

Variational derivation of energy-conserving schemes for geophysical fluid equations

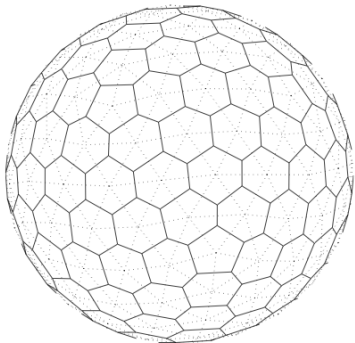
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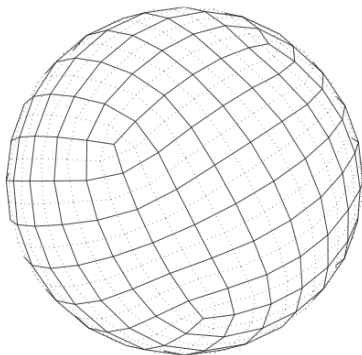
Energy-conserving schemes

- Arakawa (1966) : non-divergent, + enstrophy
- Sadourny et al. (1968) : non-divergent, icosahedron, + enstrophy
- Sadourny (1972) : rotating shallow-water, icosahedron/cubed sphere, collocated A-grid
- Sadourny (1975) : RSW, Cartesian staggered C-grid
- Simmons & Burridge (1981) : hydrostatic, hybrid vertical coordinate
- Janjic (1977, 1984), Rancic (1988, 2009) : RSW, staggered E-grid, cubed sphere / octagonal
- Arakawa & Lamb (1982) : RSW, C-grid, + enstrophy
- Hollingsworth et al. (1983) : RSW, Cartesian staggered C-grid
- Taylor et al. (2010) : RSW / hydrostatic, cubed-sphere, high-order “collocated” finite elements
- Ringler et al. (2010) : RSW, unstructured C- grid with orthogonal dual
- Thuburn & Cotter (2012) : RSW, unstructured C- grid with non-orthogonal dual
- Gassmann (2012) : z-based coordinate, non-hydrostatic, unstructured C-grid with orthogonal dual

Energy-conserving C-grid schemes



- orthogonal Delaunay/Voronay meshes
- too many velocity DOFs \Rightarrow numerical modes



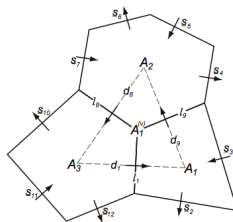
- good balance of mass/velocity DOFs
- no quasi-uniform orthogonal primal/dual pair

- 1 Energy conservation on a non-orthogonal C-grid
 - Non-orthogonal C-grid
 - A non-diagonal discrete Hodge star
 - Connection to the discrete Poisson bracket approach
- 2 Revisiting previous energy-conserving C-grid schemes
 - Rotating shallow-water Poisson bracket
 - Sadourny and related schemes
 - TRiSK scheme
- 3 Primitive equations in a general vertical coordinate
 - Variational principle in a general vertical coordinate
 - Energy-conserving schemes

Vector field on a non-orthogonal C-grid (Thuburn & Cotter, 2012)

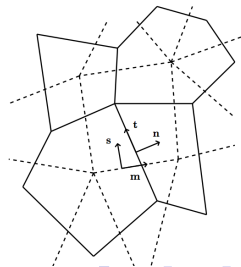
Describe a vector field by a finite set of scalars ?

- 1 cell-averaged components
- 2 pointwise components
- 3 integrals along curves
- 4 integrals across surfaces



Not orthogonal \Rightarrow distinguish between :

- circulations along dual mesh edges Γ_e
 \Rightarrow discrete vorticity budget
- fluxes across primal mesh faces
 \Rightarrow discrete mass budget



Discrete vorticity budget

prognose circulations $v_e = \int_{\Gamma_e} \underline{u} \cdot d\underline{l}$
 \Rightarrow diagnose mass fluxes $u_e = \int_{\Sigma_e} \underline{u} \cdot \underline{n} ds$

Conservation of energy

Linear wave equation

$$\partial_t \mathbf{p} + \text{div } \underline{\mathbf{u}} = 0, \quad \partial_t \underline{\mathbf{u}} + \nabla \mathbf{p} = 0$$

define column-vectors $\mathbf{p} = (p_i)$ and $\mathbf{v} = (v_e)$

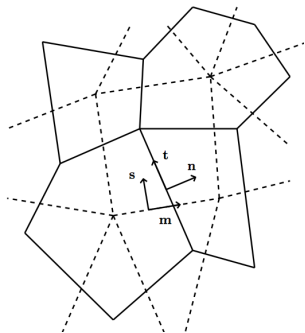
$$p_i = \int_{V_i} p dA, \quad v_e = \int_{\Gamma_e} \underline{\mathbf{u}} \cdot d\mathbf{l}$$

$$\partial_t \mathbf{p} = -\mathbf{D} \cdot \mathbf{H} \cdot \mathbf{v}, \quad \partial_t \mathbf{v} = -\mathbf{G} \cdot \mathbf{A}^{-1} \cdot \mathbf{p}$$

with V_i primal mesh cells, A diagonal matrix

$$A_{ii} = \int_{V_i} dA$$

G, D incidence matrices : ${}^t G + D = 0$



H symmetric positive definite \Rightarrow conservation of energy

$$\begin{aligned} E(\mathbf{p}, \mathbf{v}) &= \frac{1}{2} \mathbf{p}^* \cdot \mathbf{A} \cdot \mathbf{p} + \frac{1}{2} \mathbf{v}^* \cdot \mathbf{H} \cdot \mathbf{v} \\ \partial_t E &= \partial_t \mathbf{p}^* \cdot \mathbf{A} \cdot \mathbf{p} + \partial_t \mathbf{v}^* \cdot \mathbf{H} \cdot \mathbf{v} \\ &= -\mathbf{v}^* \cdot \mathbf{H} \cdot \mathbf{D}^* \cdot \mathbf{A} \cdot \mathbf{p} - \mathbf{p}^* \cdot \mathbf{A}^{-1} \cdot \mathbf{G}^* \cdot \mathbf{H} \cdot \mathbf{v} = 0 \end{aligned}$$

A 2D non-diagonal discrete Hodge star

H symmetric positive definite \Rightarrow conservation of energy

$$\begin{aligned} E(\mathbf{p}, \mathbf{v}) &= \frac{1}{2} \mathbf{p}^* \cdot A^{-1} \cdot \mathbf{p} + \frac{1}{2} \mathbf{v}^* \cdot H \cdot \mathbf{v} \\ \partial_t E &= \partial_t \mathbf{p}^* \cdot A^{-1} \cdot \mathbf{p} + \partial_t \mathbf{v}^* \cdot H \cdot \mathbf{v} \\ &= -\mathbf{v}^* \cdot H \cdot D^* \cdot A^{-1} \cdot \mathbf{p} - \mathbf{p}^* \cdot A^{-1} \cdot G^* \cdot H \cdot \mathbf{v} = 0 \end{aligned}$$

Strategy (inspired by Perot, Vidovic & Wesseling)

- Estimate the kinetic energy $K(\mathbf{v}) \simeq \frac{1}{2} \int \underline{\mathbf{u}} \cdot \underline{\mathbf{u}} d\Omega$
- Define $\mathbf{u} = \partial K / \partial \mathbf{v} = H \cdot \mathbf{v}$
- Find the primal mesh such that $u_e \simeq \int_{\Sigma_e} \underline{\mathbf{u}} \cdot \underline{\mathbf{n}} ds$!

Here \simeq means that $=$ holds when $\underline{\mathbf{u}}$ is uniform (consistency).

Corner-wise velocity reconstruction

Consider two consecutive edges AB and BC of a dual cell, counter-clockwise :

$$v_{AB} = \int_{AB} \underline{u} \cdot d\underline{l} \simeq \underline{u} \cdot \underline{AB}$$

$$v_{BC} = \int_{BC} \underline{u} \cdot d\underline{l} \simeq \underline{u} \cdot \underline{BC}$$

Define

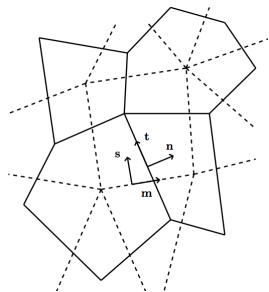
\underline{z} = unit normal vector

$$ABC = \underline{z} \cdot (\underline{AB} \times \underline{BC})$$

$$\underline{u}_{ABC}(v_{AB}, v_{BC}) = \frac{1}{ABC} \underline{z} \times (v_{AB} \underline{BC} - v_{BC} \underline{AB})$$

Then

$$\underline{u}_{ABC}(v_{AB}, v_{BC}) \simeq \underline{u}$$



Discrete Hodge star operator

Triangular dual cell

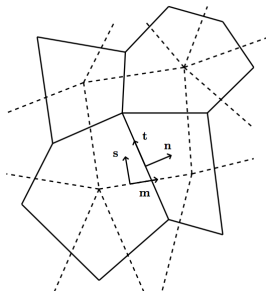
$$\text{area}(ABC) = \frac{1}{2} ABC$$

$$K_{ABC} = \frac{ABC}{6} (\underline{u}_{ABC}^2 + \underline{u}_{BCA}^2 + \underline{u}_{CAB}^2)$$

Quadrangular dual cell

$$\text{area}(ABCD) = \frac{1}{4} (ABC + BCD + CDA + DAB)$$

$$K_{ABCD} = \frac{1}{8} (ABC \underline{u}_{ABC}^2 + BCD \underline{u}_{BCD}^2 + CDA \underline{u}_{CDA}^2 + DAB \underline{u}_{DAB}^2)$$



Algebra shows that

$$K(\mathbf{v}) = \sum_{\text{dual cells}} K_{\text{cell}} \Rightarrow \frac{\partial K}{\partial v_e} \simeq \int_{\Sigma_e} \underline{u} \cdot \underline{n} ds$$

where the primal mesh vertices are barycenters of dual mesh cells.

Connection to the discrete Poisson bracket approach

e.g. Gassmann (2012)

Discrete

$$E(\mathbf{p}, \mathbf{v}) = \frac{1}{2} \mathbf{p}^* \cdot \mathbf{A}^{-1} \cdot \mathbf{p} + \frac{1}{2} \mathbf{v}^* \cdot \mathbf{H} \cdot \mathbf{v}$$

$$\partial_t \mathbf{p} = -\mathbf{D} \cdot \frac{\partial E}{\partial \mathbf{v}}, \quad \partial_t \mathbf{v} = -\mathbf{G} \cdot \frac{\partial E}{\partial \mathbf{p}}$$

$$\begin{aligned} \partial_t F(\mathbf{p}, \mathbf{v}) &= \frac{\partial F}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{p}}{\partial t} + \frac{\partial F}{\partial \mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial t} \\ &= -\frac{\partial F}{\partial \mathbf{p}} \cdot \mathbf{D} \cdot \frac{\partial E}{\partial \mathbf{v}} - \frac{\partial F}{\partial \mathbf{v}} \cdot \mathbf{G} \cdot \frac{\partial E}{\partial \mathbf{p}} \\ &= -\left(\frac{\partial F}{\partial \mathbf{v}} \cdot \mathbf{G} \cdot \frac{\partial E}{\partial \mathbf{p}} - \frac{\partial E}{\partial \mathbf{v}} \cdot \mathbf{G} \cdot \frac{\partial F}{\partial \mathbf{p}} \right) \end{aligned}$$

$$\partial_t F(\mathbf{p}, \mathbf{v}) = \{F, E\}$$

Continuous

$$E[p, \underline{u}] = \frac{1}{2} \int (p^2 + \underline{u} \cdot \underline{u}) d\Omega$$

$$\delta E = \int (p \delta p + \underline{u} \cdot \delta \underline{u}) d\Omega$$

$$\partial_t p + \nabla \cdot \frac{\delta E}{\delta \underline{u}} = 0, \quad \partial_t \underline{u} + \nabla \frac{\delta E}{\delta p} = 0,$$

$$\begin{aligned} \partial_t F[p, \underline{u}] &= \int \left(\frac{\delta F}{\delta p} \cdot \frac{\partial p}{\partial t} + \frac{\delta F}{\delta \underline{u}} \cdot \frac{\partial \underline{u}}{\partial t} \right) d\Omega \\ &= -\int \left(\frac{\delta F}{\delta \underline{u}} \cdot \nabla \frac{\delta E}{\delta p} - \frac{\delta E}{\delta \underline{u}} \cdot \nabla \frac{\delta F}{\delta p} \right) d\Omega \end{aligned}$$

$$\partial_t F[p, \underline{u}] = \{F, E\}$$

Caveat : here, discrete Poisson brackets only have antisymmetry : $\{F, G\} + \{G, F\} = 0$,

NOT the Jacobi property :

$$\{F, \{G, H\}\} + \{H, \{F, G\}\} + \{G, \{H, F\}\} = 0.$$

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Rotating shallow-water Poisson bracket

Hamiltonian (f -plane)

- \underline{u} : horizontal velocity ; $\underline{R}(x, y) = \Omega \underline{e}_z \times \underline{x}$: entrainment velocity
- $\underline{v} = \underline{u} + \underline{R}$: absolute velocity
- $\text{curl } \underline{R} = 2\Omega = f$, potential vorticity $q = \text{curl } \underline{v}/h$

$$H[h, \underline{v}] = \frac{1}{2} \left\langle h(\underline{v} - \underline{R}(x, y))^2 + gh^2 \right\rangle \quad \langle \cdot \rangle = \int dx dy$$

$$\Rightarrow \quad \frac{\delta H}{\delta \underline{v}} = h \underline{u}, \quad \frac{\delta H}{\delta h} = gh + \frac{\underline{u} \cdot \underline{u}}{2}$$

Vector-invariant form and Poisson bracket

$$\frac{\partial h}{\partial t} + \underline{v} \cdot \frac{\delta H}{\delta \underline{v}} = 0, \quad \frac{\partial \underline{v}}{\partial t} + \frac{\text{curl } \underline{v}}{h} \times \frac{\delta H}{\delta \underline{v}} + \nabla \frac{\delta H}{\delta h} = 0$$

$$\frac{d}{dt} F[h, \underline{v}] = \left\langle \frac{\delta H}{\delta \underline{v}} \cdot \nabla \frac{\delta F}{\delta h} - \frac{\delta F}{\delta \underline{v}} \cdot \nabla \frac{\delta H}{\delta h} + \frac{\text{curl } \underline{v}}{h} \cdot \left(\frac{\delta F}{\delta \underline{v}} \times \frac{\delta H}{\delta \underline{v}} \right) \right\rangle = \{F, H\}$$

Rotating shallow-water Poisson bracket

Vector-invariant form and Poisson bracket

$$\frac{\partial h}{\partial t} + \nabla \cdot \frac{\delta H}{\delta \underline{v}} = 0, \quad \frac{\partial \underline{v}}{\partial t} + \frac{\text{curl } \underline{v}}{h} \times \frac{\delta H}{\delta \underline{v}} + \nabla \frac{\delta H}{\delta h} = 0$$

$$\frac{d}{dt} F[h, \underline{v}] = \left\langle \frac{\delta H}{\delta \underline{v}} \cdot \nabla \frac{\delta F}{\delta h} - \frac{\delta F}{\delta \underline{v}} \cdot \nabla \frac{\delta H}{\delta h} + \frac{\text{curl } \underline{v}}{h} \cdot \left(\frac{\delta F}{\delta \underline{v}} \times \frac{\delta H}{\delta \underline{v}} \right) \right\rangle = \{F, H\}$$

Recipe for an energy-conserving scheme

- discretize in vector-invariant form
- approximate total energy as a function of DOFs
- define mass flux and Bernoulli function from derivatives of total energy
- ensure that div and grad are compatible
- antisymmetrize the Coriolis bracket

Was this recipe followed in the past for the RSW ?

Sadourny's energy-conserving scheme

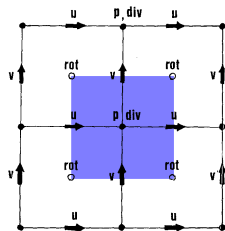
Sadourny, 1975

$$H = \frac{1}{2} \langle gh^2 + h\overline{u^2}^x + h\overline{v^2}^y \rangle$$

$$\partial_t h + \delta_x U + \delta_y V = 0 \quad U = u\overline{h}^x = \frac{\partial H}{\partial u}$$

$$\partial_t u - q\overline{V}^x{}^y + \delta_x B = 0 \quad V = v\overline{h}^y = \frac{\partial H}{\partial v}$$

$$\partial_t v + q\overline{U}^y{}^x + \delta_y B = 0 \quad B = h + \frac{\overline{u^2}^x + \overline{v^2}^y}{2} = \frac{\partial H}{\partial h}$$



$$\frac{dF}{dt} = - \left\langle \frac{\partial F}{\partial u} \delta_x \frac{\partial H}{\partial h} - \frac{\partial H}{\partial u} \delta_x \frac{\partial F}{\partial h} + \frac{\partial F}{\partial v} \delta_y \frac{\partial H}{\partial h} - \frac{\partial H}{\partial v} \delta_y \frac{\partial F}{\partial h} + \frac{\partial F^x}{\partial v} q \frac{\partial H^y}{\partial u} - \frac{\partial F^y}{\partial u} q \frac{\partial H^x}{\partial v} \right\rangle$$

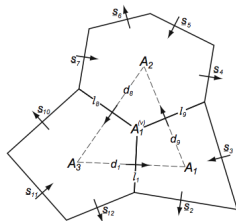
Hollingsworth et al., 1983 : Modified kinetic energy to control a numerical instability

$$H = \frac{1}{2} \left\langle gh^2 + \frac{h}{3} (\overline{u^2}^x + \overline{v^2}^y) + \frac{2h}{3} (\overline{u^2}^{xyy} + \overline{v^2}^{yxx}) \right\rangle$$

$$\Rightarrow U = \left(\frac{1}{3} \overline{h}^x + \frac{2}{3} \overline{h}^{xyy} \right) u = \frac{\partial H}{\partial u}, \quad V = \left(\frac{1}{3} \overline{h}^y + \frac{2}{3} \overline{h}^{yxx} \right) v = \frac{\partial H}{\partial v}$$

TRiSK scheme : Ringler et al. (2010)

	primal		dual
i	\Leftrightarrow cell V_i	\Leftrightarrow	vertex
v	\Leftrightarrow vertex \mathbf{x}_v	\Leftrightarrow	cell
e	\Leftrightarrow face $l_e = \mathbf{E}_e $	\Leftrightarrow	edge $d_e = \Gamma_e $



$$M_i = \int_{V_i} h dA, \quad u_e = \int_{\Gamma_e} \mathbf{u} \cdot d\mathbf{l}$$

$$\partial_t M_i + \sum_e n_{ei} U_e = 0 \quad \partial_t u_e - \eta_e U_e^\perp + \sum_i n_{ei} B_i = 0, \quad n_{ei} = -1, 0, 1$$

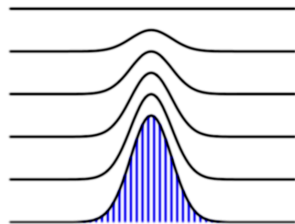
$$H = \frac{1}{2} \sum_i A_i g \left(\frac{M_i}{A_i} \right)^2 + \frac{1}{2} \sum_e l_e d_e h_e \left(\frac{u_e}{d_e} \right)^2, \quad h_e = \sum_i w_{ei} \frac{M_i}{A_i}, \quad \sum_i w_{ei} = 1$$

$$U_e = h_e l_e \frac{u_e}{d_e} = \frac{\partial H}{\partial u_e}, \quad B_i = g \frac{M_i}{A_i} + \frac{1}{A_i} \sum_e w_{ei} l_e d_e \left(\frac{u_e}{d_e} \right)^2 = \frac{\partial H}{\partial M_i}$$

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Hamiltonian in a general vertical coordinate η

- $\mathbf{R}(x, y, z)$: entrainment velocity;
- $\text{curl } \mathbf{R} = 2\boldsymbol{\Omega}$; need not be along z (complete Coriolis force, see Dellar & Salmon, 2005)
- \underline{u} : horizontal velocity ; $\underline{v} = \underline{u} + \mathbf{R}$
- pseudo-density $\mu = \rho \partial z / \partial \eta$
- mass-weighted entropy $S = \mu s$
- grad, div taken along $\eta = \text{cst}$
- mass flux W through interfaces $\eta = \text{cst}$



$$H[\mu, \underline{v}, S, z] = \left\langle \mu \left(\frac{(\underline{v} - \mathbf{R})^2}{2} + U \left(\frac{1}{\mu} \frac{\partial z}{\partial \eta}, \frac{S}{\mu} \right) + \Phi(z) \right) \right\rangle,$$

$$\frac{\delta H}{\delta \mu} = \frac{\underline{u} \cdot \underline{u}}{2} + \Phi + U + p v - T s, \quad \frac{\delta H}{\delta \underline{v}} = \mu \underline{u}, \quad \frac{\delta H}{\delta S} = T$$

$$\mu \frac{\partial}{\partial \eta} \left(\frac{\delta H}{\delta \mu} \right) + \Theta \frac{\partial}{\partial \eta} \left(\frac{\delta H}{\delta \Theta} \right) - \frac{\partial \underline{v}}{\partial \eta} \cdot \frac{\delta H}{\delta \underline{v}} - \frac{\partial z}{\partial \eta} \frac{\delta H}{\delta z} = 0$$

Vector-invariant form

$$\frac{\delta H}{\delta \underline{\mu}} = \frac{\underline{u} \cdot \underline{u}}{2} + \Phi + U + p\underline{v} - Ts, \quad \frac{\delta H}{\delta \underline{v}} = \underline{\mu} \underline{u}, \quad \frac{\delta H}{\delta S} = T$$

$$\begin{aligned} \frac{\partial \underline{\mu}}{\partial t} + \frac{\partial W}{\partial \eta} + \operatorname{div} \frac{\delta H}{\delta \underline{v}} &= 0 \\ \frac{\partial S}{\partial t} + \frac{\partial}{\partial \eta} (sW) + \operatorname{div} \left(s \frac{\delta H}{\delta \underline{v}} \right) &= 0 \\ \frac{\partial \underline{v}}{\partial t} + \frac{W}{\underline{\mu}} \frac{\partial \underline{v}}{\partial \eta} + \frac{\operatorname{curl} \underline{v}}{\underline{\mu}} \times \frac{\delta H}{\delta \underline{v}} + \nabla \frac{\delta H}{\delta \underline{\mu}} + T \nabla \frac{\delta H}{\delta S} &= 0 \\ \frac{\delta H}{\delta z} &= 0 \end{aligned}$$

Energy-conserving schemes

$$\begin{aligned} \frac{d}{dt} F[\mu, \mathbf{v}, S, z] = & \left\langle \frac{\delta H}{\delta \mathbf{v}} \cdot \nabla \frac{\delta F}{\delta \mu} - \frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta \mu} + \frac{\text{curl } \mathbf{v}}{\mu} \cdot \left(\frac{\delta F}{\delta \mathbf{v}} \times \frac{\delta H}{\delta \mathbf{v}} \right) \right\rangle \\ & + \left\langle \theta \left(\frac{\delta H}{\delta \mathbf{v}} \cdot \nabla \frac{\delta F}{\delta \Theta} - \frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta \Theta} \right) \right\rangle + \left\langle \frac{\delta F}{\delta z} \cdot \frac{\partial z}{\partial t} \right\rangle \\ & + \left\langle W \left(\frac{\partial}{\partial \eta} \left(\frac{\delta F}{\delta \mu} \right) + \theta \frac{\partial}{\partial \eta} \left(\frac{\delta F}{\delta \Theta} \right) - \frac{1}{\mu} \frac{\delta F}{\delta \mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial \eta} \right) \right\rangle \end{aligned}$$

Finite-Difference

- Define $H(\mu, \mathbf{v}, S, z)$ and $\mathbf{U} = \partial H / \partial \mathbf{v}, \dots$
- **Poisson bracket** \Rightarrow **Coriolis and compatible div/grad**
- Find W according to type of vertical coordinate
- Solve $\partial H / \partial z = 0$ for z
- **Hydrostasy** defines θ at layer interfaces (Simmons & Burridge, 1981)

Galerkin

- Define spaces $\mathcal{M}, \mathcal{V}, \mathcal{S}, \mathcal{Z}$ and $H(\mu, \mathbf{v}, S, z)$
- Define dual spaces $\mathcal{B}, \mathcal{U}, \mathcal{I}, \mathcal{W}$ for $\delta H / \delta \mu, \dots$,
- **Poisson bracket** \Rightarrow **weak form**
- Find $W \in \mathcal{W}$ according to type of vertical coordinate
- Enforce $\delta H / \delta z = 0$ weakly, solve for z
- $\mathcal{W} = \mathcal{Z} \Rightarrow$ **Hydrostasy**

Summary

Rotating shallow-water equations

- Energy-conserving shallow-water scheme on a non-orthogonal C-grid
- Interpreted as a discrete Poisson bracket
- Sadourny's scheme and TRiSK are discrete Poisson brackets !

3D geophysical equations

- Variational principles for HPE in a general vertical coordinate (generalizes Holm & Long, Brice & Roulstone, Bokhove)
- Prognose absolute velocity / angular momentum
- Several possible paths (FD/FE) to energy conservation
- Applications : deep-atmosphere QHE, non-hydrostatic, variable gravity, arbitrary equation of state, moist dynamics, ocean

Conserving energy is "easy", work is needed for :

- good *linear* properties : numerical modes, dispersion, geostrophic balance
- higher-order