Numerical Error Estimation through Local Error Learning

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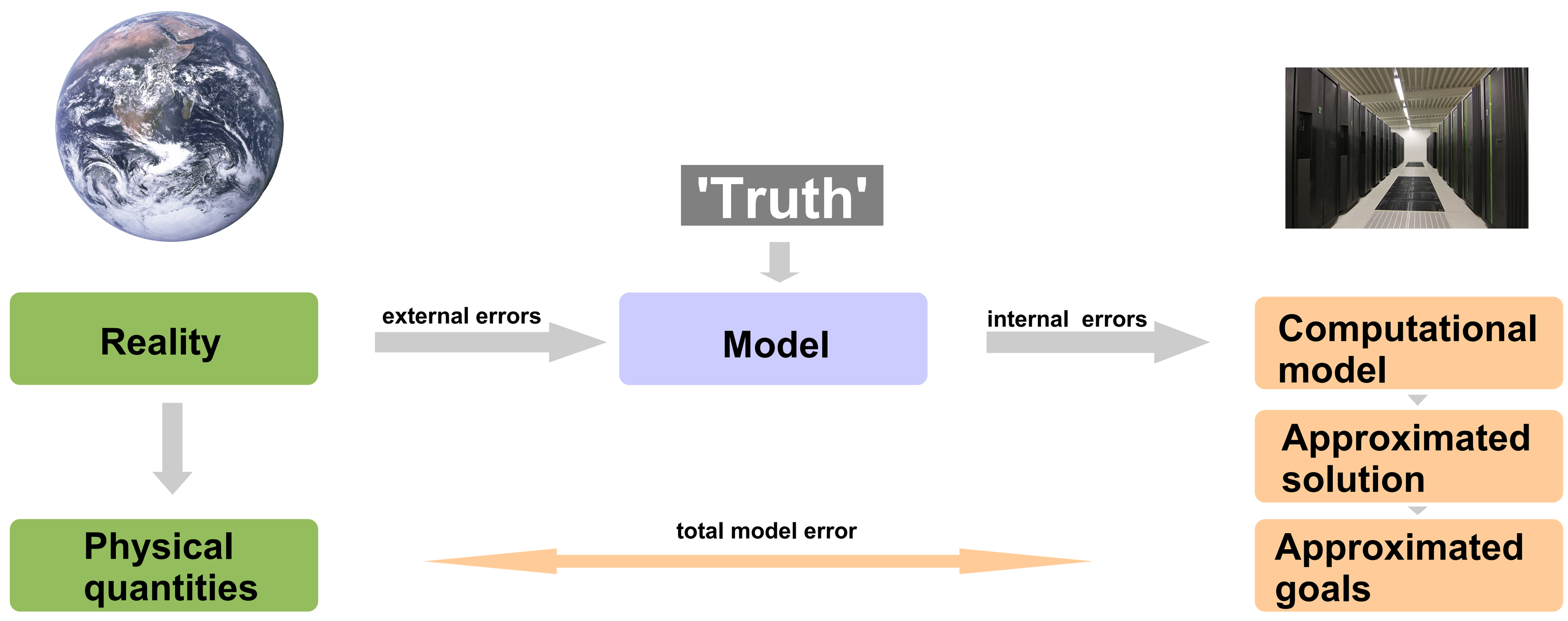
1. Problem Statement



Computational models approximate mathematical descriptions that itself approximate physical processes. We want to quantify the errors in physical quantities of interest for given solutions of computational models. The knowledge of these computational errors in physical quantities is essential to their scientific interpretation, comparable to the necessity of error bars in measurements.

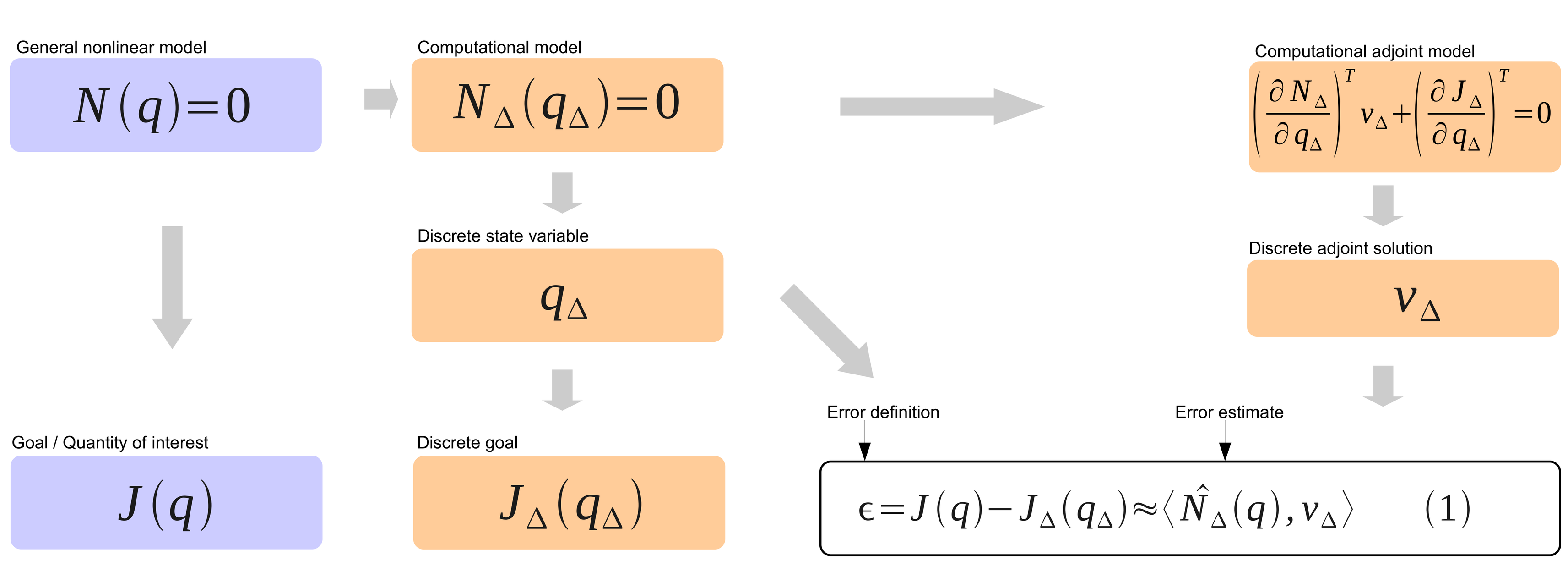
We estimate the error in approximated physical quantities, called goals. To do so, we construct local error descriptions that learn the model error characteristics by analyzing model behavior on varying resolutions.

Our algorithm allows a variety of local error descriptions; this poster focuses on stochastic local error descriptions, leading to an ensemble of error estimates, the posterior goal ensemble.

Reference

Rauser, et al., Predicting goal error evolution from near-initial-information: A learning algorithm, Journal of Computational Physics, Vol. 230, Issue 19, 2011, Pages 7284-7299

2. Goal Errors as Weighted Sum of Local Errors



We approximate goal errors for a given problem as the weighted sum of local model errors. The weights are the solution of a dual problem to the given model.
The solution of this dual problem shows the sensitivity of output goals to changes in the solution itself. This sensitivity is used to connect local errors in the solution with the final output error in physical goals.

The goal error estimate (1) is a scalar product of two components:

1) a **local error estimator** $\hat{N}_\Delta(q)$
2) the solution of a **dual problem** v_Δ .

Our algorithm shows a way to obtain both components for generic models of geophysical fluid dynamics.

References

Giles, et al., Progress in adjoint error correction for integral functionals, Computing and Visualization in Science 6 (2004) 113–121.

R. Rannacher, et al., An optimal control approach to a posteriori error estimation in finite element methods, Acta Numerica 10 (2002) 1–102.

3. Posterior Goal Ensembles: the Algorithm

The new idea:

Our algorithm allows us to use a wide class of error descriptions and learn model specific properties. This learning involves the solution of the model on varying resolutions for a single time step and the comparison between the solutions.
If we choose a stochastic error description, the resulting goal error estimates are stochastic as well; we call the resulting ensemble of goal approximations **posterior goal ensemble**.

Local Error Learning

1. Choose local error description.
2. Learn properties of this description.

Error Estimation

1. Run numerical model, calculate goals.
2. Compute weights for each goal with AD.
3. Calculate goal error estimate(s) as sum of weighted local errors.

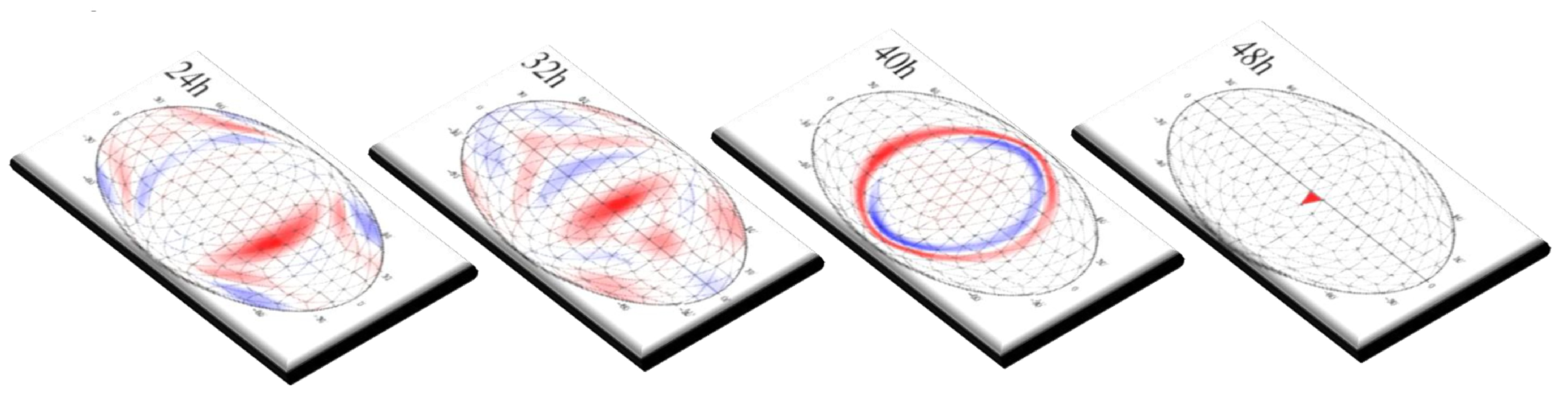


Figure 1: Typical goal sensitivities are shown for a 48h backward run after a 48h forward integration. The plots are normalized.

Reference

Rauser, et al, On the use of discrete adjoints in goal error estimation for shallow water equations, Procedia Computer Science, Volume 1, Issue 1, Pages 107-115, ICCS 2010

4. Evaluation Testbed: Shallow Water Equations

Model:

We use a discrete model of the nonlinear shallow water equations on the sphere. The discretization is a c-type staggered finite volume / difference hybrid on a triangular spherical grid with semi-implicit time-stepping (ICON-SW).

Two Test Cases:

TC1: Time-evolving solid body rotation. This test case represents a regular global flow.
TC2: Zonal flow against a mountain (Williamson TC5). This test case represents a regional perturbation and the onset of turbulence.

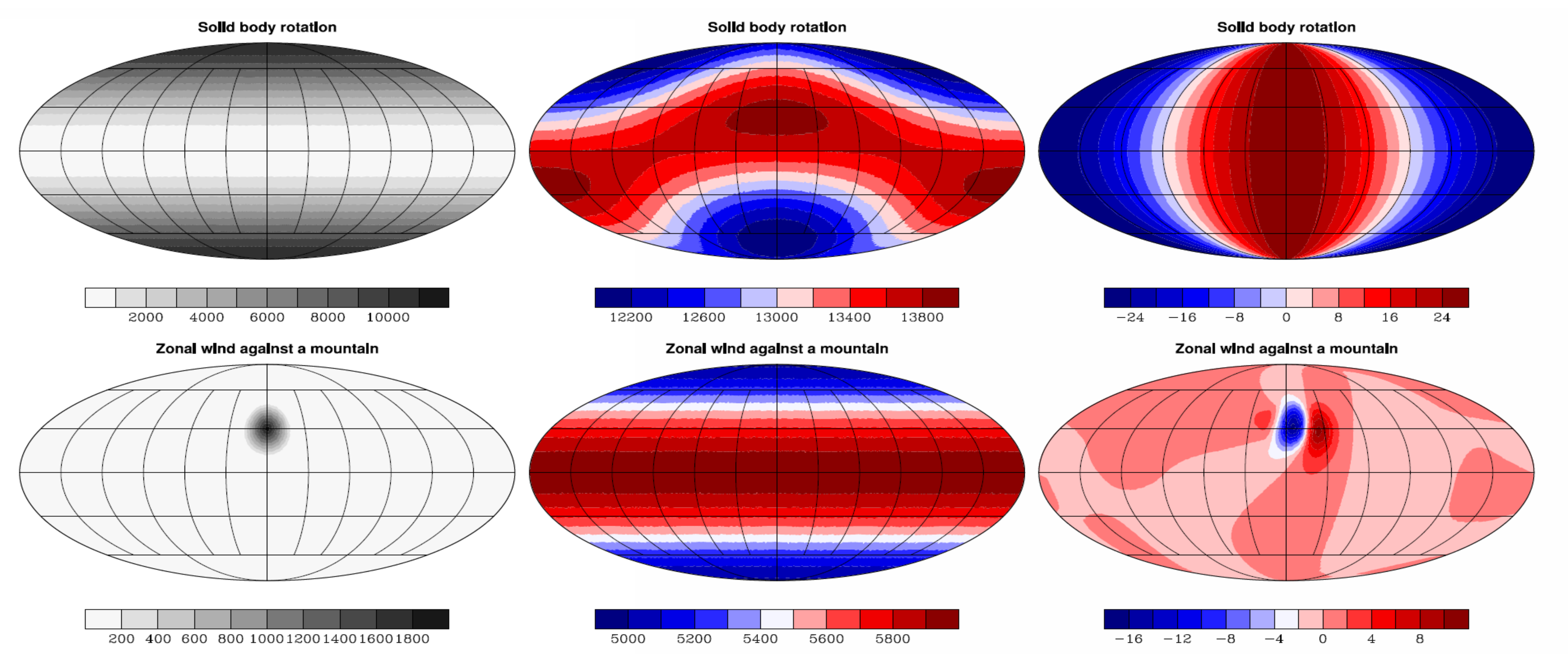


Figure 2: TC1 is shown in the top row, TC2 in the bottom row. The left column shows the analytical topography, the middle column shows the initial condition of the height field and the right column the meridional velocity after 12 hours.

5. The Central Limit Theorem and Local Errors

The choice of description of the local error random process is a priori free. As a test, we assume either a Gaussian or an exponential distribution. The resulting goal error distribution becomes normal for both local error distributions. This can be explained by the central limit theorem: if the local error processes are independent, symmetric and have zero mean, the resulting distribution is Normal and has also zero mean. Our method is an efficient and cheap way to analyze the linear propagation of local errors and investigate the influence of non-symmetric error distributions in the future.

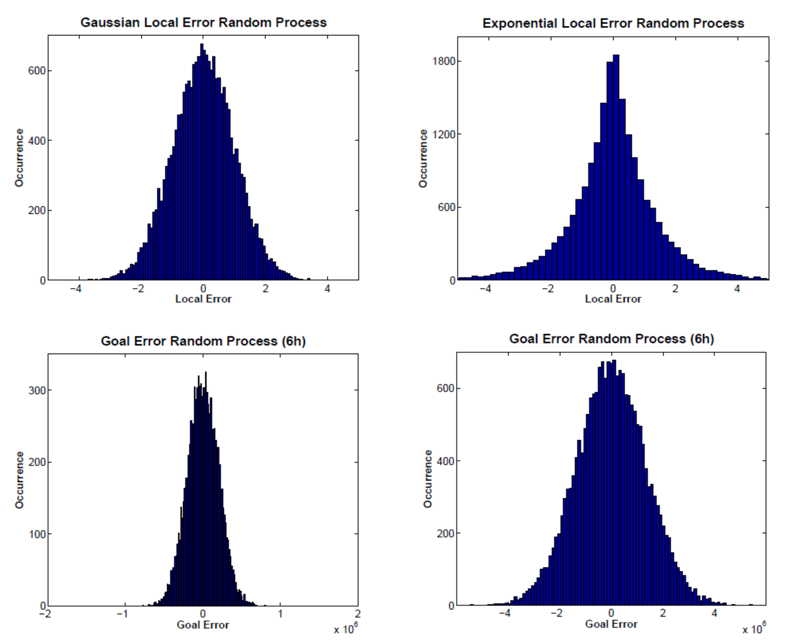


Figure 3:
Top: Local error random process (Gaussian and Exponential).
Bottom: Goal error random process for TC1 after 6 hours.

6. Results: Posterior Goal Ensembles as Error Bounds

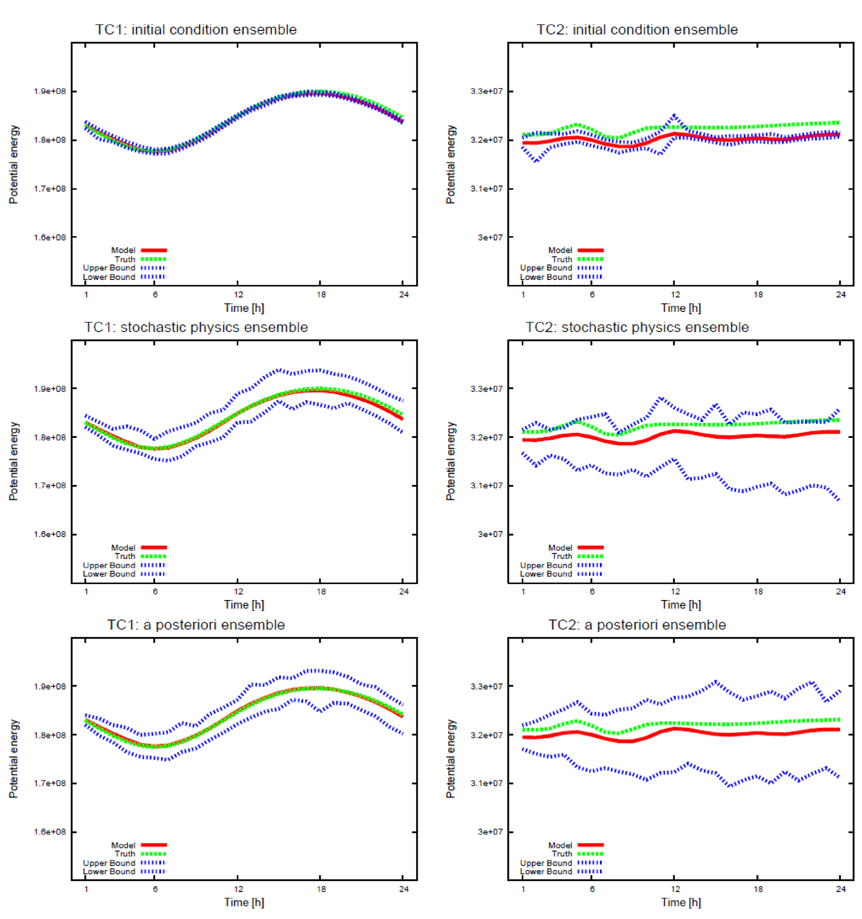


Figure 4: On the x-axis is time. On the y-axis is regional potential energy for TC1 (resolution~1000km). Top row shows an initial condition ensemble (ICE), middle row shows a stochastic physics ensemble (SPE), bottom row shows a posterior ensemble (PE).

We compare our posterior ensembles (PE) to standard prior ensembles, i.e., initial condition ensemble and stochastic physics ensemble (SPE). We observe a similar development of ensemble spread for PE/SPE. The SPE spread shows higher variability, probably because the ensemble size is too low for a converged goal PDF.

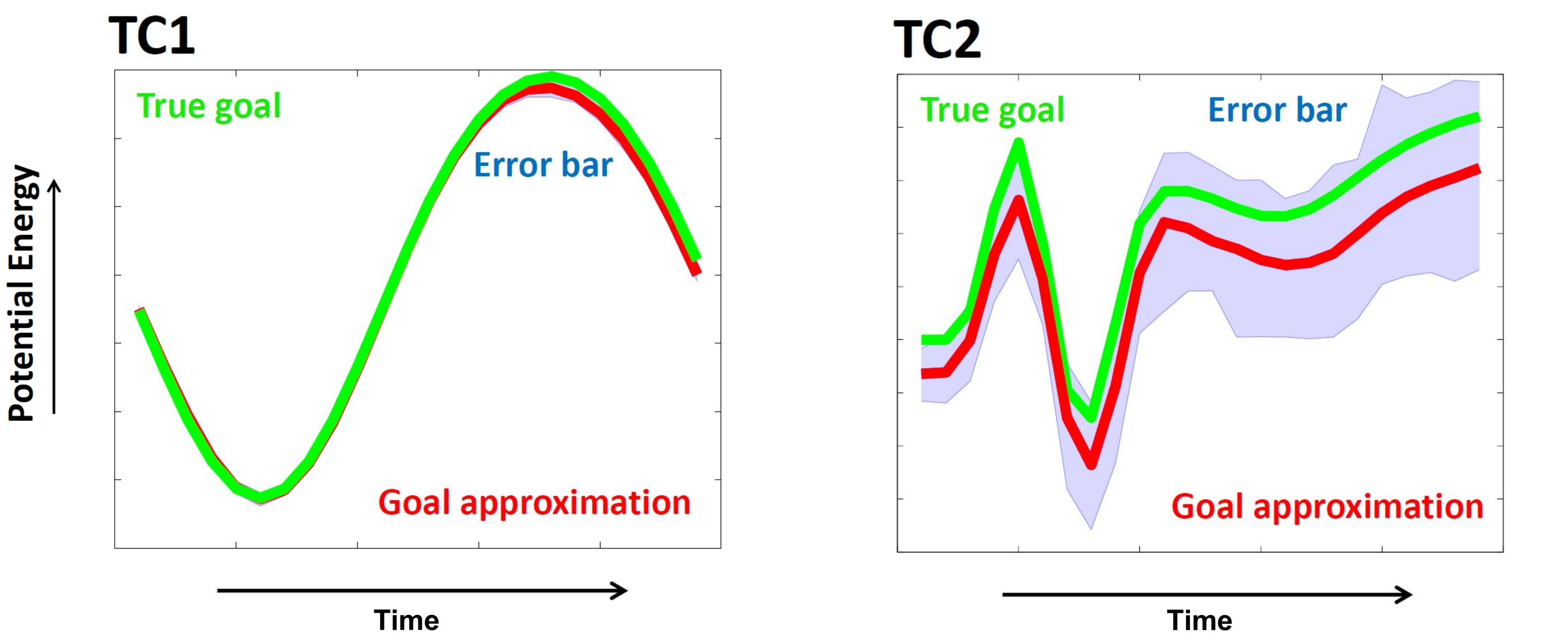


Figure 5: On the x axis is time, on the y axis potential energy for TC1 and TC2. We show the development of the goal and the corresponding error bounds derived from the posterior goal ensemble (resolution~500 km average grid cell distance).

7. Synthesis

• We adopt a numerical error estimation method from computational fluid dynamics to a new and challenging time-evolving problem in a geophys-ical fluid dynamics context.

• We introduce the idea of local errors as a stochastic process whose properties can be learned. The influence of the local errors on the goal is calculated with Algorithmic Differentiation.

• We derive an ensemble from a single model run.

8. Summary

• We show a new method to estimate numerical errors that employs a concept of local learning to estimate goal errors.

• We evaluate this method with promising results for test cases of the spherical shallow water equations.

• The posterior ensemble from one model run is comparable to a multi-run stochastic physics forward ensemble.

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