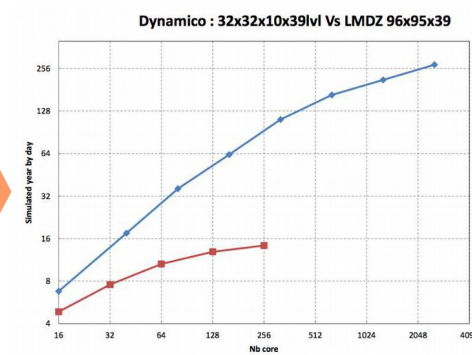
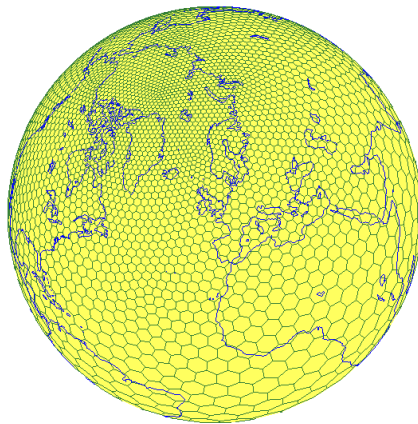


High-performance climate modelling : mimetic finite differences, and beyond ?

Thomas Dubos
École Polytechnique, LMD/IPSL

*with F. Hourdin, Marine Tort (LMD/IPSL), S. Dubey (IIT Delhi),
Yann Meurdesoif (LSCE/IPSL), Evaggelos Kritsikis (LAGA/Paris XIII), ...*

$$\delta \int \mathcal{L} dt = 0$$



Background on climate modelling

- Weather vs climate
- Characteristic scales
- Equations for atmospheric flow motion

DYNAMICO, an energy-conserving finite difference/finite volume atmospheric solver

- Conservation of energy : why ?
- Hamiltonian formulation
- Preliminary results

Finite elements, the path to higher-order accuracy ?

Background on climate modelling

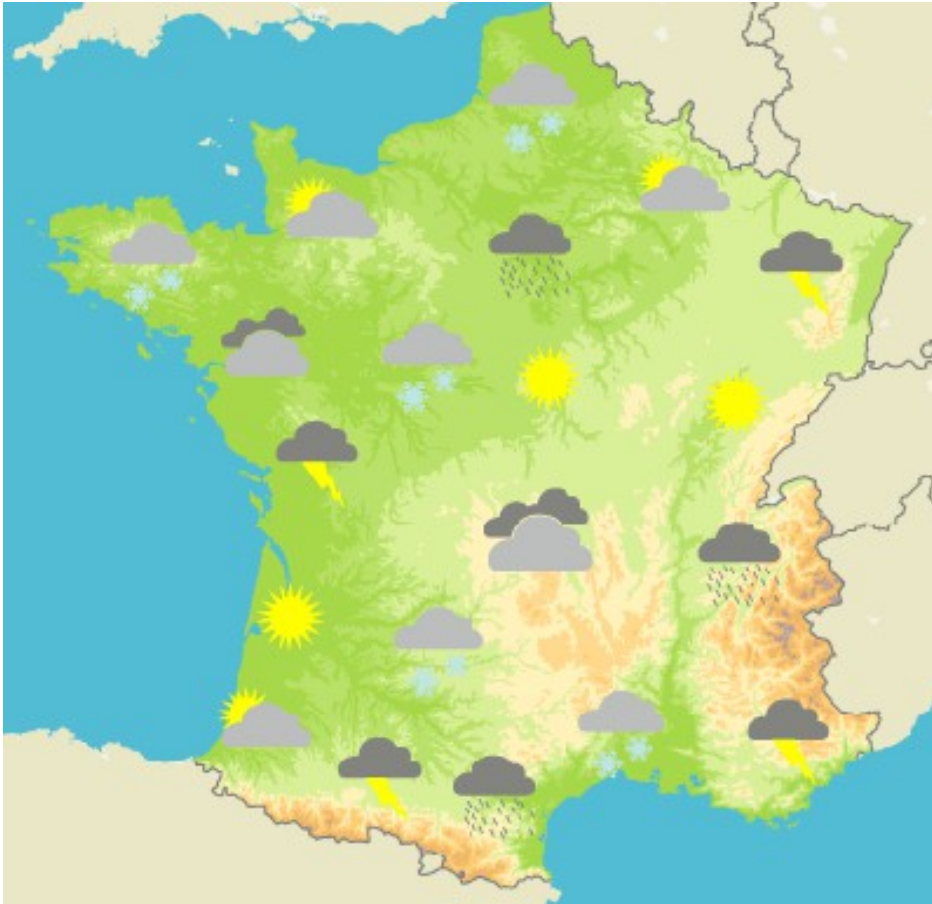
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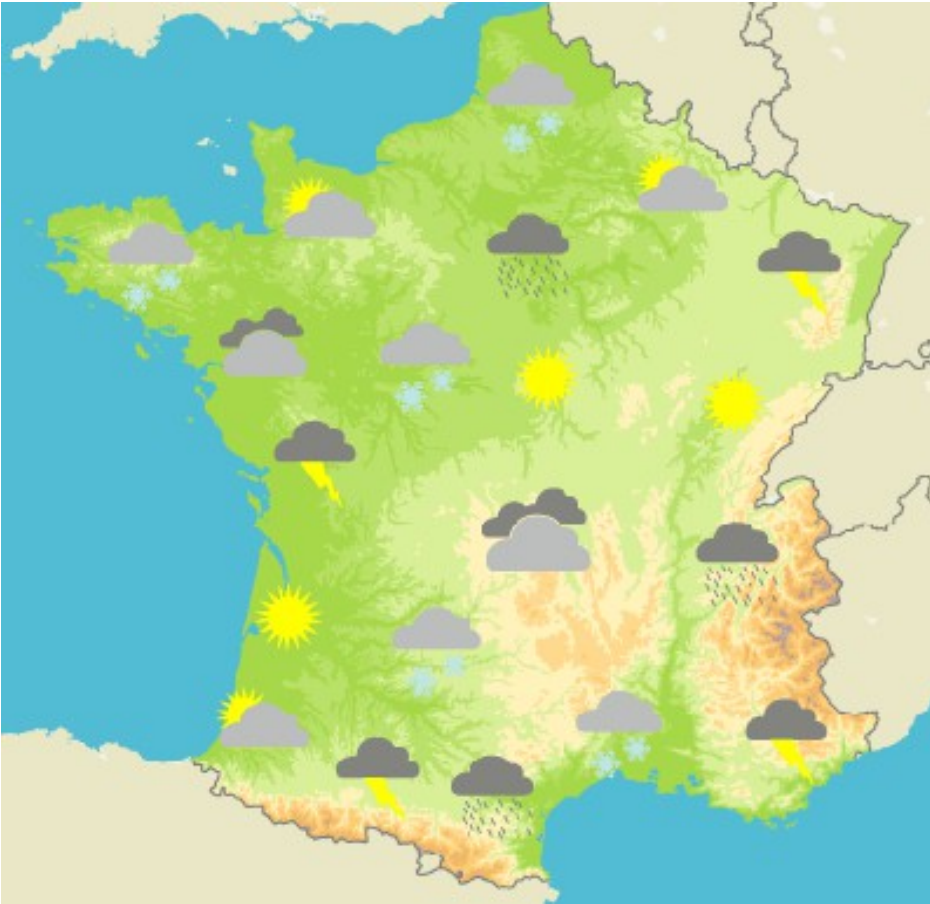
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Finite elements, the path to higher-order accuracy ?

Weather forecasting

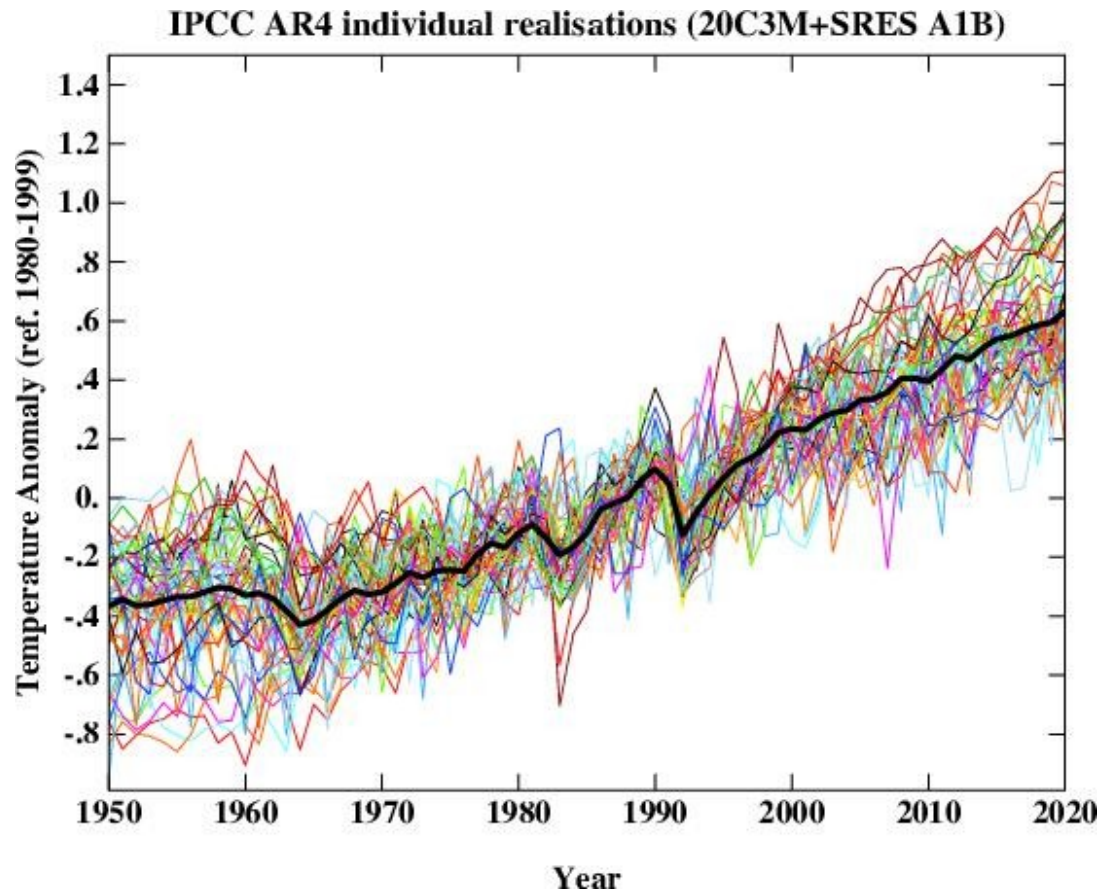


Weather forecasting



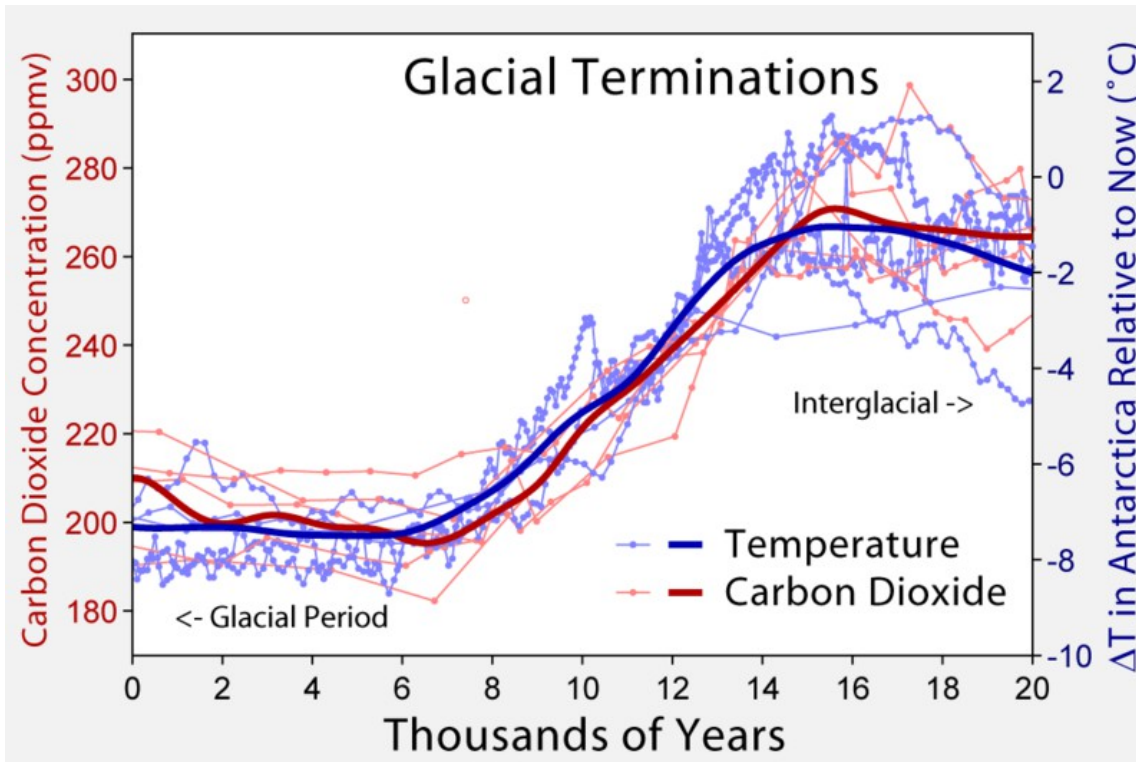
$\frac{4 \text{ simulated days}}{1 \text{ h of walltime}} = \mathbf{x 100}$

Modern climate

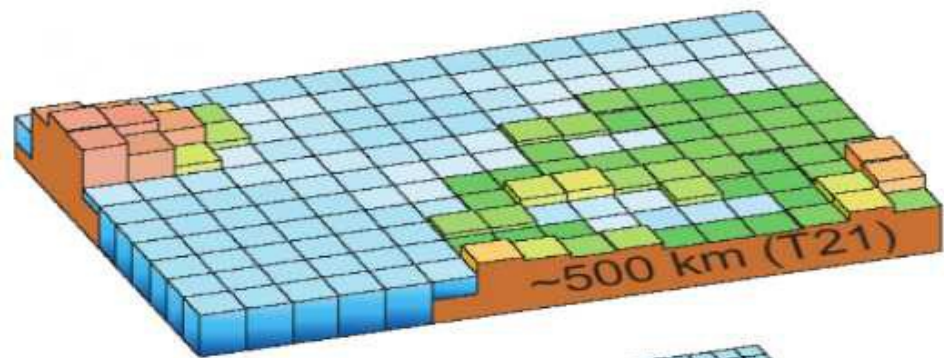


$\frac{100 \text{ simulated years}}{1 \text{ month of walltime}} = \mathbf{x 1000}$

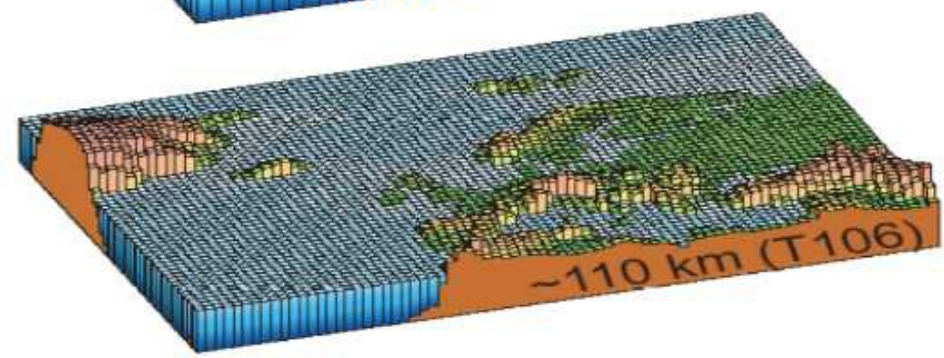
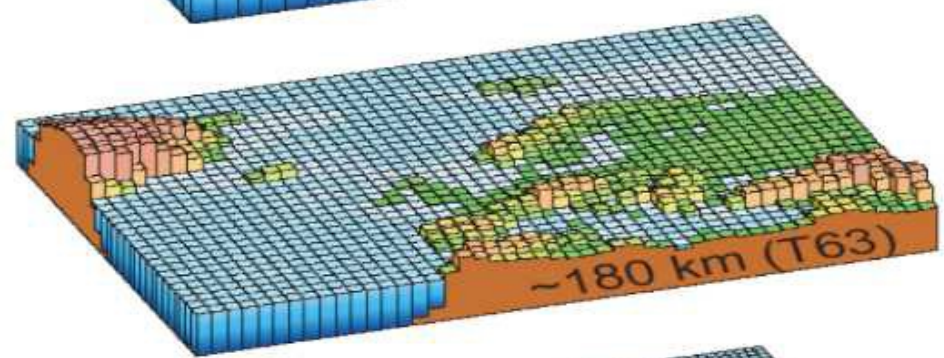
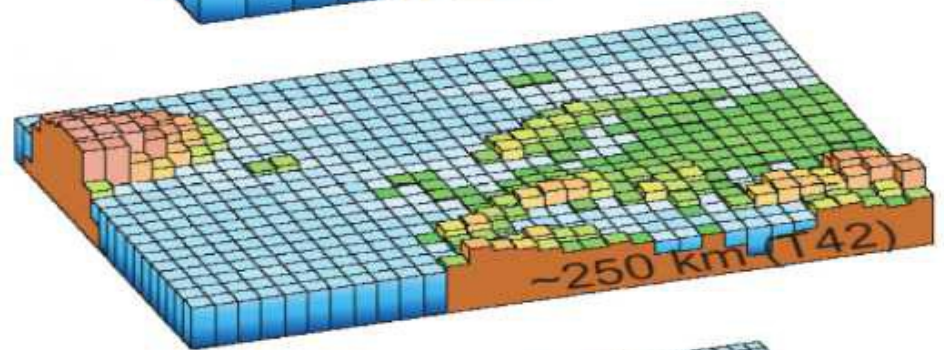
Paleoclimate



$\frac{10000 \text{ simulated years}}{1 \text{ year of walltime}} = \times 10000$



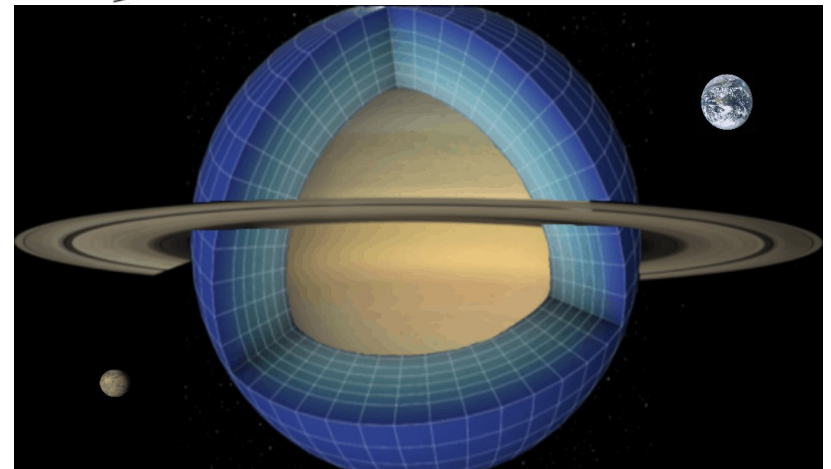
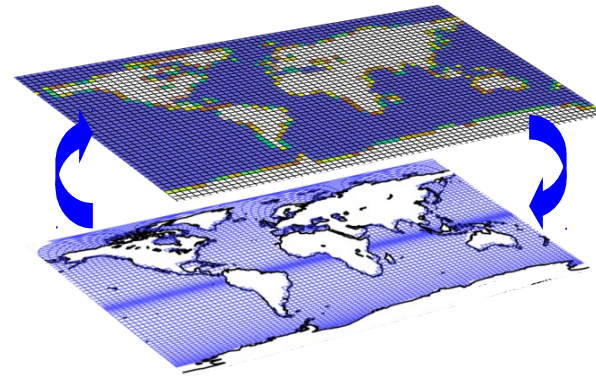
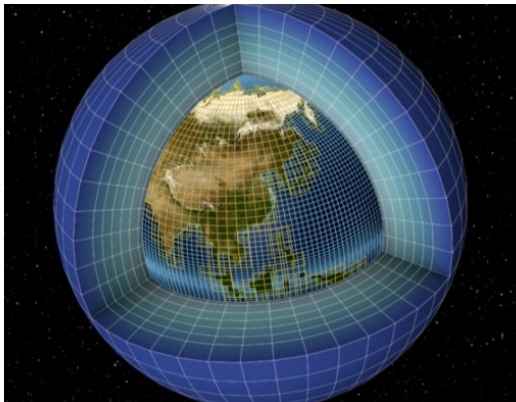
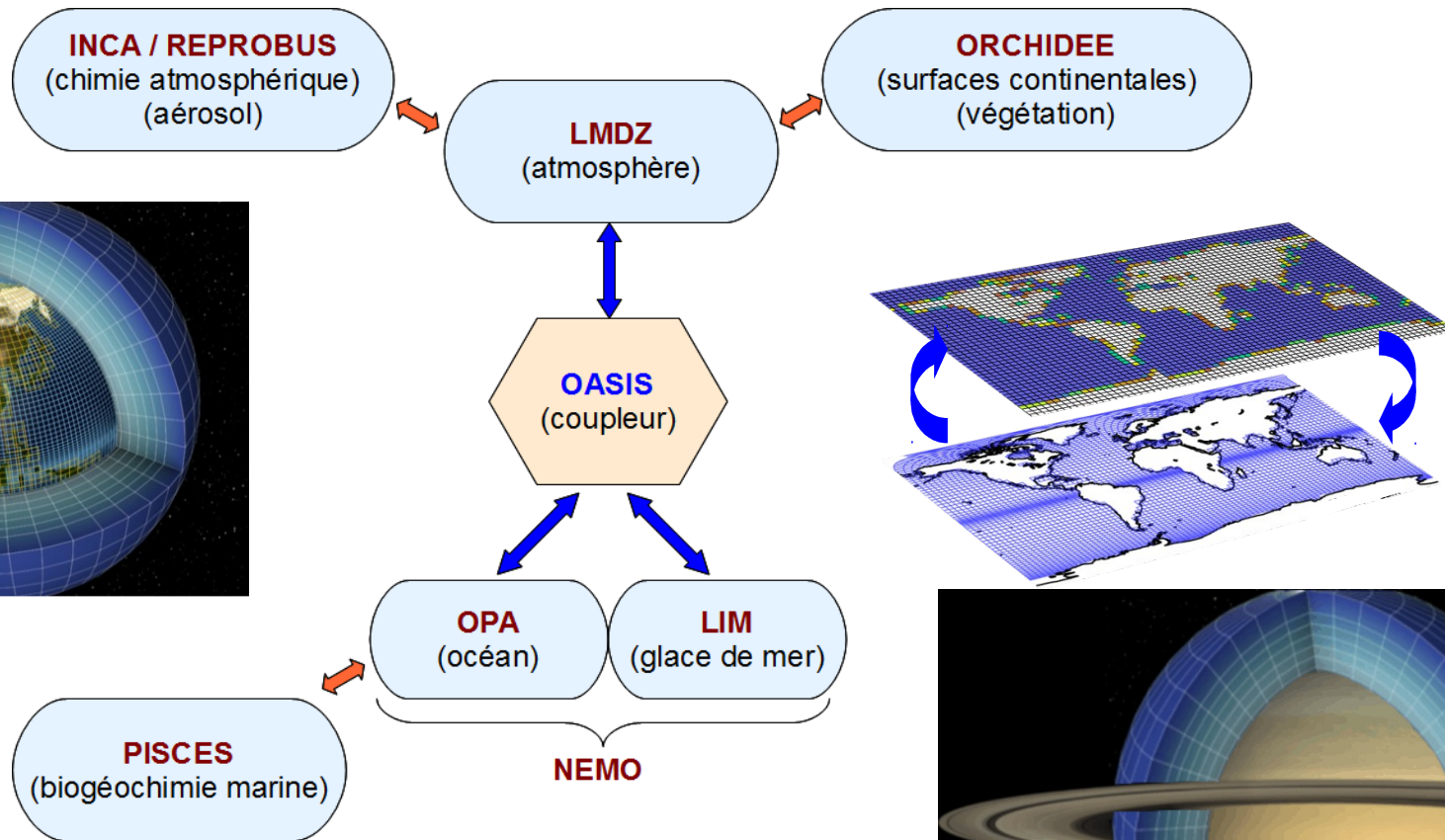
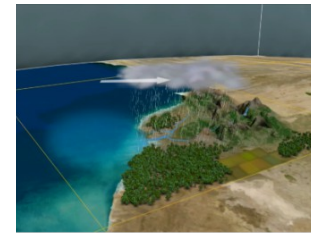
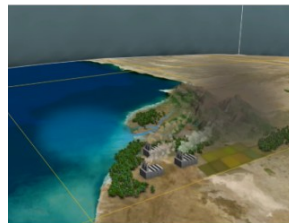
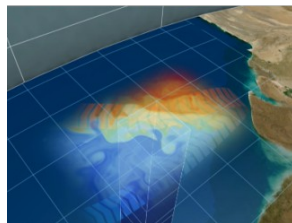
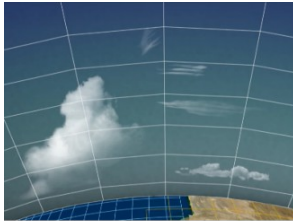
1980s



2010s



Earth System Modelling at IPSL

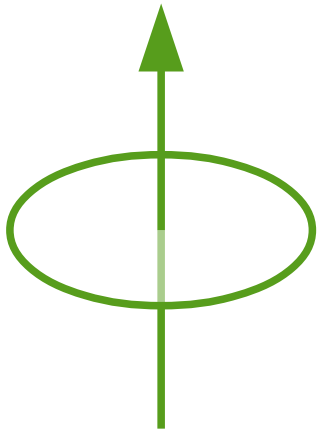


+ planetary atmospheres
(F. Forget, ...)

- Newton's fundamental principle of dynamics
- Forces : pressure and gravity
- Pseudo-forces : Coriolis and centrifugal

Planetary velocity

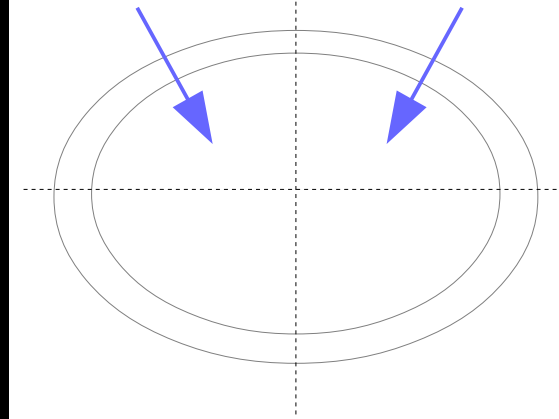
$$\mathbf{R} = \boldsymbol{\Omega} \times \mathbf{x}$$



Geopotential

$$\Phi = V - \frac{1}{2} \mathbf{R} \cdot \mathbf{R}$$

$$\mathbf{g} = -\nabla \Phi$$



$$\frac{D\dot{\mathbf{x}}}{Dt} + \text{curl } \mathbf{R} \times \dot{\mathbf{x}} + \frac{1}{\rho} \nabla p + \nabla \Phi = 0$$

$$\frac{\partial \rho}{\partial t} + \text{div } \rho \dot{\mathbf{x}} = 0 \quad \frac{Ds}{Dt} = \frac{q}{T}$$

Characteristic scales

- *Velocity* : Sound $c \sim 340\text{m/s}$ Wind $U \sim 30\text{m/s}$
- *Time* : Buoyancy oscillations $N \sim g/c \sim 10^{-2} \text{ s}^{-1}$ Coriolis $f \sim 10^{-4} \text{ s}^{-1}$
- *Length* : **Scale height $H=c^2/g=10\text{km}$** **Rossby radius : $R=c/f \sim 1000 \text{ km}$**
Planetary radius $a=6400\text{km}$

Flatness

$$af^2/g \ll 1$$

Shallowness

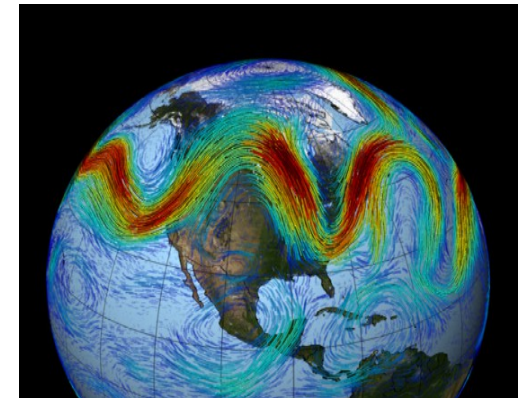
$$H/a \ll 1$$

Mach number

$$M=U/c \ll 1$$

Scale separation

$$f/N \sim H/R \ll 1$$



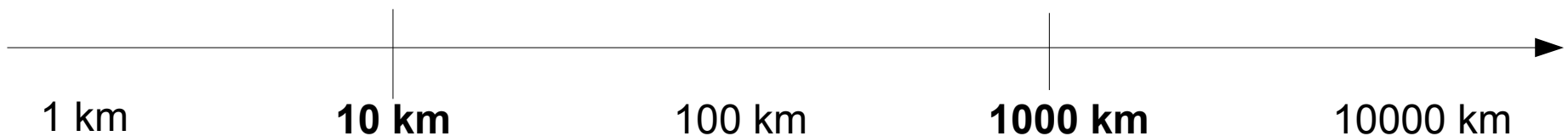
small-scale

scale height

mesoscale

synoptic

planetary



Hydrostatic approximation

Vertical momentum budget

$$\frac{dw}{dt} = -g - \frac{1}{\rho} \frac{\partial p}{\partial z}$$

If vertical acceleration is small ... $\frac{dw}{dt} \ll g, \frac{1}{\rho} \frac{\partial p}{\partial z}$

... then

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

Hydrostatic balance

When does this approximation work ?

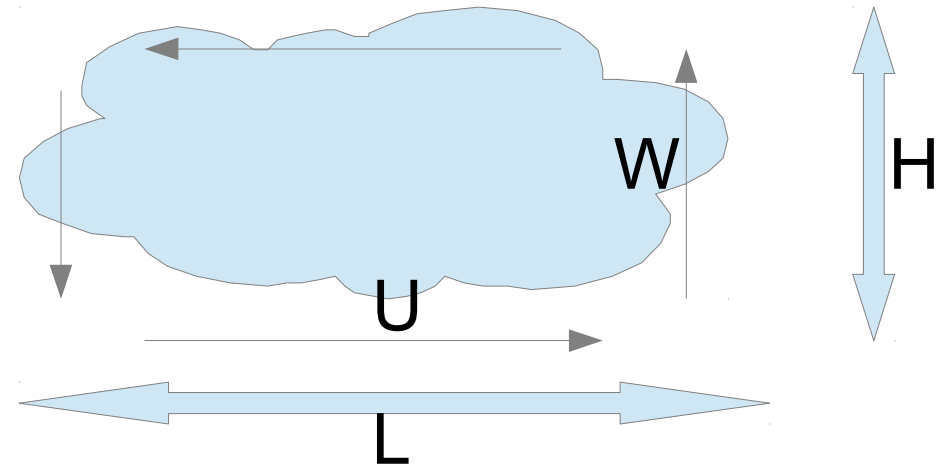
$$\frac{d}{dt} \sim \frac{W}{H} \sim \frac{U}{L}$$

$$\frac{\partial p}{\partial x} \sim \rho \frac{du}{dt} \sim \rho \frac{U}{L} U$$

$$\frac{\partial p}{\partial z} \sim \frac{L}{H} \frac{\partial p}{\partial x} \sim \frac{\rho U^2}{H}$$

$$\frac{dw}{dt} \sim \frac{W^2}{H}$$

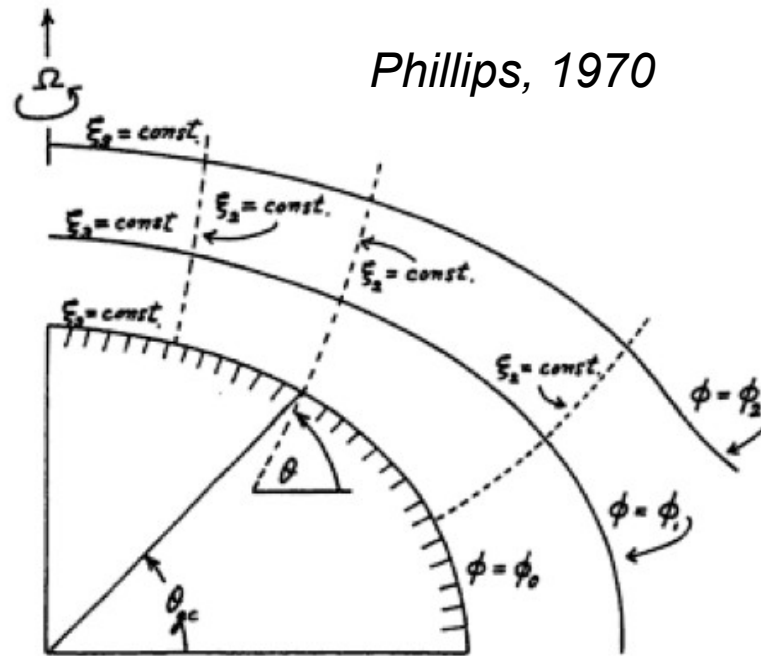
$$\frac{dw}{dt} / \rho \frac{\partial p}{\partial z} \sim \left(\frac{W}{U} \right)^2 \sim \left(\frac{H}{L} \right)^2$$



Works for circulations with a large horizontal scale ($L \gg H \sim 10\text{km}$)

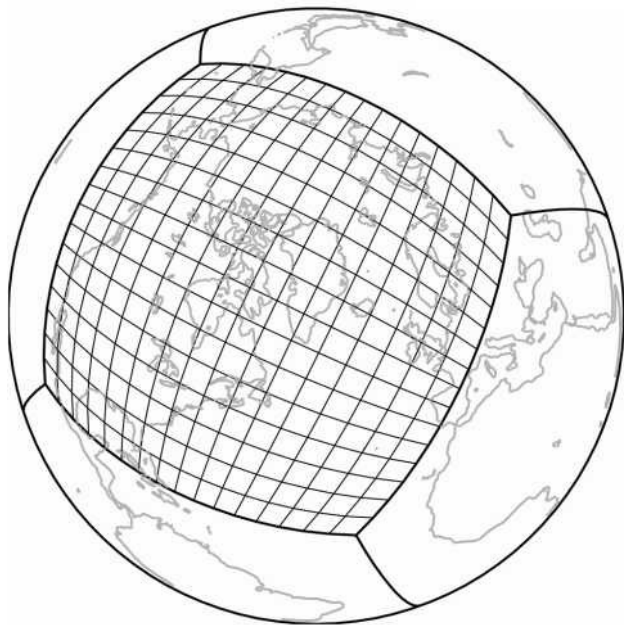
Incorrect for convection (storms), mountain flow, ...

Geopotential (curvilinear) coordinates

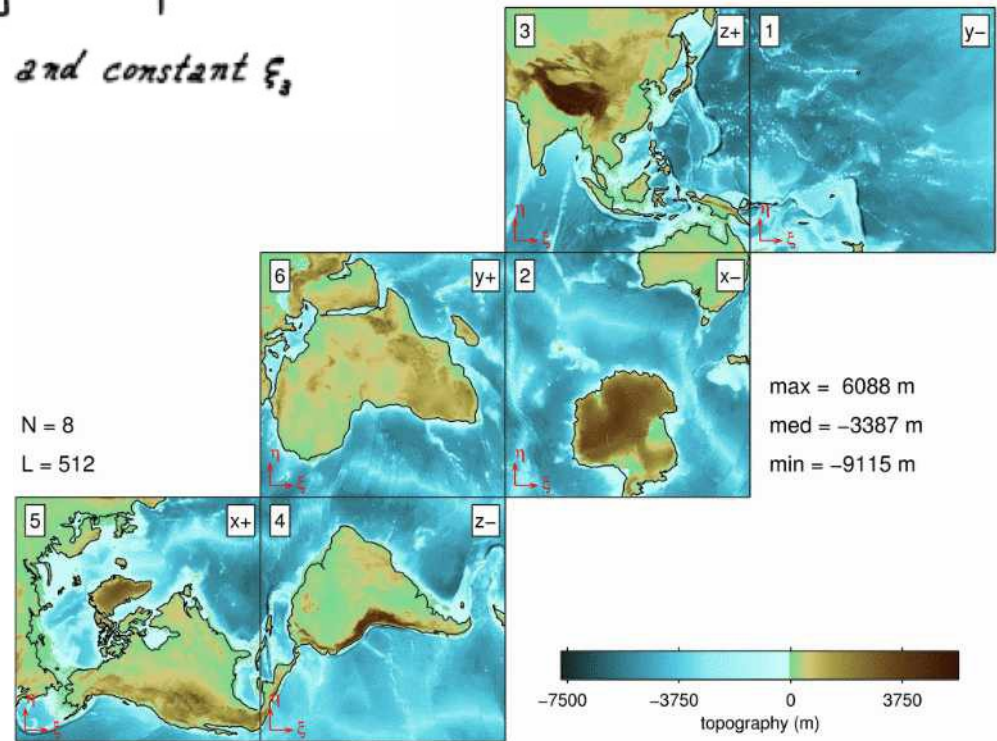


Phillips, 1970

Surfaces of constant ξ_2 and constant ξ_3



N = 8
L = 512



Transport in curvilinear coordinates

$$(x, y, z) \rightarrow (\xi^1, \xi^2, \Phi)$$

Transport in curvilinear coordinates

$$(x, y, z) \rightarrow (\xi^1, \xi^2, \Phi)$$

$$\dot{x} \longrightarrow u^i = \frac{D\xi^i}{Dt}$$

contravariant velocity components

Transport in curvilinear coordinates

$$(x, y, z) \rightarrow (\xi^1, \xi^2, \Phi)$$

$$\dot{\mathbf{x}} \longrightarrow u^i = \frac{D\xi^i}{Dt}$$

contravariant velocity components

$$\begin{aligned} J(\xi^i) d\xi^1 d\xi^2 d\xi^3 &= dx dy dz \\ dm = \mu d\xi^1 d\xi^2 d\xi^3 &= \rho dx dy dz \\ \mu &= \rho J \end{aligned}$$

pseudo-density

Transport in curvilinear coordinates

$$(x, y, z) \rightarrow (\xi^1, \xi^2, \Phi)$$

$$\dot{x} \longrightarrow u^i = \frac{D\xi^i}{Dt}$$

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pseudo-density

$$\begin{aligned} \frac{\partial s}{\partial t} + \dot{\lambda} \partial_\lambda s + \dot{\phi} \partial_\phi s + \dot{r} \partial_r s &= \frac{q}{T} \\ \rho r^2 \cos \phi &= \mu \\ \frac{\partial \mu}{\partial t} + \partial_\lambda (\mu \dot{\lambda}) + \partial_\phi (\mu \dot{\phi}) + \partial_r (\mu \dot{r}) &= 0 \end{aligned}$$

- *Contravariant formulation independent from the coordinate system*
- *No information about the geometry needed*
- *Easily in conservative form (flux-form)*

Dynamics in curvilinear coordinates

$$\frac{D\dot{\mathbf{x}}}{Dt} + \text{curl } \mathbf{R} \times \dot{\mathbf{x}} + \frac{1}{\rho} \nabla p + \nabla \Phi = 0$$

Dynamics in curvilinear coordinates

$$\frac{D\dot{\mathbf{x}}}{Dt} + \text{curl } \mathbf{R} \times \dot{\mathbf{x}} + \frac{1}{\rho} \nabla p + \nabla \Phi = 0$$



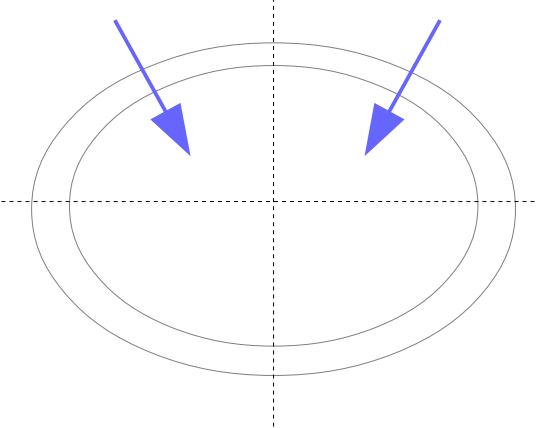
$$G_{ij} \frac{Du^j}{Dt} + \frac{1}{2} (\partial_j G_{ik} + \partial_k G_{ij} - \partial_i G_{jk}) u^j u^k + [\partial_j R_i - \partial_i R_j] u^j + \frac{J}{\mu} \partial_i p + \partial_i \Phi = 0$$

Spherical geoid approximation

- Ellipticity of geoids \sim centrifugal / gravitational $\sim 1/300$
- Spherical geoid approximation : pretend that the metric in geopotential coordinates is actually spherical !



Geopotential

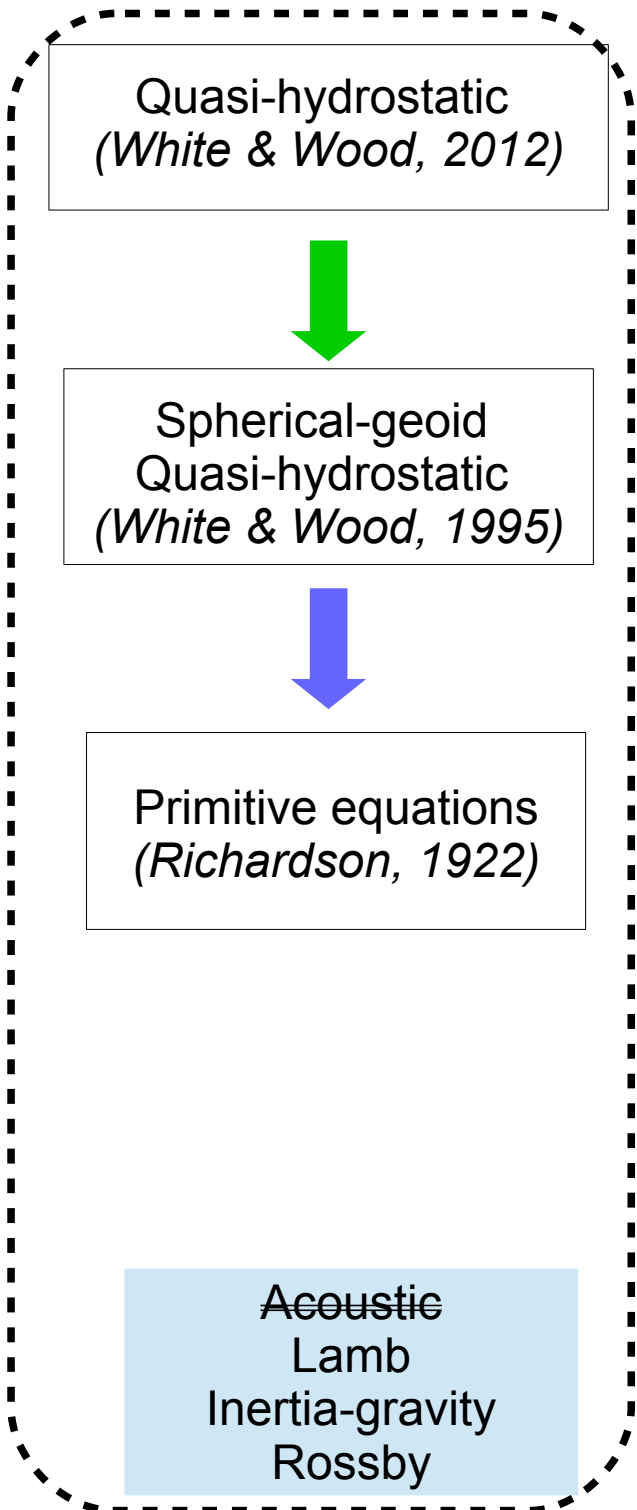
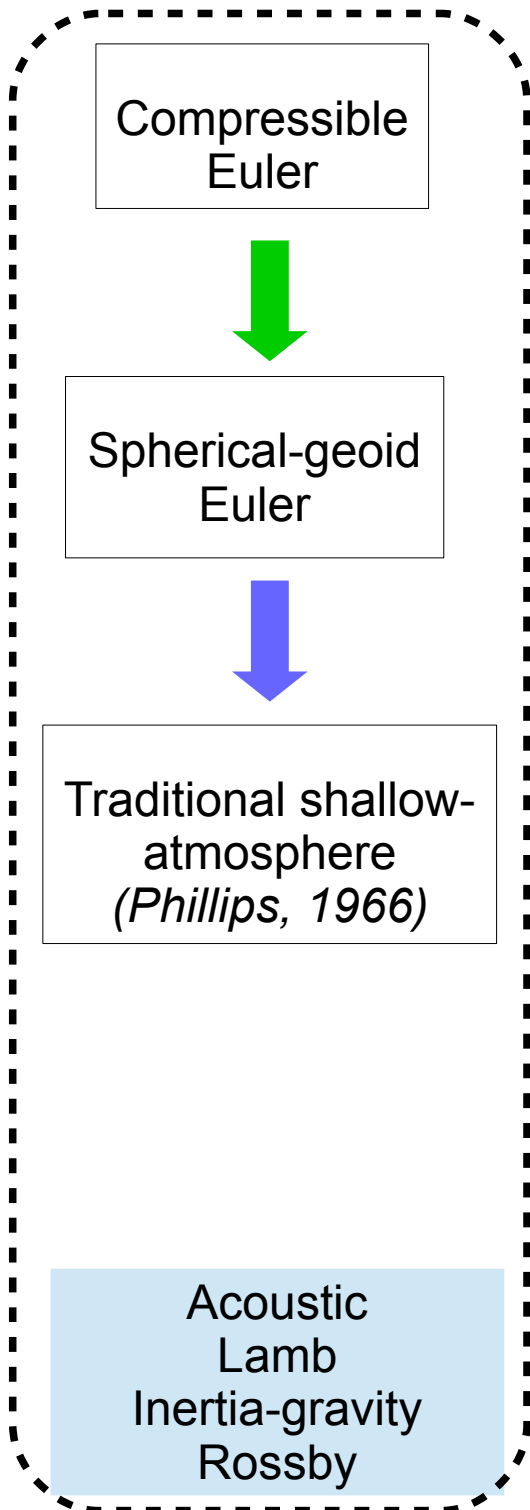
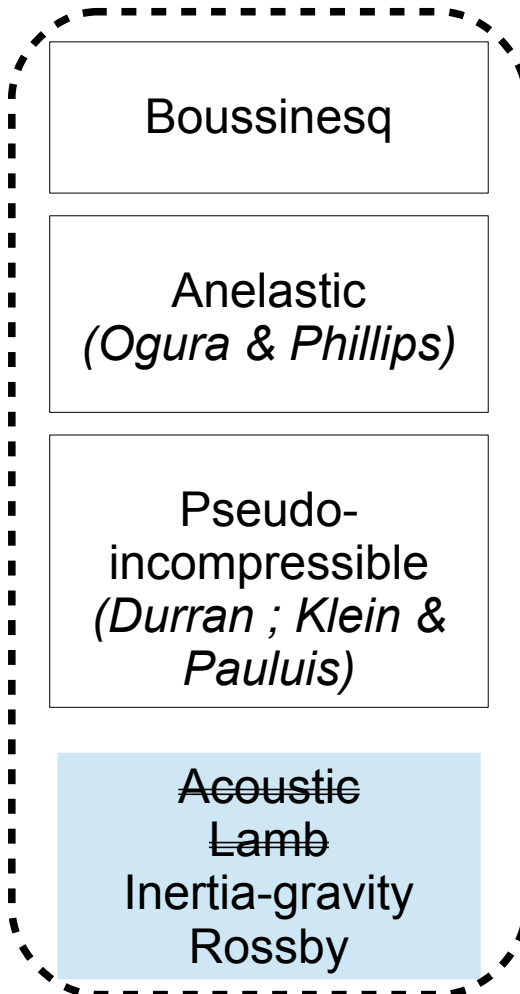
$$\Phi = V - \frac{1}{2} \mathbf{R} \cdot \mathbf{R}$$
$$\mathbf{g} = -\nabla \Phi$$


Spherical geoid

Shallow-atmosphere +
traditional

(Quasi-)Hydrostatic

Boussinesq / Anelastic /
Pseudo-incompressible



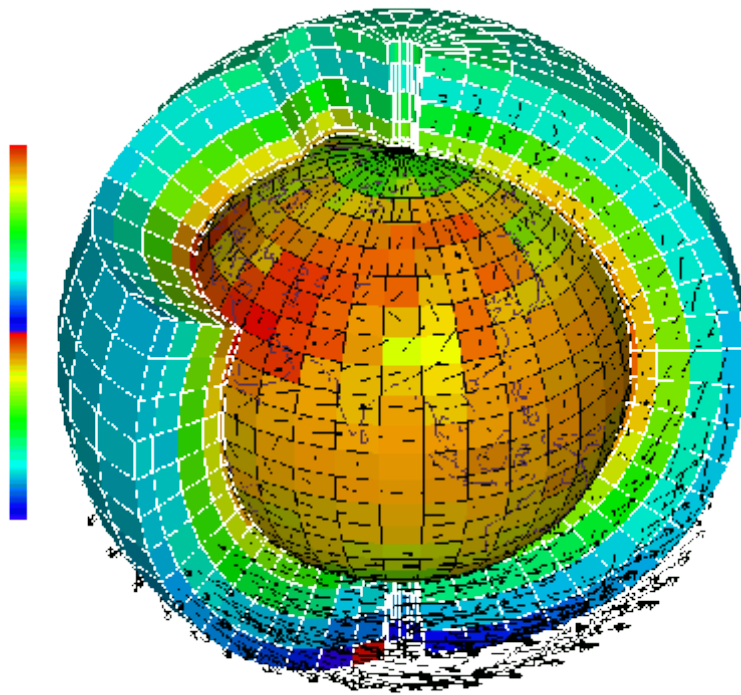
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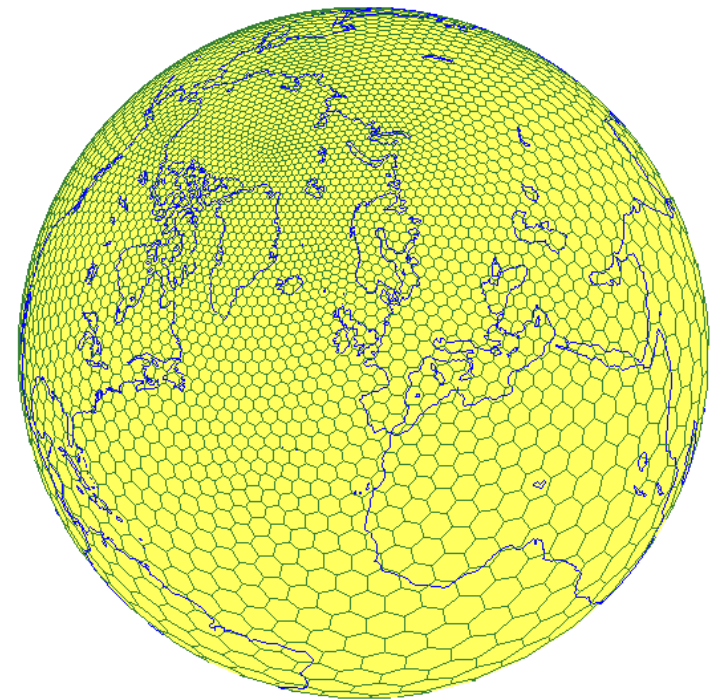
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LMD-Z lon-lat core



Enstrophy-conserving finite differences on lon-lat mesh (Sadourny, 1975)

Positive definite finite-volume transport (Hourdin & Armengaud, 1999)



Scalability

Consistency

discrete conservation laws

Versatility

not tied to a unique equation set

Why would a numerical model want to conserve energy ?

$$\mathcal{H} = \int \rho \left(\underbrace{\frac{u^2}{2} + \frac{v^2}{2} + \frac{w^2}{2}}_{\text{kinetic}} + e \left(\underbrace{\frac{1}{\rho}}_{\text{specific volume}}, \underbrace{s}_{\text{specific entropy}} \right) + \underbrace{gz}_{\text{potential}} \right) dx dy dz$$

Energy minimum given total mass and entropy ?

$$\mathcal{M} = \int \rho dx dy dz \quad \mathcal{S} = \int \rho s dx dy dz$$

$$\delta (\mathcal{H} - G_0 \mathcal{M} - T_0 \mathcal{S}) = 0$$



$$u = v = w = 0 \quad \text{Resting}$$

$$T = T_0 \quad \text{Isothermal}$$

$$e + \frac{p}{\rho} - Ts + gz = G_0 \quad \text{Hydrostatic}$$

(discrete) conservation limits
dynamically accessible states
=> stability

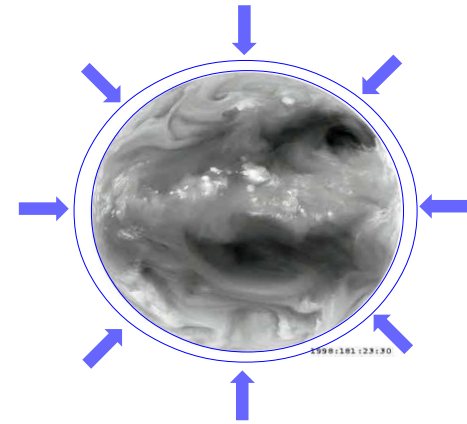
numerics conserve energy, mass ,
entropy

=> isothermal state of rest is stable

Adiabatic equations of motion imply **conservation laws** because they derive from a least **action principle**

inertia Coriolis pressure gravity

$$\frac{D\dot{\mathbf{x}}}{Dt} + 2\boldsymbol{\Omega} \times \dot{\mathbf{x}} + \frac{1}{\rho} \nabla p + \nabla \Phi = 0$$



$$\delta \int \mathcal{L} dt = 0$$



$$\frac{D}{Dt} \frac{\partial L}{\partial \dot{\mathbf{x}}} = \frac{1}{\rho} \nabla \left(\rho^2 \frac{\partial L}{\partial \rho} \right) + \frac{\partial L}{\partial \mathbf{x}}$$

$$\mathcal{L} = \mathcal{K} + \mathcal{C} - \mathcal{P} = \int L(\mathbf{x}, \dot{\mathbf{x}}, \rho, s) dm$$

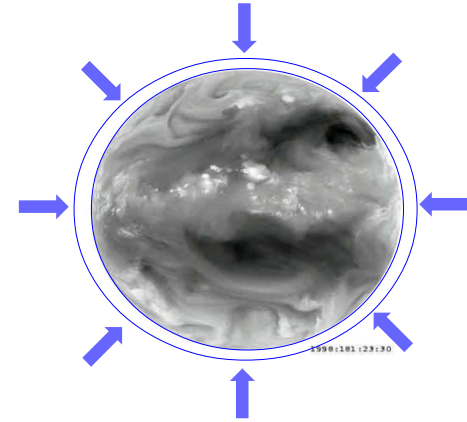
$$\mathcal{K} = \frac{1}{2} \int \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} dm \quad \text{Kinetic energy}$$

$$\mathcal{C} = \int (\boldsymbol{\Omega} \times \mathbf{x}) \cdot \dot{\mathbf{x}} dm \quad \text{Planetary velocity}$$

$$\mathcal{P} = \int \left(e \left(\frac{1}{\rho}, s \right) + \Phi(\mathbf{x}) \right) dm \quad \begin{array}{l} \text{Internal energy} \\ \text{Potential energy} \end{array}$$

Adiabatic equations of motion imply **conservation laws** because they derive from a least **action principle**

$$G_{ij} \frac{Du^j}{Dt} + \frac{1}{2} (\partial_j G_{ik} + \partial_k G_{ij} - \partial_i G_{jk}) u^j u^k + [\partial_j R_i - \partial_i R_j] u^j + \frac{J}{\mu} \partial_i p + \partial_i \Phi = 0$$



$$\delta \int \mathcal{L} dt = 0$$



$$\frac{D}{Dt} \frac{\partial L}{\partial u^i} = \frac{1}{\hat{\rho}} \partial_i \left(\hat{\rho}^2 \frac{\partial L}{\partial \hat{\rho}} \right) + \frac{\partial L}{\partial \xi^i}$$

$$\mathcal{L} = \int L(\xi^i, u^i, \hat{\rho}) dm$$

$$\mathcal{K} = \frac{1}{2} \int G_{ij} u^i u^j dm$$

Kinetic energy

$$\mathcal{C} = \int R_j u^j dm$$

Planetary velocity

$$\mathcal{P} = \int \left(e \left(\frac{J}{\hat{\rho}}, s \right) + \Phi(\xi^3) \right) dm$$

Internal energy
Potential energy

Hamiltonian formulation

- Suppose evolution equations are known for all prognostic variables. Then how an arbitrary functional of those prognostic variables evolves is entirely known :

$$\frac{d}{dt}\mathcal{F} = \int \left(\frac{\delta\mathcal{F}}{\delta v_i} \partial_t v_i + \frac{\delta\mathcal{F}}{\delta\mu} \partial_t \mu + \frac{\delta\mathcal{F}}{\delta S} \partial_t S \right) dx^1 dx^2 dx^3$$

- *Conversely, such an evolution equation contains all the equations of motion*
- A Hamiltonian formulation is such an evolution equation of the special form :

$$\frac{d}{dt}\mathcal{F} = \{\mathcal{F}, \mathcal{H}\}$$

where \mathcal{H} is total energy and the Poisson bracket is bilinear, antisymmetric and satisfies the Jacobi identity

- nice, but what is the Hamiltonian formulation for fluid flow ?

Hamiltonian formulation

$$\frac{d}{dt}\mathcal{F} = \{\mathcal{F}, \mathcal{H}\}$$

means that all tendencies can be written as expressions that are *linear in the functional derivatives of total energy*

To identify the Hamiltonian formulation let us first find those functional derivatives :

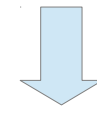
$$\mathcal{H}[v_i, \mu, S] = \int \left(\frac{1}{2} g^{ij} (v_i - R_i)(v_j - R_j) + \Phi + e \left(\frac{J}{\mu}, \frac{S}{\mu} \right) \right) \mu dx^1 dx^2 dx^3$$

$$v_i = g_{ij} u^j + R_i, k = \frac{1}{2} g_{ij} u^i u^j$$

$$\frac{d}{dt}\mathcal{H} = \int \left(\underbrace{\mu u^i \partial_t v_i}_{\frac{\delta \mathcal{H}}{\delta v_i}} + \underbrace{(k + \Phi + G)}_{\frac{\delta \mathcal{H}}{\delta \mu}} \partial_t \mu + \underbrace{T \partial_t S}_{\frac{\delta \mathcal{H}}{\delta S}} \right) dx^1 dx^2 dx^3$$

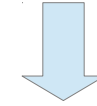
...then transform the equations of motion until they are linear in the functional derivatives

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \mathbf{f} \times \mathbf{u} + \nabla \Phi + \frac{1}{\rho} \nabla p = 0$$



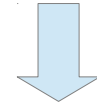
$$(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \times \mathbf{u} \times \mathbf{u} + \nabla \frac{\mathbf{u} \cdot \mathbf{u}}{2}$$

$$\partial_t \mathbf{u} + (\mathbf{f} + \nabla \times \mathbf{u}) \times \mathbf{u} + \nabla \left(\frac{\mathbf{u} \cdot \mathbf{u}}{2} + \Phi \right) + \frac{1}{\rho} \nabla p = 0$$

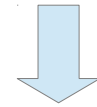


$$dG = v dp - s dT$$

$$\partial_t \mathbf{v} + (\nabla \times \mathbf{v}) \times \mathbf{u} + \nabla \left(\frac{\mathbf{u} \cdot \mathbf{u}}{2} + \Phi + G \right) + s \nabla T = 0$$



$$\partial_t v_i + \frac{\partial_j v_i - \partial_i v_j}{\mu} \mu u^j + \partial_i (k + \Phi + G) + s \partial_i T = 0$$



$$\partial_t v_i + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}}{\delta v_i} + \partial_i \frac{\delta \mathcal{H}}{\delta \mu} + s \partial_i \frac{\delta \mathcal{H}}{\delta S} = 0$$

$$\partial_t \mu + \partial_i \frac{\delta \mathcal{H}}{\delta v_i} = 0$$

$$\partial_t S + \partial_i \left(s \frac{\delta \mathcal{H}}{\delta v_i} \right) = 0$$

Hamiltonian formulation in non-Eulerian vertical coordinates

(Dubos & Tort, MWR 2014)

$$\partial_t \mu + \partial_\eta (\mu \dot{\eta}) + \partial_i \frac{\delta \mathcal{H}}{\delta v_i} = 0,$$

$$\partial_t \Theta + \partial_\eta (\Theta \dot{\eta}) + \partial_i \left(\theta \frac{\delta \mathcal{H}}{\delta v_i} \right) = 0,$$

$$\partial_t v_i + \dot{\eta} \partial_\eta v_i + v_3 \partial_i \dot{\eta} + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}}{\delta v_j} + \partial_i \frac{\delta \mathcal{H}}{\delta \mu} + \theta \partial_i \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) = 0,$$

$$\partial_t V_3 + \partial_\eta (V_3 \dot{\eta}) + \frac{\delta \mathcal{H}}{\delta \Phi} = 0,$$

$$\partial_t \Phi + \dot{\eta} \partial_\eta \Phi - \frac{\delta \mathcal{H}}{\delta V_3} = 0.$$

Integration by parts

+ invariance of Hamiltonian (total energy) w.r.t. vertical coordinate

=> conservation of energy

Hamiltonian formulation in non-Eulerian vertical coordinates

(Dubos & Tort, MWR 2014)

$$\partial_t \mu + \partial_\eta (\mu \dot{\eta}) + \partial_i \frac{\delta \mathcal{H}}{\delta v_i} = 0,$$

$$\partial_t \Theta + \partial_\eta (\Theta \dot{\eta}) + \partial_i \left(\theta \frac{\delta \mathcal{H}}{\delta v_i} \right) = 0,$$

$$\partial_t v_i + \dot{\eta} \partial_\eta v_i + v_3 \dot{\eta} + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}}{\delta v_j} + \partial_i \frac{\delta \mathcal{H}}{\delta \mu} + \theta \partial_i \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) = 0,$$

Hydrostatic $v_3 \equiv \frac{\partial L}{\partial u^3} = 0$

$$\partial_t V_3 + \partial_\eta (V_3 \dot{\eta}) + \frac{\delta \mathcal{H}}{\delta \Phi} = 0,$$

$$\partial_t \Phi + \dot{\eta} \partial_\eta \Phi - \frac{\delta \mathcal{H}}{\delta V_3} = 0.$$

Integration by parts

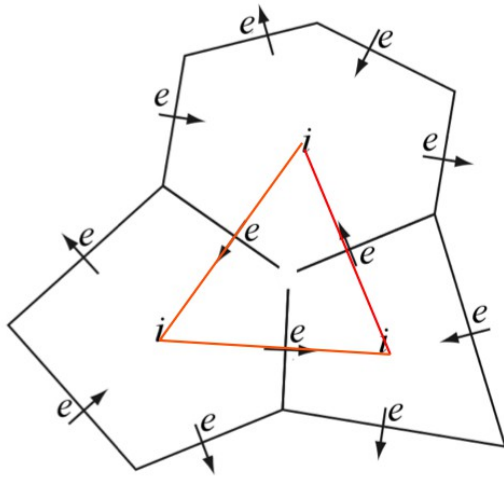
+ invariance of Hamiltonian (total energy) w.r.t. vertical coordinate

=> conservation of energy

Computational space $S^2 \times [0,1]$

n

η

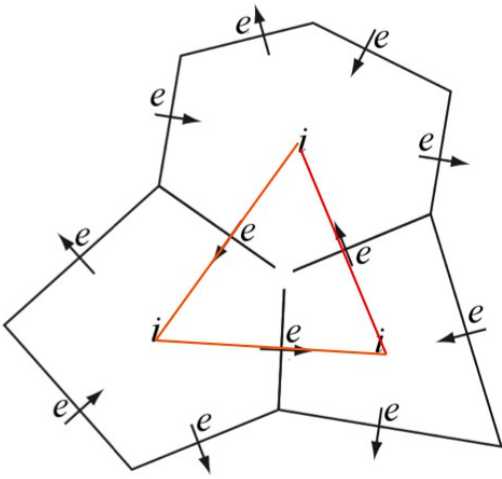


Computational space $S^2 \times [0,1]$

\mathbf{n}

η

Horizontal mesh
Icosahedral C-grid

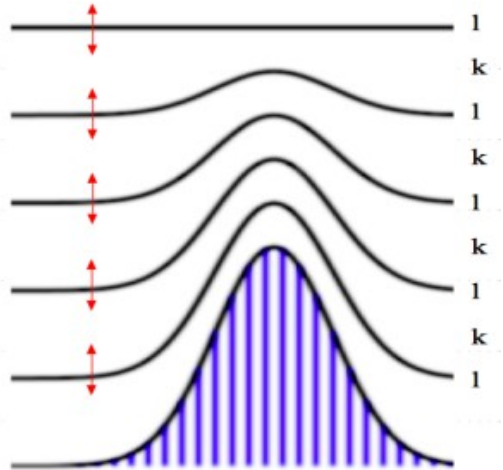


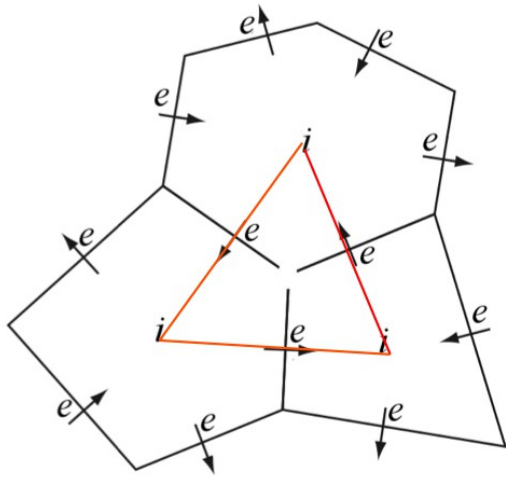
Computational space $S^2 \times [0,1]$

n **η**

Horizontal mesh
Icosahedral C-grid

Vertical mesh
Lorenz



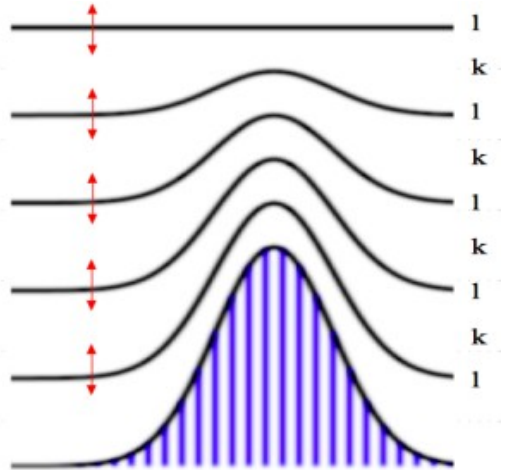


Computational space $S^2 \times [0,1]$

n η

Horizontal mesh
Icosahedral C-grid

Vertical mesh
Lorenz



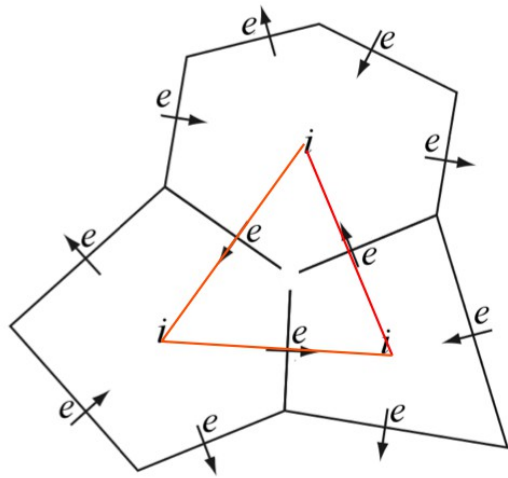
Discrete representation

$$m_{ik} = \int \int \int \mu dn d\eta$$

$$W_{il} = \int \int \mu \eta dn$$

$$v_{ek} = \int \mathbf{v} \cdot d\mathbf{n}$$

$$\alpha_{ik} = \alpha(p_{ik}, s_{ik}),$$

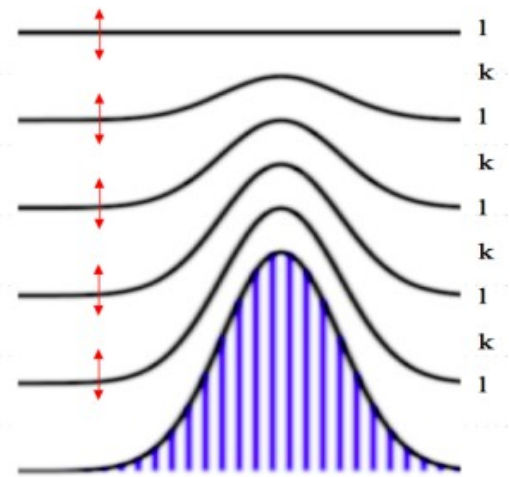


Computational space $S^2 \times [0,1]$

n **η**

Horizontal mesh
Icosahedral C-grid

Vertical mesh
Lorenz



Discrete representation

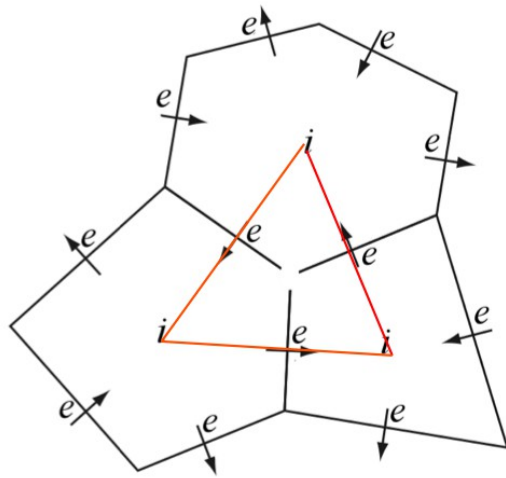
$$m_{ik} = \int \int \int \mu d\mathbf{n} d\eta$$

$$W_{il} = \int \int \mu \dot{\eta} d\mathbf{n}$$

$$v_{ek} = \int \mathbf{v} \cdot d\mathbf{n}$$

$$\alpha_{ik} = \alpha(p_{ik}, s_{ik}),$$

- Discrete Exterior Calculus : discrete exterior derivatives (grad, curl, div) are *exact*
- curl grad = 0

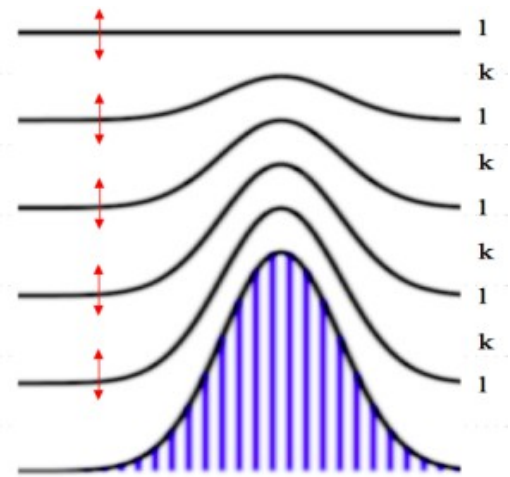


Computational space $S^2 \times [0,1]$

\mathbf{n} η

Horizontal mesh
Icosahedral C-grid

Vertical mesh
Lorenz



Discrete representation

$$m_{ik} = \int \int \int \mu d\mathbf{n}d\eta$$

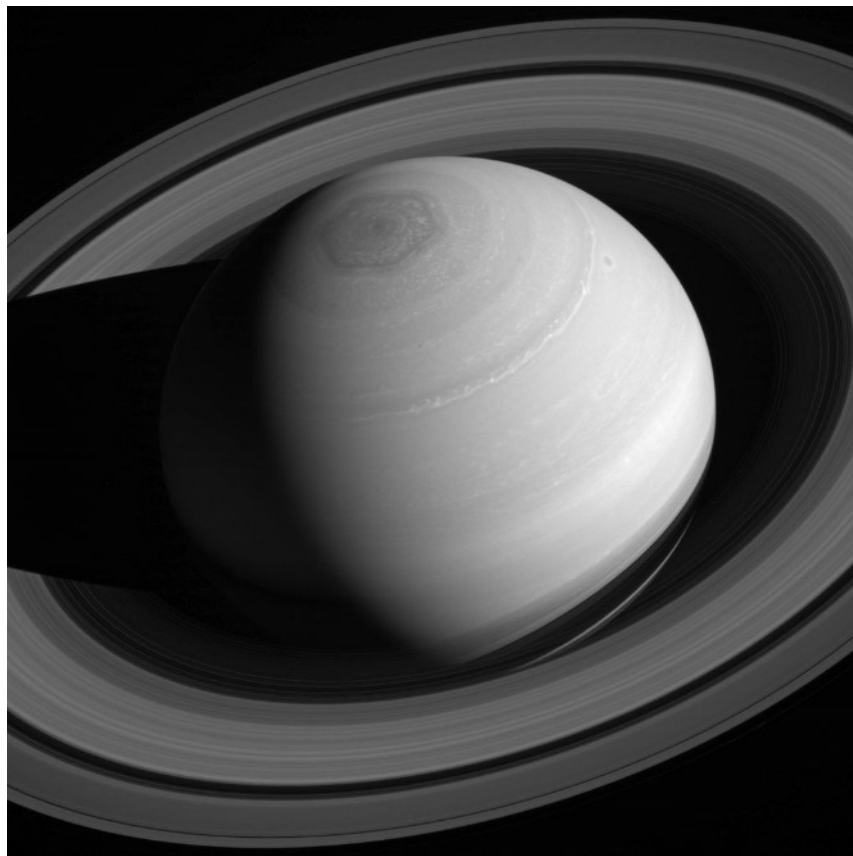
$$W_{il} = \int \int \mu \dot{\eta} d\mathbf{n}$$

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$$\alpha_{ik} = \alpha(p_{ik}, s_{ik}),$$

- Discrete Exterior Calculus : discrete exterior derivatives (grad, curl, div) are *exact*
- curl grad = 0
- Discrete integration by parts (Bonaventura & Ringler, 2005)
- Energy- and vorticity- conserving Coriolis discretization (TRiSK : Thuburn et al., 2009 ; Ringler et al., 2010)

Energy-conserving 3D solver



Saturn GCM simulations

Grid

- Horizontal resolution: $1/2^\circ$ (+ tests $1/4^\circ$ & $1/8^\circ$)
- Vertical levels: 32 levels from 3 bars to 1 mbar

Boundary conditions

- Initial: steady-state temperature from 1D run, no winds
- Dissipation (SGS): very strong (\mathcal{D}^+), strong ($\mathcal{D}^=$), regular (\mathcal{D}^-)
- Type 1: 64 levels + sponge layer on uppermost 4 levels
- Type 2: Bottom drag $|\lambda| > 33^\circ$: $\tau = 100\text{d}$ (\mathcal{F}^+), 1000d (\mathcal{F}^-)

[Liu and Schneider JAS 2010]

Machinery

- MPI+openMP code run on Occigen cluster in CINES
- cores: 1200 ($1/2^\circ$), 9000 ($1/4^\circ$), 11520-30000 ($1/8^\circ$)
- Results are shown after 20000 Saturn days integrations

1 Sat day = 10 h ; 1 Sat year = 30 Earth yr

Physical parameterizations \Rightarrow 1D computations of forcings on each grid point

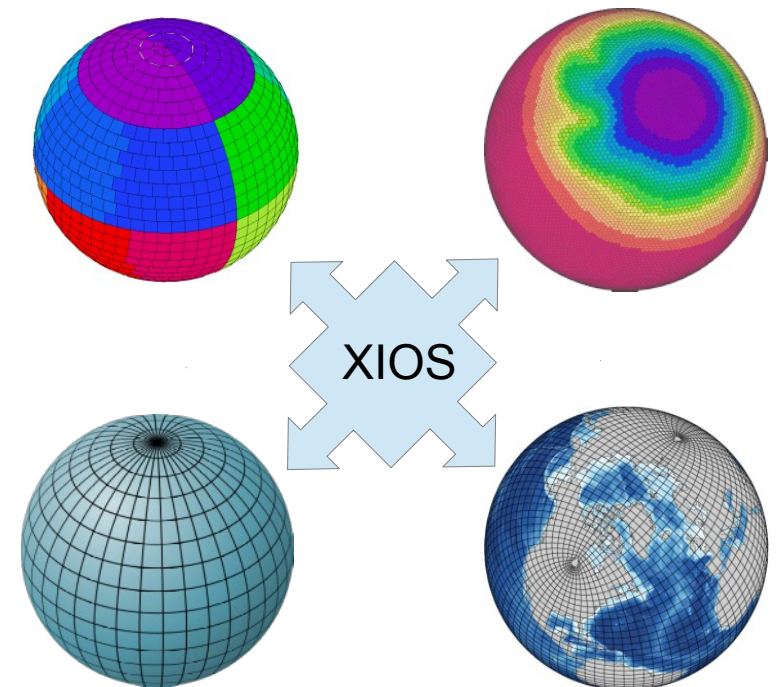
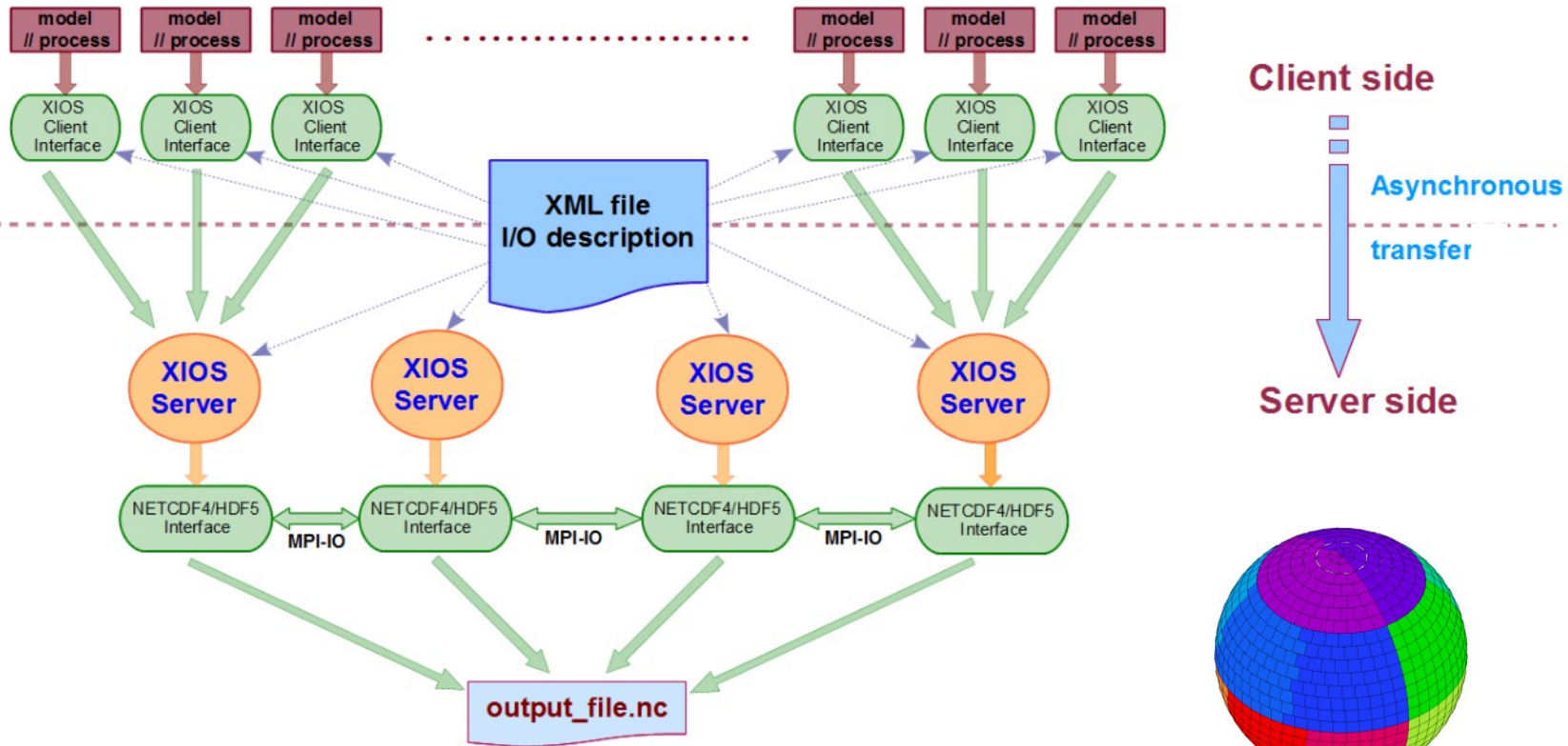
☞ Radiative transfer \Rightarrow Guerlet et al. Icarus 2014

- correlated- k scheme for IR and VIS heating rates [Wordsworth et al. 2010]
- gases CH_4 , C_2H_6 , C_2H_2 with optimized spectral discretization
- HITRAN 2012 database + Karkoschka and Tomasko 2010 for CH_4 around $1\mu\text{m}$
- collision-induced absorption $\text{H}_2\text{-H}_2$ and $\text{H}_2\text{-He}$ [Wordsworth et al. 2012]
- Rayleigh scattering H_2 , He
- simple two-layer aerosol model [constrained by Roman et al. 2013]
 - tropospheric haze layer 180 – 660 mbar / $\tau \sim 8$ / $r = 2\mu\text{m}$
 - stratospheric haze layer 1 – 30 mbar / $\tau \sim 0.1$ / $r = 0.1\mu\text{m}$
- free bottom surface with internal heat flux
- incoming flux: ring shadowing, oblateness

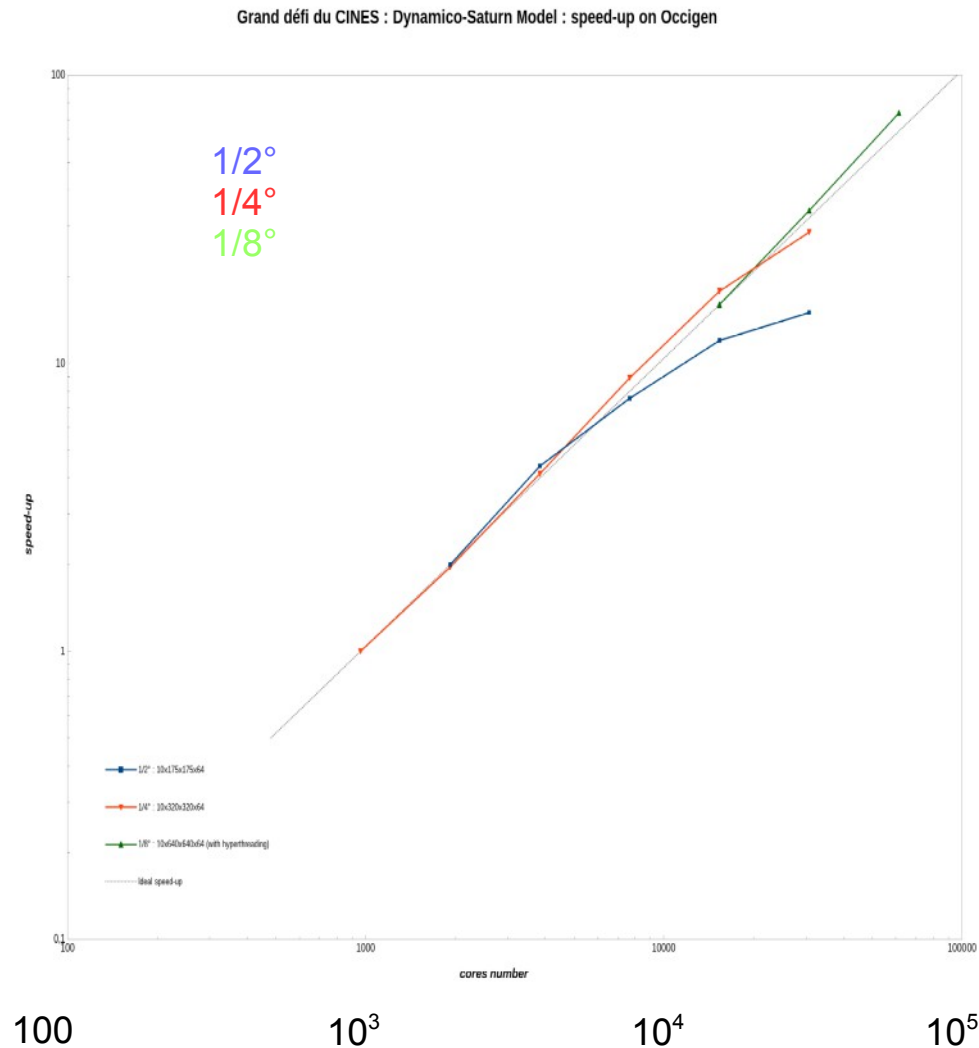
☞ Turbulent diffusion + dry convective adjustment [Hourdin et al. 1993]

XIOS (Y. MEURDESOLF) : XML I/O SERVER

PARALLEL ASYNCHRONOUS I/O - ONLINE POST-PROCESSING LIBRARY AND SERVER



- Throughput on OCCIGEN (dycore only) for 60 vertical levels :
 - 1° : 500 cores ~ 40yr/day
 - 1/4° : 8000 cores ~10yr/day, 2Mh/century
- LMDZ CMIP6 physics now coupled, aquaplanet evaluation under way
- expect at least a few yr/day at 1/4 ° for full GCM



Background on climate modelling

- Weather vs climate
- Characteristic scales
- Equations for atmospheric flow motion

DYNAMICO, an energy-conserving finite difference/finite volume atmospheric solver

- Conservation of energy : why ?
- Hamiltonian formulation
- Preliminary results

Finite elements, the path to higher-order accuracy ?

- Finite elements and conservation of energy
- A-HA

- Finite differences on unstructured meshes are low-order (1~2)
- FEM methods can be higher-order
- But will energy be conserved ?
- Illustrative sketch with a minimal model : 1D nonlinear wave equation

$$\partial_t h + \partial_x(Hu) = 0 \quad \partial_t u + \partial_x F(h) = 0$$

$$\mathcal{H}[h, u] = \int \left(G(h) + H \frac{u^2}{2} dx \right) \quad F(h) = \frac{dG}{dh}$$

$$\partial_t h + \partial_x \frac{\delta \mathcal{H}}{\delta u} = 0 \quad \partial_t u + \partial_x \frac{\delta \mathcal{H}}{\delta h} = 0$$

Conservation of energy / antisymmetry of the bracket result from integration by parts :

$$\{\mathcal{F}, \mathcal{H}\} \equiv \partial_t \mathcal{F} = - \int \left(\frac{\delta \mathcal{F}}{\delta h} \partial_x \frac{\delta \mathcal{H}}{\delta u} + \frac{\delta \mathcal{F}}{\delta u} \partial_x \frac{\delta \mathcal{H}}{\delta h} \right) dx$$

Energy-conserving FEM

$$\partial_t h + \partial_x \frac{\delta \mathcal{H}}{\delta u} = 0 \quad \partial_t u + \partial_x \frac{\delta \mathcal{H}}{\delta h} = 0$$

- We need to pick finite element spaces $H^\varepsilon, U^\varepsilon, B^\varepsilon, F^\varepsilon$

for approximations $h^\varepsilon, u^\varepsilon, b^\varepsilon, f^\varepsilon$ of $h, u, b = \frac{\delta \mathcal{H}}{\delta h}, f = \frac{\delta \mathcal{H}}{\delta u}$

- By definition
$$\delta \mathcal{H} = \int \left(\frac{\delta \mathcal{H}}{\delta h} \delta h + \frac{\delta \mathcal{H}}{\delta u} \delta u \right) dx$$

hence $b^\varepsilon, f^\varepsilon$ are obtained by projection :

$$\begin{aligned} \forall \hat{b} \in B^\varepsilon, \int \hat{h} b^\varepsilon dx &= \int \hat{h} \frac{u^2}{2} dx \\ \forall \hat{u} \in U^\varepsilon, \int \hat{u} f^\varepsilon dx &= \int \hat{u} H u dx \end{aligned}$$

- Therefore spaces $H^\varepsilon, U^\varepsilon, B^\varepsilon, F^\varepsilon$ must be in duality ; simplest choice is $B^\varepsilon = H^\varepsilon, F^\varepsilon = U^\varepsilon$

- At least one among $H^\varepsilon, U^\varepsilon$ must be in H^1 ; say it is H^ε

- Then define $\partial_x b$ as a weak derivative :
$$\forall \hat{h} \in H^\varepsilon \int \left(\hat{H} \partial_t h^\varepsilon + \partial_x f^\varepsilon \right) = 0$$

$$\forall \hat{u} \in U^\varepsilon \int \left(\hat{u} \partial_t u - \partial_x \hat{u} u^\varepsilon \right) dx = 0$$

=> discrete integration by parts => conservation of energy

Computational efficiency of FEM : the A-HA project

- Many possible choices of spaces, some giving high-order accuracy (e.g. spectral elements)
- Compared to a finite-difference method, a FEM method involves many more operations :
 - Assemble mass / stiffness matrices
 - Assemble right-hand-sides
 - Solve mass matrix (typically N-diagonal with $N > 1$)
- High-order methods require quadrature rules with more quadrature points
- CEMRACS project A-HA explores different approaches to perform matrix assembly / matrix-vector multiply, including an approach proposed by Kirby (2014) which rearranges the computation in order to formulate compute-critical parts as dense matrix-matrix products to be offloaded to an optimized BLAS library

Summary

- The atmospheric component of a climate model solves approximate equations of compressible fluid motion in a thin nearly-spherical shell.
- For climate applications where the model evolves freely over long time scales, conservation properties are desirable in order to physically constrain its evolution.
- Conservation of energy can be achieved in a systematic way at the discrete level by exploiting the Hamiltonian formulation of the equations
- The Hamiltonian formulation combines very well with mimetic finite differences and with finite element discretization methods
- However computational performance of FEM is potentially an issue, especially with higher-order FEM

Thanks for your attention !

Extra slides

Hydrostatic primitive equations : discrete

(Lagrangian vertical coordinate – extra terms for vertical transport when mass-based)

mass-weighted
potential temperature



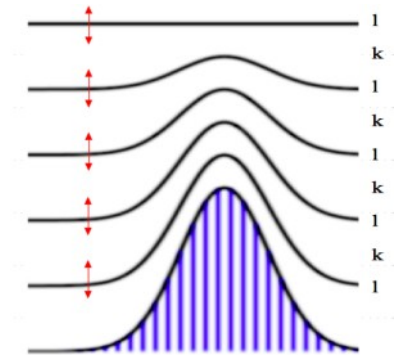
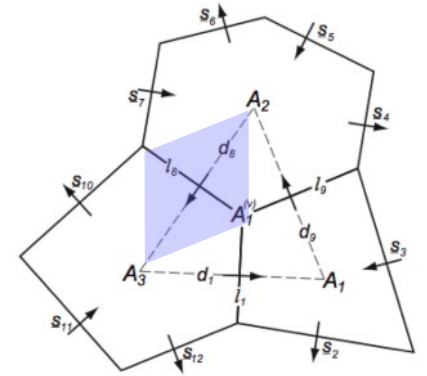
$$H = K(m_{ik}, v_{ek}) + P(m_{ik}, \Theta_{ik}, \Phi_{il})$$

$$K = \sum_{ike} m_{ik} \frac{A_{ie}}{A_i} \left(\frac{v_{ek} - R_e}{a d_e} \right)^2 \quad \leftarrow \text{normal velocity}$$

$$P_{HPE} = \sum_{ik} m_{ik} \left[\overline{\Phi}_i^k + e \left(\alpha_{ik} = \frac{A_i \delta_k (a^2 \Phi_i / g)}{m_{ik}}, \theta_{ik} = \frac{\Theta_{ik}}{m_{ik}} \right) \right]$$

TRISK

shallow-atmosphere metric
planetary velocity



$$\begin{array}{cc} \text{mass flux} & \text{centered/upwind flux} \\ \partial_t m_{ik} + \delta_i \frac{\partial H}{\partial v_{ek}} = 0 & \partial_t \Theta_{ik} + \delta_i \left(\theta_{ek}^* \frac{\partial H}{\partial v_{ek}} \right) = 0 \end{array}$$

$$\partial_t v_{ek} + \left(\frac{\delta_v v_k}{m_k^v} \frac{\partial H}{\partial v_{ek}} \right)^\perp + \delta_e \frac{\partial H}{\partial m_{ik}} + \theta_{ek}^* \delta_e \frac{\partial H}{\partial \Theta_{ik}} = 0$$

SW pot. Vort.

Bernoulli function

Exner function

Discrete energy budget : Lagrangian vertical coordinate

$$\begin{array}{l}
 \text{mass flux} \qquad \qquad \qquad \text{centered/upwind} \\
 \partial_t m_{ik} + \delta_i \frac{\partial H}{\partial v_{ek}} = 0 \qquad \partial_t \Theta_{ik} + \delta_i \left(\theta_{ek}^* \frac{\partial H}{\partial v_{ek}} \right) = 0 \\
 \\
 \partial_t v_{ek} + \left(\frac{\delta_v v_k}{\overline{m_k^v}} \frac{\partial H}{\partial v_{ek}} \right)^\perp + \delta_e \frac{\partial H}{\partial m_{ik}} + \theta_{ek}^* \delta_e \frac{\partial H}{\partial \Theta_{ik}} = 0 \\
 \text{SW pot. Vort.} \qquad \qquad \qquad \text{Bernoulli function} \qquad \qquad \text{Exner function}
 \end{array}$$

discrete div
 \updownarrow discrete integration by parts
 discrete grad

$$\frac{dH}{dt} = \sum \left(\frac{\partial H}{\partial m_{ik}} \partial_t m_{ik} + \frac{\partial H}{\partial \Theta_{ik}} \partial_t \Theta_{ik} + \frac{\partial H}{\partial v_{ek}} \partial_t v_{ek} + \frac{\partial H}{\partial \Phi_{il}} \partial_t \Phi_{il} \right) = 0$$

Discrete energy budget : Lagrangian vertical coordinate

mass flux	centered/upwind	
$\partial_t m_{ik} + \delta_i \frac{\partial H}{\partial v_{ek}} = 0$	$\partial_t \Theta_{ik} + \delta_i \left(\theta_{ek}^* \frac{\partial H}{\partial v_{ek}} \right) = 0$	
$\partial_t v_{ek} + \left(\frac{\delta_v v_k}{\overline{m_k^v}} \frac{\partial H}{\partial v_{ek}} \right)^\perp$	$+ \delta_e \frac{\partial H}{\partial m_{ik}} + \theta_{ek}^* \delta_e \frac{\partial H}{\partial \Theta_{ik}} = 0$	
SW pot. Vort.	Bernoulli function	Exner function

discrete div
↑ discrete integration by parts
↓ discrete grad

$$\frac{dH}{dt} = \sum \left[\frac{\partial H}{\partial m_{ik}} \partial_t m_{ik} + \frac{\partial H}{\partial \Theta_{ik}} \partial_t \Theta_{ik} + \frac{\partial H}{\partial v_{ek}} \partial_t v_{ek} + \frac{\partial H}{\partial \Phi_{il}} \partial_t \Phi_{il} \right] = 0$$

↑
 Hydrostatic balance

$$\Rightarrow p_{ik} \Rightarrow \alpha_{ik} \Rightarrow \Phi_{il}$$

Discrete energy budget : Lagrangian vertical coordinate

$$\begin{array}{l}
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 \partial_t m_{ik} + \delta_i \frac{\partial H}{\partial v_{ek}} = 0 \qquad \partial_t \Theta_{ik} + \delta_i \left(\theta_{ek}^* \frac{\partial H}{\partial v_{ek}} \right) = 0 \\
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 \partial_t v_{ek} + \left(\frac{\delta_v v_k}{\overline{m_k^v}} \frac{\partial H}{\partial v_{ek}} \right)^\perp + \delta_e \frac{\partial H}{\partial m_{ik}} + \theta_{ek}^* \delta_e \frac{\partial H}{\partial \Theta_{ik}} = 0 \\
 \text{SW pot. Vort.} \qquad \qquad \text{Bernoulli function} \qquad \qquad \text{Exner function}
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discrete div
 \updownarrow discrete integration by parts
 discrete grad

$$\frac{dH}{dt} = \sum \left(\frac{\partial H}{\partial m_{ik}} \partial_t m_{ik} + \frac{\partial H}{\partial \Theta_{ik}} \partial_t \Theta_{ik} + \frac{\partial H}{\partial v_{ek}} \partial_t v_{ek} + \frac{\partial H}{\partial \Phi_{il}} \partial_t \Phi_{il} \right) = 0$$

Hydrostatic balance

$$\Rightarrow p_{ik} \Rightarrow \alpha_{ik} \Rightarrow \Phi_{il}$$

Non-Lagrangian vertical coordinate : also possible to cancel additional contributions from vertical transport (Tort et al., QJRMS 2015)

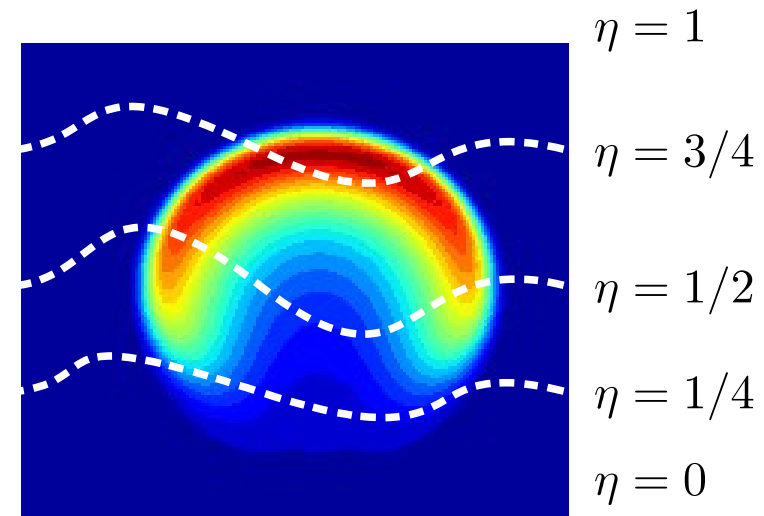
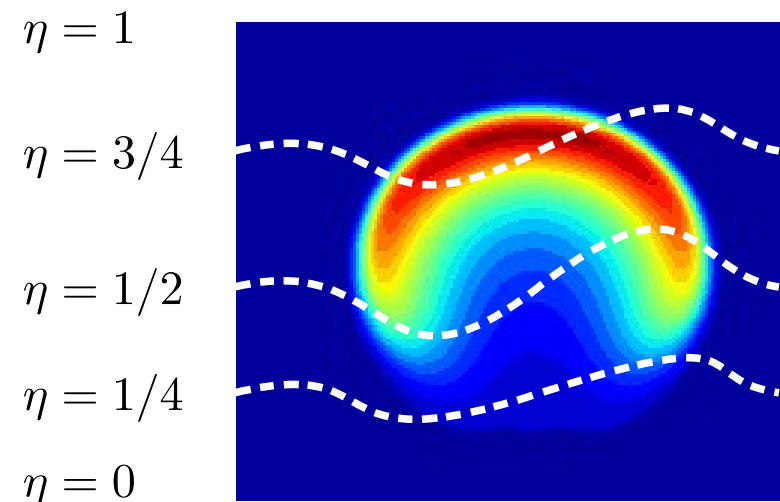
Functional derivatives and redundancy in the flow description

(Dubos & Tort, MWR 2014)

$$\mathcal{H} [\mu, \Theta, \Phi, v_1, v_2, V_3]$$



$$\delta\mathcal{H} = \int \left(\frac{\delta\mathcal{H}}{\delta\mu} \delta\mu + \frac{\delta\mathcal{H}}{\delta\Theta} \delta\Theta + \frac{\delta\mathcal{H}}{\delta\Phi} \delta\Phi + \frac{\delta\mathcal{H}}{\delta v_i} \delta v_i + \frac{\delta\mathcal{H}}{\delta V_3} \delta V_3 \right) d\xi^i d\eta$$

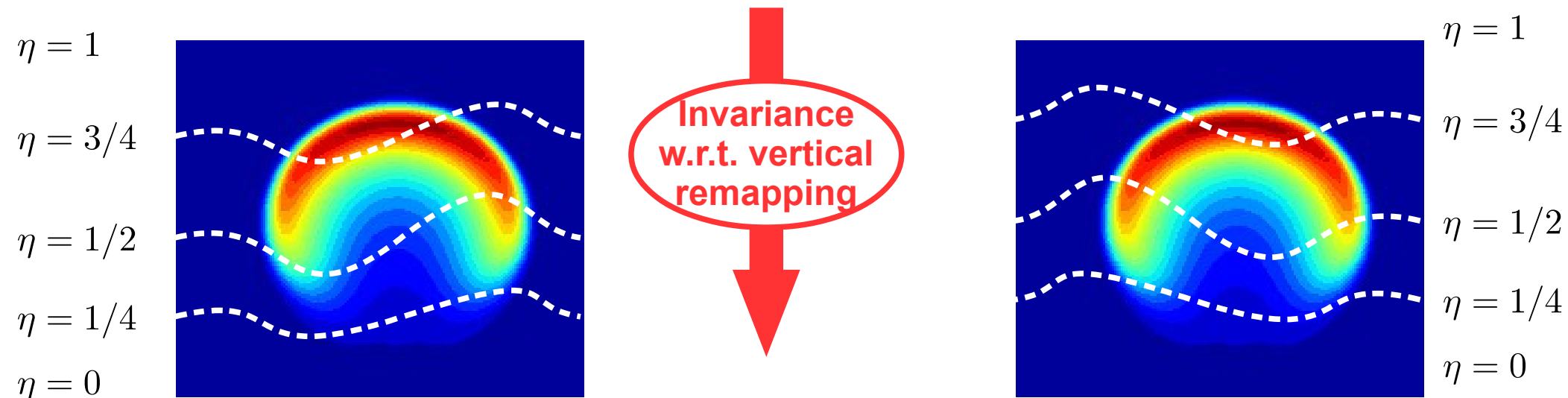


Functional derivatives and redundancy in the flow description

(Dubos & Tort, MWR 2014)

$$\mathcal{H} [\mu, \Theta, \Phi, v_1, v_2, V_3]$$

$$\delta\mathcal{H} = \int \left(\frac{\delta\mathcal{H}}{\delta\mu} \delta\mu + \frac{\delta\mathcal{H}}{\delta\Theta} \delta\Theta + \frac{\delta\mathcal{H}}{\delta\Phi} \delta\Phi + \frac{\delta\mathcal{H}}{\delta v_i} \delta v_i + \frac{\delta\mathcal{H}}{\delta V_3} \delta V_3 \right) d\xi^i d\eta$$



$$\mu \partial_\eta \frac{\delta\mathcal{H}}{\delta\mu} = (\partial_\eta v_i) \frac{\delta\mathcal{H}}{\delta v_i} - \partial_i \left(v_3 \frac{\delta\mathcal{H}}{\delta v_i} \right) + (\partial_\eta \Phi) \frac{\delta\mathcal{H}}{\delta\Phi} - V_3 \partial_\eta \frac{\delta\mathcal{H}}{\delta V_3} - \Theta \partial_\eta \frac{\delta\mathcal{H}}{\delta\Theta}$$