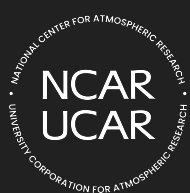


CESM-DART

Updates on **Assimilation** for Earth System Models

Helen Kershaw
DAReS NSF NCAR



SIParCS

DART NUOPC

CROCODILE

pyDART

Terminology

SIParCS Summer Internships in Parallel Computing

DART Data Assimilation Research Testbed

NUOPC National Unified Operational Prediction Capability

CROCODILE CESM Regional Ocean and Carbon cOnfigurator with Data assimilation and Embedding

CESM Community Earth System Model

Ensemble Data Assimilation

Ensemble Data Assimilation



Group of model forecasts

Ensemble Data Assimilation



Group of model forecasts

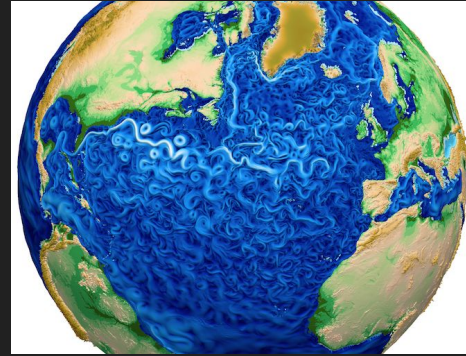
Measurements



Ensemble Data Assimilation



Group of model forecasts



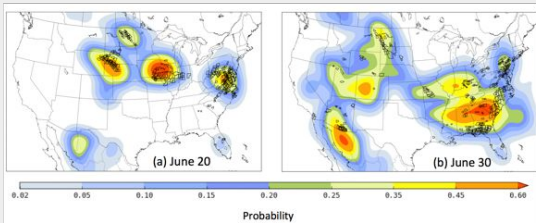
Improved estimate

Measurements

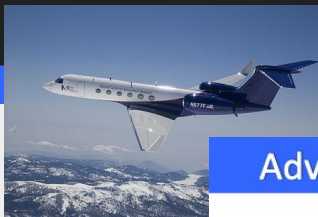


NCAR Real-time ensemble prediction system

Severe weather forecast for two days compared to NWS warnings



- WRF, 10 member ensemble, GFS for boundary conditions
- Continuous operation from April 2015 to December 2017
- 48 hour forecasts at 3km resolution
- First continuously cycling ensemble system for CONUS
- CISL Dedicated Queues and Computing Support were Vital



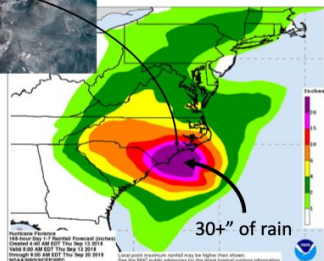
CISL Seminar: 6 Nov 2019 page 28

WRF-Hydro/DART: Florence 2018



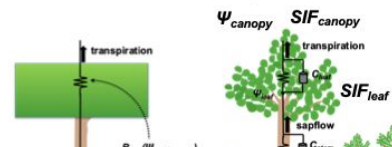
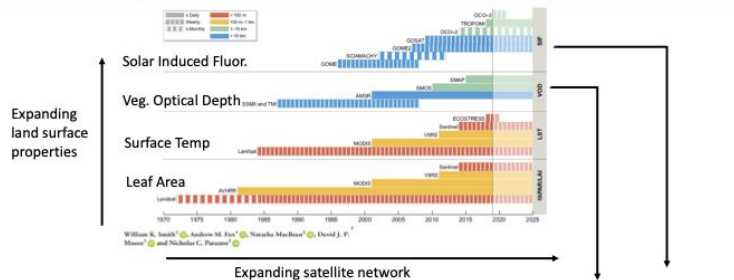
Hurricane Florence made landfall near Wrightsville Beach, North Carolina at 7:15 a.m. ET September 14. The GOES East satellite captured this geocolor image at 7:45 a.m. ET

Winds up to 150 mph (240 km/hr)
Damage: \$24.23 billion
NOAA/NWS/NCEP/WPC



CISL Seminar: 6 Nov 2019 page 38

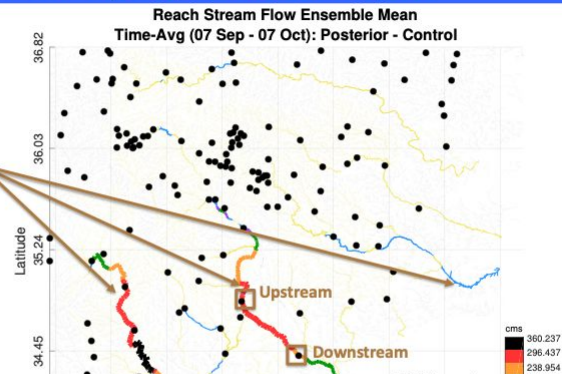
Advancing models & observations together



WRF-Hydro/DART: DA Impact

Assimilation happens every hour

Correction along major reaches. DA is adding water to the stream channels.



5

Featured project: Computational & Information Systems Lab & Research Applications Lab Collaboration

PREDICTING FLOODS AND PROTECTING LIVES



DATA ASSIMILATION FOR THE ENTIRE EARTH SYSTEM

Use ensemble DA techniques with geophysical models spanning the



USE DATA FROM ANY SOURCE, TEST MANY ALGORITHMS

Assimilate any suitable observations. Swap out filter and



LEARN ON LAPTOPS, RUN ON SUPERCOMPUTERS

Compile without MPI for conceptual models or with MPI for GCMs on

Featured project: NC State, UC San Diego, MIT & KAUST Collaboration

UNDERSTANDING GULF OF MEXICO EDDY DYNAMICS



DATA ASSIMILATION FOR THE ENTIRE EARTH SYSTEM

Use ensemble DA techniques with models spanning the



USE DATA FROM ANY SOURCE, TEST MANY ALGORITHMS

Assimilate any suitable observations. Swap out filter and



LEARN ON LAPTOPS, RUN ON SUPERCOMPUTERS

Compile without MPI for conceptual models or with MPI for GCMs on

Featured project: University of Michigan, NCAR, NASA & NRL Collaboration

NEXT-GENERATION SPACE WEATHER PREDICTION



DATA ASSIMILATION FOR THE ENTIRE EARTH SYSTEM



USE DATA FROM ANY SOURCE, TEST MANY ALGORITHMS



LEARN ON LAPTOPS, RUN ON SUPERCOMPUTERS

dart.ucar.edu

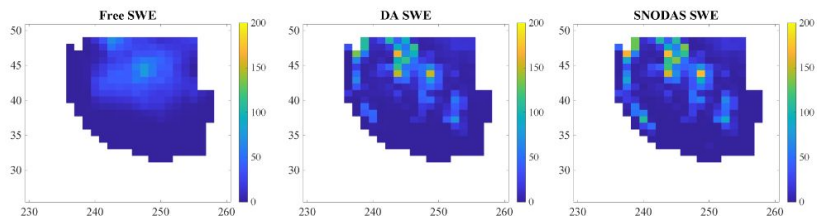
Shout out: Xueli's talk

Monday, June 10th, 2024 CESM Land Agenda

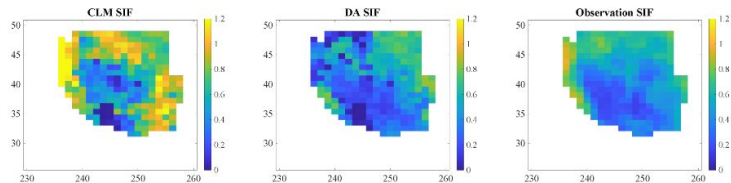
2:08pm- **Assimilating SIF and SWE observations into CLM using DART to improve GPP over the high mountains in the Western US**

Xueli Huo

Despite challenges with snow input and melting, DA successfully corrects Snow Water Equivalent over the Western US



Though the regional average of SIF aligns well with the observation, SIF is overcorrected along the Cascade Range and in Montana



Need to refine the way of leaf nitrogen altered by DA to effectively impact GPP

Shout out: Moha & Kevin's posters

The Data Assimilation Research Testbed: Recent Advances and Tools for CESM



Moha Gharantmi¹ (dAREs/TDD/CISL; gharantmi@ucar.edu), J. Anderson¹, B. Gaubert¹, D. Amrhein¹, A. RafieeNasabi¹, Y.-C. Noh²

¹U.S. National Science Foundation National Center for Atmospheric Research (NSF NCAR), Boulder CO, USA

²Korea Polar Research Institute, Incheon, South Korea

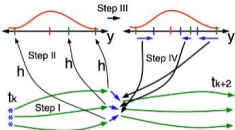
DART Algorithm and Tools

The Data Assimilation Research Testbed (DART) is an ensemble community facility, developed and maintained by the Data Assimilation Research Section at NSF NCAR.

DART's sequential filtering algorithm (Anderson, 2009) solves the following Bayesian problem:

$$p(x_t, \theta | Y_t) \propto p(x_t | x_{t-1}, \theta, Y_{t-1}) p(x_{t-1} | \theta, Y_{t-1})$$

$$x_t: \text{state}, \theta: \text{parameters}, y_t: \text{observations}$$



- Step I: A model integration step using 3 members
- Step II: Forward operator (h) computes expected obs
- Step III: Ensemble increments in obs space are computed
- Step IV: Linear regression of obs increments onto the state

What capabilities DART provides:
 Ensemble forecasting/reanalysis,
 Observation design/analysis,
 Parameter estimation,
 Predictability,
 OSE, OSSE,
 Extensive teaching and tutorial material with exercises!

Additional DA Tools

- Inflation to increase the spread
- Localization to limit the impact of observations in space
- Others: Sampling error correction, Spread restoration, Hierarchical groups, diagnostics...

References

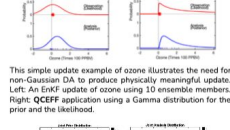
- Anderson, J., 2009. A sequential Monte Carlo approach to data assimilation. *Journal of Applied Meteorology*, 48, 1291-1302.
- Anderson, J., 2012. A particle-ensemble Kalman filter. *Journal of Applied Meteorology*, 51, 1515-1534.
- Anderson, J., 2015. A particle-ensemble Kalman filter. *Journal of Applied Meteorology*, 54, 1515-1534.
- Anderson, J., 2018. A particle-ensemble Kalman filter. *Journal of Applied Meteorology*, 57, 1515-1534.
- Anderson, J., 2021. A particle-ensemble Kalman filter. *Journal of Applied Meteorology*, 60, 1515-1534.
- Anderson, J., 2024. A particle-ensemble Kalman filter. *Journal of Applied Meteorology*, 63, 1515-1534.

Non-Gaussian DA

Quantile Conserving Ensemble Filtering Framework (Anderson, 2022, 2023, 2024)

QCEFF: is a general framework for ensemble DA. It serves as an alternative to traditional ensemble Kalman filter (EnKF). DART's sequential filtering algorithm (Anderson, 2009) solves the following Bayesian problem:

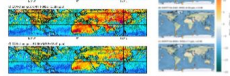
$$p(x_t, \theta | Y_t) \propto p(x_t | x_{t-1}, \theta, Y_{t-1}) p(x_{t-1} | \theta, Y_{t-1})$$



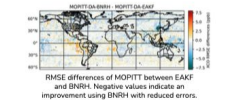
This simple update example of ozone illustrates the need for non-Gaussian DA to produce physically meaningful updates. Left: An EnKF update of ozone using 10 ensemble members. Right: QCEFF application using a Gamma distribution for the prior and the likelihood.

Another example demonstrating the need for nonlinear and non-Gaussian DA update. Displayed are the joint prior (left) and posterior (right) distributions of an observed temperature and unobserved ice fraction variables.

CAM-Chem-DART (Gaubert et al., 2024)



A 1° CAM-Chem (CESM2) with 32 vertical layers is coupled to DART to assimilate MOPITT V01 CO retrievals (left) and in-situ surface CO using NDACC station network (right). Three DA experiments are compared: Control (no CO, EnKF Gaussian filter) and the BNRH (in QCEFF variant).

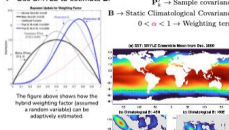


Hybrid EnKF & 3D-Var/OI

An Adaptive Hybrid Ensemble-Variational Scheme (Gharantmi, 2021)

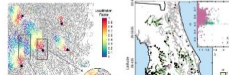
EnKF-OI: is a hybrid filtering scheme combining the ensemble flow-dependent covariances with time-invariant background covariances from 3D-Var or OI. The weight on each covariance term is adaptively estimated.

The static background covariance?
 > Sophisticated NWP methods
 > Use SMYLE to estimate B



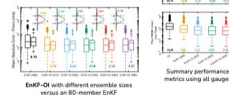
Utilizing SMYLE ensemble covs available for the last 50 years to estimate B and the climatological covariance of the ocean's SST.

Streamflow and Flooding Application in DART (Gharantmi et al., 2024)



The adaptive hybrid EnKF-OI scheme is tested in a regional flooding domain due to hurricane Ian (Florida, 2022). The static background covariance is estimated using a 40 year retrospective model run.

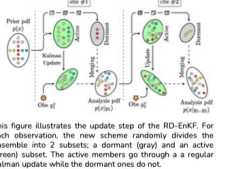
Highly efficient - 4 times less expensive
 Excellent accuracy compared to the EnKF
 Robust against forecast-observation mismatch
 Enhance of predictability by up to 18 hours



Extreme Sampling Errors

A Randomized Dormant Ensemble Kalman Filter (Gharantmi, 2023)

RD-EnKF: is a new variant of the EnKF, specifically designed to tackle extreme sampling errors when the ensemble size is considerably smaller than the size of the state.



This figure illustrates the update step of the RD-EnKF. For each observation, the new scheme randomly divides the ensemble into 2 subsets: a dormant (gray) and an active (light) subset. The active members go through a regular Kalman update while the dormant ones do not.

The RD-EnKF formulation uses a mixture likelihood in which the Bayesian likelihood is scaled by $(1-\alpha)$ and incremented by a factor of α .

CIce-DART (Noh et al., 2024)



Difference in monthly-mean sea ice concentration for the control run (no DA), EnKF (midnight), and RD-EnKF (right). The RD-EnKF yields larger ensemble spread than the EnKF.

Acknowledgements

This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977. Any opinions, findings and conclusions or recommendations expressed in this material do not necessarily reflect the views of NSF.

Essential Tools for Predictability Studies Provided by the Data Assimilation Research Testbed

Importance of ensemble forcing to land assimilations and a couple showing what happened to the Reanalysis during COVID (aircraft obs disappeared, both biases increased).

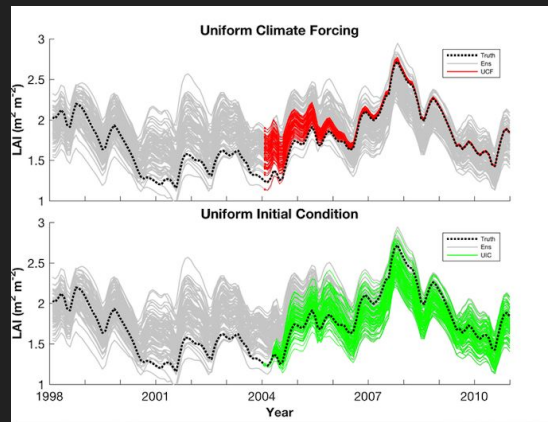


Figure courtesy of Andy Fox.

SIParCS

DART NUOPC

CROCODILE

pyDART

SIParCS project

"Optimizing ensemble data assimilation performance for coupled Earth System models" investigating the use of **NUOPC/ESMF** for **DA**, and comparing this to traditional 'offline' modes of Data Assimilation.

Anh Pham

Suman Shekhar



SIParCS project

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Anh Pham
Suman Shekhar

Mentors:
Dan Amrhein
Helen Kershaw



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Anh Pham
Suman Shekhar

Mentors:
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Helen Kershaw

Thanks to the **ESMF** team and Alper Altuntas



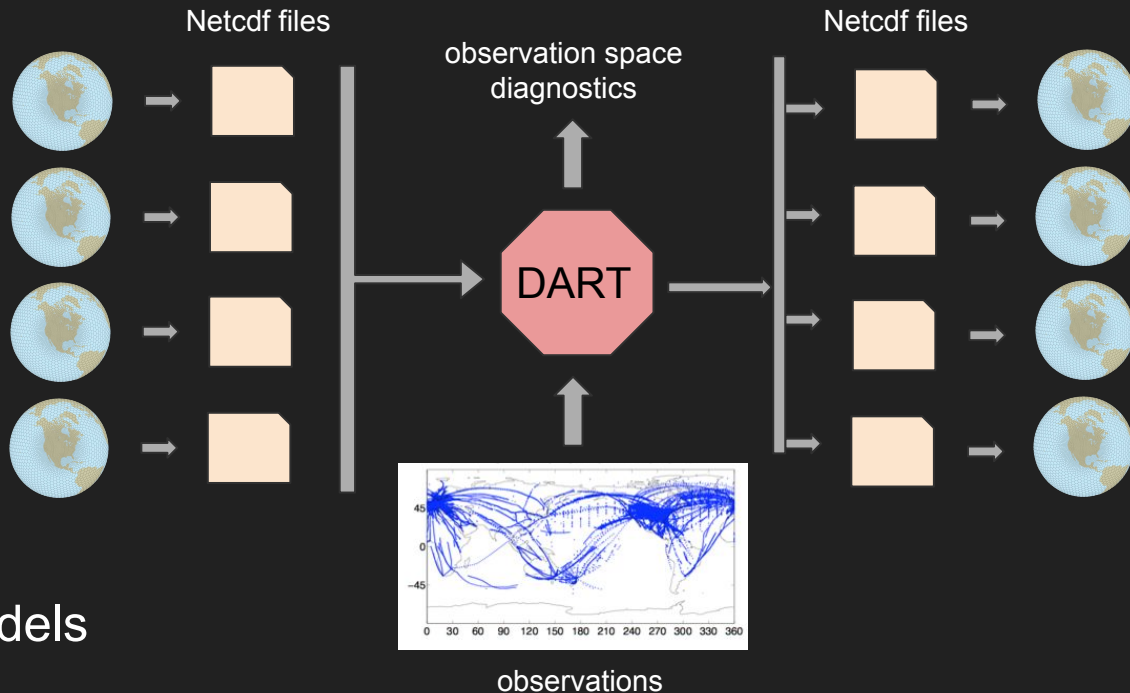
SIParCS project

Every assimilation window:

- Advance the ensemble of models
- Every model writes their state to file
- DART reads all model states and observations for the time window
- Assimilation updates the ensemble of states
- DART writes updated state files
- Models restart with updated states

Lots of data movement
“transpose”

IO: Models -> DART -> Models



SIParCS project

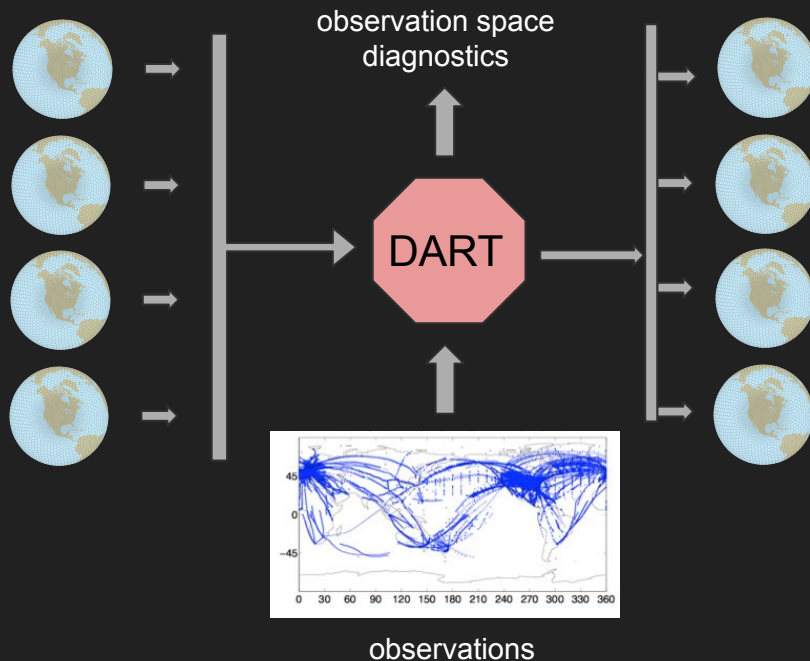
Every assimilation window:

- Advance the ensemble of models
- DART reads the observations for the time window
- Assimilation updates the ensemble of states
- Models continue with updated states

Lots of data movement

“transpose”

Not going to disk



CROCODILE



WOODS HOLE
OCEANOGRAPHIC
INSTITUTION®



5 year collaboration between NSF
NCAR and WHOI

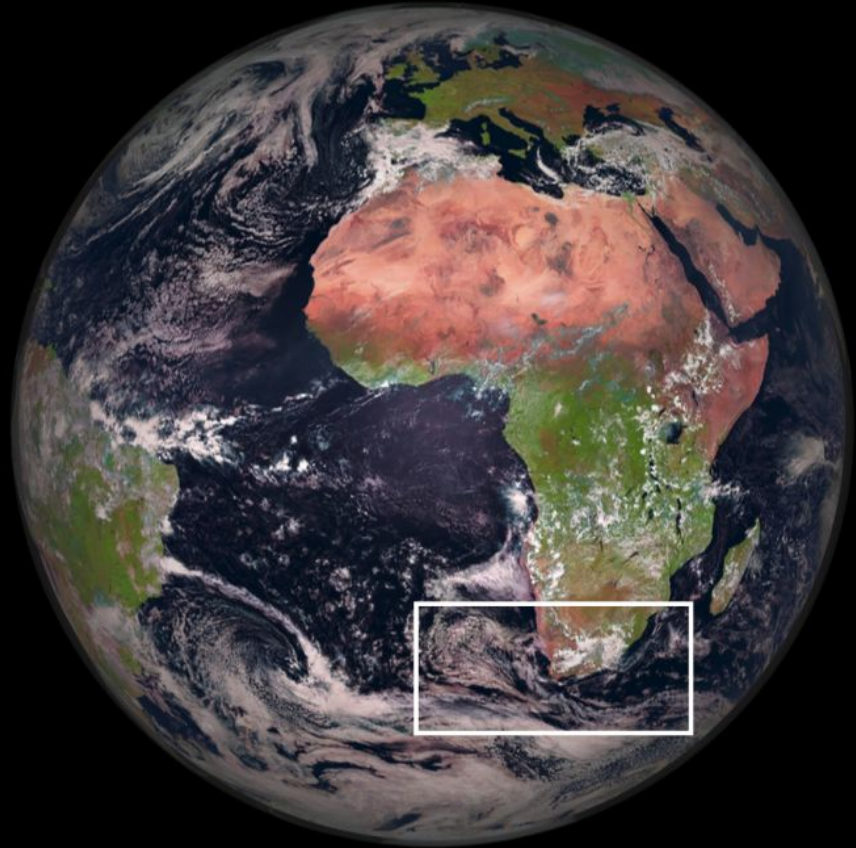
Motivation

How do we increase usability of infrastructure that translates global dynamics to human / actionable scales?

Regional model configuration requires setup and tuning.

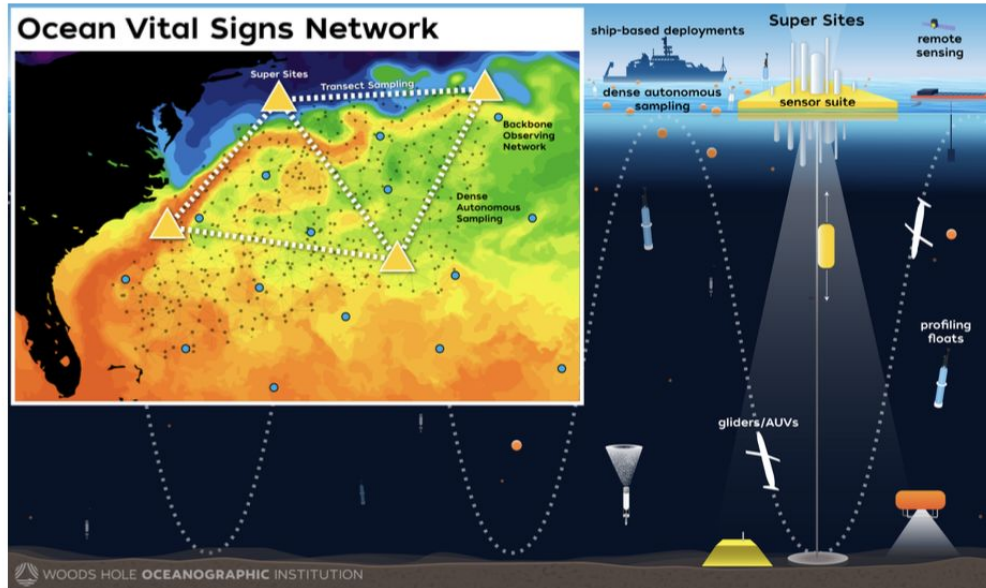
Data assimilation requires years of effort and technical capacity building.

Few have **access** to the computational resources and tools required for configuring and running these systems and then analyzing the relatively large data sets they generate.



Dan Amrhein

Use case 1: The Ocean Vital Signs Network (OVSN) and ocean CDR

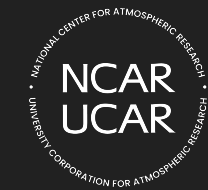


Designing next-generation ocean observing systems



Dan Amrhein

CROCODILE DART

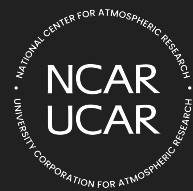


5 year collaboration between NSF
NCAR and WHOI

CROCODILE (py)DART



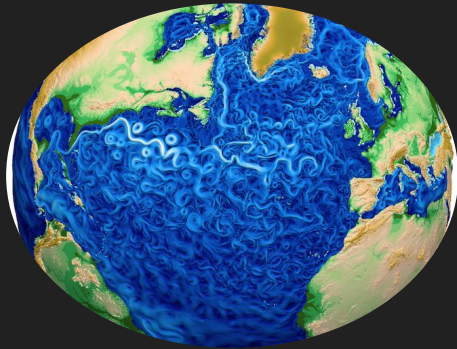
WOODS HOLE
OCEANOGRAPHIC
INSTITUTION®



5 year collaboration between NSF
NCAR and WHOI

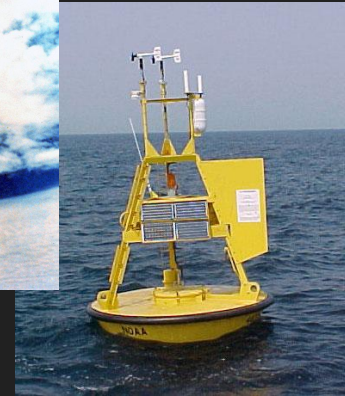
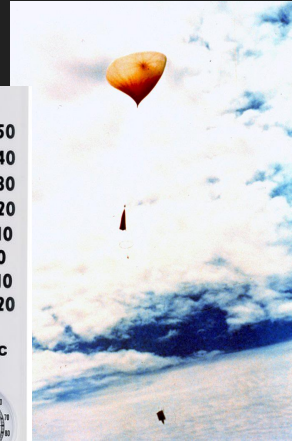
Data Assimilation Research Testbed

Models: MOM6



State Space

Observations

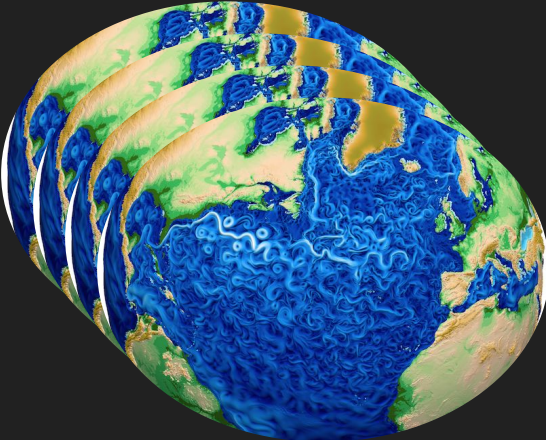


Observation Space

Data Assimilation Research Testbed

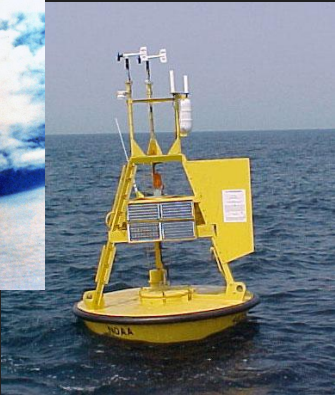
Models: MOM6

Ensemble



State Space

Observations



Observation Space

DART-MOM6



latest

GETTING STARTED

System requirements

Fortran90 compiler

Locating netCDF library

Downloading DART

Compiling DART

Verifying installation

WHAT IS DATA ASSIMILATION?

Introduction to ensemble data assimilation

The Lorenz 63 model and its relevance to data assimilation

Data assimilation in DART using the Lorenz 63 model

WHAT IS DART?

What is DART?

The benefits of using DART

A brief history of DART

Home / MOM6

[Edit on GitHub](#)

MOM6

A new ocean component model based on the Modular Ocean Model version 6 (MOM6) has been incorporated into [CESM](#) and is anticipated to replace POP2 as the default ocean component in CESM3. An early functional release of the MOM6 ocean component has been made available to users beginning with CESM2.2. Instructions for using MOM6 in CESM are available on the [MOM_interface GitHub Wiki](#).

This DART-MOM6 interface was developed for [MOM6](#) within the CESM framework.

MOM6 time

The default in CESM is to run with no leap years. To assimilate real observations, we need to switch to the Gregorian calendar to account for leap years.

```
./xmlchange CALENDAR=GREGORIAN
```

To illustrate what happens if you do not set CALENDAR=GREGORIAN, here is an example where the RUN_STARTDATE is set to 2015-02-01 and MOM6 is run for 10 days.

```
./xmlchange RUN_STARTDATE=2015-02-01
```

The MOM6 restart file has the following meta data, where Time is days from year 1.

Observation Sequence

World Ocean Database example

DA Input: obs_seq.out

- The observation types in the file
- Locations of the observations
- Quality control value(s) for each observation
- Observation + any observation specific metadata
- Time and order of observations

```
obs_sequence
obs_kind_definitions
  13
  15 FLOAT_SALINITY
  16 FLOAT_TEMPERATURE
  23 GLIDER_SALINITY
  24 GLIDER_TEMPERATURE
  27 MOORING_SALINITY
  28 MOORING_TEMPERATURE
  30 BOTTLE_SALINITY
  31 BOTTLE_TEMPERATURE
  32 CTD_SALINITY
  33 CTD_TEMPERATURE
  43 XBT_TEMPERATURE
  46 APB_SALINITY
  47 APB_TEMPERATURE
num_copies:          1 num_qc:          1
num_obs:           66643 max_num_obs:    66643
WOD observation
WOD QC
  first:             1 last:             66643
OBS                 1
2.704750061035156E-002
0.000000000000000E+000
          -1                2                -1
obdef
loc3d
          3.753021682990578          1.345058936474565          10.000000000000000          3
kind
          32
43322          151163
2.500000000000000E-007
OBS                 2
2.7048099951782227E-002
0.000000000000000E+000
          1                3                -1
obdef
loc3d
          3.753021682990578          1.345058936474565          15.000000000000000          3
kind
          32
43322          151163
2.500000000000000E-007
OBS                 3
2.704929924011230E-002
0.000000000000000E+000
          2                4                -1
obdef
loc3d
          3.753021682990578          1.345058936474565          20.000000000000000          3
kind
          32
```

Observation Sequence

Radiance example

DA Output: obs_seq.final

- various 'copies' of each observation
 - Observation value
 - Truth
 - Prior and Posterior Forward Operators, mean, standard deviation

```
obs_sequence
obs_type_definitions
  1
    216 GOES_16_ABI_RADIANCE
    num_copies:      4  num_qc:      2
    num_obs:      77042  max_num_obs: 77042
observation
prior ensemble mean
prior ensemble spread
prior ensemble member 1
GOES QC
DART quality control
  first:      1  last:      77042
OBS      1
  2.546181000000000
  2.67347519169475
  8.220037240577385E-002
  2.70210881859020
  0.000000000000000E+000
  0.000000000000000E+000
      -1      2      -1
obdef
loc3d
  4.102617740631104      0.6268096566200256      35000.00000000000
kind
  216
visir
  125.8291000000000      68.2444100000000      -888888.000000000
  -888888.000000000
      4      16      44      2
  -888888.000000000
      1
43072      152809
  6.250000000000000E-002
OBS      2
  2.610124000000000
  2.72617267485070
  8.868187079127991E-002
  2.73930031819035
  0.000000000000000E+000
```

Observation Sequence

Radiance example

DA Output: obs_seq.final

- various 'copies' of each observation
 - Observation value
 - Truth
 - Prior and Posterior Forward Operators, mean, standard deviation

Observations can have additional metadata

```
obs_sequence
obs_type_definitions
  1
    216 GOES_16_ABI_RADIANCE
    num_copies:      4  num_qc:      2
    num_obs:        77042  max_num_obs: 77042
observation
prior ensemble mean
prior ensemble spread
prior ensemble member 1
GOES QC
DART quality control
  first:      1  last:      77042
OBS          1
  2.54618100000000
  2.67347519169475
  8.220037240577385E-002
  2.70210881859020
  0.00000000000000E+000
  0.00000000000000E+000
    -1          2          -1
obdef
loc3d
  4.102617740631104      0.6268096566200256      35000.0000000000
kind
  216
visir
  125.829100000000      68.2444100000000      -888888.000000000
  -888888.000000000
    4          16          44          2
  -888888.000000000
  1
43072      152809
  6.25000000000000E-002
OBS          2
  2.61012400000000
  2.72617267485070
  8.868187079127991E-002
  2.73930031819035
  0.00000000000000E+000
```

Fortran + **Matlab** Observation Space Diagnostics

Detailed structure of an obs_seq file

Creating an obs_seq file of synthetic observations

Creating an obs_seq file from real observations

Available observation converter programs

Manipulating obs_seq files with the obs_sequence_tool

The difference between observation TYPE and QUANTITY

Adding support for a new observation TYPE

Radiances

OBSERVATION CONVERTERS

DART Observations

Converter programs

DIAGNOSTICS

Checking your initial assimilation

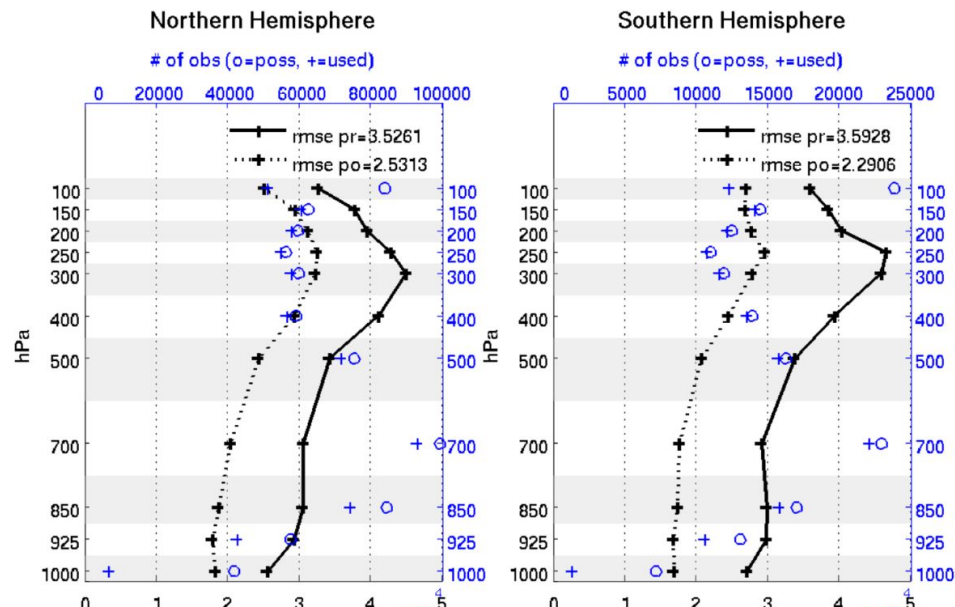
Computing filter increments

Computing filter increments using a complex model

DART missing data value

`plot_profile.m` plots the spatial and temporal average of any specified quantity as a function of height. The number of observations possible and used are plotted on the same axis.

```
fname      = 'POP11/obs_diag_output.nc';      % netcdf file produced by 'obs_diag'  
copystring = 'rmse';                          % 'copy' string == quantity of interest  
plotdat    = plot_profile(fname,copystring);
```



Fortran + **Matlab** Observation Space Diagnostics

```
5  !> The programs defines a series of epochs (periods of time) and geographic
6  !> regions and accumulates statistics for these epochs and regions.
7  !> All 'possible' observation types are treated separately.
8  !> The results are written to a netCDF file.
9  !> If the rank histogram is requested (and if the data is available),
10 !> only the PRIOR rank is calculated.
```

```
11
12 program obs_diag
13
```

4370 lines of Fortran

Matlab

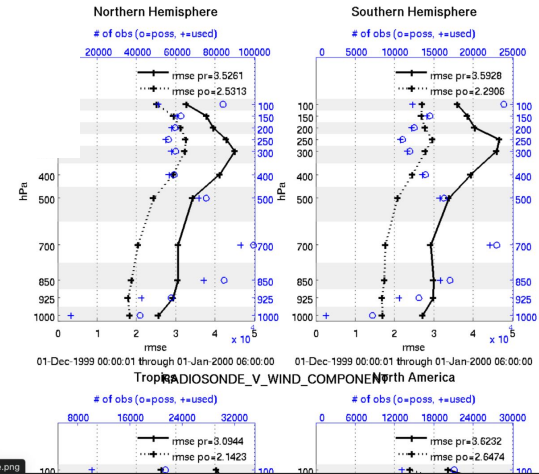
- not open source
- not freely available

- DART Observations
- Converter programs
- DIAGNOSTICS
 - Checking your initial assimilation
 - Computing filter increments
 - Computing filter increments using a complex model
 - DART missing data value
 - DART quality control field
 - Examining the obs_seq final file
- MATLAB observation space diagnostics
 - Configuring MATLAB

https://docs.dart.ucar.edu/en/latest/_images/plot_profile_example.png

the spatial and temporal average of any specified quantity as a function of height. The conditions possible and used are plotted on the same axis.

```
!1/obs_diag_output.nc'; % netcdf file produced by 'obs_diag'
e'; % 'copy' string == quantity of interest
_profile(fname,copystring);
```



Fortran + **Matlab** Observation Space Diagnostics

```
5  !> The programs defines a series of epochs (periods of time) and geographic
6  !> regions and accumulates statistics for these epochs and regions.
7  !> All 'possible' observation types are treated separately.
8  !> The results are written to a netCDF file.
9  !> If the rank histogram is requested (and if the data is available),
10 !> only the PRIOR rank is calculated.
```

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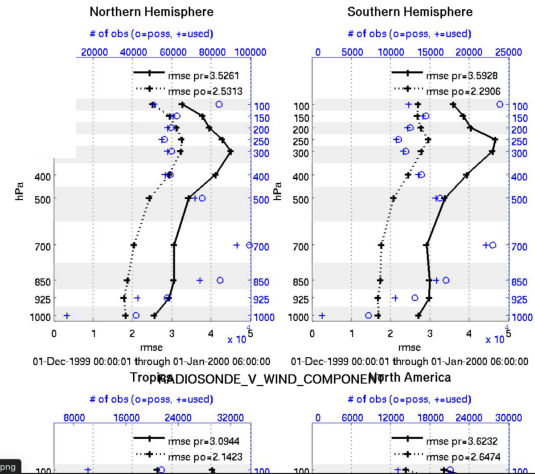


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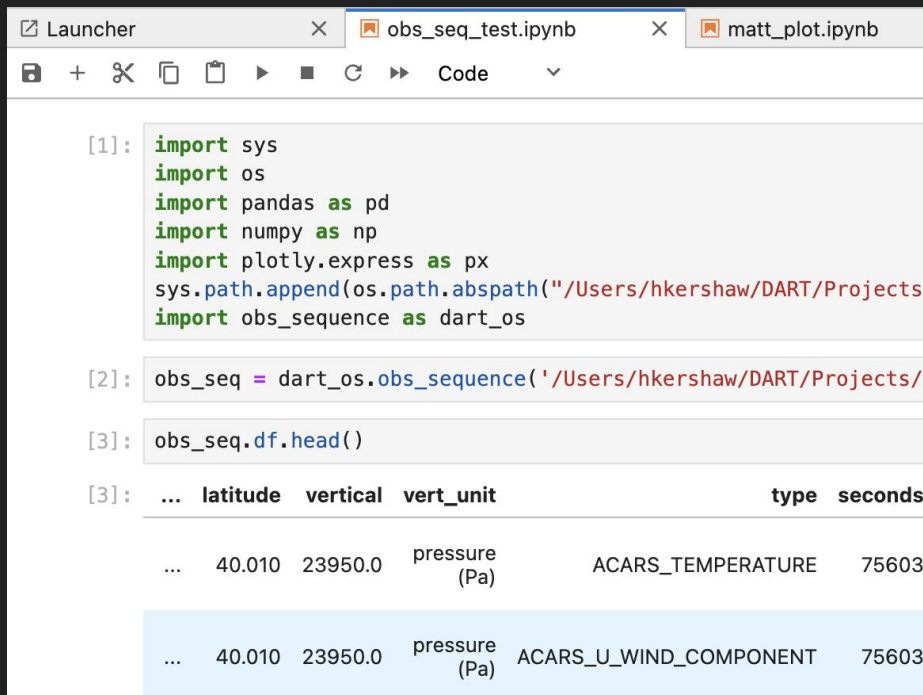


pyDARTdiags

obs_seq.{out/final} -> pandas dataframe

- Interactive python **Observation Space Diagnostics**: language of data science
- User extensible, & allows us to improve obs_seq format
- Observation preprocessing in be done in python?

github.com/NCAR/pyDARTdiags



```
[1]: import sys
import os
import pandas as pd
import numpy as np
import plotly.express as px
sys.path.append(os.path.abspath("/Users/hkershaw/DART/Projects/..."))
import obs_sequence as dart_os

[2]: obs_seq = dart_os.obs_sequence('/Users/hkershaw/DART/Projects/...')

[3]: obs_seq.df.head()
```

...	latitude	vertical	vert_unit	type	seconds
...	40.010	23950.0	pressure (Pa)	ACARS_TEMPERATURE	75603
...	40.010	23950.0	pressure (Pa)	ACARS_U_WIND_COMPONENT	75603

Next Steps

- What diagnostics are people interested in?
- What existing tools can we plug in to?
- Xarray + dask
 - Test case 20 year DART-CAM reanalysis
- pyDARTdiags as a preprocessing tool
- Pipeline of ocean data into CESM-DART

The screenshot shows a GitHub repository page for 'NCAR / pyDARTdiags' with the 'Discussions' tab selected. The discussion is titled 'Collection of software out there #4' and was started by user 'hkershaw-brown'. The main content of the discussion is a list of software for model, observation comparison:

- [MELODIES MONET](https://github.com/NOAA-CSL/MELODIES-MONET)
<https://github.com/NOAA-CSL/MELODIES-MONET>
- [MetPy](https://github.com/Unidata/MetPy)
<https://github.com/Unidata/MetPy>

There is one comment by 'hkershaw-brown' from 2 weeks ago, which lists several tools and resources:

- CUPID: CESM Unified Postprocessing and Diagnostics
[2024 CESM SEWG Group](https://ncar.github.io/CUPID/)
<https://ncar.github.io/CUPID/>
- ADF (CAM)
<https://justin-richling.github.io/ADF-Tutorial/README.html>
- MOM6 tools (dead?)
<https://github.com/NCAR/mom6-tools>
- IO
pyNIO GFDL using this
<https://www.pyngl.ucar.edu/Nio.shtml>

The right sidebar shows the discussion was converted from issue #3 on April 23, 2024, and includes notification options like 'Unsubscribe', 'Lock conversation', and 'Transfer this discussion'.

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hkershaw@ucar.edu

The screenshot shows a GitHub repository page for 'NCAR / pyDARTdiags'. The 'Discussions' tab is active, displaying a thread titled 'Collection of software out there #4'. The thread was started by user 'hkershaw-brown' on April 23. The main content of the discussion is a list of software for model, observation comparison:

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The right sidebar shows the discussion's category as 'Show and tell', with 1 participant and a notification to 'Unsubscribe'.