Parcel and Particle Eulerian–Lagrangian Methods for Geophysical Flows

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B. (2005b). . . Popular article (in English). Subm. *Nieuw Archief voor Wiskunde*

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1. Introduction

Parcel Euler-Lagrangian (EL) Hamiltonian formulations have recently been used in:

- structure-preserving numerical schemes (Frank, Gottwald and Reich, 2002; Frank and Reich, 2004);
- asymptotic calculations; and,
- alternative explanations parcel (in)stabilities (B., 2005ab).

What is a Parcel EL Hamiltonian formulation?

A parcel formulation describes the dynamics of a single fluid parcel with a Lagrangian kinetic energy but an Eulerian potential, prescribed or given by an integral relation, evaluated at the parcel's position.

Goals

- Show geometric link of variational and Hamiltonian dynamics; Eulerian PDE's ↔ parcel EL dynamics; *Examples:* 2D vortical flows, shallow water equations, 3D compressible Euler equations, Vlasov equations.

  2. From parcel to continuum Hamiltonian/variational dynamics

- Essentials of structure-preserving numerical EL schemes.

  3. Hamiltonian Particle-Mesh Method (HPM)

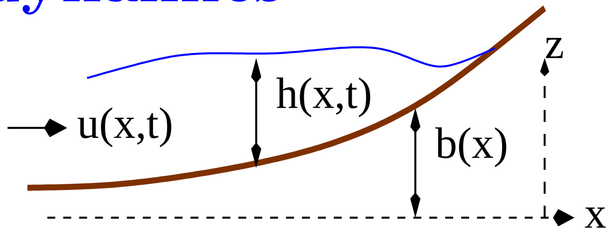
- Relevance to NWP and climiate simulations?

  4. Discussion: HPM for forced-dissipative climate simulations?

Why in Wye?

- *Curiosity.*
- Understanding *link* between *numerics HPM* and *continuum* geometric fluid dynamics.
- *Easiest proof Jacobi identity* for Hamiltonian formulation of (some) fluid PDE's, that I know.
- . . . ?

Rotating shallow water dynamics



Equations of motion

- *Eulerian* form, 2D,

$$\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} + f\,\boldsymbol{u}^{\perp} + g\,\boldsymbol{\nabla}(h+b) = 0\,, \tag{1a}$$

$$\partial_t h + \boldsymbol{\nabla}\cdot(h\,\boldsymbol{u}) = 0\,. \tag{1b}$$

- *Eulerian* Hamiltonian formulation $\mathrm{d}\mathcal{F}/\mathrm{d}t = \{\mathcal{F},\mathcal{H}_\mathrm{s}\}$ with

$$\{\mathcal{F},\mathcal{G}\} = \int_D \left(q_\mathrm{s}\,\frac{\delta\mathcal{F}}{\delta\boldsymbol{u}}^{\perp}\cdot\frac{\delta\mathcal{G}}{\delta\boldsymbol{u}} - \frac{\delta\mathcal{F}}{\delta\boldsymbol{u}}\cdot\boldsymbol{\nabla}\frac{\delta\mathcal{G}}{\delta h} + \frac{\delta\mathcal{G}}{\delta\boldsymbol{u}}\cdot\boldsymbol{\nabla}\frac{\delta\mathcal{F}}{\delta h}\right)\mathrm{d}\boldsymbol{x}$$

  with potential vorticity $q_s = (f + \boldsymbol{\nabla}^{\perp}\cdot\boldsymbol{u})/h$.

- Hamiltonian, factor $1/2$ of potential energy term,

$$\mathcal{H}_\mathrm{s} = \int_D \frac{1}{2}\,h\,|\boldsymbol{u}|^2 + \frac{1}{2}\,g\,(h+b)^2\,\mathrm{d}\boldsymbol{x}\,. \tag{2}$$

Parcel Eulerian-Lagrangian rotating SWE

Parcel form of dynamics used in Hamiltonian particle mesh method (HPM) of Frank and Reich (2003, 2004):

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = \boldsymbol{\nabla}_{\boldsymbol{U}} H_{\mathrm{s}} = \boldsymbol{U}\,, \tag{3a}$$

$$\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = -f\,\boldsymbol{\nabla}_{\boldsymbol{U}}^{\perp} H_{\mathrm{s}} - \boldsymbol{\nabla}_{\boldsymbol{X}} H_{\mathrm{s}} = -f\,\boldsymbol{U}^{\perp} - g\,\boldsymbol{\nabla}(h+b)\,, \tag{3b}$$

$$\mathbf{h}(\boldsymbol{X},\mathbf{t}) = \int_{\mathbf{D}} \mathbf{h_0}(\boldsymbol{a})\,\delta\big(\boldsymbol{X} - \boldsymbol{\chi}(\boldsymbol{a},\mathbf{t})\big)\,\mathrm{d}\boldsymbol{a}\,, \tag{3c}$$

$$\text{Hamiltonian} \quad H_{\mathrm{s}}(\boldsymbol{X},\boldsymbol{U},t) = \frac{1}{2}\,|\boldsymbol{U}|^2 + g\,\big(h(\boldsymbol{X},t) + b(\boldsymbol{X})\big)\,. \tag{3d}$$

- In single parcel Hamiltonian: no factor 1/2 in potential energy.
- $\boldsymbol{X}$ and $\boldsymbol{U}$ Lagrangian horizontal position and velocity.
- *Lagrangian position* $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{a},t)$ fluid parcel.
  Special variation: $\delta\boldsymbol{\chi}(\boldsymbol{a},t) = \delta(\boldsymbol{a} - \boldsymbol{A})\,\delta\boldsymbol{X}$.

- Parcel Hamiltonian formulation

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H_\mathrm{s}\} \tag{4a}$$

with

$$\{F,G\} = f\,\boldsymbol{\nabla}_{\boldsymbol{U}}^{\perp} F \cdot \boldsymbol{\nabla}_{\boldsymbol{U}} G + \boldsymbol{\nabla}_{\boldsymbol{X}} F \cdot \boldsymbol{\nabla}_{\boldsymbol{U}} G - \boldsymbol{\nabla}_{\boldsymbol{X}} G \cdot \boldsymbol{\nabla}_{\boldsymbol{U}} F \tag{4b}$$

for arbitrary functions F and G of $\boldsymbol{X}, \boldsymbol{U}$ and t.

- Single parcel Hamiltonian reads

$$H_\mathrm{s}(\boldsymbol{X}, \boldsymbol{U}, t) = \frac{1}{2}\,|\boldsymbol{U}|^2 + g\left(h(\boldsymbol{X}, t) + b(\boldsymbol{X})\right). \tag{5}$$

Rotating shallow water equations 1^{st} *continuation*

From parcel to continuum Eulerian Hamiltonian dynamics

- *Relate functions* $F(\boldsymbol{U},\boldsymbol{X})$ *for single fluid parcel to functionals*

$$\begin{aligned}\mathcal{F}[\boldsymbol{u},h] &= \int h(\boldsymbol{x},t)\, F(\boldsymbol{u}(\boldsymbol{x},t),\boldsymbol{x})\ \mathrm{d}\boldsymbol{x} \\ &= \int F\big(\dot{\boldsymbol{\chi}}(\boldsymbol{a},t),\boldsymbol{\chi}(\boldsymbol{a},t)\big)\,\mathrm{d}\boldsymbol{a}\,. \qquad (6)\end{aligned}$$

- Relate partial derivatives of F to ones of $\mathcal{F}$

$$\delta\mathcal{F} = \int \frac{\delta\mathcal{F}}{\delta\boldsymbol{u}}\cdot\delta\boldsymbol{u} + \frac{\delta\mathcal{F}}{\delta h}\,\delta h\,\mathrm{d}\boldsymbol{x}\,. \qquad (7)$$

$$\delta\mathcal{F} = \int h(\boldsymbol{x},t)\,\boldsymbol{\nabla}_{\boldsymbol{u}}F\big(\boldsymbol{u}(\boldsymbol{x},t),\boldsymbol{x}\big)\cdot\delta\boldsymbol{u} + F\big(\boldsymbol{u}(\boldsymbol{x},t),\boldsymbol{x}\big)\,\delta h\,\mathrm{d}\boldsymbol{x}\,. \qquad (8)$$

- Since $\delta\boldsymbol{u}$ and δh are independent:

$$\frac{\delta\mathcal{F}}{\delta\boldsymbol{u}} = h\,\boldsymbol{\nabla}_{\boldsymbol{u}}F \qquad \text{and} \qquad \frac{\delta\mathcal{F}}{\delta h} = F\,, \qquad (9)$$

and

$$\boldsymbol{\nabla}\frac{\delta\mathcal{F}}{\delta h} = \boldsymbol{\nabla}F\big(\boldsymbol{u}(\boldsymbol{x},t),\boldsymbol{x}\big) = \boldsymbol{\nabla}_{\boldsymbol{u}}F\cdot\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}_{\boldsymbol{x}}F$$

$$= \frac{1}{h}\,\frac{\delta\mathcal{F}}{\delta\boldsymbol{u}}\cdot\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}_{\boldsymbol{x}}F\,. \qquad (10)$$

- Moreover,

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \int \frac{\partial}{\partial t}F(\dot{\boldsymbol{\chi}},\boldsymbol{\chi})\,\mathrm{d}\boldsymbol{a} = \int h(\boldsymbol{x},t)\,\frac{\mathrm{d}}{\mathrm{d}t}F\big(\boldsymbol{u}(\boldsymbol{x},t),\boldsymbol{x}\big)\,\mathrm{d}\boldsymbol{x}$$

$$= \int h(\boldsymbol{x},t)\,\{F,H_{\mathrm{s}}\}\,\mathrm{d}\boldsymbol{x}\,. \qquad (11)$$

- Substitution (9) & (10) into (11) using (4b) yields Hamiltonian formulation (e.g., Shepherd, 1990).

3. Hamiltonian Particle-Mesh Method (HPM)

Discretize the parcel equation to $k = 1, \ldots, N$ *particles*

$$\frac{\mathrm{d}\boldsymbol{X}_k}{\mathrm{d}t} = \boldsymbol{U}_k \,, \tag{12a}$$

$$m_k \frac{\mathrm{d}\boldsymbol{U}_k}{\mathrm{d}t} = -f\, m_k\, \boldsymbol{U}_k^{\perp} - g\, m_k\, \boldsymbol{\nabla}(\tilde{h} + b)_{\boldsymbol{x}=\boldsymbol{X}_k} \,, \tag{12b}$$

$$\tilde{h}(\boldsymbol{x}, t) = \bar{h}^{ij}\, S_{ij}^{mn}\, \psi_{nm}(\boldsymbol{x}) = \bar{h}^{ij}\, \hat{\psi}_{ij}(\boldsymbol{x}) \tag{12c}$$

$$\text{Hamiltonian} \quad \mathcal{E} = \sum_k \frac{1}{2} m_k |\boldsymbol{U}_k|^2 + \frac{1}{2} g \sum_{i,j} \tilde{h}^{ij} \bar{h}^{ij} \tag{12d}$$

- $h(\boldsymbol{X}, t) = \int_D \delta\big(\boldsymbol{X} - \boldsymbol{\chi}(\boldsymbol{a}, t)\big)\, h_0(\boldsymbol{a})\, \mathrm{d}\boldsymbol{a} \approx \sum_l m_l \psi(\boldsymbol{X} - \boldsymbol{X}_l(t))$ (continuity) and $\sum_{i,j} \psi(\boldsymbol{x}_{ij} - \boldsymbol{x}) = 1$ (enforced using splines)
- $\bar{h}^{ij} = \sum_k m_k \psi(\boldsymbol{x}_{ij} - \boldsymbol{X}_k(t))$ on a regular grid $\boldsymbol{x}_{ij}$ and *meshed* $\bar{h}(\boldsymbol{x}, t) = \bar{h}^{ij}\, \psi(\boldsymbol{x}_{ij} - \boldsymbol{x})$

- A smoothed version $\tilde{h}^{nm}$ of $\bar{h}^{ij}$ is used for numerical stability $\tilde{h}^{nm} = \bar{h}^{ij}\, S_{ij}^{nm}$ such that

  $$\tilde{h}(\boldsymbol{x}, t) = \tilde{h}^{nm}\, \psi_{nm}(\boldsymbol{x}) = \bar{h}^{ij} \hat{\psi}_{ij}(\boldsymbol{x})$$

  with the matrix representation S_{ij}^{nm} of the smoothing operator $\mathcal{S} = (1 - \alpha \boldsymbol{\nabla}^2)^{-p}$ and $\hat{\psi} = \mathcal{S}\, \psi$ $(\alpha, p > 0)$.

- Numerical example (Courtesy Frank, Gottwald and Reich, 2002; HPM website) barotropic instability in rotating double-periodic plane over 15 days. Shown are: the potential vorticity contours (top left), the particle velocity field (top right), the geopotential height (bottom left), and diagonostics total energy(blue), potential (green) and kinetic (red) energies and the ageostrophic kinetic energy(cyan), an adiabatic invariant (lower right).

- http://www.cwi.nl/projects/gi/HPM

Summary

- Geometric link shown between continuum parcel and PDE Hamiltonian formulations.
- Also achieved: link between variational principles (B. & Oliver, 2006).
- AR: *"Why is something so fundamental so irksome to demonstrate? Is it really equivalent to something else that would be easier to verify?"* New, easier proof Jacobi identity.
- Essentials HPM explained: Hamiltonian, conservation mass and circulation.

Discussion: HPM for forced-dissipative climate simulations?

Objective of research is to assess how important numerical preservation of the limiting Hamiltonian structure actually is in (idealized) climate models in which climatological forcing and dissipation mechanisms are present.

Investigated in three ways:

- Difference in performance between Hamiltonian and non-Hamiltonian based numerical discretizations for *low-order models*.
- Symplectic Hamiltonian Particle-Mesh methods with *many degrees of freedom* constructed for hydrostatic stratified models on the sphere using isentropic or mixed vertical and isentropic coordinates.

- Performance of *extended HPM models tested* by simulating one of following atmospheric applications:
  - dynamics of stratospheric chemical species such as ozone; and,
  - coupling between troposphere and stratosphere for benchmark calculation proposed by Held and Suarez (1994).
- **Ph.D. position available in Twente**; collaboration with Jason Frank (biweekly visits anticipated, Amsterdam) and Sebastian Reich (Potsdam).

Preliminaries

- *Lagrangian position* $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{a}, t)$ fluid parcel.
- *Euleriam velocity* $\boldsymbol{u}(\boldsymbol{x}, t)$ parcel passing location $\boldsymbol{x}$ time t.

  Lagrangian velocity fluid parcel

$$\dot{\boldsymbol{\chi}}(\boldsymbol{a}, t) \equiv \partial_t \boldsymbol{\chi}(\boldsymbol{a}, t) = \boldsymbol{u}(\boldsymbol{\chi}(\boldsymbol{a}, t), t) \quad \text{or} \quad \dot{\boldsymbol{\chi}} = \boldsymbol{u} \circ \boldsymbol{\chi}\,. \tag{13}$$

- Height h and initial height h_0

$$\boldsymbol{\chi}^* h \equiv (\det \boldsymbol{\nabla} \boldsymbol{\chi})\, h \circ \boldsymbol{\chi} = h_0. \tag{14}$$

- Integral form height

$$\begin{aligned} h(\boldsymbol{x}, t) &= \int_D h(\boldsymbol{x}', t)\, \delta(\boldsymbol{x} - \boldsymbol{x}')\, \mathrm{d}\boldsymbol{x}' \\ &= \int_D h_0(\boldsymbol{a})\, \delta\big(\boldsymbol{x} - \boldsymbol{\chi}(\boldsymbol{a}, t)\big)\, \mathrm{d}\boldsymbol{a}\,. \end{aligned} \tag{15}$$

- By differentiating (14), continuity equation

$$\partial_t h + \boldsymbol{\nabla} \cdot (h\boldsymbol{u}) = 0\,. \tag{16}$$

- In analogy to $\dot{\boldsymbol{\chi}} = \boldsymbol{u} \circ \boldsymbol{\chi}$, *Eulerian variation* $\boldsymbol{w}$ via

$$\delta\boldsymbol{\chi} = \boldsymbol{w} \circ \boldsymbol{\chi}\,. \tag{17}$$

- $\boldsymbol{u}$ and $\boldsymbol{w}$ satisfy same boundary conditions.
- Just as (16) emerges from (13), we derive from (17):

$$\delta h + \boldsymbol{\nabla} \cdot (h\boldsymbol{w}) = 0. \tag{18}$$

- Localize to distinguished single fluid parcel with label $\boldsymbol{A}$

$$\begin{aligned} \boldsymbol{X}(t) =& \boldsymbol{\chi}(\boldsymbol{A},t) \quad \text{and} \quad \boldsymbol{U}(t) = \dot{\boldsymbol{\chi}}(\boldsymbol{A},t) \\ \delta\boldsymbol{\chi}(\boldsymbol{a},t) =& \delta(\boldsymbol{a}-\boldsymbol{A})\,\delta\boldsymbol{X} \quad \text{and} \quad \delta\dot{\boldsymbol{\chi}}(\boldsymbol{a},t) = \delta(\boldsymbol{a}-\boldsymbol{A})\,\delta\boldsymbol{U}\,. \end{aligned} \tag{19}$$

Jacobi identity

- We derived before:

$$\frac{\delta\mathcal{K}}{\delta\boldsymbol{u}} = h\,\boldsymbol{\nabla}_{\boldsymbol{u}}K \qquad \text{and} \qquad \frac{\delta\mathcal{K}}{\delta h} = K\,, \tag{20}$$

$$\begin{aligned}\{\mathcal{F},\mathcal{G}\} &= \int h\,\{F,G\}\,\mathrm{d}\boldsymbol{x} \\ &= \int\left(q_{\mathrm{s}}\,\frac{\delta\mathcal{F}}{\delta\boldsymbol{u}}^{\perp}\cdot\frac{\delta\mathcal{G}}{\delta\boldsymbol{u}} - \frac{\delta\mathcal{F}}{\delta\boldsymbol{u}}\cdot\boldsymbol{\nabla}\frac{\delta\mathcal{G}}{\delta h} + \frac{\delta\mathcal{G}}{\delta\boldsymbol{u}}\cdot\boldsymbol{\nabla}\frac{\delta\mathcal{F}}{\delta h}\right)\mathrm{d}\boldsymbol{x}\,.\end{aligned} \tag{21}$$

- Hence,

$$\frac{\delta\{\mathcal{F},\mathcal{G}\}}{\delta\boldsymbol{u}} = h\,\boldsymbol{\nabla}_{\boldsymbol{u}}\{F,G\} \qquad \text{and} \qquad \frac{\delta\{\mathcal{F},\mathcal{G}\}}{\delta h} = \{F,G\}\,. \tag{22}$$

- We can transform the nested bracket in the Jacobi identity for functionals backward to an integrated one for functions

$$\{\mathcal{K},\{\mathcal{F},\mathcal{G}\}\} = \int h\,\{K,\{F,G\}\}\,\mathrm{d}\boldsymbol{x}. \tag{23}$$

- Hence, this proves the Jacobi identity (since the Jacobi identity holds for the ODE bracket $\{F,G\}$)

$$\begin{aligned}\{\mathcal{K},\{\mathcal{F},\mathcal{G}\}\} + \text{cyclic terms} = \int h\,\big(\{K,\{F,G\}\}+ \\ \text{cyclic terms}\big)\mathrm{d}\boldsymbol{x} = 0.\end{aligned} \tag{24}$$

Rotating shallow water equations 2^{nd} *continuation*

From continuum to parcel variations

Rotating SWE arise from variational principle (e.g., Salmon, 1988)

$$\begin{aligned}\delta\mathcal{S}_{\mathrm{s}} &= \delta\int_{t_0}^{t_1}\mathcal{L}_{\mathrm{s}}\,\mathrm{d}t\\ &= \delta\int_{t_0}^{t_1}\int\left[\boldsymbol{R}\circ\boldsymbol{\chi}\cdot\dot{\boldsymbol{\chi}}+\tfrac{1}{2}\,|\dot{\boldsymbol{\chi}}|^2-g\,(\tfrac{1}{2}\,h+b)\circ\boldsymbol{\chi}\right]\mathrm{d}\boldsymbol{a}\,\mathrm{d}t\,. \qquad (25)\end{aligned}$$

- $\boldsymbol{\nabla}^{\perp}\cdot\boldsymbol{R}=f$.
- Variations $\delta\boldsymbol{\chi}$ that vanish at the temporal end points.
- At solid boundaries: $\boldsymbol{n}\cdot\boldsymbol{w}=0=\boldsymbol{n}\cdot\boldsymbol{u}$.
- Eulerian form

$$0=\delta\int_{t_0}^{t_1}\int h\left[\boldsymbol{R}\cdot\boldsymbol{u}+\tfrac{1}{2}\,|\boldsymbol{u}|^2-g\,(\tfrac{1}{2}\,h+b)\right]\mathrm{d}\boldsymbol{x}\,\mathrm{d}t. \qquad (26)$$

- Using (18) and integration by parts

$$
\begin{aligned}
\delta \int \left(\tfrac{1}{2}\, h^2 + b\, h\right) \mathrm{d}\boldsymbol{x} = \int (h+b)\, \delta h \, \mathrm{d}\boldsymbol{x} \overset{(18)}{=} - \int (h+b)\, \boldsymbol{\nabla} \cdot (h\boldsymbol{w})\, \mathrm{d}\boldsymbol{x} \\
= \int \boldsymbol{\nabla}(h+b) \cdot \boldsymbol{w}\, h\, \mathrm{d}\boldsymbol{x} \\
= \int (\boldsymbol{\nabla}(h+b)) \circ \boldsymbol{\chi} \cdot \delta\boldsymbol{\chi}\, \mathrm{d}\boldsymbol{a}\,. \qquad (27)
\end{aligned}
$$

- Restrict variational principle to single “fluid parcel” $\boldsymbol{A}$.
- Consider h given height, last term in (25) and (27) is perfect variation w.r.t. parcel coordinates,

$$
\begin{aligned}
\int (\boldsymbol{\nabla}(h+b)) \circ \boldsymbol{\chi} \cdot \delta\boldsymbol{\chi}\, \mathrm{d}\boldsymbol{a} = \boldsymbol{\nabla}_{\boldsymbol{X}} \big(h(\boldsymbol{X},t) + b(\boldsymbol{X})\big) \cdot \delta\boldsymbol{X} \\
= \delta \left(h(\boldsymbol{X},t) + b(\boldsymbol{X})\right). \qquad (28)
\end{aligned}
$$

- First two terms in (25) give

$$
\begin{aligned}
\delta \int \left(\boldsymbol{R}\circ\boldsymbol{\chi}\cdot\dot{\boldsymbol{\chi}}+\tfrac{1}{2}\,|\dot{\boldsymbol{\chi}}|^2\right) \mathrm{d}\boldsymbol{a} &= \int \left[(\boldsymbol{R}\circ\boldsymbol{\chi}+\dot{\boldsymbol{\chi}})\cdot\delta\dot{\boldsymbol{\chi}}+(\nabla\boldsymbol{R})\circ\boldsymbol{\chi}\,\delta\boldsymbol{\chi}\cdot\dot{\boldsymbol{\chi}}\right] \mathrm{d}\boldsymbol{a} \\
&= (\boldsymbol{R}+\boldsymbol{u})\cdot\delta\dot{\boldsymbol{X}} + \nabla\boldsymbol{R}\,\delta\boldsymbol{X}\cdot\dot{\boldsymbol{X}} \\
&= \delta\left(\boldsymbol{R}(\boldsymbol{X})\cdot\dot{\boldsymbol{X}} + \tfrac{1}{2}\,|\dot{\boldsymbol{X}}|^2\right). \qquad (29)
\end{aligned}
$$

- Parcel variational principle

$$
\begin{aligned}
0 = \delta S_{\mathrm{s}} &= \delta \int_{t_0}^{t_1} L_{\mathrm{s}}\,\mathrm{d}t \\
&= \delta \int_{t_0}^{t_1} \left[(\boldsymbol{R}(\boldsymbol{X})\cdot\dot{\boldsymbol{X}} + \tfrac{1}{2}\,|\dot{\boldsymbol{X}}|^2 - g\left(h(\boldsymbol{X},t)+b(\boldsymbol{X})\right)\right] \mathrm{d}t.
\end{aligned}
$$

Open questions or wishful thinking?

Parcel EL Hamiltonian dynamics:

- Compressible 3D Euler equations air? B. & O. 2005.
- Generalized 2D vorticity streamfunction dynamics? B. & O. 2005.
- Compressible→hydrostatic→isopycnic/isentropic/isothermal layer model on plane? Done. B. 2005a.
- Compressible Euler equations general EoS?
- Parcel dynamics use curvilinear coordinates? Use Buitendijk 2003?
- Recast shallow layer, (quasi-)hydrostatic approximations on sphere? Use White 1999?
- Where does the simplicity end? Specialties fluid structure.
- Warning: must clearly distinguish between Eulerian and Lagrangian framework.

Parcel/particle instabilities

Static (in)stability (3D compressible Euler passive):

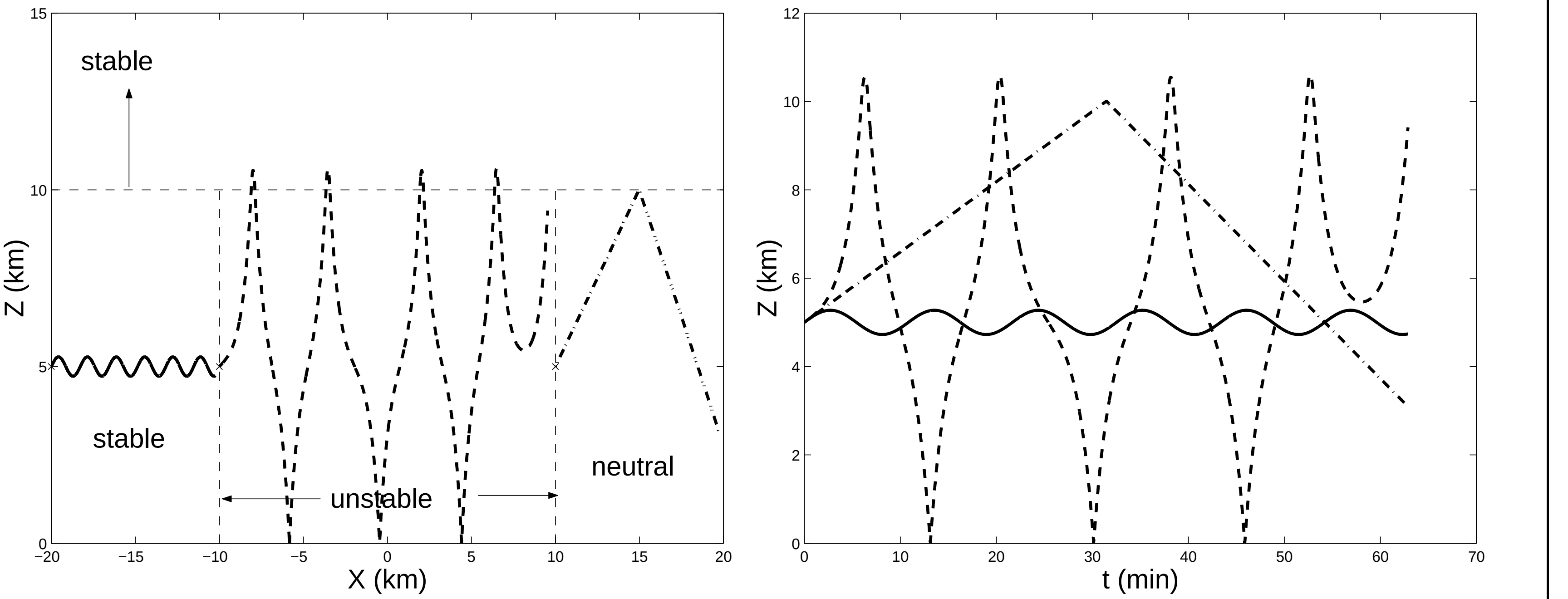


Figure 1: Stable and unstable fluid particle trajectories for statically stable oscillatory flow (solid thick line), unstable flow (dashed thick line), and neutrally stable flow (dashed-dotted thick line). Particle trajectories: (a) in vertical cross section, and (b) as function of z and t.

Inertial (in)stability (SWE passive):

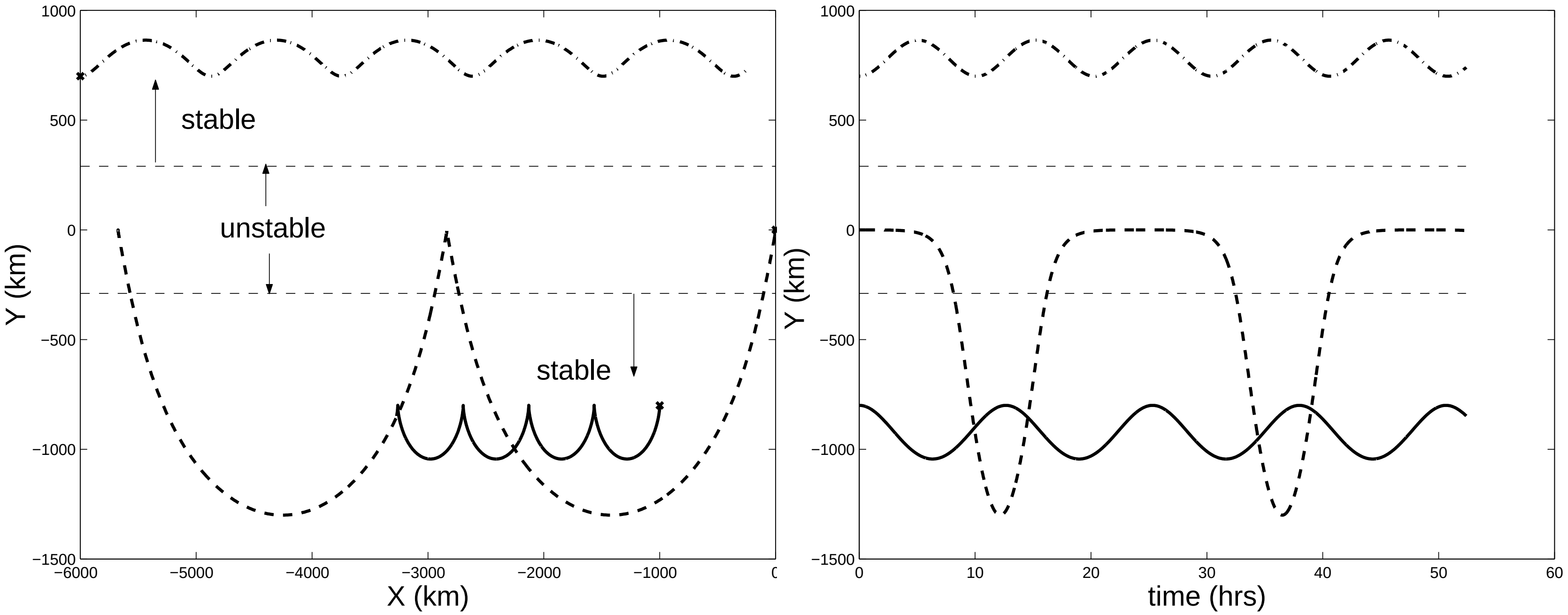


Figure 2: Three fluid particle trajectories are shown for inertially stable oscillatory flow (solid and dashed-dotted thick lines) and unstable flow (dashed thick lines) in a horizontal plane (Holton, 2004). (a) Trajectories are displayed in the X–Y-plane. (b) Trajectories are displayed in the t–Y-plane. Initially, 3 particles placed at $X = (X, Y)^T = (0, 0)^T, (-6, 0.7)^T, -(1, 0.8)^T \times 10^3\, km$.

Summary

- B. & Oliver (2006); link between Hamiltonian formulation of parcel EL dynamics and continuum PDE exemplified for:
  (i) 2D generalized vorticity streamfunction dynamics,
  (ii) **2D rotating shallow water dynamics,** and
  (iii) 3D rotating compressible dynamics for air.
- B. (2005ab) description in particle/parcel EL framework of:
  - static (in)stability, and
  - inertial (in)stability.

More open questions and wishful thinking!

Parcel EL Hamiltonian dynamics:

- Incompressible case?
- Asymptotics, balanced dynamics?
- Other instabilities & (linear) waves with parcel picture?
- Hybrid Eulerian-Lagrangian formulation. Numerical integration?
- Vlasov bracket from parcel dynamics.
- Extension with forcing and dissipation?
- Numerical "Hamiltonian" integration parcel dynamics with forcing and damping? B. and Frank (2006), NWO Climate proposal funded.

  Idelsohn et al. (non-Hamiltonian basis).

Compressible Euler general EoS

- Parcel form 3D Euler equations for ideal gas:

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = \boldsymbol{\nabla}_{\boldsymbol{u}} H_{\mathrm{c}} = \boldsymbol{U}\,, \tag{30a}$$

$$\begin{aligned}\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = -2\,\boldsymbol{\Omega}\times\boldsymbol{\nabla}_{\boldsymbol{u}} H_c - \boldsymbol{\nabla} H_c = -2\,\boldsymbol{\Omega}\times\boldsymbol{U}\\ -\Theta\,\boldsymbol{\nabla}\Pi\big(p(\boldsymbol{X},t)\big) - \boldsymbol{\nabla}\Phi(\boldsymbol{X})\,,\end{aligned} \tag{30b}$$

$$\frac{\mathrm{d}\Theta}{\mathrm{d}t} = 0\,, \tag{30c}$$

$$\rho(\boldsymbol{X},t) = \int_D \rho_0(\boldsymbol{a})\,\delta\big(\boldsymbol{X} - \boldsymbol{\chi}(\boldsymbol{a},t)\big)\,\mathrm{d}\boldsymbol{a}\,, \tag{30d}$$

$$\theta(\boldsymbol{X},t)\,\rho(\boldsymbol{X},t) = \int_D \theta_0(\boldsymbol{a})\,\rho_0(\boldsymbol{a})\,\delta\big(\boldsymbol{X} - \boldsymbol{\chi}(\boldsymbol{a},t)\big)\,\mathrm{d}\boldsymbol{a}\,, \tag{30e}$$

- Hamiltonian

$$H_{\mathrm{c}}(\boldsymbol{X},\boldsymbol{U},\Theta,t) = \frac{1}{2}\,|\boldsymbol{U}|^2 + \Theta\,\Pi\big(p(\boldsymbol{X},t)\big) + \Phi(\boldsymbol{X})\,. \tag{30f}$$

- $\Phi = \phi(\boldsymbol{X})$ external potential.
- $\theta = T\,(p/p_r)^{-\kappa}$ Eulerian, $\Theta(t) = \theta(\boldsymbol{X}(t), t)$ parcel potential temperature with temperature T, pressure p, reference pressure p_r, gas constant R, specific heat at constant pressure c_p, and $\kappa = R/c_p$.
- System closed via Exner function

$$\Pi(p) = c_p \left(\frac{p}{p_r} \right)^{\kappa} \tag{30g}$$

and ideal gas law $p = \rho R T$, such that:

$$p(\boldsymbol{X}, t) = \left(\frac{R\,\theta(\boldsymbol{X}, t)\,\rho(\boldsymbol{X}, t)}{p_r^{\kappa}} \right)^{\frac{1}{1-\kappa}} . \tag{30h}$$

- Can we write
$$-\frac{1}{\rho}\,\boldsymbol{\nabla} p = -\theta\,\boldsymbol{\nabla}\Pi \tag{31}$$
for a general Equation of State?
- Use law of thermodynamics $\mathrm{d}U = T\,\mathrm{d}s - p\,\mathrm{d}(1/\rho)$.
- Use Maxwell's relations.
- For ideal gas: $\mathrm{d}H = T\,\mathrm{d}s + (1/\rho)\,\mathrm{d}p$ and $p = \rho R T$. Hence, $\theta = T_0\,e^{(s-s_0)/c_p}$.
- What is the solution for general EoS $p = p(\rho, s)$?

Compressible Euler curvilinear coordinates

- Given compressibele Euler equations in curvilinear coordinates, can we find the parcel Hamiltonian formulation?

- Spherical case:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = -\frac{U\,W}{R} + \frac{U\,V\,\tan\phi}{R} - 2\,\Omega\,W\,\cos\phi \tag{32a}$$

$$+2\,\Omega\,V\,\sin\phi - \frac{1}{\rho\,R\,\cos\phi}\,\frac{\partial p}{\partial\lambda}, \tag{32b}$$

$$\frac{\mathrm{d}V}{\mathrm{d}t} = -\frac{V\,W}{R} - \frac{U^2\,\tan\phi}{r} - 2\,\Omega\,U\,\sin\phi - \frac{1}{\rho\,R}\,\frac{\partial p}{\partial\phi}, \tag{32c}$$

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{U^2+V^2}{R} + 2\,\Omega\,U\,\cos\phi - \frac{\partial\Phi}{\partial R} - \frac{1}{\rho}\,\frac{\partial p}{\partial\lambda}, \tag{32d}$$

$$\frac{\mathrm{d}\lambda}{\mathrm{d}t} = \frac{U}{R\,\cos\phi}, \qquad \frac{\mathrm{d}\phi}{\mathrm{d}t} = \frac{V}{R}, \qquad \frac{\mathrm{d}R}{\mathrm{d}t} = W \tag{32e}$$

with rotation Ω and (gravitational) potential $\Phi = \Phi(R)$.

- Approximate: quasi-hydrostatic, *hydrostatic* $(R = a)$, TRL equations $(R = a)$: scale and use shallowness parameter $\delta = H/L \ll 1$. Simplification in a review.
- β– and f–plane approximations, leading- and higher order.
- Isopycnic, isentropic, isothermal layer/stratified approximations.

Balanced dynamics

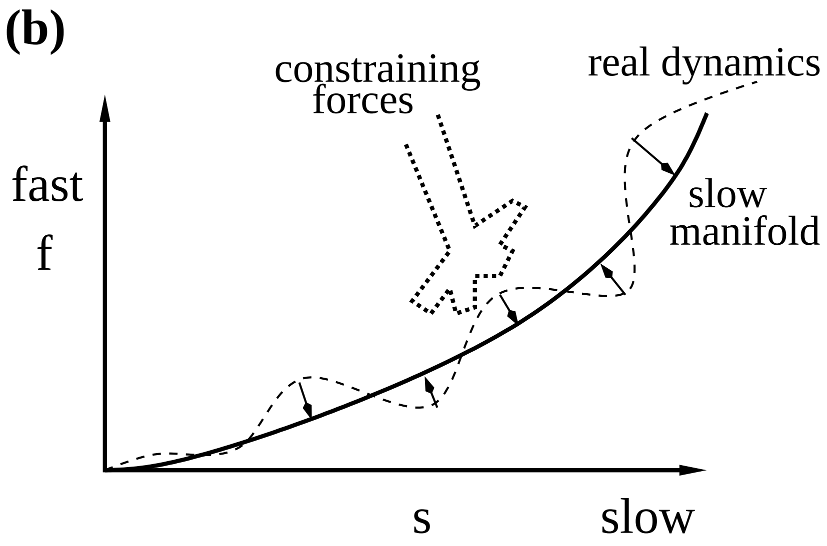
- Concept of balanced large-scale flow arises from observation that at mid-latitudes the atmosphere and oceans are in approximate geostrophic balance.

- Locally balance often fails.

- Notion of balance may be formalized in various ways: small Rossby and Froude numbers identified from measurements, observations or simulations; used in scaling arguments.

- Subsequently, perturbative or iterative approach applied to approximate full or parent model. Resulting dynamics evolves on approximate slow or slaving manifold of reduced dimensionality: slow manifold has a third (or half) of the dimension of the entire Eulerian (or Lagrangian) phase space, with fast f and slow s variables.

- Constraining forces, “hand”, place dynamics on manifold.



- Preservation variational or Hamiltonian structure, imposed heuristically in balanced approximations.
- Whether conservative or non-conservative approach to balanced dynamics better? Undecided; depends on value placed on accuracy and long-term stability.

Perturbation analysis

- Geostrophic balance denotes alignment of the velocity vectors along height contours.
- Leading order balance, we scale and rewrite shallow water equations (3)

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = \boldsymbol{\nabla}_{\boldsymbol{U}} H_{\mathrm{s}} = \boldsymbol{U}\,, \tag{33a}$$

$$\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = -\frac{f}{R}\,\boldsymbol{\nabla}^{\perp}_{\boldsymbol{U}} H_{\mathrm{s}} - \frac{1}{R}\,\boldsymbol{\nabla}_{\boldsymbol{X}} H_{\mathrm{s}} = -\frac{f}{R}\,\boldsymbol{U}^{\perp} - \frac{g}{R}\,\boldsymbol{\nabla}(h+b)\,, \tag{33b}$$

- Rossby number $R = U/(f\,L) \ll 1$: ratio of inertial time scale $1/f$ and vortical time scale L/U with typical length and velocity scales L and U.
- Leading order in R: geostrophic balance from (33a) and (33b) $U = -g\,\frac{\partial(h+b)}{\partial Y}/f$ and $V = g\,\frac{\partial(h+b)}{\partial X}/f$.

- In general, (higher-order) velocity constraints obtain form

$$\boldsymbol{\phi} = \boldsymbol{U} - \boldsymbol{U}^C[h(\boldsymbol{X})]. \tag{34}$$

- Constrained velocity $u^C[h]$ denotes a possibly non-local operator working on h and, hence, through h on parcel coordinates $\boldsymbol{X}$.

Conservative balance models: a slaved Hamiltonian approach

We illustrate the derivation of Hamiltonian balanced models in the hybrid parcel framework.

- Variables $(\boldsymbol{X}, \boldsymbol{U})$ are transformed to $(\boldsymbol{X}, \boldsymbol{\phi})$ using (34)
- Constrained variational derivative is introduced

$$\left.\frac{\partial H}{\partial X_i}\right|^C = \frac{\partial H}{\partial X_i} + \frac{\partial H}{\partial U_j}\frac{\partial U_j^C}{\partial X_i}, \tag{35}$$

  where $(\cdot)|^C$ denotes that $\phi_i = 0$ in derivatives of $\boldsymbol{X}$.

- The evolution on the slow manifold of reduced dimensionality becomes, via (3a) and (3b)

$$\frac{dX_i}{dt} = \{X_i, X_j\} \frac{\partial H^C}{\partial X_j} + \{X_i, \phi_j\} \frac{\partial H}{\partial U_j} = \frac{\partial H}{\partial U_i} = U_i \quad \text{and} \tag{36a}$$

$$\begin{aligned} 0 = \frac{d\phi_i}{dt} &= \{\phi_i, X_j\} \frac{\partial H^C}{\partial X_j} + \{\phi_i, \phi_j\} \frac{\partial H}{\partial U_j} \\ &= -\frac{\partial H^C}{\partial X_i} + \epsilon_{ij}\, hQ^C\, U_j . \end{aligned} \tag{36b}$$

with $hQ^C = f + \partial_X V^C - \partial_Y U^C$.

- The slaved Hamiltonian dynamics on the slow manifold is

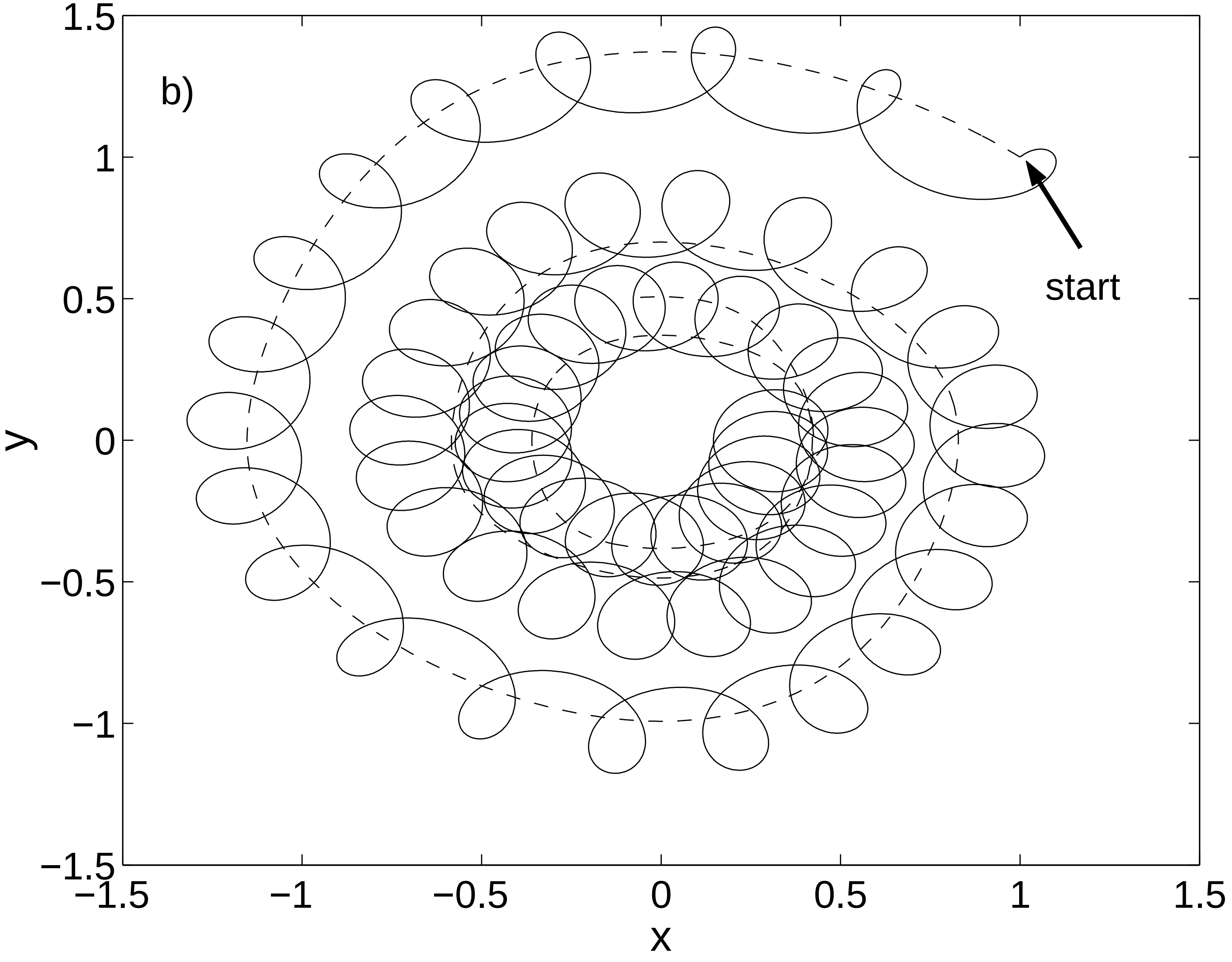
$$\frac{dX_i}{dt} = (L^{-1})_{ij} \frac{\partial H^C}{\partial X_j} \quad \text{or} \tag{37a}$$

$$\frac{\mathrm{d}F^C}{\mathrm{dt}} = \{F^C, H^C\} = \frac{\partial F^C}{\partial X_i} (L^{-1})_{ij} \frac{\partial H^C}{\partial X_j} \tag{37b}$$

[cf. Dirac (1958)] skew $L_{ij} = \epsilon_{ij}\, hQ^C$ and $F^C = F^C(\boldsymbol{X})$ and $H^C = H(\boldsymbol{X}, \boldsymbol{U}^C)$.

- Open question whether parcel balanced dynamics (37) presented is a simplified illustration or equivalent to the results for the Eulerian Hamiltonian balanced equations of Vanneste and B. (2002).
- Can we transform the function bracket to the functional bracket and prove the Jacobi identity?

- 41.7 days of (dimensionless) geostrophically balanced and unbalanced Hamiltonian motion of a particle in a simple potential $h(\boldsymbol{X})$. $(\boldsymbol{X})(0) = (1, 1)$. Predictability horizon lies around 14 days when the balanced and unbalanced trajectories depart.


b)
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1.5
x

Hybrid Eulerian-Lagrangian formulation

- Eulerian-Lagrangian bracket in terms of Lagrangian velocity $\mathbf{u}^L(\mathbf{a},t)$ and Eulerian depth $h(\mathbf{x},t)$

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \iint f\,\hat{\mathbf{z}} \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{u}^L} \times \frac{\delta \mathcal{H}}{\delta \mathbf{u}^L} + \left(\boldsymbol{\nabla} \frac{\delta \mathcal{F}}{\delta h} \right) \circ \chi \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{u}^L} - \left(\boldsymbol{\nabla} \frac{\delta \mathcal{H}}{\delta h} \right) \circ \chi \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{u}^L}\,\mathrm{d}\boldsymbol{a}. \tag{38}$$

- Hamiltonian quadratic

$$\mathcal{H} = \iint \frac{1}{2}\,|\mathbf{u}^L|^2\,\mathrm{d}\boldsymbol{a} + \iint \frac{1}{2}\,g\,(h+b)^2\,\mathrm{d}\boldsymbol{x}. \tag{39}$$

- Variation of (39) gives

$$\frac{\delta \mathcal{H}}{\delta h} = g\,(h + h_b) \qquad \text{and} \qquad \frac{\delta \mathcal{H}}{\delta \mathbf{u}^L} = \mathbf{u}^L. \tag{40}$$

- Substitute variations (40) into (38) for $\mathcal{F} = h(\mathbf{x}, t), \mathbf{u}^L(\boldsymbol{a}, t)$.
- Use $h\,\mathrm{d}\boldsymbol{x} = \mathrm{d}\boldsymbol{a}$ to swap between the Eulerian and Lagrangian framework .
- Gives Eulerian continuity and Lagrangian momentum equations

$$
\begin{aligned}
\frac{\partial h}{\partial t} + \boldsymbol{\nabla} \cdot (h\,\mathbf{u}) &= 0 \\
\frac{\partial \mathbf{u}^L}{\partial t} + f\,\hat{\mathbf{z}} \times \mathbf{u}^L &= -\,g\,\boldsymbol{\nabla}(h + b).
\end{aligned}
\tag{41}
$$

- Require map between Eulerian and Lagrangian space:

$$\mathbf{u}^L = \mathbf{u} \circ \chi.$$

Vlasov dynamics

- Kinetic or Vlasov equation with probability distribution D

$$\frac{\mathrm{d}\mathsf{D}}{\mathrm{d}t} + \boldsymbol{\nabla}\cdot(\bar{\zeta}\,\mathsf{D}) - \boldsymbol{\nabla}_{\zeta}\cdot[(f\,\hat{\mathbf{z}}\times\bar{\zeta} + g\,\boldsymbol{\nabla} h_b)\,\mathsf{D}] = 0 \tag{42}$$

distribution function $\mathsf{D} = \mathsf{D}(\bar{x}, \bar{\zeta}, t)$, $\bar{x} = (x, y) = (x_1, x_2)$, velocity coordinates $\bar{\zeta} = (\zeta_1, \zeta_2)$, and time t; spatial operator $\boldsymbol{\nabla}$; potential $g\,h_b(\bar{x})$; and velocity operator $\boldsymbol{\nabla}_{\zeta}$.

- Parcel Hamiltonian formulation

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} &= \bar{\zeta} = \frac{\partial H_p}{\partial \bar{\zeta}} \qquad \frac{\mathrm{d}\bar{\zeta}}{\mathrm{d}t} + f\,\hat{\mathbf{z}}\times\bar{\zeta} = -g\,\boldsymbol{\nabla}_{\boldsymbol{X}} h_b = -\frac{\partial H_p}{\partial \boldsymbol{X}} \\ H_p &= \frac{1}{2}\,\bar{\zeta}^2 + g\,h_b(\boldsymbol{X}). \end{aligned} \tag{43}$$

- For $f = 0$, function $F = F(\bar{x}, \bar{\zeta})$ is related to the functional

$$\mathcal{F} = \iint \mathsf{D}\,F(\bar{x}, \bar{\zeta})\,\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{\zeta}. \tag{44}$$

- Relation of functional and function derivatives

$$\delta\mathcal{F} = \iint \frac{\delta\mathcal{F}}{\delta \mathsf{D}}\,\delta\mathsf{D}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{\zeta} = \iint F\,\delta\mathsf{D}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{\zeta}. \tag{45}$$

- Hence

$$\begin{aligned}\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} =& \{\mathcal{F},\mathcal{H}_p\} = \iint \mathsf{D}\,\frac{\mathrm{d}F}{\mathrm{d}t}(\bar{x},\bar{\zeta})\,\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{\zeta}\\ =& \iint \mathsf{D}\,\{F,H_p\}\,\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{\zeta}\\ =& \iint \mathsf{D}\left(\boldsymbol{\nabla}\frac{\delta\mathcal{F}}{\delta\mathsf{D}}\cdot\boldsymbol{\nabla}_\zeta\frac{\delta\mathcal{H}_p}{\delta\mathsf{D}} - \boldsymbol{\nabla}\frac{\delta\mathcal{H}_p}{\delta\mathsf{D}}\cdot\boldsymbol{\nabla}_\zeta\frac{\delta\mathcal{F}}{\delta\mathsf{D}}\right)\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{\zeta}.\end{aligned} \tag{46}$$

- Since $\delta\mathcal{H}_p/\delta\mathsf{D} = H = |\boldsymbol{\zeta}|^2/2 + g\,h_b(\boldsymbol{x})$, we find

$$\mathcal{H}_p = \iint \mathsf{D}\left(|\boldsymbol{\zeta}|^2/2 + g\,h_b(\boldsymbol{x})\right)\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{\zeta}. \tag{47}$$

- For $f \neq 0$, follow ideas in B. (2005, *Applied Math. Lett.*).