Numerical Finite Volume Methods for Global Multiscale Models

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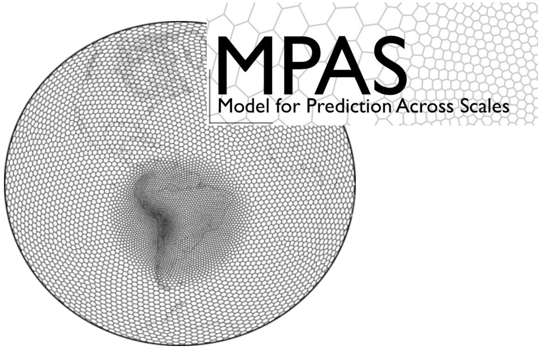
Métodos de Volumes Finitos para Modelos Globais Multiescala
(Numerical Finite Volume Methods for Global Multiscale Models)

- **Início**: 16 de Outubro de 2023
- **Fim**: 16 de Novembro de 2023 - Se tudo der certo e não perdermos nenhuma aula ;-)

- **Aulas:** Seg/Ter/Qui 16h-18h - Online
- **Monitoria:** Sex 16h-17h - Online

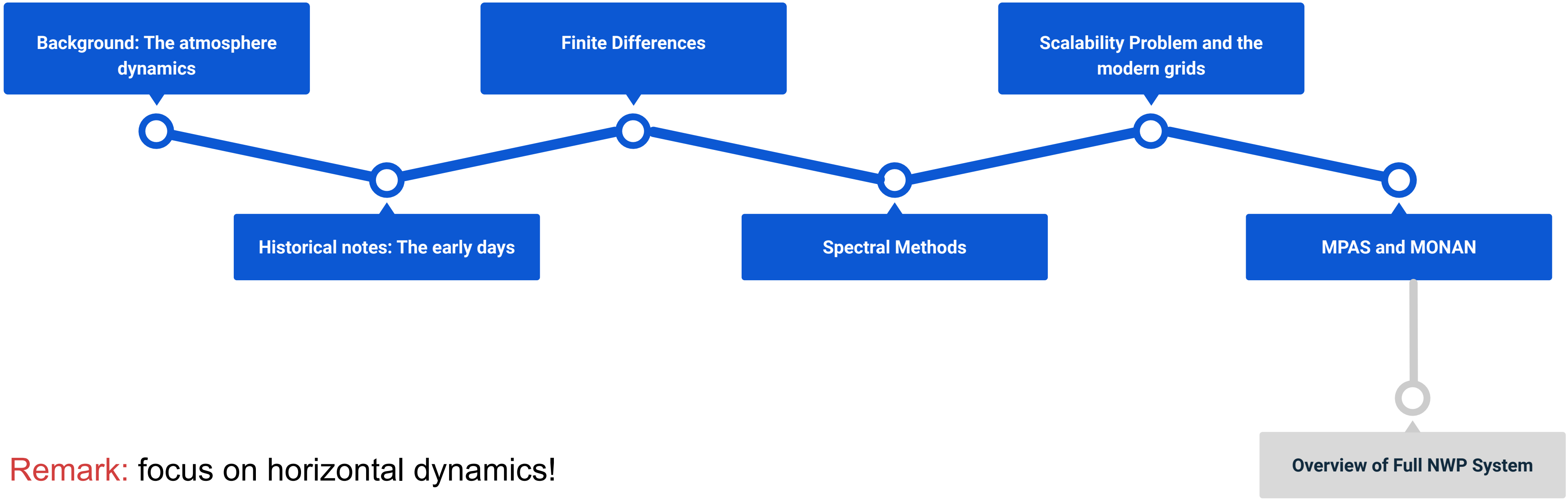
Tópicos Principais: Métodos numéricos de volumes finitos usados na discretização horizontal de modelos globais como o Model for Prediction Across Scales (MPAS).

MONAN



Overview

Today's class:



Remark: focus on horizontal dynamics!

Overview

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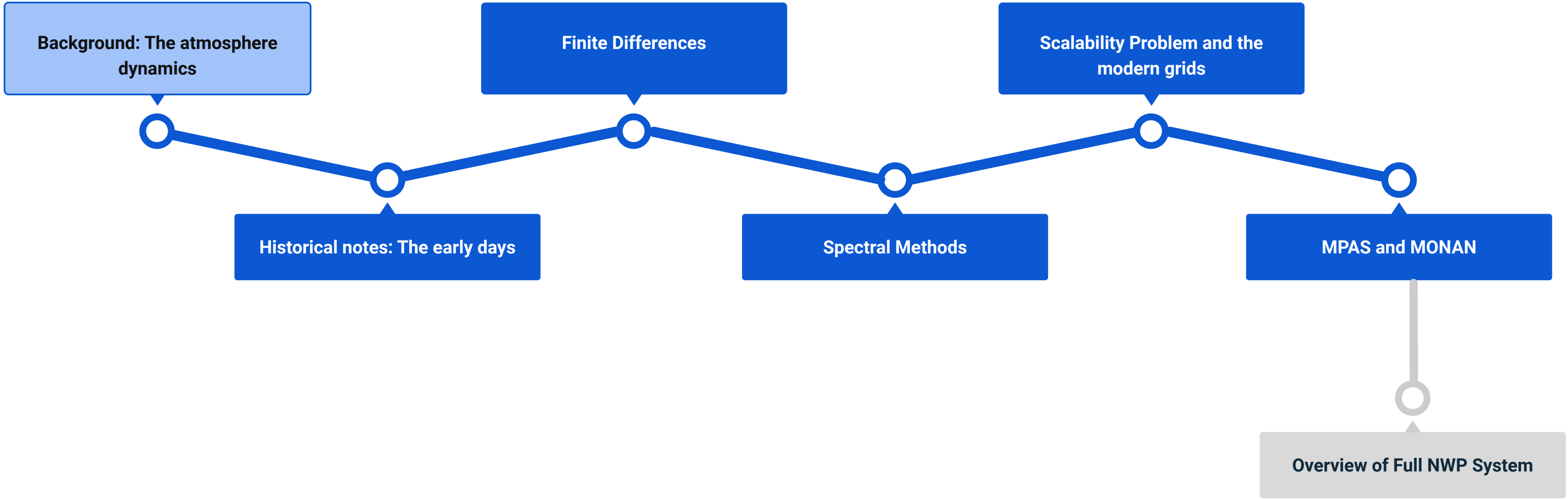
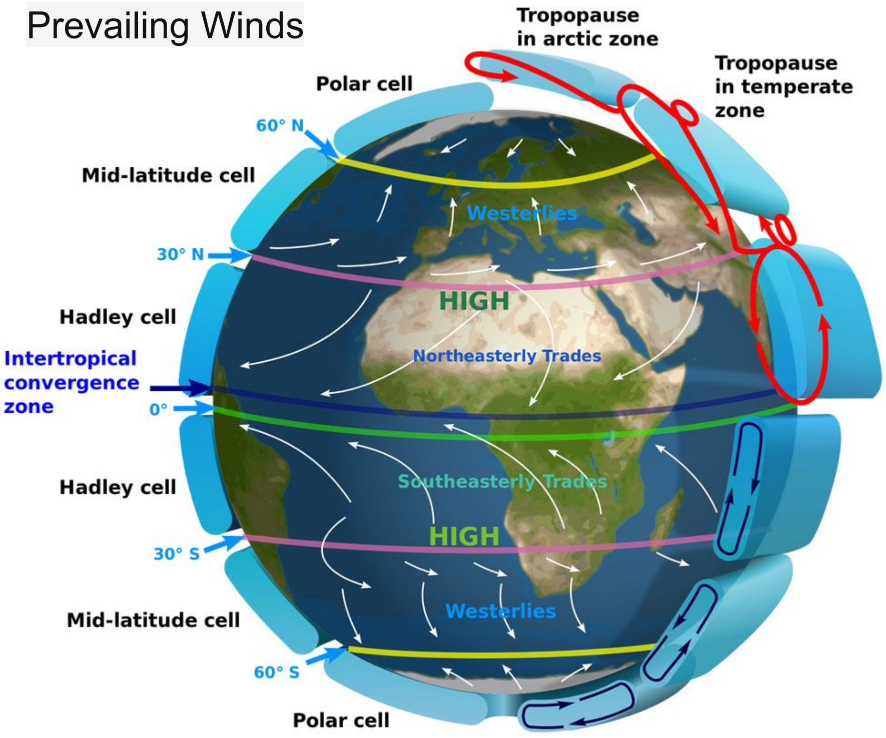
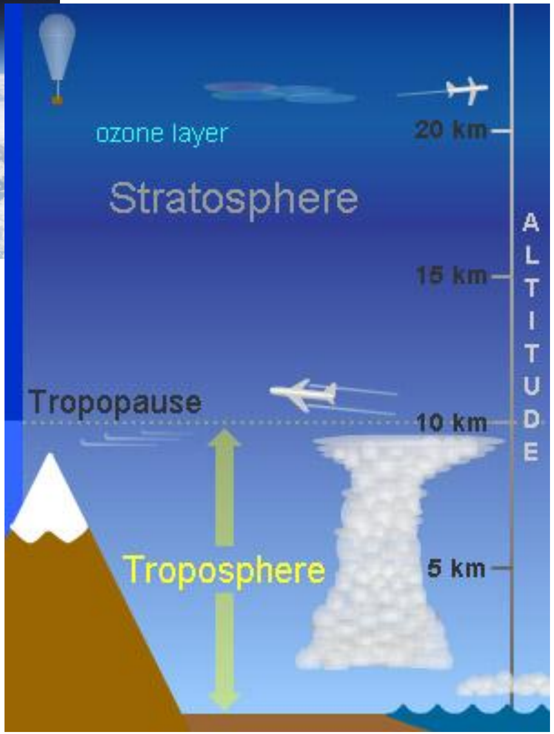


Centrepiece of study: Atmosphere

The atmosphere is a layered fluid (gas)



Images: Nat. Geo. / Wikimedia/Nasa ^

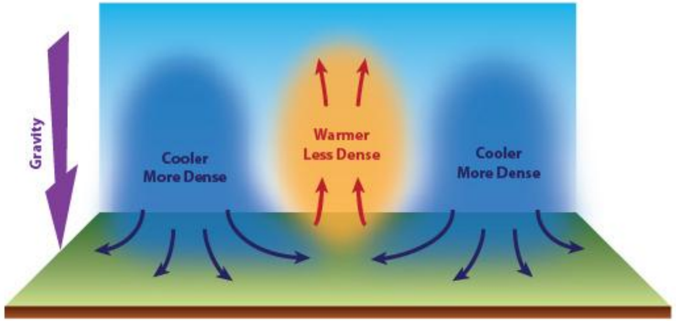


Remark: Many topics discussed in this course are also valid for **ocean** models.

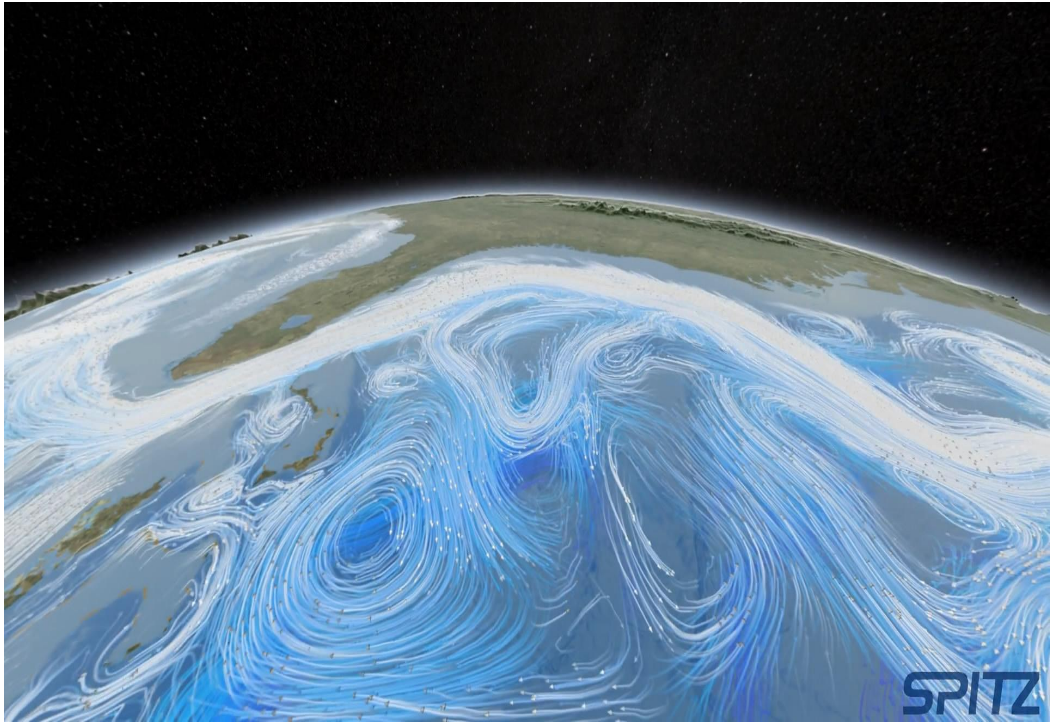
Images: < Nasa, ^ NCAR-UCAR

Atmosphere Dynamics

- Assume continuity
- Thermodynamics/Newton's law

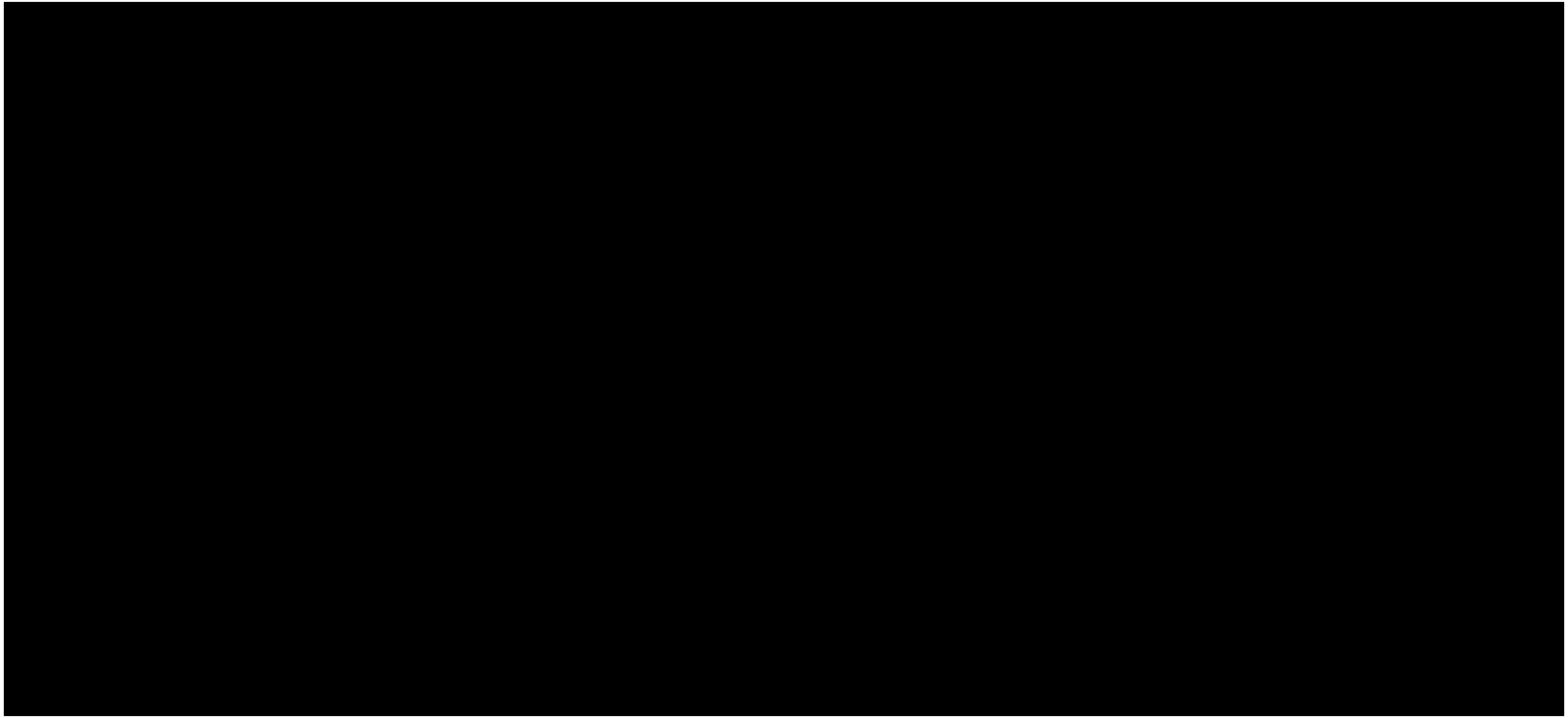


- Waves
- Circulation
- Turbulence
- Convection
- Cyclones ...

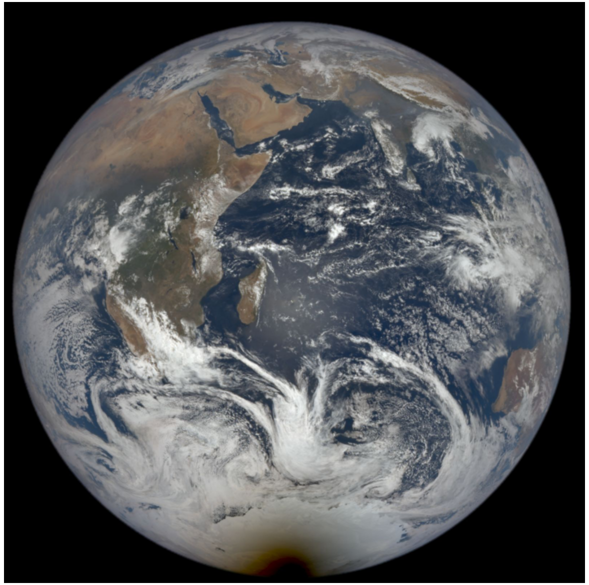


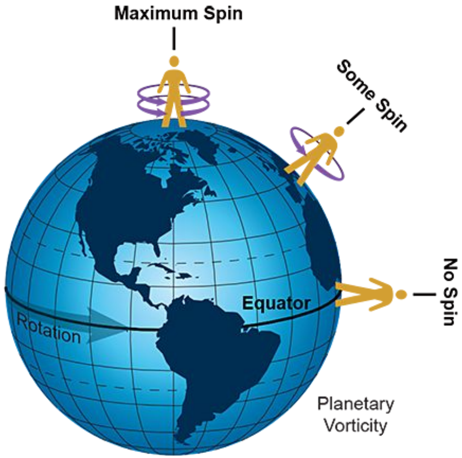
Wallace, J.M. and Hobbs, P.V., 2006. *Atmospheric science: an introductory survey* (Vol. 92). Elsevier.

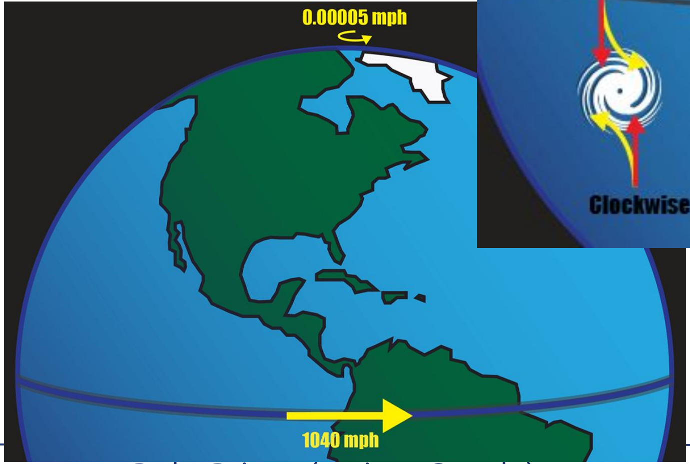
What are we trying to model?



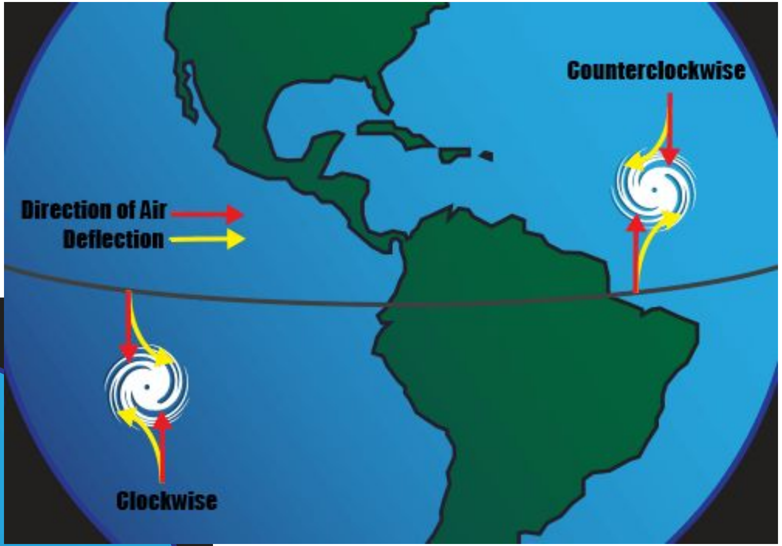
Earth: A rotating “sphere”







Coriolis Effect



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

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

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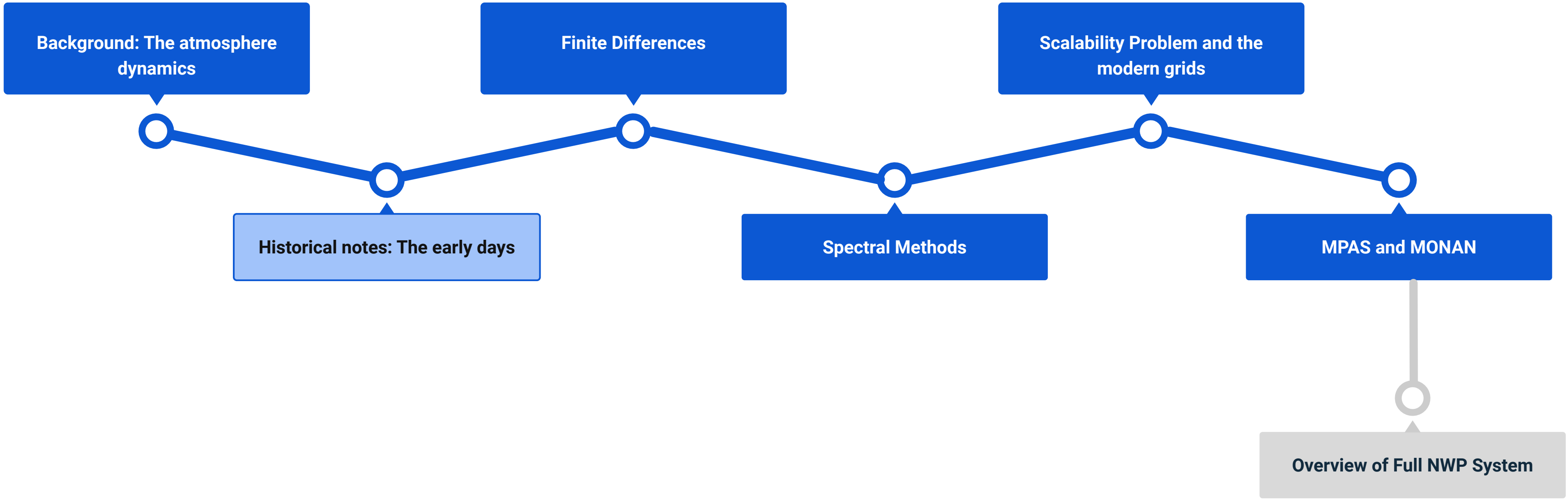


History

“The alien sciences of meteorology and oceanography”

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 $\boldsymbol{\Omega}$)

$$\frac{\mathrm{D}\Gamma}{\mathrm{D}t} = 0$$

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

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

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

Barotropic Vorticity Equation

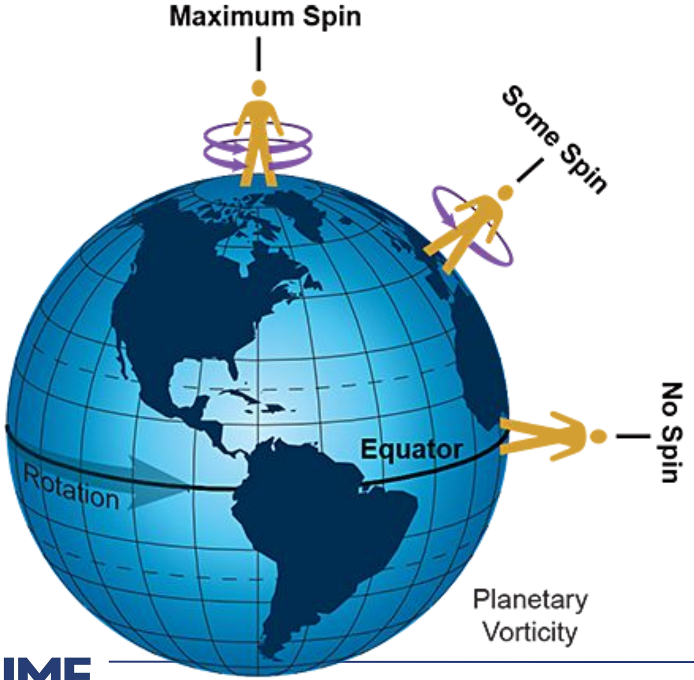
Conservation of absolute vorticity

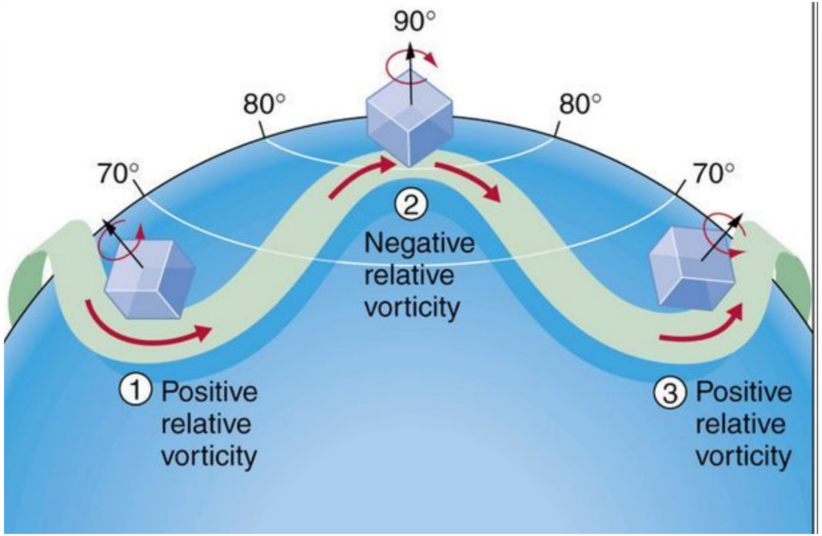
$$\frac{D\eta}{Dt} = 0$$

Material Derivative (along with flow)

$$\eta = \zeta + f$$ Absolute vorticity (Relative + Coriolis)

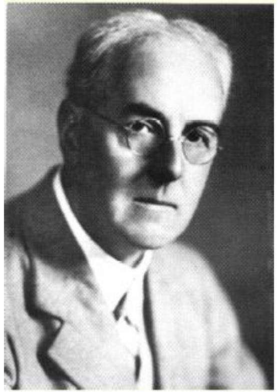
Single layer, non-divergent horizontal flow





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

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)

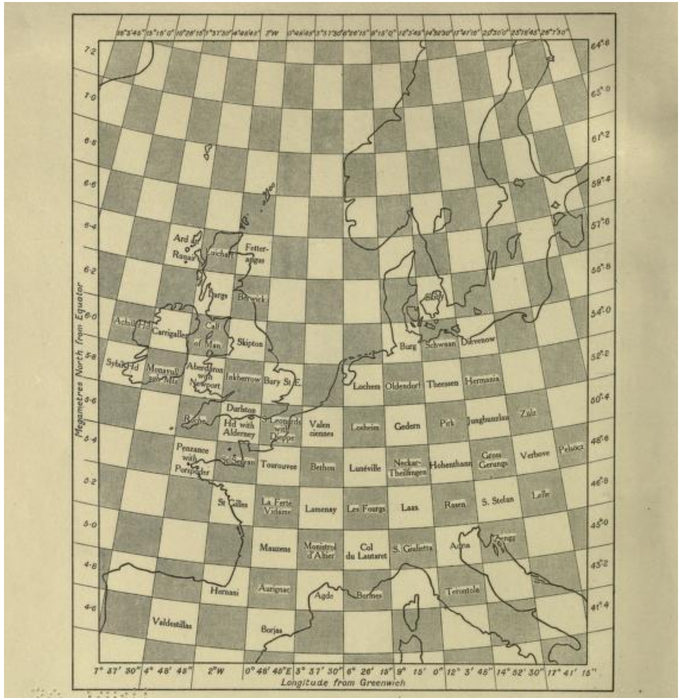
$$p = \rho R T$$

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

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

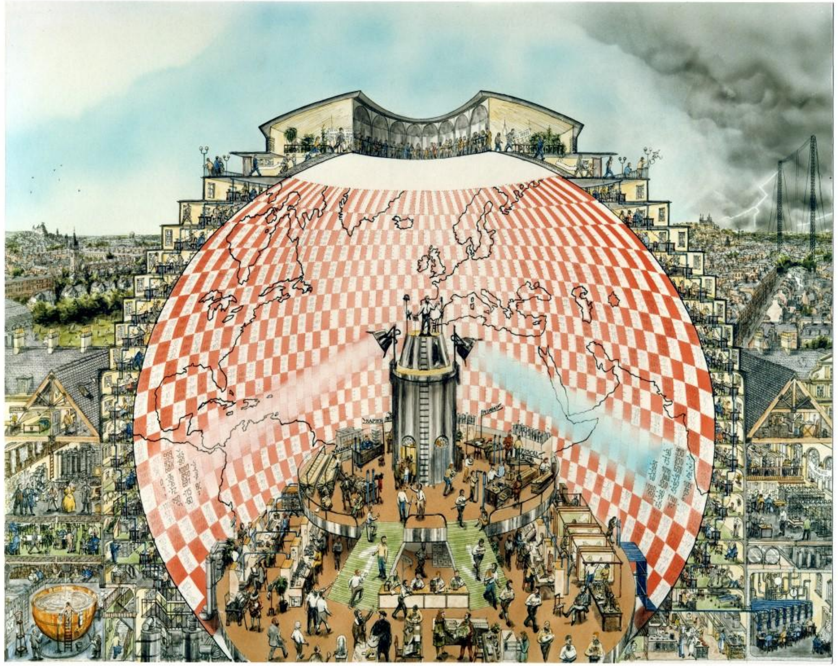
…. we will see details of these equations later in the course.

Weather prediction by numerical process



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

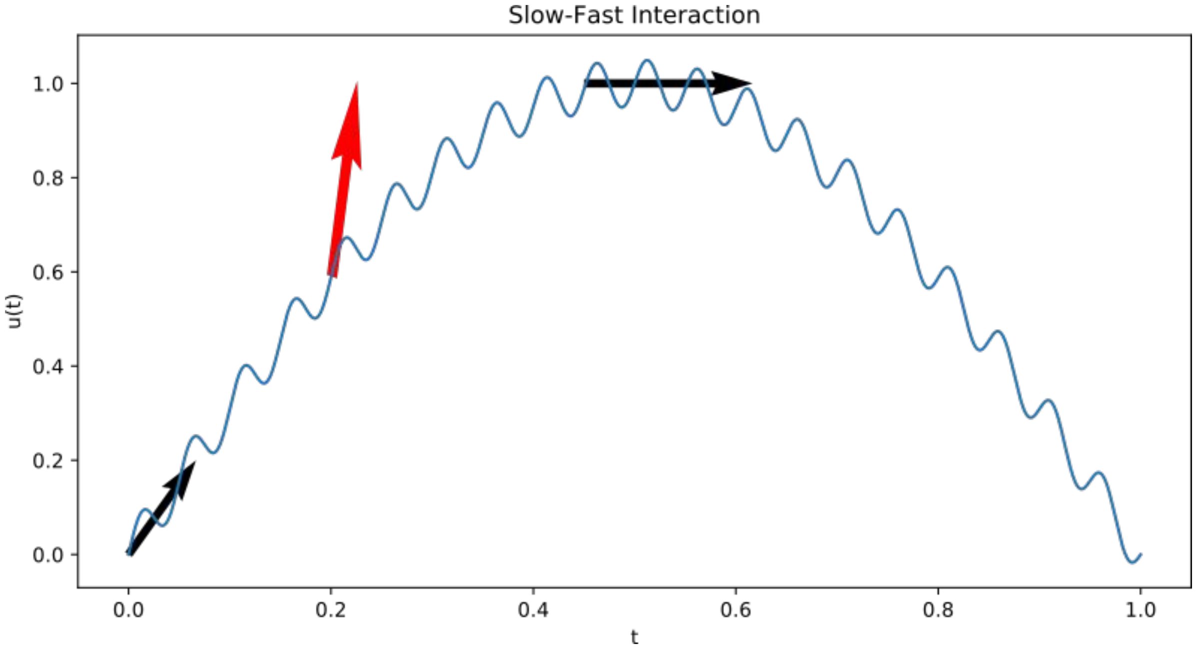
- Two years of hand calculation while in ambulance trips (driver) in WW-I



“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)**

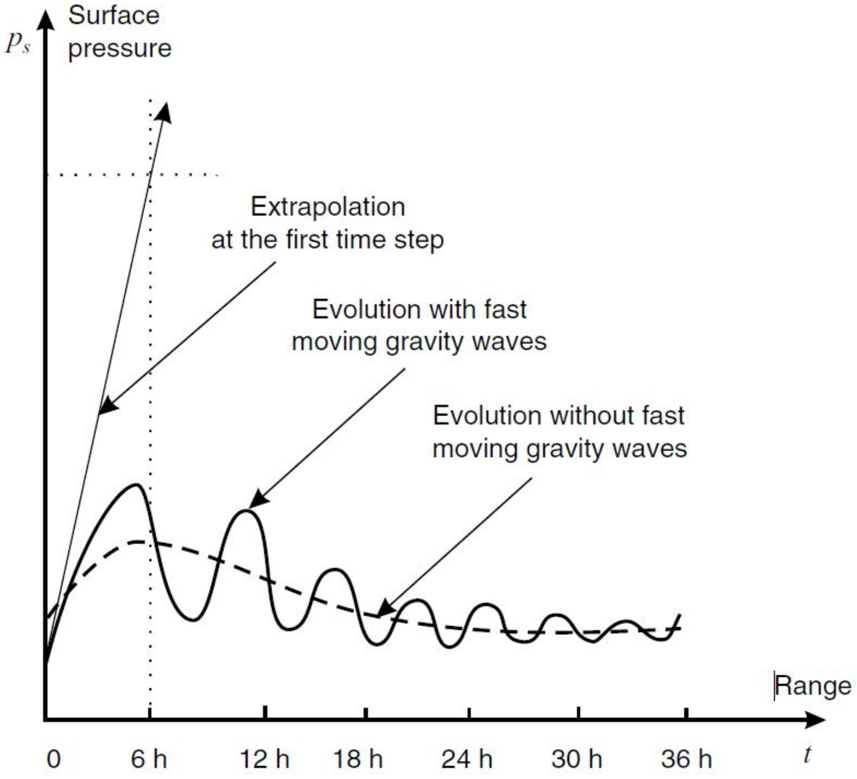
Lynch, P., 1999. Richardson's marvelous forecast. In The life cycles of extratropical cyclones. American Meteorological Society, Boston, MA.

Model Initialization

Initial conditions

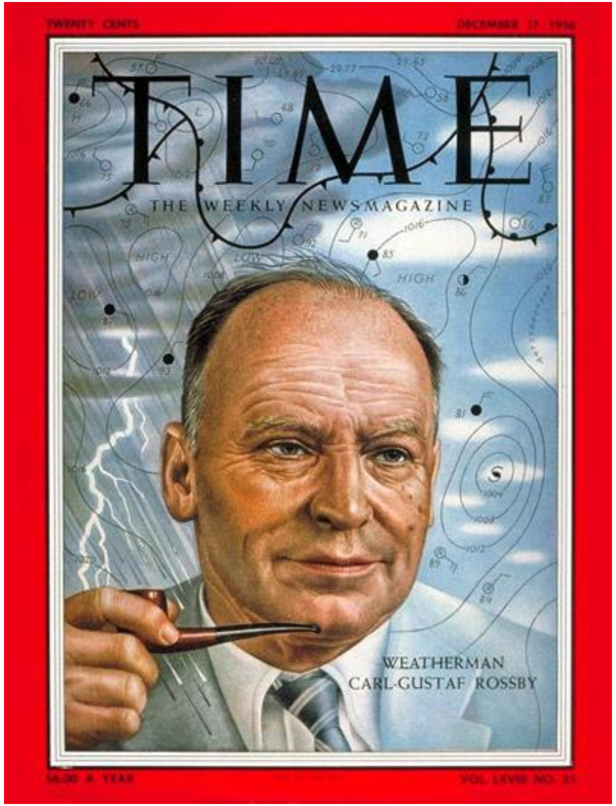
Normal mode initialization

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).

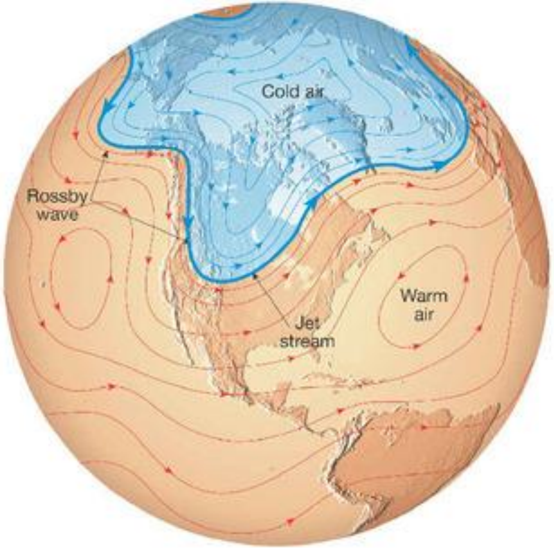
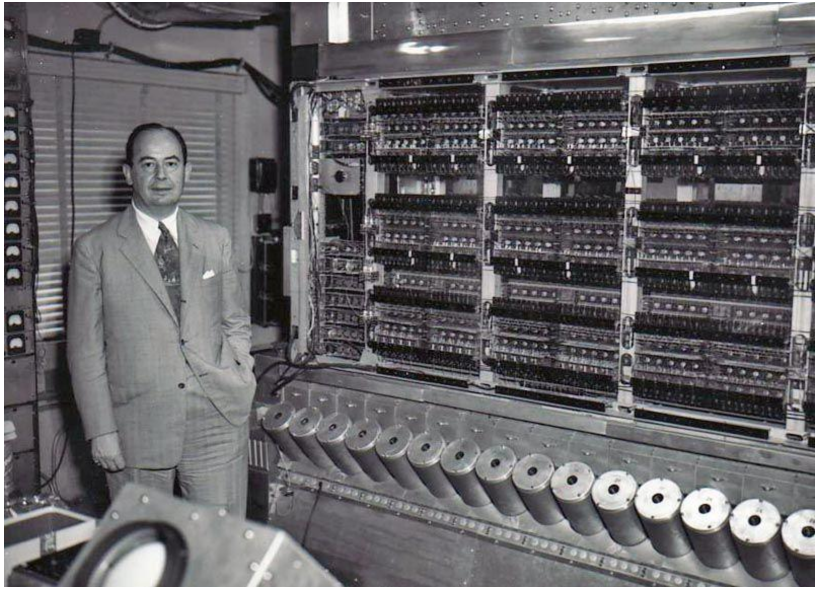


Image credit: stephenleahy.net

History



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:

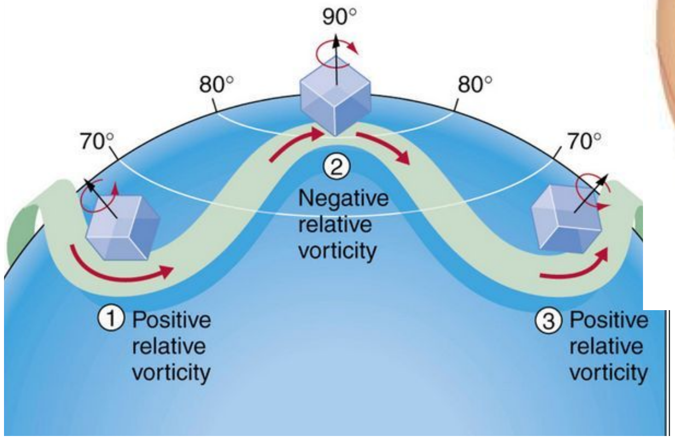
$$\frac{D\eta}{Dt} = 0$$

Material Derivative (along with flow)

$$\eta = \zeta + f$$

Absolute vorticity (Relative + Coriolis)

Remark:
No gravity waves, so initialization is “easier”



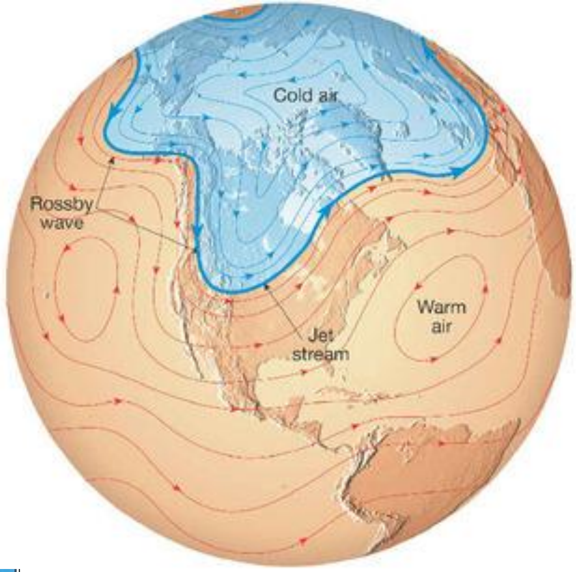
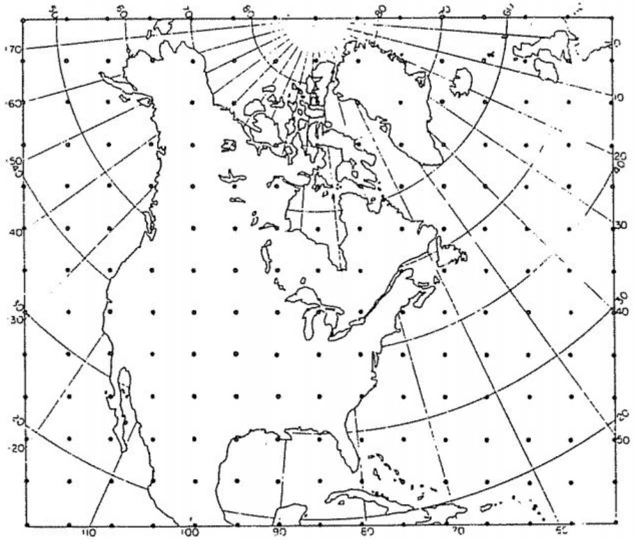
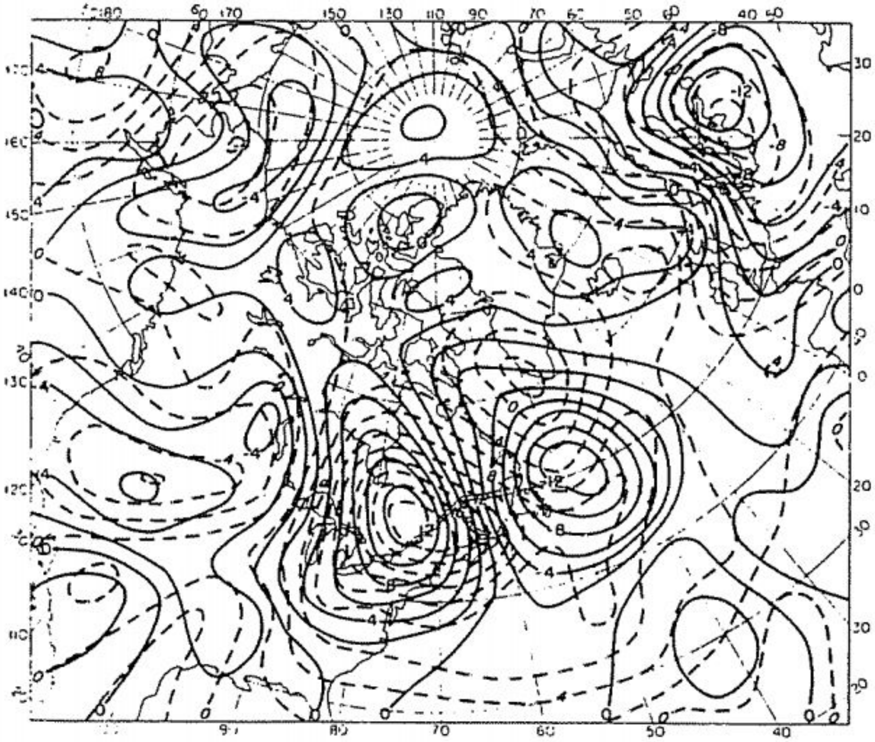


Image credit: stephenleahy.net ^ <http://homework.uoregon.edu/pub/class/atm/ross1.html

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

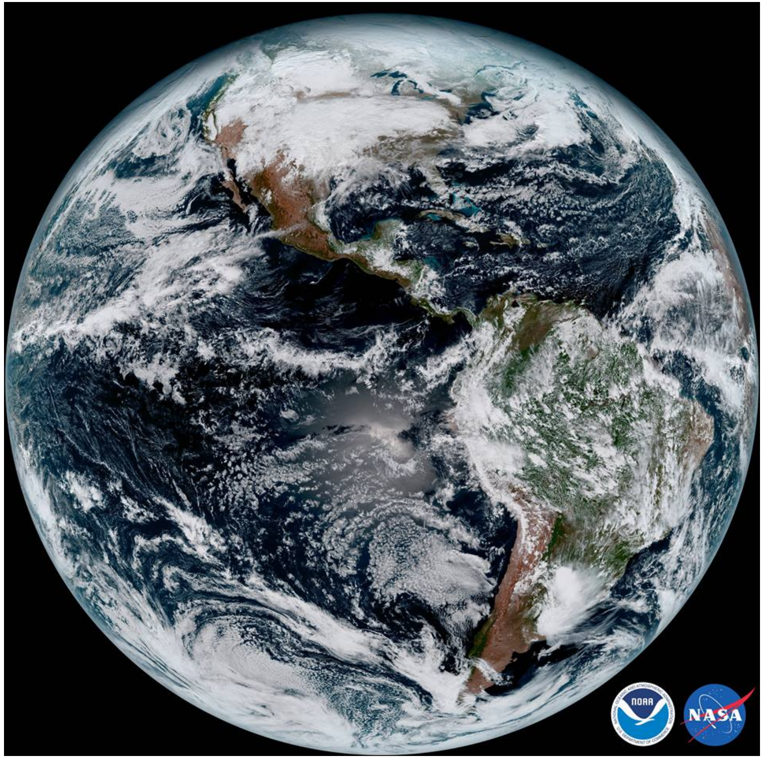


Image: GOES-16 Jan 2017

Three-dimensional Navier-Stokes equations

$\Downarrow$

Nonhydrostatic models

$\Downarrow$

Primitive equations
(hydrostatic equations)

$\Downarrow$

Shallow water equations

$\Downarrow$

Quasi-geostrophic models

$\Downarrow$

Two-dimensional barotrophic 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 << 10km):

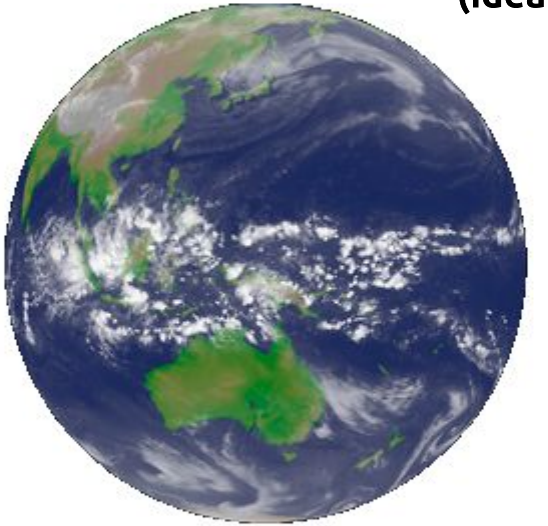


Image: NICAM Model (Japan)

Compressible Euler equations for atmosphere (ideal gas)

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

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

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

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

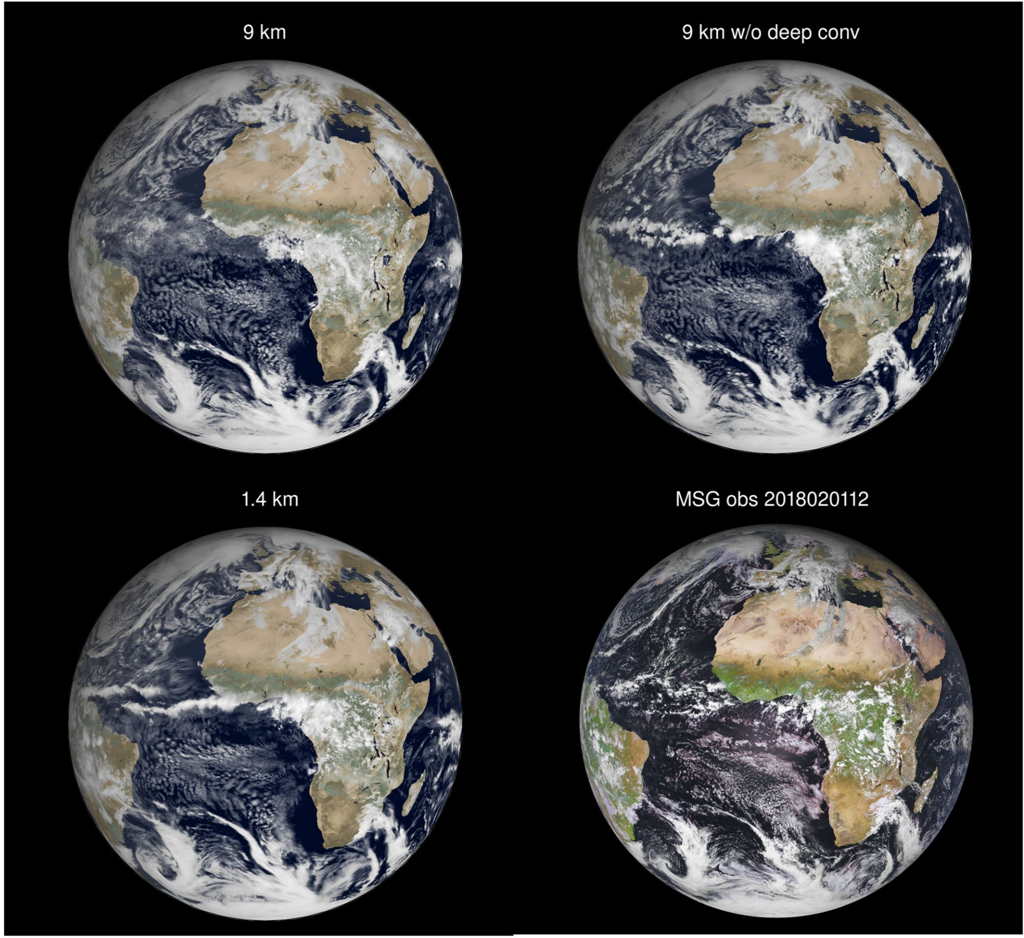
Non-hydrostatic!

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.

Overview

Today's class:

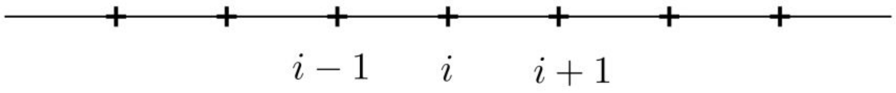
- Background: The atmosphere dynamics
- Historical notes: The early days
- Finite Differences
- Spectral Methods
- Scalability Problem and the modern grids
- MPAS and MONAN
- Overview of Full NWP System

Finite Differences

Change derivatives for finite differences

- 1D:

$$\frac{\partial q}{\partial x} \approx \frac{q_{i+1} - q_{i-1}}{2\Delta x}$$



- 2D on the sphere (λ, θ) = (longitude, 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?

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

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 unfeasible 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

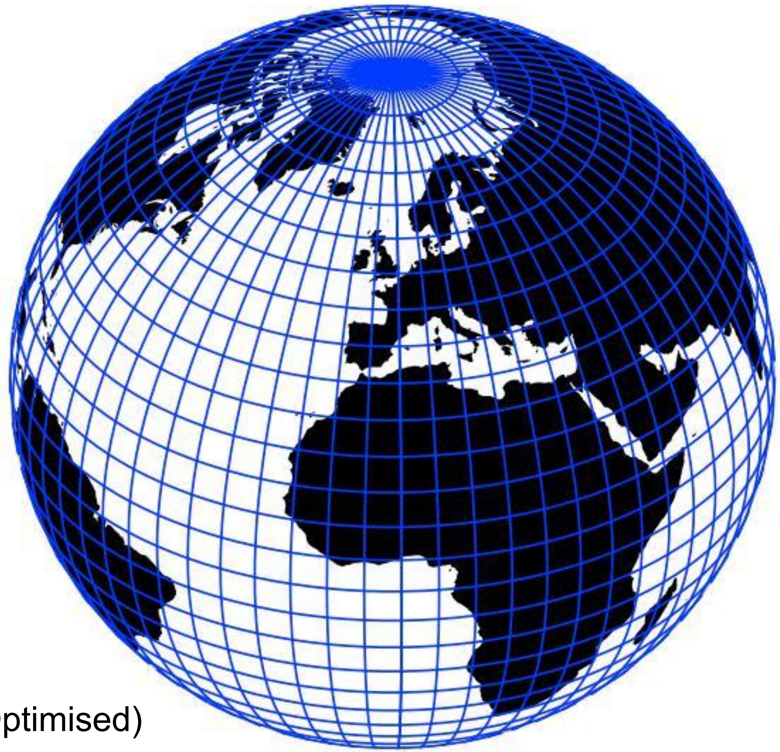
Wood, N., Staniforth, A., White, A., Allen, T., Diamantakis, M., Gross, M., Melvin, T., Smith, C., Vosper, S., Zerroukat, M. and Thuburn, J., 2014. An inherently mass-conserving semi-implicit semi-Lagrangian discretization of the deep-atmosphere global non-hydrostatic equations. *Quarterly Journal of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

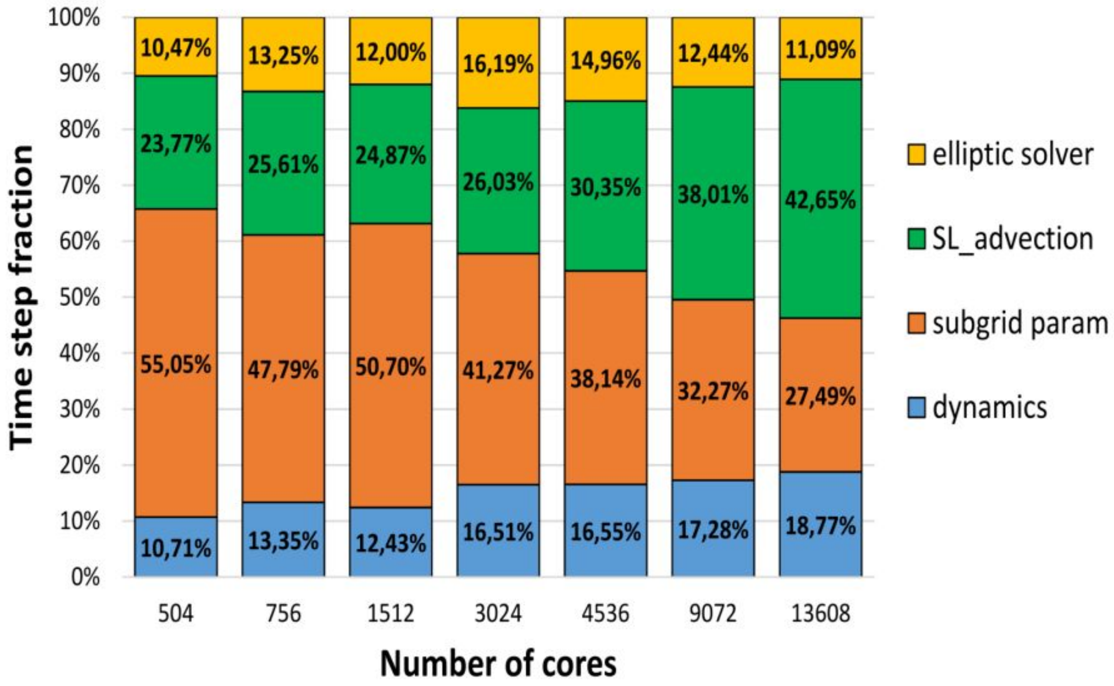
Scalability issues

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

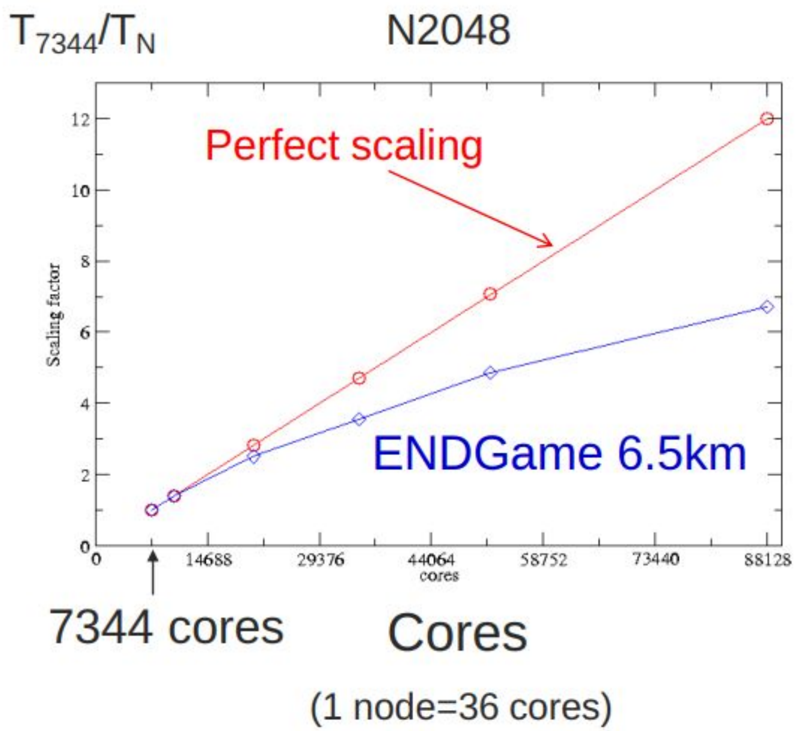


- https://wgne.net/wp-content/uploads/2019/10/WED_Wedi_WGNE34_scalabilitymixed.pdf

Scalability issues

An example: **UKMetOffice: Endgame**

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



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- Background: The atmosphere dynamics
- Historical notes: The early days
- Finite Differences
- **Spectral Methods**
- Scalability Problem and the modern grids
- MPAS and MONAN
- Overview of Full NWP System

Spectral Models

Main idea:

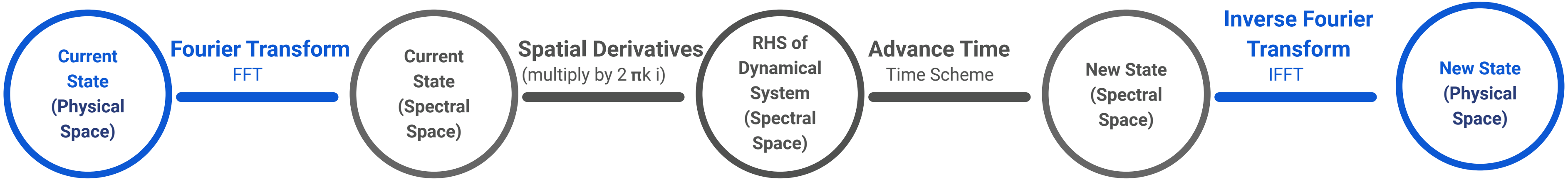
- Expand unknown functions as series of "simpler" basis functions (e.g. Fourier Series/transform)

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

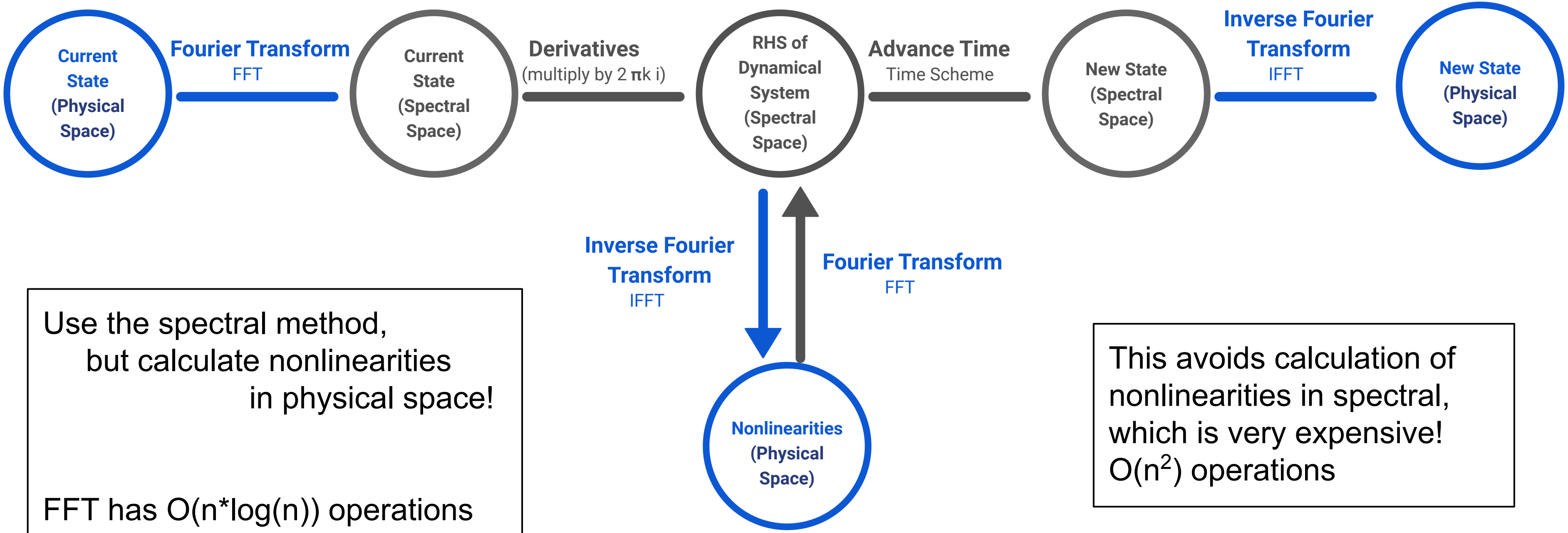
- Calculate derivatives in "spectral space" : derivatives are transformed into multiplications by 2πik.
- Calculate inverse transform to recover an algebraic equation with respect to spatial derivatives.
- Advance in time (pick your favourite time integrator)
- Use inverse transform to recover new state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

Very accurate and fast for linear equations!

Very expensive for nonlinear equations!



Pseudo-Spectral Models



Use the spectral method,
but calculate nonlinearities
in physical space!

FFT has $O(n*\log(n))$ operations

This avoids calculation of nonlinearities in spectral, which is very expensive! $O(n^2)$ operations

- Eliasen, 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:

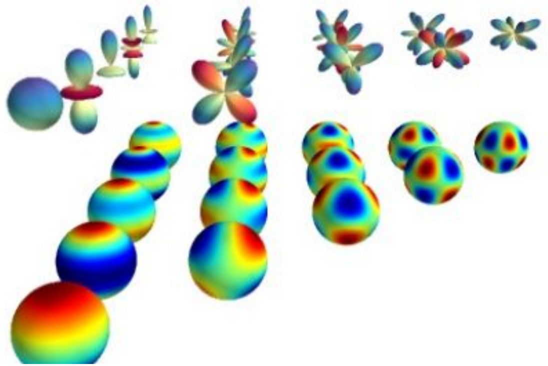
- Fourier expansion for each latitude circle
- Legendre polynomials on meridians

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

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

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)



- Eliasen, 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, 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

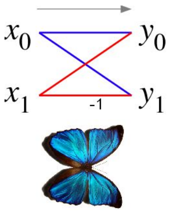
- **Resolution increases of the deterministic 10-day medium-range Integrated Forecast System (IFS) over ~28 years at ECMWF:**
  - 1983: T 63 (~316km)
  - 1987: T 106 (~188km)
  - 1991: T 213 (~95km)
  - 1998: T_L319 (~63km)
  - 2000: T_L511 (~39km)
  - 2006: T_L799 (~25km)
  - 2010: T_L1279 (~16km)
  - 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…

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

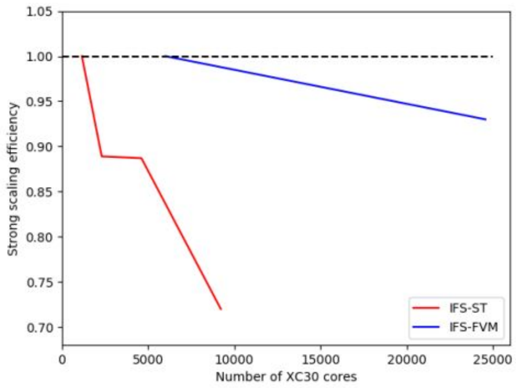
Scalability



Drawbacks:

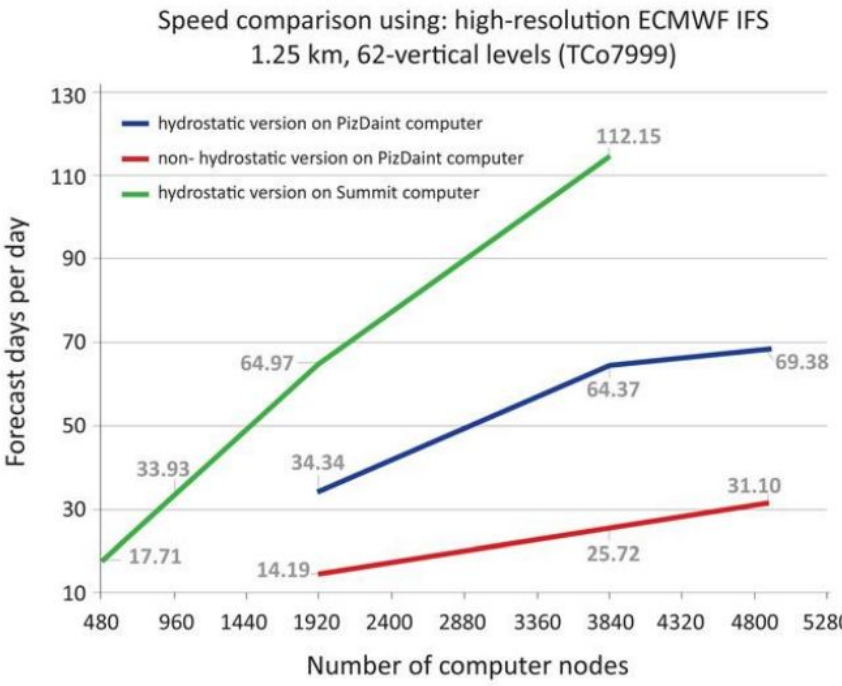
- Legendre Transform is O(N^2) operations
  –> use "fast" Legendre transforms (Butterfly Algorithm)
- Spectral transforms require global communication
  –> reduces scalability (parallelism has communication bottlenecks)

IFS-ECMWF
Example:



Strong scaling

Time-to-solution



- Wedi, N.P., Hamrud, M. and Mozdzynski, G., 2013. A fast spherical harmonics transform for global NWP and climate models. Monthly Weather Review, 141(10), pp.3450-3461.
- Bauer, P., Quintino, T., Wedi, N., Bonanni, A., Chrust, M., Deconinck, W., Diamantakis, M., Düben, P., English, S., Flemming, J. and Gillies, P., 2020. The ECMWF scalability programme: Progress and plans. European Centre for Medium Range Weather Forecasts.
- https://wgne.net/wp-content/uploads/2019/10/WED_Wedi_WGNE34_scalabilitymixed.pdf

Overview

Today's class:

- Background: The atmosphere dynamics
- Historical notes: The early days
- Finite Differences
- Spectral Methods
- Scalability Problem and the modern grids
- MPAS and MONAN
- Overview of Full NWP System

The scalability problem

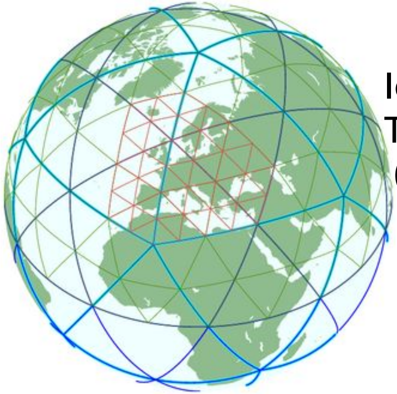
Weather forecasting needs to be done within a short time windows (1 or 2 hours wall clock time)

TUPÃ-CPTEC/INPE (~30k cores)

Massively Distributed Memory Parallel Machines

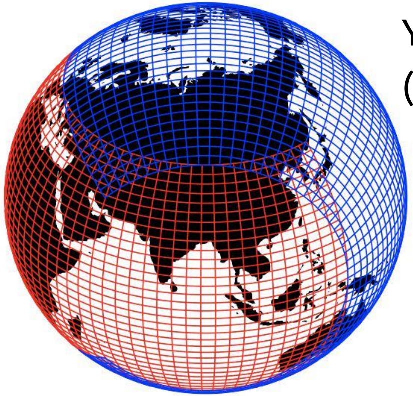
- Finite Differences: Pole communicates with many other computer nodes
- Semi-implicit: A lot of global communication required for the solution of the global linear system or spectral transforms
- Limited scalability on large supercomputers (cannot do the forecast within the time window for high resolutions)

Search for alternatives - more isotropic grids



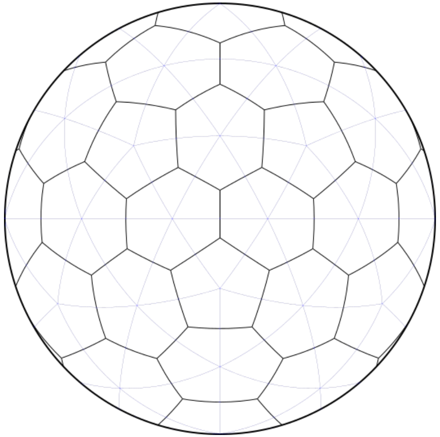
Icosahedral/
Triangular
(ICON-Germany)

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

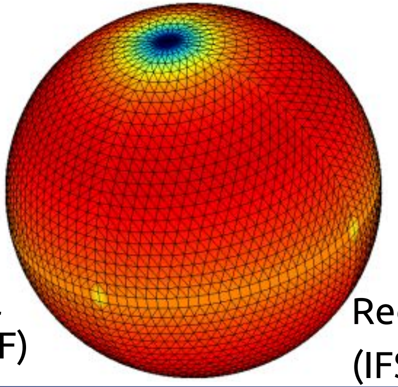


Yin-Yang
(GEM-Canada)

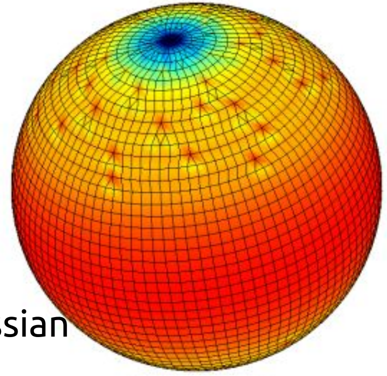
Voronoi
(MPAS/FIM/
OLAM-USA
NICAM-Japan)



Octahedral
(IFS-ECMWF)

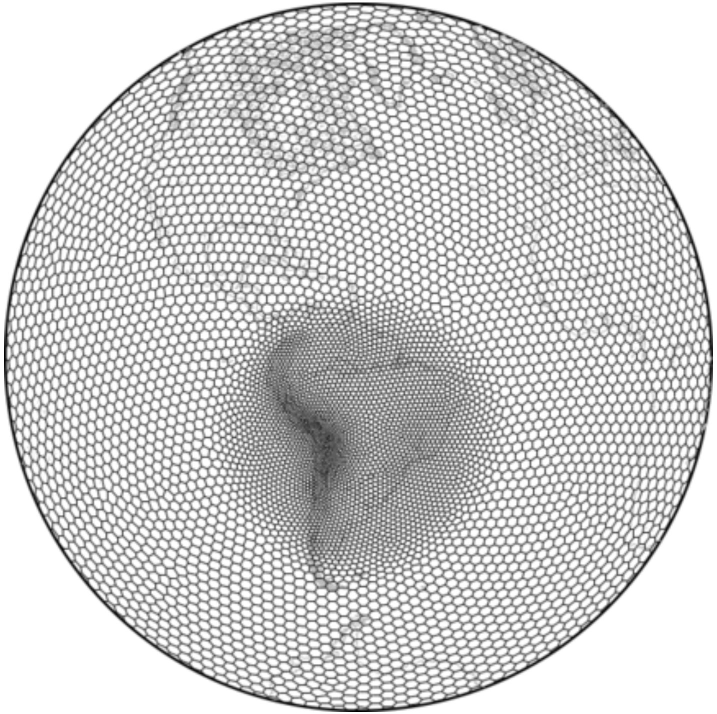


Reduced Gaussian
(IFS-ECMWF)



New generation of models

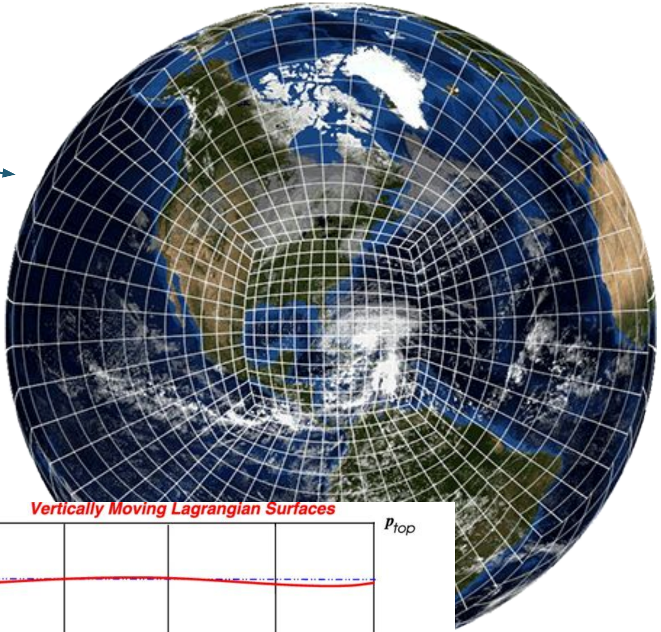
- Grids:
  - Cubed sphere - logically rectangular
  - Triangular/Voronoi - flexible for refinement
- Methods:
- Finite Volume
  - Low order/grid effects with good properties
  - Higher order with less mimetic properties
- Finite Element
  - Mixed finite elements: Mimetic properties
  - Spectral elements/DG: Accuracy, scalable
- HPC
  - Scalability and energy efficiency
  - Maintainability
  - Hybrid architectures, GPUs, ...
  - Massively parallel computing

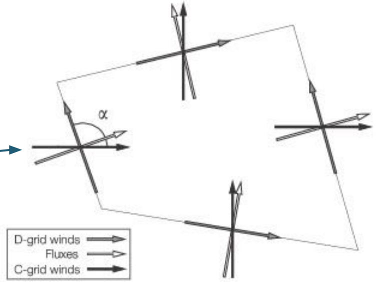


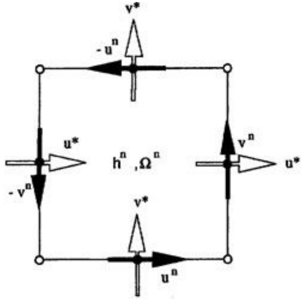
Several open problems!

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

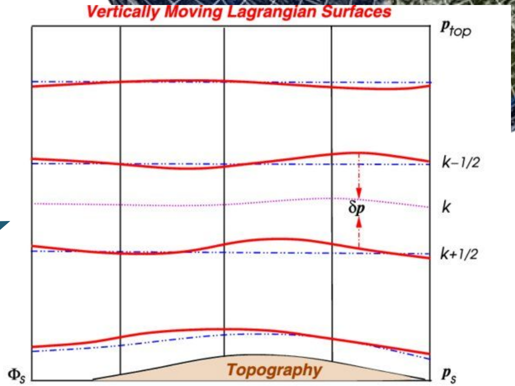
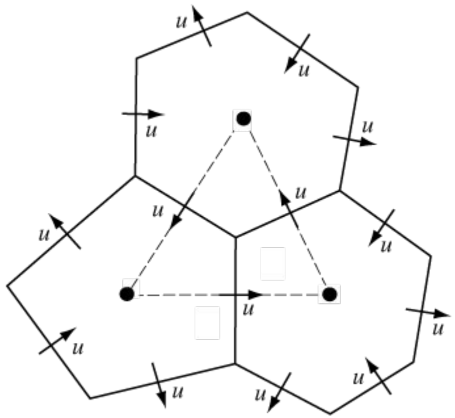


Figure Ref: Nair, Choi, Tufo (2009). Computers & Fluids, 38(2), 309-319.

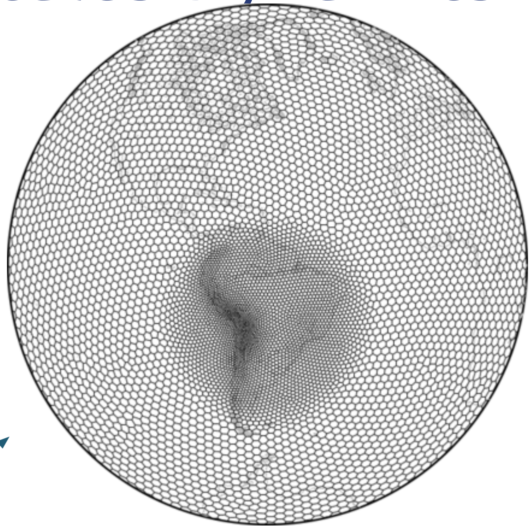
References: https://www.gfdl.noaa.gov/fv3/

Model for Prediction Across Scales Dynamics



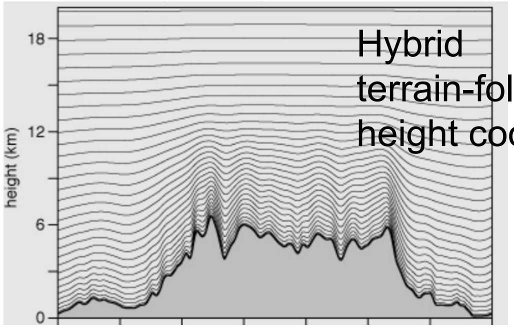
MPAS
Model for Prediction Across Scales

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/)

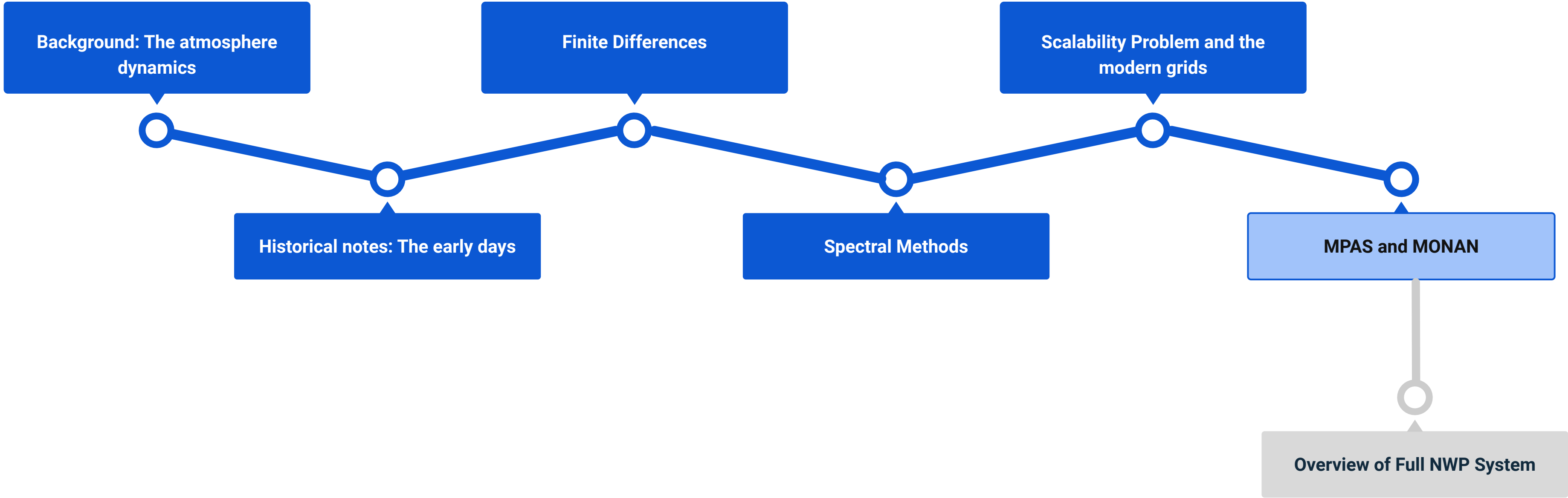


Hybrid terrain-following height coordinate

- 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 tesselations and C-grid staggering. Monthly Weather Review, 140(9)

Overview

Today's class:



MONAN

MONAN – Model for Ocean-laNd-Atmosphere predictioN

Modelo para Previsão dos Oceanos, Superfícies Terrestres e Atmosfera

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) >= 2nd order of global and effective accuracy.

-https://monanadmin.github.io/monan_cc_docs/

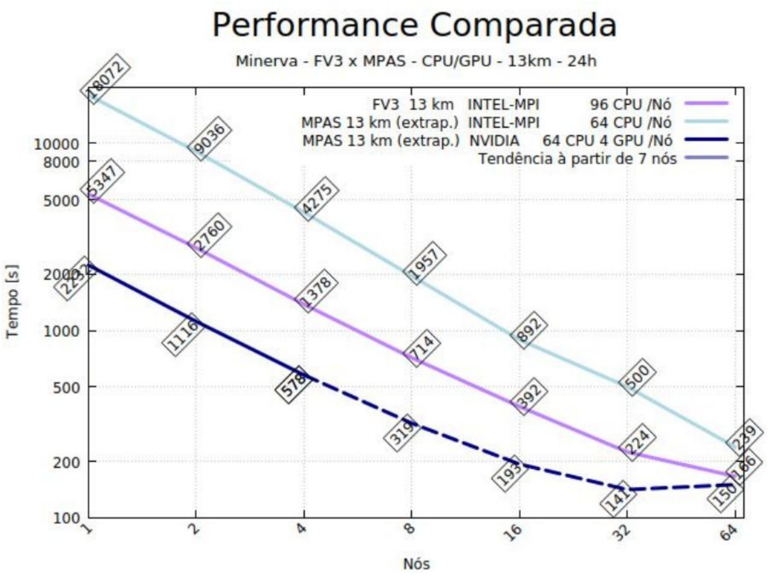
MONAN

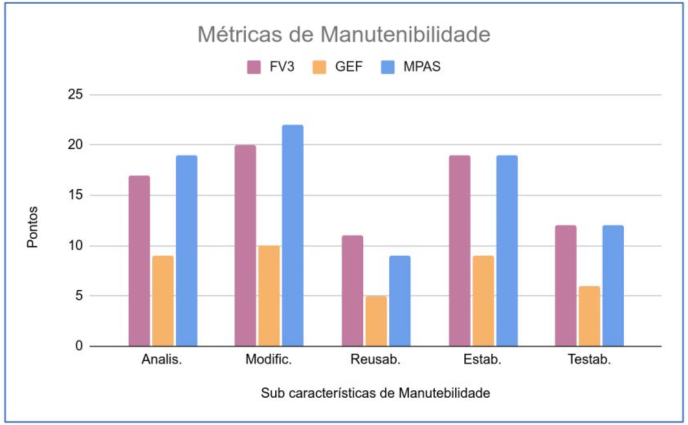
9a reunião do Comitê Científico do MONAN (03/08/2023):

- 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.



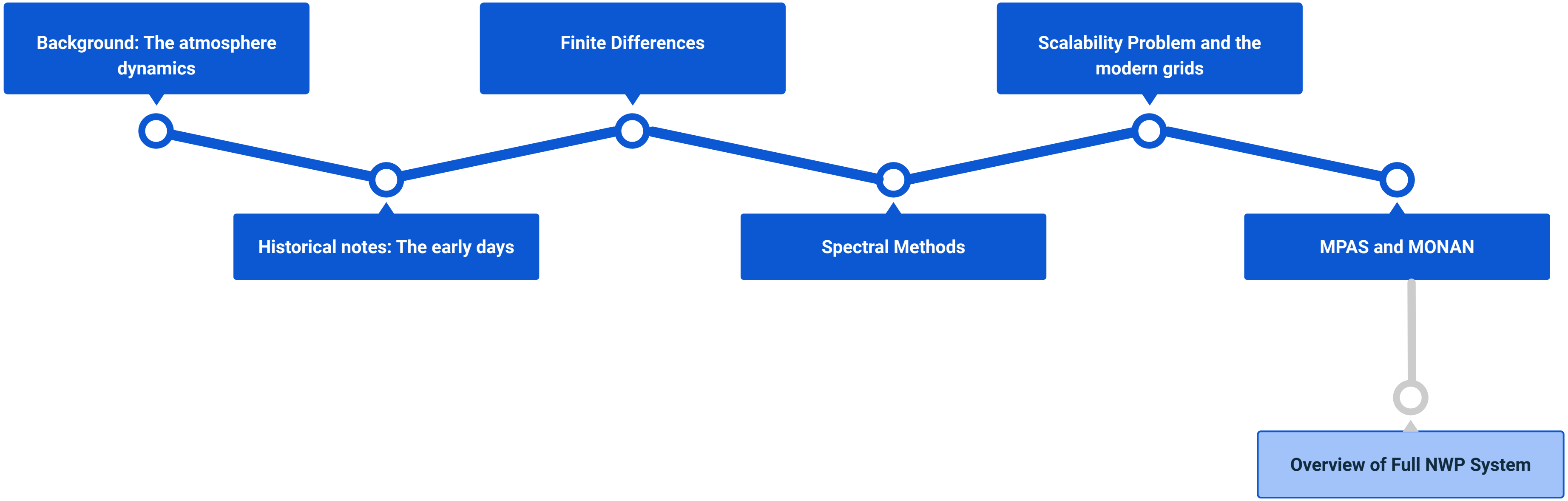


MPAS
Model for Prediction Across Scales

-https://monanadmin.github.io/monan_cc_docs/

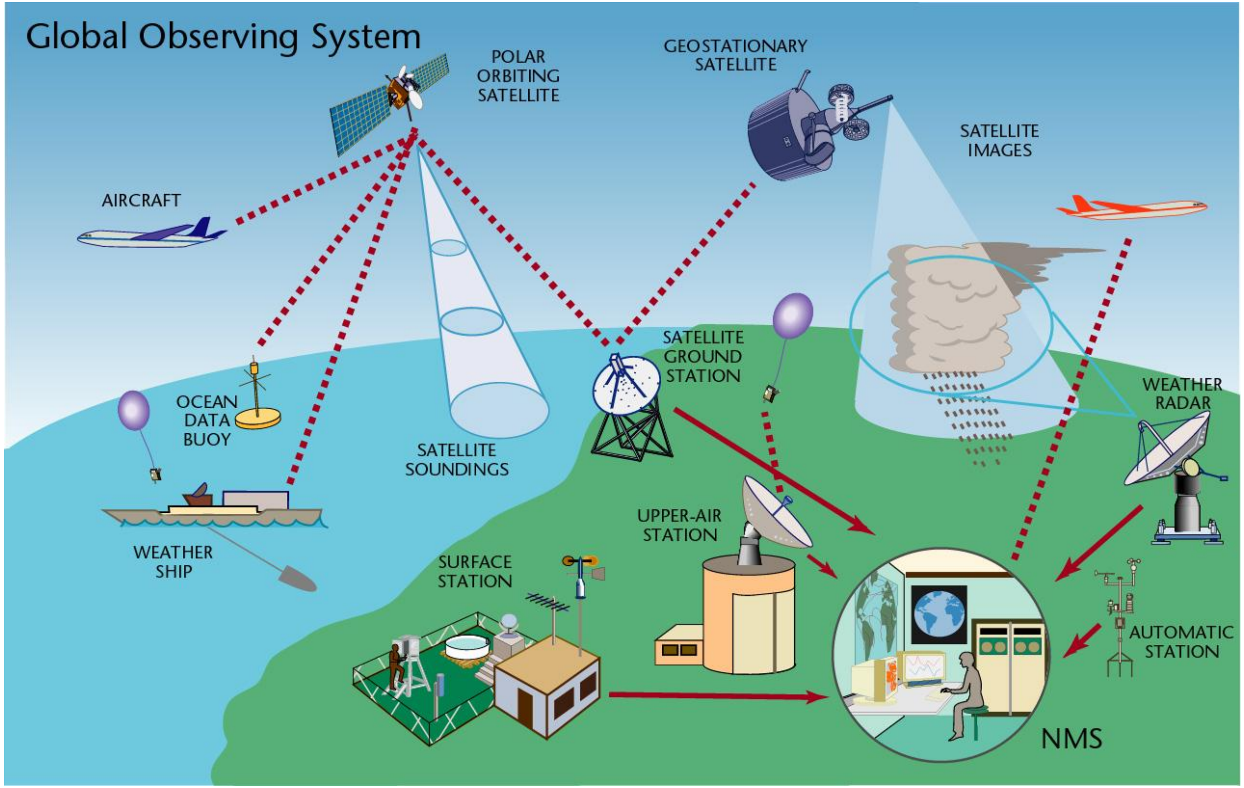
Overview

Today's class:



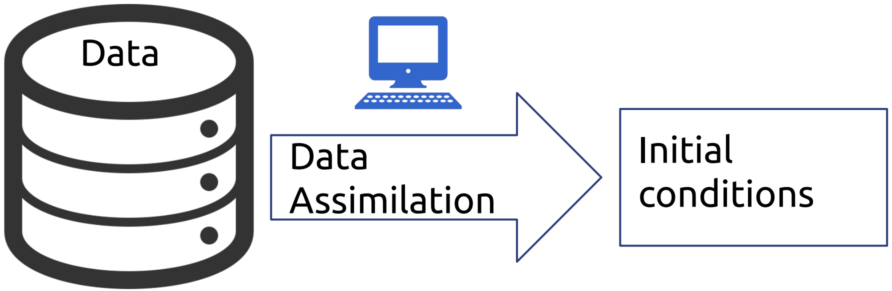
Operational Weather Forecasting

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

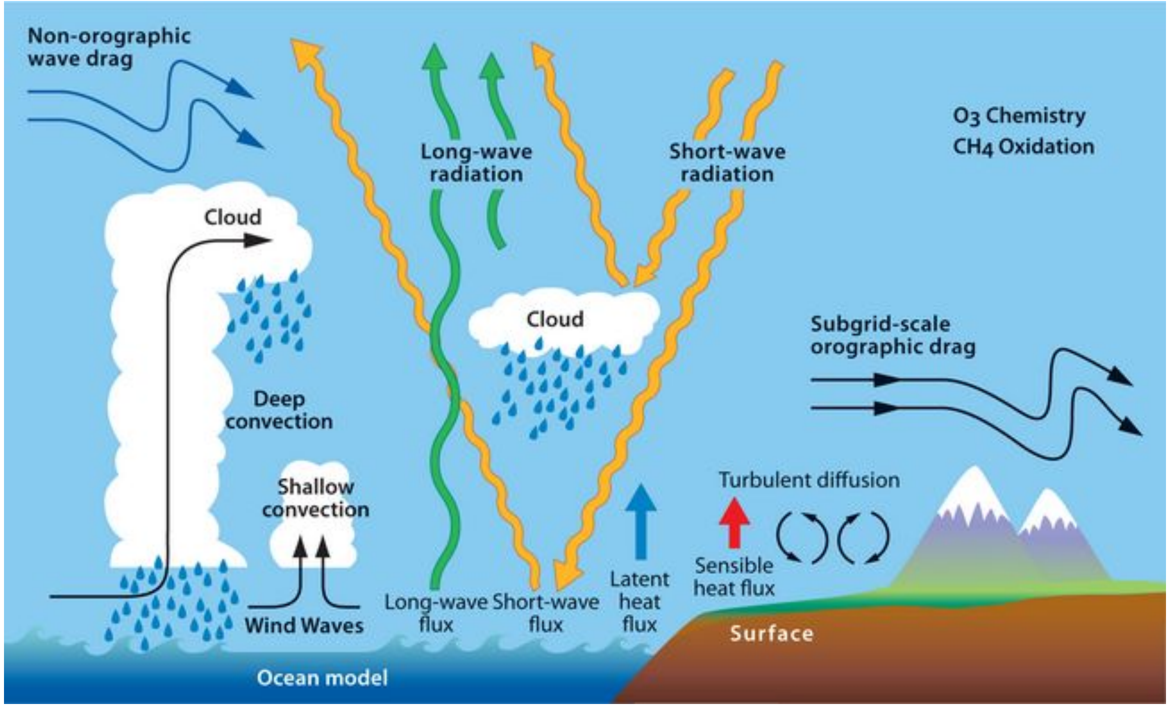
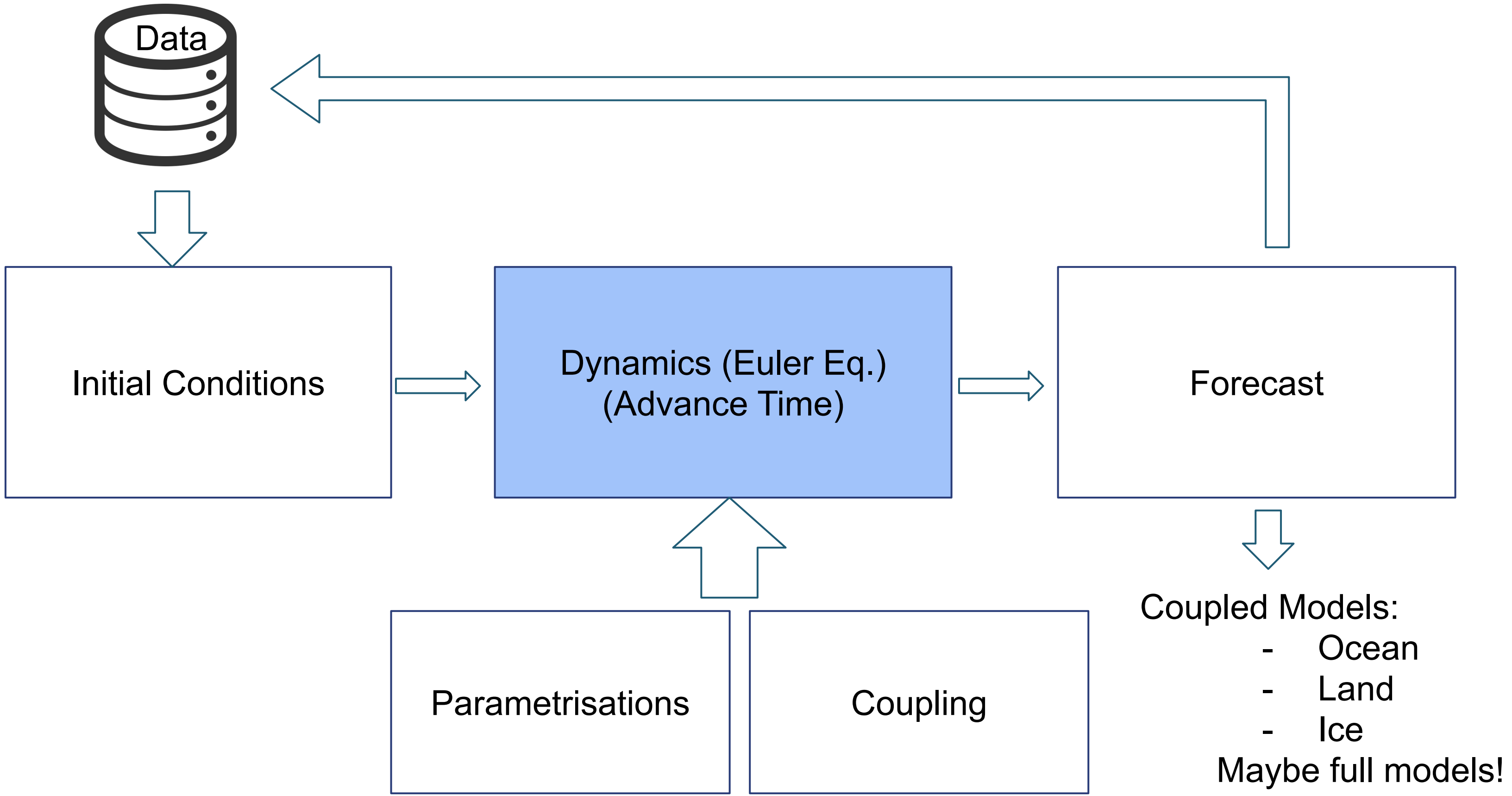


Image: ECMWF

Operational Weather Forecast



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Next classes

This course

Numerical Finite Volume Methods for Global Multiscale Models

General goal:

Provide graduate students and researchers a theoretical and practical introduction to the main Finite Volume methods used in dynamical cores of global geophysical fluids models (atmosphere and ocean) discretized geodesic unstructured grids targeting multiscale resolutions.

Practical goal:

Provide understanding of the underlying numerical methods used in the future dynamical core of MONAN, which is based on MPAS.

Disclaimer:

- Focus on atmosphere dynamics (no physics, parametrizations, real data, assimilation)
- Focus on horizontal dynamics (vertical dynamics will not be discussed)
- “Mixed” Finite Volumes - Finite Difference methods (focused on MPAS dynamics)

Semana 1

Seg - 16 Out

Introdução

- Conceitos iniciais/gerais
- Histórico
- Fundamento de métodos numéricos

Ter - 17 Out

Dinâmica Temporal

- Eq. diferenciais ordinárias
- Convergência
- Estabilidade
- Runge-Kutta do MPAS

- Atividade para 24 Out

Qui - 19 Out

Transporte

- Diferenças Finitas 1D
- Volumes finitos 1D
- Estabilidade (CFL)
- Advecção do MPAS

- Atividade para 26 Out

Sex - 20 Out

Monitoria

Discussão das atividades

Semana 2

Seg - 23 Out

Shallow Water Eq.

- Dedução SWE na esfera
- Formulação de vetor invariante
- Diferenças finitas 1D
- Volumes Finitos 1D

- Atividade para 30 de Out

Ter - 24 Out

SWE - 2D

- Diferenças Finitas 2D
- Volumes Finitos 2D
- Estabilidade
- Conservação de Energia
- Jato instável

- Atividade para 31 Out

Qui - 26 Out

Malhas

- Voronoi/Delaunay 2D
- Voronoi na Esfera
- Refinamento local na esfera
- Malhas do MPAS

- Atividade para 6 Nov

Sex - 27 Out

Monitoria

Discussão das atividades

Semana 3

Seg - 30 Out	Ter - 31 Out	Qui - 2 Novembro	Sex - 3 Nov
FV na esfera • Estrutura de Dados • Operadores de Volumes Finitos do MPAS	**SWE na esfera** • Fortran • Simulação SWE • Jato instável - Atividade para 7 de Nov (Simulação SWE)	**Finados**	**Finados**

Semana 4

Seg - 6 Nov	Ter - 07 Out	Qui - 9 Novembro	Sex - 10 Nov
MPAS • Instalação • Equações Governantes • Estrutura do código	**MPAS** • Inicialização • Experimentos clássicos • Pós-processamento - Atividade para 13 Nov (Simulação)	**Sem aula (Seminário meio-termo CAPES)**	**Sem aula (Seminário meio-termo CAPES)**

Semana 5

Seg - 13 Nov	Ter - 14 Nov	Qui - 16 Novembro	Sex - 17 Nov
Revisão e Atividades • Discussão das atividades realizadas	**Perspectivas** • Questões ainda em aberto sobre o MPAS e MONAN • Pesquisas em curso • Colaborações	**Aula se necessário**	

Atendimento por e-mail: ppeixoto@usp.br

- **Aulas e atividades**: Google Classroom, Google Colaboratory

  https://classroom.google.com/c/NjI1NTk1Mzk4NDcx

- **Material:** Via Google Classroom e depois disponibilizado no site

  https://www.ime.usp.br/~pedrosp/modelagem-numerica-atmosfera/

- **Presença e Nota:** Computadas via atividades.

É fortemente recomendado assistir o curso de forma síncrona!!!

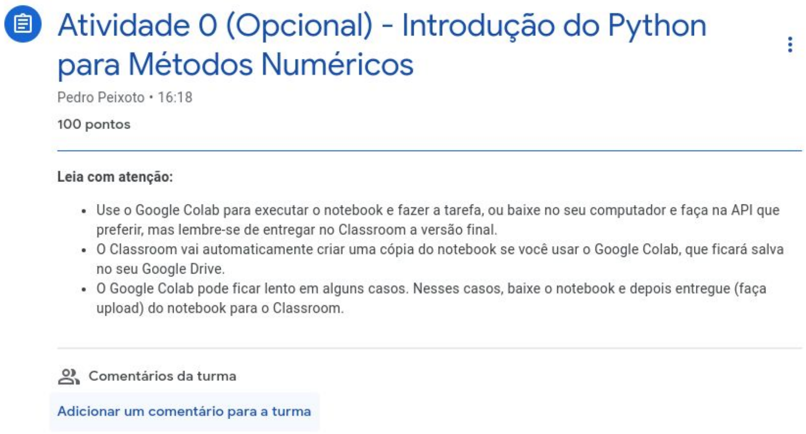
Se não conseguir todas as aulas, tudo bem, assista o vídeo depois e faça as atividades.

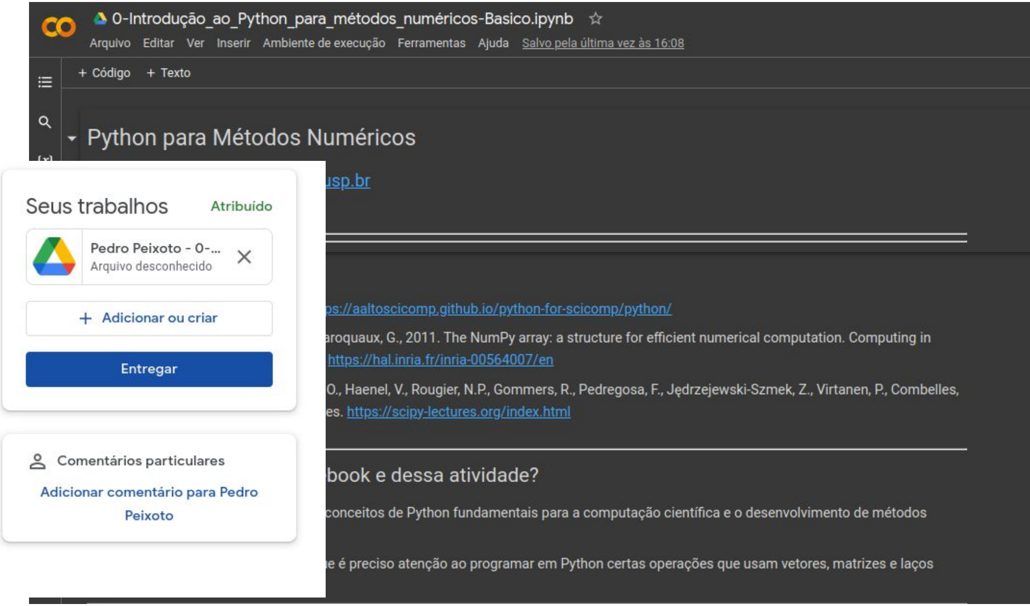
Atividade de hoje

Opcional!

Revisão de Python

Estudar e fazer as atividades do notebook sobre Python para Métodos Numéricos (ver no Google Classroom)





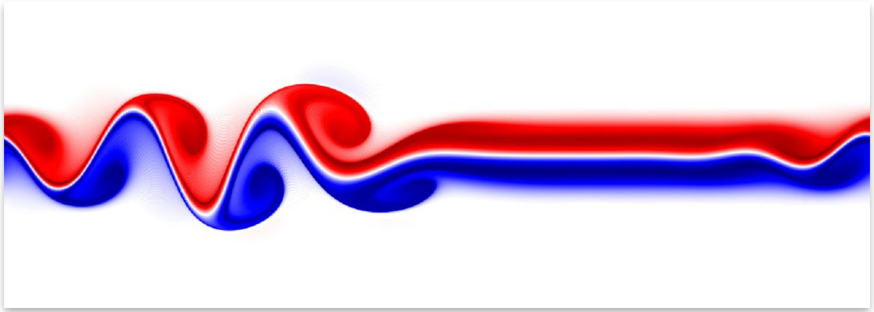
That is all for today…

“All models are wrong, but some are useful”

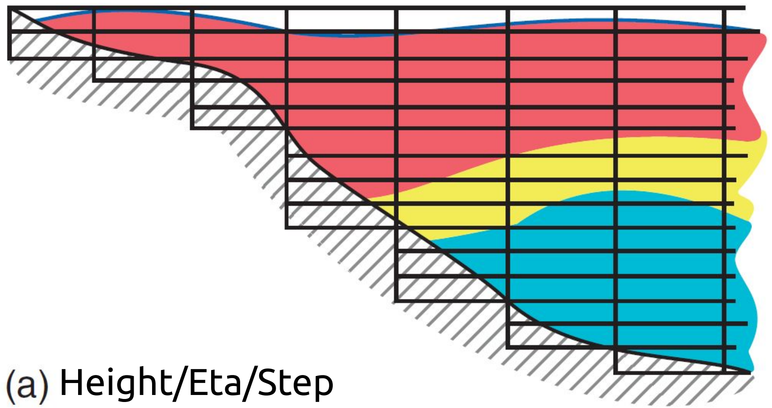
— George Box

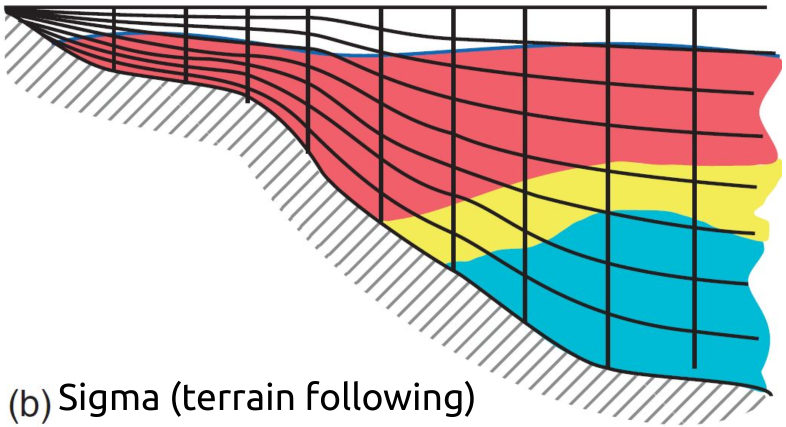
More at: www.ime.usp.br/~pedrosp

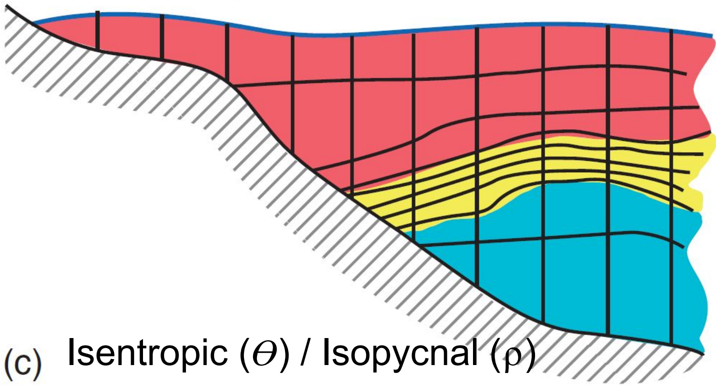
Thanks!



Vertical Coordinates/Grid







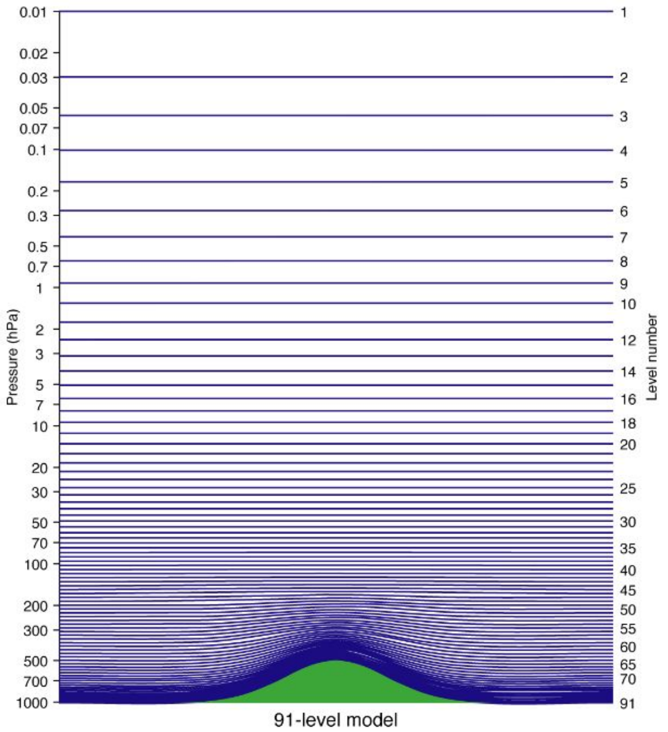
Usually column based!

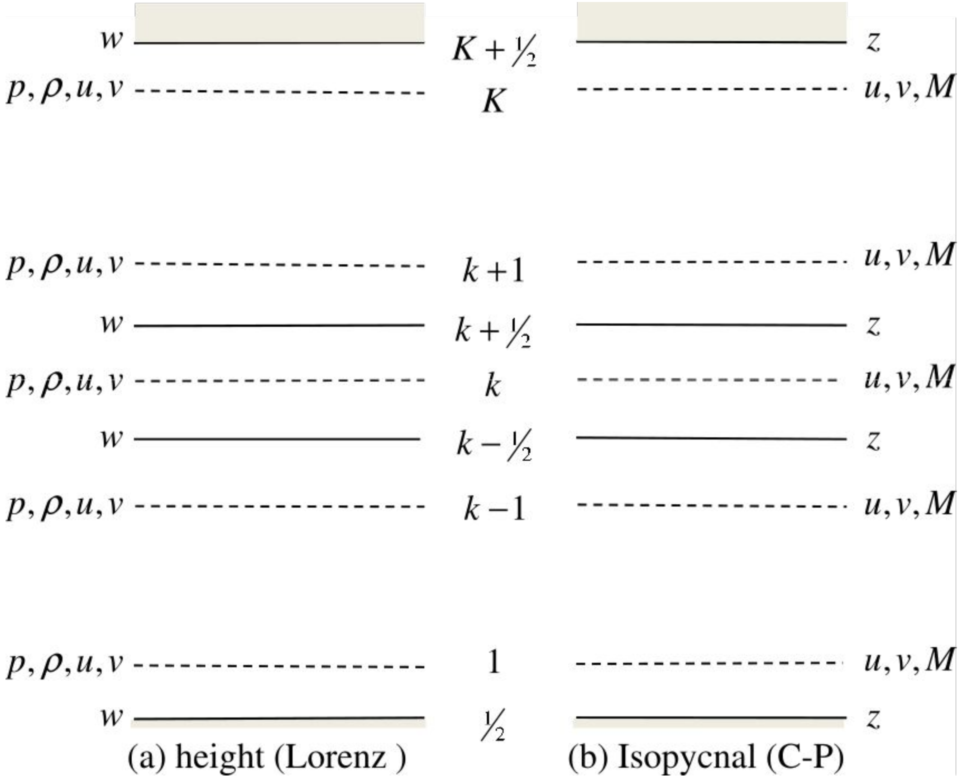
Hodges, B., 2009. Hydrodynamical Modeling.(EL Gene, Ed.) Encyclopedia of Inland Waters. *Academic Press-Elsevier. doi*, *10*, pp.B978-012370626.

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.

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)

Intermediate step

3D Incompressibility (constant density):

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

Vertical Integration (Mean Flow)

Hydrostatic balance:

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

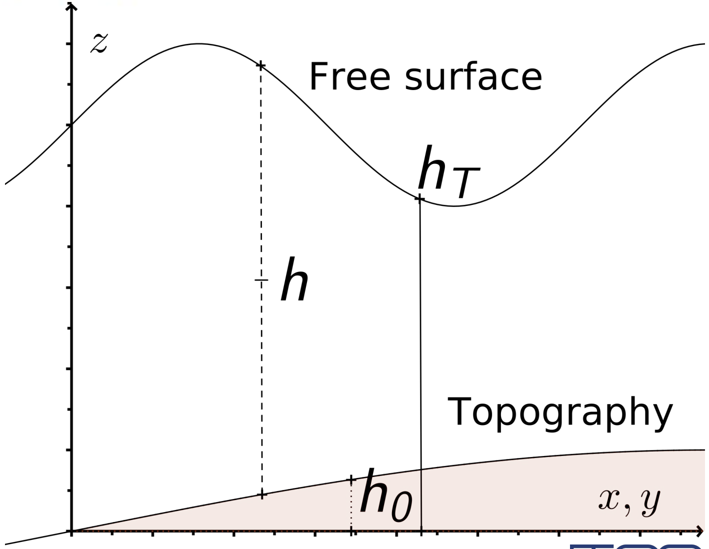
Free surface $h_T(x, y, t)$ where $h_T = h_0 + h$, with $h_0(x, y)$ topography, $h(x, y, t)$ fluid depth.

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

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

Pressure gradient:

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



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 surfave must have w velocity:

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

Topography height must have w_0 velocity:

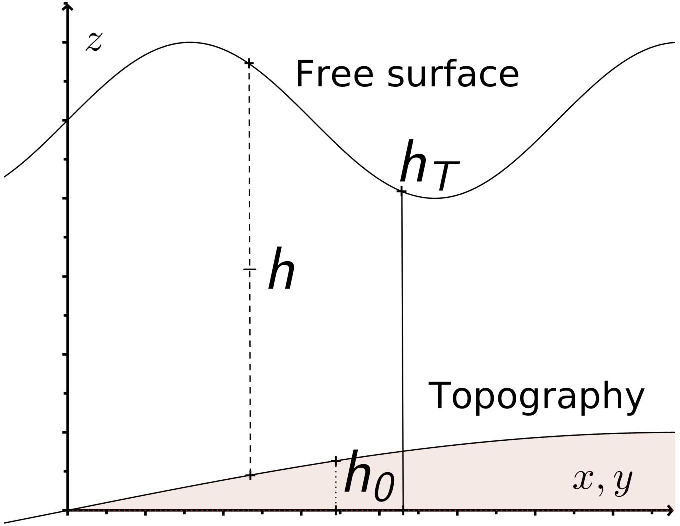
$$\frac{Dh_0}{Dt} = w(x, y, h_0, t) \Rightarrow w(x, y, h_0, t) = \vec{v} \cdot \nabla h_0$$

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

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

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

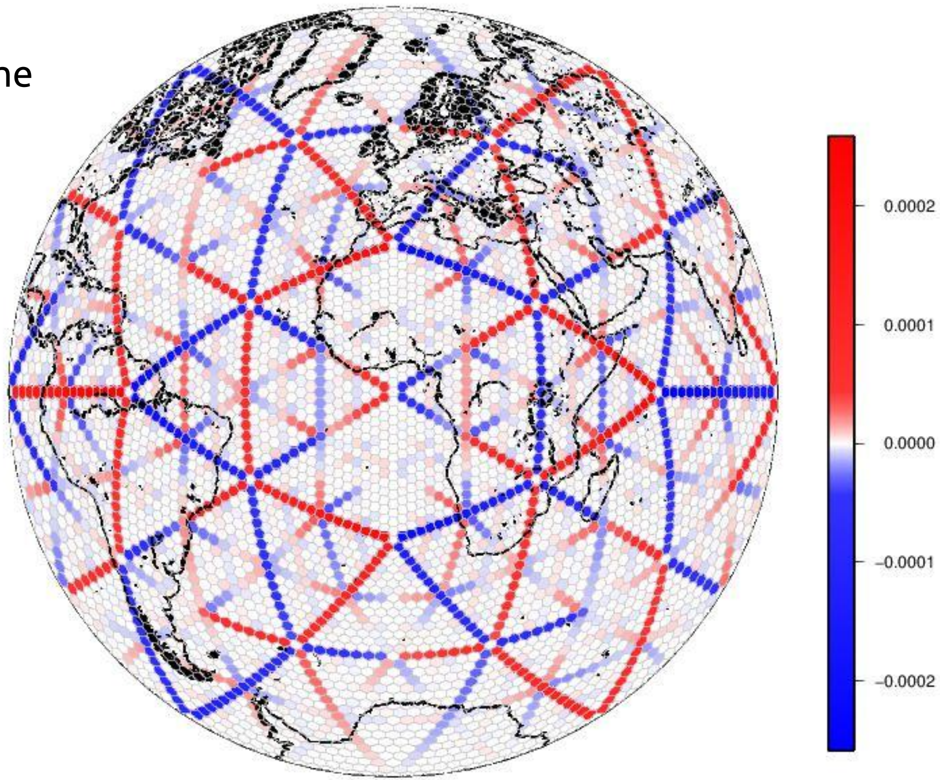
- Example of desired properties for horizontal shallow water equations:
  - Accurate and stable
  - Scalable (Local operators - no global operations)
  - Mass and energy conservation
  - Accurate representation slow/fast waves (staggering)
  - Curl-free pressure gradient $\nabla \times \nabla \psi = 0$
  - 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



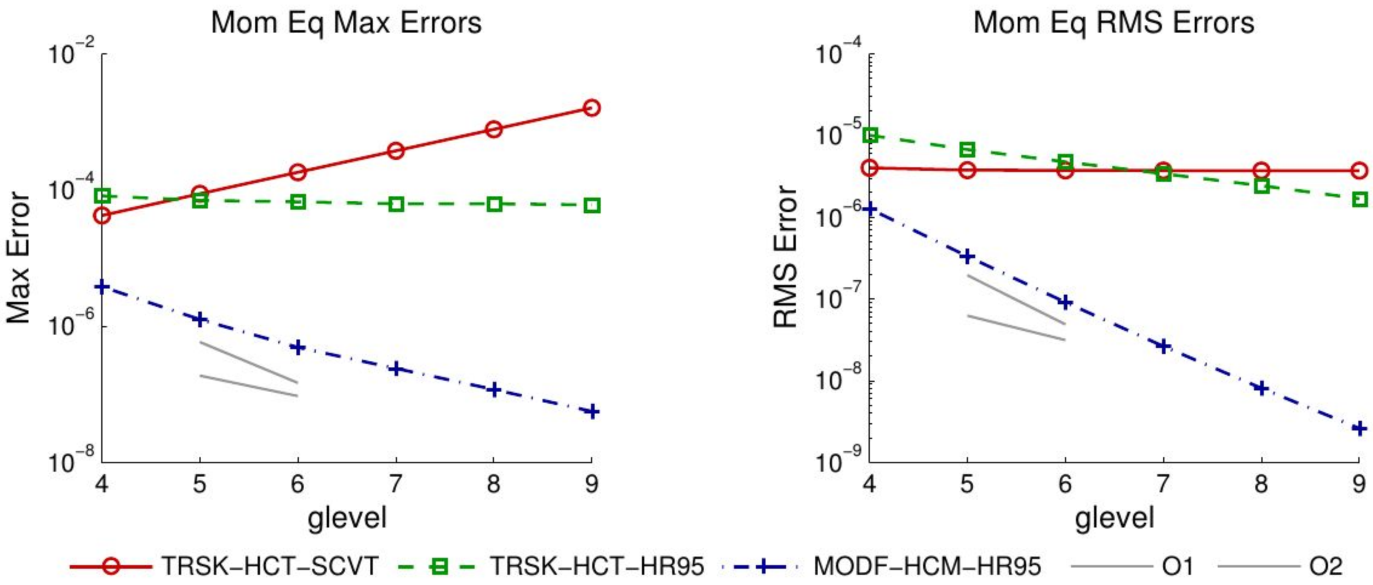
Classic Finite Volume Discretization error for 2D divergence of solid body rotation (should be zero everywhere!)

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

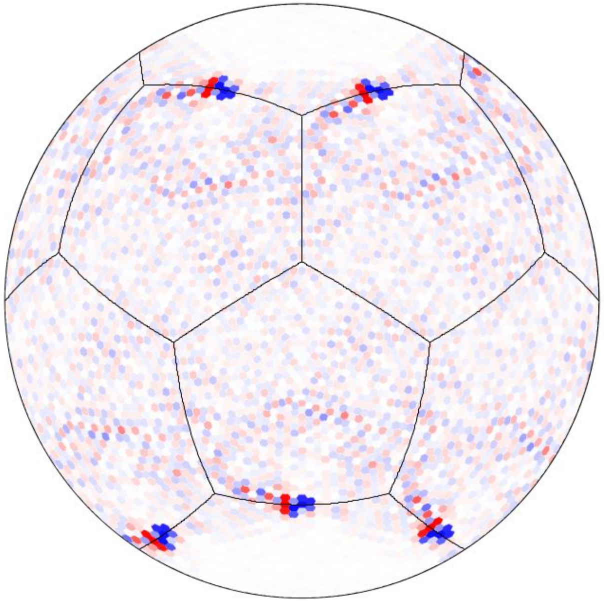
- Energy conserving schemes on polygonal grids use vector relation

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

Equivalently for 2D:

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

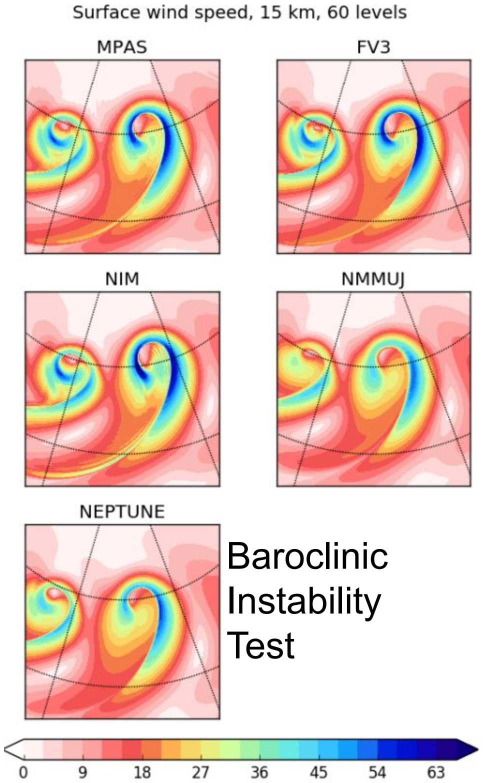
$$uv_x + vv_y = \left(\frac{u^2 + v^2}{2}\right)_y + (v_x - u_y)(u)$$



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

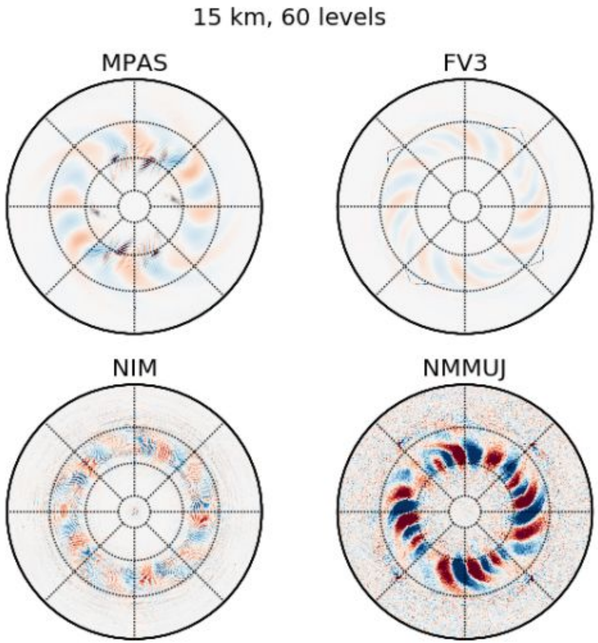
Peixoto, P.S., Thuburn, J. and Bell, M.J., 2018. Numerical instabilities of spherical shallow-water models considering small equivalent depths. *Quarterly Journal of the Royal Meteorological Society, 144(710), pp.156-171.*

High Impact Weather Prediction Project



Baroclinic Instability Test

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



Be careful with grid related noise...

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.cmalibrary.cn/ztwxk/zyyjjg/201803/P020180313393622242811.pdf

High Impact Weather Prediction Project

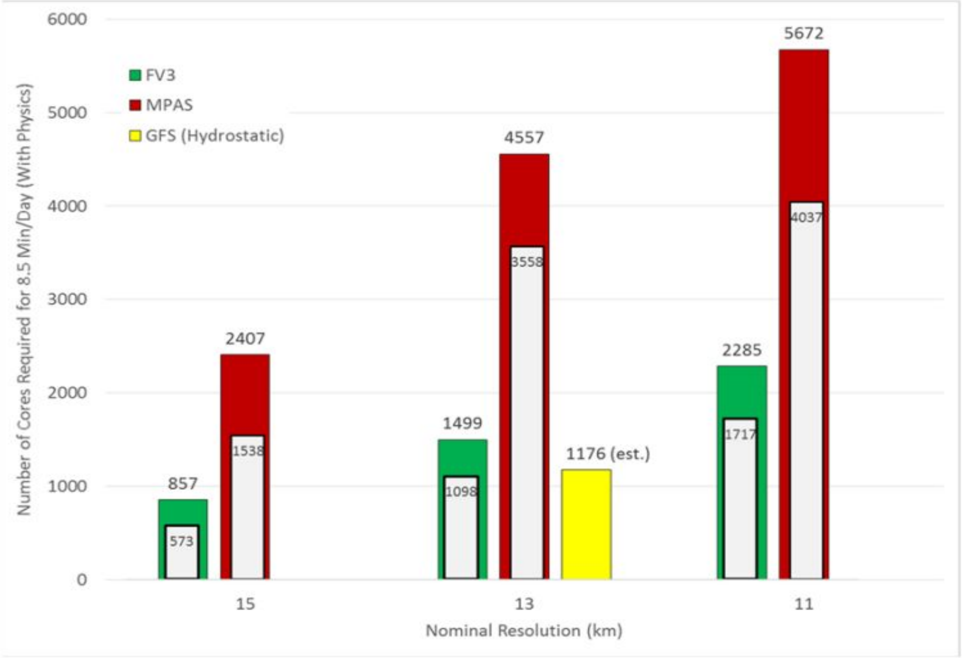


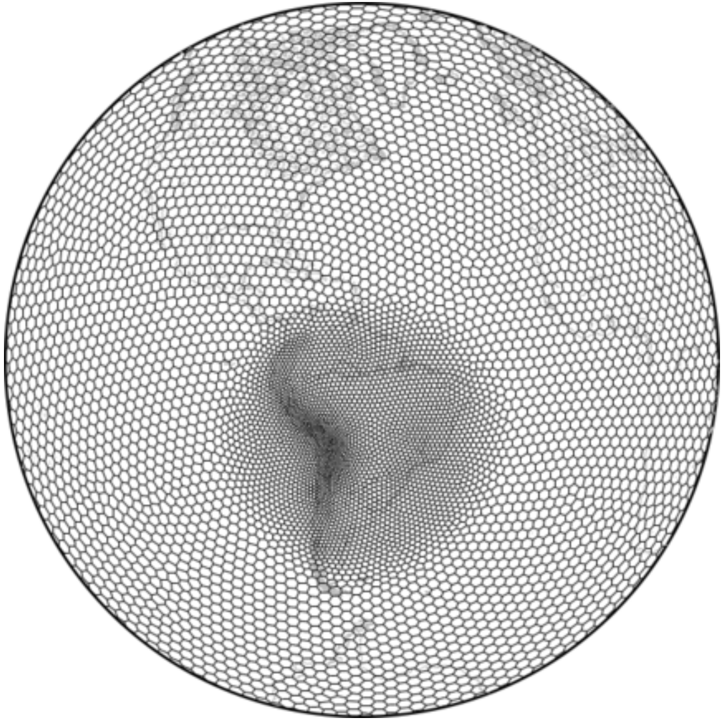
Figure 2: Cores required to meeting 8.5 minutes per day forecast speed requirement for operations at 15, 13, and 11 km horizontal resolution. All cases used 63 vertical levels. Colored bars show time with GFS physics; insets show the fraction of cores required by the dycore alone. The estimated number of cores required to run the 13 km operational GFS in 8.5 minutes on NCEP's WCOSS Cray XC40 is shown for comparison.

- FV3 was selected, as MPAS was at the time still working to improve its computational efficiency
- FV3 does not have the grid flexibility of MPAS

MPAS has gone through major computational improves since then...

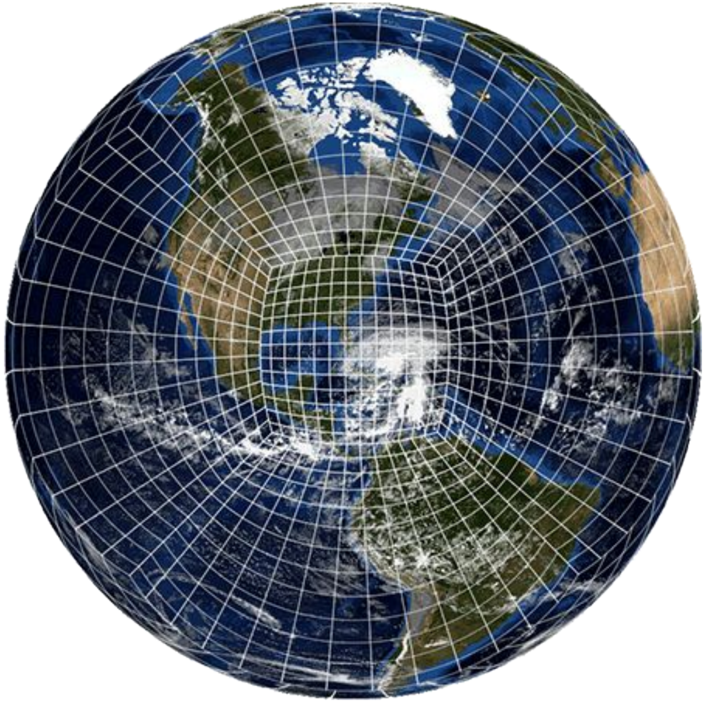
Michalakes , Whitaker. Talk at 17th ECMWF HPC for Meteorology
https://www.ecmwf.int/sites/default/files/elibrary/2016/16813-testing-performance-and-scaling-noaas-next-generation-global-modeling-system.pdf

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.