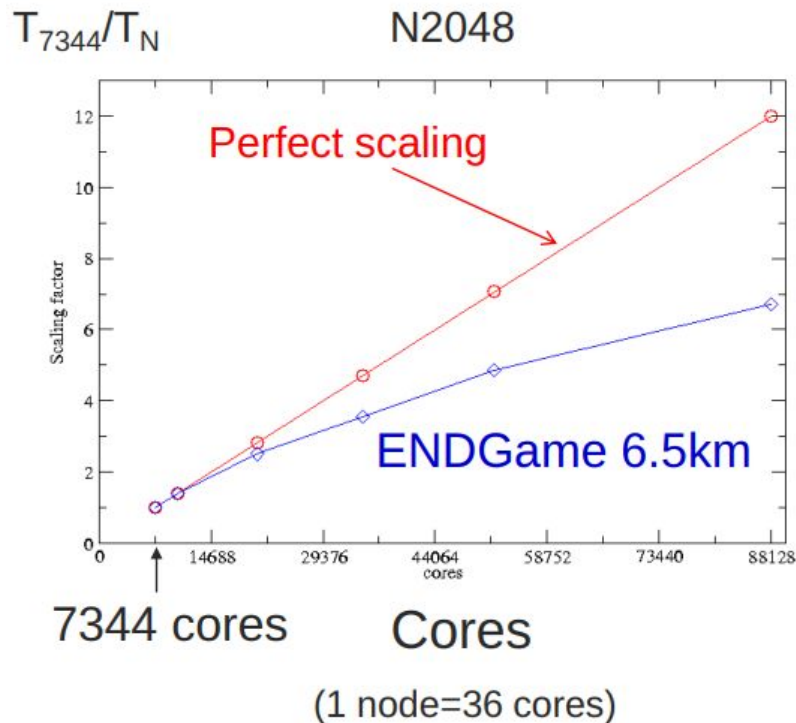
Computationally not feasible in practice...



Scalability issues

An example: UKMetOffice: Endgame

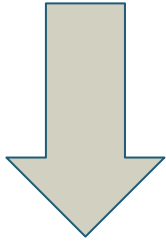
- Latitude-Longitude grid
- Semi-Lagrangian
- Implicit solver



- https://wgne.net/wp-content/uploads/2019/10/WED_Wedi_WGNE34_scalabilitymixed.pdf

Model Initialization

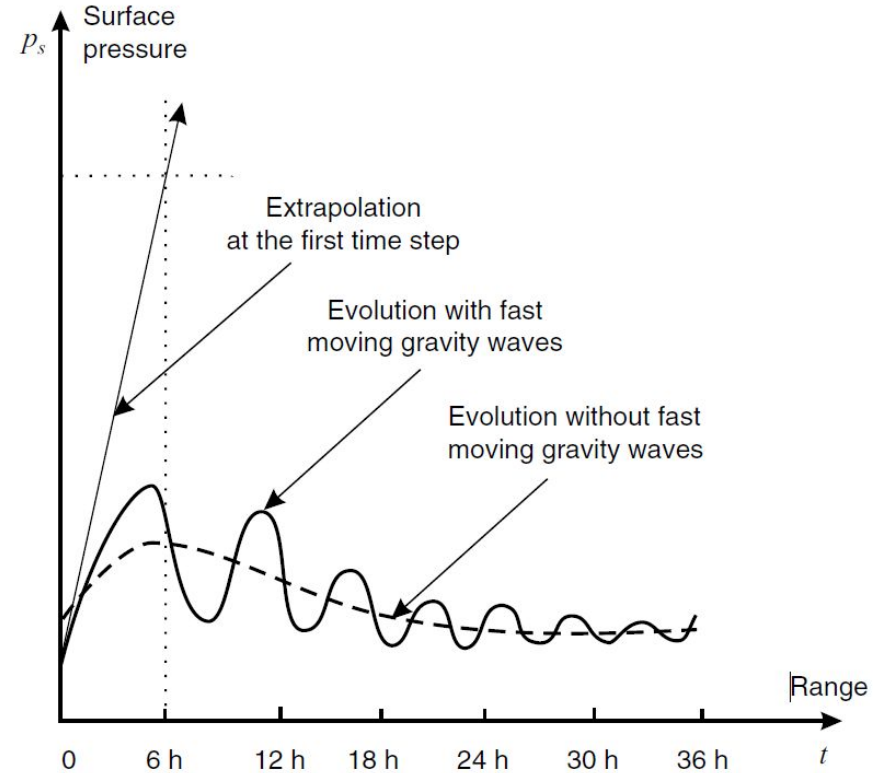
Initial conditions



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.

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).

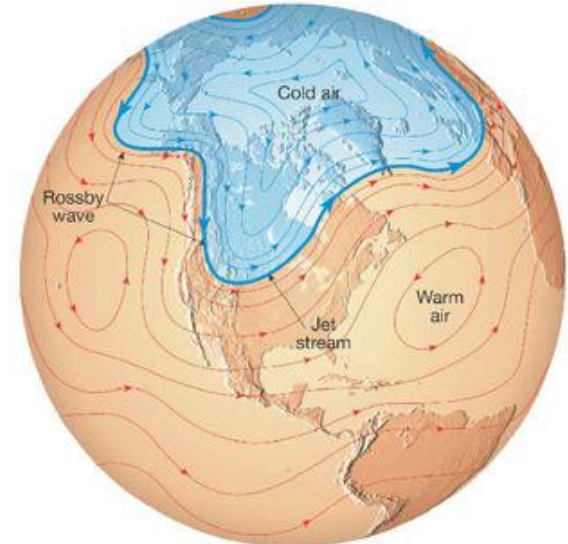
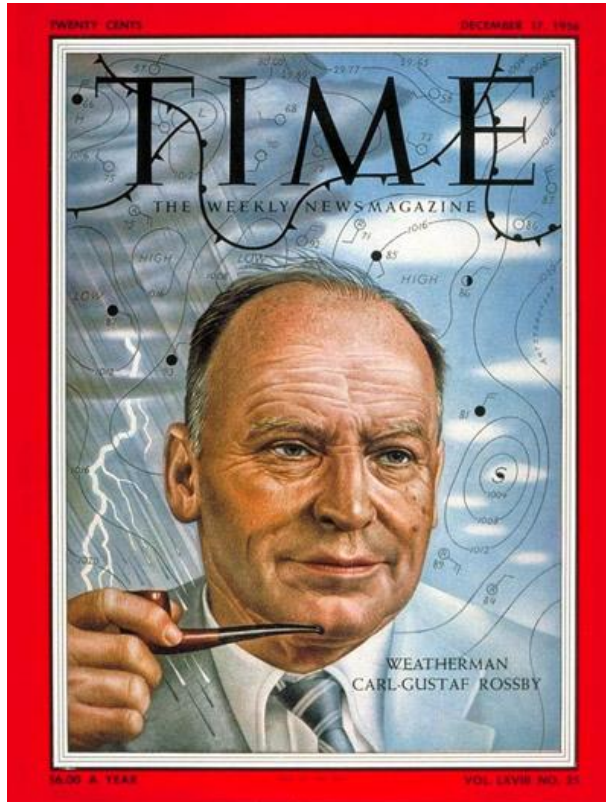


Image credit: stephenleahy.net

History

“The alien sciences
of meteorology and
oceanography”



Vilhem Bjerknes (Norway 1862-1951)

- ~ 1890 Bjerknes's circulation theorem
- Barotropic fluid: density is a function of pressure only
- 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)

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

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

$$= \int_A \nabla \times (\mathbf{u} + \Omega \times \mathbf{r}) \cdot \mathbf{n} dS = \int_A (\nabla \times \mathbf{u} + 2\Omega) \cdot \mathbf{n} dS$$

- 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.

Eliassen, A. 1999. Vilhelm Bjerknes's Early Studies of Atmospheric Motions ...

Barotropic Vorticity Equation

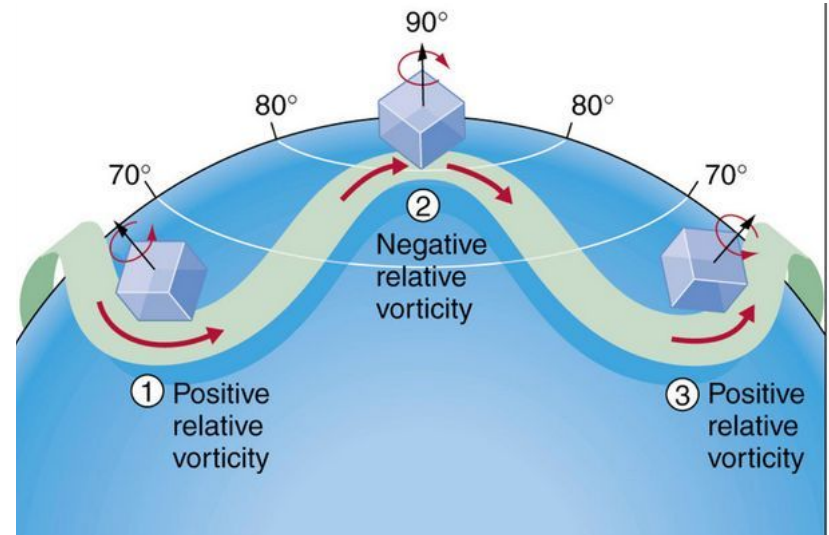
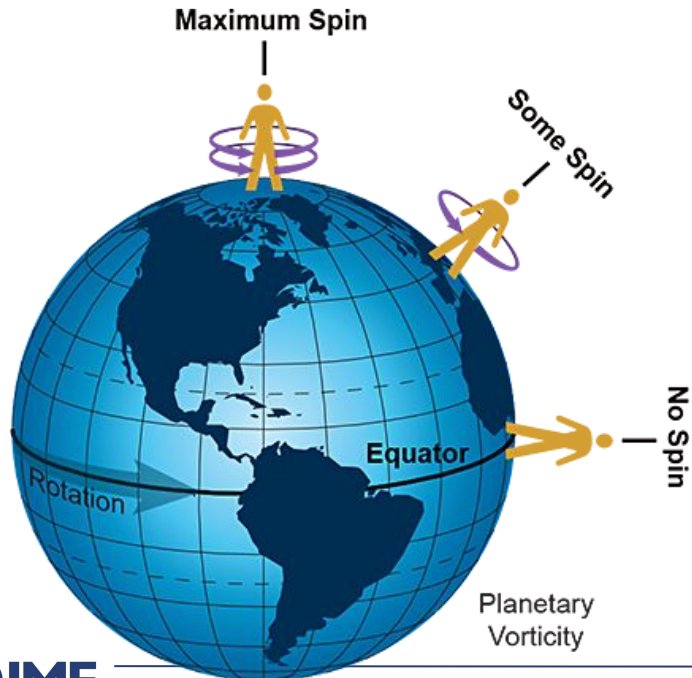
Conservation of absolute vorticity

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

Material Derivative (along with flow)

$$\eta = \zeta + f \quad \text{Absolute vorticity (Relative + Coriolis)}$$

Single layer, non-divergent horizontal flow



Images: < NOAA (https://www.weather.gov/jetstream/climate_v_wx)
<http://homework.uoregon.edu/pub/class/atm/ross1.html> ^

Time discretization

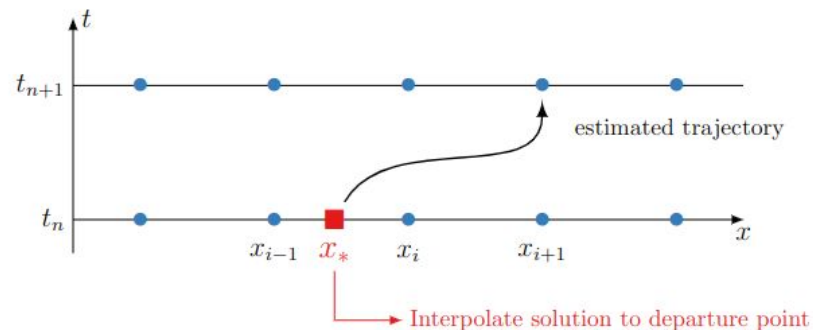
Historically:

- Semi-Lagrangian Semi-Implicit
with *Finite-differences or spectral methods*
(potential scalability issues)



Modern models (quasi-uniform grids):

- Explicit Finite-Differences/Volumes in Time
with *Finite-volumes/elements in space*
(small time steps)



Is it possible to make the Semi-Lagrangian Spectral models more efficient improving the time discretization?

Time discretization

Historically:

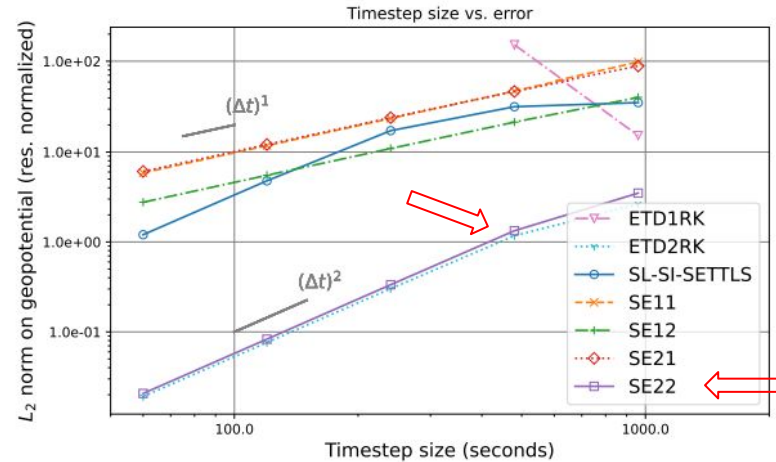
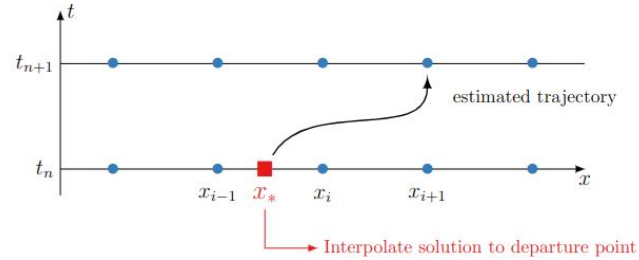
- Semi-Lagrangian Semi-Implicit
with *Finite-differences or spectral methods*
(potential scalability issues)

New methods: Improve accuracy of fast processes
with large time-steps

Exponential Integrator in Lagrangian Trajectories

$$\frac{dU}{dt} = LU + N(U),$$

$$U(t_{n+1}) = e^{\Delta t L} U(t_n) + \int_{t_n}^{t_{n+1}} e^{-(s-t_n)L} N(U(s)) ds.$$



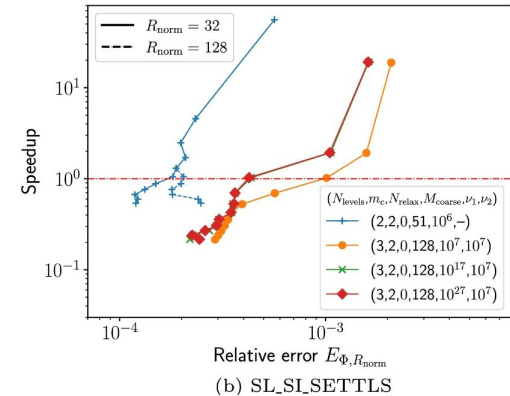
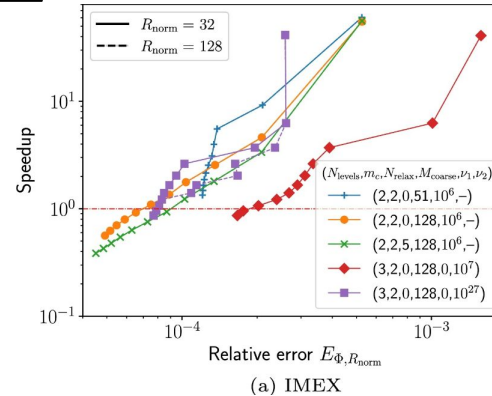
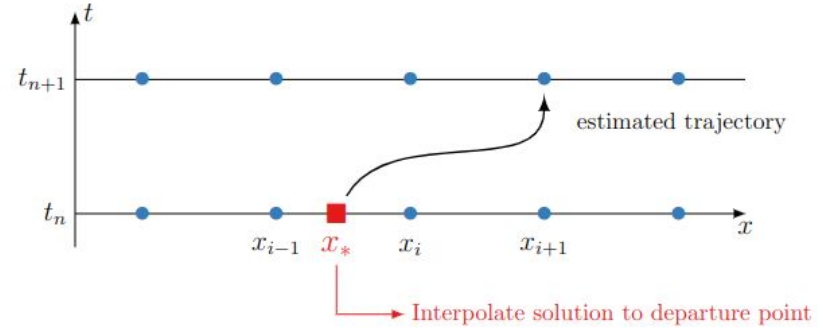
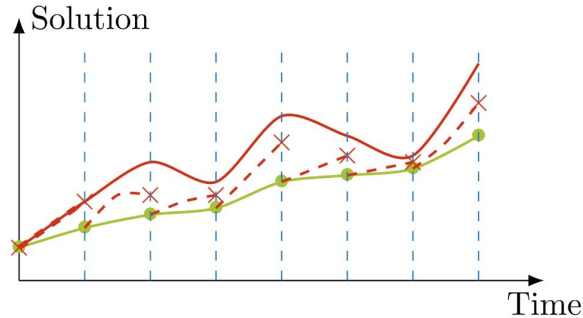
-Peixoto, P.S. and Schreiber, M., 2019. Semi-Lagrangian exponential integration with application to the rotating shallow water equations. SIAM J. Scientific Computing
-Steinstraesser, J.G.C., Peixoto, P.D.S. and Schreiber, M., 2024. A second-order semi-Lagrangian exponential scheme with application to the shallow-water equations on the rotating sphere. arXiv preprint arXiv:2405.02237.

Time discretization

Historically:

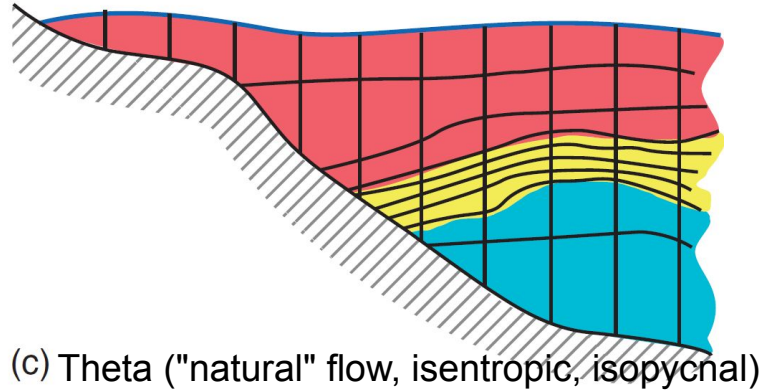
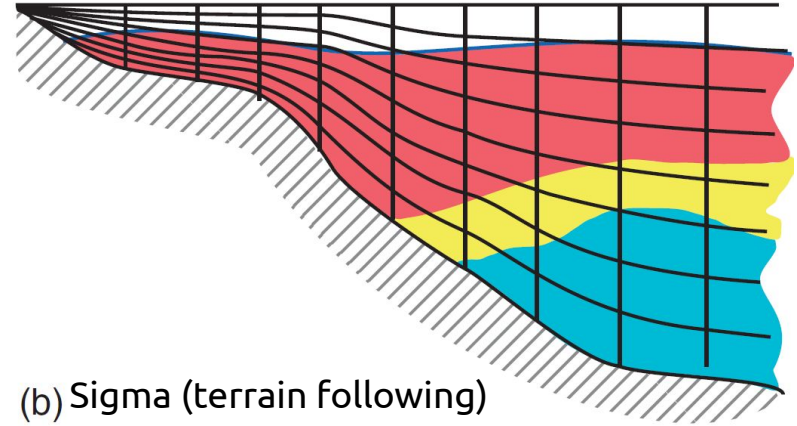
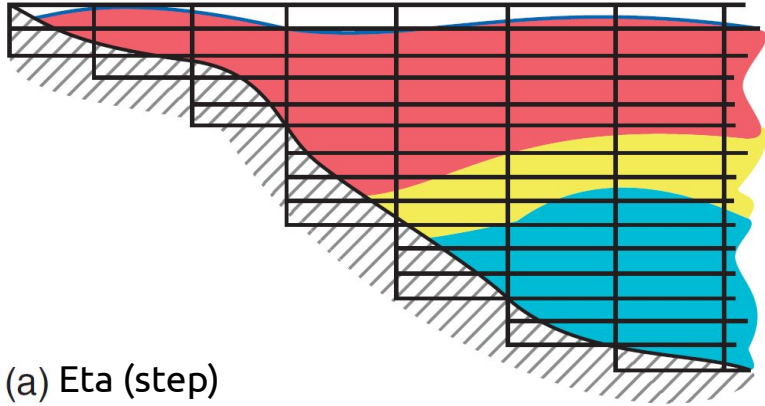
- Semi-Lagrangian Semi-Implicit
with *Finite-differences or spectral methods*
(potential scalability issues)

Parallel-in-time: Exploit some degree of parallelism in time dimension.



Steinstraesser, J.G.C., Peixoto, P. and Schreiber, M., 2024. Parallel-in-time integration of the shallow water equations on the rotating sphere using Parareal and MGRIT. *Journal of Computational Physics*, 496, p.112591.

Vertical Coordinates/Grid



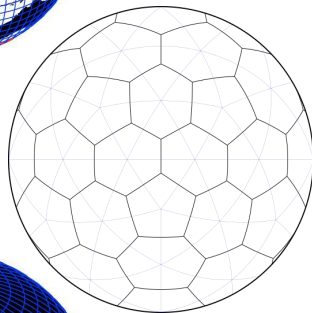
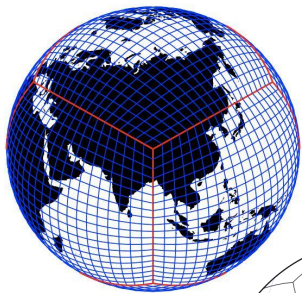
Usually column based!

Hydrostatic: Pressure based or isentropic
Non-hydrostatic: Geometric Height

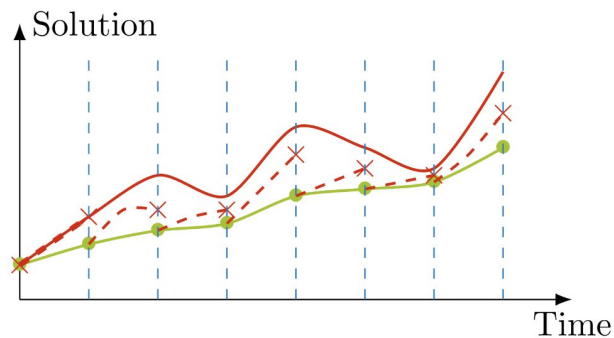
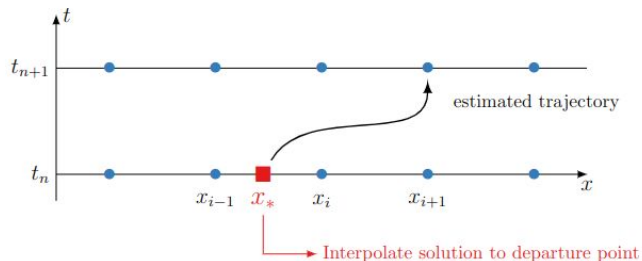
Hodges, B., 2009. Hydrodynamical Modeling.(EL Gene, Ed.) Encyclopedia of Inland Waters. *Academic Press-Elsevier*. doi, 10, pp.B978-012370626.

In summary...

Horizontal scheme/grid



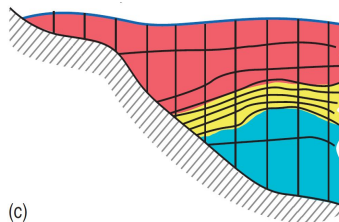
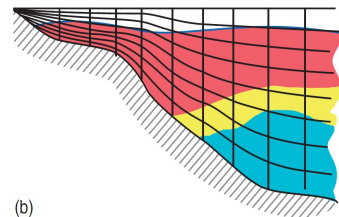
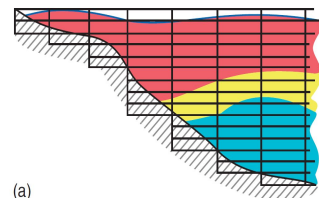
Temporal scheme/grid



Solve:

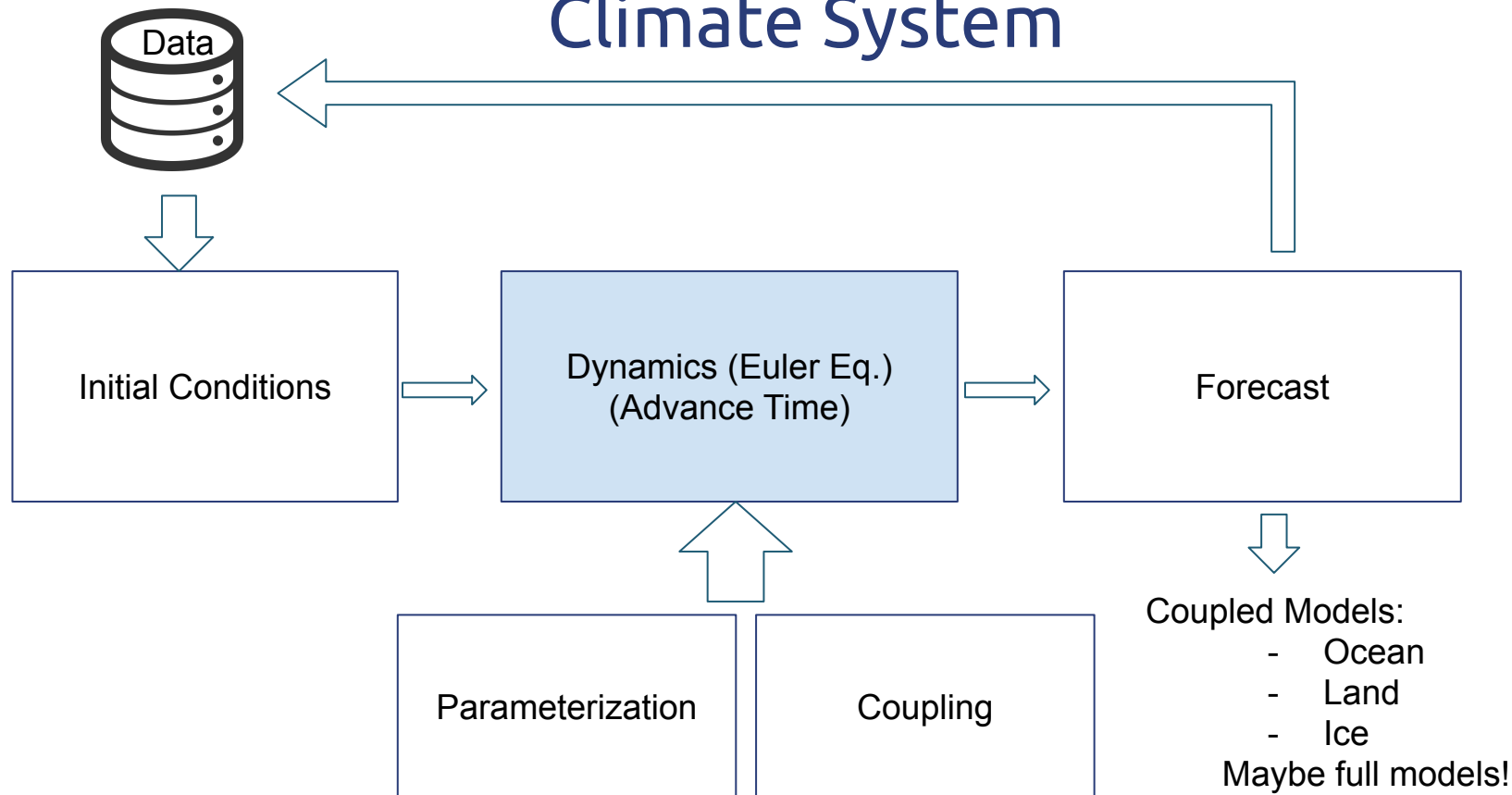
$$\begin{aligned} \frac{D\mathbf{u}}{Dt} &= -2\boldsymbol{\Omega} \times \mathbf{u} - \frac{1}{\rho} \nabla p + \mathbf{g} + \mathbf{F}_r \text{ (Momentum)} \\ \frac{D\rho}{Dt} &= -\rho \nabla \cdot \mathbf{u} \text{ (Continuity)} \\ c_v \frac{DT}{Dt} &= -\frac{p}{\rho} \nabla \cdot \mathbf{u} \text{ (Thermodynamics)} \end{aligned}$$

Vertical scheme/grid



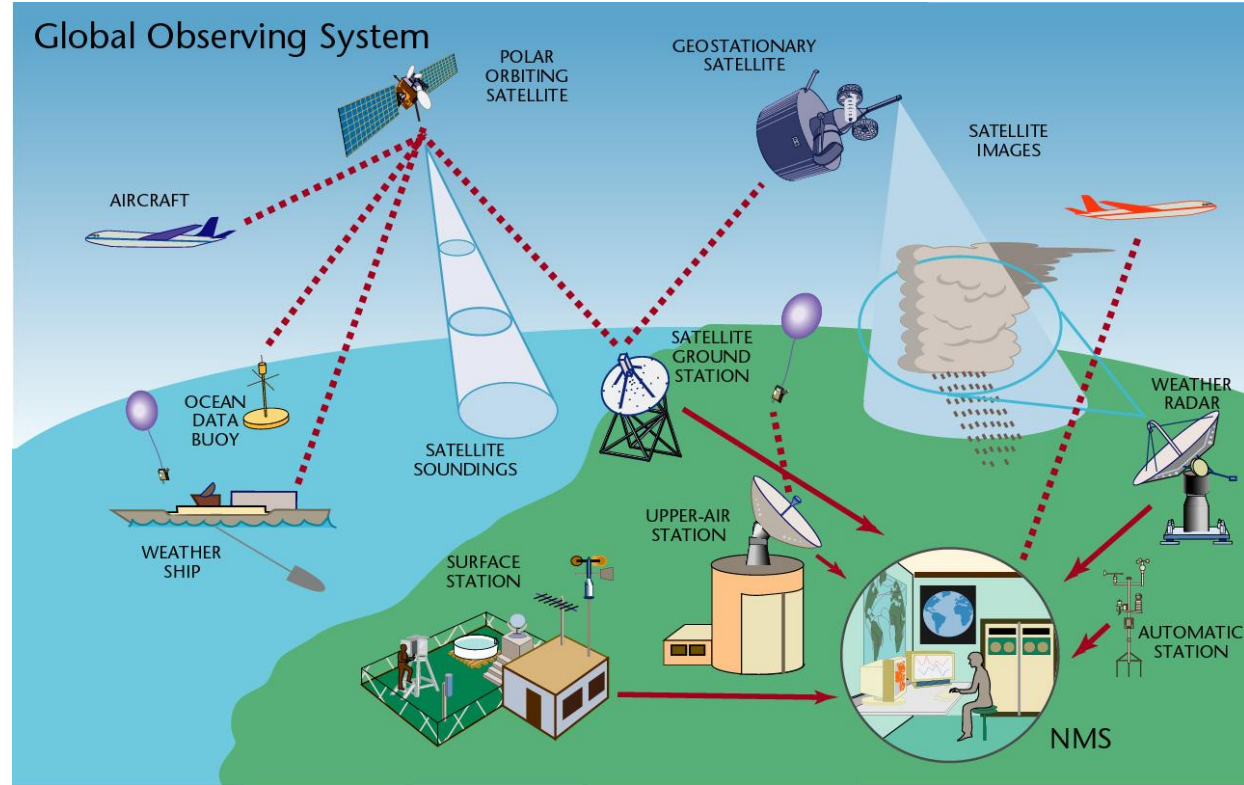
(c)

Operational Weather Forecast / Climate System



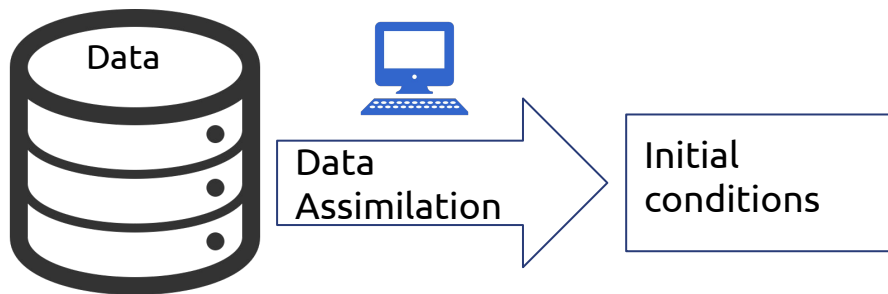
Operational Weather Forecasting

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.

Parameterised processes

Sub-grid scale physics:

- Moist/Clouds
- Radiation
- Boundary layer
- Land/Sea/Ice
- Turbulence

Chemistry:

- Aerosols
- Greenhouse Gases
- Reactive Gases

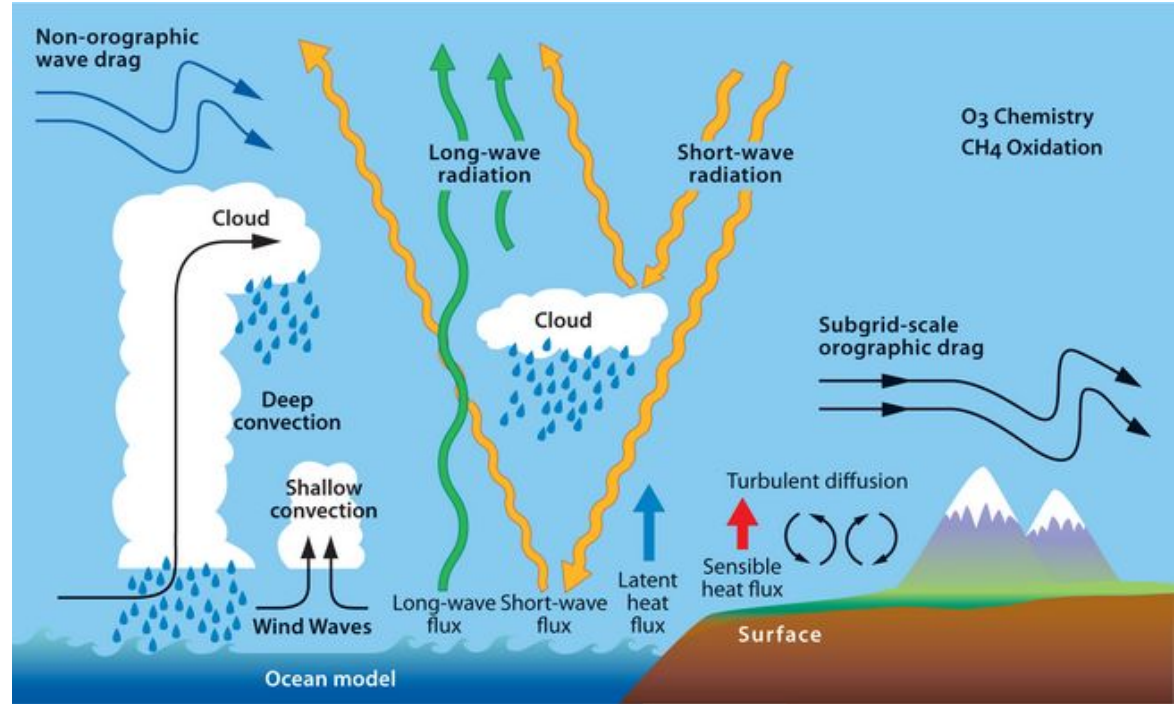
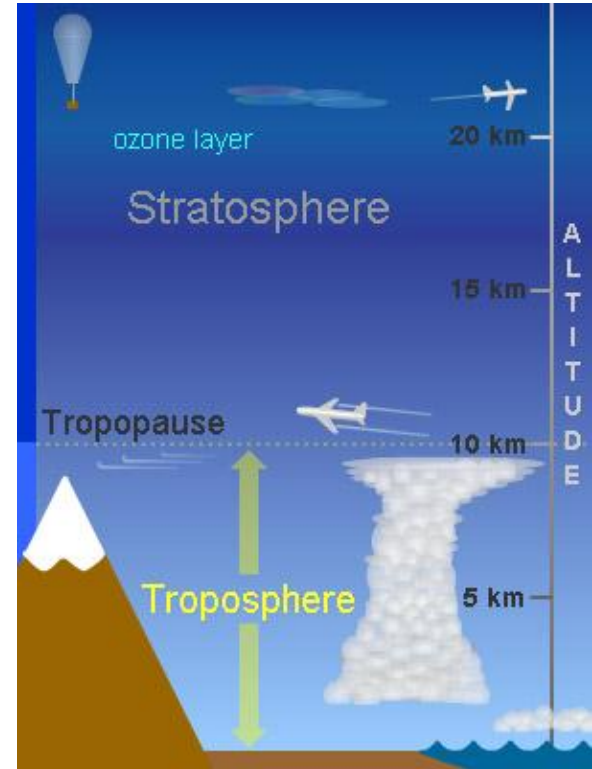


Image: ECMWF

Atmosphere

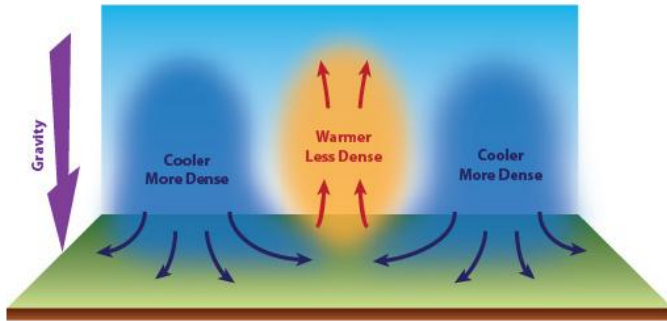
- The atmosphere is layered fluid (gas)



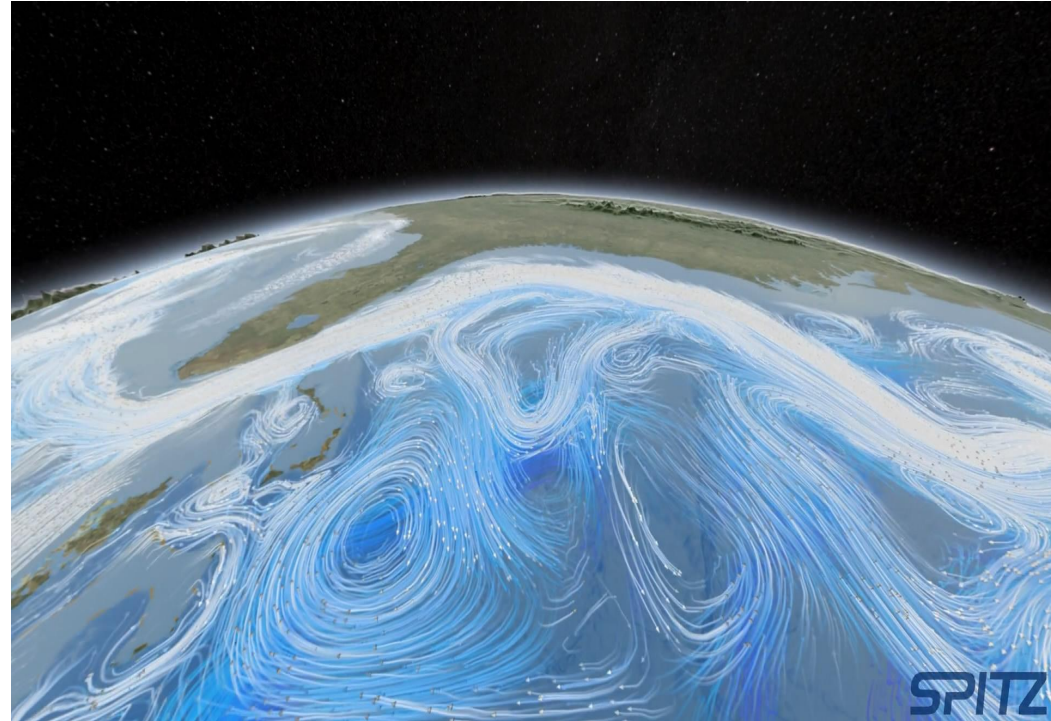
Images: < Nasa, ^ NCAR-UCAR

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.

Theoretical/Mathematical Challenges

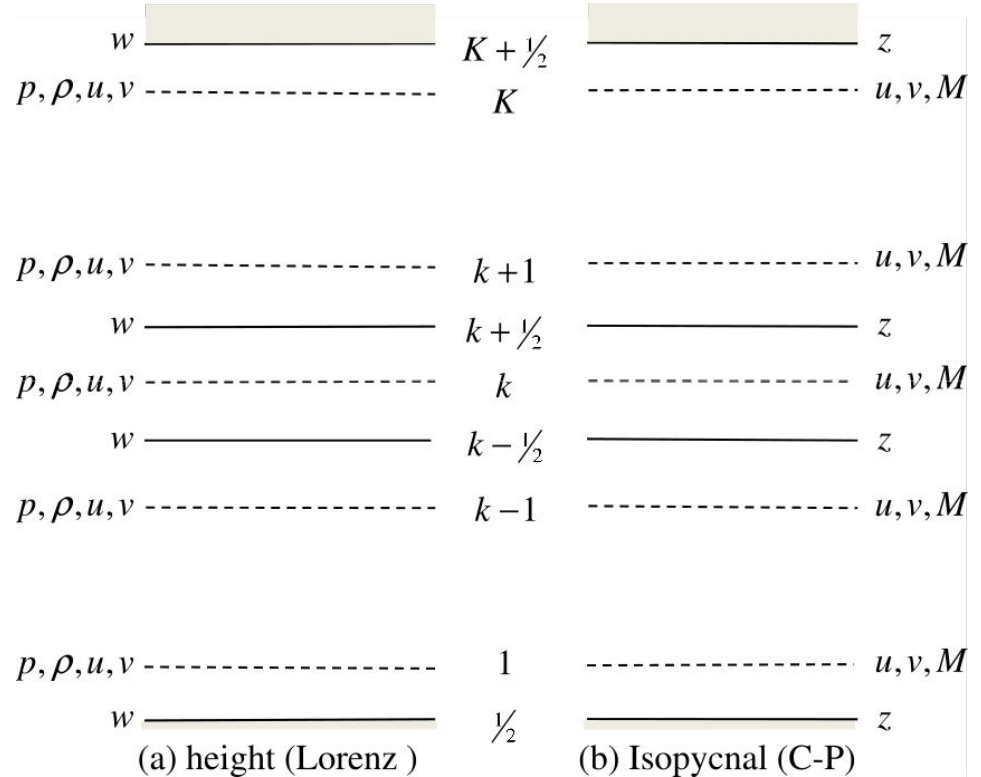
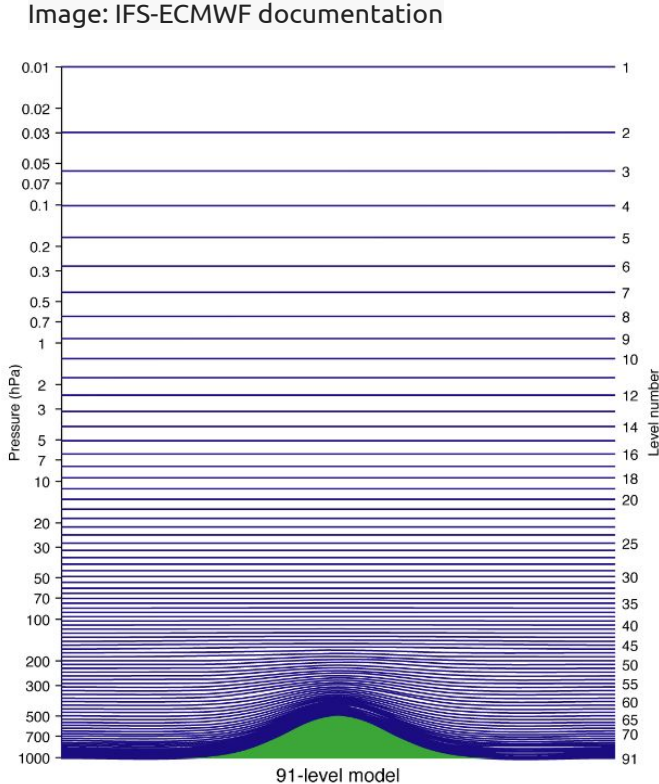
Nonlinear dynamics: Interaction of linear modes.

Can fast linear waves interact to generate slow (low frequency) climate related waves?

Raphaldini, Peixoto, Raupp, Teruya, Bustamante, 2022. Precession resonance of Rossby wave triads and the generation of low frequency atmospheric oscillations (Physics of Fluids). [ARXIV](#), [DOI](#)

Vertical

Ex: Hybrid sigma (terrain following)/pressure



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.

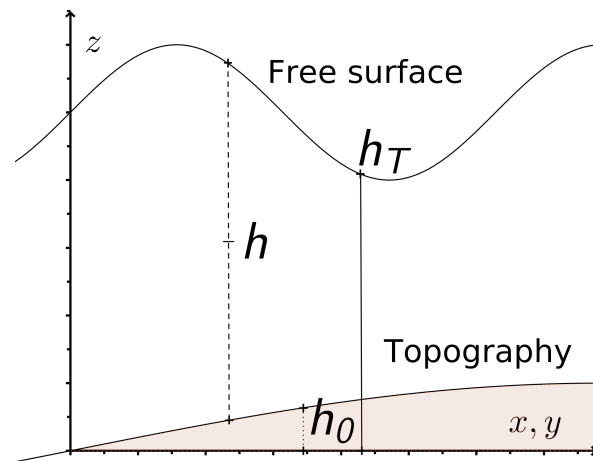
Shallow Water Equations

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

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

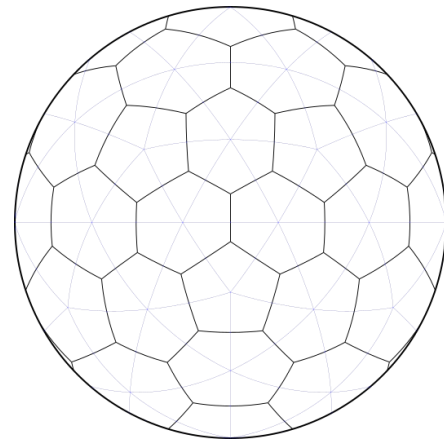
(f -plane approximation)

Vertical
Integration
(Mean Flow)



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.

Intermediate step

3D Incompressibility (constant density):

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

Hydrostatic balance:

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

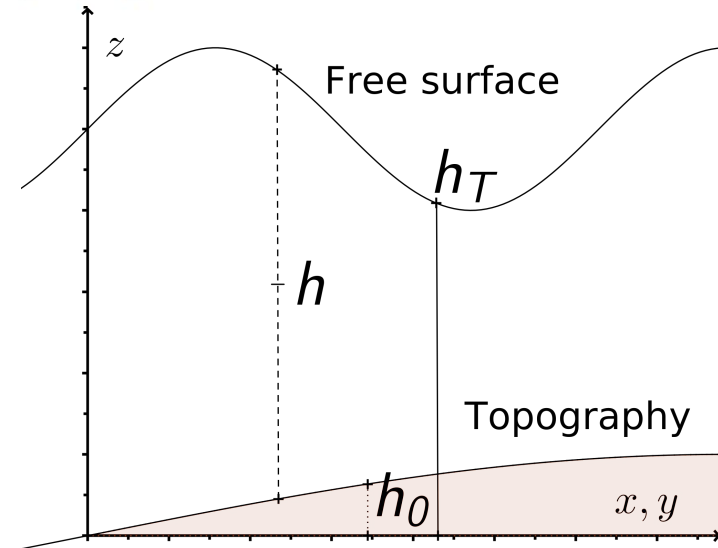
Free surface $h_T(x, y, t)$ where $h_T = h_0 + h$, with $h_0(x, y)$ topography, $h(x, y, t)$ fluid depth.

$$\int_z^{h_T} \frac{\partial p}{\partial z} dz = - \int_z^{h_T} \rho_0 g dz$$
$$p(z) = \rho_0 g (h_T - z) + \underbrace{p(h_T)}_{\text{Constant}}$$

Pressure gradient:

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

Vertical
Integration
(Mean Flow)



Intermediate Model

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 surface must have w velocity:

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

Topography height must have w_0 velocity:

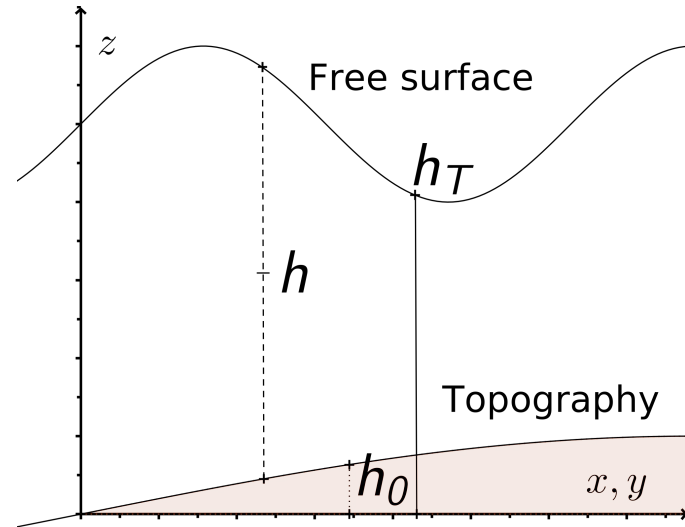
$$\frac{Dh_0}{Dt} = w(x, y, h_0, t) \Rightarrow w(x, y, h_0, t) = \vec{v} \cdot \nabla h_0$$

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

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 on the Sphere

Vector invariant form:

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

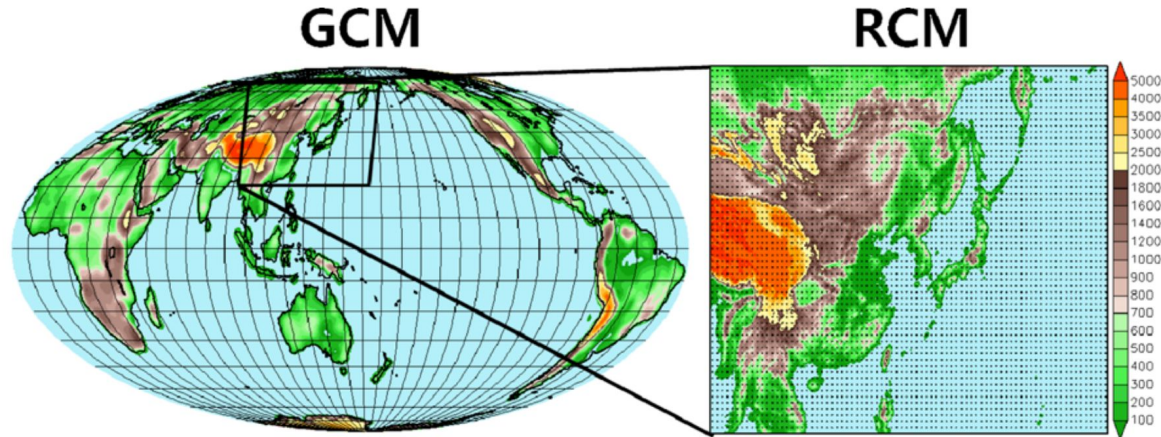
$$\frac{\partial \vec{v}}{\partial t} + \eta \vec{k} \times \vec{v} = -\nabla K - g\nabla(h + h_0)$$

- \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...

Regional -> Global ?



High resolution global model is very computational demanding,....

Dynamical downscaling:

Use coarse global model as input for boundaries of high resolution regional model

Regional (Climate or Weather) models:

Requires Lateral Boundary conditions
(use GCM or Reanalysis data)

Hong, S. Y., & Kanamitsu, M. (2014). Dynamical downscaling: Fundamental issues from an NWP point of view and recommendations. Asia-Pacific Journal of Atmospheric Sciences, 50(1), 83-104.

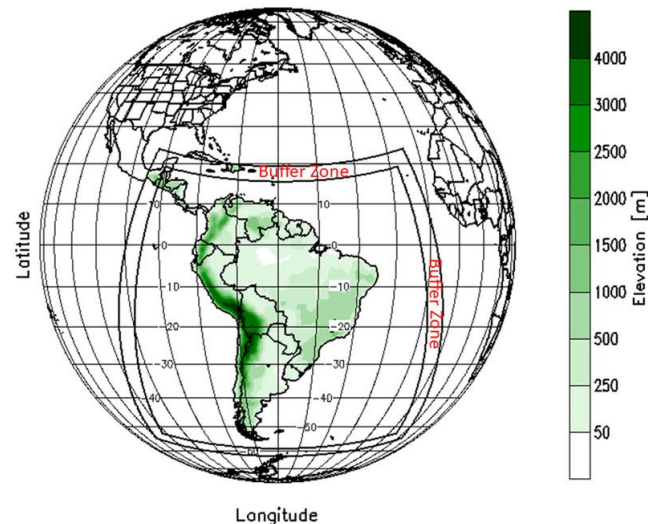
Regional Models

Wide range of success in weather and climate analysis !

- Regular grids (latitude and longitude)
- Simpler numerics (differential operators)
- Good scalability (computational performance)
- Better representation of details (high resolution scales) at acceptable computational cost

Many flavors (stand alone or full climate systems)

- ETA (NCEP, CPTEC et al)
- RAMS (CSU) -> BRAMS (CPTEC/USP/et al)
- WRF (NCAR, NCEP, et al)
- COSMO->ICON (Germany et al)
- HIRLAM/ECHAM/HIRHAM (Denmark/Germany/et al)
- ALADIN/AROME/ALARO (Euro consortium)
- HADGEM3 (UK et al)
- Many, many, others...



Giorgi, F. (2019). Thirty years of regional climate modeling: where are we and where are we going next?. Journal of Geophysical Research: Atmospheres, 124(11), 5696-5723.

Ambrizzi, T., Reboita, M. S., da Rocha, R. P., & Llopart, M. (2019). The state of the art and fundamental aspects of regional climate modeling in South America. Annals of the new york academy of sciences, 1436(1), 98-120.

Regional Models

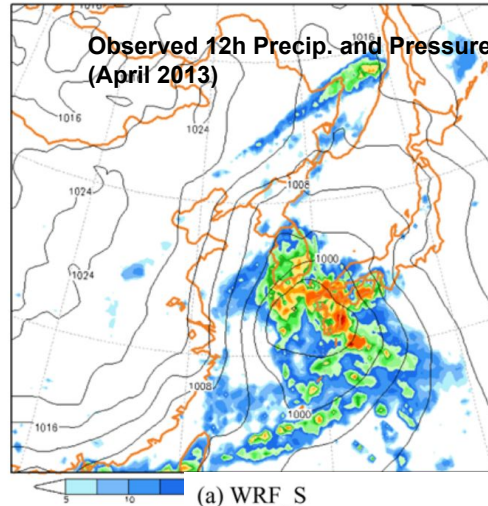
Caution required!

- Requires lateral boundary conditions
- Coarse grid global model provides large
- Consistency between global and region.
- Nudging? Domain size?
- Multiscale representation
- In/out wave propagation

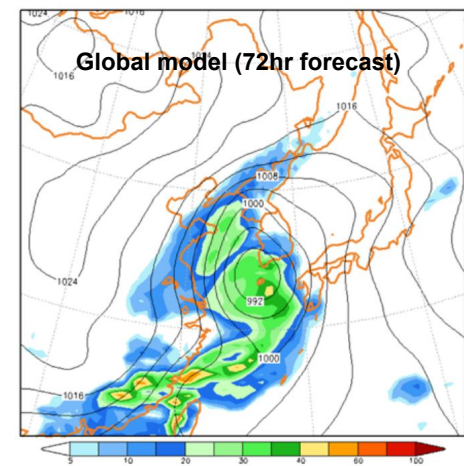
The atmosphere dynamics is a globally coupled chaotic (nonlinear) multiscale system

Hong, S. Y., & Kanamitsu, M. (2014). Dynamical downscaling: Fundamental issues from an NWP point of view and recommendations. *Asia-Pacific Journal of Atmospheric Sciences*, 50(1), 83-104.

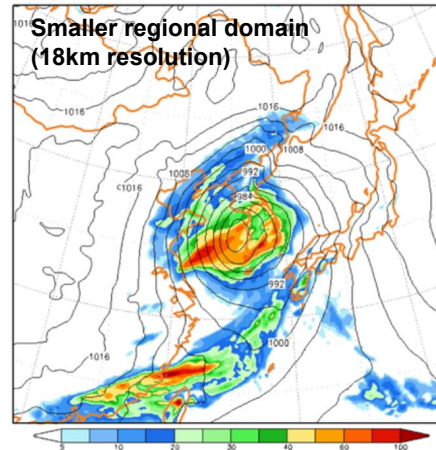
(a) TMPA and FNL



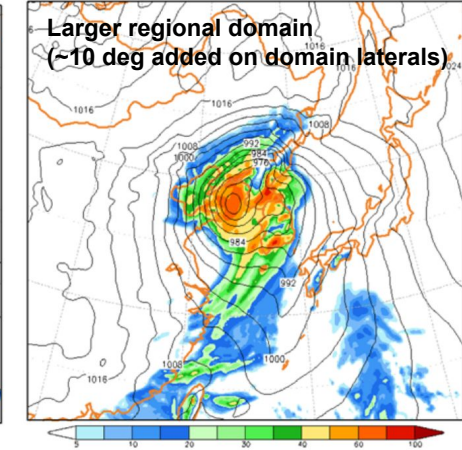
(b) GFS forecast

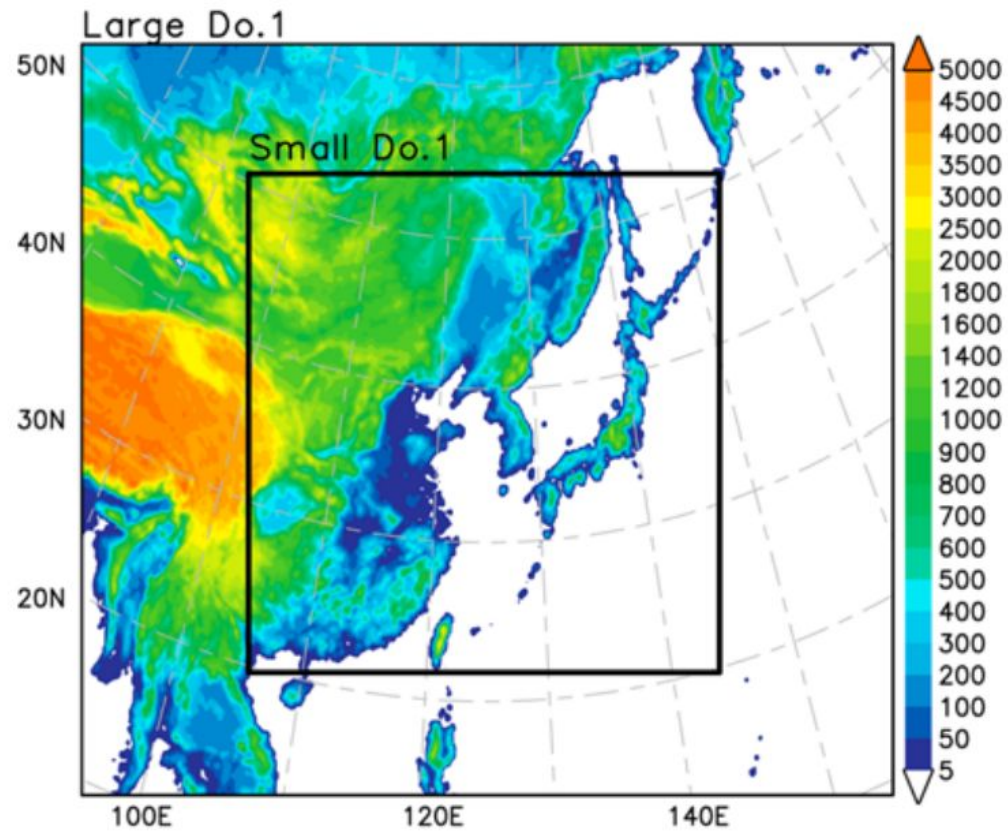


(a) WRF_S

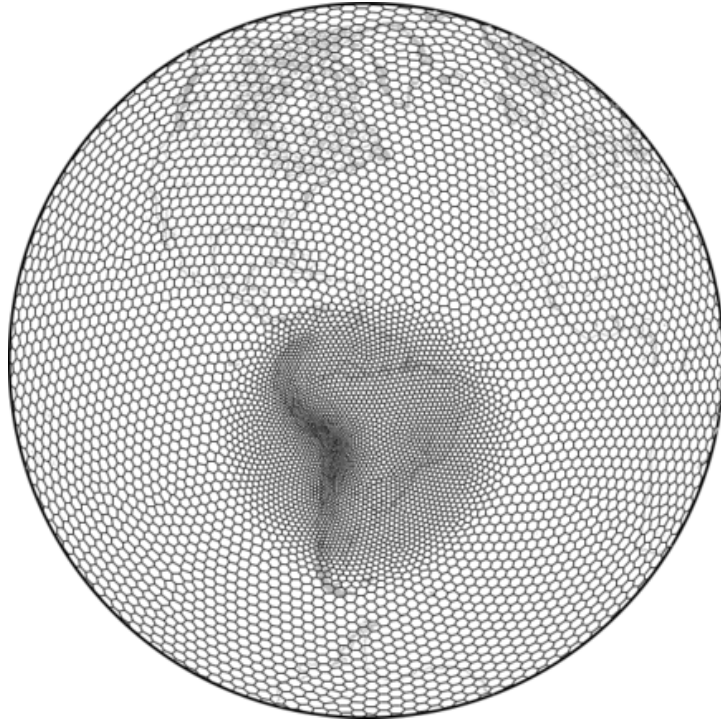


(b) WRF_L



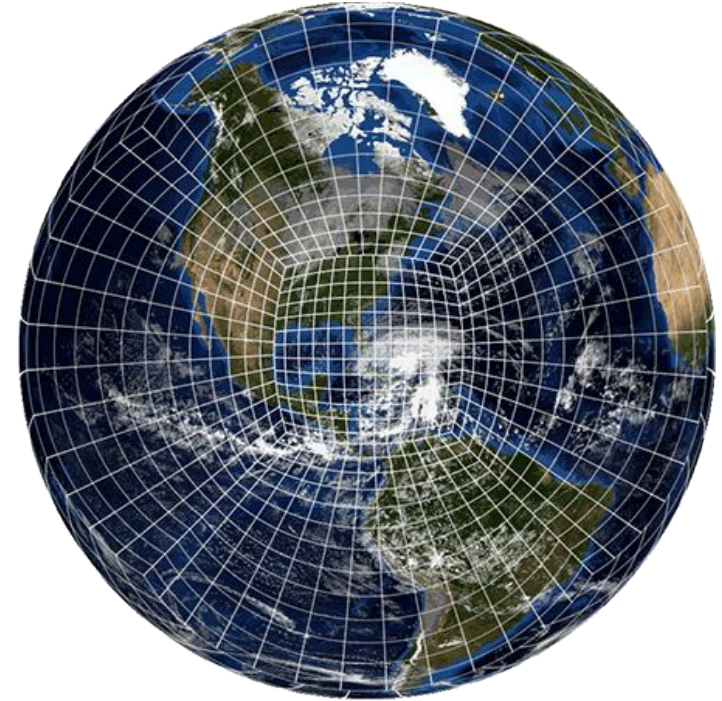


New regional?



Smooth dynamical
downscaling

Single multiscale
global to regional
model



Santos, L.F. and Peixoto, P.S., 2021. Topography based local spherical Voronoi grid refinement on classical and moist shallow-water finite volume models. Geoscientific Model Development Discussions, pp.1-31.

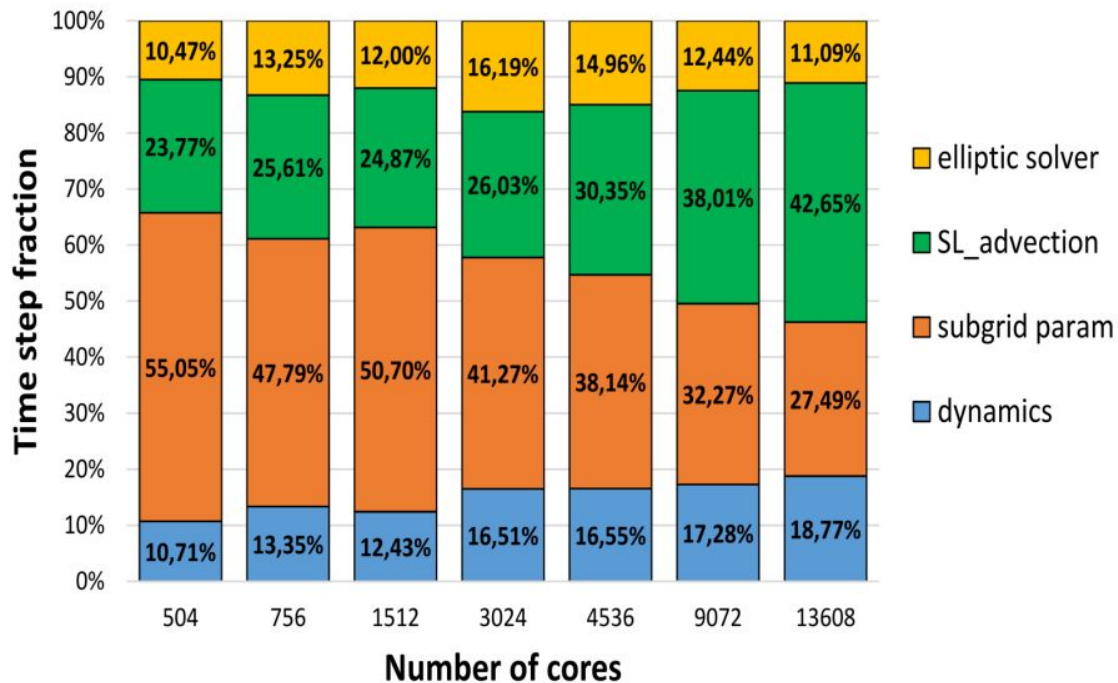
Scalability issues

An example: Hydrometeorological Centre of Russia – SL-AV

- Percentage of different dynamics part in elapsed time vs. # of cores

Model:

- (4th-order) finite-difference, semi-implicit, semi-Lagrangian (on lat-lon, optionally reduced grid)
- Hybrid parallelization optimisations using MPI/OpenMP
- Parallel efficiency of semi-Lagrangian (and elliptic solver) reduced at high core counts

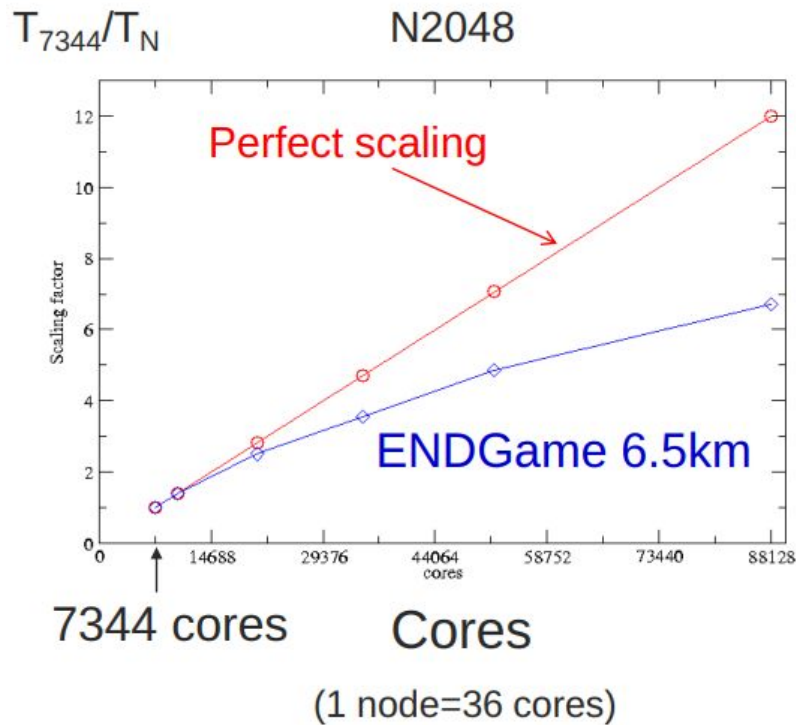


- https://wgne.net/wp-content/uploads/2019/10/WED_Wedi_WGNE34_scalabilitymixed.pdf

Scalability issues

An example: UKMetOffice: Endgame

- Latitude-Longitude grid
- Semi-Lagrangian
- Implicit solver



- https://wgne.net/wp-content/uploads/2019/10/WED_Wedi_WGNE34_scalabilitymixed.pdf

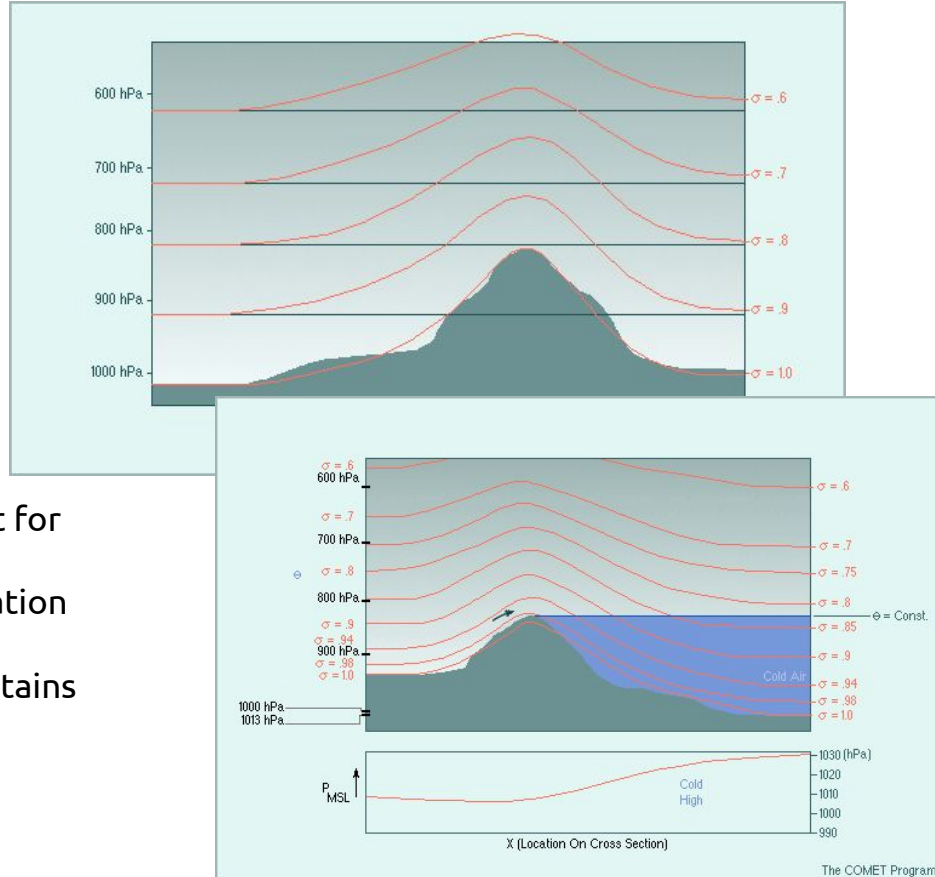
Sigma (terrain following):

Based on **Pressure**, **Height**, (or others)

Uses surface value as reference (e.g. p/p_s)

Results in terrain following coordinate

- + Simpler equation formulations
 - + Conforms to sloping terrain
 - + Same number of layers in model domain
 - + No intersection of coordinate with terrain
 - + Good to represent flows along mountains
-
- Bad with flows hitting topography (barrier)
 - Difficulties in obtaining pressure gradient to account for steep terrain slopes
 - Steepness maybe smoothed, inducing misrepresentation (in mountain or even coastal areas)
 - Misrepresentation of events on the lee side of mountains



COMET Program UCAR - NWP Essentials: Structure and Dynamics
https://lqvx.sinaapp.com/wfiles/mstructure_dynamics/index.htm
(<http://www.dca.ufcg.edu.br/mna/Anexo-MNA-modulo02b.pdf>)

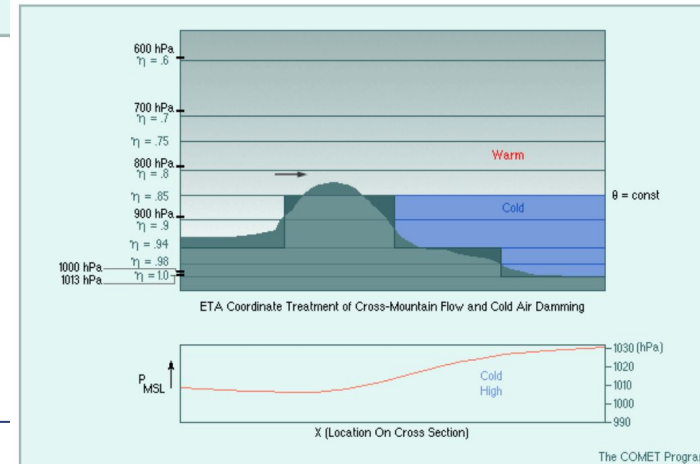
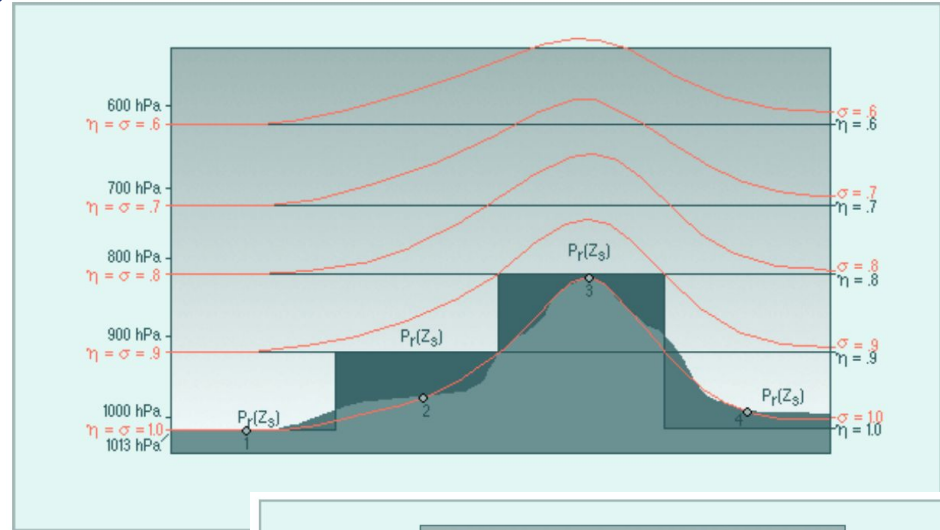
The COMET Program

Eta (step):

Like sigma it is based on **Pressure** or **Height** as well,...
But uses mean sea level as reference instead of
surface pressure (e.g. $(p - p_{\text{top}})/(p_{\text{sea}} - p_{\text{top}})$)

Results in step mountain coordinate

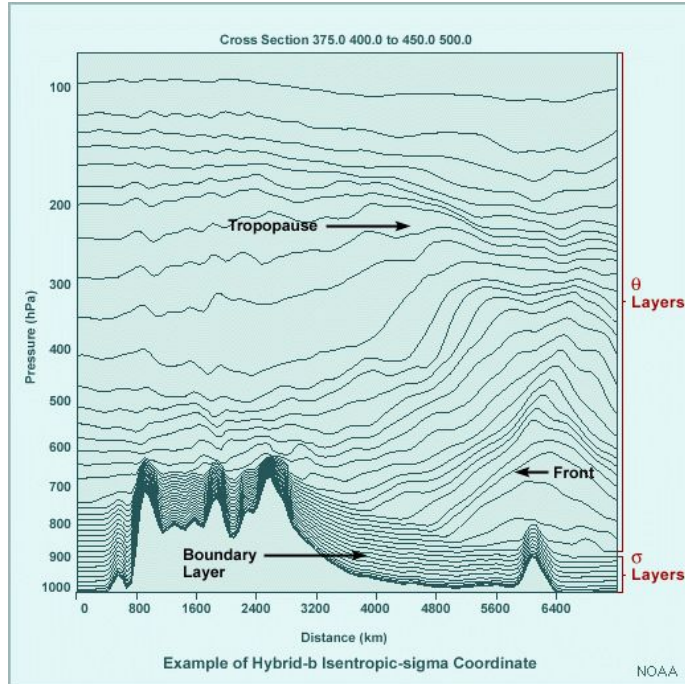
- + Accurate pressure gradient representation in steep terrain
- + Better representation of near surface events
- + Better representation of lee mountain related events
- Number of layers vary depending on topography (worst representation of boundary layer on high grounds)
- Requires high vertical/horizontal resolution to represent well smooth slopes realistically (step -> smooth)
- Steps can create spurious wave effects
- Can require more costly numerics



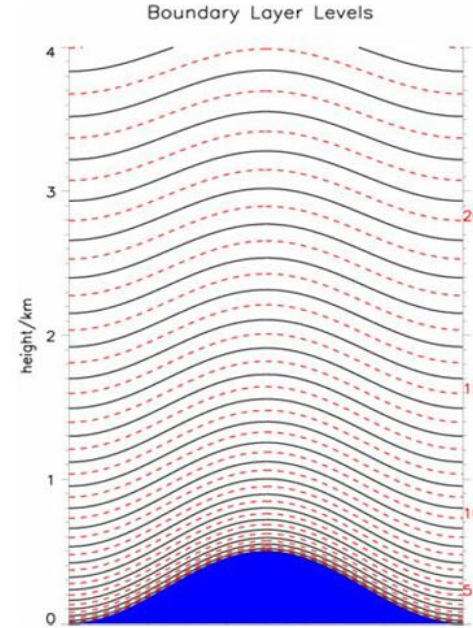
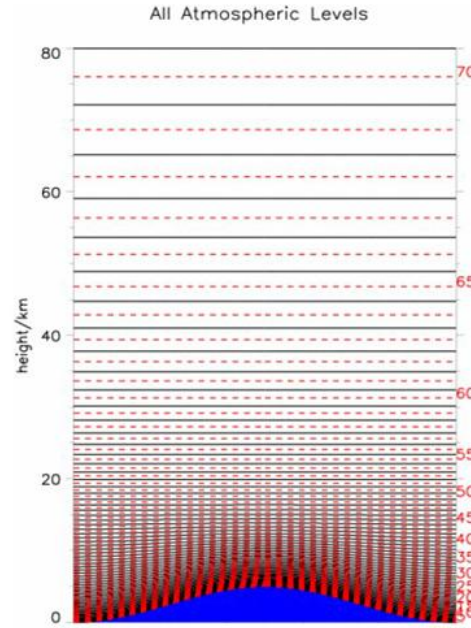
COMET Program UCAR - NWP Essentials: Structure and Dynamics
https://vqx.sinaapp.com/wfiles/mstructure_dynamics/index.htm
(<http://www.dca.ufcg.edu.br/mna/Anexo-MNA-modulo02b.pdf>)

Hybrid coordinates

Smoothly vary from one formulation to another

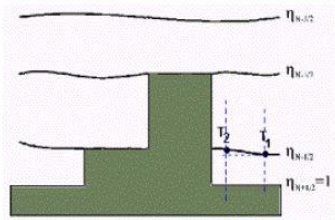


COMET Program UCAR - NWP Essentials: Structure and Dynamics
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(<http://www.dca.ufcg.edu.br/mna/Anexo-MNA-modulo02b.pdf>)



Terrain following coordinates near the surface to constant geopotential surfaces in the upper atmosphere

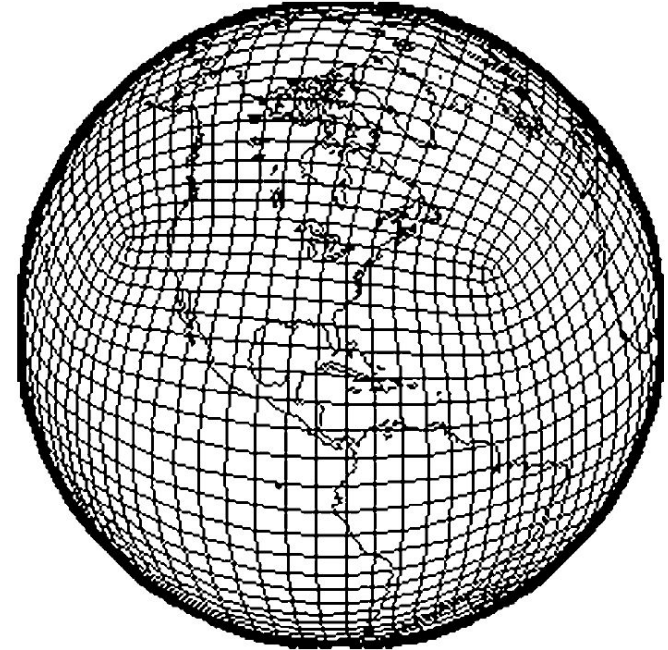
Eta Model and GEF



eta $\eta = \left(\frac{P - P_T}{P_S - P_T} \right) * \eta_S$

$$\eta_s = \frac{P_{ref}(z_s) - P_T}{P_{ref}(0) - P_T}$$

GEF - Global Eta Framework



Eta

- Regional
- Eta vertical coordinates
- Finite Differences: E-Staggering (as Richardson!) but with C-grid features...
- Energy/entropy conservation properties
- Non-hydrostatic option

<http://etamodel.cptec.inpe.br/>

Zhang, H. and Rančić, M., 2007. A global Eta model on quasi-uniform grids. Quarterly Journal of the Royal Meteorological Society: A journal of the atmospheric sciences, applied meteorology and physical oceanography, 133(623), pp.517-528.