# What should an "Outer Loop" for ensemble data assimilation look like?


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# Motivation

- When observations clearly indicate feature but none of the ensemble members has the feature, rerunning ensemble in outer loop provides opportunity to obtain a “better” ensemble.
- Features of interest might include clouds, precip or ribbons of chemicals/PV in the stratosphere.

# What we've done

- Algebraically derived *error form* or *observation space form* of weak and strong constraint incremental 4D-VAR
- Based on interpretations of the *meaning* of the outer loop in observation space, proposed ensemble based analogues to incremental 4D-VAR.
- Tested proposals on simple model of solitary waves.

# Things to consider

- If ensemble gives distribution of truth given forecast then 4D ensemble covariance equals true 4D forecast error covariance matrix. In this case, (ensemble) Kalman smoother gives minimum error variance estimate (BLUE). What can an outer loop add to this?
- Would an outer loop turn an ensemble that is not the distribution of truth given the forecast into one that does?
- Bishop and Shanley (2008, MWR) argue that some ensembles better approximate distribution of historical forecasts given that today's ensemble mean is the truth than the *prior* distribution of truth. Does an ensemble outer loop make more sense from this perspective?

# Weak constraint 4D-VAR

Minimize

$$J(\underline{\mathbf{x}}) = J_b(\underline{\mathbf{x}}) + J_m(\underline{\mathbf{x}}) + J_o(\underline{\mathbf{x}}),\ \text{where}$$

$$J_b(\underline{\mathbf{x}}) = \frac{1}{2}\left(\underline{\mathbf{x}}^f - \underline{\mathbf{x}}\right)^T \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \mathbf{P}_0^{g-1} \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}^T \left(\underline{\mathbf{x}}^f - \underline{\mathbf{x}}\right),$$

$$J_m(\underline{\mathbf{x}}) = \frac{1}{2}\sum_{i=1}^{2}\left[M_{(i-1)i}(\mathbf{x}_{i-1}) - \mathbf{x}_i\right]^T \mathbf{Q}^{-1}\left[M_{(i-1)i}(\mathbf{x}_{i-1}) - \mathbf{x}_i\right],\ \text{and}$$

$$J_o(\underline{\mathbf{x}}) = \frac{1}{2}\left[\underline{\mathbf{y}} - \underline{H}(\underline{\mathbf{x}})\right]^T \mathbf{R}^{-1}\left[\underline{\mathbf{y}} - \underline{H}(\underline{\mathbf{x}})\right]$$

# Linearize about guess field

$$\underline{\delta\mathbf{x}} = \underline{\mathbf{x}} - \underline{\mathbf{x}}^g = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} - \begin{bmatrix} \mathbf{x}_0^g \\ \mathbf{x}_1^g \\ \mathbf{x}_2^g \end{bmatrix}, \quad \underline{\delta\mathbf{x}^f} = \underline{\mathbf{x}}^f - \underline{\mathbf{x}}^g = \begin{bmatrix} \mathbf{x}_0^f \\ \mathbf{x}_1^f \\ \mathbf{x}_2^f \end{bmatrix} - \begin{bmatrix} \mathbf{x}_0^g \\ \mathbf{x}_1^g \\ \mathbf{x}_2^g \end{bmatrix},$$

$$\underline{\mathbf{y}}' = \underline{\mathbf{y}} - \underline{H}\left(\underline{\mathbf{x}}^g\right),$$

$$\underline{H}\left(\underline{\mathbf{x}}\right) - \underline{H}\left(\underline{\mathbf{x}}^g\right) = \underline{\mathbf{H}}\underline{\delta\mathbf{x}}, \quad \text{where } \frac{\partial\left[\underline{H}\left(\underline{\mathbf{x}}^g\right)\right]}{\partial\left(\underline{\mathbf{x}}^g\right)^T} = \underline{\mathbf{H}}$$

$$\mathbf{M}_{(i-1)i}\delta\mathbf{x}_{i-1} = \left[M_{(i-1)i}\left(\mathbf{x}_{i-1}\right) - M_{(i-1)i}\left(\mathbf{x}_{i-1}^g\right)\right], \text{ where } \mathbf{M}_{(i-1)i} = \frac{\partial\left[M_{(i-1)i}\left(\mathbf{x}_{(i-1)}^g\right)\right]}{\partial\left(\mathbf{x}_{i-1}^g\right)^T}$$

# Incremental form

$$J\left(\underline{\delta \mathbf{x}}\right) = J_b\left(\underline{\delta \mathbf{x}}\right) + J_m\left(\underline{\delta \mathbf{x}}\right) + J_o\left(\underline{\delta \mathbf{x}}\right), \text{ where}$$

$$J_b\left(\underline{\delta \mathbf{x}}\right) = \frac{1}{2}\left(\underline{\delta \mathbf{x}}^f - \underline{\delta \mathbf{x}}\right)^T \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \mathbf{P}_0^{g-1} \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}^T \left(\underline{\delta \mathbf{x}}^f - \underline{\delta \mathbf{x}}\right),$$

$$J_m\left(\underline{\delta \mathbf{x}}\right) = \frac{1}{2}\sum_{i=1}^{2}\left\{\left[\mathbf{M}\delta \mathbf{x}_{i-1} + M\left(\mathbf{x}_{i-1}^g\right) - \mathbf{x}_i^g\right] - \delta \mathbf{x}_i\right\}^T \mathbf{Q}^{-1}$$

$$x\left\{\left[\mathbf{M}\delta \mathbf{x}_{i-1} + M\left(\mathbf{x}_{i-1}^g\right) - \mathbf{x}_i^g\right] - \delta \mathbf{x}_i\right\}, \text{ and}$$

$$J_o\left(\underline{\delta \mathbf{x}}\right) = \frac{1}{2}\left[\underline{\mathbf{y}}' - \underline{\mathbf{H}}\underline{\delta \mathbf{x}}\right]^T \mathbf{R}^{-1}\left[\underline{\mathbf{y}}' - \underline{\mathbf{H}}\underline{\delta \mathbf{x}}\right].$$

# Algebraic derivation shows that minimum of cost function occurs when

$$\left(\underline{\mathbf{x}}^a - \underline{\mathbf{x}}^g\right) = \left(\underline{\mathbf{x}}^f - \underline{\mathbf{x}}^g\right) + \underline{\mathbf{P}}^g \underline{\mathbf{H}}^T \left(\underline{\mathbf{H}}\underline{\mathbf{P}}^g \underline{\mathbf{H}}^T + \underline{\mathbf{R}}\right)^{-1} \left[\underline{\mathbf{y}}' - \underline{\mathbf{H}}\underline{\delta \mathbf{x}^f}\right], \text{ where}$$

$$\underline{\mathbf{P}}^g = \begin{bmatrix} \mathbf{P}_0^g & \mathbf{P}_0^g\mathbf{M}^{\mathrm{T}} & \mathbf{P}_0^g\mathbf{M}^{\mathrm{T}}\mathbf{M}^{\mathrm{T}} \\ \mathbf{M}\mathbf{P}_0^g & \mathbf{M}\mathbf{P}_0^g\mathbf{M}^{\mathrm{T}} + \mathbf{Q} & \mathbf{M}\mathbf{P}_0^g\mathbf{M}^{\mathrm{T}}\mathbf{M}^{\mathrm{T}} + \mathbf{Q}\mathbf{M}^{\mathrm{T}} \\ \mathbf{M}\mathbf{M}\mathbf{P}_0^g & \mathbf{M}\mathbf{M}\mathbf{P}_0^g\mathbf{M}^{\mathrm{T}} + \mathbf{M}\mathbf{Q} & \mathbf{M}\mathbf{M}\mathbf{P}_0^g\mathbf{M}^{\mathrm{T}}\mathbf{M}^{\mathrm{T}} + \mathbf{M}\mathbf{Q}\mathbf{M}^{\mathrm{T}} + \mathbf{Q} \end{bmatrix}, \text{ and}$$

$$\underline{\mathbf{y}}' - \underline{\mathbf{H}}\underline{\delta \mathbf{x}^f} \approx \underline{\mathbf{y}} - H\left(\underline{\mathbf{x}}^f\right), \text{ hence}$$

$$\underline{\mathbf{x}}^a = \underline{\mathbf{x}}^f + \underline{\mathbf{P}}^g \underline{\mathbf{H}}^T \left(\underline{\mathbf{H}}\underline{\mathbf{P}}^g \underline{\mathbf{H}}^T + \underline{\mathbf{R}}\right)^{-1} \left[\underline{\mathbf{y}} - H\left(\underline{\mathbf{x}}^f\right)\right]$$

Because $\mathbf{P}_0^g$ is fixed, the outer loop only affects the analysis if changes to the guess and linearization state change $\underline{\mathbf{H}}$ and $\mathbf{M}$.

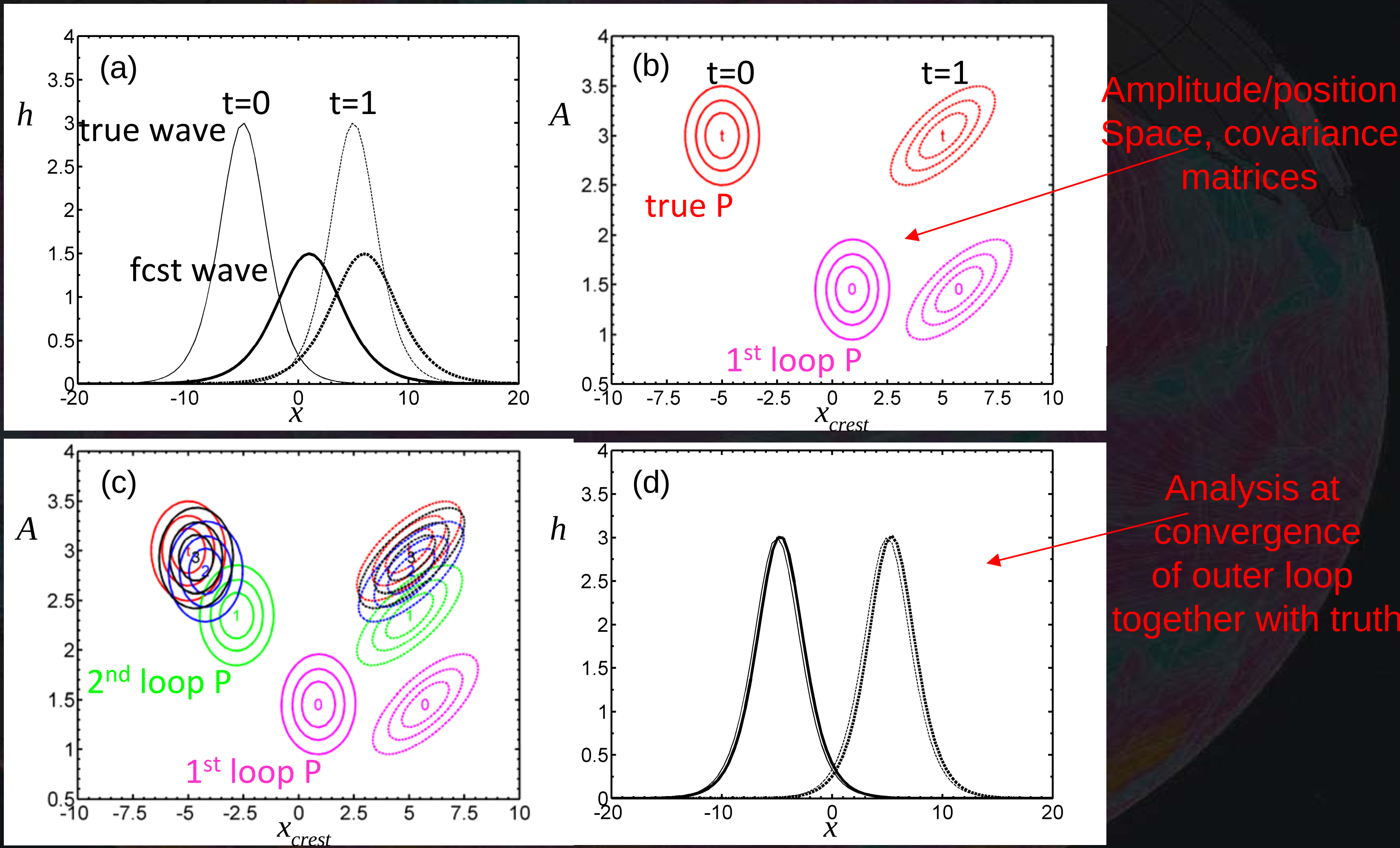
# Interpretation of outer loop

Outer loop will consistently help analysis if it causes $\underline{\mathbf{P}}^g$, $\underline{\mathbf{P}}^g\underline{\mathbf{H}}^T$ and $\underline{\mathbf{H}}\underline{\mathbf{P}}^g\underline{\mathbf{H}}^T$ to better approximate the corresponding true forecast error covariance matrices.

Improvement guaranteed if $\underline{\mathbf{P}}^g$ gives distribution of historical forecasts given that the guess field was equal to the truth because, in this case, each improvement of the guess field causes $\underline{\mathbf{P}}^g$ to better approximate a true forecast error covariance matrix.

Improvement not guaranteed if $\underline{\mathbf{P}}^g$ represents distribution of truth given today's forecast because, in this case, it is not clear that centering it closer to the analysis would improve its accuracy.

# Solitary wave example (strong constraint)




Example of effect of outer loop on analysis of solitary wave. Observations are of wave amplitude at every second grid point at the final time position of the wave.

# Ensemble Analogue

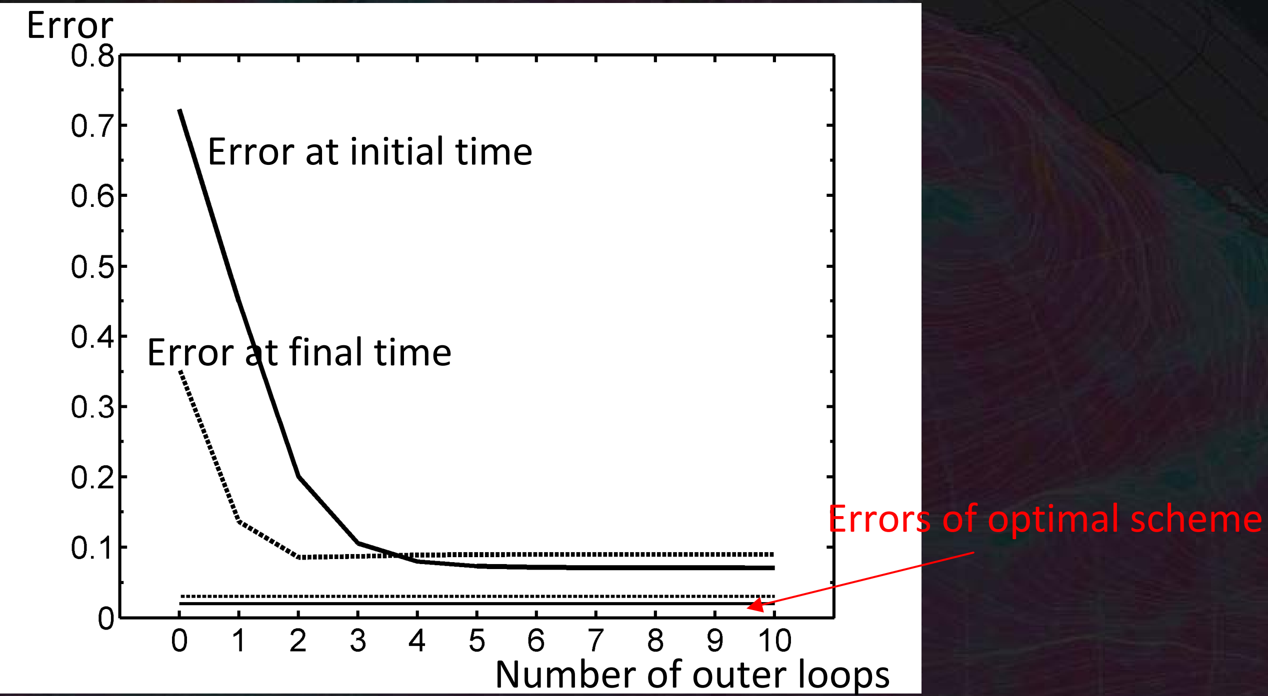
Approximate $\underline{\mathbf{P}}^g$, $\underline{\mathbf{P}}^g\underline{\mathbf{H}}^T$ and $\underline{\mathbf{H}}\underline{\mathbf{P}}^g\underline{\mathbf{H}}^T$ using ensemble counterparts centered on guess field.

In the first inner loop, the initial ensemble perturbations are added to the mean of the ensemble forecast from the previous analysis at the beginning of the window. The covariances from this ensemble are then used to obtain guess field.

In the second outer loop, the initial ensemble perturbations are added to the guess field and then propagated using the non-linear model. If model error is present the evolving perturbations need to be recentered around the evolving guess field from time to time.

And so on until convergence.

# Solitary wave example (strong constraint)




Ensemble outer loop profoundly reduces analysis error

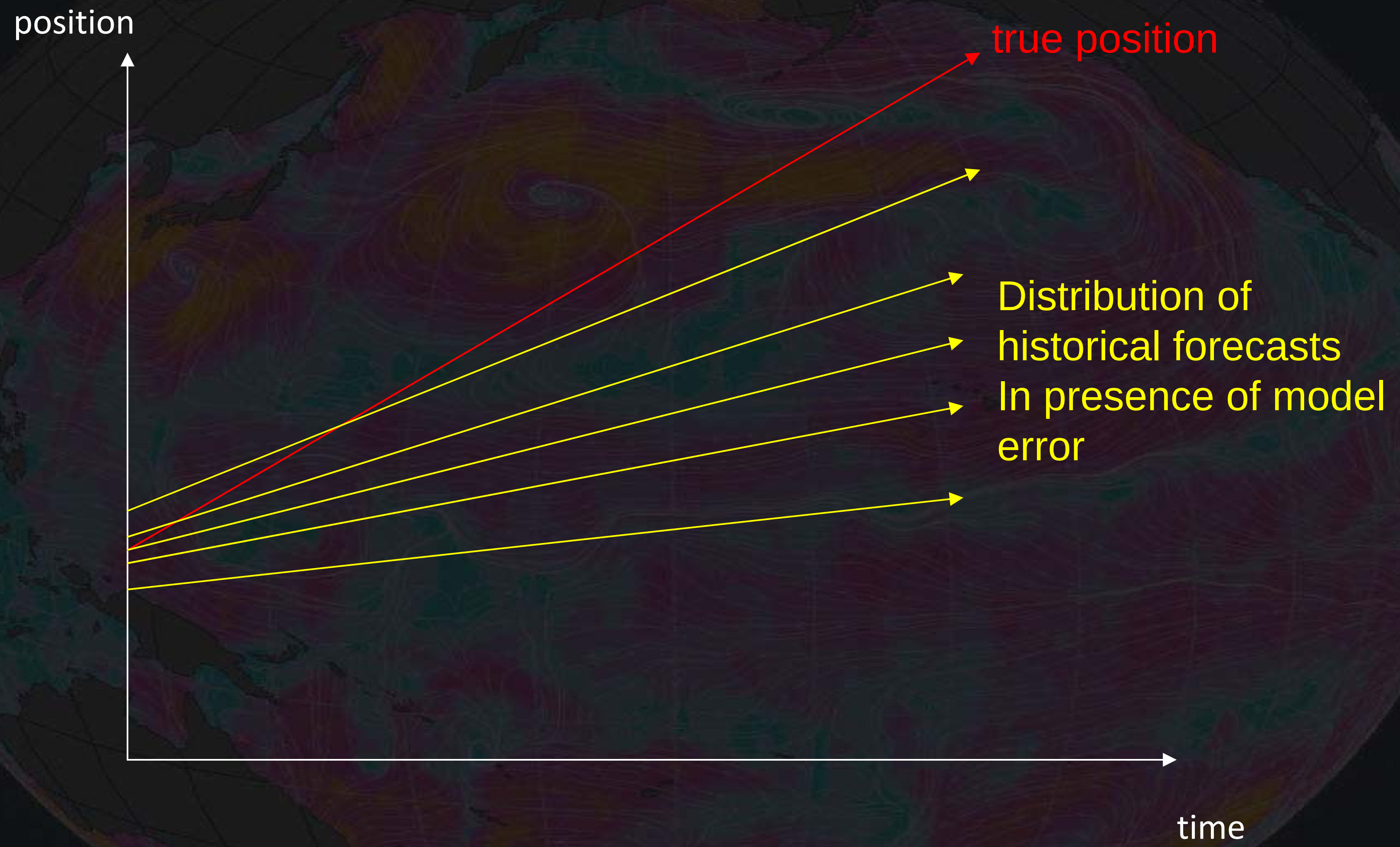
# Ensemble outer loop for strong constraint case

1. Make an analysis using raw ensemble
2. Create new ensemble by re-centering initial perturbations on latest analysis rather than first guess and then integrating using non-linear model.
3. Make new analysis using new ensemble
4. Repeat steps 2 and 3 until convergence.
5. (Note: At no point in the iteration should the innovation be altered).

# Issues for weak constraint case

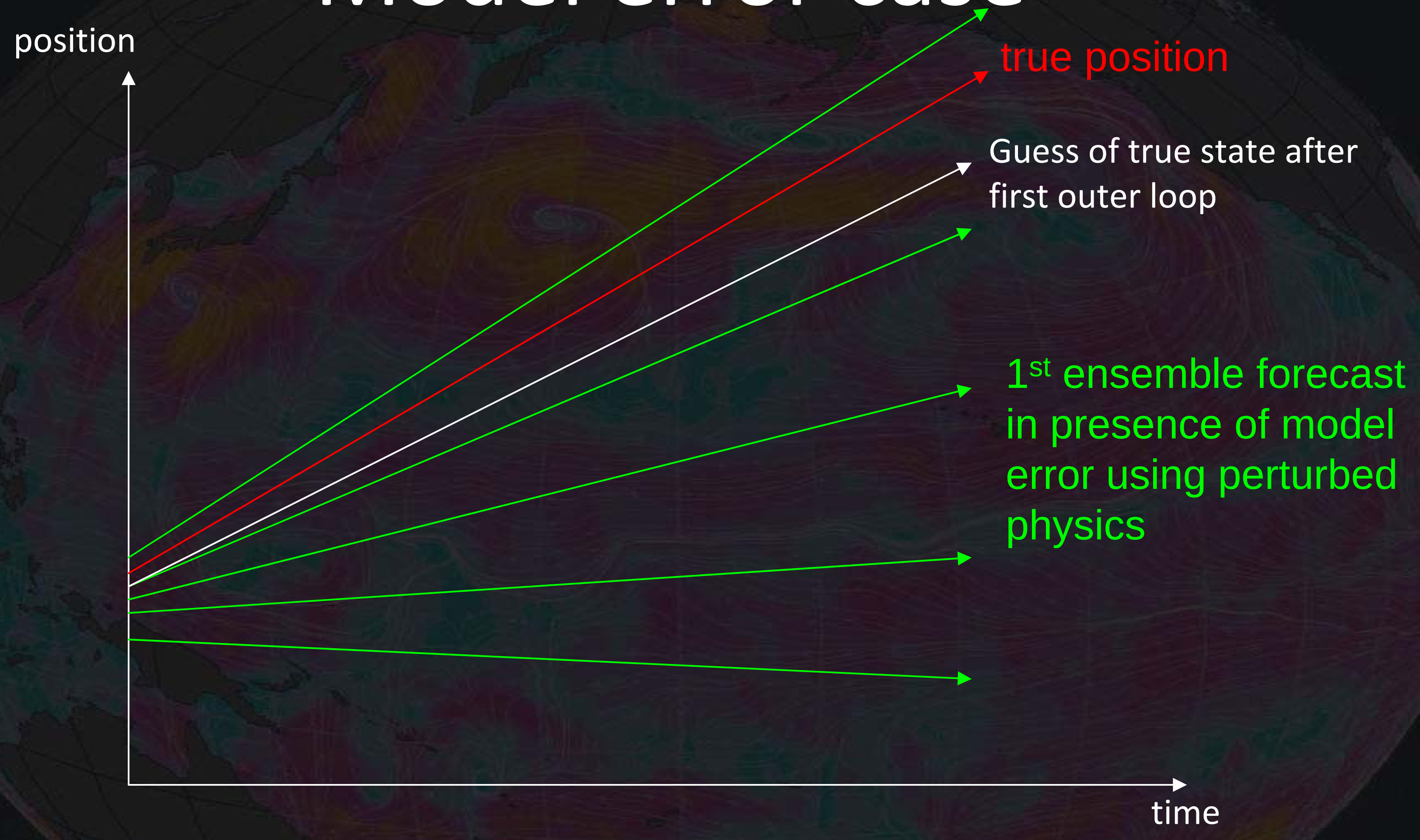
- Simple minded analogue of weak constraint 4D-VAR involves continual re-centering of ensemble about guess field.
- Depending on type of model error, it is not obvious that this approach would yield the best approximation to the distribution of historical forecasts given the truth.

# Model error case



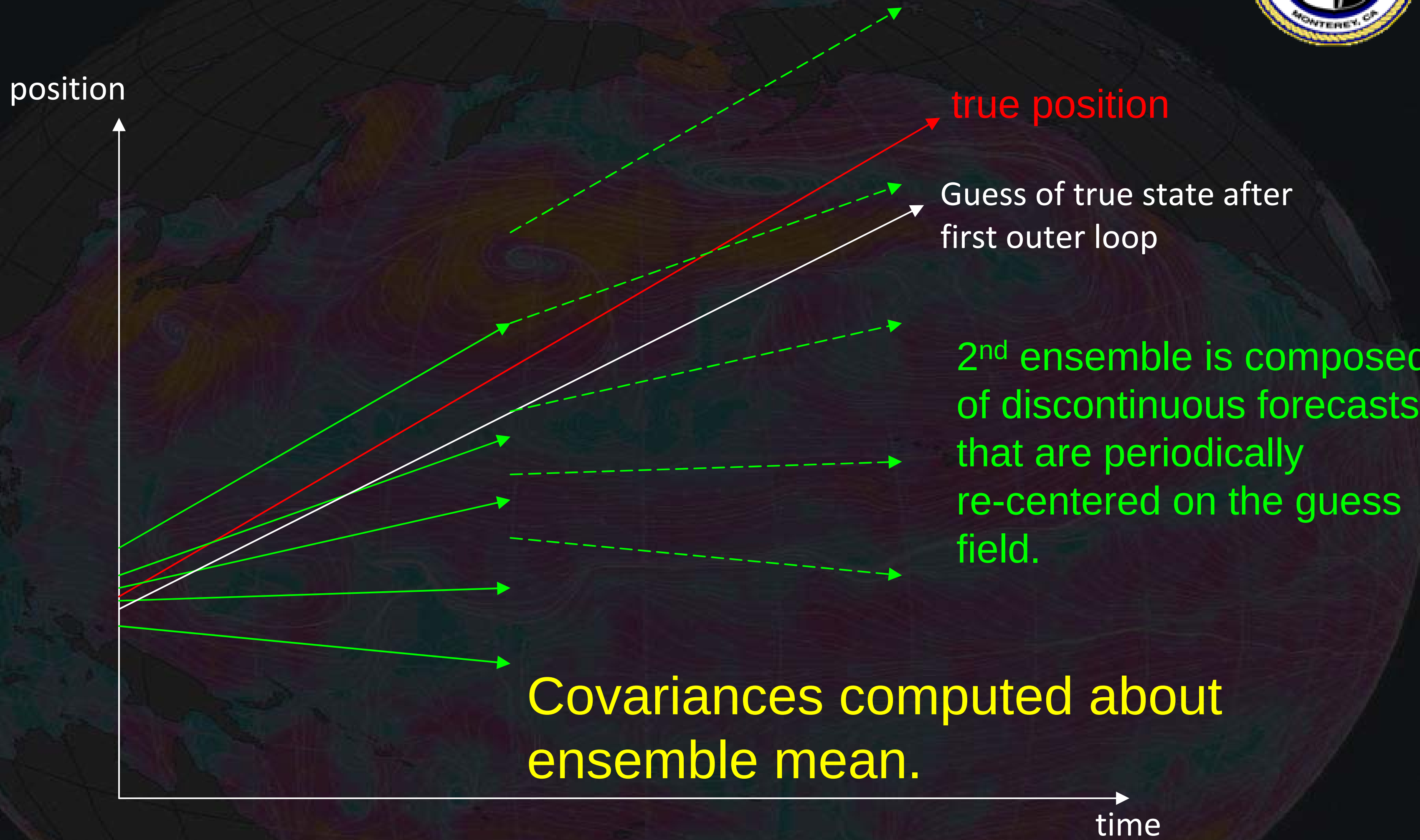

The forecasts are biased in the sense that their positions have not advanced as far as the truth. However, in general, such biases are unknown. In this case, the minimum error variance is obtained using a covariance matrix of the actual errors of these biased forecasts.

# Model error case



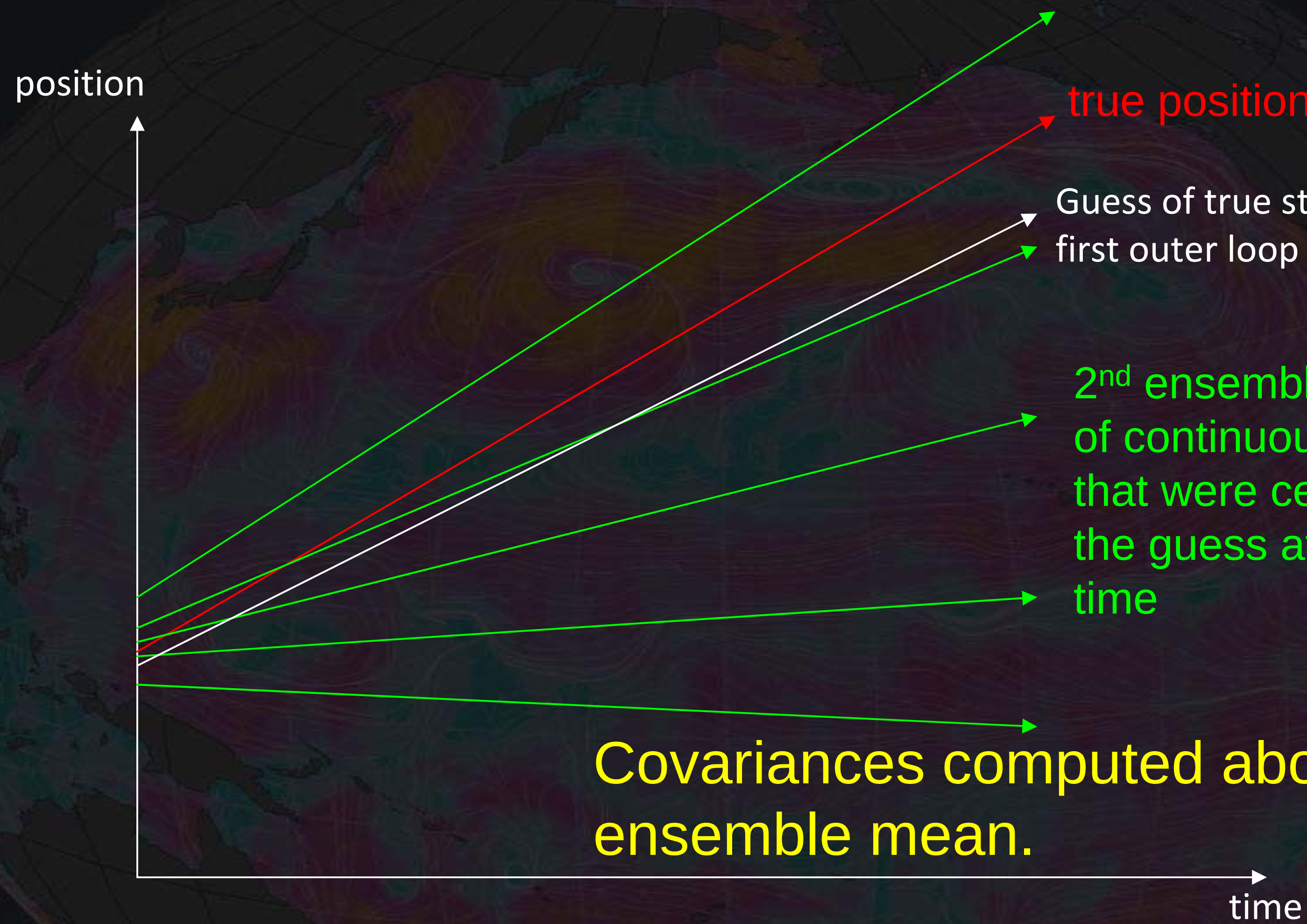

Initial ensemble is not centered on the truth. It has more spread than the ensemble of historical control/mean forecasts because each model has a different set of parameters. How can the outer loop be used to generate a covariance similar to that on the previous slide?

# Option 1 for 2nd ensemble (breaks)



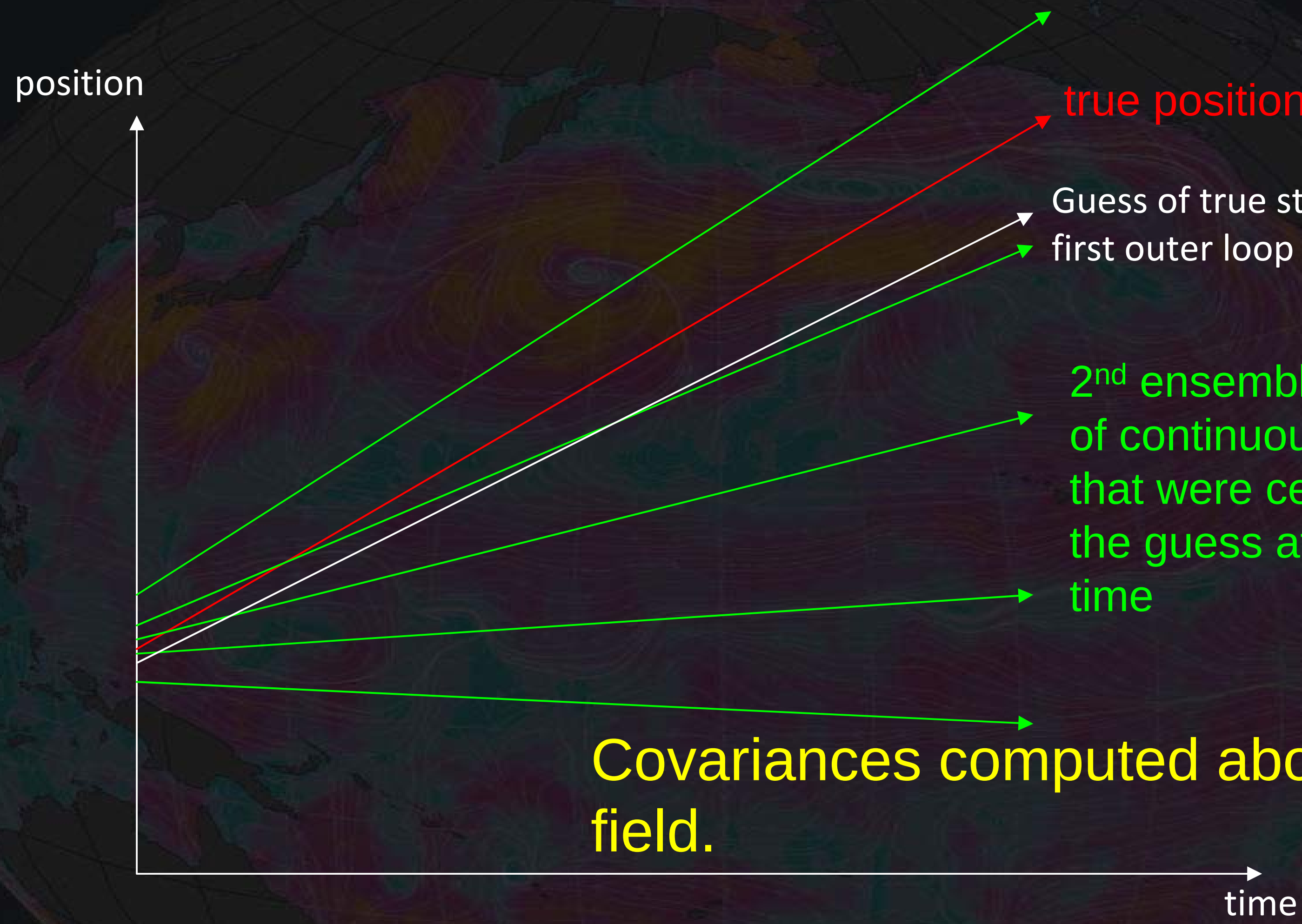

This option is the closest ensemble approximation to what happens in weak constraint 4D-VAR with TLM/adjoint. Note that it does not preserve the time continuity of the actual errors.

# Option 2 for $2^{nd}$ ensemble (no breaks)




This option preserves the continuity of the errors but the computation of covariances is still computed using differences about the mean rather than the best available estimate of the truth.

# Option 3 for 2nd ensemble (no breaks)

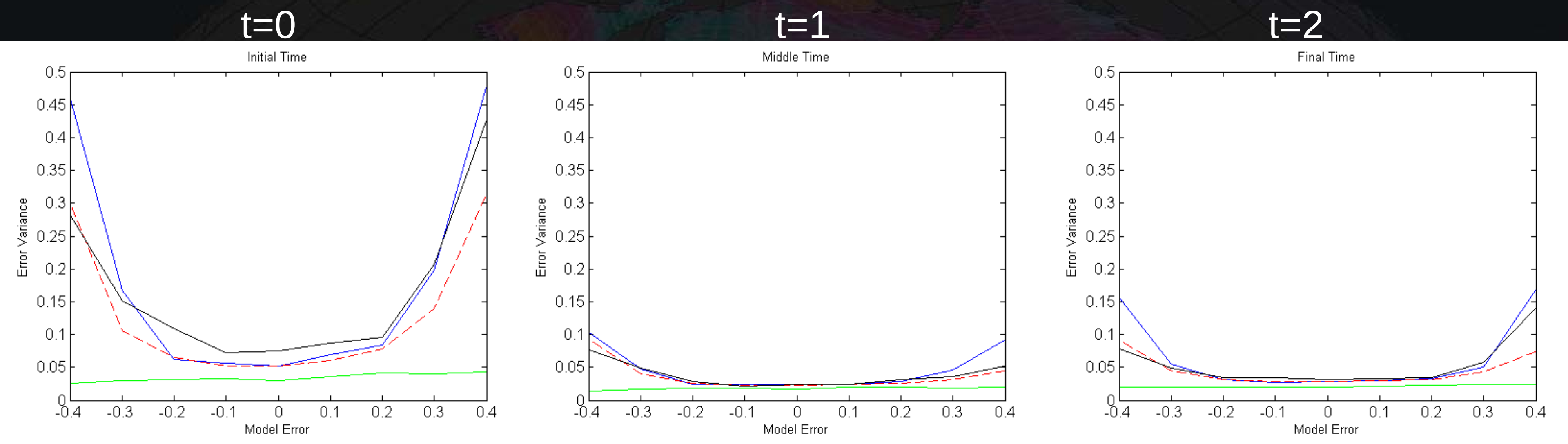



2nd ensemble is composed of continuous forecasts that were centered on the guess at the initial time

Covariances computed about guess field.

This option preserves the continuity of the errors and covariances are computed using differences about the best available estimate of the truth – (the latest guess).

# Test of Options




Variation of 0.1 in model error corresponds to a 1 sigma deviation of a parameter that affects propagation of solitary wave

Green line: Analysis obtained using covariance of historical forecasts about truth.

Option 1: Black line (Weak constraint 4D-VAR analogue with breaks in ensemble)

Option 2: Blue line (No breaks but differences about mean)

Option 2/3: Dashed red line (as in option 2 but differences about guess after 5$^{th}$ loop)

There are a number of options for weak constraint form of the ensemble outer loop. The one that is closest to TLM/adjoint weak constraint 4D-VAR is not necessarily the best.

# Concluding Remarks

- Outer loop for ensemble DA provides potential mechanism for dealing with problem of "feature in obs but not in ensemble"
- Experiments with simple soliton model show how rerunning ensemble in outer loop allows the ensemble covariance to better approximate the covariance of the distribution of historical forecasts given the truth.
- Ensemble outer-loop offers possibility of basing covariances on differences of non-linear forecasts around best guess field rather than the ensemble mean. Soliton experiments show that "difference about guess" can be superior to "difference about mean". There is no TLM/adjoint analogue of the "difference about guess" framework.