

NRL Atmospheric Data Assimilation Science Strategy

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EXECUTIVE SUMMARY

Data assimilation (DA) connects observations of the Earth system to the warfighter to enable accurate and timely decision-making using numerical weather prediction. The Marine Meteorology Division is committed to providing data-assimilation solutions that leverage the intrinsic capabilities of Navy models and make optimal use of new, novel, and Navy-unique observations, as well as providing guidance to both developing and providing specifications for new observing systems that meet the emerging needs of NWP and DA. We aim to readily assimilate new observation types and to rapidly adapt to a changing global observing system in terms of both satellite and conventional data. DA challenges unique to NRL include adapting to both observation-dense and communications-limited environments, optimally exploiting information provided by classified observations or observations of opportunity, operating within Navy time constraints and information assurance requirements, assessing risk to the warfighter associated with loss of observational information, and exploring forward-deployed prediction solutions.

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NRL ATMOSPHERIC DATA ASSIMILATION SCIENCE STRATEGY

1. INTRODUCTION

Data assimilation (DA) is a multidisciplinary science combining Earth science, remote sensing, instrumentation, mathematics, data science, computer science, and electrical engineering. The goal of DA is to produce an optimal combination of information from a previous forecast and new information from observations to create an optimal estimate of the current global atmospheric state. This estimate is then used as an initial condition to launch a forecast to predict future atmospheric states. The quality of this forecast is heavily dependent on the initial state provided by the DA. The global observing system is in a state of perpetual flux, with new and old instrumentation entering and exiting the system. Forecast models continuously improve as the understanding of physical phenomena and numerical methods are incorporated. The DA system links these two evolving systems and therefore must constantly evolve itself.

1.1 Mission of NRL Data Atmospheric Data Assimilation

Data assimilation (DA) connects observations of the Earth system to the warfighter to enable accurate and timely decision-making using numerical weather prediction. The Marine Meteorology Division is committed to providing data-assimilation solutions that leverage the intrinsic capabilities of Navy models and make optimal use of new, novel, and Navy-unique observations, as well as providing guidance to both developing and providing specifications for new observing systems that meet the emerging needs of NWP and DA. We aim to readily assimilate new observation types and to rapidly adapt to a changing global observing system in terms of both satellite and conventional data. DA challenges unique to NRL include adapting to both observation-dense and communications-limited environments, optimally exploiting information provided by classified observations or observations of opportunity, operating within Navy time constraints and information assurance requirements, assessing risk to the warfighter associated with loss of observational information, and exploring forward-deployed prediction solutions.

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1.2 The Data Assimilation Problem

The goal of data assimilation is to provide optimal initial conditions for the forecast model. In other words, data assimilation is how we link observational information to decisions. DA combines observations, y^o , with error assumptions and a background state provided by short-range forecasts from an NWP model, x^f , to determine the best estimate of the current state of the atmosphere, x^a , also known as the analysis. To achieve this, data assimilation must transfer information from the unevenly distributed locations and times of the observations to the model grid while preserving physical, dynamical, and numerical consistency. DA is an iterative process and information from past observations is accumulated into all subsequent forecasts. DA is formulated as an optimization problem that is different from other forms of machine learning and statistical methods in that it utilizes the dynamical model of the system being analyzed.

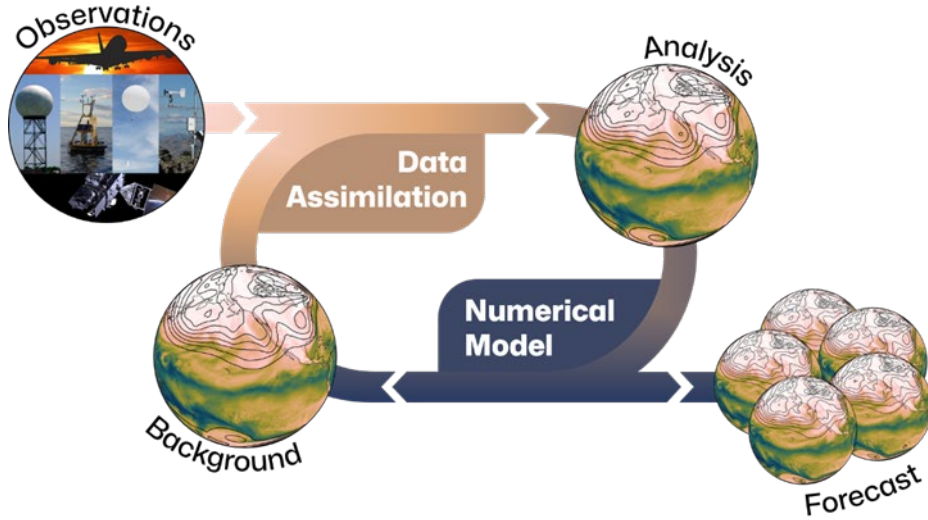


Fig. 1—Data assimilation is an essential component of operational weather prediction. DA combines environmental observations with a short-range forecast from the numerical model (known as the "background" estimate) to create an "analysis" that serves as initial conditions for the numerical model. This cycle is repeated as often as several times per day and is continued day after day to provide relevant and skillful forecasts for the warfighter.

If the model were linear, and the underlying statistics of both the forecast error and the observation error were Gaussian, then the Kalman filter equation yields the optimal analysis,

$$x^a = x^f + BH^T(HBH^T + R)^{-1}(y^o - Hx^f), \quad (1)$$

where \mathbf{B} and \mathbf{R} represent the background and observation error covariance matrices, respectively, and \mathbf{H} is the forward model, or observation operator, used to map model variables into observation space. Most research and operational data-assimilation systems are either ensemble based, variational, or a combination of the two. The solution to both of these methods may be written as Eq. (1). More recently, attempts to use particle filters combined with techniques from ensemble methods have been tested in regional models (Poterjoy et al. 2019). However, a vast majority of research being undertaken is related to the variational and ensemble methods.

Ensemble-based methodologies use statistical sampling to form a Kalman filter. Ensemble sizes are typically limited due to computational constraints, and difficulties arise with properly prescribing initial conditions and model perturbations. Mitigating the effects of undersampling is an active research area. Variational methods are maximum-likelihood estimates cast in the form of a cost function spanning across a time window. 4D-variational methods require linearized models and their adjoints and are generally more difficult to develop. Combinations of the ensemble and variational techniques are often referred to as hybrid methods.

Whether ensemble-based, variational, or hybrid, most operational systems make common assumptions of Gaussianity, linearity, unbiased states and observations, and mutually uncorrelated observation and background error when using Eq. (1) or state estimation; the differences are in implementation. Typically, many simplifying assumptions are also made in specification of the error covariance matrices as well. For example, until recently, \mathbf{R} was typically assumed to be diagonal, even though observation errors are often correlated (Campbell et al. 2017, among others).

1.3 The Data Problem

Observational data comes from a wide variety of platforms and can be collected in situ or remotely sensed through passive or active sensors. In situ observations can be collected by radiosondes (weather balloons), dropsondes, aircraft, ships, surface stations, and buoys; remotely sensed observations can be collected by Doppler radar, satellite-based imagers and sounders, lidar, and GNSS receivers. Environmental observations have irregular or unpredictable errors that are introduced during sensing, reporting, translation, truncation, and unit conversion that must be handled through the quality-control algorithms. Many platforms do not directly observe the state variables of the atmospheric model and require the development of complex observation operators for their observations to be used in Navy data-assimilation systems. The observation operators have their own simplifying set of assumptions, which can lead to the introduction of further errors. Additionally, the observation operators require model states as inputs, which may lead to state-dependent errors, biases, and correlation between observation and model errors.

Operational observations arrive at FNMOC through multiple redundant communication pathways. Most nonradiance operational observations arrive at FNMOC through a subscription to the Global Telecommunications System (GTS) through the NWS Telecommunication Gateway (NWSTG), through the Air Force Automated Weather Network (AWN), from the National Oceanic and Atmospheric Administration (NOAA)-Port satellite receiver, or directly from the Naval Oceanographic Office (NAVO). A few nonradiance observations may also arrive through the NOAA public website, from the Cooperative Institute for Meteorological Satellite Studies (CIMSS), through Command and Control Official Information Exchange (C2OIX) message traffic, or through the Joint Observations Submission Portlet (J-OBS). Operational radiance observations may be downloaded locally at FNMOC directly from the satellite through fixed meteorological equipment (FMQ) receivers, transmitted through the National Environmental Satellite, Data and Information Service (NESDIS) Production Distribution and Access (PDA) System, the Air Force Satellite Control Network (AFSCN), or collected from Mark-IVB receivers operated by the 557th Weather Wing and transmitted through the Defense Information Systems Agency (DISA) Optical Transport Network (OTN).

Observational challenges stem from the constantly evolving nature of the Global Observing System (GOS), as changes to instruments, sensing methods, sensing platforms, data providers, reporting frequency, and data formatting happen frequently. Ideally, these changes are presented well in advance through technical notices from individual countries' weather agencies, bulletins from the World Meteorological Organization (WMO), messages from NOAA's Office of Satellite and Product Operations, NWS Service Change Notices, or scientific presentations at international workshops. Sufficient notice provides NRL the opportunity to plan implementation as part of the traditional 3-year project arc, to coordinate and prioritize

execution with other observing system changes, and potentially to evaluate early-release data to provide feedback to the observation providers. Unfortunately, some changes happen with relatively short or no notice, which may require NRL to alter existing project milestones for high-impact observation changes or to implement necessary changes without fully testing the capability. Unplanned or unannounced changes are usually discovered by monitoring observation counts, radgrams, and innovation and observation impact statistics from the operational runs, which requires continuous vigilance on the part of scientists to detect and correct for GOS changes. Short-notice or no-notice observation changes can also be hindered by how quickly the transition partner is able to promote data-assimilation software changes to operations. The Fleet Numerical Meteorology and Oceanography Center (FNMOC), which is the transition partner for NRL's atmospheric data-assimilation systems, has requested an update schedule of no more than once per quarter for the global system and once per year for the regional system due to increasing operational support requirements and limited personnel. This prescribed regular schedule will not generally align with unannounced observational changes, resulting in a potentially long gap between detection and operational mitigation, as well as the potential for a temporary loss of critical observations during this gap.

Note that these changes to the observing system include not only adding new observations, but also accommodating changes to existing observations. In the past two years, the observation processing for NAVGEM and COAMPS has needed modifications to reflect four geostationary satellite swaps (Meteosat-8 to Meteosat-9, Himawari-8 to Himawari-9, GOES-17 to GOES-18, and Meteosat-11 to Meteosat-10), the loss of the Metop-A polar-orbiter and the addition of Metop-C, and NESDIS products switching from on-premises computing to cloud computing, all of which affected both satellite-derived winds as well as radiances. Even though these satellite changes were between similar satellites, the changes still required testing to ensure that the performance was similar. Also, in situ observations are not immune to change; the change from ASCII formats to the WMO-defined binary BUFR formats for aircraft, buoy, land surface, and radiosonde data began nearly a decade ago and is still in process. The most dramatic of these was the switch to BUFR for radiosonde data, with BUFR radiosonde profiles including up to roughly 6,000 levels, compared to 150 levels or fewer reported in ASCII. The WMO-mandated change from using five-digit "block-station" numbers as identifiers to using four-part "WIGOS" identifiers that can be up to 30 characters long is a potentially disruptive impending change that must be accommodated in the near future for surface and radiosonde stations. As stated above, changes to the existing observing system such as these must be accounted for in the observation processing for Navy models to avoid the loss of critical observations, in addition to working on the assimilation of new observing systems.

The data source itself poses an additional challenge. A large percentage of observations assimilated into Navy numerical weather prediction systems are part of the Global Observing System (GOS) and do not originate within the Navy or from the Department of Defense. Instead, these observations originate from a variety of organizations that can be academic, commercial, or governmental and can come from allied, adversarial, or nonaligned countries. As the Navy requires more software to be built using zero-trust architecture, it is expected that additional project efforts will be required to implement new cybersecurity requirements into new or existing observation ingestion software.

2. NRL CURRENT STATUS

The Atmospheric Data Assimilation Section at NRL supports an array of Navy atmospheric models:

Global Atmospheric Data Assimilation (Hybrid 4DVar operational)

- Naval Research Laboratory Atmospheric Variational Data Assimilation System-Accelerated Representer (NAVDAS-AR, Hybrid 4DVar) for Navy Global Environmental Model (NAVGEM)

- Development of Flexible Assimilation Linking Collaborations to Operations for Neptune (FALCON, 3DVar) Data Assimilation for Navy Environmental Prediction sysTem Utilizing a Nonhydrostatic Engine (NEPTUNE), which will utilize Joint Effort for Data assimilation Integration (JEDI) infrastructure

Regional Atmospheric Data Assimilation for Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS, 3DVar operational)

- 4DVar (research mode)
- EnKF for COAMPS-TC (research mode)
- Radar DA: hourly 3DVar, EnKF, 4DVar (research mode)
- All-Sky EnKF (research mode)

Weakly coupled DA for Navy Earth System Predictive Capability (ESPC) Coupled Global Atmospheric/Ocean Data Assimilation

- Atmosphere: NAVDAS-AR (Hybrid 4D-Var)
- Ocean/Sea Ice: NCODA (3D-Var)
- DA systems use fully coupled state as background (weakly coupled)

Aerosol Data Assimilation for Navy Aerosol Analysis and Prediction System (NAAPS, 2DVar operational)

- 3DVar (research mode)
- E-NAAPS (EnKF)

2.1 Global Atmospheric Data Assimilation

Naval Research Laboratory Atmospheric Variational Data Assimilation System-Accelerated Representer (NAVDAS-AR) is a weak-constraint observation-space (dual-form) four-dimensional variational (4DVar) formulation (Rosmond and Xu 2006, Xu et al. 2005). That is, it evaluates a four-dimensional cost function (three spatial dimensions plus time) with model error (weak-constraint). The accelerated representer method propagates the background error covariance across the assimilation window using linearized models without explicitly forming the covariance in its entirety. Since its adoption, several methodological upgrades have been incorporated into the system. One of the most impactful has been the adoption of a hybrid background error covariance. Prior to this, a static climatological background covariance was used to represent the uncertainty in the current state estimate. The hybrid error covariance linearly combines this static error covariance with a sample error covariance created from ensembles. In this way, “errors of the day” may be included. A Hybrid 4D-Var system (Kuhl et al. 2013) was implemented within this framework and was transitioned to operations in 2016. Hybridization follows Hamill and Snyder (2000), e.g., covariances are hybridized at the beginning of the data-assimilation window and are propagated throughout the data-assimilation window using the tangent linear and adjoint models. This formulation was shown by Wang (2007) to be equivalent to the extended control variable form (Lorenc 2003).

The static component of the background error covariance matrix is a covariance model based on the formulation of Daley and Barker (2001), which was designed to provide balance to the observation space 3DVar (NAVDAS) and representer form of 4DVar (NAVDAS-AR). In this formulation, the background geopotential and temperature error variances are specified to be in exact hydrostatic balance. The wind and geopotential background error variances are set to be approximately geostrophically coupled in the extratropics and uncoupled in the tropics following Lorenc (1981). The background error correlations are specified using separable vertical and horizontal components based on a second-order autoregressive (SOAR, Daley and Barker 2001) function that varies as a function of distance between points as well as

with interactions between velocity potential and streamfunction following approximate hydrostatic and geostrophic balance. Errors in the relative humidity field are univariate and have shorter specified horizontal and vertical length scales (Franke and Barker 2000). Errors in the ozone field are also assumed univariate.

The flow-dependent component of the hybrid covariance is provided by the operational ensemble (McLay *et al.* 2008, 2010), which is based on a local formulation of the Ensemble Transform (Bishop and Toth 1999). A short-term cycling ensemble of 80 members applied at NAVDAS-AR inner loop solver resolution of T119 (~110 km) provides a fully multivariate covariance matrix. The ensemble-based error covariance matrix is localized in physical space using correlation functions that are dependent on horizontal and vertical position (details in Kuhl *et al.* 2013). Although NAVDAS-AR can accommodate a range of representations of model error covariance, in operations this term is set to zero (i.e., strong constraint, or the perfect model assumption). Our dual form 4DVar uniquely positions us to be able to fully explore the weak constraint formulation; however, we have not currently leveraged this capability.

2.2 Regional Data Assimilation

The Navy Atmospheric Variational Data Assimilation System (NAVDAS) is the operational 3DVar DA system that supports initialization of the Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS®) model (Naval Research Laboratory 2003). The system was adapted from its global equivalent that supported the previous generation NWP model Navy Operational Global Atmospheric Prediction System (NOGAPS). NAVDAS 3DVar is an observation-space algorithm, so the computational cost of the assimilation is strongly dependent on the number of observations. For this reason, the number of satellite radiances that can be assimilated is severely limited by operational timing considerations. The observation-space algorithm was chosen as a developmental shortcut to the representer form of NAVDAS-AR. The background error covariance used within NAVDAS forms the basis of the static background error covariance used in NAVDAS-AR, where error correlation length scales have been reduced to support mesoscale NWP.

COAMPS can also be initialized using COAMPS-4DVar, a 4DVar regional data-assimilation system. The COAMPS-4DVar system is typically used in research applications due to its larger computational expense compared to NAVDAS. COAMPS-4DVar utilizes the same accelerated representer algorithms used by its global DA NAVDAS-AR counterpart but uses a much simpler univariate initial background error covariance. While the 4DVar algorithm outperforms its 3DVar counterpart, the limited improvement from the currently supported conventional observation data sources did not justify a transition to FNMOC operations. It is believed that the univariate initial background error covariance significantly limited forecast improvements provided by the more advanced data-assimilation method.

An ensemble Kalman filter (EnKF) was also developed for COAMPS and COAMPS-TC (Tropical Cyclone). This research system is able to assimilate conventional weather observations, surface-based and airborne Doppler radar data, aircraft dropsonde and flight-level data, and derived satellite products. Recently, a new capability to assimilate all-sky (clear-sky plus cloud-affected) infrared (IR) water vapor (WV) imagery data from geostationary satellites, through a collaboration with Penn State University, has been added into COAMPS-TC to improve TC forecasts (see Section 2.1.8). The EnKF approach naturally develops cross-variable correlations between the observed parameter and the model state variables of temperature, humidity, winds, and hydrometeors. This experimental system is showing promise for more accurately capturing tropical cyclone intensification and track forecasts.

The ability to assimilate radar data is also a feature of the operational 3DVar system and the research-based 4DVar system. In the operational system, radar reflectivity and radial velocity are assimilated in a separate 3DVar solver outside of the NAVDAS solver. This framework is the basis for the operational COAMPS Rapid Environmental Assessment, which can assimilate data from traditional surface-based

radars, such as NEXRAD or the Navy's land-based Supplemental Weather Radars (SWR), as well as the Navy's shipboard tactical Doppler radars (SPS-48). Investments were also made to directly assimilate radar reflectivity and radial velocity directly into COAMPS-4DVar while it was being developed. When assimilating radar reflectivity, a 3DVar cost function is used within the 4DVar framework due to the lack of microphysics in the COAMPS adjoint. The 4DVar system also assimilates retrieved radar refractivity from clutter (RFC) observations into COAMPS initial fields. Numerical experiments have shown impressive impacts from radar data assimilation, which has improved forecasts of atmospheric electromagnetic (EM) propagation conditions near the ocean surface and convective storm prediction. Radar data assimilation remains a capability found only within the Navy's regional data assimilation.

The Navy's efforts in regional data assimilation are likely to undergo significant changes as the Navy's next-generation NWP system is operationalized and further developed. Current regional atmospheric modeling uses nested domains with an outer nest resolution between 15 and 45 km (depending on the area); the 3DVar system performs its analysis using variable resolutions corresponding to the resolution of the nest (which can be as high as 2/3 km) while the 4DVar system performs its analysis using the outer nest resolution. The targeted resolution for NEPTUNE is 9 km resolution with data assimilation performed on a roughly 0.5 degree grid (see Section 2.1.7); as NEPTUNE's data-assimilation system becomes more advanced and is performed at higher resolutions, it may become unnecessary to run a separate regional data-assimilation system except for specific tactical cases run at extremely high resolutions or on computational hardware where the necessary number of CPUs to run the full global system are unavailable due to classification or edge computing.

2.3 NAVY ESPC Coupled Global Atmospheric/Ocean Data Assimilation

Since August 2020, the Navy's global coupled forecasting system (Navy ESPC v1) has been used operationally to generate 16-member ensemble forecasts out to 45 days. In the Navy ESPC v1 system, deterministic and ensemble-based forecasts are initialized from analyses generated by a weakly coupled DA system. In the weakly coupled system, the DA minimization for the varying model components is isolated. The ocean/ice DA system (NCODA) does not directly utilize observations of the atmosphere and, similarly, the atmospheric DA system (NAVDAS-AR) does not incorporate observations of the ocean or ice. However, information propagates across the model interface during the model forecast, allowing observations in one component to influence the background state of the other components in the subsequent DA cycle. Note also that there are underutilized surface-sensitive channels on CrIS, IASI, and AIRS that could show extra benefit for coupled DA and would not be difficult to implement and test. The Navy ESPC ensemble is generated using an ensemble of data assimilations (EDA) framework where the observations are perturbed using their observation error characteristics.

2.4 Aerosol Data Assimilation

Prediction of scattering and absorbing aerosol particles is a component of numerical weather prediction important for Navy applications. NRL has an active effort to develop new methods for the prediction of atmospheric aerosols including dust, sea salt, smoke, and pollution. These particles are relevant in terms of their direct effects on atmospheric transmission and electro-optical propagation; prediction of these properties is critical to aviation, target visibility, sensor performance, and laser weapons system performance. Aerosols are also important in terms of their impacts on other weather phenomena, including tropical cyclones, cloud formation and properties, and surface-energy budgets at medium-range to seasonal prediction scales. NRL conducts basic and applied research on atmospheric particles ranging from laboratory studies, to measurement field campaigns, to global and mesoscale modeling and data assimilation. NRL supports operational implementation of aerosol prediction and data assimilation for aerosol and is the lead developer for the operational Navy models used for these applications.

The strategic emphasis for NRL in this area centers on three aspects: observations, data-assimilation methods, and aerosol-NWP interactions.

Observations: NRL closely collaborates with partner agencies to test and deploy the most advanced space-based and ground-based observations in support of aerosol prediction. Applied research at NRL develops and refines methods for processing observations to obtain maximum forecast improvement. NRL research leverages existing aerosol DA systems to quantify the impact of new observations and updated observation-processing techniques.

Data-assimilation methods: The characteristic properties of atmospheric aerosols impact the efficacy of different numerical methods of data assimilation. NRL research leverages internal NRL DA development as well as outside collaborations with the wider DA community to build and test advanced methods for aerosol data assimilation, leveraging scientific advancements from both the aerosol and DA communities. Using state-of-the-art tools such as the JEDI framework from JCSDA, NRL intends to advance the skill of aerosol DA for forecast initialization and to leverage tighter coupling between DA for aerosol and other NWP components.

Aerosol-NWP interactions: Interactions between aerosol particles and other components of the weather system permeate all aspects of NWP DA, from corrections for aerosol effects applied to observations of atmospheric and oceanic temperatures to correlated errors in ensemble predictions of aerosol and other phenomena. NRL conducts basic research into these aerosol-NWP interactions as well as applied research aimed at capturing aerosol effects to improve NWP DA outcomes, and vice versa.

2.5 MW Sensor Systems Engineering, Cal/Val, Monitoring, and Radiative Transfer

NRL has a long-standing heritage of supporting space-based environmental monitoring (SBEM), specifically in the realm of the microwave (MW) radiometer systems and the calibration and validation (CalVal) of MW sensor data and derived products. The NRL MMD CalVal team is nationally recognized in microwave remote-sensing hardware, software, and environmental retrieval algorithms. Our extensive NRL radiance analysis software, sensor models, and databases are utilized to conduct comprehensive calibration and validation of MW imaging and sounding instruments with the goal of providing the highest-caliber MW data possible for Navy operational users and DoD warfighters.

Our current technical approach includes the full spectrum of MW sensor development, from preflight proposal evaluation and systems engineering, sensor-specific radiative transfer model development and coordination with US civilian and international partners, to postlaunch CalVal. Postlaunch efforts include long-term sensor health monitoring, anomaly detection and mitigation, and the development of sensor-specific radiance quality control and preprocessing strategies required to meet the stringent requirements of DA systems. We are actively involved in the development of new machine learning methods to detect radio frequency interference (RFI) and in assessing impact of frequency impingements due to potential FCC selloffs of protected passive MW SBEM bands to support 5G cellphone communications. Recently, we have been tasked to perform the CalVal of new MW CubeSat sensors and to evaluate their performance as part of the USAF SBEM Technology Demonstrations and Commercial Weather Data Program (CWDP), from sensor development to assessing the impact to our Navy DA and NWP systems, and to provide technical expertise and guidance to NOAA's development of their Hyperspectral MW radiometer (HyMS) demonstration projects.

2.6 FALCON DA for NEPTUNE

The data-assimilation section is currently developing the FALCON (Flexible Assimilation Linking Collaborations to Operations for NEPTUNE) unifying DA system. This DA system utilizes the JCSDA

JEDI (Joint Effort for Data assimilation Integration) infrastructure to provide a flexible and modular system for NEPTUNE (Navy Environmental Prediction sysTem Utilizing a Nonhydrostatic Engine) applications. The first application will be the global forecast model with future capabilities tailored for each application (NEPTUNE-LAM, ESPC, etc.).

Efforts during the past several years have focused on the development of NRL-specific DA components relating to the NRL observation stream and atmospheric model. This includes the incorporation of the NRL observation API, the NEPTUNE-JEDI interface, a reworking of the NAVDAS-AR static B, continual development of diagnostics (METplus, reworked NAVGEM, and JCSDA Skylab), assimilation configurations (yamls), and cylc. We have also made contributions to the JCSDA's JEDI development relating to observations and infrastructure.

The FALCON DA system currently consists of an incremental 3DVar/3DVar FGAT solver with observations preprocessed from NAVGEM. The system is currently ingesting ~2.4 million observations per cycle point and is capable of multiple-month cycling. The DA is performed on the native NEPTUNE atmosphere grid at approximately 1-degree resolution for current testing; we are targeting half-degree resolution for transition. Efforts in the modeling sections are underway to improve its vertical integration method as well as select a final physics suite. Changes to the model dynamics and physics as well as changes to the evolving JEDI infrastructure will be continuously incorporated into the system. We will also add refinements of the DA system including dual resolution and the new instruments. Note that the TLM/ADJ for NEPTUNE are under development and there are plans to move to 4DVar in the future.

The FALCON DA system consists of a combination of community software packages and NRL-unique packages:

- NEPTUNE BUNDLE: This is the NWP system in its entirety and includes everything required to run experiments using data assimilation with the forecast model or the stand-alone forecast model.
- DIAGNOSTICS: Collection of DA diagnostics ported from NAVGEM for use in FALCON.
- VERIFICATION: ADS and MET scripts.
- ND-STATIC-B (NRL Static B): Grid-agnostic, configurable version of the NAVDAS-AR static B.
- NEPTUNE-JEDI: Links the atmospheric model and the DA and provides the model-aware components of the DA. It also contains the drivers and configures templated applications for the DA (HofX, LETKF, 3DVar, 4DVar...)
- CYLC: Developed by 7531/7533/7532: Controls the cycling experiment and contains configurations for running the NWP system.
- NEPTUNE ATMOS: Developed by 7533/7532 spectral/finite-element forecast model.

From the JCSDA:

- OOPS (Object Oriented Prediction System): Top-level, model-agnostic, abstract framework that implements DA applications: variational solvers, ensemble DA solvers, HofX applications, etc. It is primarily written in C/C++ and comes prepackaged with single-threaded Lorenz95 and quasi-geostrophic models. FALCON DA creates OOPS drivers with NEPTUNE objects to create the DA applications. The linear solve and the horizontal interpolation are also done as part of OOPS.
- UFO (Unified Forward Operator): Provides the framework for HofX computations. It includes many observation operators and interfaces to the CRTM and ROPP. The UFO and observation operators also perform vertical interpolation. The UFO is model agnostic but requires

information from the forecast model depending on the types of observations being used in applications. FALCON DA uses the UFO for all HofX computations.

- IODA (Interface for Observational Data Access): This ingests and processes observational data. FALCON DA uses IODA conventions and formatting for observation files so that they may be ingested into the system through IODA.
- IODA-Converters: Observation file format converters for IODA compatibility.
- CRTM (Community Radiative Transfer Model): Observation operator for radiative transfer.

Other Community Packages:

- ESMF (Earth System Modeling Framework): Used in the DA for grid remapping between resolutions. ESMF was developed as part of a collaboration between NASA, NOAA, the Navy, NCAR, and ESPC.
- ROPP (Radio Occultation Processing Package): Observation operator for bending angles. Developed by EUMETSAT.

There are other packages that the JCSDA has created that are not currently part of the FALCON DA system. These include SABER (System Agnostic Background Error Representation) and VADER (VARIABLE DERIVATION Repository) that may provide future opportunities for research and code simplification. Note that the JCSDA packages rely heavily on ECMWF packages (ecbuild, Atlas, ecKit, fcKit).

The observation ingestion, preprocessing and quality-control software is being revised to follow coding “best practices,” and these components will be directly used for FALCON DA. Moreover, the modular approach will allow us to isolate and restrict (as appropriate) Navy controlled unclassified information while still drawing on community expertise.

The payoff for this approach to DA software is that antiquated, computationally slow, difficult-to-follow-and-upgrade computer code is replaced by code that is easier to compartmentalize, improve, and maintain and is more computationally efficient. This will significantly 1) increase the pool of new employees already familiar with aspects of our system, enabling them to more readily contribute to 6.4 operational systems through 6.1 R&D, 2) decrease the roadblocks associated with being able to develop and test new DA ideas in an operationally relevant environment, 3) increase opportunities for thoughtful collaborations with external partners, 4) enhance our ability to rapidly exploit new observations and DA methodologies, and 5) help maintain a competitive edge against our near-peer competitors.

3. CURRENT SCIENCE PLAN

NRL conducts basic research into data assimilation methodology, including research on ensemble construction, background uncertainty estimation, parameter estimation using ensemble DA, and refinement of models of observation uncertainty.

3.1 Maintenance and Development of Current Systems

3.1.1 Navy Unique

The Navy and the Marine Corps’s mission makes its METOC needs unique compared to other nonmilitary costumers. Current operations require the ability to configure the Navy’s regional NWP model to run over any region in the world; the data-assimilation systems that support COAMPS or future regional NWP models will need to have this same capability. Future DA and NWP systems used by the Navy will

need to be able to run on both edge computing (relatively few processors, limited memory, and limited bandwidth) and HPC resources (thousands to tens of thousands of processors and no limitations of bandwidth). Future Navy DA methods will also need to be robust against extreme variations of data densities: certain regions of interest may be extremely data sparse, or mission requirements may significantly limit the observation availability for data assimilation. Navy DA systems must be able to run at multiple classification levels and appropriately handle classified datasets.

3.1.2 Observation Preprocessing

Much of the code within the Navy's data-assimilation systems is focused on observation processing and quality control. Although the observation processing and quality control were originally built within separate repositories (one for each NWP system) due to limitations with the previous code-management systems, advancements in these tools have rendered this separation unnecessary. Efforts are currently underway to create model-agnostic observation-processing and quality-control systems that will be hosted in a single repository. The global and limited-area NWP systems both will utilize this repository as a common library for observation decoding, processing, and quality control. The goals of this effort are fourfold: modernizing the code to take advantage of newer Fortran constructs, adapting the code for all Navy modeling systems, streamlining the code to make adding new observations easier, and making the code easier to run for historic cases or reanalyses that are dependent on obsolete observation types or satellites. The latter two goals will be accomplished by putting details related to specific observation types or satellites in external files for past, current, and future observation types or satellites. Options that will be configurable in these external files include data selection and thinning, super-observation generation, the use of the NWP prior for quality control, and data quality-control options. The overarching goal is to maintain support for NAVGEM, COAMPS, and Navy ESPC while supporting the observation requirements for FALCON.

3.1.3 Improved Observation Error Statistics

A recent active area of research has been with the improved specification of observation error covariance matrices. We have recently implemented interchannel correlations for radiance assimilation (Campbell et al. 2017). Although horizontal correlation has not presently been implemented, we expect we will need to explore such methods to effectively assimilate more modern high-resolution observations or observations of opportunity. The dominant contribution to correlated error is due to representation error, rooting from the fact that the observations typically observe a higher-resolution state than the model. There have been efforts to better understand and quantify this error (e.g., Hodyss and Satterfield 2017, Satterfield et al. 2017). In addition, this work demands more effective strategies for preconditioning and a better understanding of convergence properties.

Another active area of research is to better account for temporal and spatial variability of the observation uncertainty. Presently, all the observation uncertainty is assumed invariant in the Navy's NWP systems. This assumption will likely need reassessment for emerging SmallSat sensors. SmallSats typically have modular compact designs and have less mass, which means they can be subject to more thermal effects on performance. This, in turn, can pose challenges to characterizing the sensor precision and noise performance. In particular, their observation uncertainty might be seasonal, might have orbital heating and cooling dependence, and might be spatially variant. Innovation-based techniques, such as the Desroziers method (Desroziers et al. 2005), or machine learning-based algorithms could be used to provide spatial and temporal variability of the observation uncertainty. Full understanding of the sensor hardware is essential for developing physically based uncertainty characteristics and quality-control strategies. Extensive testing and evaluation of these new techniques are warranted.

As the volume of satellite data continues to grow, it becomes increasingly necessary to update our current thinning algorithm with a more sophisticated method that can predict optimal observation locations and to prioritize those that provide the greatest impact. Conversely, especially with SmallSats, there may be situations in which particular observations are detrimental, and we would like to predict and avoid those situations as well. This problem has similarities to the observation uncertainty estimation discussed in the previous paragraph, and we plan to work on both problems in parallel.

3.1.4 *Data Assimilation for Conventional Data and Satellite-Derived Winds*

While data from radiosondes, aircraft, and surface platforms have been used in NWP since its inception, today's conventional data are quite different in character and quality from those used even 20 years ago.

NRL has been a leader in assimilating high-resolution radiosonde data that have only become available in near real time within roughly the past 5 to 10 years (Ingleby et al. 2016). These profiles typically have thousands of levels and include balloon drift times and locations that are most often derived from GPS. In addition, some countries now provide radiosonde descent profiles, which are also assimilated in Navy DA systems. Today's observations from commercial aircraft include those taken primarily for the meteorological community and those taken for air traffic control purposes. Perhaps the most exciting development is meteorological observations derived from Mode-S EHS transponder reports, which are extremely dense and are currently available primarily over Europe; these are not yet used in Navy DA, although a preliminary COAMPS-based study demonstrated their value. Hourly surface land reports are available for many countries, but not yet for the U.S. in the standard WMO forms. However, hourly airport observations are available for the U.S. in a dense network that is not yet being utilized for Navy DA. Finally, the latest generation of geostationary satellites permits atmospheric motion vectors derived from imagery to be available hourly (and in some cases subhourly) from an increased set of channels. Satellite wind datasets from both geostationary satellites and polar orbiters also change primarily as satellites change, requiring research to determine their characteristics and optimal use.

Conventional data are messy, as they come from a large number of data providers. These datasets are quite heterogeneous, with differences in observing methods (e.g., radar vs. GPS wind finding for radiosondes) and data formats (e.g., binary vs. text) as well as other aspects (Pauley and Ingleby 2022). Irregular observation errors arise not only from the sensors, but also in converting measured quantities into meteorological quantities and other filtering/processing applied at the source. Both sensors and processing can differ among manufacturers and countries, leading to different error characteristics in different types of radiosondes. Errors can also be introduced in encoding observations in standard formats for transmission, sometimes by differing interpretations of the WMO formatting rules by disseminating countries. Standard formats differ in the units and precision used, something that is also true of the internal formats used by FNMOC after decoding observations from WMO formats. These differences in formats can also make duplicate checking challenging — conventional observations are commonly received at FNMOC in more than one format. While some errors in observations are large and require little subtlety to detect, others are large enough to potentially lead to forecast errors but small enough not to be detected by generic error checking. Thus, there is a need for quality control tailored for each observing system.

However, this heterogeneity is unrecognized in terms of observation errors, which are currently a function only of observation type (e.g., radiosonde or aircraft) and pressure level, making this an area for future research. Conventional data in general and radiosonde data in particular are also a critical source of anchor observations for the variational bias correction for radiances and play an important role in model verification. However, verification, at present, focuses on using mandatory level radiosonde data (approximately 20 standard levels). Enhanced verification should be developed to use additional vertical

levels extracted from high-resolution radiosonde profiles. In summary, conventional data play an important role in Navy DA and verification despite their small numbers compared to satellite data.

3.1.5 Improved Radiance Assimilation

The assimilation of cloud- and precipitation-affected radiances are being explored for both microwave (MW) and infrared (IR) sensors. Our approach is twofold. Currently, we are assimilating the $\sim 6.7\text{-}\mu\text{m}$ water vapor (WV) channel from geostationary advanced baseline imagers (ABI) into COAMPS-TC to improve TC intensity and track forecasts. For the global hybrid NAVDAS-AR system, cloud-affected MW radiance assimilation will be incrementally employed starting with nonprecipitating and stratiform regimes. The quality control will be adapted for increased flexibility to allow ease in thinning, error assignment, and channel/level selection. This will ease the multiple use for global, regional, or ensemble systems, which may have different requirements for data. A plan to assimilate geostationary IR WV raw radiances from both clear- and cloudy-sky (all-sky) regions into the Navy's next-generation high-resolution global model (NEPTUNE) is under development. This new capability is to assimilate satellite-observed cloud and storm information into NEPTUNE to improve storm forecasts in the tropics, especially over tropical oceans, where weather observations from other sensors are limited.

Future plans include increased use of surface sensitivity satellite radiances over difficult surfaces, such as land and sea ice. These frequencies are also sensitive to water vapor and lower-atmosphere temperature, and this should help improve the characterization of the boundary layer.

3.1.6 Radio Occultation Assimilation

The assimilation of radio occultation (RO) data is becoming an increasingly important data source at most NWP centers, including FNMOC. The RO data assimilated within NAVGEM is made up of bending angle observations of Global Navigation Satellite System (GNSS) signals as they pass through the Earth's atmosphere. RO observations provide important high-resolution vertical profile information of temperature and humidity to the analysis, as the bending angles of GPS signals are directly related to these atmospheric variables. This data is particularly valuable in regions where other profiled observations of these variables are sparse or nonexistent. RO data may be collected by satellite-based receivers, which has been the dominant form of this data for the past decade, or by ground-based stations, the increasingly prevalent zenith total delay observations. RO data may also be provided by public, such as government organizations, or private entities, as in the case of the NOAA RO commercial purchase data. The number of commercial RO observations is expected to increase significantly in the next several years. NRL is involved in an international experiment to study the potential impacts of the enormous data volume that is likely to come from new RO sensors. Additionally, some commercial entities are also advertising that they will be able to produce observations that sample the boundary layer, which is of extreme importance to the Navy. These observations will require further evaluation.

In addition to the direct GNSS RO assimilation, we also utilize a new data source from the ground stations that track the GNSS transmitters. The observable is the ground-based zenith total delay (ZTD) at each ground station. This ground-based GNSS ZTD represents the tropospheric delay of the propagation of GNSS radio L-band signal between the transmitters and the ground stations after correcting for ionospheric effects. Significant effort was devoted to implement this assimilation capability, which includes quality control (e.g., ground station height correction), single observation test, bias correction scheme, and data impact assessment (Christophersen et al. 2023). Initial testing indicates that the ground-based ZTD data have a significant positive impact on the Southern Hemisphere's forecasts beyond 3 days. When evaluating each ZTD observation's impact on the 24-hr model forecasts, the impact of a single zenith total delay measurement is comparable to that of the average impact of a single GNSS radio occultation data at a single

tangent point. This capability was delivered to FNMOC in June 2022 and operational assimilation of the data is scheduled to begin in April 2023.

3.1.7 Coupled Data Assimilation

In recent years, development on the Navy ESPC system has continued with the first transition of the deterministic ESPC system (ESPC-D v2) to operations in FY23 and upgrades to the ESPC ensemble (ESPC-E v2) transitioning to operations in FY24. Upgrades provided in the version 2 update have led to demonstrable improvements to the performance of the ESPC system. As we look toward the next version of ESPC (v3), of particular interest is progress toward strongly coupled data assimilation. While many operational centers have seen benefits from implementing coupled systems in which the DA schemes are weakly coupled, it is recognized that moving to strongly coupled DA can lead to further improvement, having been shown in both operational (Sluka et al. 2016, Laloyaux et al. 2018) and simplified (Smith et al. 2015) systems. Strongly coupled DA is not without significant challenges, particularly regarding the development and maintenance of coupled tangent linear and adjoint models required for variational approaches.

Given the challenges associated with implementing a strongly coupled DA system in Navy ESPC, we aim our sights instead on a more intermediate level of coupling between NCODA and NAVDAS-AR. One potential intermediate solution provides an approximation to strongly coupled DA by running separate DA solvers in the atmosphere and ocean/ice, but allowing each to incorporate observations from the other component that are close to the model interface. It is assumed that observations in the upper (lower) layers of the atmosphere (ocean) exhibit very little influence on the forecast of the other model component during the short data-assimilation cycle and can therefore be ignored. This assumption has been explored using an approximation of strongly coupled DA that utilizes existing well-developed uncoupled DA capabilities in a block-iterative approach (Yaremchuk et al. 2021). The block-iterative approach is significant because it does not require the development of a new coupled solver; rather, it applies the current uncoupled solvers to a series of innovations to approximate to the strongly coupled solution. Coupled correlations from the Navy ESPC 16-member ensemble are used to produce a coupled increment by projecting the coupled innovation onto the model grid. Use of generalized coupled innovations in this approach ensures that coupled update information is consistent between the NAVDAS-AR and NCODA components of the system and helps to reduce initialization shocks within the coupled forecast. Testing of the block-iterative approximation to strongly coupled DA within the Navy ESPC system has already been conducted on an array of points around the globe and is shown to reduce the error to within 3% of the strongly coupled solution within one iteration (Yaremchuk et al. 2023). The block-iterative framework will be implemented on a global scale with plans to incorporate into Navy ESPC v3. The additional cost is estimated to be the equivalent of running the uncoupled DA solvers.

It is important to note that because the block-iterative approach relies only on the uncoupled DA systems, it is relatively system agnostic. This point becomes increasingly important as we continue to develop out

3.2 Development Pathway for FALCON

At the end of FY24, FALCON DA will consist of the JEDI-enabled 3DVar FGAT solver with an observation stream supported by NAVGEM. As we prepare for the initial transition, we will see development toward hybrid 4Dvar in parallel. Initial testing of the NEPTUNE atmosphere TLM/ADJ models in FALCON DA will begin and parallel development of a LETKF will proceed. Capability replacement of the current NAVDAS-AR system is targeted for FY 26 with subsequent transitions of 4DVar, Hybrid4DVar.

The planned resolution for the NEPTUNE deterministic forecast is 9 km, and this may reduce the dependence on regional/basin scale limited domain applications for NEPTUNE DA. The JEDI 3DVar algorithm is in model space — as such, it will not have the strong dependence on the number of assimilated

observations. At these scales, it is unclear whether specialized procedures for tropical cyclone initialization will be required. If so, we plan to assimilate information from the TC warning messages directly as opposed to generated pseudo-raob profiles as is currently done in NAVGEM.

3.2.1 Bias Correction — Variational (VarBC) and Alternatives

Correction of systemic bias is essential to obtain benefit from satellite radiance observations, which now constitute the majority (~80%) of assimilated data in global atmospheric models. The most successful system to date is variational bias correction (VarBC), which relies on a flawed assumption that the model prior is unbiased. As a result, some amount of model bias is improperly mapped into the set of assimilated radiance innovations and thus into each new analysis. The accumulation of the model bias through the increments eventually locks the model into a permanently biased state. A review of this topic is provided by Eyre (2016). For NAVGEM, efforts are being made to mitigate this problem by using a “trusted analysis cycle” (TAC) to define a less-biased model prior, or background, to be used in the radiance-bias-correction procedure. TAC works reasonably well in a mature global DA system like NAVGEM, with an abundance of trusted observations. But for developing systems such as NEPTUNE/JEDI, or for regional or forward-deployed systems, trusted observations may not be available in time, or the DA system may not have the sophistication or computational resources need to run the extra analyses required by TAC. We are currently working on a simpler, lightweight approach to decouple the feedback between model error and VarBC by performing a separate model bias-removal step prior to VarBC. Toy model tests using Lorenz96 show promise.

In the meantime, for NEPTUNE/JEDI, there are options for both static (offline) and variational (VarBC) bias corrections. These options have been tested with several trials assimilating data from the ATMS and MHS instruments, and testing with hyperspectral IR instruments (CrIS and IASI) will soon be underway. A combination of both approaches may mitigate bias drift that occurs with pure VarBC while retaining most of its advantages, while the model bias-removal system is being developed.

3.2.2 Improvements to Static Background Error Component

Specification of model background-error covariance is critical in the data-assimilation process to obtain a proper balance of information from observations and forecast prior and is in need of updating to be made consistent with current model accuracy. The NAVDAS-AR static B (Daley and Barker 2001, Xu et al. 2005) has been modified as part of FALCON DA to allow for unstructured, decomposed grids as an input. It has also been modified to accept yaml configurations, making it more flexible.

Our suite of metrics for tuning the static B for NEPTUNE includes single ob testing, fit-to-obs (described in Section 3.3) and innovation-based methods such as Desroziers et al (2005) and Hollingsworth-Lönnberg (1986). This is an area where development of new techniques could produce a significant payoff in analysis quality. One new concept involves intercomparison (such as mean-square differences) of large sets of atmospheric analyses produced by different centers (Langland et al. 2008). This information provides a proxy for actual error in the analysis and short-range background forecast, which, in general, is difficult to accurately quantify by regular forecast-verification methods.

3.2.3 All-Sky Radiance Assimilation for NEPTUNE

A new capability is under development to assimilate all-sky satellite raw radiance data into NEPTUNE to improve cloud and convective storm prediction in the tropics. Currently, we assimilate ABI water vapor channels 8, 9, 10 data from GOES-16, 18, and Himawari-9 using ensemble approach. The Community Radiative Transfer Model (CRTM) is used as the forward operator. A multiscale ensemble localization algorithm has been developed for updating model state variables at both convective scale for storms and large scale for the environment in which the storms develop. High-pass and low-pass filters were also

developed to select the observed radiance data at the scales needed. To ensure the scalability and efficiency of the system, we used the LETKF parallelization algorithm to divide the all-sky DA domain into many subdomains. These subdomains are relatively small and contain a limited number of observations, allowing for timely completion of the ensemble data assimilation. For each subdomain, we use the LETKF parallelization procedures to select the observational data, the NEPTUNE ensemble forecasts, and to optimize number of CPUs assigned to the subdomain. Then we use the EnKF data-assimilation technique for each of the subdomains to assimilate the radiance data into NEPTUNE in a manner similar to limited-area data assimilation. The EnKF technique enables the ability to use satellite radiance data from multiple channels with different frequencies and vertical weighting functions. It also allows the system to use different scales for different model state variables in the multiscale ensemble data-assimilation algorithm. Currently, the all-sky radiance assimilation for NEPTUNE focuses on addressing scientific issues at a 6.2 level. After successful testing of the system with satisfied results from experiments, we will transition the system to a 6.4 program (FALCON or a similar project), where it will be further tested and integrated into the NEPTUNE-JEDI for potential transition to Navy operations for NEPTUNE data assimilation.

In the future, we also plan to add microwave (WV) data into the assimilation. MW all-sky radiance assimilation must consider different hydrometer scattering and emissions in the CRTM forward calculations. NEPTUNE explicit microphysics (with the integration of CCPP) is suitable to perform all-sky radiance assimilation. Many operational centers have pioneered the all-sky assimilation of MW imagers, MW humidity sounders, and MW temperature sounders (Geer et al. 2018). Hence, all-sky radiance assimilation will be one of the top priorities to further improve environmental characteristics and forecast skill.

3.2.4 4DVar

After 3DVar, our next major transition update will be 4Dvar. The 4Dvar cost function in the FALCON DA system is an incremental cost function in the state space. The incremental cost function is defined around a nonlinear trajectory that is updated in the outer loop. The tangent linear model (TLM) and adjoint (ADJ) modules propagate the increment across the DA window. The TLM/ADJ for the dynamical core of NEPTUNE, a spectral element model, have been developed and have undergone preliminary testing (Zaron et al. 2022). The development of the TLM/ADJ for NEPTUNE has been led by Code 7533.

3.2.5 Hybrid 4DVar

Many practical tests (Etherton and Bishop 2004, Wang et al. 2008a, b, and 2013, Yaremchuk et al. 2011, Clayton et al. 2013, Kuhl et al. 2013, Ménétrier and Auligné 2015) all suggest that hybrid error covariance models (Hamill and Snyder 2000, Lorenc 2003) yield superior data-assimilation performance to either just-localized ensemble covariances (Hamill et al. 2001) or quasistatic climatological error covariance models. Work by Bishop and Satterfield (2013) and Satterfield et al. (2018) offer theoretical justification for hybrid covariance models and show that in a simplified scenario, a hybrid covariance model produces the minimum posterior variance.

For NEPTUNE, we plan to use an implementation of the Hybrid 4D-Var that involves forming a hybrid background-error covariance matrix (e.g., Hamill and Snyder 2000, Lorenc 2003) that is propagated through the DA window using TLM and Adjoint models. This form is consistent with what is currently operational in NAVGEM.

We note that hybrid variants that do not use a TLM and Adjoint have not been able to match the performance of those that do. Lorenc and Jarda (2018) offer the explanation that the time-evolved covariances are responsible for a large portion of the benefit of 4DVar over 3DVar and allow the static covariances to produce structures that are tilted with the atmospheric flow and resemble singular vectors. The isotropic static background error covariance model (as used in 3DVar) cannot give preference to such

growing structures. Evolving the ensemble-based error covariances within the DA window using the TLM is typically less impactful, as they already have a well-formed state-dependent structure at the beginning of the window.

3.2.6 Ensemble Methods

Our ensemble components of FALCON will utilize the local ensemble transform Kalman filter (LETKF) (Hunt et al. 2007, Szunyogh et al. 2008). The LETKF will initially be developed for Thermosphere DA by collaborators in Code 7227. Eventually, the application will be extended for use in FALCON to provide the flow-dependent component of the hybrid background error covariance and to serve as initial conditions for long forecast ensembles for probabilistic prediction.

The LETKF will be implemented to run in tandem with the Hybrid-4DVar, with the analysis being recentered on the higher-resolution Hybrid-4DVar analysis, and the flow-dependent component of the covariance being updated, at each analysis time. The majority of the LETKF implementation is being undertaken by collaborators in Code 7227.

3.3 Verification and Diagnostics for DA

The requirements for diagnostics and verification in data assimilation differ from those used to assess forecast model changes and corresponding skill changes. Diagnostics for both are required to be able to adequately assess data assimilation changes and the resulting forecast skill. In the past, more emphasis has been put toward the assessment of forecast skill. Differences in the analysis due to changes in the observation suite or other aspects of the DA system are often small, as are the subsequent forecast error changes, even at longer forecast ranges. Moreover, it is possible to improve the data-assimilation system and the quality of atmospheric analyses (and to qualify upgrades for transition to operations) while not necessarily providing statistically significant improvements to forecast metrics. In some cases, improved analyses may create forecast degradations because the forecast model is improperly tuned to compensate for biases in the current analysis products (initial conditions and verification fields). We also note that the quantification of analysis errors must be more rigorous than for forecast errors because we cannot make use of simplifying assumptions (e.g., error in a proxy for true state is much smaller than forecast error). The classification of analysis errors is critical for improving the analysis, simulating observations, and providing an analysis with proper error representation to serve as forecast verification. Therefore, developing new metrics of analysis and forecast skill is required to support data-assimilation development and basic research.

NRL-Monterey has a strong history of developing adjoint-based techniques for data-assimilation diagnostics. These include the forecast sensitivity to observation impact (FSOI) (Langland and Baker 2004) now used at many operational forecast centers, and sensitivity-based methods for tuning observation error covariance and Kalman gain of assimilated innovations (Daescu and Langland 2013, 2017). FSOI is a capability that utilizes the adjoint and TLM of the forecast model and the adjoint of the data-assimilation system to propagate forecast errors backward in time to attribute them to the individual observations that were assimilated. FSOI statistics can be computed for both 3DVar- and 4DVar-based systems; however, it is most often seen with 4DVar systems, as 4DVar methodologies require the adjoints and TLM of the forecast model and data-assimilation systems. We plan to implement FSOI capability for NEPTUNE DA once the NEPTUNE TLM/ADJ have been completed.

One metric that has come into increasing prominence is the evaluation of fit to observations. The metric uses the vast quantities of available satellite radiance data to measure how close the background (typically a 6-hour forecast) is to new observations that have not yet been assimilated. Because the forecast is short, model error should be small, so we are effectively measuring how good our previous analysis was.

Unlike most verification metrics, it is computed in observation space rather than model space. ECMWF uses background fit to observations as their primary metric in evaluating short-range forecasts, and NRL has a fully developed fit to observations capability. A major reason to use the metric is that it can reach statistical significance very rapidly to determine improvement or degradation of a numerical experiment versus a control run, often on the order of a week of simulation, rather than the 2 or 3 months required by traditional forecast-verification metrics.

4. FUTURE DEVELOPMENT

In order to further develop our FALCON DA hybrid-4DVar approach, as well as to move out in new directions of data assimilation at cloud-resolving scales, exploiting Navy-unique observations and coupled DA, we will continue to leverage partnerships, or to participate in community activities, in the following research directions.

4.1 Initializing Multiple Scales

The notion that the data-assimilation system must be able to accurately estimate both the large scales and the small scales simultaneously has historically been a substantial challenge in state estimation for the multiscale phenomena. While the rapid increase in computational power has led to a substantial increase in the resolution of the numerical weather prediction models used by the Navy, we have not seen parallel multiscale efforts in DA. Typically, the components of a global DA system have been broadly constructed to work adequately at coarser resolutions. A scale-aware approach becomes more important as we move to higher-resolution, highly coupled systems.

Operational resolutions for DA have tended to be around three times as coarse as the forecast model. The initial operational resolution for FALCON DA will be four to five times as coarse. The impact of this is unknown. In future, higher resolutions, the hydrostatic balance approximations may be less representative of the dynamical system. It is computationally expensive to run high-resolution ensembles for data assimilation. Running relatively few members means also means that the undersampling of the state space will be exacerbated. The AGR filter (King et al. 2020) represents a potential path to reducing the number of ensemble members needed to resolve the DA problem.

The next generation of global NWP models is cloud-resolving, which presents new challenges for current DA methodologies and practices. Current solver methodologies are built on quasilinear and Gaussian approximations. These approximations provide a tractable approach for DA and have led to useful results. These approximations are less representative of cloud-resolving systems and should therefore be reevaluated and improved. Machine learning (ML) methods for either approximating or transforming non-Gaussian distributions present a path forward for using current methods in this DA regime.

4.2 Multiple Outer Loops

ECMWF utilizes a multiple-outer-loops strategy whereby the model and observation operators are repeatedly linearized about the updated (possibly more accurate) nonlinear trajectory. This outer-loop mechanism has recently been shown to be one of the key drivers of analysis and forecast accuracy in the IFS (Bonavita et al. 2018). More recently, ECMWF has implemented continuous DA. Rather than waiting for most of the relevant observations to arrive (1 hour after the end of the assimilation window) to begin the 4DVar minimization, this solver process is started earlier, and late-arriving observations are added to the next outer-loop minimization. In addition, ECMWF was able both to add an additional outer loop minimization and to increase the assimilation window length while still meeting the operational time constraints for their early delivery schedule. This continuous DA approach, with approximately 14% more

observations, was found to improve the forecast quality significantly. Furthermore, multiple outer loops can facilitate implicit coupling between fluids in coupled data-assimilation systems (Laloyaux et al. 2018); however, it is shown to be most effective when used in systems with longer DA windows (i.e., > 6 hours). We anticipate FALCON DA will have the ability to perform multiple outer loops pending the addition of features to NEPTUNE atmosphere.

4.3 Improvements to Hybridization and Localization

There has been a recent push to use more quantitative methods in defining covariance matrices. To that end, we are exploring methods for optimal hybridization and localization. B. Ménétrier and T. Auligné (2015) outline methods of hybridization and localization that are dependent on the ensemble's being random draws from the true distribution. Satterfield et al. (2018) discusses how to incorporate observational information to determine optimal hybridization.

The region of influence of the observation, or how observational information is spread to neighboring areas, is determined by the structure of error correlations. Ensemble localization is used to reduce spurious correlations caused by sampling error. Inherently, it is clear that such statistics should be dependent on the scale of the analyzed feature. Buehner and Shylaeva (2015) and Caron and Buehner (2018) used overlapping wavenumber bands to define scale-dependent correlations. In particular, Caron and Buehner (2018) implemented this multiscale methodology in a global NWP model by defining three wavenumber bands to coarsely define small, medium, and large scales and a weighting function ranging between 0 and 1 to allow for between-scale interactions. The forecast impact results indicated that the multiscale correlation schemes yielded improved forecast skill over using fixed correlations.

Exploring such approaches of hybridization and localization, likely implemented in an adaptive and scale-aware manner, is necessary to achieve optimal use of flow-dependent information.

4.4 Weak-Constraint 4DVar

In the incremental weak-constraint cost function, formulation the error covariance explicitly contributes to the cost function. The key question that we are facing is how to define a model-error covariance matrix. Current proposed methods have ranged from modeling model error following the same formulation used to model the static portion of the static background error covariance, using statistical information from innovations and increments, or analyzing between model differences.

4.5 Observational Information

The nature of environmental observations is changing as the global observing network evolves, as does the need for continued improvements in the global observing system's sensors and derived geophysical variables to meet the expected performance improvements models such as NEPTUNE and full ESPC models are to provide. We are witnessing significant increases in resolution for the vertical, horizontal, and temporal dimensions of the observational data, and we expect this trend to continue. Since DA systems have a computational limit to the amount of data they can process, we must be thoughtful in our approach for selecting or thinning data to have optimal impact on the analysis. The focus will be to prioritize sensors and platform observation types with larger FSOI observed and expected based upon instrument performance specifications. We must also adapt to shorter sensor timelines of the new SmallSats and the associated need for increased observation monitoring. There will be new opportunities to make timely use of high-resolution datasets more effectively and even assimilating new types of derived observations, for example, assimilating boundary-layer height estimates derived from measured profiles of the atmosphere obtained from high-resolution rawinsondes or aircraft, ceilometers, GPS-RO, etc.

4.6 Coupled Earth System Data Assimilation (Ocean, Sea-Ice, Land, Aerosols)

The growth of coupled modeling has been dramatic, as the Navy Earth System Prediction Capability (ESPC) shows the ability for skillful prediction at subseasonal timescales of 45–60 days. Though the environmental prediction models have seen full coupling between the ocean, the sea ice and the atmosphere, the data-assimilation components for these systems continue to be run independently, with the interaction occurring as the increments are applied in unison. The land assimilation, historically by the Navy atmospheric system, was done as a direct insertion of fields from the USAF surface analysis or surface and soil temperature and wetness. These surface fields are used to provide radiative fluxes at the atmosphere/surface interface. In the future, we look toward incorporating the Land Information System (LIS) into the Navy ESPC, which will allow a coupling of the land model explicitly with the other model components. Also, the LIS system comes with an assimilative component for the land, which can readily ingest surface station observations, and some satellite products.

As the complexity of Earth system models increases, the Navy’s operational DA schemes will need to adapt. Information (and errors) will increasingly flow between different Earth system subcomponents, and it will be crucial to optimize the DA approach in order to make the most of the information coming from observational data. Improvements to the coupled data assimilation can be achieved through research focused on 1) knowing when and where strongly coupled DA is of the most benefit to the Navy, 2) optimizing the assimilation of observations within coupled system, particularly from new, satellite-based observations that often sense multiple Earth system components, 3) developing effective space/time localization for ensemble and/or hybrid error covariances, and 4) developing adaptive meshes for limited-area applications. The outcomes of these short- to long-term research efforts are expected to enhance NRL’s coupled global and regional analysis/reanalysis and forecasting capabilities by accelerating the research leading ultimately to operational transitions.

4.7 Machine Learning for Data Assimilation

DA is uniquely positioned to integrate ML techniques because the two fields share a common theoretical foundation. We anticipate expanded use of AI/ML techniques throughout the prediction system. In particular, we recognize the opportunities presented by AI/ML with regard to uncertainty quantification and estimation, smart thinning/data selection, representation of physical processes, handling of unknown probability distributions, and data preprocessing and quality control. The current 6.2 Microsats project is one effort that is already leveraging ML for uncertainty quantification and smart thinning.

5. COMMUNITY PARTNERSHIPS

We realize that we are a relatively small group and need to be strategic in how we collaborate with the community. We aim to align our focus and expertise on naval need and capability. We are choosing to leverage community development for infrastructure so we can allow our world-class scientists to focus on science and naval need.

5.1 JCSDA

The Joint Center for Satellite Data Assimilation (JCSDA) was established by NASA and NOAA in July 2001. The Department of the Navy and the Department of the Air Force were subsequently added as full partners by 2002. The mission of JCSDA is to “to accelerate and improve the quantitative use of research and operational satellite data in weather, ocean, climate, and environmental analysis and prediction systems.” NRL Monterey has adopted the JEDI framework to provide a unified framework for upcoming and future DA capabilities. The JEDI consists of a series of abstracted data-assimilation and observation

processing packages: OOPS, SABER, UFO, IODA, and VADER. The JCSDA also develops the Community Radiative Transfer Model (CRTM), which is used with microwave and IR instruments. The JCSDA has also released JEDI-SKYLAB, which represents an end-to-end NWP system.

We engage with the JCSDA through a seat on the executive team (ET), by contributing to the JEDI, and by participating in workshops and special sessions. Additionally, our collaboration includes a supporting a liaison position between NRL and JCSDA.

5.2 METplus

Community verification packages have recently reached a high level of maturity with a large, active user base. In particular, the METplus system developed by NCAR's Developmental Testbed Center (DTC) has been adopted by many of our US colleagues, including the National Weather Service/Environmental Modeling Center. NOAA's Next Generation Global Prediction System (NGGPS) verification framework is entirely based on the METPlus software. We are in the process of adapting the METplus system to Navy atmospheric models, including NEPTUNE, to develop a division-wide system for verification and validation. Such a framework will allow us to make use of more modern, feature-based analysis and forecast verification metrics that can assist with identification and diagnosis of specific sources of model error. In addition, this modern framework would allow NRL to better tailor our verification products to inform data assimilation and model development, as well as to meet the needs of the end user. A consistent model verification framework would aid in collaboration with other U.S. partners (e.g., NCAR, EMC, JCSDA for JEDI) who are employing the same community tools. Additionally, we have transitioned some of our in-house-developed diagnostics to the METplus software package and anticipate additional collaboration with DTC. We engage with DTC through the METPlus governance meetings, by contributing to the METPlus repositories, and by participating in workshops.

5.3 International Collaboration/Coordination Groups

NRL scientists are actively involved in multiple World Meteorological Organization (WMO) and Coordination Group for Meteorological Satellites (CGMS) science working groups. These include the International Winds Working Group (IWWG), the International TOVS Working Group (ITWG), the International Radio Occultation Working Group (IROWG), and the Global Cryosphere Watch (GCW) of the WMO, as well as the Working Group on Observational Data, a subgroup of the Committee for Operational Processing Centers under the U.S. Interagency Council for Advancing Meteorological Services. These groups are critical to help monitor the global observing system, to decrease the time to delivery of new capabilities, to be made aware of critical methodology improvements, and to learn details of instruments, future instruments, and influence agencies on what observables are most critical for impact on Navy data-assimilation and NWP systems.

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