How mathematical structures can help designing (numerical) models of the atmosphere (and ocean)

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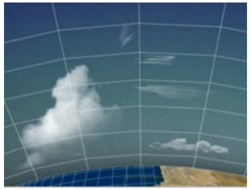
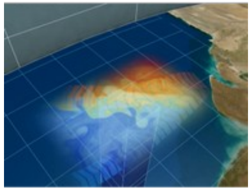
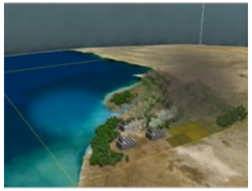
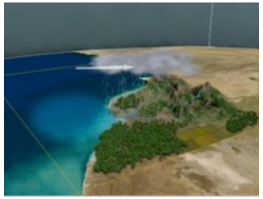
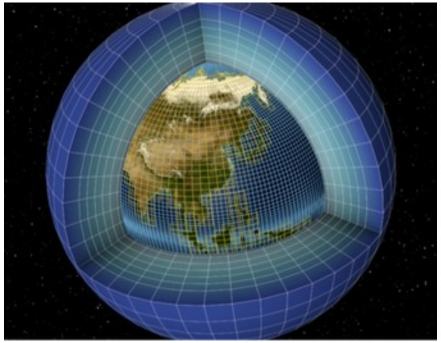
Earth System Modelling at IPSL

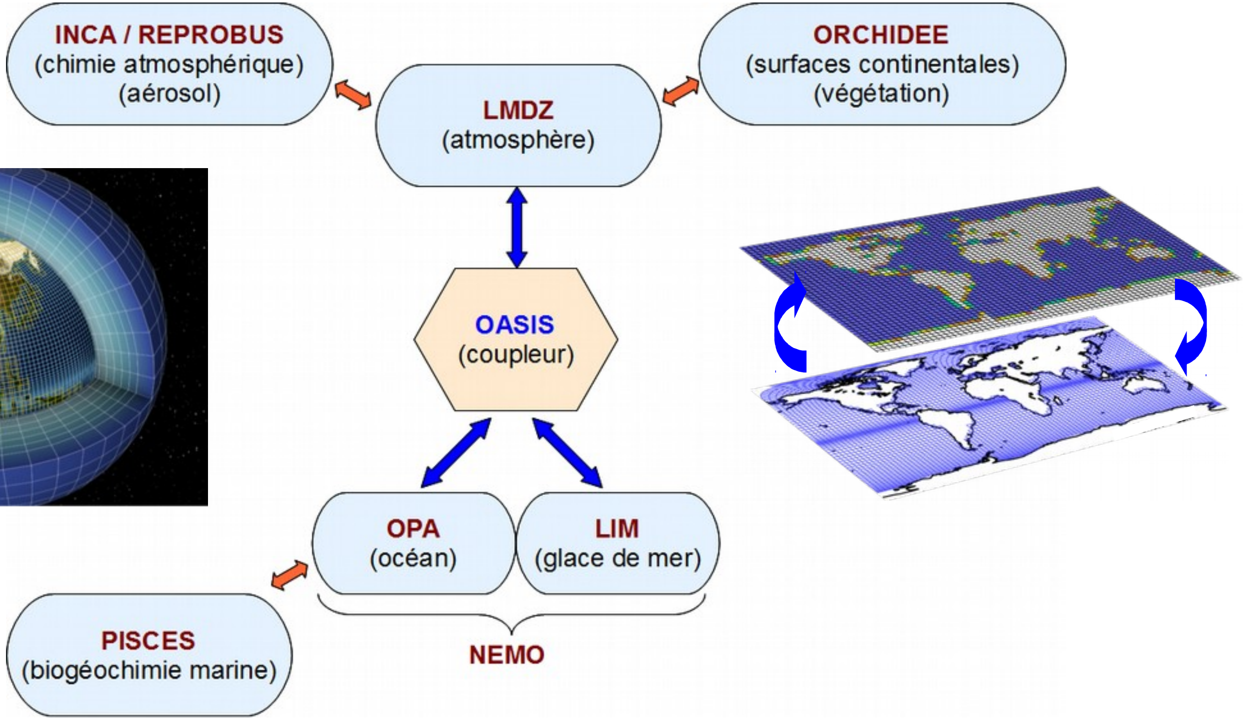


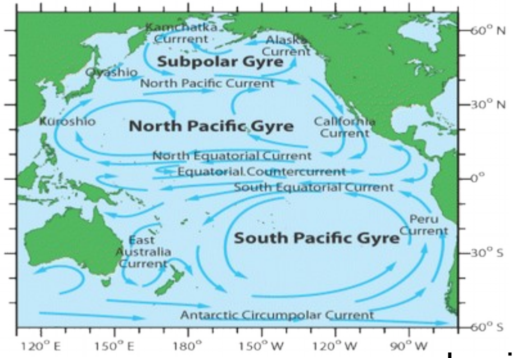












submesoscale | Rossby radius | basin

R=c/f~30 km | 10000 km

Unresolved ~irreversible « physics » | **Resolved reversible « dynamics »**

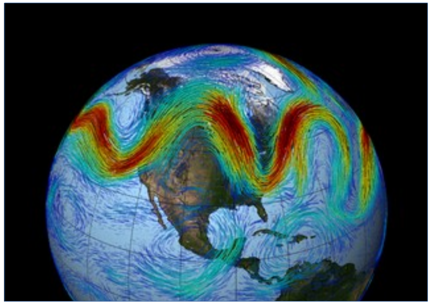
inviscid Boussinesq fluid

+ gravity, rotation

+ hydrostatic balance

$$\frac{\partial X}{\partial t} = \left.\frac{\partial X}{\partial t}\right|_{phys} + \left.\frac{\partial X}{\partial t}\right|_{dyn}$$

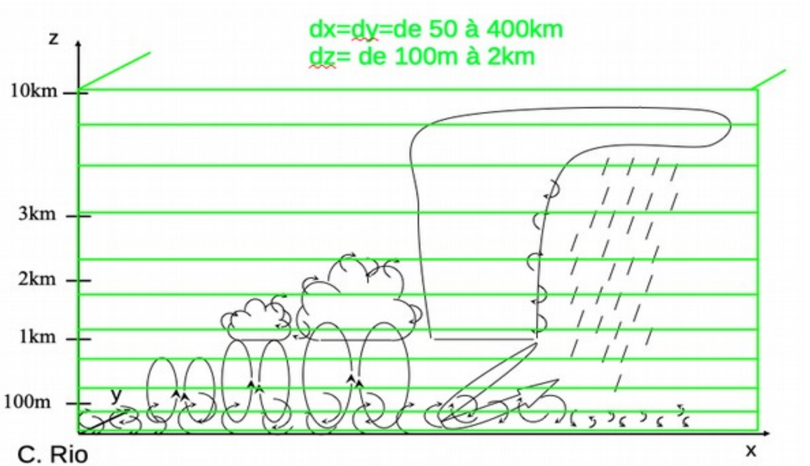


small-scale | scale height | mesoscale | Rossby radius | planetary

1 km | $H=c^2/g=10km$ | 100 km | $R=c/f=1000$ km | 10000 km

Unresolved ~irreversible « physics » | **Resolved reversible « dynamics »**



C. Rio

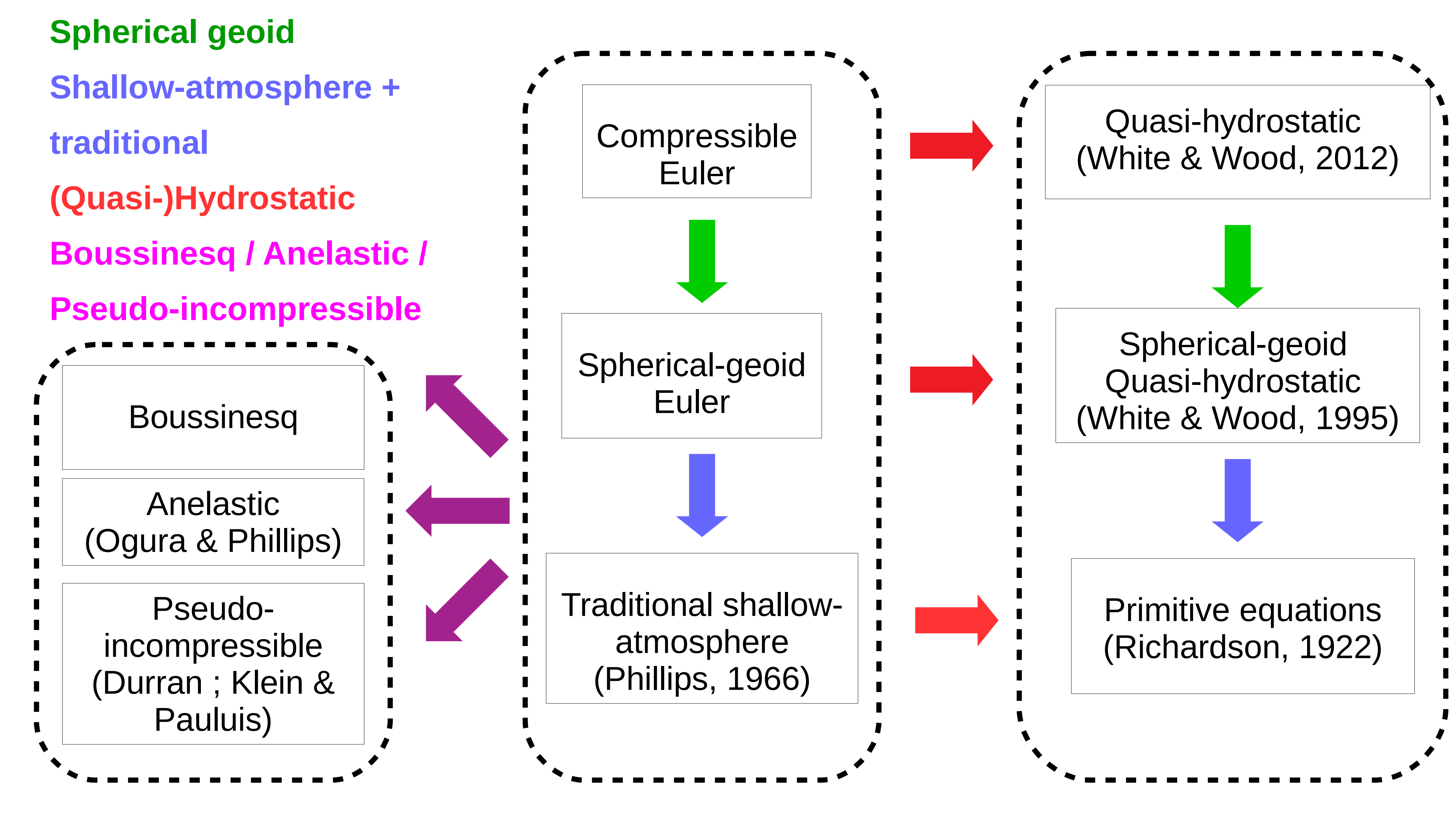
inviscid compressible fluid

(low-Mach)

+ gravity, rotation

+ hydrostatic balance

$$\frac{\partial X}{\partial t} = \left.\frac{\partial X}{\partial t}\right|_{phys} + \left.\frac{\partial X}{\partial t}\right|_{dyn}$$


Spherical geoid
Shallow-atmosphere + traditional
(Quasi-)Hydrostatic
Boussinesq / Anelastic / Pseudo-incompressible
Compressible Euler
Spherical-geoid Euler
Traditional shallow-atmosphere (Phillips, 1966)
Quasi-hydrostatic (White & Wood, 2012)
Spherical-geoid Quasi-hydrostatic (White & Wood, 1995)
Primitive equations (Richardson, 1922)
Boussinesq
Anelastic (Ogura & Phillips)
Pseudo-incompressible (Durran ; Klein & Pauluis)

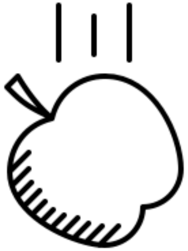
- Structure vs phenomenology for « dynamics »
  What we gain by identifying them

- What is the structure of « physics » ?

- Efforts towards a tighter cooperation between maths, physics and climate ?

The structure of the laws of free fall

$$\ddot{\mathbf{x}} = -\boldsymbol{\nabla} V$$



$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \ell}{\partial \dot{\mathbf{x}}} = \frac{\partial \ell}{\partial \mathbf{x}}$$

$$\ell(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2}\dot{\mathbf{x}}^2 - V(\mathbf{x})$$

$$\dot{\mathbf{v}} = -\frac{\partial E}{\partial \mathbf{x}} \qquad \dot{\mathbf{x}} = \frac{\partial E}{\partial \mathbf{v}}$$

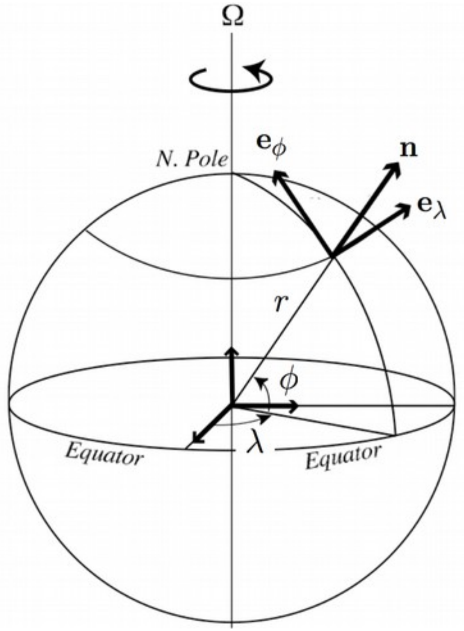
$$E(\mathbf{x}, \mathbf{v}) = \frac{1}{2}\mathbf{v}\cdot\mathbf{v} + V(\mathbf{x})$$

structural

+

phenomenological

Spherical-geoid approximation



Approximate geoid $\Phi = cst$ by sphere of radius $r(\Phi) = -\frac{a\, g_0}{\Phi}$.

$$\ell = \frac{1}{2}\left(r^2 \cos^2\phi\,\dot{\lambda}^2 + r^2\dot{\phi}^2 + \dot{r}^2\right) + \Omega r^2 \cos^2\phi\,\dot{\lambda} - \Phi(r)$$

$$\Rightarrow \quad v_\lambda = r^2 \cos^2\phi\,\left(\Omega + \dot{\lambda}\right)$$

AAM depends on *r*
vertical motion => horizontal Coriolis acceleration

Deep-atmosphere equations, see White & Wood (1995)

Traditional shallow-atmosphere approximation

On Earth, ocean and atmosphere are **very thin** fluid layers

$$r = a + z$$
$$z \ll a$$

	Earth	Titan
ratio	~ 1%	~ 25%
g variability	~ 2.8%	~ 53.4%

$$\ell = \frac{1}{2}\left(a^2 \cos^2\phi\,\dot{\lambda}^2 + a^2\dot{\phi}^2 + \dot{z}^2\right) + \Omega a^2 \cos^2\phi\,\dot{\lambda} - g_0\, z$$

$$\Rightarrow \quad v_\lambda = a^2 \cos^2\phi\,\left(\Omega + \dot{\lambda}\right)$$

AAM independent from *z*
Coriolis acceleration purely horizontal *:* **traditional approximation**

The structure of thermodynamics relationships

Systematic approach (Ooyama, 1990 ; Bannon, 2003 ; Feistel, 2008)

- State variables :

  specific volume/pressure

  specific entropy / temperature

  composition / chemical potential (mixtures)

- All thermodynamic relationships derive from a single ***thermodynamic potential,*** function of **canonical variables**

Internal energy

$$\mathrm{d}U = T\mathrm{d}S - p\mathrm{d}V + \mu^a \mathrm{d}N_a$$

$$H - U = pV$$

Enthalpy

$$\mathrm{d}H = T\mathrm{d}S + V\mathrm{d}p + \mu^a \mathrm{d}N_a$$

$$H - G = TS$$

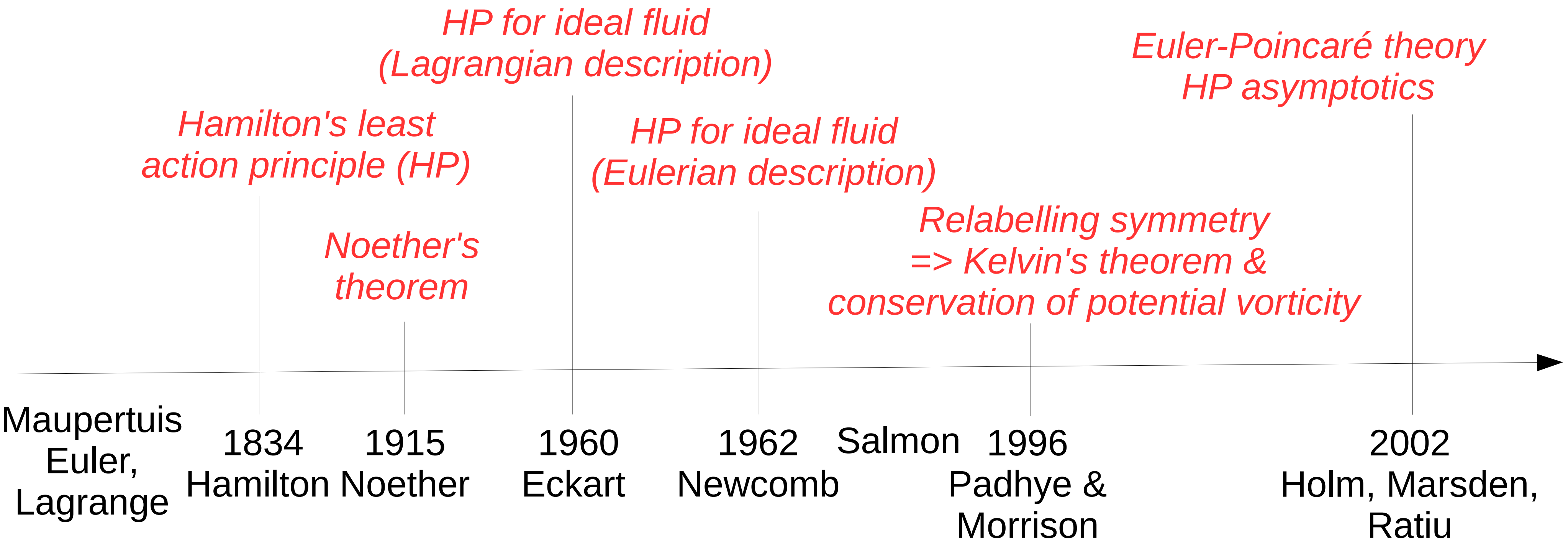
Gibbs function

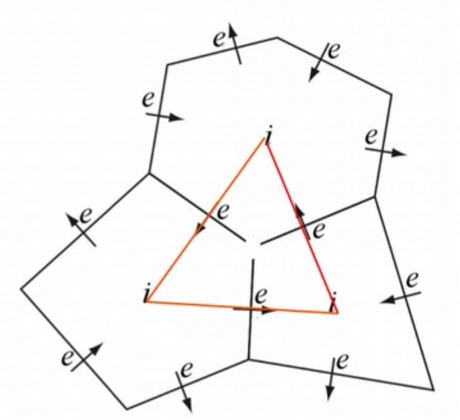
$$\mathrm{d}G = -S\mathrm{d}T + V\mathrm{d}p + \mu^a \mathrm{d}N_a$$

Legendre transform

Conjugate variables

Least action principle for fluids



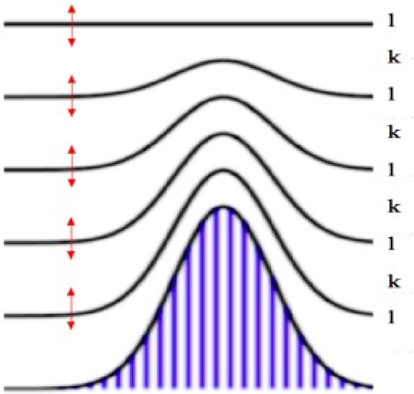


Computational space $S^2 \times [0,1]$

$\mathbf{n}$ η

Horizontal mesh
Icosahedral C-grid

Vertical mesh
Lorenz



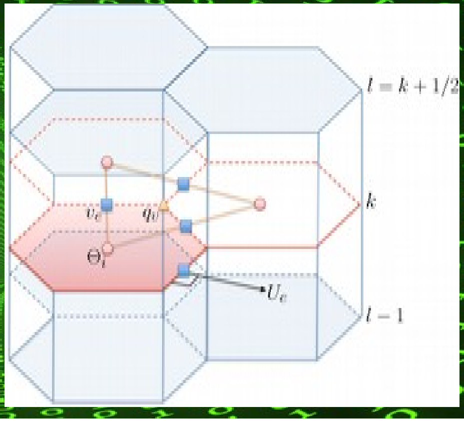
Discrete representation

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

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

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

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



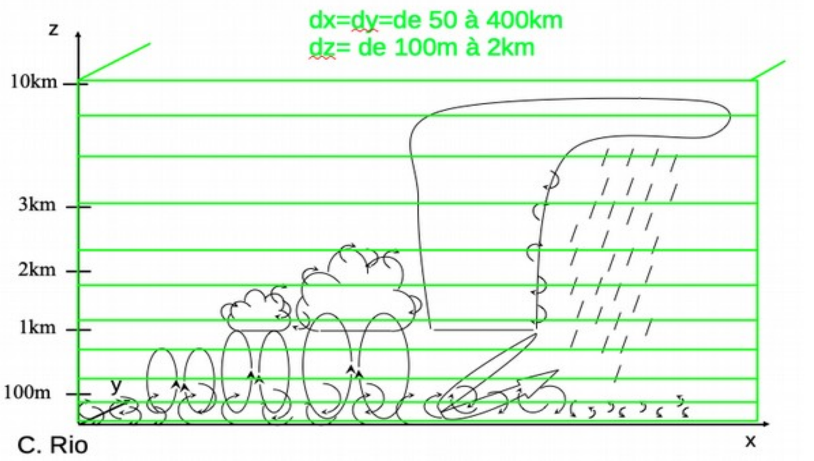
- Discrete Exterior Calculus : discrete exterior derivatives (grad, curl, div) are *exact,* curl grad = 0
- Discrete integration by parts *(Bonaventura & Ringler, 2005)*
- Energy- and vorticity- conserving Coriolis discretization (*Thuburn et al., 2009 ; Ringler et al., 2010*)

Energy-conserving 3D solver

?

- Structure *(Tort & Dubos 2015, ...)* :
  least action principle <=> Poisson bracket
- Phenomenology :
  thermodynamic potential + metric tensor
  + dynamical approximation(s)
- Numerics : *Salmon(1983), Gassmann (2013), Dubos et al. (2015), Tort et al. (2015) Cotter & Shipton (2012), Taylor et al. (2019)*

Unresolved ~irreversible « physics »



Resolved reversible « dynamics »

inviscid compressible fluid

(low-Mach)

+ gravity, rotation

+ hydrostatic balance

How to teach machines about conservations laws ?

Subfilter-scale turbulence

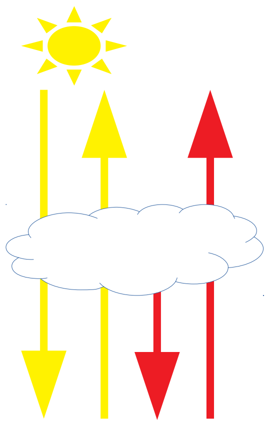
$$\frac{\partial \overline{\mathbf{u}}}{\partial t} + (\overline{\mathbf{u}} \cdot \nabla)\overline{\mathbf{u}} = \overline{\mathbf{F}} + \overline{\mathbf{D}} + \mathbf{S},$$

$$\text{where } \mathbf{S} = \underbrace{(\overline{\mathbf{u}} \cdot \nabla)\overline{\mathbf{u}} - \overline{(\mathbf{u} \cdot \nabla)\mathbf{u}}}_{\text{Subfilter eddy momentum forcing}}.$$

$$\mathbf{S} = \nabla \cdot \underbrace{\left(\overline{\mathbf{u} \otimes \mathbf{u}} - \overline{\mathbf{u}} \otimes \overline{\mathbf{u}}\right)}_{\text{Subfilter stress}}$$

*Learning stresses rather than their divergence (= force) would **structurally** enforce **conservation of momentum***

Radiative transfer



Radiative heating rate

Radiative energy flux

$$\rho c_p \delta T = \delta Q = -F_{rad} z$$

*Learning energy fluxes rather than their divergence (= heating rate) would **structurally** enforce **conservation of energy***

Structure of turbulent closures ?

composition	$\rho D_t q + \nabla \cdot \rho \overline{q' \mathbf{u}'} = 0$

Potential or conservative temperature	$\rho D_t \theta + \nabla \cdot \rho \overline{\theta' \mathbf{u}'} = \sigma_\theta$
Entropy	$\rho D_t s + \nabla \cdot \rho \overline{s' \mathbf{u}'} = \sigma_s$
Internal energy	$\nabla_t (\rho U) + \nabla \cdot \rho \overline{h' \mathbf{u}'} = -\rho \overline{b' w'} + \varepsilon$

Question : how much freedom do we have to *close* turbulent fluxes **and** :

- Conserve energy
- Produce entropy

Issue : some thermodynamic functions are **sensitive** to reference values while others are **insensitive**. The closed system should be **insensitive**.

Structure of turbulent closures ?

- Recently developed formalism extends Hamilton's principle to include irreversible processes

  Gay-Balmaz & Yoshimura (2017)

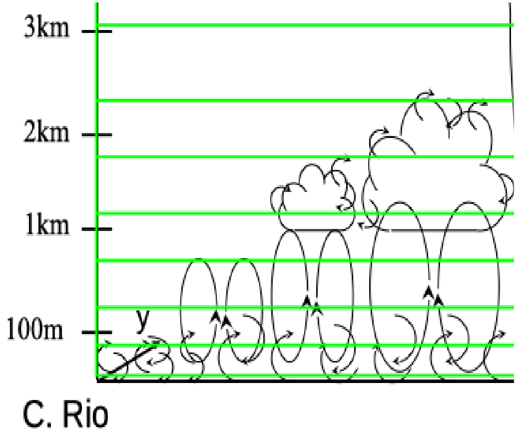
- Applied to conduction and diffusion in geophysical fluid models

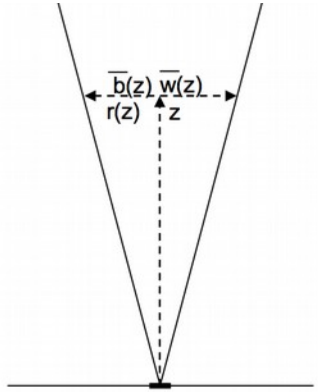
  Eldred & Gay-Balmaz (2021)

WIP (with R. Tailleux, C. Eldred) :

- define **insensitive** reduced fluxes and gradients. K-diffusion closures are generally energetically consistent, even with different diffusivities and cross-diffusion.
- Extend formalism to accomodate turbulent closures, possibly with prognostic TKE / Reynolds stress ?

Structure of convective parameterizations ?





« Mass-flux » (convective plume) approach :

- Energetic constraints on entrainment closures ?
- Universality of entrainment closures ?

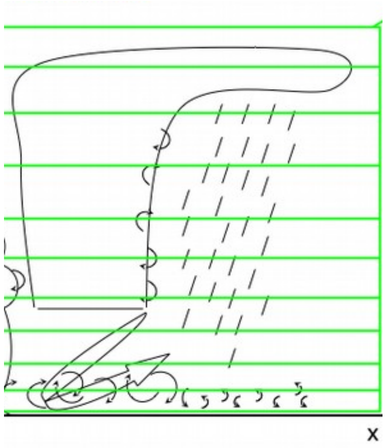
Beyond mass-flux :

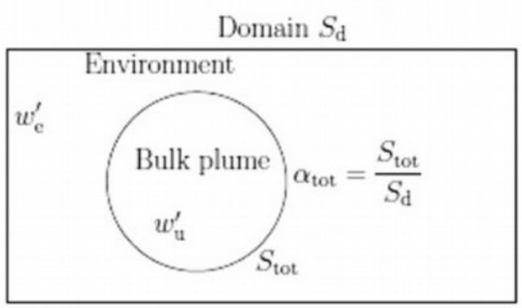
- Multiple-fluid approaches

  (Thuburn et al., 2018)

Well-posedness of hydrostatic + parameterized convection ?

Structure of deep convective parameterizations ?





Deep convection is made possible by the condensation of water vapor. It is akin to the quasi-instantaneous transition from a metastable state to a new stable state.

Two main elements :

- Triggering : whether the transition occurs
- New state after convection

Transition to new state can be :

- Abrupt (discontinuity in time)
- Continuous (relaxation towards new state)

Triggering can be :

- Deterministic
- Stochastic
- Stochastic + resolution-dependent *(Rochetin et al. 2014)*

Is the full model resolving a PDE ? A SPDE ? Something else ? What are the adequate numerics and adequate notions of convergence ?

- Structure vs phenomenology for « dynamics »
  What we gain by identifying them

- What is the structure of « physics » ?

  More generally, many open questions regarding the physics and mathematics of « physics » : admissible closures, well-posedness, stability, adequate numerics ...

- Efforts towards a tighter cooperation between maths, physics and climate ?

Efforts towards a tighter cooperation between maths, physics and climate sciences ?

There is a need
- to *learn* from the other community/discipline to understand each other.
- to transfer of results from toy models to « real models »
  => tools, especially numerical

How to achieve this ?
- scientific literature : scattered, inhomogeneous, evolving
- books : a few recent (Muller, Staniforth), several under way
- schools : modnumoa (LEFE/MANU), ML... ; parameterizations ?
- Numerical models :
    - intricate, realistic community models
    - one-shot, one-person simple models

  => composable models ? (TRACCS)

Quid des enthalpies et entropies de référence ?

$$g(p,T,q) = g_*(p,T,q) + (1-q)\left(h_0^d - Ts_0^d\right) + q\left(h_0^w - Ts_0^w\right).$$

$$s = -g_T \qquad \delta s = (1-q)\delta s_0^d + q\delta s_0^w$$

$$h = g - Tg_T \qquad \delta h = (1-q)\delta h_0^d + q\delta h_0^w$$

$$v = g_p, \quad c_p = -Tg_{TT} \qquad \delta v = 0, \quad \delta c_p = 0$$

Les fermetures sont des lois ***phénoménologiques*** *et devraient être (équivalentes à) des relations entre grandeurs* ***observables****. Or si on ne mesure que* $v(p,T,q)$ *et* $c_p(p,T,q)$*, les enthalpies et entropies de référence, et donc en général les* ***variables conservatives*** $\theta(s,q)$*, sont* ***inobservables****...*

Flux turbulents : observables ou inobservables ?

$$\rho D_t q + \nabla \cdot \rho\, \overline{q'\mathbf{u}'} = 0$$

$$\rho D_t s + \nabla \cdot \rho\, \overline{s'\mathbf{u}'} = \sigma_s$$

$$\rho D_t \theta + \nabla \cdot \rho\, \overline{\theta'\mathbf{u}'} = \sigma_\theta$$

$$\nabla_t\,(\rho U) + \nabla \cdot \rho \overline{h'\mathbf{u}'} = -\rho \overline{b'w'} + \varepsilon$$

$$\rho D_t s + \nabla \cdot \rho \left(\overline{s_q}\, \overline{q'\mathbf{u}'} + \widetilde{s'\mathbf{u}'} \right) = \sigma_s$$

*Flux turbulent d'entropie **réduit***

$$\nabla_t\,(\rho U) + \nabla \cdot \rho \left(\overline{h_q}\, \overline{q'\mathbf{u}'} + \widetilde{h'\mathbf{u}'} \right) = -\rho\, \overline{b'w'} + \varepsilon$$

Flux turbulent de chaleur sensible

Conservation de l'énergie + production d'entropie par un jeu de fermetures "down-gradient"

$$\nabla q,\ \nabla\theta(s,q) \longmapsto \widehat{q'w'},\ \widehat{b'w'},\ \widehat{\theta'w'},\ \widehat{h'w'}$$

$$\nabla q,\ \tilde{\nabla} s \longmapsto \widehat{q'w'},\ \widehat{b'w'},\ \widetilde{s'w'},\ \widetilde{h'w'}$$

Étant donnée une fermeture pour $\widehat{q'w'}$ et $\widetilde{s'w'}$, l'énergie est conservée si :

$$\widehat{b'w'} = b_s \widehat{s'w'} + b_q \widehat{q'w'} \qquad \widetilde{h'w'} = T\widetilde{s'w'}$$

$$T\widehat{\sigma}_s = \varepsilon - \rho \left(\underbrace{h_{ss}\widetilde{s'w'}\tilde{\nabla}_z s + g_{qq}\widehat{q'w'}\nabla_z q}_{\text{Mélange isobare}} \right)$$

NB : on peut toujours choisir une autre variable conservative comme variable prognostique

$$\widehat{\theta'w'} = \theta_s \widehat{s'w'} + \theta_q \widehat{q'w'}$$

$$\sigma_\theta = \ldots$$

	NEMO	**ROMS**	**IFS/ARPEGE**	**MesoNH**	**WRF**	**EndGAME**	**LMDZ**	**DYNAMICO**
Geometry	SG+TSA	SG+TSA	SG+TSA	SG+TSA	SG+TSA	SG	SG+TSA	SG+TSA
Dynamics	HB	HB	FCE	A	FCE	FCE	HPE	HPE/(FCE)
Grid	CC	CC	LL	CC	CC	LL	LL	HEX
Disc. Dyn	FD	FV	SP	FD	FV	FD	FD	FD
Transport	FV	FV	SL	FV	FV	FV	FV	FV
Conserv.	M, E/Z	M		M	M	M	M, E/Z	M, E
Time	Split-EX	Split-EX	SI	EX	Split-HEVI	SI	EX	EX/HEVI
Helmholtz			Direct	Direct		Iter		

SG	Spherical-Geoid
TSA	Traditional Shallow-Atmosphere
FCE	Fully Compressible Euler
HPE	Hydrostatic Primitive Eq.
HB	Hydrostatic Boussinesq
A	Anelastic
EX	Explicit
SI	Semi-Implicit
Split	Split
HEVI	Horizontally Explicit, Vertically Implicit
Direct	Direct (spectral)
Iter	Iterative

CC	Cartesian Curvilnear
LL	Latitude-Longitude
HEX	Icosahedral-Hexagonal
FD	Finite Difference
FV	Finite Volume
FE	*Finite Element*
SE	*Spectral Element*
SL	Semi-Lagrangian
SP	Spectral
M	Mass and scalars
E	Energy
Z	Enstrophy

Transported fields

Transported fields may be scalars ...

$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = 0$$

densities ...

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$

or *tensors* but the transport equations are ***always the same***,
even in ***arbitrary coordinate systems***

$$\frac{\partial X}{\partial t} + \mathcal{L}_{\mathbf{u}} X = 0$$

Lie derivative

Consider a small variation of the *velocity field*. How does a *transported field* vary in a way compatible with its transport equation ?

Variations of transported fields

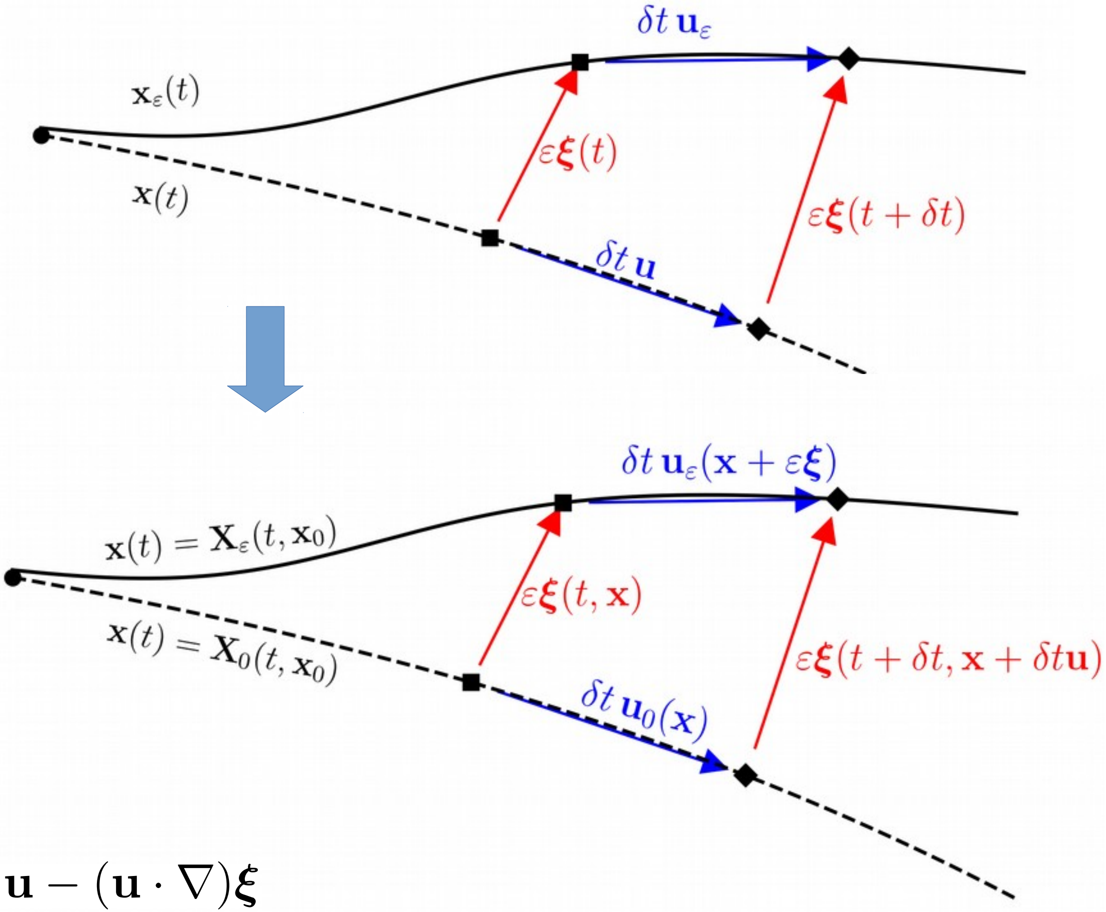
Variations of all fields derive from the perturbation of Lagrangian trajectories

$$(f + \varepsilon \delta f)(t, \mathbf{x} + \varepsilon \boldsymbol{\xi}) = f(t, \mathbf{x})$$

$$\delta f = -\boldsymbol{\xi} \cdot \nabla f = -\mathcal{L}_{\boldsymbol{\xi}} f$$

$$\delta \rho = -\nabla \cdot \rho \boldsymbol{\xi} = -\mathcal{L}_{\boldsymbol{\xi}} \rho$$

$$\delta \mathbf{u} = \frac{D\boldsymbol{\xi}}{Dt} - (\boldsymbol{\xi} \cdot \nabla)\mathbf{u} = \frac{\partial \boldsymbol{\xi}}{\partial t} - \mathcal{L}_{\boldsymbol{\xi}} \mathbf{u}$$



$$\mathcal{L}_{\boldsymbol{\xi}} \mathbf{u} \equiv (\boldsymbol{\xi} \cdot \nabla)\mathbf{u} - (\mathbf{u} \cdot \nabla)\boldsymbol{\xi}$$

Eulerian least action principle for fluids

$$\frac{\partial L}{\partial \mathbf{u}} = \rho \mathbf{v} \qquad L + E = \rho \mathbf{u} \cdot \mathbf{v} \qquad \frac{\partial E}{\partial \mathbf{v}} = \rho \mathbf{u}$$

$$\mathcal{L}\left[\mathbf{u}, \rho, \ldots\right] = \int L\left(\mathbf{x}, \mathbf{u}, \rho, \ldots\right) \mathrm{d}\mathbf{x} \quad \longleftrightarrow \quad \mathcal{E}\left[\mathbf{v}, \rho, \ldots\right] = \int E\left(\mathbf{x}, \mathbf{v}, \rho, \ldots\right) \mathrm{d}\mathbf{x}$$

$$\delta \mathcal{S} = \int \left(\frac{\partial L}{\partial \mathbf{u}} \left(\frac{\partial \boldsymbol{\xi}}{\partial t} - \mathcal{L}_{\boldsymbol{\xi}} \mathbf{u} \right) - \frac{\partial L}{\partial \rho} \nabla \cdot \rho \boldsymbol{\xi} + \ldots \right) \mathrm{d}\mathbf{x}\mathrm{d}t$$

$$= - \int \rho \boldsymbol{\xi} \cdot \left(\frac{\partial \mathbf{v}}{\partial t} + (\nabla \times \mathbf{v}) \times \mathbf{u} \right) + \nabla \frac{\partial E}{\partial \rho} + \ldots \right) \mathrm{d}\mathbf{x}\mathrm{d}t$$

To be done once for all !

- Equations for momentum in *vector-invariant form* (a.k.a curl form)
- Budgets for energy, momentum/AAM, potential vorticity
- Energy-conserving numerics : Salmon (since 80s), Gassmann (2012), Cotter & Shipton (2013), Dubos et al. (2015), Eldred et al (2020) ...

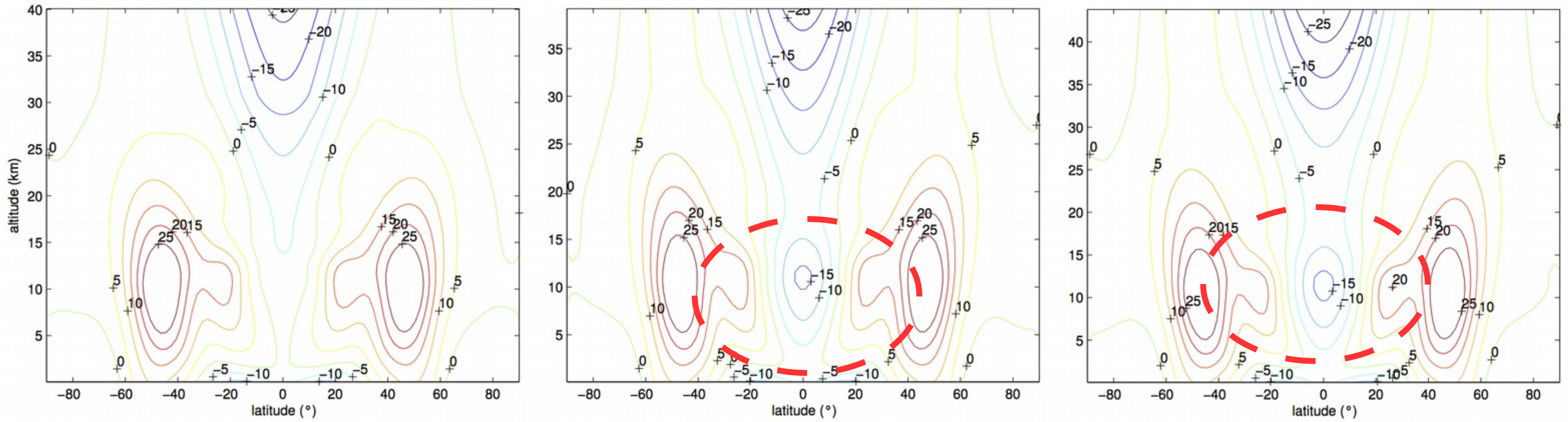
Non-traditional shallow-atmosphere approximation

$$\ell = \frac{1}{2}\left(a^2\cos^2\phi\,\dot\lambda^2 + a^2\dot\phi^2 + \dot z^2\right) + \Omega(a^2+2az)\cos^2\phi\,\dot\lambda - g_0\, z$$

$$\Rightarrow\ v_\lambda = \cos^2\phi\left((a^2+2az)\Omega + a^2\dot\lambda\right)$$

AAM depends on *z* => *non-traditional Coriolis acceleration*
Tort & Dubos QJRMS 2014

Zonal-mean zonal flow in idealized climate experiments on an rapidly-rotating Earth (Tort et al., 2014)



shallow, traditional

shallow, non-traditional

deep-atmosphere