POP + DART

Parallel Ocean Program + Data Assimilation Research Testbed

Accelerated Scientific Discovery Presentation
NCAR HPC User Group May 2022 Meeting

NCAR

Ben Johnson & Moha Gharamti
DAReS · TDD · CISL · NCAR

Anna-Lena Deppenmeier
OS · CGD · NCAR

Ian Grooms
CU-Boulder

Scientific Background

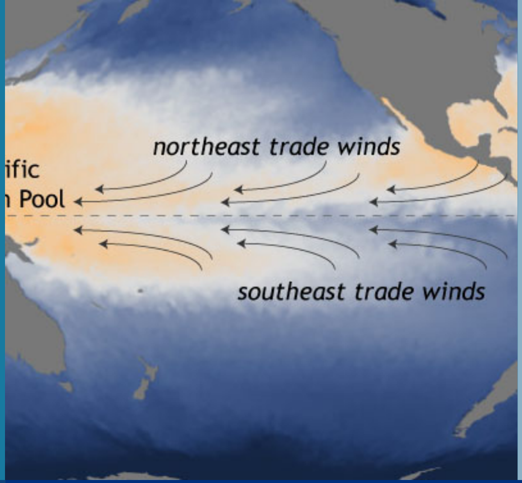
Emergent Phenomena

IN THE ATMOSPHERE				
Dynamical or Physical Regime	LAMINAR / BAROTROPIC	BAROCLINIC RESOLVING	CYCLOSTROPHIC / SUBMESOSCALE	SMALL-SCALE THERMODYNAMICS
IN THE OCEAN				

IN THE ATMOSPHERE				
Dynamical or Physical Regime	LAMINAR / BAROTROPIC	BAROCLINIC RESOLVING	CYCLOSTROPHIC / SUBMESOSCALE	SMALL-SCALE THERMODYNAMICS
IN THE OCEAN				

Increasing resolution →

IN THE ATMOSPHERE



Dynamical or Physical Regime

Increasing resolution →

LAMINAR / BAROTROPIC	BAROCLINIC RESOLVING	CYCLOSTROPHIC / SUBMESOSCALE	SMALL-SCALE THERMODYNAMICS

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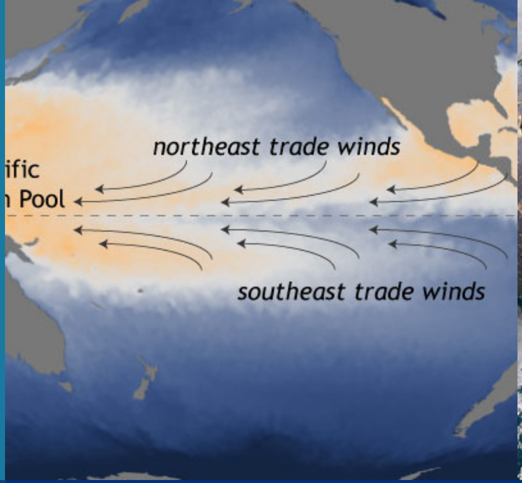

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LAMINAR / BAROTROPIC	BAROCLINIC RESOLVING	CYCLOSTROPHIC / SUBMESOSCALE	SMALL-SCALE THERMODYNAMICS

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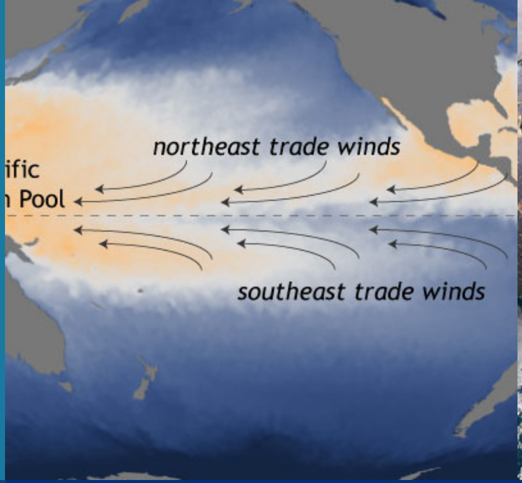

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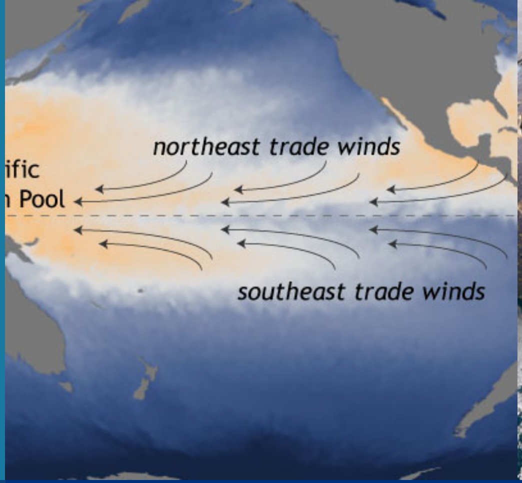

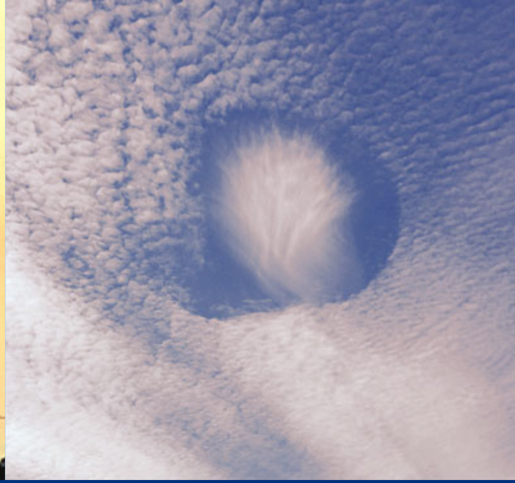

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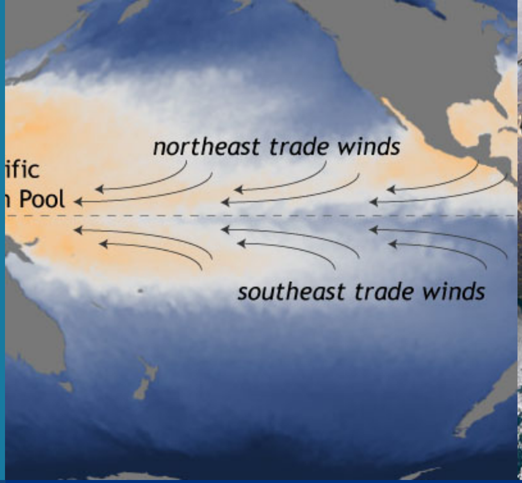

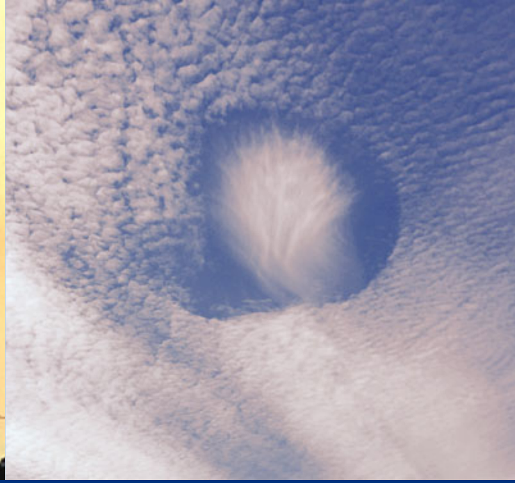

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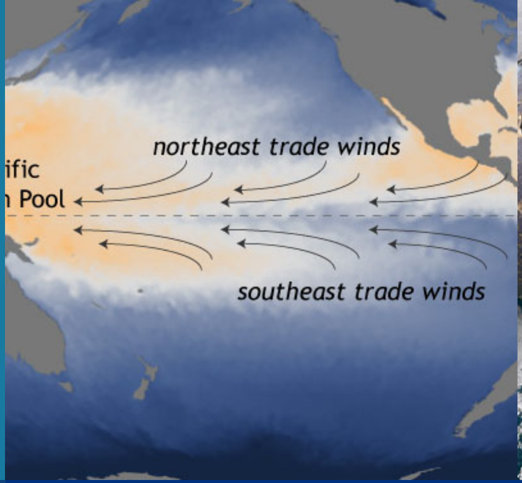

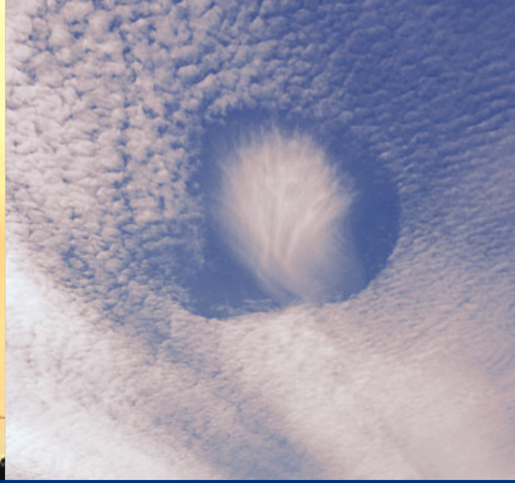

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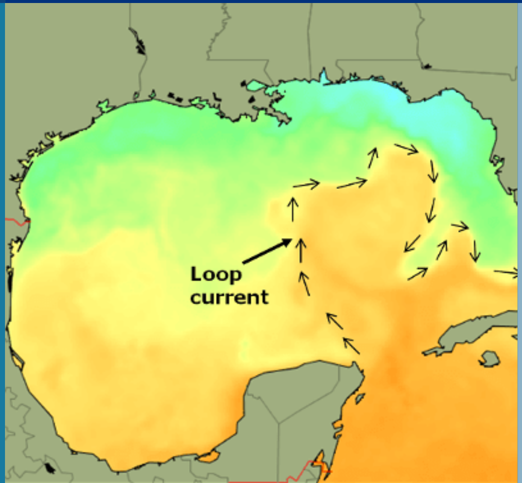

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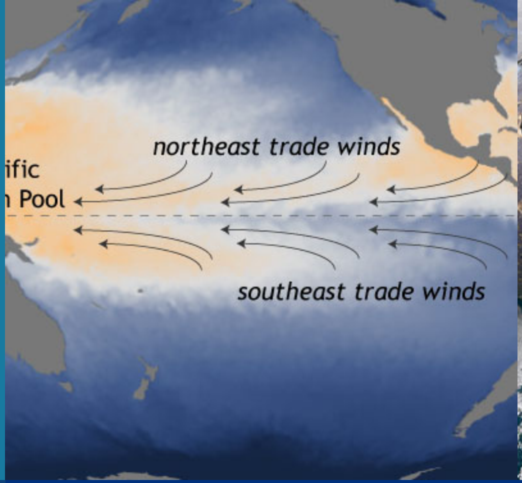

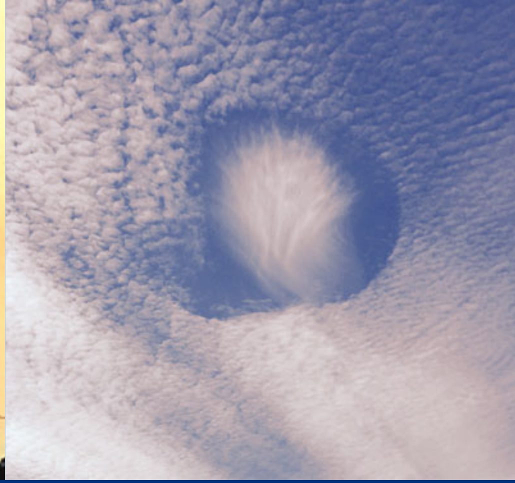

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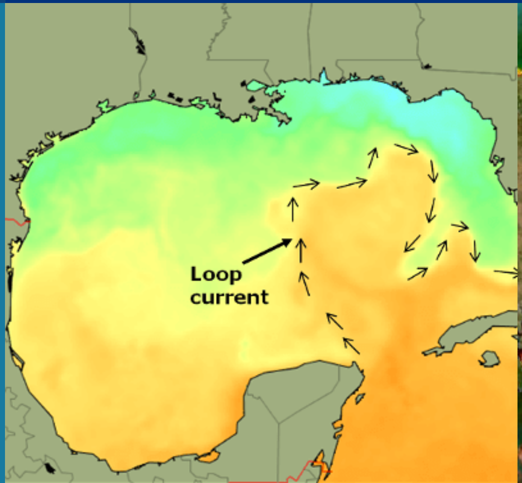

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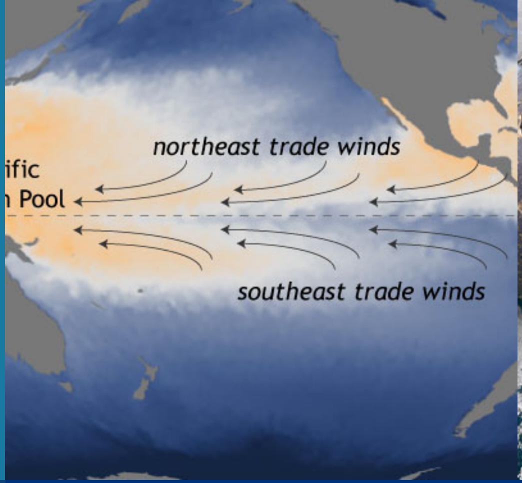

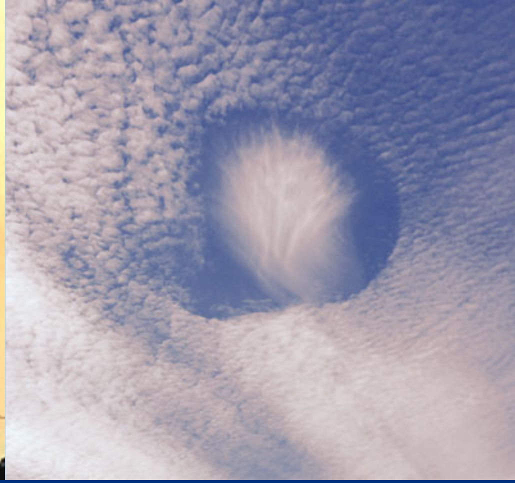

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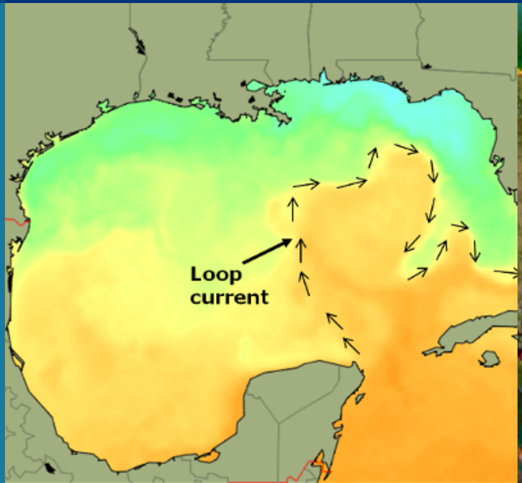

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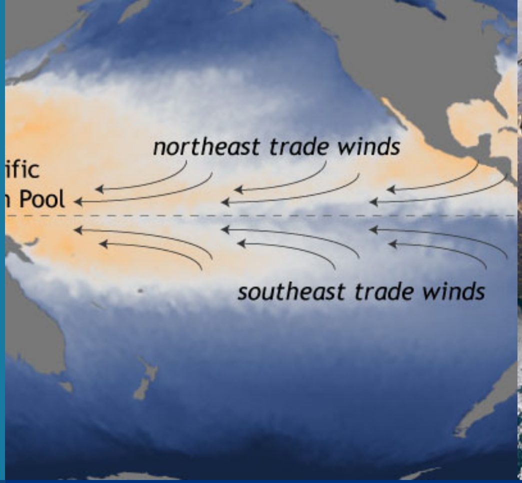

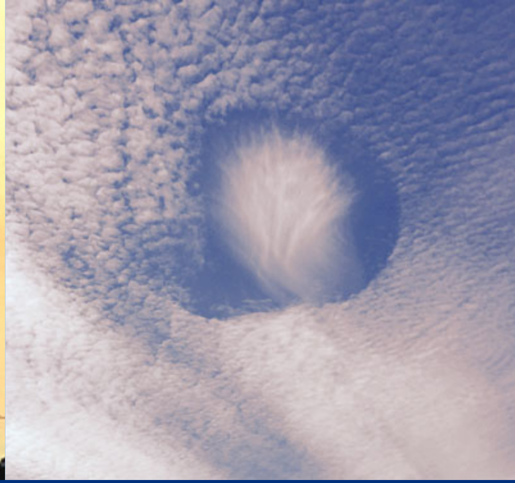

Dynamical or Physical Regime

Increasing resolution →

LAMINAR / BAROTROPIC

BAROCLINIC RESOLVING

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Increasing resolution →

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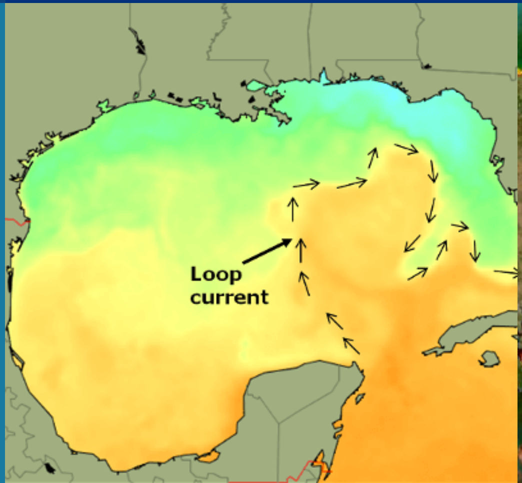
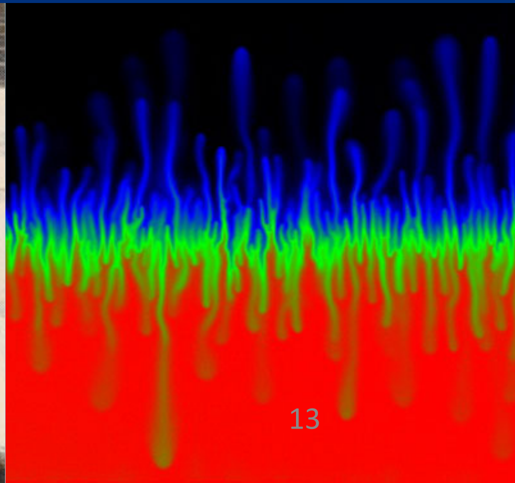
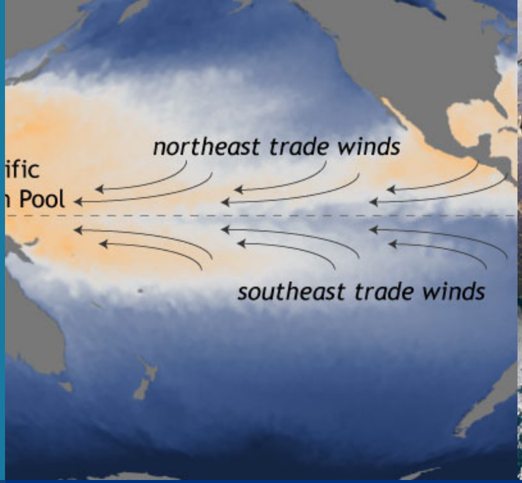
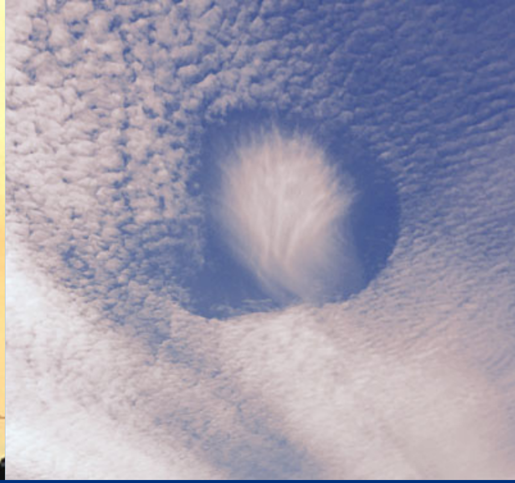




IN THE
ATMOSPHERE





Horizontal resolution

Dynamical or
Physical
Regime

Horizontal resolution

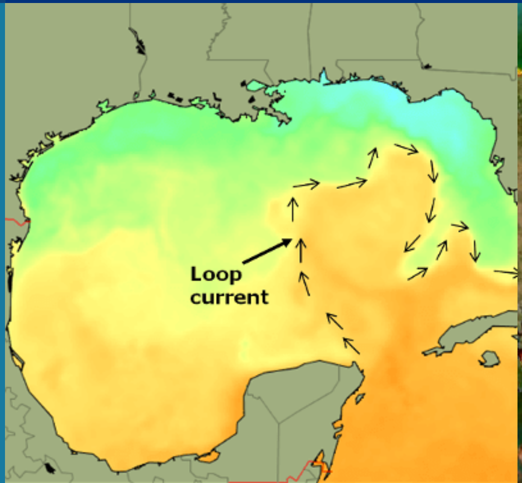
LAMINAR /
BAROTROPIC

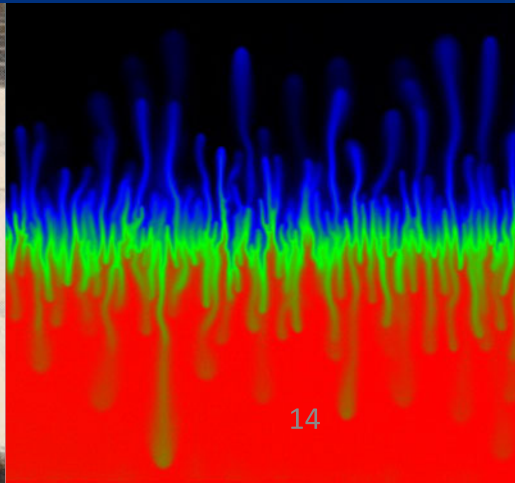
BAROCLINIC
RESOLVING

CYCLOSTROPHIC /
SUBMESOSCALE

SMALL-SCALE
THERMODYNAMICS

IN THE
OCEAN





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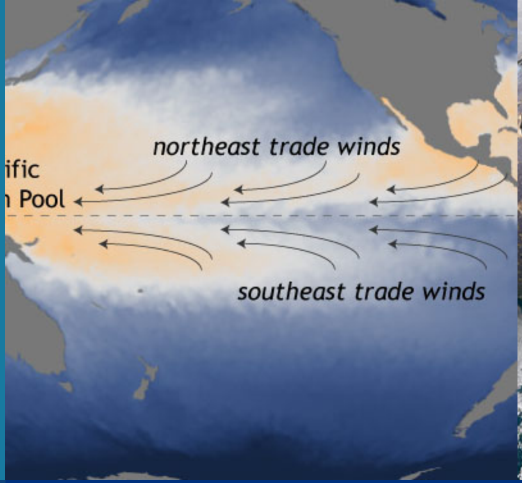

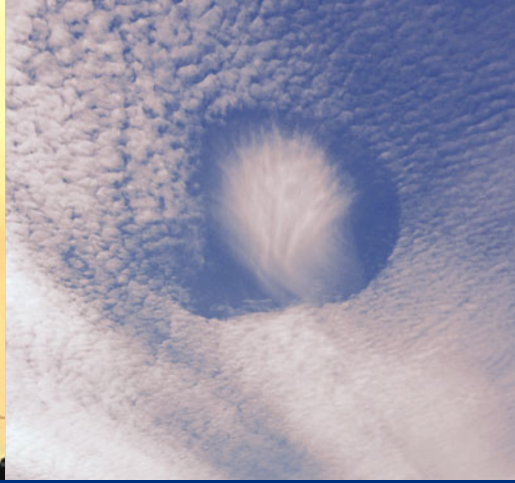

Horizontal resolution	~10° latitude/longitude	1° latitude/longitude	100 – 1 km	> 100 m
Dynamical or Physical Regime	**LAMINAR / BAROTROPIC**	**BAROCLINIC RESOLVING**	**CYCLOSTROPHIC / SUBMESOSCALE**	**SMALL-SCALE THERMODYNAMICS**
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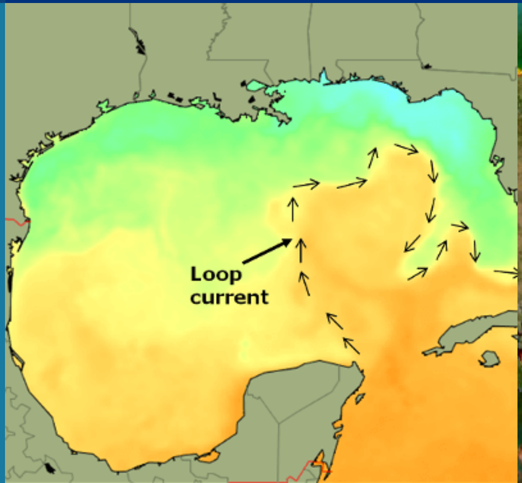
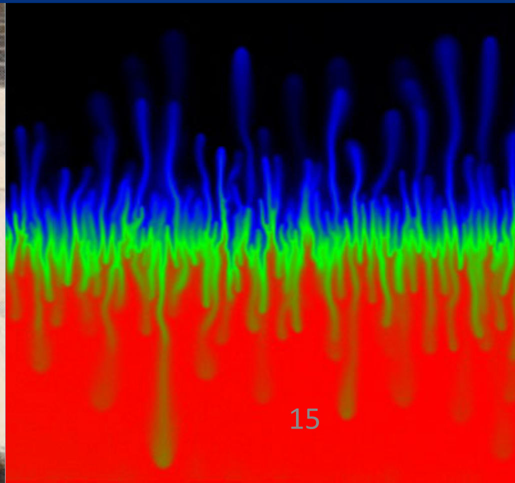
IN THE OCEAN





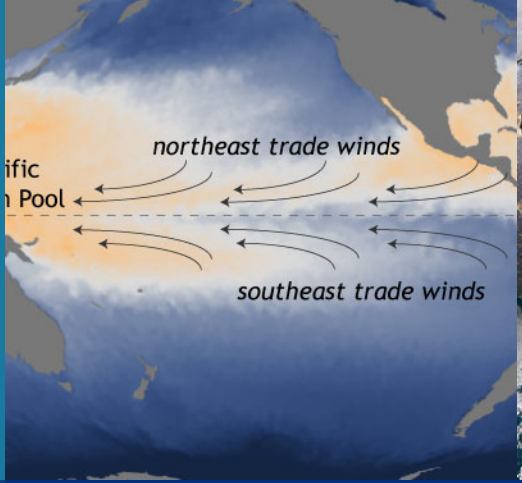
Software Components

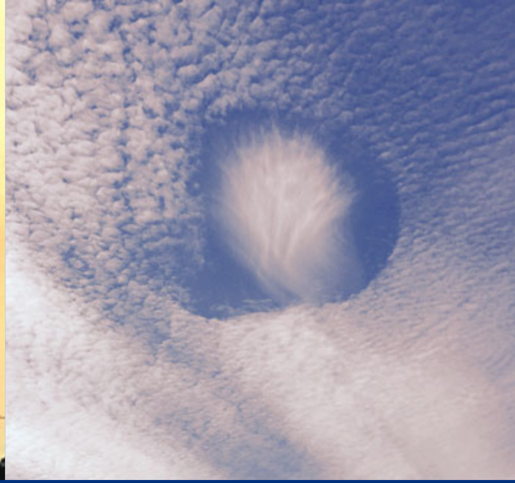
Community Earth System Model + Data Assimilation Research Testbed

Model Hierarchy

Parallel Ocean Program (POP) in Eddy-Resolving and Eddy-Parameterizing Configurations

IN THE ATMOSPHERE





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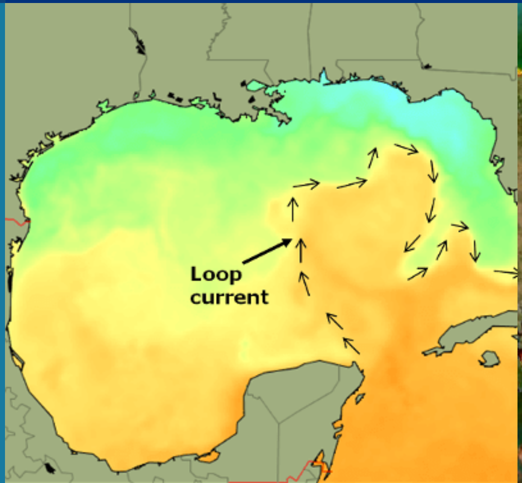

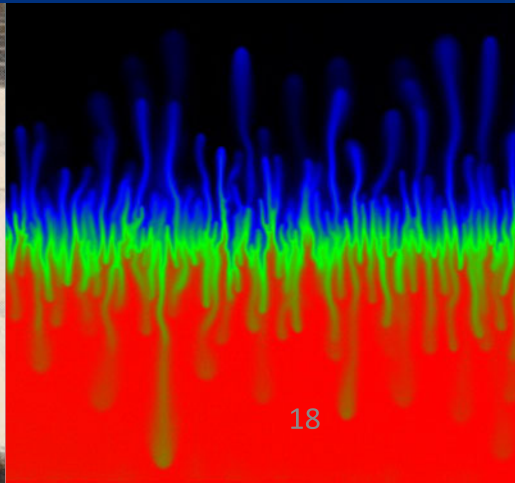

Horizontal resolution

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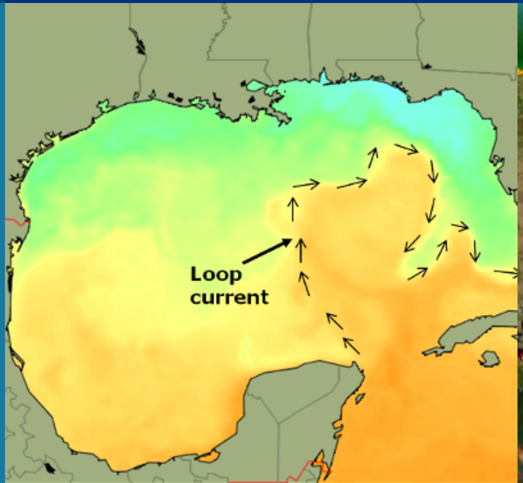
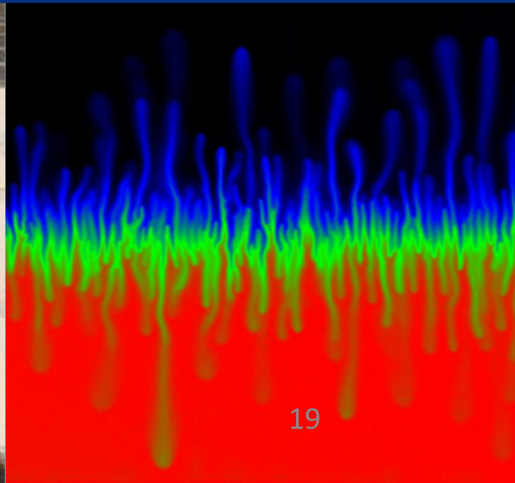
IN THE OCEAN				

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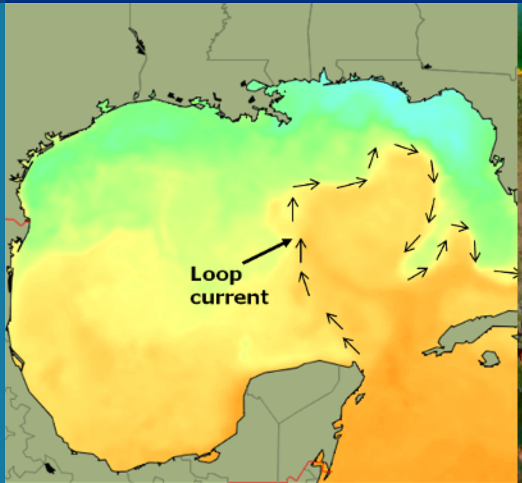
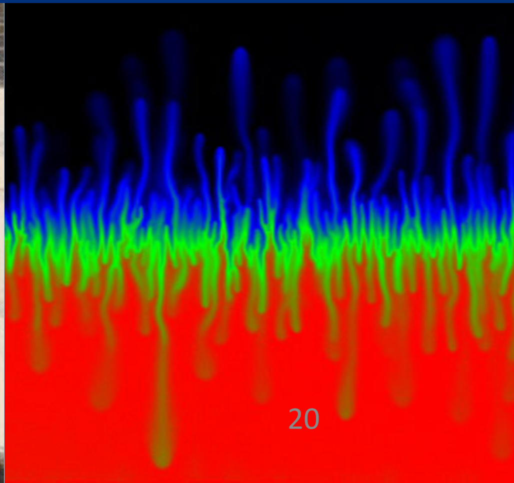
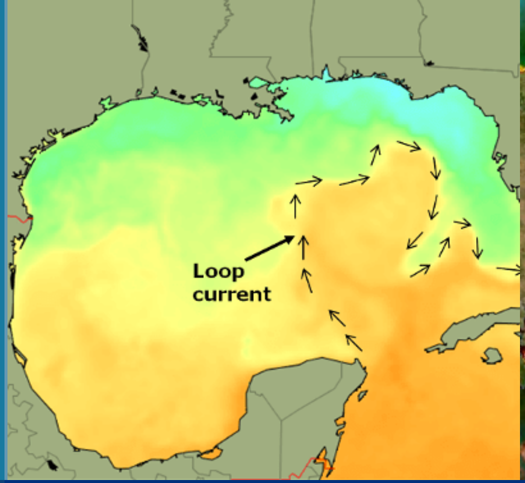
Low Resolution Ocean Configuration (g17 grid)

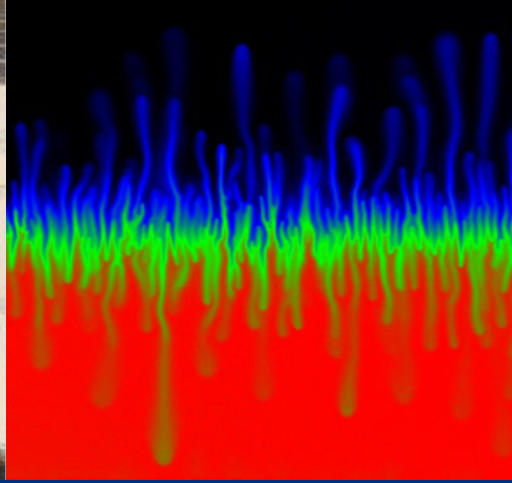






High Resolution Ocean Configuration (t13 grid)





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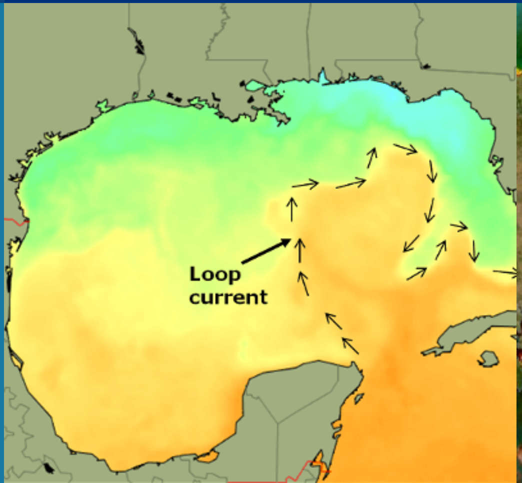

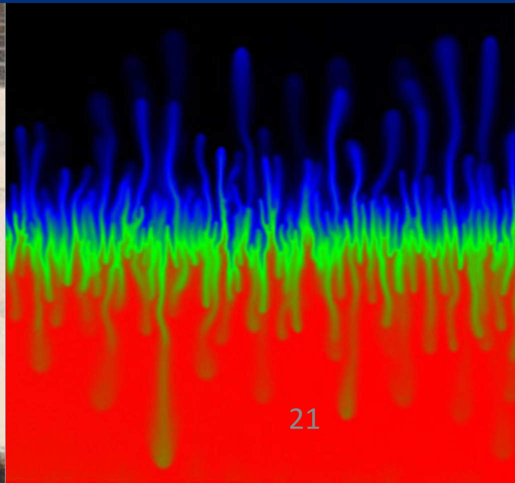

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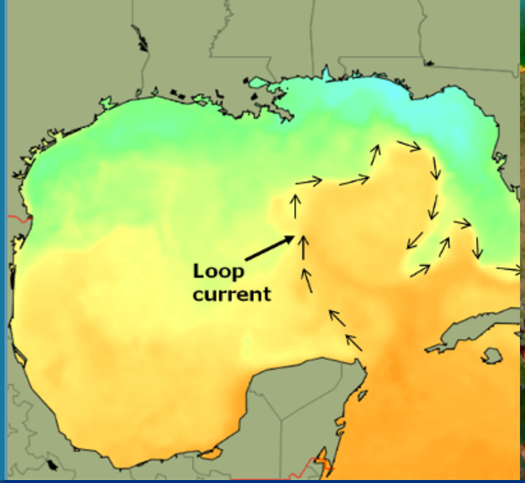

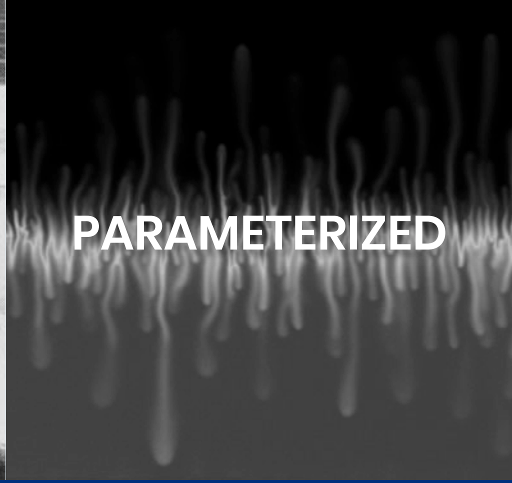

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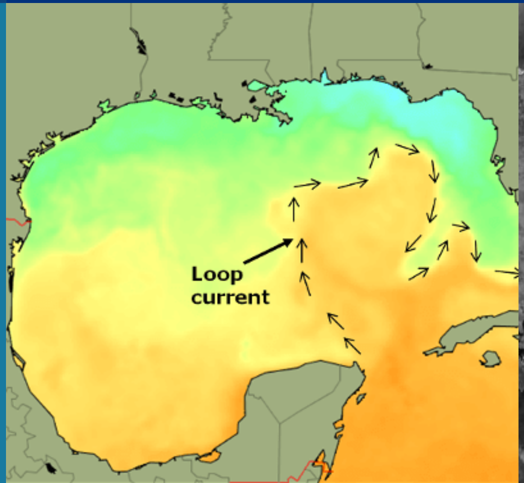

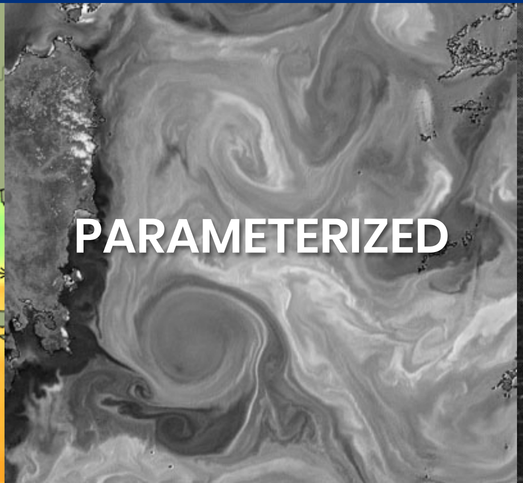

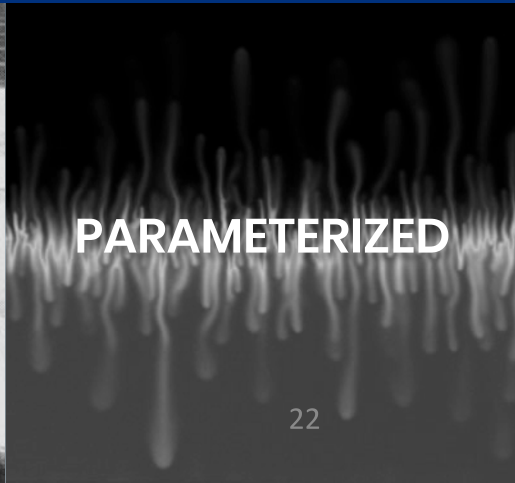

Detecting Model Error

Using Data Assimilation to Diagnose where the Model Physics Produce Improbable Outcomes

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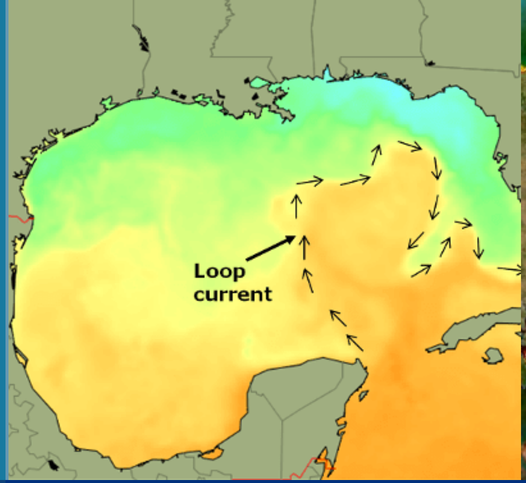

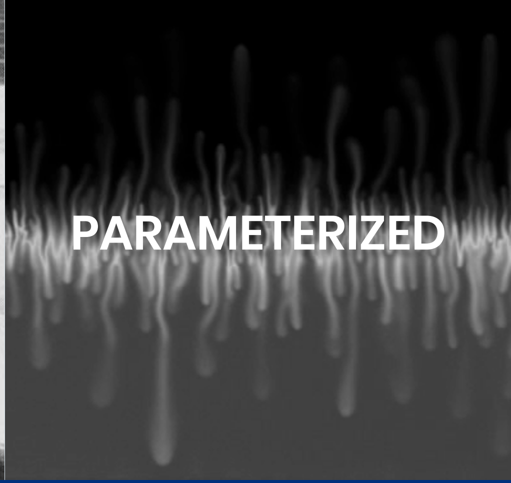

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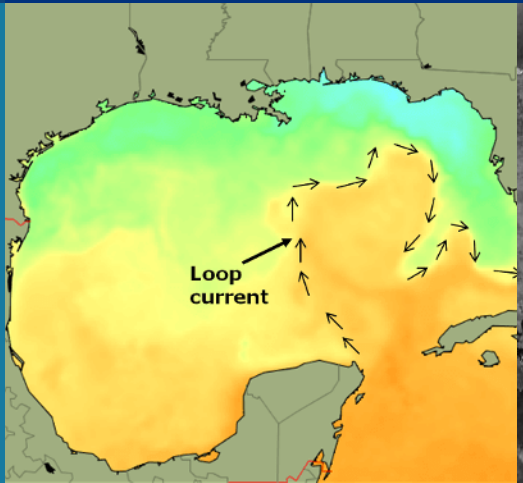

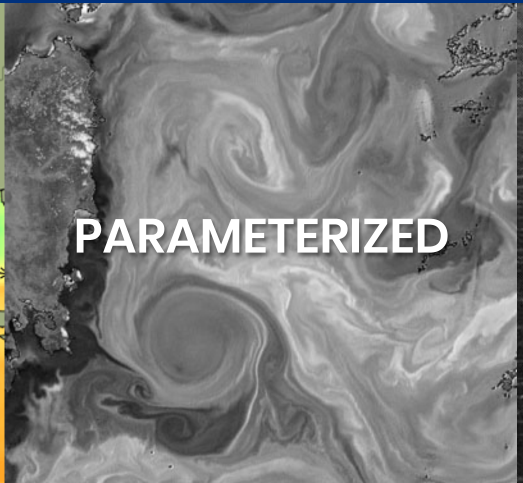

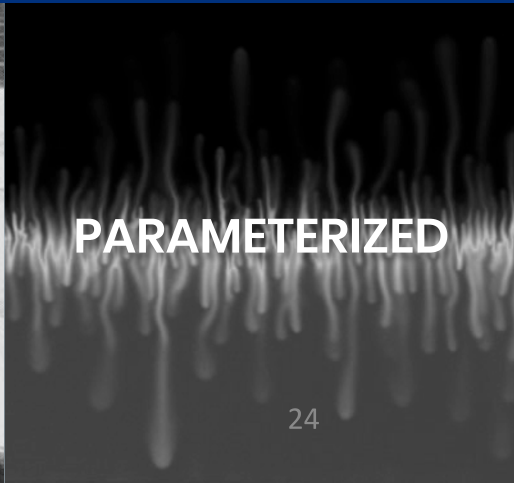

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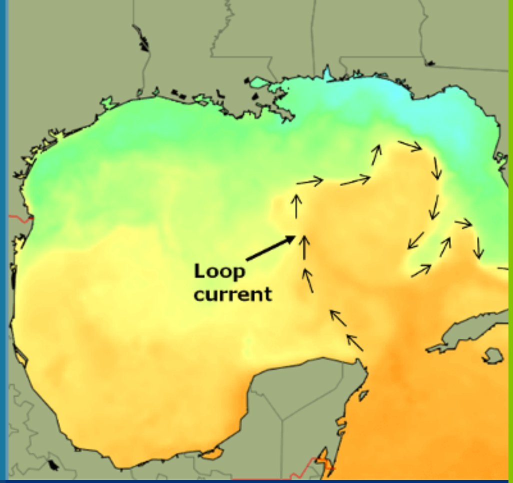

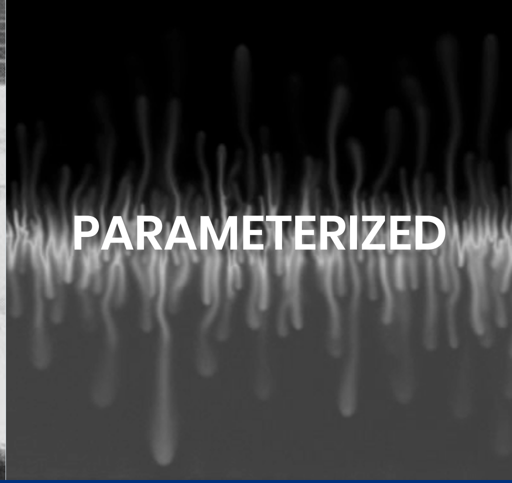

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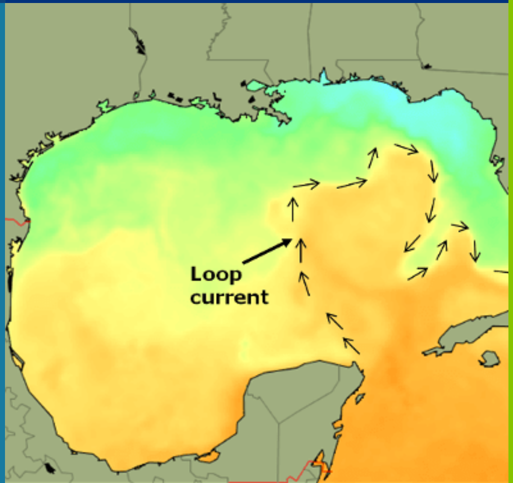
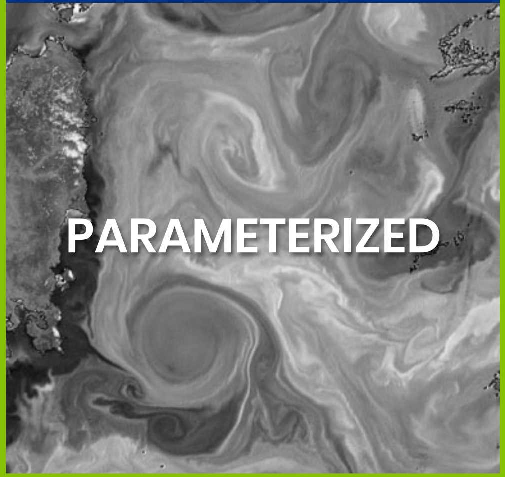
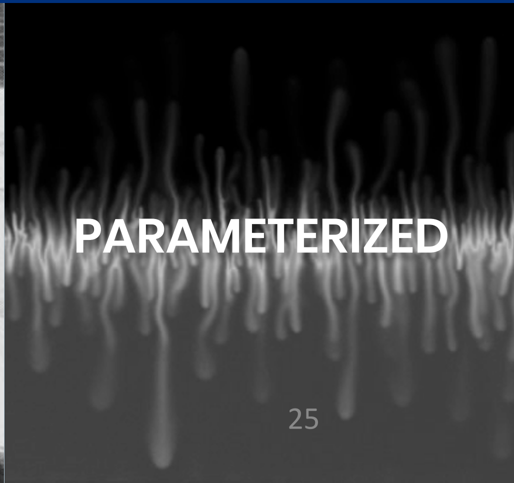


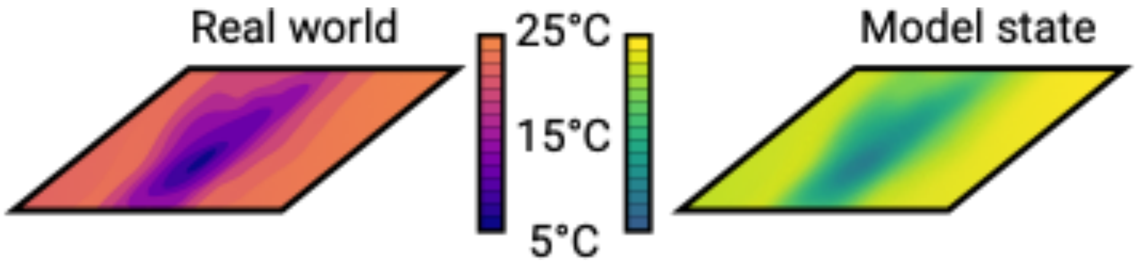




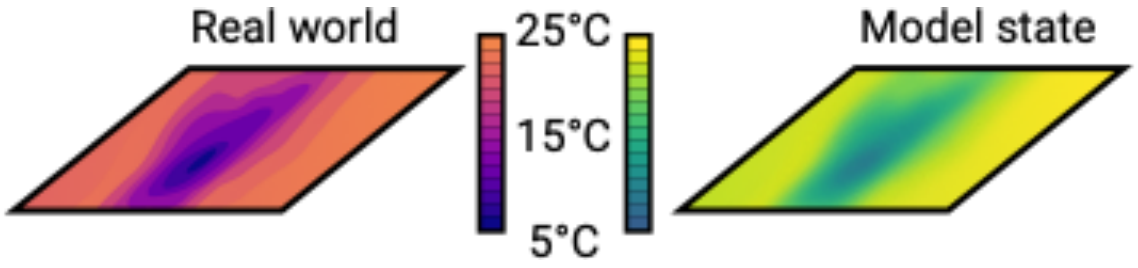
Scientific Workflow

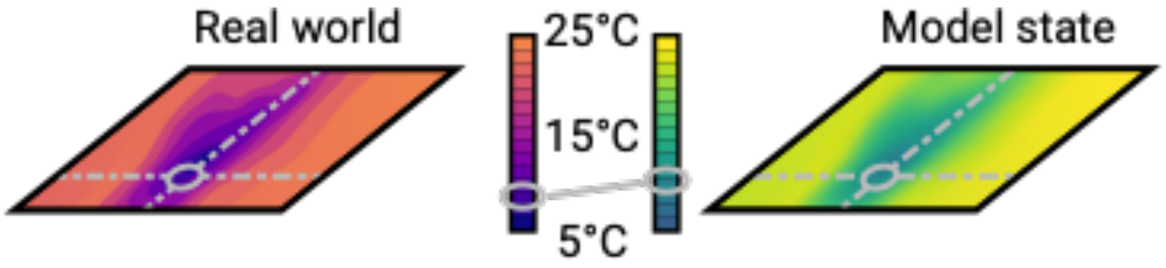
Data Assimilation Cycling

Ensemble Data Assimilation 101



Ensemble Data Assimilation 101





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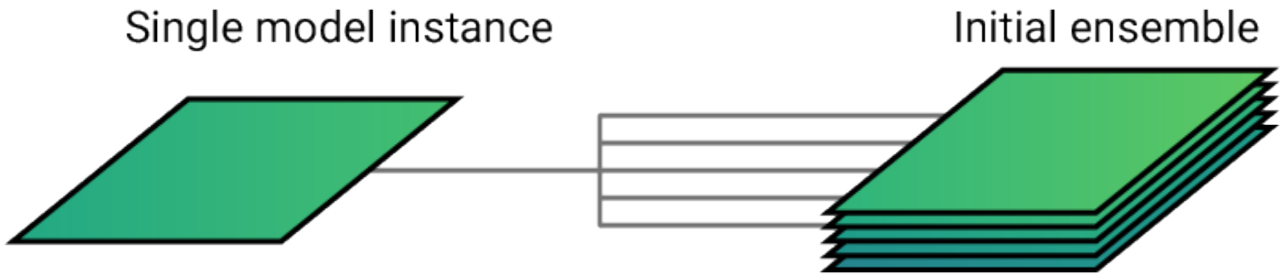

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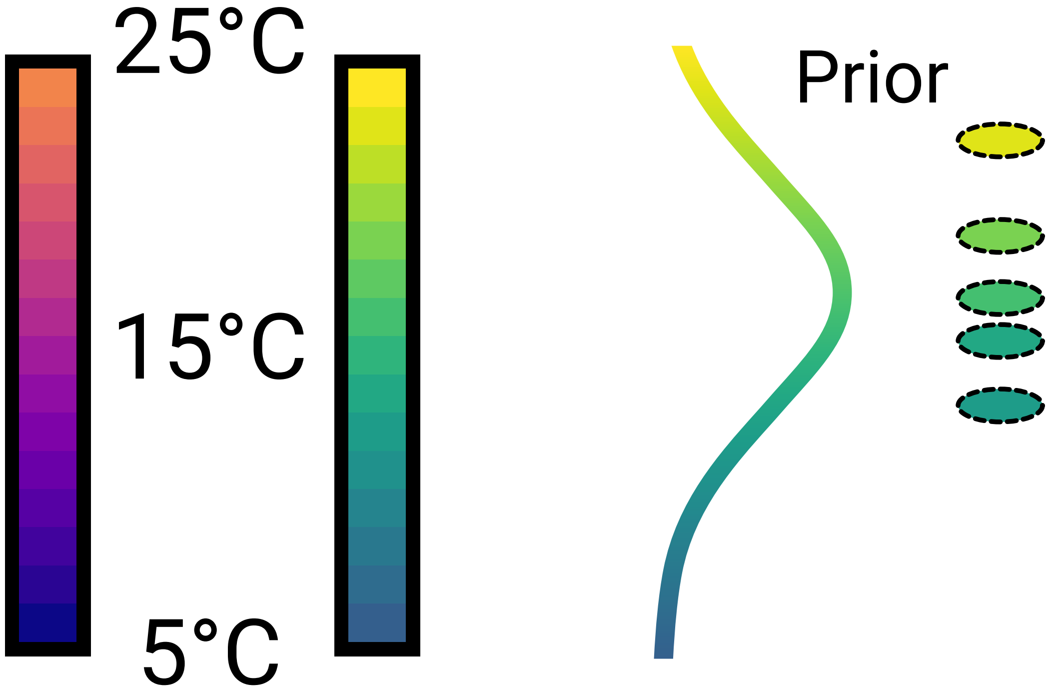

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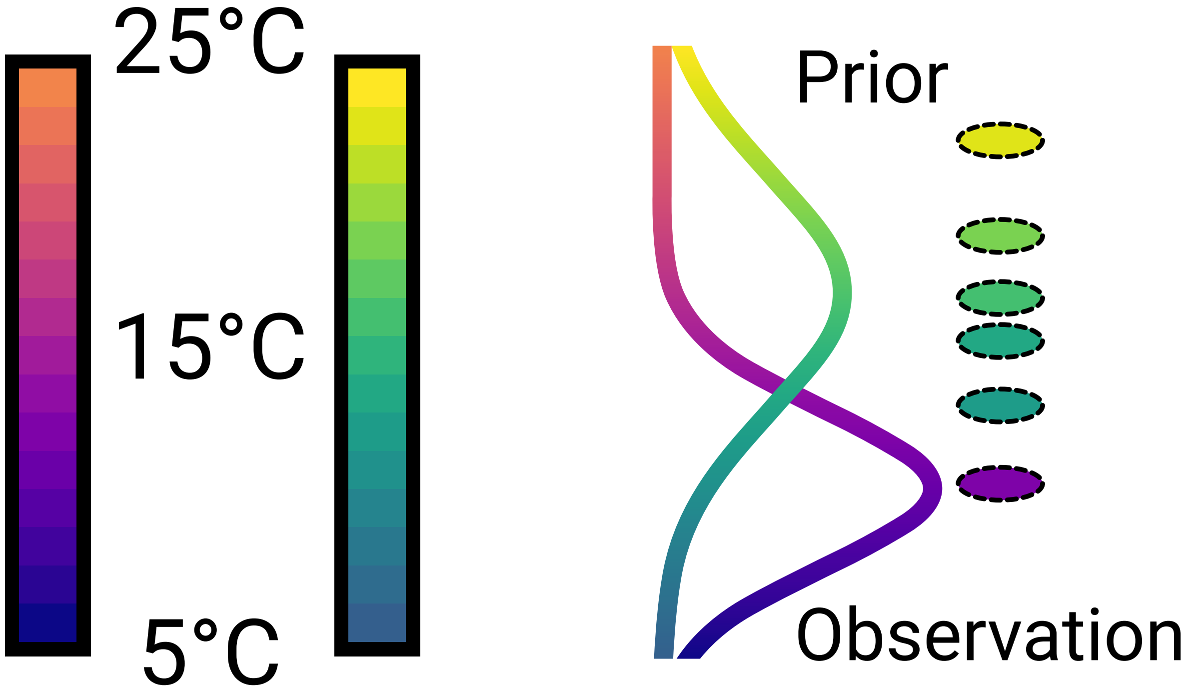

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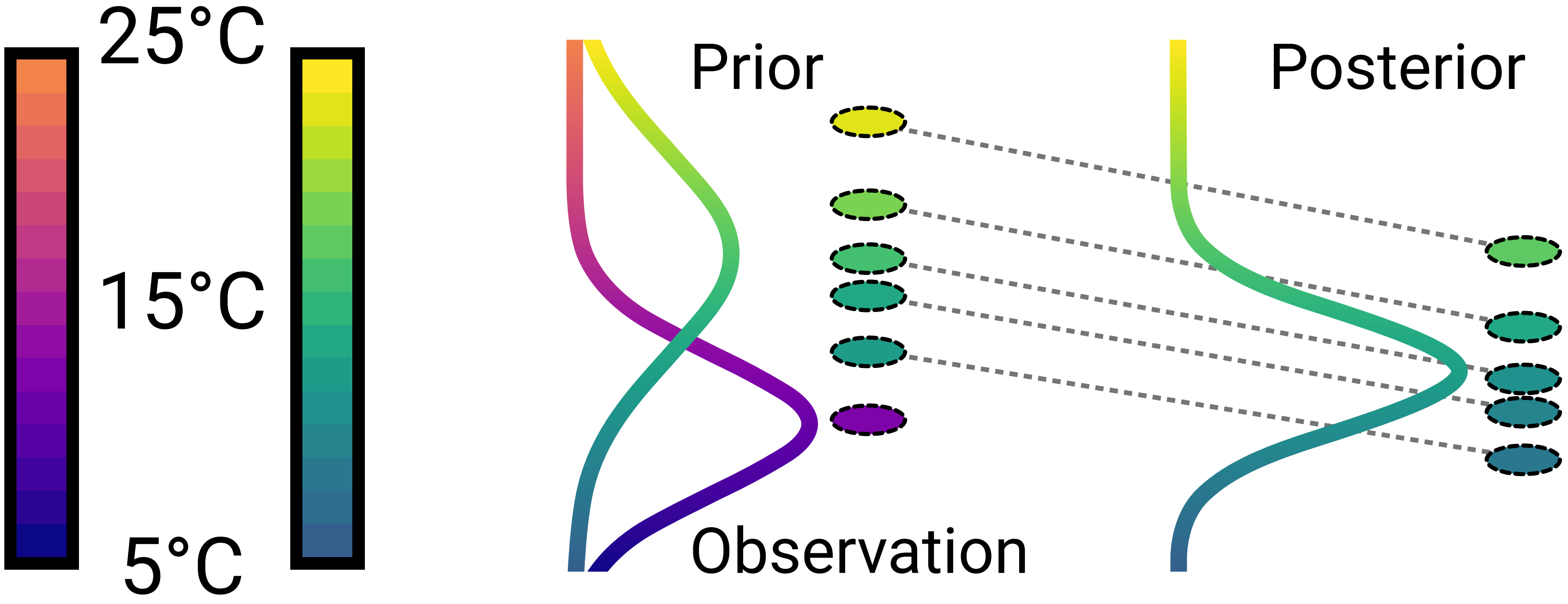

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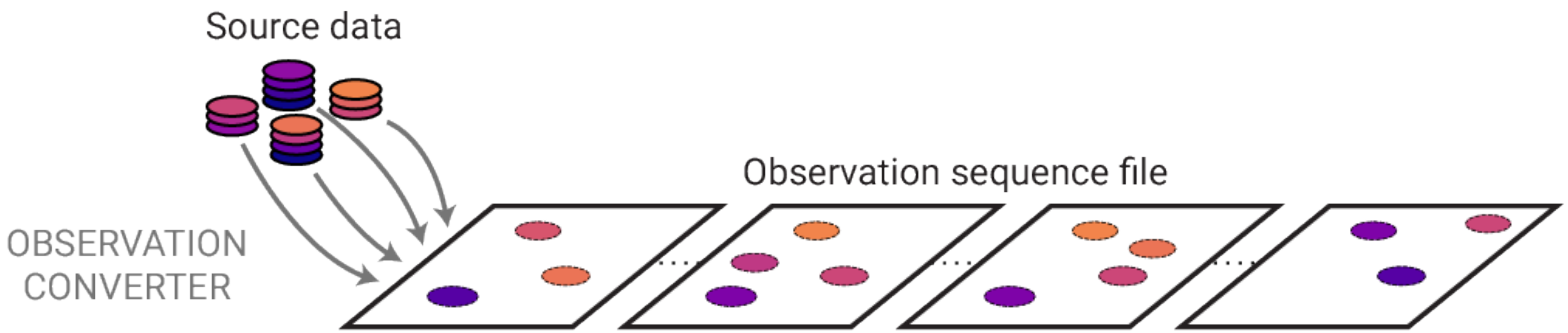

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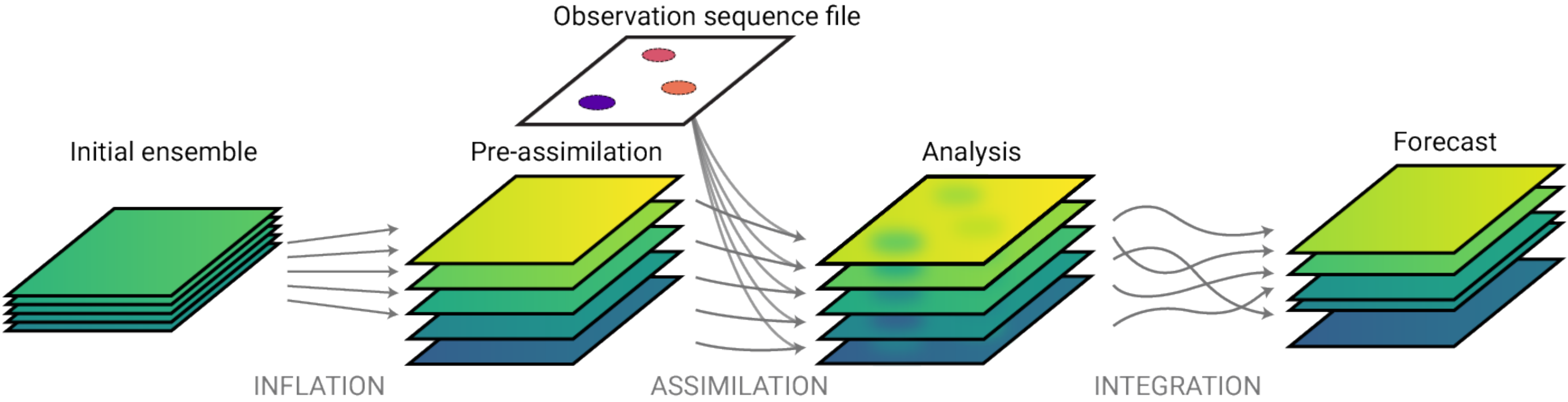

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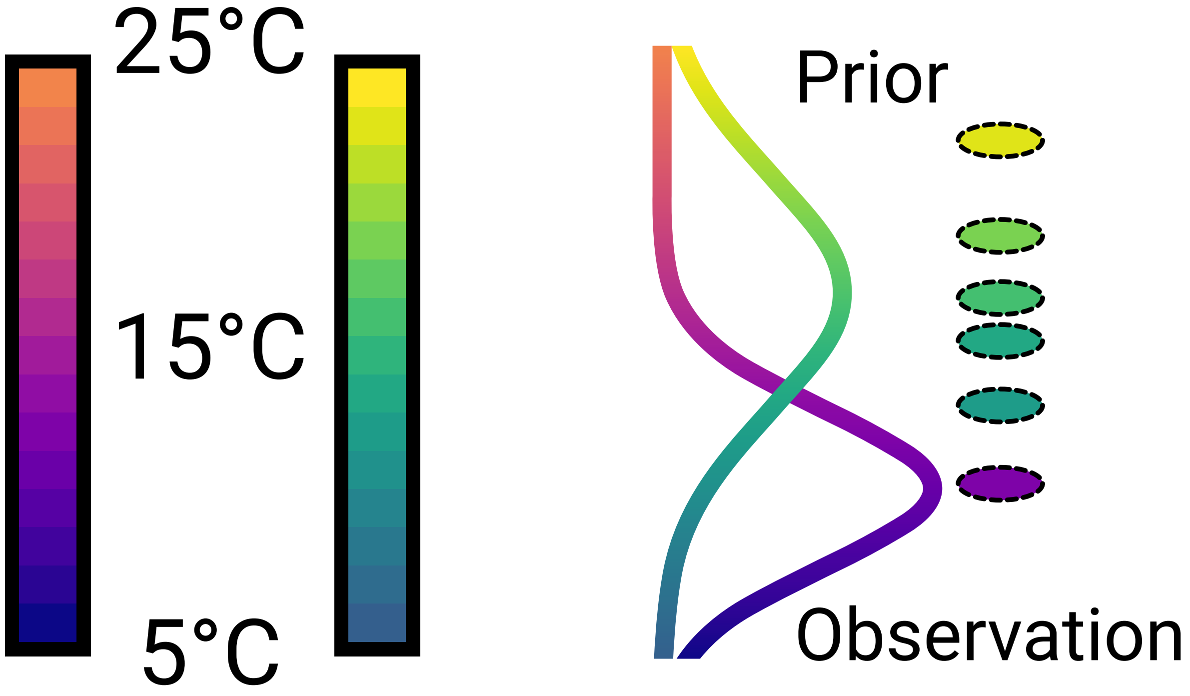
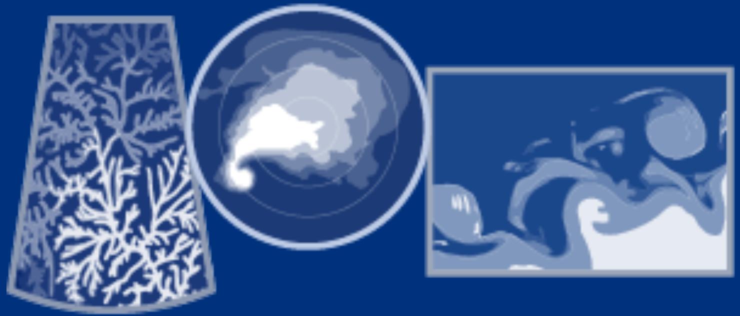
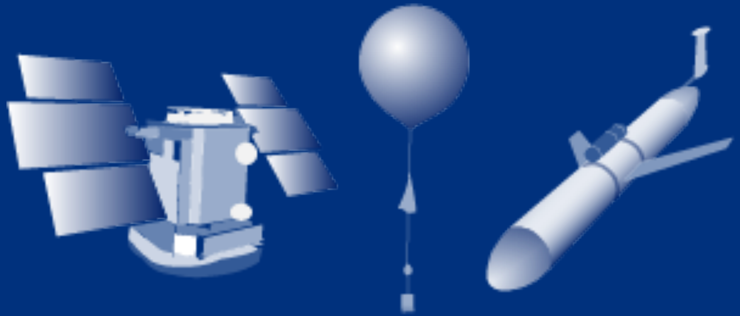


DART Overview



General-purpose codebase
Interfaces with atmospheric, oceanographic, cryospheric, land surface & space weather models.



Works with any type of observation
Satellites, weather balloons, undersea gliders, radar stations, GPS, etc. Each type can pose unique challenges.

Range of users
Can be compiled without MPI for use on laptops; can be compiled with MPI for running on thousands of nodes

Written in FORTRAN

Implements algorithms currently used in weather forecasting and experimental techniques

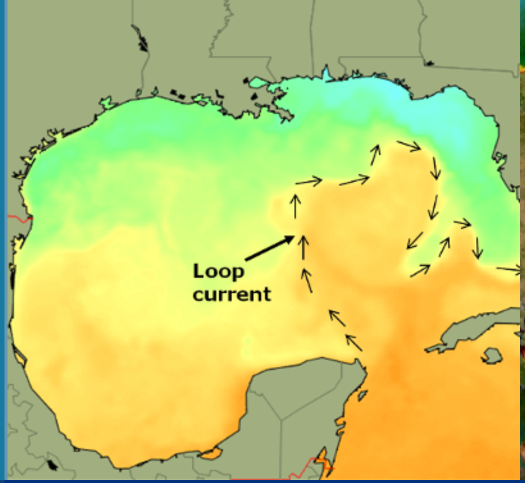
Accommodates huge state vectors; one-way MPI communications

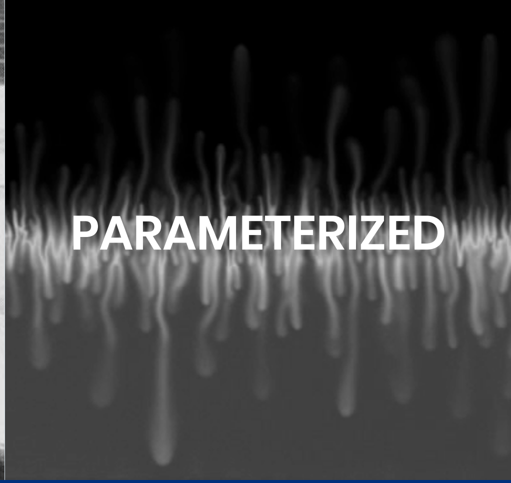
https://dart.ucar.edu

Computational Background

Experimental Setup

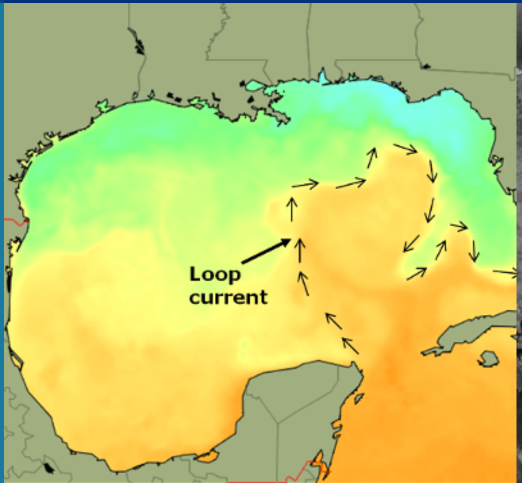
High Resolution Ocean Configuration (t13 grid)

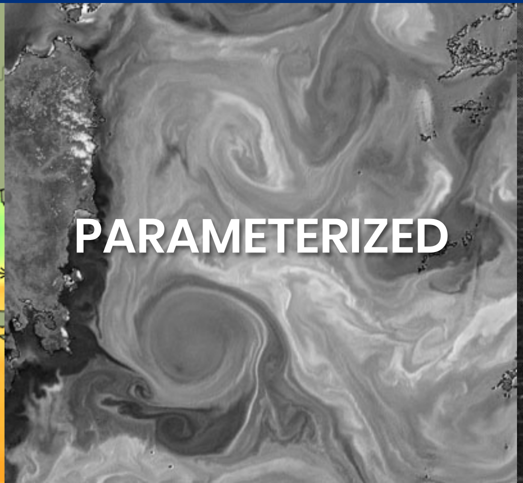


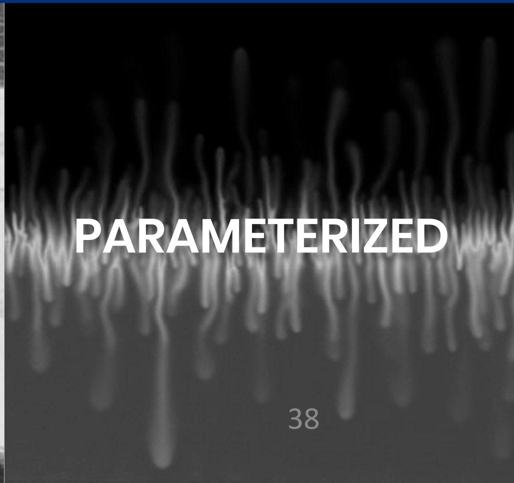


Horizontal resolution	1° latitude/longitude	0.1° latitude/longitude	1 km – 100 m	> 10 m
Dynamical or Physical Regime	**LAMINAR / BAROTROPIC**	**BAROCLINIC RESOLVING**	**CYCLOSTROPHIC / SUBMESOSCALE**	**SMALL-SCALE THERMODYNAMICS**
Horizontal resolution	1° latitude/longitude	0.1° latitude/longitude	1 km – 100 m	> 10 m

Low Resolution Ocean Configuration (g17 grid)







Model Configuration

Model Configuration	Low-resolution (g17)	High-resolution (t13)
Model Grid	Offset Greenland	Poseidon Tripole
Grid points in 1 instance	5,160,960	535,680,000
Derecho CPU hours	135,924	44,142,416
Long term archiving	3.7 TB	87.9 TB
Forcing	CAM6 Reanalysis (f09)	CAM6 Reanalysis (f09)

Team Experience

Precursor Projects

Yellowstone ASD t12 Runs

- Two long-term integrations of POP in its high-resolution, eddy-resolving configuration were completed using the Yellowstone ASD period and a University Large Allocation using roughly 5M core hours on Yellowstone.
- These experiments are described in Bryan and Bachman (2015) and Johnson et al. (2016).
- The output has been heavily studied and the experiments are colloquially known as the "ASD Runs" in CGD's Oceanography Section.

Isohaline Salinity Budget of the North Atlantic Salinity Maximum

FRANK BRYAN
Climate and Global Dynamics Division, National Center for Atmospheric Research, Boulder, Colorado*

SCOTT BACHMAN
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge, United Kingdom

(Manuscript received 21 August 2014, in final form 4 November 2014)

In this study, the salinity budget of
volumes bounded by isohaline surfaces
a high-resolution numerical simulatio
of hydrography and surface fluxes. V
instantaneous volume-integrated salt
uated from time-averaged data. In thi
variability of the salinity maximum ar
instantaneous and time-averaged moc
water mass is determined. This study fi
by the mesoscale eddies is approxima
climatological-mean conditions. The i
rates associated with surface forcing a
the surface net evaporation in the No
7 Sverdrups (Sv; 1 Sv = 10^6 m^3 s^{-1}) of
the simulation, whereas the estimate

1. Introduction

In each of the subtropical gyres of the g
there exists a distinct surface salinity max
closed isohaline contours. They are an ex
the coupling of the ocean and atmosphere
hydrologic cycle. The surface salinity max
cated in the vicinity of regional extrema i
oration but are not exactly collocated
These surface features connect to equato
westward-extending subsurface salinity max
core depths of 100–150 m) sometimes i

* The National Center for Atmospheric Researc
by the National Science Foundation.

Corresponding author address: Frank Bryan, NC
3000, Boulder, CO 80307-3000.
E-mail: bryan@ucar.edu

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Climatological Annual Cycle of the Salinity Budgets of the Subtropical Maxima

BENJAMIN K. JOHNSON
Department of Atmospheric and Oceanic Science, University of Maryland, College Park, College Park, Maryland

FRANK O. BRYAN
National Center for Atmospheric Research,[a] Boulder, Colorado

SEMYON A. GRODSKY AND JAMES A. CARTON
Department of Atmospheric and Oceanic Science, University of Maryland, College Park, College Park, Maryland

(Manuscript received 19 October 2015, in final form 17 June 2016)

ABSTRACT

Six subtropical salinity maxima (S_{max}) exist: two each in the Pacific, Atlantic, and Indian Ocean basins. The north Indian (NI) S_{max} lies in the Arabian Sea while the remaining five lie in the open ocean. The annual cycle of evaporation minus precipitation ($E - P$) flux over the S_{max} is asymmetric about the equator. Over the Northern Hemisphere S_{max}, the semiannual harmonic is dominant (peaking in local summer and winter), while over the Southern Hemisphere S_{max}, the annual harmonic is dominant (peaking in local winter). Regardless, the surface layer salinity for all six S_{max} reaches a maximum in local fall and minimum in local spring. This study uses a multidecade integration of an eddy-resolving ocean circulation model to compute salinity budgets for each of the six S_{max}. The NI S_{max} budget is dominated by eddy advection related to the evolution of the seasonal monsoon. The five open-ocean S_{max} budgets reveal a common annual cycle of vertical diffusive fluxes that peak in winter. These S_{max} have regions on their eastward and poleward edges in which the vertical salinity gradient is destabilizing. These destabilizing gradients, in conjunction with wintertime surface cooling, generate a gradually deepening wintertime mixed layer. The vertical salinity gradient sharpens at the base of the mixed layer, making the water column susceptible to salt finger convection and enhancing vertical diffusive salinity fluxes out of the S_{max} into the ocean interior. This process is also observed in Argo float profiles and is related to the formation regions of subtropical mode waters.

1. Introduction

The broad patterns of surface layer salinity (SLS) are set by the interaction of surface waters with the atmosphere (Wüst 1935). The descending branch of the Hadley cell drives anticyclonic flow over the ocean basins, causing evaporation to exceed precipitation, elevating SLS and creating six subtropical salinity maxima (hereinafter S_{max}). Five of the S_{max} lie primarily in the open ocean: the Pacific and Atlantic S_{max} are located around 25°N and 20°S; the south Indian S_{max} is around 30°S (Gordon et al. 2015). The north Indian (NI) S_{max} lies in the Arabian Sea and Gulf of Oman around 18°N. It is bounded by coasts to the north and west. For brevity, we will refer to each S_{max} by the first initial of its hemisphere and ocean basin, for example, NA S_{max} denotes the North Atlantic subtropical salinity maxima. The S_{max} are bounded by different isohaline values given in Table 1. We selected these values as those that define the maximum volume that is confined to the subtropical region of each basins' corresponding hemisphere.

The annual cycle of evaporation minus precipitation ($E - P$) flux over the subtropical regions is asymmetric about the equator (Large and Yeager 2009). Over the

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[a] The National Center for Atmospheric Research is sponsored by the National Science Foundation.

Corresponding author address: Benjamin Johnson, Department of Atmospheric and Oceanic Science, University of Maryland, College Park, 3424 Computer and Space Science Bldg., College Park, MD 20742.
E-mail: bjohnson@atmos.umd.edu

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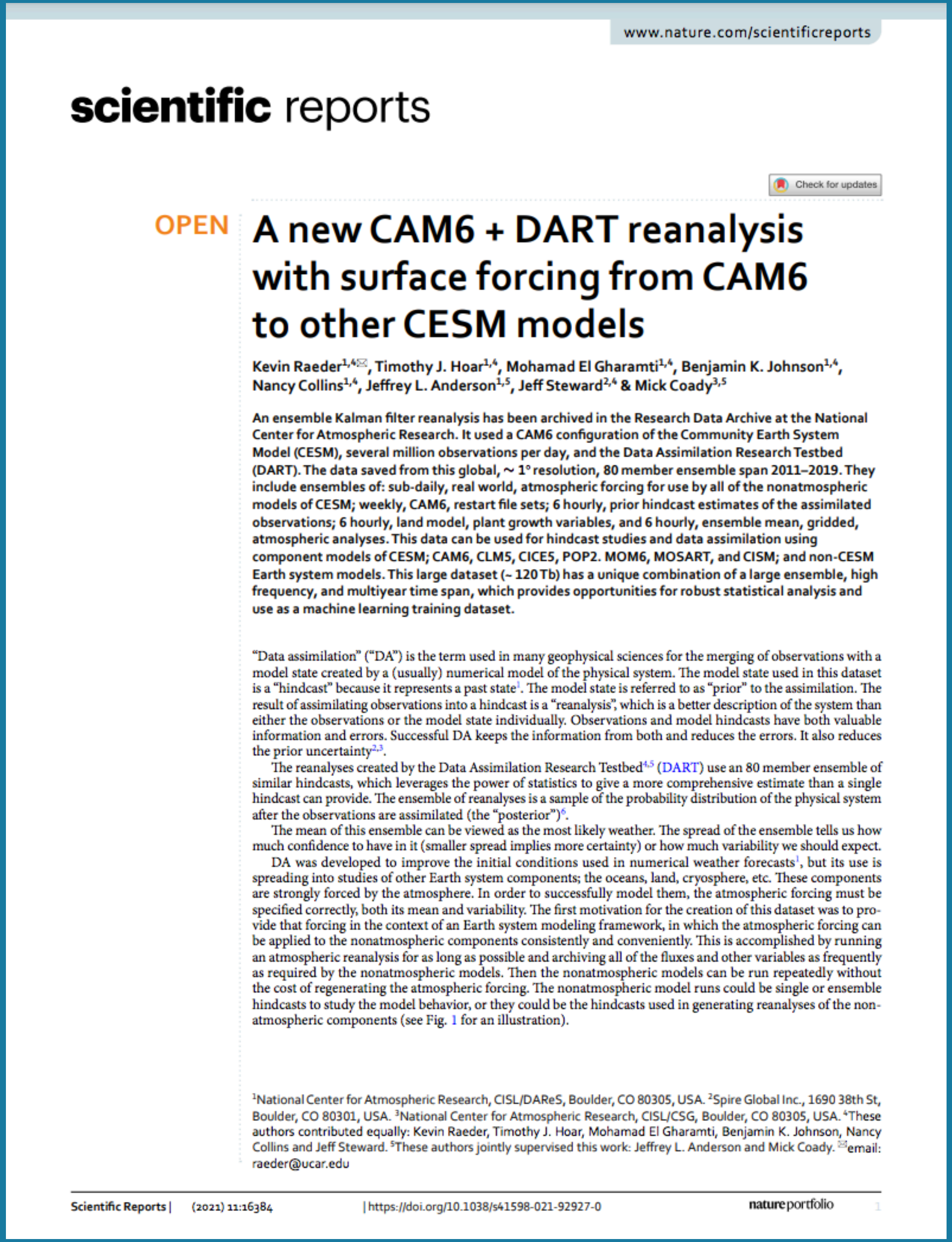
CAM6 + DART Reanalysis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A new CAM6 + DART reanalysis with surface forcing from CAM6 to other CESM models

Kevin Raeder[1,4✉], Timothy J. Hoar[1,4], Mohamad El Gharamti[1,4], Benjamin K. Johnson[1,4], Nancy Collins[1,4], Jeffrey L. Anderson[1,5], Jeff Steward[2,4] & Mick Coady[3,5]

An ensemble Kalman filter reanalysis has been archived in the Research Data Archive at the National Center for Atmospheric Research. It used a CAM6 configuration of the Community Earth System Model (CESM), several million observations per day, and the Data Assimilation Research Testbed (DART). The data saved from this global, ~ 1° resolution, 80 member ensemble span 2011–2019. They include ensembles of: sub-daily, real world, atmospheric forcing for use by all of the nonatmospheric models of CESM; weekly, CAM6, restart file sets; 6 hourly, prior hindcast estimates of the assimilated observations; 6 hourly, land model, plant growth variables, and 6 hourly, ensemble mean, gridded, atmospheric analyses. This data can be used for hindcast studies and data assimilation using component models of CESM; CAM6, CLM5, CICE5, POP2. MOM6, MOSART, and CISM; and non-CESM Earth system models. This large dataset (~ 120 Tb) has a unique combination of a large ensemble, high frequency, and multiyear time span, which provides opportunities for robust statistical analysis and use as a machine learning training dataset.

"Data assimilation" ("DA") is the term used in many geophysical sciences for the merging of observations with a model state created by a (usually) numerical model of the physical system. The model state used in this dataset is a "hindcast" because it represents a past state[1]. The model state is referred to as "prior" to the assimilation. The result of assimilating observations into a hindcast is a "reanalysis", which is a better description of the system than either the observations or the model state individually. Observations and model hindcasts have both valuable information and errors. Successful DA keeps the information from both and reduces the errors. It also reduces the prior uncertainty[2,3].

The reanalyses created by the Data Assimilation Research Testbed[4,5] (DART) use an 80 member ensemble of similar hindcasts, which leverages the power of statistics to give a more comprehensive estimate than a single hindcast can provide. The ensemble of reanalyses is a sample of the probability distribution of the physical system after the observations are assimilated (the "posterior")[6].

The mean of this ensemble can be viewed as the most likely weather. The spread of the ensemble tells us how much confidence to have in it (smaller spread implies more certainty) or how much variability we should expect.

DA was developed to improve the initial conditions used in numerical weather forecasts[1], but its use is spreading into studies of other Earth system components; the oceans, land, cryosphere, etc. These components are strongly forced by the atmosphere. In order to successfully model them, the atmospheric forcing must be specified correctly, both its mean and variability. The first motivation for the creation of this dataset was to provide that forcing in the context of an Earth system modeling framework, in which the atmospheric forcing can be applied to the nonatmospheric components consistently and conveniently. This is accomplished by running an atmospheric reanalysis for as long as possible and archiving all of the fluxes and other variables as frequently as required by the nonatmospheric models. Then the nonatmospheric models can be run repeatedly without the cost of regenerating the atmospheric forcing. The nonatmospheric model runs could be single or ensemble hindcasts to study the model behavior, or they could be the hindcasts used in generating reanalyses of the nonatmospheric components (see Fig. 1 for an illustration).

[1]National Center for Atmospheric Research, CISL/DAReS, Boulder, CO 80305, USA. [2]Spire Global Inc., 1690 38th St, Boulder, CO 80301, USA. [3]National Center for Atmospheric Research, CISL/CSG, Boulder, CO 80305, USA. [4]These authors contributed equally: Kevin Raeder, Timothy J. Hoar, Mohamad El Gharamti, Benjamin K. Johnson, Nancy Collins and Jeff Steward. [5]These authors jointly supervised this work: Jeffrey L. Anderson and Mick Coady. ✉email: raeder@ucar.edu

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nature portfolio

- Raeder et al., (2021) completed a 10-year atmospheric reanalysis using DART and the atmospheric component of CESM, the Community Atmosphere Model 6
- Reanalysis spans 2011-2019 with 2020 currently underway
- Required roughly 17M CPU hours on Cheyenne
- Revealed inefficiencies in model build scripts due to directory locking

KiloCAM Experiment

- Johnson and Gharamti are conducting a thousand-member CAM6 ensemble experiment to test DART algorithms on Shaheen II, a Cray XC40 at King Abdullah University of Science and Technology.

- Shaheen II has 6174 nodes with Intel Haswell processors and can theoretically compute 7.2 Pflop/s. The thousand-member experiment uses up to 3000 nodes at one time, nearly 50% of the system’s nodes.

Closing Remarks

Desired Outcomes

Desired Outcomes

- Produce a hierarchical reanalysis spanning four complete years, 2012-2015, that encompasses the termination of the 2012 La Niña event, the transition of PDO from its cool to warm phase in 2014 and the onset of the subsequent 2015 El Niño event.
- Allow for enhanced understanding of mode water formation, continuing the work of Johnson et al. (2016)
- Sensitivity testing of adaptive inflation algorithms, continuing the work of Gharamti (2018)
- Studying interannual variability of the Equatorial Pacific Cold Tongue, continuing the work of Deppenmeier et al. (2021)
- Improved parameterization of mesoscale eddies, continuing the work of Grooms and Kleiber (2019).

Deppenmeier, A.-L., F. O. Bryan, W. S. Kessler, and L. Thompson, 2021: Modulation of Cross-Isothermal Velocities with ENSO in the Tropical Pacific Cold Tongue. *J. Phys. Oceanogr.*, **51**, 1559–1574, https://doi.org/10.1175/JPO-D-20-0217.1.

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Gharamti, M., 2018: Enhanced Adaptive Inflation Algorithm for Ensemble Filters. *Mon. Wea. Rev.*, **146**, 623–640, https://doi.org/10.1175/MWR-D-17-0187.1.

Grooms, I., and W. Kleiber, 2019: Diagnosing, modeling, and testing a multiplicative stochastic Gent-McWilliams parameterization. *Ocean Modelling*, **133**, 1–10, https://doi.org/10.1016/j.ocemod.2018.10.009.

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Thanks For Your Attention

Any Questions?