Current challenges and future directions in data assimilation and reanalysis

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CAPSULE: Joint WCRP-WWRP Symposium on Data Assimilation and Reanalysis

What: Scientists from the three research areas data assimilation, reanalyses and observing systems came together to discuss current progress and future challenges and to highlight the synergies between the communities.

When: 13-17 September 2021

Where: Online

1. Introduction

The first Joint WCRP[1]-WWRP[2] Symposium on Data Assimilation and Reanalysis took place on 13-17 September 2021, and it was organized in conjunction with the ECMWF Annual Seminar on observations. The last WCRP/WWRP-organized meetings were held separately for data assimilation and reanalysis in 2017 (Buizza et al. 2018; Cardinali et al. 2019). Since then, common challenges and new emerging topics have increased the need to bring these communities together to exchange new ideas and findings. Thus, a symposium involving the aforementioned communities was jointly organized by DWD[3], HErZ[4], WCRP, WWRP, and the ECMWF annual seminar. Major goals were to increase diversity, provide early career scientists with opportunities to present their work and extend their professional network, and bridge gaps between the various communities.

The online format allowed more than 500 participants from over 50 countries to meet in a virtual setting, using the gathertown [5] platform as the central tool to access the meeting. A virtual conference center was created where people could freely move around and talk to other close-by participants. A lobby served as the main hub and it connected the poster halls and the conference rooms for the oral presentations and the ECMWF seminar talks. The feedback from the participants was overwhelmingly positive.

Scientifically, the meeting offered opportunities to bring together the communities of Earth system data assimilation, reanalysis and observations to identify current challenges, seek opportunities for collaboration, and strategic planning on more integrated systems for the longer term. The contributions totalled 140 oral and over 150 poster presentations covering a large variety of topics with increased interest in Earth system approaches, machine learning and increased spatial

[1]World Climate Research Programme
[2]World Weather Research Programme
[3]German Meteorological service
[4]Hans-Ertel-Centre for Weather Research
[5]https://www.gather.town/

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resolutions. Key findings of the symposium and the ECMWF annual seminar are summarized in section 2. Section 3 highlights the common and emerging challenges of these communities.

2. Topics

a. Operational Data Assimilation and infrastructure

Many participants were affiliated with operational numerical weather prediction centers and thus a significant portion of the program focused on related updates. One common theme was moving beyond medium-range forecasts. National centers have focused their data assimilation (DA) developments on both operational coupled Earth system models and new or improved high-resolution regional systems (cf. sections c and d). Other areas of interest included the viability of higher-frequency updating and increased use of observations from the private sector (reported in sections c and e).

Several operational centers have embraced community model developments including data assimilation infrastructure, allowing more focus on scientific advancements and a significant reduction of duplication of efforts. The U.S.-based Joint Center for Satellite Data Assimilation (JCSDA), the MetOffice, NOAA, NASA, and the U.S. Navy are collaborating on the Joint Effort for Data assimilation Integration, or JEDI (Auligne T. 2021) which received a lot of attention. However, the development of generic DA infrastructure is not limited to JEDI, as additional examples were shown featuring both the Parallel Data Assimilation Framework (PDAF, Nerger L. 2021) and the Data Assimilation Research Testbed (DART, Raeder K. 2021). The progress presented at the symposium underlines the ongoing, successful efforts for collaborations among operational as well as non-operational centers.

b. Reanalysis

Since its first implementations for the atmosphere, reanalyses have expanded to include more components of the Earth system (land, ocean, sea-ice, composition) as well as regional specializations (continents, seas and the Arctic).

Reanalyses represent the synthesis between models and observations to produce the best possible Earth system representation over multiple decades while assimilating observations at small spatio-temporal scales. Global reanalyses continue to be a foundation for global climate analysis and

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research, especially where observations are limited, such as the stratosphere with the SPARC Reanalysis Intercomparison Project (S-RIP, Fujiwara M. (2021)). Continuity in space and time is a great asset for users to study an ever-growing and diversified number of applications of physical or socio-economic nature. Heatwaves (Thomas N. (2021a)), droughts (Arshad A. (2021)) or weather/climate interactions with dust (Mytilinaios M. (2021), Sara B. (2021)) and other aerosols (Franke P. (2021)) represent active research topics related to reanalyses. Further, renewable energy applications have lead to a growing interest in wind data from reanalyses (Morris M. (2021), Niermann D. (2021), Thomas N. (2021b), Spangehl T. (2021)).

Major international centers continue both forward production of existing systems and developing new projects, given the user interests. Examples of atmospheric global reanalysis systems discussed in the symposium's sessions are JRA-3Q at JMA (Kobayashi C. 2021; Kosaka Y. 2021; Harada Y. 2021; Naoe H. 2021), ERA5 and planned ERA6 at ECMWF (Hersbach H. 2021; Bell A. 2021; Munoz-Sabater J. 2021) as well as MERRA2, the planned MERRA-3 and GEOS-R21C at NASA GMAO (Bosilovich M. 2021; El-Akkraoui A. 2021). Many of these current and future full-observing system reanalyses include an ensemble component to also provide an uncertainty estimate. Further, they exhibit a progressively increased resolution for longer time periods up to three quarters of a century (e.g., 20Km JRA-3Q, 30Km ERA5). With continuing data rescue efforts (Andersson A. 2021), reconstructions of even longer periods become possible such as 20CRv3 from NOAA-CIRES-DOE (Slivinski L. 2021) reaching back to 1836. Several ocean reanalysis products were also presented, such as the CMCC Global Ocean Reanalysis System (Banerjee D. 2021) and the ECMWF ORAP6 ocean and sea-ice reanalysis (Zuo H. 2021).

Due to growing computing capabilities and ongoing research, regional reanalyses are expanding into many areas at higher resolutions. Examples covered were regional reanalysis activities at DWD (Kaspar F. 2021), the Copernicus regional reanalysis (Schimanke S. 2021), a 5-km regional reanalysis over Japan (Fukui S. 2021), the IMDAA regional reanalysis over the Indian monsoon region (Rani I. 2021), a high resolution reanalysis for the Mediterranean Sea (Aydogdu A. 2021) and a 20-year high-resolution Red Sea Reanalysis (Sanikommu S. 2021). These data sets allow for the in-depth evaluation and study of the local weather and climate, not readily captured in global systems. Further, the Arctic continues to be of interest for reanalysis efforts (e.g., C3S

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Copernicus Arctic Regional Reanalysis, Schyberg H. 2021), owing to the limited observations, changing environment and development of sea-ice and glacial representations in models.

As regional reanalyses are reaching kilometer-scale resolutions, significant interactions not only with the reanalysis producers (e.g., Kaspar F. 2021; Fourrie N. 2021), but also with the convective-scale DA community are envisaged.

c. Convective-scale Data Assimilation

While convective-scale DA (CSDA) has been a focus of NWP research and developments for a while, the interaction between CSDA and reanalysis communities is expected to continue and grow. Further, CSDA is moving beyond regional applications as global NWP approaches the kilometer scales and high-resolution observational systems such as Doppler velocities (Lippi D. (2021)) can be utilized. CSDA continues to be improved and fostered by the development of regional NWP and the inclusion of corresponding observing systems at kilometer-scales (e.g., Hu M. 2021; Carley J. 2021; Hernandez-Banos I. 2021).

The symposium included discussions on specific challenges of CSDA, such as error representation of fine-resolution observations compared to coarse-resolution simulations, multi-scale and non-Gaussian errors, and model errors that contribute to nonlinear error growth. Assimilating observations at CSDA scales, such as radar, satellite, and lightning observations, can improve analyses and forecasts (Miyoshi T. 2021; Combarnous P. 2021; Deppisch T. 2021). Further, innovative observations, such as crowd-sourced data, have also shown promising results (Paschalidi Z. 2021, and presentations in section e).

Convective-scale dynamics are driven by instabilities that require increased spatial resolutions O(0.1-1 km) and temporal resolution from hours to minutes. For non-linear regimes, non-Gaussianity can become more severe, leading to suboptimal solutions in ensemble filters conditioned on Bayesian assumptions. In this regard, advanced DA strategies, like nowcasting objects, grafting look-alike storms, and warm bubbles, were proposed (Neef L. 2021; Sodhi J. 2021; Janjic T. 2021).

Another strategy that has proven to be effective is the use of high-frequency observations through smaller perturbations and more linear error growth (Ruiz J. 2021). Along these lines Miyoshi T. (2021) assimilated phased-array radar observations every 30s with 1000 ensemble-members and

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at 500m spatial resolution in real-time. Advances have also been reported for non-Gaussian DA algorithms which may bring significant benefits for CSDA in years to come (see section d for more details)

A major issue for high-resolution observations are significant observation error correlations. Yang X. (2021) investigated this effect in Doppler velocities and found that including these correlations explicitly improves the representation of extreme precipitation events. Similar positive impacts have been reported by Fujita T. (2021). To represent model errors in CSDA, other strategies were also proposed, including additive noise, uncertainties in physical parameterizations, and errors resulting from unresolved scales (Janjic T. 2021; Waller J. 2021).

Further, multi-scale features of CSDA can be addressed by blending algorithms that combine large- and small-scale analyses from a global model and a regional model (Schwartz C. 2021). In addition, adaptive localization approaches including scale-dependent localization, variable-dependent localization, and correlation-dependent localization as well as the impact of large ensembles on localization were discussed (Wang H. 2021; Necker T. 2021; Duc L. 2021).

d. Data Assimilation developments

A wide variety of topics were presented in the broader area of methodological advances in DA, from the ongoing research of ensemble approaches to machine learning methods to coupled systems. As in previous symposia, there were submissions focusing on more theoretical aspects of the DA generally split between algorithms and information flow. For NWP applications, Kalman filters were very present in ensemble DA (e.g., Pannekoucke O. (2021) with the parametric Kalman filter, Raboudi N. (2021) with the time-dependent observation noise inclusion or Wang X. (2021) with the multi-scale local Gain Form Ensemble Transform). Also, hybrid DA algorithms were popular with applications such as integrated hybrid EnKF (Lei L. 2021) or a 20-year eddy-resolving reanalysis for the Red Sea (Sanikommu S. 2021). Further, the non-Gaussian DA algorithms presented include non-Gaussian hybrid data assimilation (e.g., the Maximum Likelihood Ensemble Filter Fletcher S. 2021), non-Gaussian observation errors (Hu C. 2021), and particle filters. The latter approach continues to show great progress and potential as it is transitioned to more complex model applications. Examples of particle filters were given by, Schenk N. (2021) with a 4D-localized version, Feng J. (2021) with an improved local non-linear ensemble transform filter, Kawabata T.

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(2021) with an implementation of non-Gaussian assimilation methods for error estimation at the convective-scale, and Kotsuki S. (2021) who showed increased stability for a local particle filter with a Gaussian mixture extension in intermediate global circulation model.

The emergence of machine learning (ML) and deep learning (DL) techniques in recent years were also visible at the symposium. The major aim was to use ML to support specific DA aspects, accelerate/improve parts of the DA or to address model errors and parameter uncertainties. ML was used to support computationally expensive traditional DA methods by Barthelemy S. (2021), who proposed to use a neural-network to emulate a high-resolution background from a low-resolution NWP. Further, ML was employed to improve error estimates (e.g., Farchi A. 2021) or ensure more consistent error models also in non-Gaussian DA (Hossen M. 2021). The more classical ML use of model parameter estimation was addressed by Legler S. (2021) in a shallow-water convective-scale model, or Bocquet M. (2021), who used the dual EnKF to learn the state, global and local parameters based on either covariance or domain localisation.

Coupled DA in Earth system models was discussed with respect to strengths and current limitations. Bhargava K. (2021) showed the benefit of weakly-coupled atmosphere-ocean SST assimilation, Reichle R. (2021) presented atmosphere-land DA with the assimilation of SMAP brightness temperature, Kleist D. (2021) detailed the recent and future updates for weakly-coupled DA in the NOAA GFS, and O'kane T. (2021) showed a 60-years retrospective product using a strongly-coupled DA with ocean-sea ice and biogeochemistry components. Other work presented focused on the important topic of coupled covariances within the different Earth system compartments (e.g., Tang Q. 2021; Smith P. 2021). Several authors mentioned the problems of underdispersed land ensembles (e.g., Reichle R. 2021), with Draper C. (2021) presenting vegetation and soil parameter perturbations as a possible way forward. Several authors also outlined methodological considerations of the choices between strongly and weakly coupled DA, e.g., different timescales in the components (de Rosnay 2021) or tuning of the pre-existing system degrading overall efficacy of coupled model state estimates (Reichle R. 2021).

Some contributions highlighted issues of assimilating new spatial observations in coupled DA (for more on observations, refer to section e). However, neglecting new observing systems in one compartment may imply benefits to other quantities. In fact, the assimilation of surface temperatures for the ocean (While J. 2021) and land (Valmassoi A. 2021) show an improvement in

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the assimilated variable, but also an increase in biases in other parts of the system, respectively at the base of the ocean mixed layer and the 2-meter temperature.

e. Observations

A more detailed look at the state of observations for Earth system sciences was enabled by the joint aspects of the symposium with the concurrent ECMWF Annual Seminar, where recent Observing System Experiment results were shown for different Earth System components (Bormann 2021; Remy 2021; Kolassa 2021). Advances in data assimilation are enabling an even better utilization of observations, as exemplified by Laloyaux (2021) (estimating model error) and Prigent (2021) (surface observations). Whilst observations for non-atmospheric components of the Earth System do not yet, in general, fully meet requirements, encouraging progress was reported for land, ocean, sea-ice, snow and composition by several Annual Seminar speakers (Inness 2021; Benedetti 2021; Charlton-Perez 2021).

Several presentations in the symposium discussed new or not yet fully exploited satellite observations. The assimilation of targeted geostationary hyperspectral sounder observations with high temporal resolution was shown to be beneficial for typhoon forecasts (Han W. 2021) and visible satellite channels improved convective scale cloud and radiation forecasts (Scheck L. 2021). Chandramouli K. (2021) presented an online method for estimating nonlinear biases to improve the assimilation of all-sky satellite observations. The rising number and importance of GNSS observations was noted by (Bormann 2021), while impressive results with the Aeolus research mission was shown as well (Koepken-Watts 2021). Aeolus lidar wind observations revealed to be in good agreement with ECCC forecasts and ERA5 reanalyses (Chou C. 2021) with their assimilation in NWP exhibiting a significant positive impact at DWD (Cress A. 2021).Contributions also addressed the potential impacts on planned satellite missions such as the Meteosat Third Generation (MTG) and the potential for assimilation of the flash extent accumulation (Combarnous P. 2021) or infrared and microwave channels (Villeneuve E. 2021).

While 99% of observations assimilated in global NWP are from satellites (English 2021), multiple speakers at the ECMWF annual seminar noted that in situ observations remain very important, not least for the earth's surface (Siddorn 2021; Ingleby 2021; Sandells 2021, e.g.). Recent developments using ground-based remote sensing in data assimilation were presented, especially to characterize

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the state of the atmospheric boundary layer. Here, an observation gap - especially for temperature, humidity and wind profiles - remains, as satellites are not able to resolve the ABL to the required extent. Ceilometers, Doppler lidars (Kayser M. 2021) and microwave radiometers (Knist C. 2021) were shown to be on their way to becoming operationally assimilated. For Doppler lidar networks, Nomokonova T. (2021) showed significant potential for short term wind forecasts in the ABL, especially at wind turbine hub-heights, with Observation System Simulation Experiments (OSSEs). Further, the EU COST action PROBE[6] (Profiling the Atmospheric Boundary Layer at European Scale, Loehnert U. 2021) is coordinating efforts to set standards (Lehmann V. 2021) and exploit (Merker C. 2021) newly organized ground-based remote sensing networks for data assimilation applications.

There is also a rising interest in the assimilation of crowd sourced or otherwise non-conventional observations, which are inexpensive, but may require more effort for quality control and bias correction. It was demonstrated that assimilating bias-corrected temperature and humidity observations from citizen weather stations leads to significant improvements in the first six forecast hours (Paschalidi Z. 2021). Vehicle-based sensor measurements (Acevedo W. 2021; Dance S. 2021) and commercial wind turbine data (Kelbch A. 2021) were also discussed as promising observations for data assimilation and reanalysis.

The seminar reflected a large, growing and increasingly diverse global observing system. With this increase of complexity, the number of observation anomalies also increases making quality control and cross calibration very important (Dahoui 2021; Zhang 2021; Bathmann 2021). A more continuous approach to data screening and assimilation may enable some problems to be spotted early (Lean 2021). Waller (2021) highlighted the need of a more detailed look at sources of observations' error correlation, notably the spatial one. The seminar presented also the expected future evolution of both the space sector (Coppens 2021; Donlon 2021; Donoho 2021) and in situ observations (Randriamampianina 2021).

3. Conclusions and remarks

Through its design, the first Joint WCRP-WWRP Symposium on Data Assimilation and Reanalysis together with the ECMWF annual seminar on observations allowed for the three scientific

[6]www.probe-cost.eu

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communities to come closer together highlighting the impressive progress and addressing common challenges.

A major theme of the symposium was a trend towards the consolidation of data assimilation efforts with respect to shared infrastructure. With the increasingly growing complexity of current DA, such approaches aim to share the costs and split the efforts for achieving progress without significant increases in expenses by facilitating collaboration and exploiting synergies in operational centers and research institutes. Therefore, the successful use of observation types and methodological advances can be accelerated. However, we also found that these efforts are not at its goal, as a major recommendation from the symposium was the need for data-sharing infrastructure to facilitate expensive experiments that now only a few centers are able to implement.

As model resolutions in global NWP and reanalysis is constantly increasing, the need for methods to appropriately and efficiently handle the assimilation of data at multiple spatio-temporal scales is growing further. Issues formerly related only to limited area models are becoming more relevant also for global DA, such as multi-scale features, non-Gaussian error distributions, and the model errors which contribute to fast error saturation. To tackle these challenges, several algorithms have been proposed and successfully applied. In particular, efficient non-Gaussian methods such as localized particle filters have been rapidly maturing in recent years, and may soon begin to replace the first variational- or Kalman filter-based assimilation systems.

Further, machine learning methods are being introduced to the DA community at an astonishing speed with many promising results. However, more research is required to more fully exploit these techniques and to address the high-dimensional problems for which inexpensive solutions are needed, such as the estimation of complex model errors or observation error covariances.

The advances in data assimilation are enabling an even better utilization of observations, both in their characterization and in high-frequency assimilation. Several contributions have demonstrated that there is a significant potential for new observations and under-utilized remote sensing data to be exploited in data assimilation especially at the convective scale and through exploitation of "all-surface/all-sky" radiance assimilation within the context of coupled DA.

The popularity of reanalysis is continuing to increase, due to its invaluable contribution to climate monitoring and weather forecasting as well as in research and the commercial sector, and with new fields of applications still emerging. The applications are not limited to atmospheric-related

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events, since several products are available for the ocean, land surface, atmospheric composition and cryosphere. Reanalyses are continuously improved not only by increasing their spatial resolution and assimilating more observing systems/observations types, but also by extending them from atmosphere-focused products to a more complete Earth system. Events such as this symposium help to bridge the gaps between different reanalyses, working toward the plan to provide coupled products in the coming years (e.g., ECMWF and NASA).

Coupled Earth system modeling and assimilation is also becoming more prevalent both in research and operational applications related to NWP, especially in connection with the pursuit of seamless prediction systems. The associated multi-scale challenges have to be addressed in DA: be it the necessity to adapt the algorithms to include observing systems for other Earth system components, the need for weakly or strongly coupled DA, or the challenges of properly initializing each component of the Earth system. In this regard, a close collaboration between NWP and reanalysis communities is essential to exploit existing and future synergies.

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Data availability statement. The presentations of the Joint Symposium can be accessed at `https://www.dwd.de/EN/specialusers/research_education/seminar/2021/wcrp_wwrp_symposium/wcrp_wwrp_symposium_en_node.html`. A summary of the Annual Seminar is available on the ECMWF website at `https://www.ecmwf.int/en/about/media-centre/news/2021/annual-seminar-looks-earth-system-observations`.

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