Numerical methods for global dynamical core development

Traditional and modern approaches

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CPTEC

Summary

1. Introduction
2. Finite differences
3. Spectral methods
4. Finite volume methods
5. Finite Elements
6. Conclusions

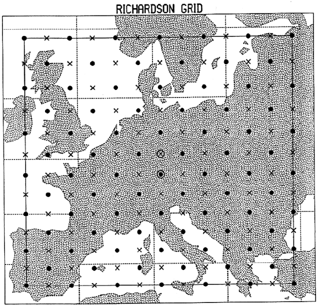
Summary

1 Introduction
- History
- Dynamics

Beginning

Lewis Fry Richardson (1922) *Weather Prediction by Numerical Process*

- Primitive equations
- Finite differences (staggered E-grid)
- 4 vertical levels
- Regional: Europe
- 2 years of (hand) calculation
- Problems with initial data

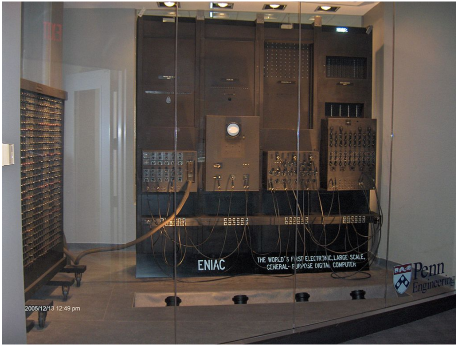


Lynch, P. (1999). Richardson's marvelous forecast. In The life cycles of extratropical cyclones (pp. 61-73). American Meteorological Society, Boston, MA.

Early days

1950-1960 - Beginning of regular computer aided forecasting

- Computers, ENIAC
- More/better surveillance data
- Primitive equations
- Finite differences



Summary

1 Introduction
- History
- Dynamics

Governing equations - Dynamics

Compressible Euler equations for atmosphere (ideal gas) in vector form:

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

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

Governing equations

- Compressible Euler
  - Hydrostatic vs Non-hydrostatic
  - Shallow atmosphere vs Deep atmosphere
- Primitive equations: hydrostatic and shallow atmosphere
  - Shallow water equations
  - Quasigeostrophic equations
  - Barotropic vorticity equations
  - Passive transport equation

Summary

2 Finite differences
- 1D Transport
- Global Models

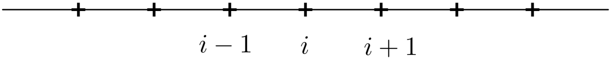
Basic Finite Difference

Example: Transport equation 1D :

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

Finite differences: Change partial derivatives with finite deviations

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



Main concerns: Accuracy and stability.

Summary

2 Finite differences
- 1D Transport
- Global Models

Global Latitude and Longitude Models

Latitude and Longitude Grids
with Finite Differences

- Traditional Eulerian
  - Stability usually requires $\Delta t \propto \Delta x$
  - Pole requires Δt very small
- Semi-Lagrangian semi-implicit
  - Allows large Δt
  - Solve a very large linear system at each time-step

EndGame - UK MetOffice

- Even Newer Dynamics for General Atmospheric Modelling of the Environment - Met. Office
- Global latitude - longitude grid
- Differences on C-Grid (with some Finite Volume)
- Semi-implicit Semi-Lagrangian
- Two-time level scheme - iterations for correction
- Non Hydrostatic / Deep Atmosphere
- Terrain Following (Height based) Vertical Coordinate
- Operational (17 km resolution from 07/2014 - time-step 450 s)

Problems...

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

Massively Distributed Memory Parallel Machines

- Pole communicates with many other computer nodes
- A lot of global communication required for the solution of the global linear system
- Limited scalability on large supercomputers (cannot do the forecast within the time window)

MetOffice Cray XC40 supercomputer with 460,000 compute cores (December 2016)

Summary

3 Spectral methods
- Main idea
- 1D Transport
- Global Models

Spectral methods

Emerged around 1960-1970.

- Derivatives are calculated in spectral space
- Fourier Transforms

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

- Derivatives ($\frac{\partial q}{\partial x}$):
  - Given a vector of values of $\boldsymbol{q} = [q_i]$
  - Calculate Fast Fourier Transform FFT to obtain $\hat{\boldsymbol{q}} = [\hat{q}_k]$
  - Calculate derivatives (in spectral space, simply multiply by $2\pi ik$)
  - Return to physical space with Inverse FFT
- 1970s: Viability for Atmosphere shown by Eliasen et al (1970) & Orszag (1970)

Summary

3 Spectral methods
- Main idea
- 1D Transport
- Global Models

1D transport

1D transport with constant speed (u) and periodic boundaries:

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

Substituting the Fourier Series $q(t,x) = \sum_k \hat{q}_k(t)e^{2\pi ikx}$ into the transport equation, results in

$$\sum_k \frac{\partial \hat{q}_k(t)}{\partial t} e^{2\pi ikx} + u\sum_k \hat{q}_k(t)\frac{\partial e^{2\pi ikx}}{\partial x} = 0$$

Using that $\frac{\partial e^{2\pi ikx}}{\partial x} = 2\pi ike^{2\pi ikx}$ we have

$$\sum_k \left(\frac{\partial \hat{q}_k(t)}{\partial t} + 2\pi iku\hat{q}_k(t)\right) e^{2\pi ikx} = 0$$

1D transport

1D transport with constant speed (u):

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

in spectral space is solved for every k (wavenumer) as

$$\frac{\partial \hat{q}_k(t)}{\partial t} + 2\pi i k u \hat{q}_k(t) = 0$$

No more spatial derivatives - it is an ODE!

Algorithm

1D transport with constant speed (u):

1. FFT $\boldsymbol{q}$ at initial time to obtain $\hat{q}_k(t_0)$
2. Solve $\frac{\partial \hat{q}_k(t)}{\partial t} + 2\pi i k u \hat{q}_k(t) = 0$ for every k with your favourite time-stepping scheme to obtain $\hat{\boldsymbol{q}}(t)$ for future times
3. IFFT $\hat{\boldsymbol{q}}(t)$ to obtain $\boldsymbol{q}(t)$

Very accurate space derivatives!

Nonlinear example

1D transport with variable speed ($v(x)$):

$$\frac{\partial q}{\partial t} + v(x)\frac{\partial q}{\partial x} = 0$$

How to calculate the transform of $v(x)\frac{\partial q}{\partial x}$ and make use of derivatives in spectral space? Transform each one separately and combine?

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

$$v(x) = \sum_l \hat{v}_l e^{2\pi ilx}$$

$$v(x)\frac{\partial q}{\partial x} = \sum_k \sum_l 2\pi ik \hat{v}_l \hat{q}_k(t) e^{2\pi ilx} e^{2\pi ikx}$$

Using this makes the method computationally intense ...

Nonlinear - pseudo-spectral

1D transport with variable speed ($v(x)$):

$$\frac{\partial q}{\partial t} + v(x)\frac{\partial q}{\partial x} = 0$$

For each time step:

1. Calculate de FFT of $\boldsymbol{q}(t)$ at current time to obtain $\hat{\boldsymbol{q}}(t)$
2. Calculate the derivative in spectral space for each mode: $\hat{q}_k^d(t) = 2\pi i k \hat{q}_k(t)$
3. Convert back to physical space and multiply v with $\boldsymbol{q}^d$ for each grid point.
4. Calculate the FFT of $v\boldsymbol{q}^d$ to obtain $[\widehat{(vq^d)_k}]$.
5. Solve for future times

$$\frac{\partial \hat{q}_k(t)}{\partial t} + (\widehat{vq^d})_k(t) = 0$$

6. Calculate IFFT of $\hat{\boldsymbol{q}}(t+\Delta t)$ to obtain $\boldsymbol{q}(t+\Delta t)$.

Summary

3 Spectral methods
- Main idea
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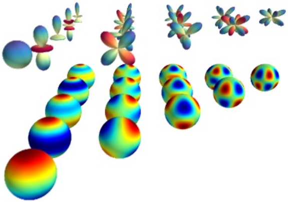
Spectral methods

What about doing this on the sphere?

- Spherical harmonics: Fourier expansion for each latitude circle, Legendre polinomials on meridians

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

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



Spectral methods

- Spherical harmonics with Fast Fourier Transform and “Fast” Legendre tramsforms
- Pseudo-spectral method
- Avoids the requirement of special treatment at the poles
- Semi-implicit is easier in spectral space
- With also Semi-Langrangian : allows large Δt!
- Very accurate!
- Used in most operational Weather Forecasting models and in many Climate models (BAM, IFS, GFS, ...).

IFS Model

- Integrated Forecasting System - ECMWF
- Global Spectral Model - Triangular Truncation
- Gaussian Reduced (Linear) Grid
- Semi-implicit Semi-Lagrangian
- Two-time level scheme
- Developed Fast Legendre Transforms

Introduction – A history

- **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…

Problems...

- Most of the computational time is spent solving the Spherical Harmonics transform (Legendre + Fourier).
- This part implies in a global communication, which reduces its scalability
- We might not be able to fit the necessary time windows for very high resolution models.

Summary

4. Finite volume methods
   - 1D Transport
   - Global Models

Basic Finite Volume

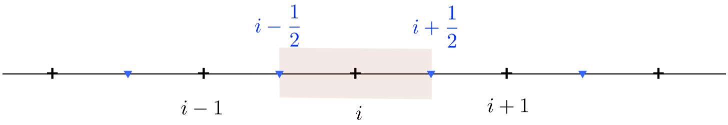
Example: Transport equation 1D :

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

Finite Volume: Integrate over cells!

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial q}{\partial t}\, dx = -\int_{x_{i-1/2}}^{x_{i+1/2}} u\frac{\partial q}{\partial x} dx$$

$$\frac{d}{dt}\int_{x_{i-1/2}}^{x_{i+1/2}} q(t,x)dx = -\underbrace{uq(t,x_{i+1/2})}_{\text{Right Flux}} + \underbrace{uq(t,x_{i-1/2})}_{\text{Left Flux}}$$



See LeVeque - FV for Hyperbolic Problems

Integrated quantities

Finite Volume (mean quantity):

$$Q_i = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} q(t,x)dx$$

$$\frac{dQ_i(t)}{dt} = \underbrace{-\frac{1}{\Delta x}\delta_x\left(uq(t,x_i)\right),}_{\text{Mean Fluxes}} \qquad \delta_x q(x) = q(x+\Delta x/2) - q(x-\Delta x/2),$$

Integrate over time

$$\int_{t_n}^{t_{n+1}} \frac{dQ_i(t)}{dt}dt = -\frac{1}{\Delta x}\int_{t_n}^{t_{n+1}} \delta_x\left(uq(t,x_i)\right)dt$$

$$Q_i(t_{n+1}) = Q_i(t_n) \underbrace{-\frac{1}{\Delta x}\delta_x \int_{t_n}^{t_{n+1}} uq(t,x_i)dt}_{F}$$

How to calculate F? This defines different FV schemes.

Transport equation 1D

$$Q_i^{n+1} = Q_i^n + F, \qquad F = -\frac{1}{\Delta x}\delta_x \int_{t_n}^{t_{n+1}} uq(t, x_i)dt$$

A first try at calculating F (explicit):

$$F \approx F^n = -\frac{\Delta t}{\Delta x}\delta_x \left(uq(t_n, x_i)\right) = \frac{\Delta t}{\Delta x}\left(uq(t_n, x_{i-1/2}) - uq(t_n, x_{i+1/2})\right)$$

But our prognostic variables are now Q_i, so $q(t_n, x_{i\pm 1/2})$ have to be calculated based on Q_i. Example:

$$Q_i^{n+1} = Q_i^n + \frac{\Delta t}{\Delta x}\left(u\frac{Q_{i-1}^n + Q_i^n}{2} - u\frac{Q_{i+1}^n + Q_i^n}{2}\right)$$

Looks like FD...but Q is an integrated quantity!
BTW: This FD scheme is unstable! Try it!

Transport equation 1D

General form for explicit scheme:

$$Q_i^{n+1} = Q_i^n + \frac{u\Delta t}{\Delta x}\left(G_{i-1/2} - G_{i+1/2}\right)$$

Where G is an interpolation operation

$$G_{i\pm 1/2} \approx q(t_n, x_{i\pm 1/2})$$

Important: This general form always gives mass conserving schemes, as left/right cell fluxes cancel out!!

Transport equation 1D

An useful scheme: Lax-Friedrichs

$$Q_i^{n+1} = Q_i^n + \frac{u\Delta t}{\Delta x}\left(G_{i-1/2} - G_{i+1/2}\right)$$

$$G_{i-1/2} = \frac{Q_{i-1}^n + Q_i^n}{2} - \frac{\Delta x}{2u\Delta t}(Q_i^n - Q_{i-1}^n)$$

$$G_{i+1/2} = \frac{Q_i^n + Q_{i+1}^n}{2} - \frac{\Delta x}{2u\Delta t}(Q_{i+1}^n - Q_i^n)$$

$$Q_i^{n+1} = \frac{Q_{i-1}^n + Q_{i+1}^n}{2} + \frac{u\Delta t}{\Delta x}\left(\frac{Q_{i-1}^n - Q_{i+1}^n}{2}\right)$$

Try it out!

Transport equation 1D

Another useful scheme (let $u > 0$): Upwind

$$Q_i^{n+1} = Q_i^n + \frac{u\Delta t}{\Delta x}\left(G_{i-1/2} - G_{i+1/2}\right)$$

Flux coming from the left:

$$G_{i-1/2} = Q_{i-1}^n$$

$$G_{i+1/2} = Q_i^n$$

$$Q_i^{n+1} = Q_i^n + \frac{u\Delta t}{\Delta x}\left(Q_{i-1}^n - Q_i^n\right)$$

Try it out!

Task 1

Problem:

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0, \quad x \in (0,1),\ t > 0,$$

with

$$u = 1, \quad q(0,x) = q_0(x) = \begin{cases} 1, & x \in [1/4, 2/4] \\ 0, & \text{otherwise} \end{cases}$$

and periodic boundary conditions ($q(t,0) = q(t,1)$).
Task:

- Look into and implement 3 schemes: the unstable, LF, upwind
- Test with different Δt, Δx.
- Plots with error vs dt and dx.
- Exact solution is $q(t,x) = q_0(x - t)$

Remember: Use Q_i, average quantities!!!

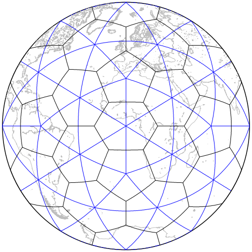
If you found this easy, try out the spectral scheme for the same problem and compare results.

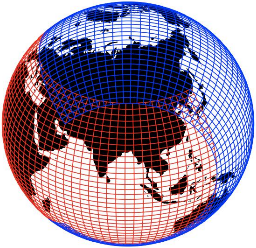
Summary

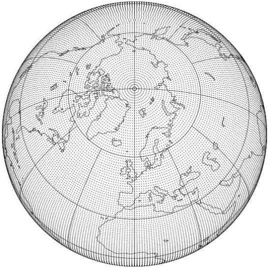
4. Finite volume methods
   - 1D Transport
   - Global Models

Quasi uniform grids

- Icosahedral (triangular / hexagonal)
- Cubed Sphere
- Yin-Yang Grids
- Reduced Gaussian grid





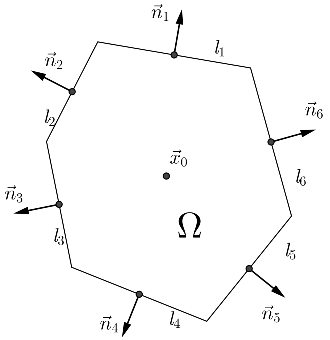


Continuity equation

Horizontal continuity equation (Shallow water model)

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

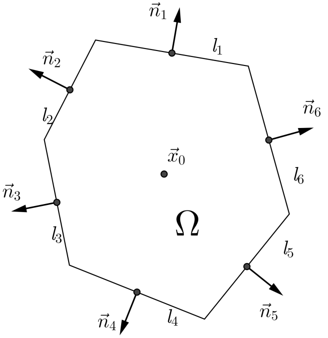
- h is the fluid depth
- $\vec{u} = (u, v)$ is the fluid horizontal velocity



Divergence theorem

$$\frac{1}{|\Omega|}\int_\Omega \frac{\partial h}{\partial t} d\Omega = -\frac{1}{|\Omega|}\int_\Omega \nabla \cdot (h\vec{u}) d\Omega$$

$$\underbrace{\frac{d}{dt}\left(\frac{1}{|\Omega|}\int_\Omega h\, d\Omega\right)}_{H_i \text{ Mean depth}} = \underbrace{-\frac{1}{|\Omega|}\int_{\partial\Omega} h\vec{u}\cdot\vec{n}\, d\partial\Omega}_{\text{Normal fluxes}}$$



Mid point rule integration:

$$\frac{d H_i}{dt} = -\frac{1}{|\Omega|}\sum_e h_e \vec{u}_e \cdot \vec{n}_e\, l_e$$

Interpolations required to obtain h_e and $\vec{u}_e$ depending on the staggering (A,C,...)

Problems...

- Can we get all the nice properties obtained in finite difference models, or the great accuracy of spectral schemes, and also scalability?

Desired:

1. Accurate
2. Stable
3. Conservative (mass, energy, PV, axial-angular momentum)
4. Mimetic Properties (spurious modes)

And also:

- Scalable on supercomputers
- Arbitrary spherical grids

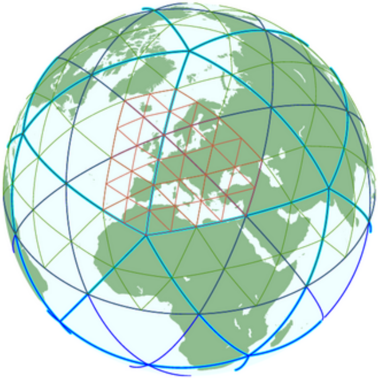
Is it possible?

Let's see some models with Finite Volume or Finite Differences on quasi uniform grids...

ICON

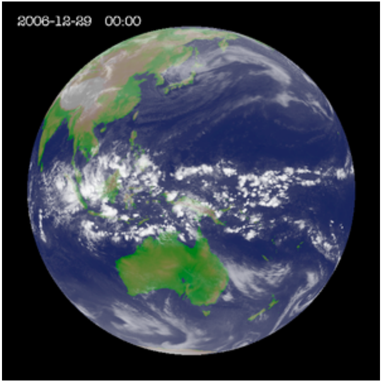
- Icosahedral non-hydrostatic
- MPI-M and DWD
- Triangular C grid
- Conservation of mass
- Highly scalable
- Hierarchically local refinement
- Spring dynamics optimization

- ICON-IAP (University of Rostock): Uses Hexagons



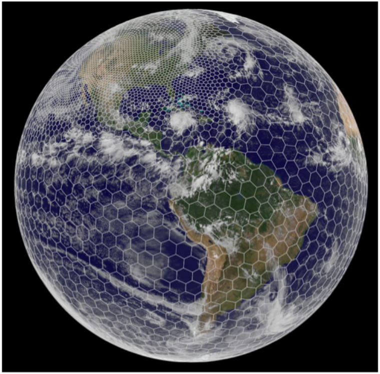
NICAM

- Nonhydrostatic ICosahedral Atmospheric Model
- RIKEN, JAMSTEC, University of Tokyo
- Hexagonal/pentagonal A grid
- Spring dynamics
- Highly scalable (3.5km, 15s)
- Operational
- JCP 2008 paper: Global cloud resolving simulations
- `https://earthsystemcog.org/projects/dcmip-2012/nicam`



MPAS

- Model for Prediction Across Scales
- NCAR and Los Alamos Nat Lab
- Spherical Centriodal Voronoi Tesselations (Smooth local refinement)
- Voronoi C grid (Hexagonal/Pentagonal)
- Fully mimetic
- Highly scalable
- Non-hydrostatic
- MWR 2012 paper: Multiscale Nonhydrostatic Atmospheric Model
- `http://mpas-dev.github.io/`

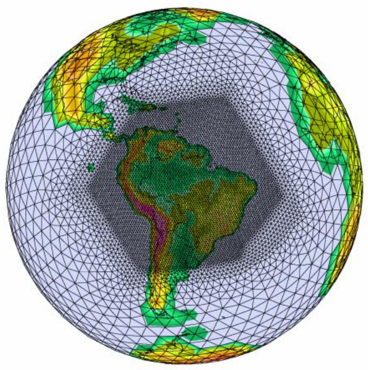


FV3

- Finite Volume Cube ([3])
- Geophysical Fluid Dynamics Laboratory-NOAA
- Shallow Atmosphere (plans for deep)
- 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

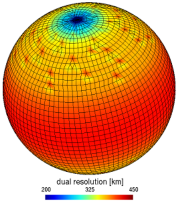
OLAM

- Ocean Land Atmosphere Model
- University of Miami / Colorado State University
- Non-hydrostatic / Deep Atmosphere
- Triangular / Hexagonal grids (possible refinements)
- Vertical Coordinate / Cut Cells
- Operational - US Environmental Protection Agency
- Split / Explicit time-stepping

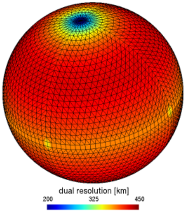


IFS-FV

ECMWF - IFS-FV : Finite Volume schemes from CFD models - Pantha-Rhei Project



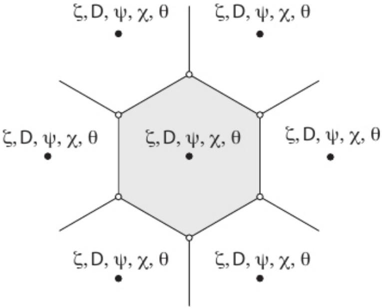
"classical" reduced Gaussian grid (N24)



reduced octahedral Gaussian grid (N24)

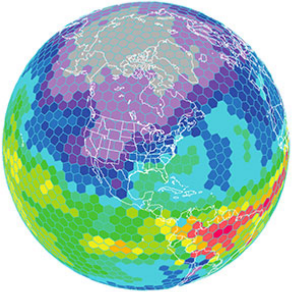
UZIM

- Unified Z-grid Icosahedral Model
- Colorado State University, Fort Collins
- Non-hydrostatic
- Heikes and Randall (1995) grid optimization
- Vorticity-Divergence Z-grid (Randall (1994))
- Less computational modes
- Multigrid solver



NIM

- Non-hydrostatic Icosahedral Model
- NOAA/ESRL
- GPU and MIC(Intel)
- Icosahedral - optimized - hexag/pentag
- Unstaggered finite-volume (A-grid)
- Local coodinate system - Flow following
- Time: RK4
- HEVI
- Vertical : Height based
- Shallow Atmosphere



Summary

5 Finite Elements
- FE basics
- Global Models

Finite elements

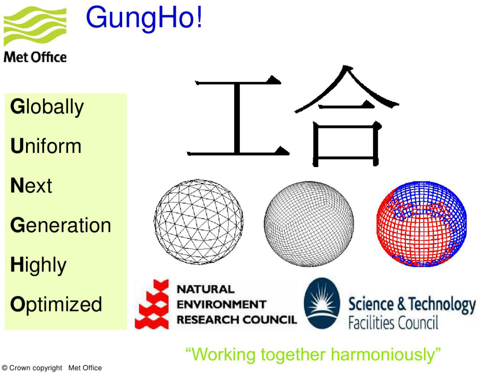
- Traditional Finite element
- Spectral Elements
- Discontinuous Galerkin
- Mixed finite elements

Details not discussed in this course...

Summary

5 Finite Elements
- FE basics
- Global Models

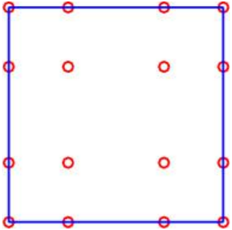
Gung Ho project- UK MetOffice



- Mixed Finite Elements - Fully mimetic - Cubed Sphere grid
- Finite Volumes advection
- Challenges: Quadrature - Mass Matrix inversion - Solver - ....

CAM-SE Model

- Community Atmosphere Model - Spectral Element - NCAR
- Operational - Hydrostatic - Shallow Atmosphere
- Continuous Galerkin Formulation - Cubic Polynomials
- Gauss-Lobato Quadrature
- Runge-Kutta time integration
- Hybrid Vertical coordinate (terrain following)
- Hyperviscosity
- Highly Scalable parallelism
- Hydrostatic



NUMA

- NRL (Navy)
- Element-based Galerkin methods (continuous or discontinuous high-order)
- Mesoscale (limited-area) or global model
- Grid: Any rectangular based (cubed sphere)
- Multiple methods (modular): IMEX, RK, ...
- Highly scalable

numa
Non-hydrostatic Unified Model of the Atmosphere

Summary

6 Conclusions
- Conclusions

That is all for today

"All models are wrong but some are useful"

— George Box

Thank you!

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