On "objective" (optimization-based) formulation of hybrid coordinate gridding

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Acknowledgement: Mohamed Iskandarani, Carlisle Thacker

- Hybrid coordinate generation (HybGen), or regridding for heterogeneous vertical coordinates at each timestep, is a highly nonlinear procedure.
- Typical data assimilation procedure is a least-squares of linear terms (equivalently, Bayesian analysis on assumed Gaussian densities).
- How can data assimilation be fixed to be (more) consistent with HybGen?

Motivation: Residual SSH over Gulf of Mexico (1/12° HYCOM data assimilation experiment)

TIME : 28-SEP-1999 00:00



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Errors over shallow areas where a *terrain-following* (depth based) coordinate is used.

Contours at 100 : 100 : 1000 meters



Hybrid coordinate specifications (simplified):

- L = 20 layers, indexed by l = 1, 2, ..., L.
- Minimum layer thickness: *h_l*,
 e.g., {3.0, 3.5, 4.0, 4.5, ... meters}.
 (terrain-based values in shallow areas.)
- Target densities (isopycnal densities): ρ_l.
 (the preferred coordinate if minimum h_l is met.)

• HYCOM:
$$(\rho, z) \longrightarrow (\alpha, p)$$

 $\alpha \equiv 1/\rho, \ p \equiv \rho g z, \ h \longrightarrow \delta p$

Mid-domain Gulf of Mexico density profiles: summer & winter density-1025 [kg/m³]



- Problem with homogeneous vertical propagation of data: $\Delta(SSH) \rightarrow \Delta(\delta p_l), \ l = 1,...,L-1$
- Cannot avoid $\delta p_l < 0$.
- Either δp_l or α_l is constant (target value): $\Delta(SSH) = \sum_{l=1}^{L} \Delta(\alpha_l \delta p_l)$

– Positivity (minimum value): $\delta p_l \ge \delta p_l^* \ge 0$.

- Mass conservation: $\int \rho dz$ or $\int dp$ fixed/known.
- Volume conservation: $\int dz$ or $\int \alpha d(\delta p)$ fixed/known.

To update model state x by data

- 1. Coordinate regimes (fixed values) need to be known.
- 2. Minimum layer-thickness (inequality) constraint: $Sx \ge c$.
- 3. Mass/volume conservation (equality) constraints: Ax = b.

Sequential assimilation: (background _b is the model forecast; y is data) $\min_{x} \|x - x_{b}\|_{P_{b}^{-1}}^{2} + \|y - Hx\|_{R^{-1}}^{2}$

becomes a *constrained* minimization.

Applying constrained optimization

- Increased computational cost:
 - Equality constraints: 2 more variables per profile.
 - Inequality constraints: combinatorial trials, 2^{*L*} cases!
- An approximation ...
 - Build around existing assimilation routine.

- 1. Identify the coordinate regimes.
- 2. Perform (typical) data assimilation steps; project the results onto the target coordinate systems. $\rightarrow \overline{x}$ (unconstrained state values);
- 3. Apply equality (mass/volume conservation) constraints:

$$\min_{\mathbf{x}} \|\mathbf{x} - \bar{\mathbf{x}}\|^2 + \text{regularization}(\mathbf{x})$$

Identify Coordinate Regimes



Coordinate Transition Line



Uncertainty/Ambiguity in Regime Transition



→ use several "regime maps".

Steps in an assimilation cycle (SSH)

Repeated trials for regime-boundaries & inequalities:

- 1. Identify the coordinate regimes.
- 1a. Make alternative regime maps by perturbing the boundaries.
- 2. Perform (classical) data assimilation steps; project the results onto the target coordinate systems.

 $\rightarrow \overline{x}$ (unconstrained state values);

2a. Repeat 2 with all regime maps; choose $\bar{\mathbf{x}}$ that minimizes $\|\bar{\mathbf{x}} - \mathbf{x}_b\|^2$.

Steps in an assimilation cycle (SSH) (cont')

3. Apply equality (mass/volume conservation) constraints: $\label{eq:min_x} \min_{\mathbf{x}} \ \|\mathbf{x} - \bar{\mathbf{x}}\|^2 + \mbox{regularization}(\mathbf{x})$

3a. If any δp_l *violates its minimum, set* δp_l *to the minimum and repeat 3.*

Application of mass & volume (equality) constraints

• Normalized layer thickness $\delta p_{\ell}/p_L$ would form a *probability mass function* (PMF).

 $ightarrow ~\delta p_\ell \geq 0$, always.

- Mass = 0th order statistical moment; Volume = 1st order statistical moment (the mean). (In *ρ-z* system, mass = 1st order and volume = 0th.)
- Existing formulas/procedures in applied probability?
 - Moment matching (0th to (L-1)st) \rightarrow regularization needed!
 - *−* "Histopolation" (area-matching interpolation).
 → provision for $\delta p_{\ell} \ge 0$?

Experiments:

• Given $p_L = \sum_{\ell=1}^L \delta p_\ell$ and $SSH = \sum_{\ell=1}^L \alpha_\ell \, \delta p_\ell$

$$\min \sum_{\ell \in \text{isobars}} (\alpha_{\ell} - \bar{\alpha}_{\ell})^2 + \sum_{\ell \in \text{isopycnal}} (\delta p_{\ell} - \overline{\delta p}_{\ell})^2$$

- 1. A reference (α, p) profile is perturbed.
- 2. Perturbed profile is re-gridded using the mass (p_L) and volume (SSH) values from the reference.

- Is the re-gridding robust/unique?
- How does it respond to $\Delta(SSH)$?

Example: re-gridding of perturbed density profile



"Errors" before & after re-gridding



"Error" as a function of perturbation size



Random variations in SSH: vertical distribution



SSH-constrained regridding over Gulf-of-Mexico (HYCOM)

 Δ (SSH): "before"



 Δ (SSH): "after"



Re-gridded layer-interfaces over Florida Shelf



<u>Summary</u>

- A modest (computationally etc) scheme for post-assimilation adjustments:
 - Coordinate regime identification
 - Lagrange multipliers
 - \rightarrow being applied to SSH (and T profile) data sets
- A more general formulation: functional/continous representations $\alpha(s), p(s), \text{ etc.}$
 - *"Histopolation"* (area-preserving spline)
 - Area-preserving sampling (!)
- Other approaches
 - Ensemble filter: constraints applied during ensemble generation.
 - 4D-Var: HybGen-conscious adjoint (linearized backward) model.