Large-scale atmospheric circulation, semi-geostrophic motion and Lagrangian particle methods

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References: R Salmon "Lectures on geophysical fluid dynamics", M Cullen "A mathematical theory of large-scale atmosphere/ocean flow", CJ Cotter & S Reich "Semi-geostrophic particle motion and exponentially accurate normal forms".

1. Hyrostatic and semi-geostrophic approximation

Euler's equations for a rotating fluid in Cartesian geometry are given by

$$\frac{D\mathbf{u}}{Dt} + f\mathbf{k} \times \mathbf{u} + \frac{1}{\rho}\nabla p + g\mathbf{k} = 0,$$

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\theta_t + \mathbf{u} \cdot \nabla \theta = 0,$$

where $\mathbf{u} \in \mathbb{R}^3$ is the velocity (wind) field, θ is the potential temperature, $k = (0, 0, 1)^T$, $f = 2\Omega \sin \phi_0$ is the Coriolis parameter, g is the gravitational constant, the ideal gas law becomes

$$\theta = T(p_0/p)^{R/c_p},$$

and material time derivative is

$$\frac{df}{dt} := f_t + \mathbf{u} \cdot \nabla f.$$



A good model for large scale circulations is provided by the hydrostatic and semi-geostrophic (SG) model:

$$\frac{D\mathbf{u}_g}{Dt} + f\mathbf{k} \times \mathbf{u} + \frac{1}{\rho}\nabla p + g\mathbf{k} = 0,$$

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\theta_t + \mathbf{u} \cdot \nabla \theta = 0,$$

with the geostrophic wind approximation

$$\mathbf{u}_g = \left[\begin{array}{ccc} u_g & v_g & \mathbf{0} \end{array} \right]^T$$

and

$$fu_g = -\frac{1}{\rho} \frac{\partial p}{\partial y}, \qquad fv_g = +\frac{1}{\rho} \frac{\partial p}{\partial x}.$$

In northern hemisphere: Stand with your back to the wind, pressure increases to the right.

2. The shallow water equations

A single layer approximation is provided by the shallow water equations (SWE):

$$\frac{Du}{Dt} - fv = -g\frac{\partial}{\partial x}(h_s + \eta),$$

$$\frac{Dv}{Dt} + fu = -g\frac{\partial}{\partial y}(h_s + \eta),$$

$$\eta_t = -\left(\frac{\partial(\eta u)}{\partial x} + \frac{\partial(\eta v)}{\partial y}\right)$$

with material time derivative

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y}.$$

Here η is the layer depth, h_S is the surface orography, g is the gravitational constant, and f is twice the Earth's angular velocity.

3. Scaling limits and SG approximation

We non-dimensionalize the equations by using scaled variables (denoted with a dash) as follows

$$(x,y) = L(x',y'), \quad t = \left(\frac{L}{U}\right)t', \quad (u,v) = U(u',v'), \quad \eta = H\eta'.$$

Upon introducing $\mathbf{u}' = (u',v')^T$, $J_2 = \begin{pmatrix} 0 & 1\\ -1 & 0 \end{pmatrix}$,

 $Ro = \frac{U}{fL}$ (Rossby number), $Fr = \frac{U}{\sqrt{gH}}$ (Froude number),

we obtain the scaled shallow water equations $(h_s = 0)$

$$\frac{D\mathbf{u}'}{Dt'} = Ro^{-1}J_2\mathbf{u}' - Fr^{-2}\nabla\eta',$$

$$\frac{\partial\eta'}{\partial t'} = -\nabla \cdot (\eta'\mathbf{u}').$$

The semi-geostrophic (SG) scaling regime is

$$\varepsilon = Fr^2 = Ro \to 0.$$

This regime is observed for global atmospheric flow patterns.

It follows that

$$\varepsilon \frac{D\mathbf{u}'}{Dt'} = J_2 \mathbf{u}' - \nabla \eta'$$

and approximate geostrophic wind balance

$$J_2\mathbf{u}'\approx\nabla\eta'$$

follows for $\varepsilon \to 0$ and bounded time-derivatives, i.e., $||D\mathbf{u}'/Dt'|| \le M$. Defining $\mathbf{u}'_q = -J_2 \nabla \eta'$, we obtain the SG equations

$$\varepsilon \frac{D\mathbf{u}'_g}{Dt} = J_2 \mathbf{u}' - \nabla \eta', \qquad \eta' = -\nabla \cdot (\eta' \mathbf{u}').$$

Historical comments:

A first mathematical use of the geostrophic wind approximation goes back to Charney (quasi-geostrophic approximation) and Eliasen (semi-geostrophic (SG) approximation) 1947-1949.

The importance of SG to frontogenesis was discovered by Hoskins (1972) who also formulated a simplifying coordinate transformation.

Its link to geometric PDEs such as the Monge-Ampere equations was pointed out by Cullen & Purser (1987).

Alternatively, Salmon (1985) has studied asymptotic expansions and coordinate transformations on the level of the Lagrangian variational principle.

Lorenz studied the existence and non-existence of slow manifolds (1992) with implications to data assimilation and initialization.

4. The single fluid-particle picture

Instead of investigating the full SWEs, we consider the following simpler model problem (Gottwald & Oliver, Cotter & Reich).

We assume that the layer depth $\mu(\varepsilon t, x, y)$ is a given function of time t and space $\mathbf{x} = (x, y)^T$. We may then investigate the motion of a single fluid parcel with coordinates $\mathbf{q} = (q_x, q_y)^T \in \mathbb{R}^2$. The corresponding Newtonian equations of motion are given by

$$\varepsilon \frac{d^2 q_x}{dt^2} = + \frac{dq_y}{dt} - \mu_{q_x}(\varepsilon t, q_x, q_y),$$

$$\varepsilon \frac{d^2 q_y}{dt^2} = - \frac{dq_x}{dt} - \mu_{q_y}(\varepsilon t, q_x, q_y),$$

We next rescale time and introduce the new time-scale $\tau = \varepsilon t$. We denote time derivatives with respect to τ by overdot, *e.g.*, $dq_x/d\tau = \dot{q}_x$. We also introducue the momentum $\mathbf{p} = (p_x, p_y)^T \in \mathbb{R}^2$ and obtain

$$\dot{p}_x = +p_y - \varepsilon \,\mu_{q_x}(\tau, q_x, q_y),$$

$$\dot{p}_y = -p_x - \varepsilon \,\mu_{q_y}(\tau, q_x, q_y),$$

$$\dot{q}_x = p_x,$$

$$\dot{q}_y = p_y.$$

These equations may be expressed in a more compact form:

$$\dot{\mathbf{p}} = J_2 \mathbf{p} - \varepsilon \nabla \mu(\tau, \mathbf{q}), \qquad J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

$$\dot{\mathbf{q}} = \mathbf{p}.$$

The associated SG equations are given by

$$\dot{\mathbf{p}}_g = J_2 \mathbf{p} - \varepsilon \nabla \mu(\tau, \mathbf{q}), \dot{\mathbf{q}} = \mathbf{p},$$

with geostrophic "wind" $\mathbf{p}_g = -\varepsilon J_2 \nabla \mu(\tau, \mathbf{q})$. For time-independent μ (which we assume from now on), the energy

$$E = \frac{1}{2} \|\mathbf{u}_g\|^2 + \varepsilon \mu(\mathbf{q})$$

is preserved.

The Hoskins' transform

$$\mathbf{q}_{\varepsilon} = \mathbf{q} + \varepsilon \nabla \mu(\mathbf{q}) = \mathbf{q} + J_2 \mathbf{p}_g$$

leads to the following equation in the transformed variable q_{ε} :

$$\dot{\mathbf{q}}_{\varepsilon} = -\varepsilon J_2 \nabla \mu(\mathbf{q}).$$

An important observation is that one may view Hoskins' transformation as an energy minimization problem in q for given q_{ε} :

$$E_{\mathbf{q}_{\varepsilon}}(\mathbf{q}) = \frac{1}{2} \|\mathbf{q}_{\varepsilon} - \mathbf{q}\|^{2} + \varepsilon \mu(\mathbf{q}).$$

The SG model in transformed variables can be derived from the Lagrangian functional

$$\mathcal{L} = \int \left[\frac{1}{2} \|\mathbf{q}_{\varepsilon} - \mathbf{q}\|^2 + \varepsilon \mu(\mathbf{q}) + \frac{1}{2} \dot{\mathbf{q}}_{\varepsilon}^T J_2 \mathbf{q}_{\varepsilon} \right].$$

Let us reconsider the energy minimization problem and denote the induced map by $\mathbf{q} = s(\mathbf{q}_{\varepsilon})$ with inverse $t = s^{-1}$. Hence

$$\int_{\mathbb{R}^2} E_{t(\mathbf{q})}(\mathbf{q}) \, dA(\mathbf{q}) = \int_{\mathbb{R}^2} \frac{1}{2} \|t(\mathbf{q}) - \mathbf{q}\|^2 dA(\mathbf{q}) + C$$
$$= \int_{\mathbb{R}^2} \frac{1}{2} \|\mathbf{q}_{\varepsilon} - s(\mathbf{q}_{\varepsilon})\|^2 \nu \, dA(\mathbf{q}_{\varepsilon}) + C$$
$$\nu = |s'| \text{ and } C = \varepsilon \int_{\mathbb{R}^2} \mu(\mathbf{q}) dA(\mathbf{q}).$$

with

This is an optimal transport/coupling problem of a measure $d\mu_1 = \nu dA(\mathbf{q}_{\varepsilon})$ into the Lebesgue measure $d\mu_2 = dA(\mathbf{x})$ on \mathbb{R}^2 in the Wasserstein metric

$$W_2(\mu_1, \mu_2) = \inf_{\lambda \in \Gamma(\mu_1, \mu_2)} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \|\mathbf{x} - \mathbf{y}\|^2 d\lambda(\mathbf{x}, \mathbf{y}).$$

5. Lagrangian and Hamiltonian framework

Hamiltonian picture. We introduce the non-canonical symplectic structure operator

$$J = \begin{pmatrix} J_2 & -I_2 \\ I_2 & 0_2 \end{pmatrix} \in \mathbb{R}^{4 \times 4},$$

so that the equations become

$$\dot{\mathbf{z}} = J\nabla H_0(\mathbf{z}),$$

with Hamiltonian

$$H_0(\mathbf{z}) = K(\mathbf{p}) + \varepsilon V(\mathbf{q}), \quad K(\mathbf{p}) := \frac{1}{2} \mathbf{p}^T \mathbf{p}, \quad V(\mathbf{q}) := \mu(\mathbf{q}),$$

and phase space variable $\mathbf{z} = (\mathbf{p}^T, \mathbf{q}^T)^T \in \mathbb{R}^4.$

Lagrangian picture. Another approach is to rewrite the system of first-order equations as a second-order equation

$$\ddot{\mathbf{q}} - J_2 \dot{\mathbf{q}} + \varepsilon \nabla \mu(\mathbf{q}) = \mathbf{0}.$$

This is the Euler-Lagrange equation for the Lagrangian functional

$$\mathcal{L} = \int d\tau \left[\frac{1}{2} \| \dot{\mathbf{q}} \|^2 + \frac{1}{2} \mathbf{q}^T J_2 \dot{\mathbf{q}} - \varepsilon \mu(\mathbf{q}) \right].$$

One may alternatively work with the degenerate Lagrangian

$$\mathcal{L} = \int d\tau \left[\left(\mathbf{p} - \frac{1}{2} J_2 \mathbf{q} \right)^T \dot{\mathbf{q}} - H_0(\mathbf{q}, \mathbf{p}) \right].$$

6. The variational approach to semi-geostrophy

Rick Salmon's derivation of semi-geostrophic models starts from the assumption that we may replace ${\bf p}$ by the geostrophically balanced

$$\mathbf{p}_g = -\varepsilon J_2 \nabla \mu(\mathbf{q})$$

in the degenerate Lagrangian formulation.

Under this assumption, we may formally collect terms of equal order in ε and rewrite the Lagrangian functional as

$$\mathcal{L} = \int d\tau \left[\varepsilon L_0 + \varepsilon^2 L_1 \right],$$

for suitably chosen Lagrangian densities L_0 and L_1 . We then ignore the $\mathcal{O}(\varepsilon^2)$ term.

To improve this approximation, we introduce transformed coordinates $\mathbf{q}_{\boldsymbol{\varepsilon}}$ via

$$\mathbf{q} = \psi_{\varepsilon}(\mathbf{q}_{\varepsilon}) = \mathbf{q}_{\varepsilon} + \varepsilon \mathbf{F}_{1}(\mathbf{q}_{\varepsilon}) + \mathcal{O}(\varepsilon^{2}).$$

Following Rick Salmon's and Marcel Oliver's work, we set

$$\mathbf{F}_1(\mathbf{q}_{\varepsilon}) = -\frac{1}{2} \nabla \mu(\mathbf{q}_{\varepsilon}) + \lambda \nabla \mu(\mathbf{q}_{\varepsilon}).$$

Upon dropping $\mathcal{O}(\varepsilon^3)$ terms, we obtain the Lagrangian

$$\mathcal{L}_{\varepsilon} = \int d\tau \left\{ \frac{1}{2} \mathbf{q}_{\varepsilon}^{T} J_{2} \dot{\mathbf{q}}_{\varepsilon} - \varepsilon \mu(\mathbf{q}_{\varepsilon}) + \varepsilon \left[\frac{1}{2} + \lambda \right] \nabla \mu(\mathbf{q}_{\varepsilon})^{T} J_{2} \dot{\mathbf{q}}_{\varepsilon} - \varepsilon^{2} \lambda \| \nabla \mu(\mathbf{q}_{\varepsilon}) \|^{2} \right\}.$$

One can set $\lambda = 0$, but the choice $\lambda = -1/2$ is of particular interest as it is close (but not identical) to Hoskins' transformation and to Rick Salmon's large-scale semi-geostrophic approximation. The associated reduced equations of motion

$$J_2 \dot{\mathbf{q}}_{\varepsilon} = \varepsilon \nabla \left\{ \mu(\mathbf{q}_{\varepsilon}) - \frac{\varepsilon}{2} \| \nabla \mu(\mathbf{q}_{\varepsilon}) \|^2 \right\}$$

can be derived from the Lagrangian functional

$$\mathcal{L}_{\mathsf{Isg}} = \int d\tau \left[\frac{1}{2} \mathbf{q}_{\varepsilon}^T J_2 \dot{\mathbf{q}}_{\varepsilon} - \varepsilon \mu(\mathbf{q}_{\varepsilon}) + \frac{\varepsilon^2}{2} \|\nabla \mu(\mathbf{q}_{\varepsilon})\|^2 \right]$$

These equations look like a "Taylor expanded" version of Hoskin's SG equation

$$J_2 \dot{\mathbf{q}}_{\varepsilon} = \varepsilon \nabla \mu(\mathbf{q}), \qquad \mathbf{q}_{\varepsilon} = \mathbf{q} + \varepsilon \nabla \mu(\mathbf{q}).$$

7. The normal form approach to semi-geostrophy

A more complete picture of the dynamics can be obtained from the Hamiltonian side of things and normal form theory. (Cotter & Reich, 2006)

Our aim is to find a canonical near-identity change of coordinates Ψ_n so that

$$H_n = H_0 \circ \Psi_n = K + \varepsilon G_n + \varepsilon^{n+1} R_n, \tag{1}$$

where

$$\{G_n, K\} = 0, \tag{2}$$

with $\{\cdot, \cdot\}$ being the Poisson bracket obtained from J.

A few key results from Cotter and Reich, 2006.

Corollary. Let us assume that the momentum $\mathbf{p} = \dot{\mathbf{q}}$ satisfies $\mathbf{p}(0) = -\varepsilon J_2 \nabla \mu(\mathbf{q}(0)) + \mathcal{O}(\varepsilon^2)$

at initial time $\tau = 0$, then

$$\mathbf{p}(\tau) = -\varepsilon J_2 \nabla \mu(\mathbf{q}(\tau)) + \mathcal{O}(\varepsilon^2)$$

for all $|\tau| < e^{c/2\varepsilon}$ provided the potential $V = \mu$ is real-analytic.

This means that provided the system is within $\mathcal{O}(\varepsilon^2)$ of the geostrophically balanced state initially, it will stay there for exponentially long time intervals.

If $p_{\varepsilon}(0) = 0$, (*i.e.*, we start on the "slow manifold") then we get the "slow equation" given in the following corollary:

Corollary. If $p_{\varepsilon}(0) = 0$ then

$$J_2 \dot{\mathbf{q}}_{\varepsilon} = \varepsilon \nabla_{\mathbf{q}} G(\mathbf{0}, \mathbf{q}_{\varepsilon}) + \mathcal{O}(e^{-c/2\varepsilon}),$$

for all $|\tau| < e^{c/2\varepsilon}$.

Corollary. To leading order the symplectic change of coordinates reduces on the slow manifold to Hoskins/Salmon tranformation (i.e., $\lambda = -1/2$ in Salmon's formula).

8. A step towards the continuum limit

So far we have assumed that the fluid depth μ is a given function of space and time and derived equations of motion for a single 'fluid parcel'.

Now we consider a numerical approximation for μ of the form

$$\mu(t, \mathbf{x}) = \sum_{i=1}^{N} m_i \psi(\|\mathbf{x} - \mathbf{q}_i(t)\|)$$

in terms of N moving 'fluid parcels', where $q_i(t) \in \mathbb{R}^2$ denotes the location of the *i*th fluid parcel at time t with mass m_i and shape function $\psi(r) \ge 0$.

The above layer-depth approximation provides the starting point for smoothed particle hydrodynamics (SPH).

Each 'fluid parcel' moves under the Newtonian equations of motion

$$\frac{d}{dt}\mathbf{p}_i = Ro^{-1}J_2\mathbf{p}_i - Fr^{-2}\nabla_{\mathbf{x}}\mu(t,\mathbf{x})|_{\mathbf{x}=\mathbf{q}_i},$$
$$\frac{d}{dt}\mathbf{q}_i = \mathbf{p}_i$$

After setting $Fr^2 = Ro = \varepsilon$ and a rescaling of time, these equations become

$$\dot{\mathbf{p}}_{i} = J_{2}\mathbf{p}_{i} - \varepsilon \nabla_{\mathbf{x}} \mu(\mathbf{x}, t)|_{\mathbf{x}=\mathbf{q}_{i}},$$

$$\dot{\mathbf{q}}_{i} = \mathbf{p}_{i}.$$

Without restriction of generality, we may also assume that all 'fluid parcels' carry a constant mass $m_i = m$. Then the equations posses the Hamiltonian function

$$H_{\mathsf{sph}}(\mathbf{z}) = K(\mathbf{p}) + \varepsilon V(\mathbf{q}) = \sum_{i=1}^{N} \frac{1}{2} \|\mathbf{p}_i\|^2 + \frac{\varepsilon m}{2} \sum_{i,j}^{N} \psi(\|\mathbf{q}_i - \mathbf{q}_j\|),$$

Note that a finite fluid depth μ implies that the particle masse m approach zero as the number of particles $N \to \infty$. More precisely, m N = const. as $N \to \infty$.

For a given basis function ψ , the SPH method converges for $N \rightarrow \infty$ to solutions of a regularized set of SWEs (Oelschläger, 1991; Di Lisio et al, 1998). Global existence and uniqueness of solutions follows.

Main findings (Cotter & Reich):

- 1. The single particle theory goes through for fixed N and $\varepsilon \to 0$ as well.
- 2. The estimates do *not* deteriorate for fixed ψ with increasing N since there is (i) only a single fast frequency determined by f = constant and (ii) mN = constant as $N \to \infty$ (conservation of total mass).
- 3. Normal form theory implies that there is hardly any tranfer between potential and kinetic energy. Particles may however exchange their kinetic energy contributions.
- 4. The analysis collapses however in case the basis functions ψ approach a Dirac delta function as $N \to \infty$. But it is perhaps feasible for sufficiently regular initial conditions.

Exchange of kinetic energy between two particles:



A particle simulation of barotropic instability:



9. Summary

The semi-geostrophic approximation is one of the most useful theoretical tools in large-scale meteorology (e.g., frontogenesis).

A lot of theory has been developed around the SG equations and interesting links to various fields have been made. We have explained some of the main points in terms of a simple single particle model.

Hamiltonian normal form theory allows for arbitrarily accurate SG models in terms of a regularized set of fluid equations and is applicable to numerical particle methods.

Frontogenesis is still rather poorly approximated by todays NWP codes (Cullen). Can better methods be devised using SG explicitly (Cullen) or implicitly (moving mesh methods (Budd); particle methods)?