An overview of future research projects within UFS-RTMA

Miodrag Rancic, R. James Purser, Manuel De Pondeca, Edward Colon, Gang Zhao, Annette Gibbs, Ting Lei

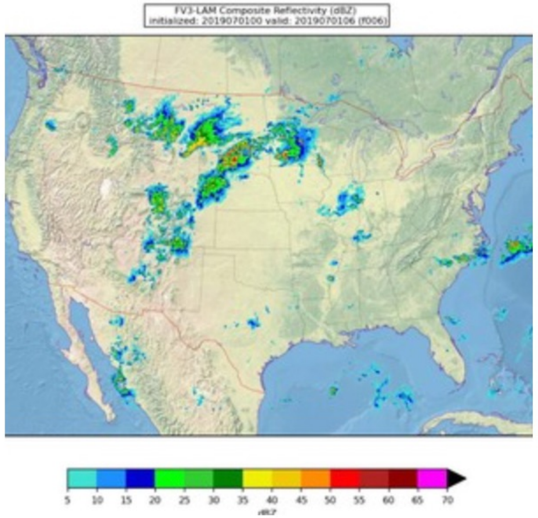
IMSG at NOAA/NCEP/EMC

Jacob Carley
NOAA/NCEP/EMC

Therese T. Ladwig
Curtis R. Alexander
NOAA/OAR/ESRL/GSL

3D RTMA/URMA Project

The Real Time Mesoscale Analysis (RTMA), and its delayed real-time companion system, UnRestricted Mesoscale Analysis (URMA) is a data assimilation project conducted jointly by NOAA's Environmental Modeling Center (EMC) and Global Systems Laboratory (GSL). It provides field forecasters with analyses for nowcasting and situational awareness, serves as an Analysis of Record (AOR) for forecast verification, calibration/bias-correction, and accelerated Unified Forecast System (UFS) development.



Major milestone: UFS Short-Range Weather Application 2.0.0 released on June 23, 2022.

The major development underway is a fully three-dimensional (3D) RTMA system which will provide analyses of a range of parameters at

- high horizontal resolutions
- (~2.5 km and beyond)
- frequent time intervals
- (~15 min)

A comprehensive plan, a roadmap for future developments, is presently being formulated. It includes a detailed outline of envisioned developments of 3DRTMA in next 10 years, consistent with GSL strategic plan, and with priorities outlined in the EMC 10 years strategy (draft) for data assimilation.

A list of targets in the 3DRTMA Roadmap (Draft)

- Improved observation processing
  - Quality control
  - Processing
  - Inclusion of new observations, such as weather cameras and uncrewed aerial systems (UAS)
- Improved analysis uncertainty
  - A versatile new multigrid tools, recently developed for the efficient representation of background error covariances might be co-opted, in combination with ML (Machine learning) for representing analysis covariances as well
- Background Error Covariance (BEC) Modeling
  - High-resolution ensemble-based BEC information

- The Multigrid-Beta Filter (MGBF) is a new method developed for the efficient application of BEC operators on a massively-parallel computational platform

- Application of Machine Learning and Artificial Intelligence (ML/AI)

- Enhanced resolution and downscaling

- Inclusion of air quality and smoke
  - Extensions to chemical and aerosol data assimilation

- Coastal and global RTMA

- Improved data visualization

The RTMA project represents ideal framework for new research and development. This talk will focus on several underlined items, some of them in mature stage of development and others, for now, just as interesting ideas worth further exploration.

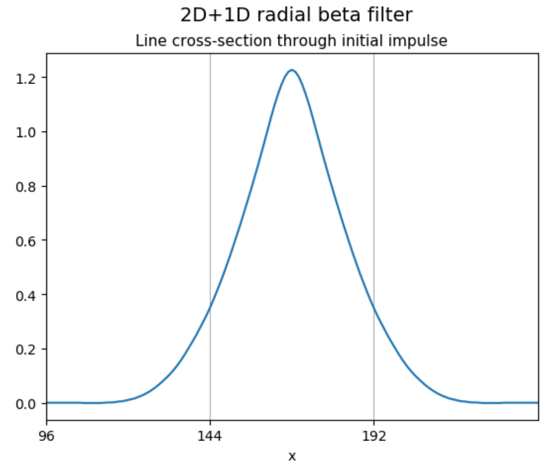
Multigrid Beta filter (MGBF)

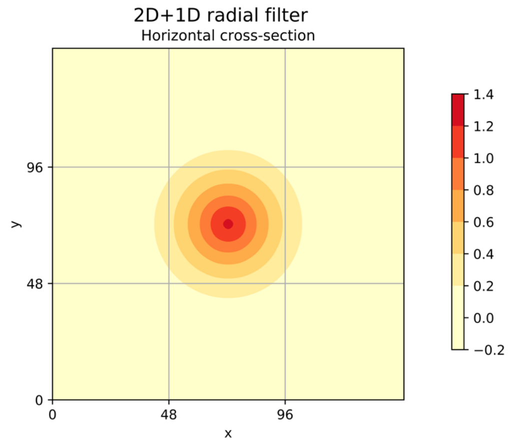
The key prerequisite for the success of RTMA enterprise is a vastly improved efficiency in producing those analyses.

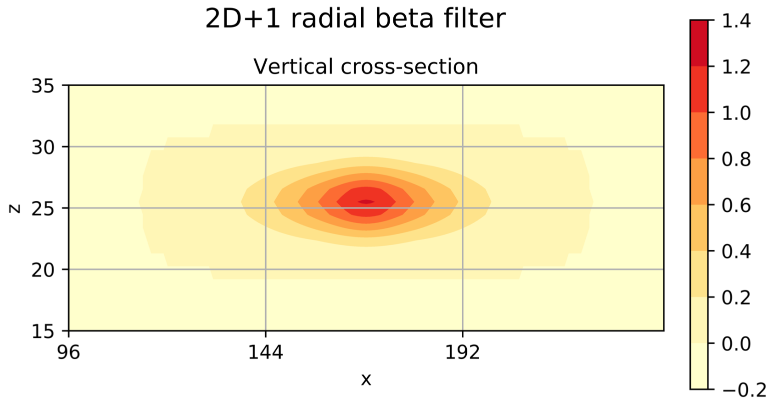
MGBF, a new approach for modeling of the background covariance error, ($\boldsymbol{B}$), is one of the key components for the success of that effort.

It is replacing the recursive filter (e.g., Wu et al. 2002; de Pondeca et al. 2011) which, despite some nice properties, being essentially a sequential operator, is very difficult to parallelize efficiently.

Technically, a single delta impulse has to producing a quasi-Gaussian response:





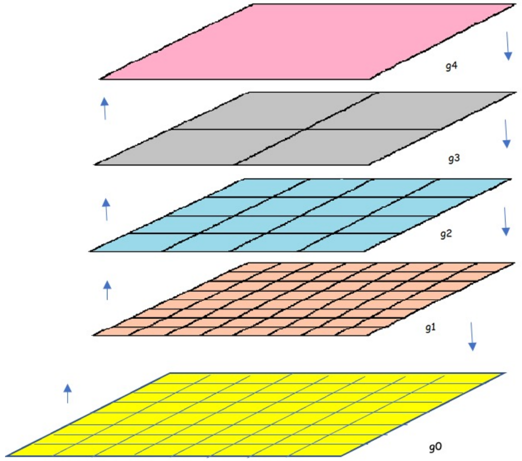


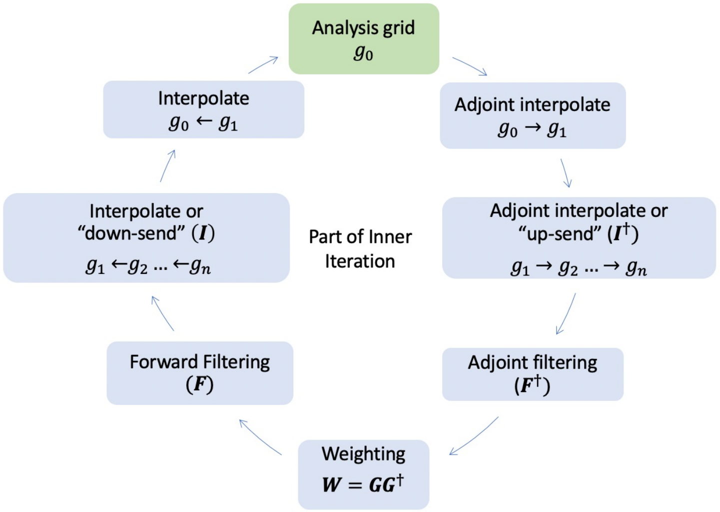
In these tests, we use a radial beta filter, defined in the special isotropic case as:

$$\beta(\boldsymbol{r}) = (1-\rho)^p \quad , \rho \leq 1 \quad \text{where} \quad \rho = \frac{K}{s^2}\boldsymbol{r}\cdot\boldsymbol{r}^T$$

Here p is a small positive integer, s is a radial scale in grid units, and K a dimensionless constant that depends upon p and the dimensionality and $\boldsymbol{r}$ the relative position vector. In the more general anisotropic case, $1/s^2$ is replaced by the inverse "aspect tensor".

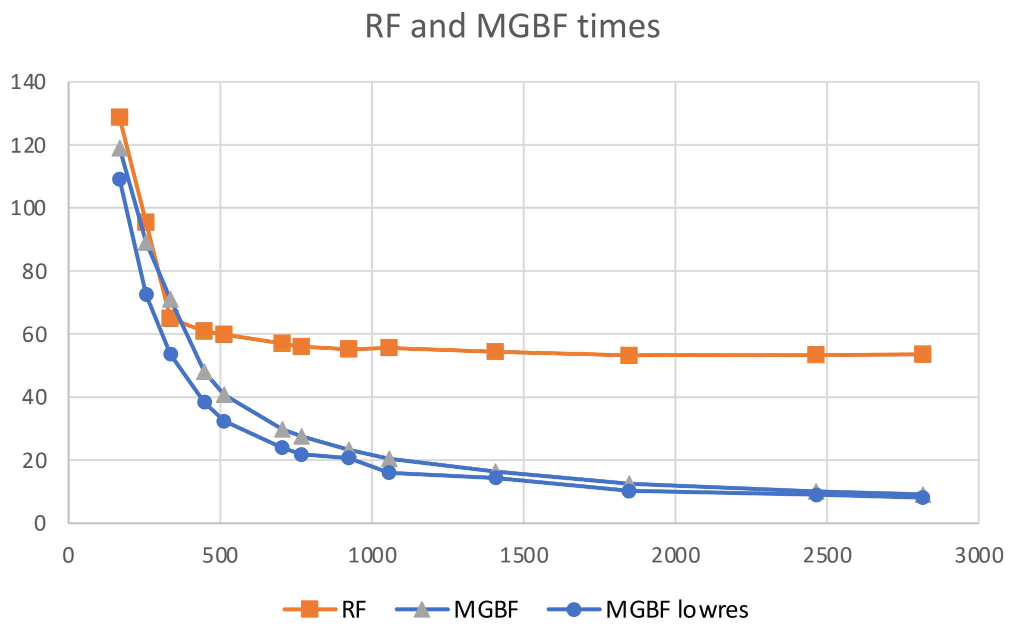
The beta filter is further used at a hierarchy of different scales, combined into a parallel multigrid scheme in order to achieve a larger coverage and potentially a more versatile synthesis of anisotropic covariances, allowing a greater control over the shape.





Schematic description of filtering procedure (From Purser et al. 2022 MWR)

Tests in GSI



Isotropic version of MGB line filter is about 3 times faster than RF and scales better. Running filter grid at some 10 % lower horizontal resolution helps, though not substantially.

Yet, that alone is not sufficient to push down execution time of GSI beyond ~ 500-700 PEs. Clearly, too much all-to-all calls and communication with discs. (From Rancic 2022 - *ResActESM)*

A series of variations of the basic radial beta filter are devised:

- line beta filter (Purser 2021 – Office Note)
  - There is a 4D version of line beta filter (potential for nowcasting, a poor man 4DVAR, …)
- planar beta filer (Purser et al. 2022 – ISDA)
- fast isotropic version (Rancic et al. 2021 - AMS)

Application of the multigrid approach gave us opportunity that through a skillful weighting of contributions from different multigrid generations, for the first time, introduce cross-covariances in the variational framework.

For example, let us symbolically express the overall contribution from the multigrid generations to a set of selected variables is as:

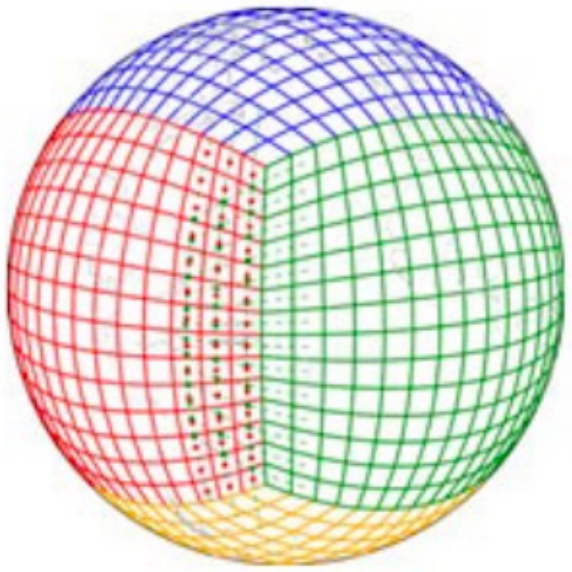
$$\begin{pmatrix} p \\ \psi \\ \chi \end{pmatrix} = \sum_i w_i \begin{pmatrix} p_i \\ \psi_i \\ \chi_i \end{pmatrix}$$

Here:

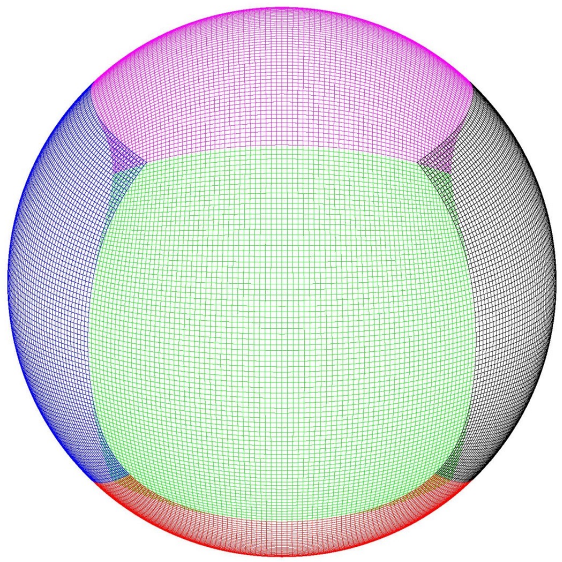
- pressure (p)
- stream function (ψ)
- velocity potential (χ)

By defining scale weights, w_i, as symmetric positive definite matrices, leads to a cross-covariance formulation. Thus, the impulse in the pressure field, for example, may lead to the response in the wind field!

Global version (JEDI)

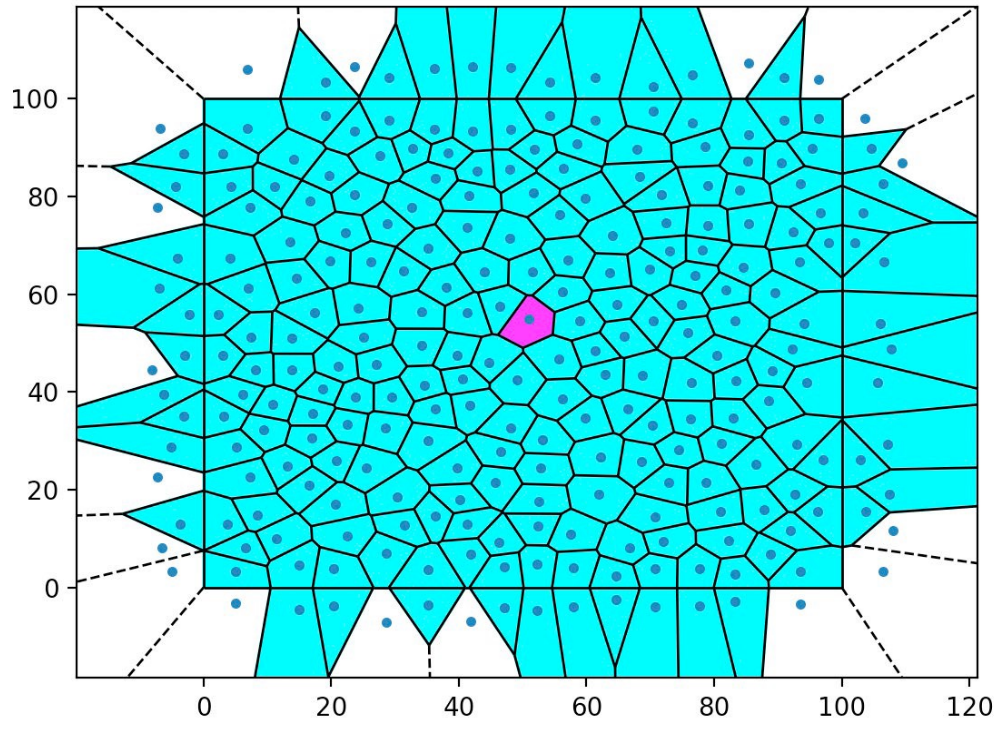


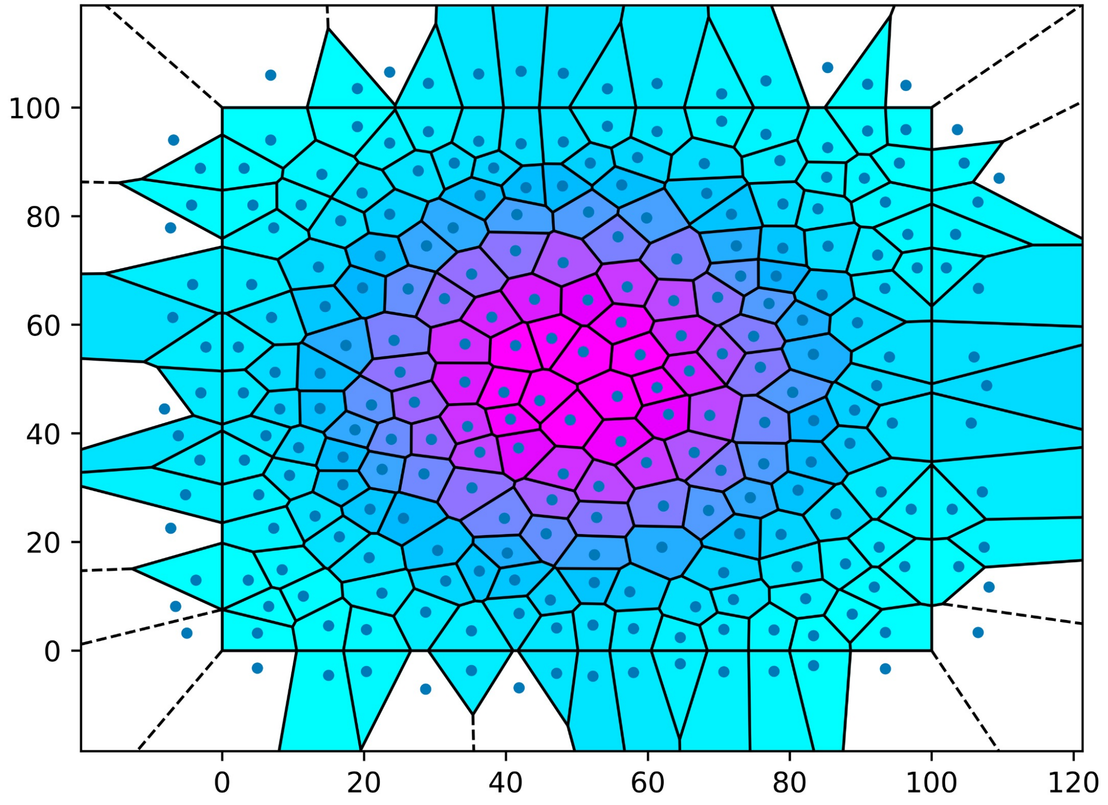
Equidistant along edges gnomonic cubed sphere used in FV3. A new radial version of beta filter under development will be able to handle edges and corners and provide calculating the analysis on the native grid.



A novel Overlapped conformal Yin-Yang grid which can be ideally used with the line version of MGB filter. (Purser et al. 2022 – ISDA 2022)

Unstructured grids





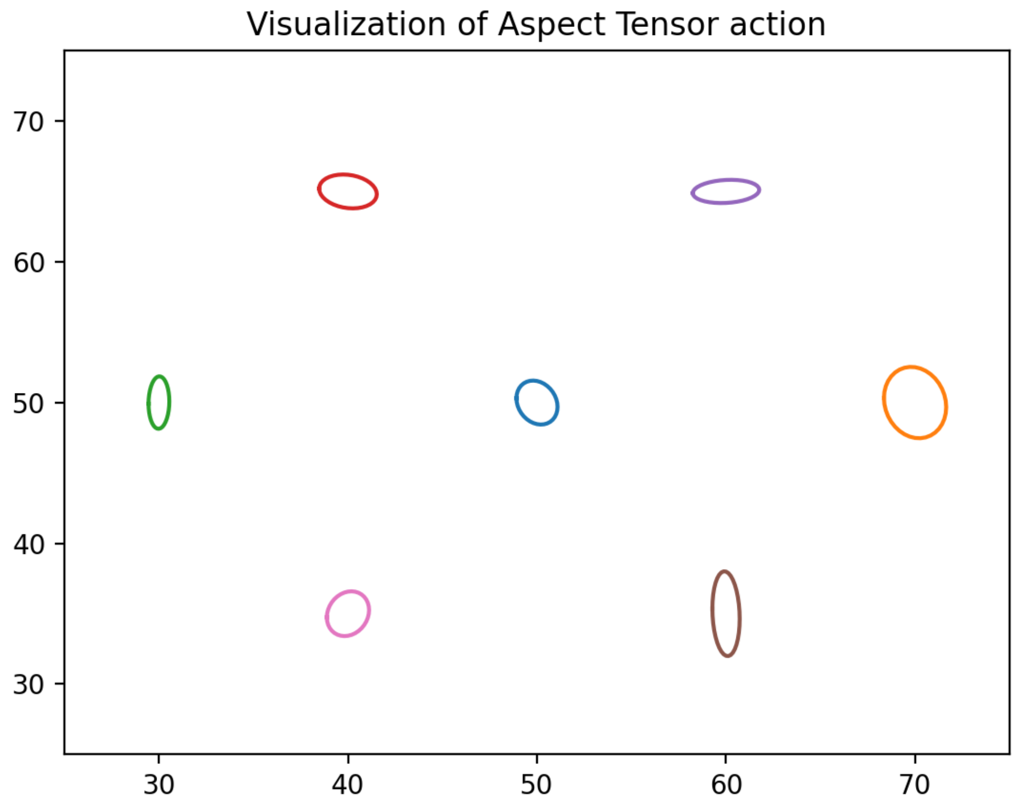
From Rancic et al. (2022a) – ISDA 2022

Inhomogeneous, anisotropic DA

We have developed a new strategy for introducing an inhomogeneous, anisotropic version of the multigrid beta filter as a function of topography and background field.

That is accomplish through formulation of a positive definite aspect tensor, which controls the shape of covariances.

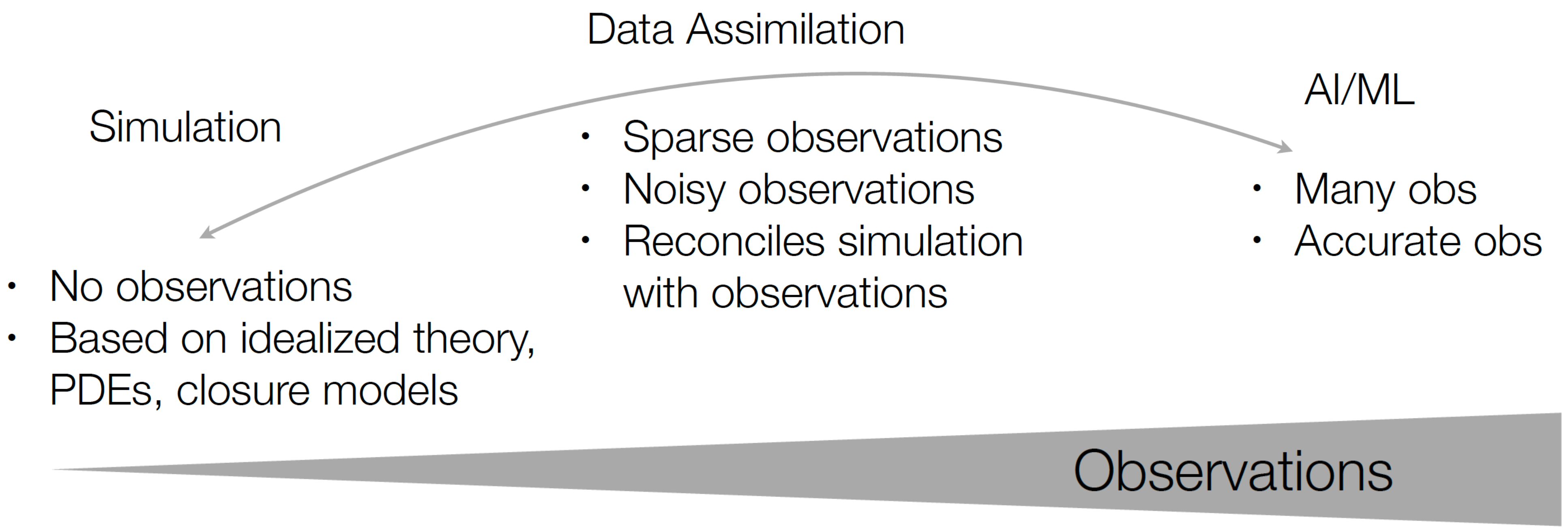
Figure shows examples of response functions as function of different scenarios of weather conditions and topography introduced though aspect tensor.



From Rancic et al. (2022b) – ISDA 2022

ML/AI in RTMA-UFS

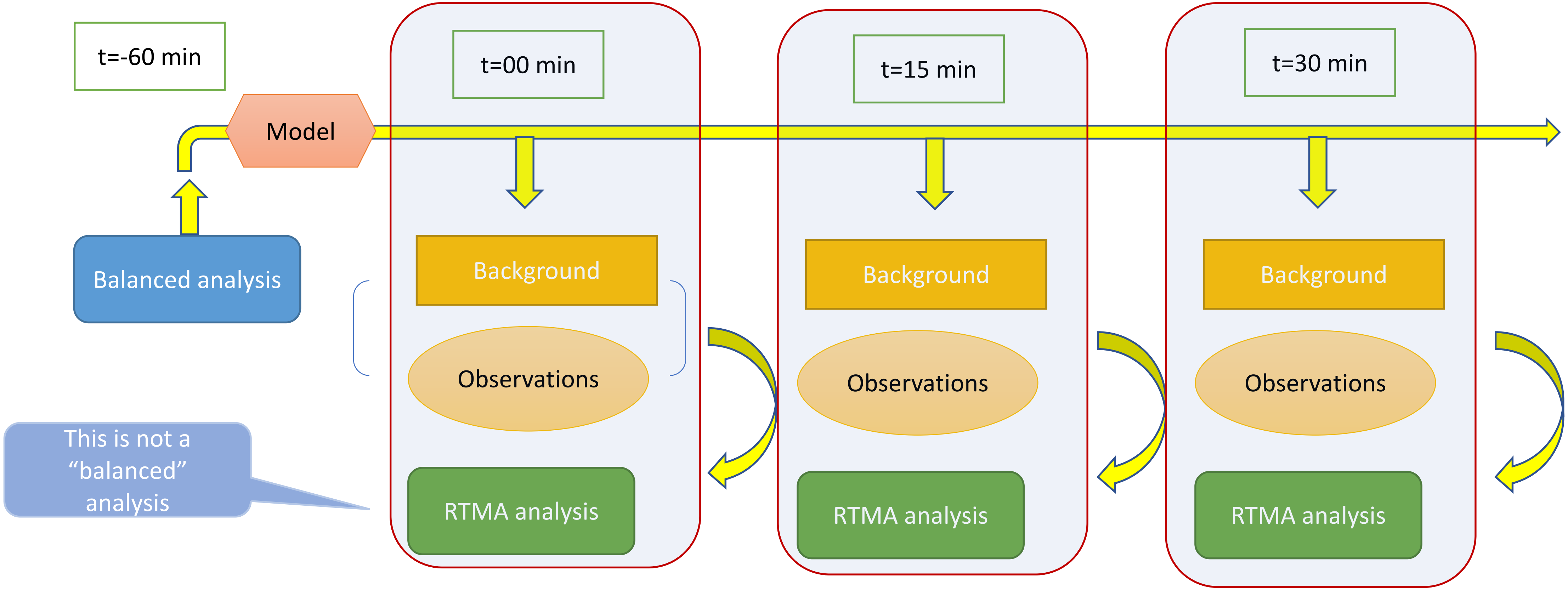
A diagram from Stephen Penny's recent keynote address at ISDA 2022 meeting best describes the rational for the paradigm switch with ML/AI in data assimilation



Anticipated ML/AI Projects

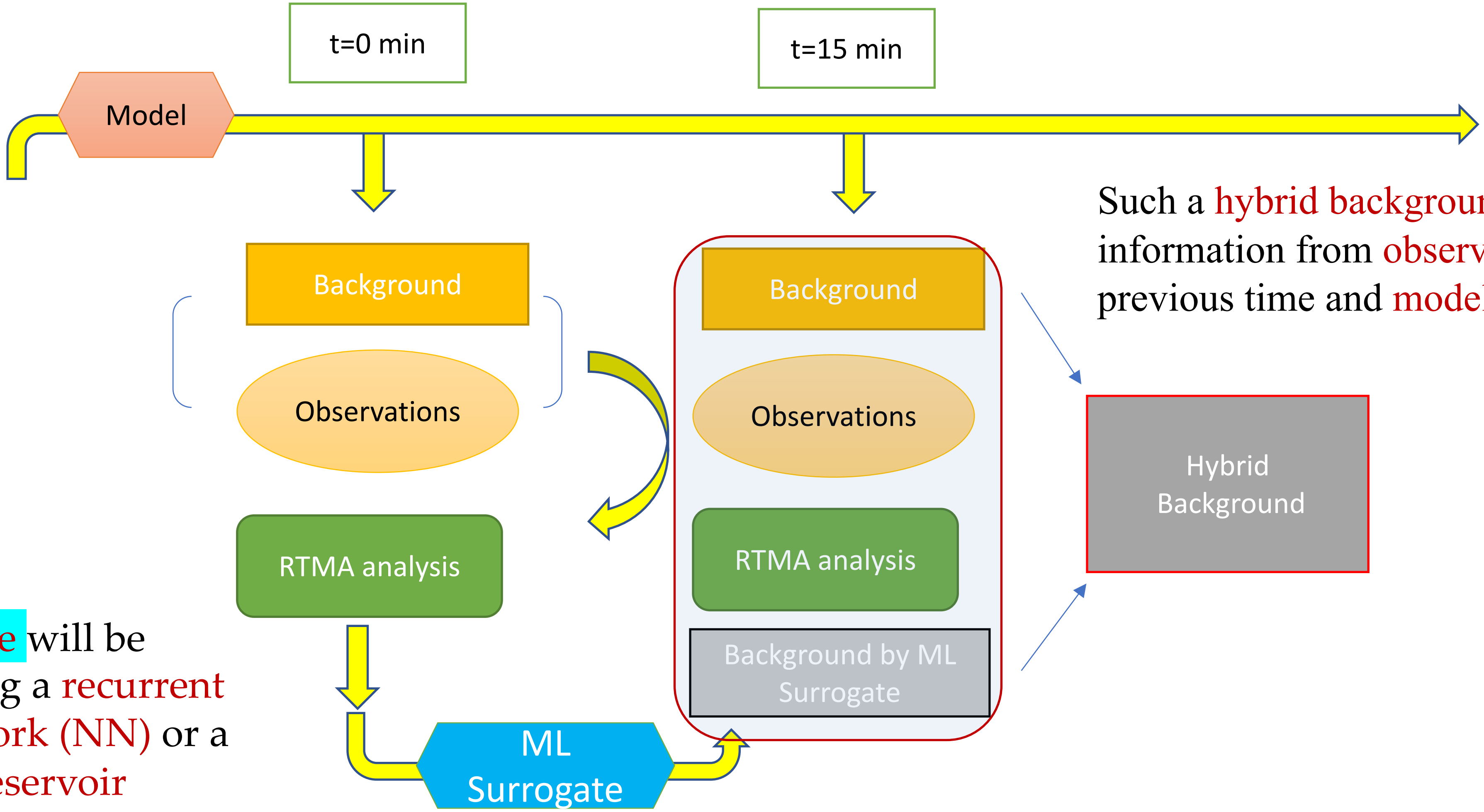
- Observation quality control (e.g., Sha et al. 2021; Mieruch et al. 2021)
- Estimation of analysis uncertainty using MGBF and ML/AI
- Improving the background field
- Downscaling
- Calibration of parameters of MGBF filter

Application of AI for improving the background field in RTMA



Model starts its run from a balanced analysis at -60 min, and its forecasts at 0, 15, 30, and 45 min are used as the background at these times. RTMA analyses at 0, 15, 30 and 45 min are produced using these backgrounds and observations at (and around) these times. Problem is that backgrounds degrade with time, because they do not take advantage of analyses and data from the previous analysis times.

We came with a method in which we combine the model background with the background derived running a ML surrogate from the previous time interval, which includes knowledge of data from previous time (Rancic et al. 2022 – AMS)

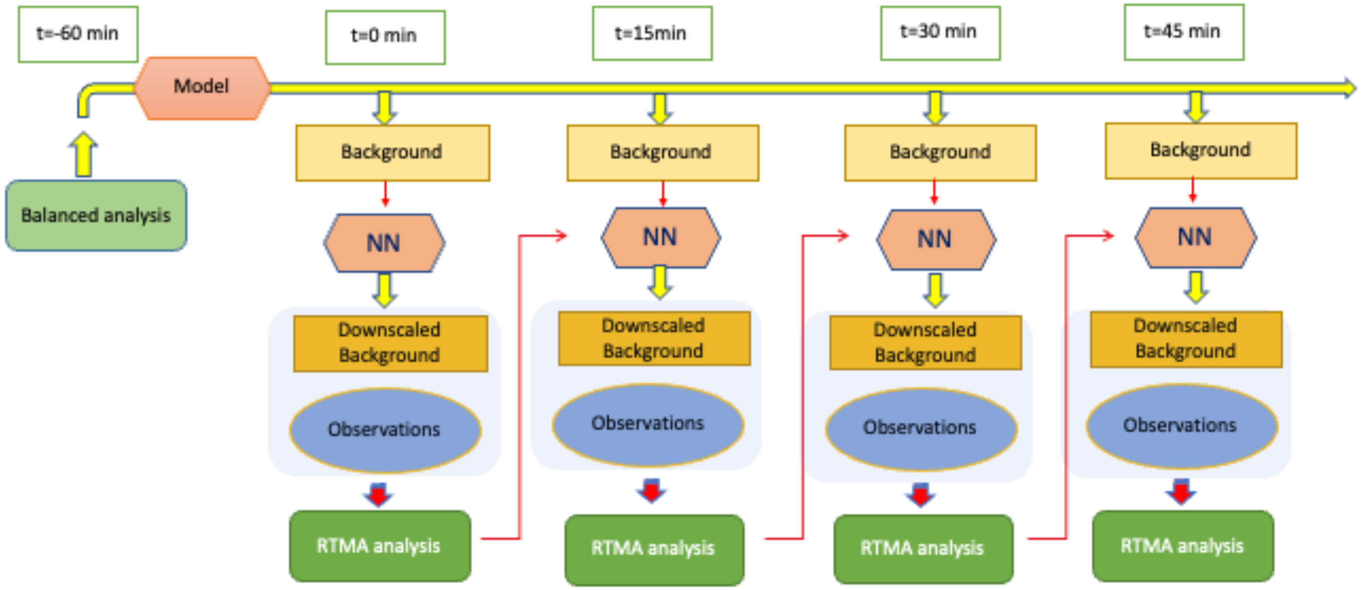


Such a hybrid background combines information from observations at the previous time and model forecast

ML surrogate will be derived using a recurrent neural network (NN) or a method of reservoir computing

Downscaling

- The background fields additionally needs to be downscaled to a higher resolution, currently from 3 km to 2.5 km (later to 1 km).
- This is now accomplished using dynamic downscaling (Gibbs et al. 2022 - AMS)
- We intend to apply the ML surrogate (NN), not only to replace 15 model forecast, but also to downscale it to the desired resolution, which should further increase the efficiency in deriving the RTMA products.



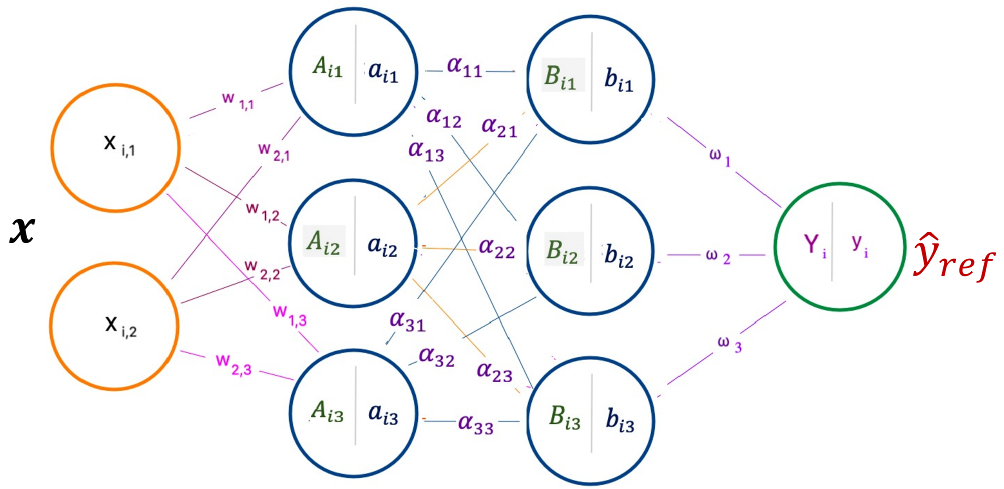
A quick, ~ 15 min ML forecast surrogate, based on RTMA analysis, could be used as an efficient tool for nowcasting

Calibration of MGBF using RF as a reference

- We assume that a set of MGBF parameters, $(w_1, w_2, w_3, w_4\,, A_o\,, \varepsilon, \delta) \equiv \boldsymbol{y}$, can be expressed as some unknow function of the background field $(\psi, \chi, T, q, O_3, w, p_s, T_s, T_l, T_i, \phi_s) \equiv \boldsymbol{x}$

$$\boldsymbol{y} = f(\boldsymbol{x})$$

- Furthermore, we formulate a deep neural net (NN) that connects causally these two sets, schematically depicted as:

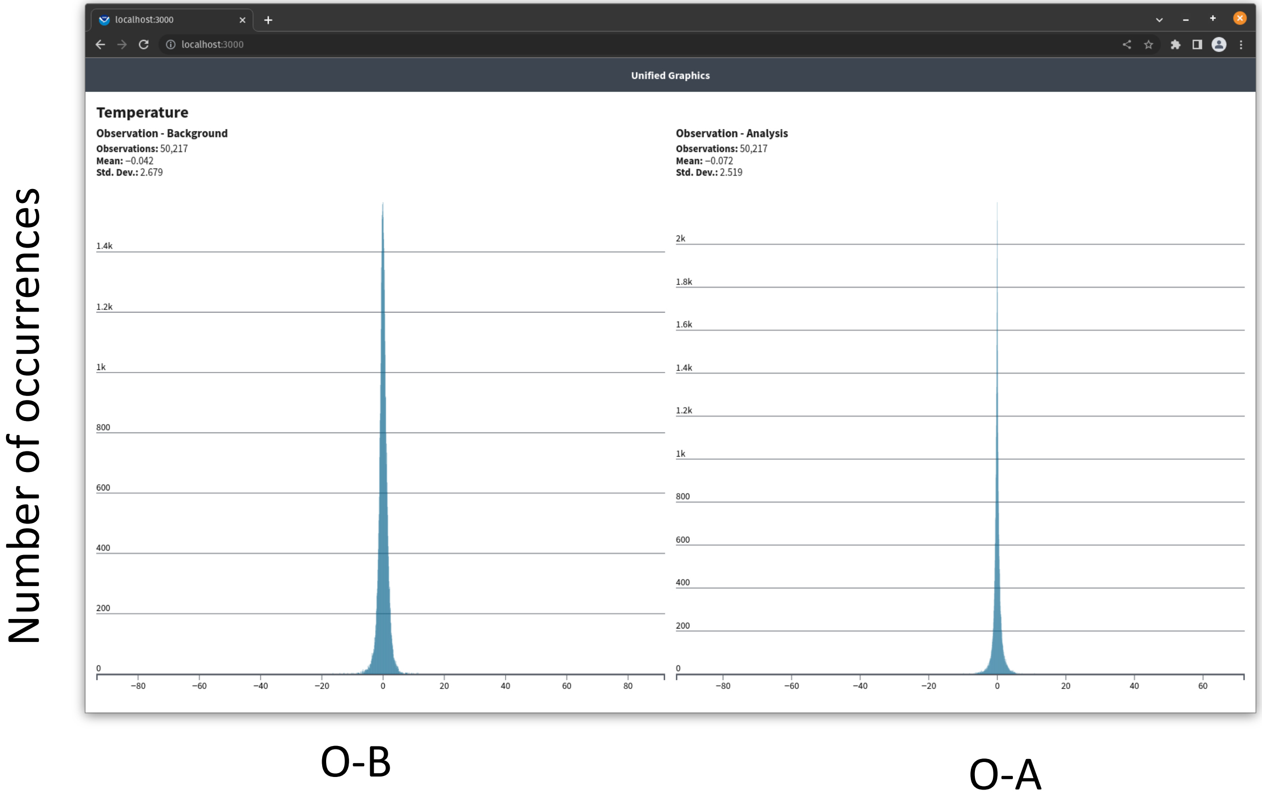


From here which we can find the unknow parameters **y,** assuming we have reference set of values, $\hat{y}_{ref}$, for training of NN.

To this end, we plan to use the analysis produced using RF, and later diagnostics coming from the ensemble.

Advanced tool for evaluation and visualization

- RRFS (Rapid Refresh Forecasting System) is the new NOAA's regional modeling system which in 2023 will replace North American Model (NAM), High Resolution Rapid Refresh (HRRR) and various derivatives.
- Both RRFS (Rapid Refresh Forecasting System) and RTMA are now being ported on the Cloud Platform (a joint project)
- A new, common packages for diagnostics, evaluation and visualization will be used to analyze results.
- The package will be potentially used in HWTs (Hazardous Weather Testbeds)

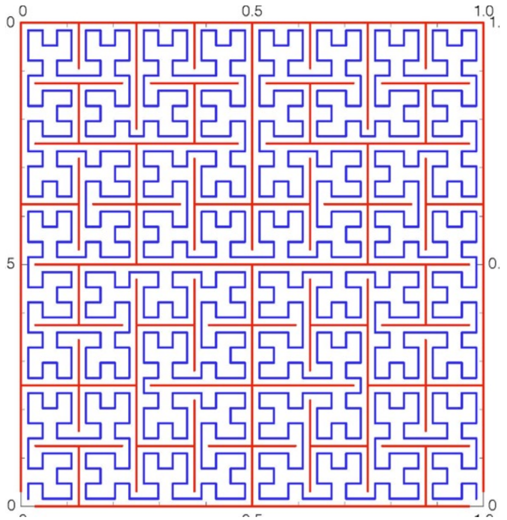


An example of new visualization of RTMA results in very early stage of development.
(Thanks to Evan Sheehan for providing this picture.)

Various other potentially useful ideas

- Preconditioning using Hilbert curves

One of the most time-consuming processes in variational analysis is the iterative minimization of the cost function. This is can be greatly accelerated if the effective condition number of the problem is somehow significantly reduced.
In the existing RTMA we have a tool, the Hilbert curve projection and sorting software, that allows observation locations to be systematically and serially ordered on a fractal "curve" parametrized so that closeness on the curve translates to geographical closeness. This property can be exploited for preconditioning.



An example of Hilbert-ordered observation space.

- Application of developed multigrid structure to speed up the conjugant gradient method (e.g., Tatebe 1993, Kang et al. 2014)

References

Gibbs, A. M., M. Pondeca, E. Colon, G. Zhao, M. Rancic, J. Purser, M. T. Morris, J. R. Carley, B. Blake, E. Rogers, and G. Gayno, 2022: 3B.4 RRFS Dynamic Downscaling in 3DRTMA. 102th Annual Meeting of American Meteorological Society, 23-27 January 2022.

Kang, Y.-H., Kwak, D. Y., and Kyungjeen, P. , 2014: Multigrid methods for improving the variational data assimilation in numerical weather prediction, Tellus A: Dynamic Meteorology and Oceanography, 66:1, 20217, DOI: 10.3402/tellusa.v66.20217

Mieruch, S., and co-authors, 2021: SalaciaML: A deep learning approach for supporting ocean data quality control. Front. Mar. Sci., April 2021, Volume 8, Article 611742. doi:10.3389/fmars.2021.611742

Pondeca, M., and co-authors, 2011: The Real-Time Mesoscale Analysis at NOAA's National Centers for Environmental Prediction: Current status and development. *WAF,* 26(5):593--612.DOI, 10.1175/WAF-D-10-05037.1

Purser, R. J., M. Rancic, M.S.F.V. De Pondeca, 2022: The Multigrid Beta function approach for modeling of background error covariance in the Real Time Mesoscale Analysis (RTMA), *Mon. Wea. Rev.,* **150,** 715-732. https://doi.org/10.1175/MWR-D-20-0405.1

Purser, R. J., Rancic, M., and De Pondeca, M., 2022: Assessing the performance of a Beta Planar Filter for anisotropic covariance modeling in a multigrid framework compared to Radial and Line forms of the filter. 8th International Symposium on Data Assimilation (ISDA), Fort Collins, Colorado, 6-10 June,2022.

Purser, R. J., Rancic, M., and De Pondeca, M., 2022: Assessing the performance of a Beta Planar Filter for anisotropic covariance modeling in a multigrid framework compared to Radial and Line forms of the filter. 8th International Symposium on Data Assimilation (ISDA), Fort Collins, Colorado, 6-10 June,2022.

Purser, R. J., *2020a: A formulation of the Hexad algorithm using the geometry of the Fano projective plane. NOAA/NCEP Office Note 499, 13 pp., https://doi.org/10.25923/xrzpx016.*

Purser, R. J., *2020b: A formulation of the Decad algorithm using the symmetries of the Galois field, GF(16). NOAA/NCEP Office Note 500, 28 pp., https://doi.org/10.25923/4nhyx681.*

Rancic, M., Purser, R. J., and De Pondeca, M., 2022a: Application of the multigrid Beta filter (MGBF) on unstructured analysis grids. 1.11. 8th International Symposium on Data Assimilation (ISDA), Fort Collins, Colorado, 6-10 June,2022.

Rancic, M., Purser, R. J., and De Pondeca, M., 2022b: Formulation of an Aspect Tensor for Inhomogeneous, Anisotropic Data Assimilations with the Multigrid Beta Filter (MGBF). 1.12. 8th International Symposium on Data Assimilation (ISDA), Fort Collins, Colorado, 6-10 June,2022.

Rancic, M., J. Purser and M. Pondeca, 2022: 15.2 Plans for Application of ML/AI within the Real Time Mesoscale Analysis (RTMA) Project. 102th Annual Meeting of American Meteorological Society, 23-27 January 2022.

Rancic, M., Purser, R. J., and De Pondeca, M., 2022: Efficiency and Scaling of the Multigrid Beta Filter for Modeling Background Error Covariance. 1-13.Research Activities in Earth System Modelling. Working Group on Numerical Experimentation. Report No. 50. WCRP Report No.12/2020. WMO, Geneva.

Tatebe, O., 1993: The Multigrid Preconditioned Conjugate Gradient Method. In Proceedings of the Sixth Copper Mountain Conference on Multigrid Methods. Copper Mountain, CO, USA, 4–9 April 1993; Melson, N.D., McCormick, S.F., Manteuffel, T.A., Eds.; NASA: Washington, DC, USA, 1993, pp. 621–634.

Wu, W.-S., R. J. Purser, and D. F. Parrish, 2002: Three-dimensional variational analysis with spatially inhomogeneous covariances. *Mon. Wea. Rev.,* **130,** 2905–2916

Yinkgai, S., and co-authors, 2021: Deep-learning-based precipitation observation quality control. *J. Atmos. Ocean. Technol.,* **38,** 1075-1091.