Assimilation of Compact Phase Space Retrievals (CPSRs): Comparison with Independent FRAPPE, IAGOS, and IASI Observations and Assimilation of Retrieval Partial Profiles

> Arthur P. Mizzi^{*}, David Edwards^{*}, and Jeffrey Anderson[#] (mizzi@ucar.edu)

> 8th International Workshop on Air Quality Forecasting Research January 10 – 12, 2017 Toronto, ON Canada

* NCAR/Atmospheric Chemistry Observations and Modeling Laboratory, Boulder, CO
NCAR/Institute for Mathematics Applied to Geosciences, Boulder, CO

IWAQFR 2017 Toronto, ON Canada



Overview

- ➤ WRF-Chem/DART (FRAPPE and 2008 Case).
- Compact phase space retrievals (CPSRs) and extension to truncated retrieval profiles.
- Comparison with independent FRAPPE, IAGOS and IASI observations.
- > Dependence on form of the retrieval forward operator.
- ➢ Summary and Conclusions.



WRF-Chem/DART: Overview

IWAQFR 2017 Toronto, ON Canada



WRF-Chem/DART

- WRF-Chem/DART a regional chemical weather forecast/ensemble data assimilation system (ensemble adjustment Kalman filter) developed by NCAR/ACOM and NCAR/IMAGe.
- WRF-Chem the Weather Research and Forecasting (WRF) model with online chemistry.
- DART the Data Assimilation Research Testbed (a flexible software environment for exploring different ensemble data assimilation methods, models, and observations.



WRF-Chem/DART cont.

> WRF-Chem/DART:

- ✓ Assimilate MOPITT and IASI CO total and partial column retrievals, IASI O₃ total and partial column retrievals (under development), OMI total column NO₂ retrievals (under testing), MODIS total column AOD retrievals, and AirNow *in situ* observations.
- ✓ Assimilate partial column retrievals as raw (RETRs), quasi-optimal (QORs), and compact phase space retrievals (CPSRs).
- ✓ State variable localization to enable joint, independent, and specified correlation assimilation of chemistry observations.
- ✓ Uses State Augmentation Method (SAM) to obtain emission updates from assimilation of chemistry observations.
- ✓ Real-time scripting system.



WRF-Chem/DART cont.

> WRF-Chem/DART:

- ✓ Being applied to 2008 Case Study (NCAR/ACOM Mizzi, Arellano, Edwards, and Anderson); FRAPPE/DiscoverAQ (NCAR/ACOM – Mizzi, Pfister, and Edwards; UC-Berkley – Cohen and Liu), and PANDA (NCAR/ACOM – Mizzi and MPI-M – Brasseur and Bouarar).
- ✓ 2008 Case Study CONUS domain with western extension 100 km (101x41x34) resolution; 20-member ensemble; June 1− 30, 2008; assimilate MOPITT and IASI CO and MODIS AOD.
- ✓ PANDA Central and East Asia nested domain with 60 km (150x112x37) and 20 km (148x157x37) resolutions; 10-member ensemble; assimilation on coarse grid; quasi-real time; assimilate MOPITT (development and testing).



WRF-Chem/DART cont.

> WRF-Chem/DART cont:

✓ FRAPPE – Western US nested domain with 15 km (180x140x37) and 3 km (321x291x37) resolutions; data assimilation on coarse grid; July 14 – August 3, 2014; 30-member ensemble; assimilate MOPITT CO; real time scripting.



FRAPPE/Discover-AQ Observation Domain

IWAQFR 2017 Toronto, ON Canada



Compact Phase Space Retrievals (CPRS): Extension to Truncated **Retrieval Profiles**

IWAQFR 2017 Toronto, ON Canada



CPSRs: Full Retrieval Profiles

- $> y_r = Ay_t + (I A)y_a + ε \implies y_r (I A)y_a ε = Ay_t$ where A is singular and its leading left singular vectors span its range.
- Project the quasi-optimal retrieval onto the leading left singular vectors of A: data compression step.
- That transform reduces the number of observations from the dimension of the retrieval profile to the number of non-zero singular values.
- ➤ The transformed E²_m is non-diagonal: use an SVD diagonalization (Anderson, 2003; Migliorini et al., 2008): diagonalization step.
- ▶ 1st SVD: A = ΩΣΨ^T = Ω₀Σ₀Ψ^T₀ Compression Transform; 2nd SVD: Ω^T₀E²_mΩ₀ = ΠΛΘ^T - Diagonalization Transform; Assimilate CPSRs:

$$\Pi^T \Lambda^{-1/2} \Omega_0^T (y_r - (I - A)y_a - \varepsilon) = \Pi^T \Lambda^{-1/2} \Sigma_0 \Psi_0^T y_t.$$



CPSRs: Extension to Truncated Retrieval Profiles

≻ Mizzi et al. (2017a):

$$y_r - (I - A)y_a - \epsilon = Ay_t$$

- ✓ Discard *m* elements of y_r . The resulting dimension is n m.
- ✓ Discard the corresponding rows of *A*, and the corresponding rows and columns of E_m (resulting dimension $(n m) \times (n m)$).
- ✓ A was a square n × n matrix. It is now a rectangular (n − m) × n matrix. Thus, assimilation of retrieval partial profiles is called "CPSRs applied to rectangular systems."
- ✓ The rest of the derivation follows Mizzi et al. (2016) due to their use of SVDs for the "compression" and "diagonalization" transformations.



Comparison with Independent Observations (IASI, IAGOS/ MOZAIC, and FRAPPE)

IWAQFR 2017 Toronto, ON Canada



2008 Case Study: (June 19, 2008 18 UTC)





Comparison with MOPITT CO



NCA

13

IWAQFR 2017 Toronto, ON Canada

Vertical Profiles (Full Retrieval Profiles)



IWAQFR 2017 Toronto, ON Canada



2008 Case Study: Forecast Verification





FRAPPE Results (July 14 – August 3, 2014)



IWAQFR 2017 Toronto, ON Canada



FRAPPE Results (July 29, 2014)



IWAQFR 2017 Toronto, ON Canada



FRAPPE/MOPITT CO Results (July 29, 2014)



IWAQFR 2017 Toronto, ON Canada



Dependence on Form of the Retrieval Forward Operator

IWAQFR 2017 Toronto, ON Canada



Dependence on the Retrieval Forward Operator

MOPITT DOFS Histograms



IWAQFR 2017 Toronto, ON Canada



Dependence on the Retrieval Forward Operator



IWAQFR 2017 Toronto, ON Canada



Summary and Conclusions

IWAQFR 2017 Toronto, ON Canada



Summary and Conclusions

- Extended CPSRs to assimilation of truncated retrieval profiles to enable discarding of elements with known errors.
- Comparison of MOPITT CPSR CO assimilation/forecasts with 2008 Case IASI partial column CO retrievals, IAGOS/MOZAIC *in situ* CO, and FRAPPE *in situ* CO confirms that CPSRs improve the fit/skill (~80%) at a computational cost reduction (30% 50%) compared to assimilation of raw or quasi-optimal retrievals.
- CPSRs can be applied to any partial column retrieval obtained through optimal estimation. Has implications to assimilation of total column retrievals.
- CPSRs successfully applied to joint assimilation (MOPITT and IASI CO CPSRs; MOPITT/IASI CO CPSRs and MODIS AOD RETRs) and emission estimation (MOPITT and IASI CO CPSRs, MODIS AOD RETRs to estimate dust and fire emissions).
- Analysis of different retrieval forward operators shows that averaging kernel sensitivities, and therefore assimilation/forecast results, depend on the form of the forward operator.



References

- Mizzi, A. P., A. F. Arellano, D. P. Edwards, J.L. Anderson, and G. G. Pfister: Assimilating compact phase space retrievals of atmospheric composition with WRF-Chem/DART: A regional chemical transport/ensemble Kalman filter data assimilation system. *Geosci. Model Dev.*, 9, 1-14, 2016.
- Mizzi, A. P., D. P. Edwards, and J. L. Anderson: Assimilating compact phase space retrievals (CPSRs): Comparison with independent observations (MOZAIC in situ and IASI retrievals) and extension to assimilation of retrieval partial profiles. [*under internal review*], 2017a.
- Mizzi, A. P., X. Liu, A. F. Arellano, J. Liang, R. C. Cohen, Y. Chen, D. P. Edwards, and J. L. Anderson: Assimilating compact phase space retrievals (CPSRs): Joint assimilation of MOPITT and IASI CO as CPSRs and MODIS AOD as raw retrievals with constrained emissions. [*in preparation*], 2017b.





IWAQFR 2017 Toronto, ON Canada



Extra Slides (2008 Case – IASI CO Comparisons)

IWAQFR 2017 Toronto, ON Canada



Comparison with IASI CO



CPSR Extension to Retrieval Partial Profiles



CPSR Extension to Truncated Retrieval Profiles



IWAQFR 2017 Toronto, ON Canada

