GPS Radio Occultation Observation Operators for NWP Models

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Overview

- Characteristics of GPS radio occultation observations
- Assimilation of GPS radio occultation data—which data product?
- Brief description of different observation operators
- Relations between some of the operators
- Summary and prospects

Characteristics of GPS occultation data

- Limb sounding geometry complementary to ground and space nadir viewing instruments
- High accuracy
- High vertical resolution
- Basically unaffected by aerosols, clouds and precipitation
- Requires no first guess sounding
- No instrumental drift

Assimilating occultation data into NWP

Challenges and potential problems:

- GPS radio occultation data (phase, amplitude, bending angle, refractivity) are non-traditional meteorological measurements (e.g., wind, temperature, moisture, pressure)
- The long ray-path limb sounding measurement characteristics are very different from the traditional meteorological measurements (e.g., radiosonde) or the nadir-viewing passive microwave/IR measurements
- The GPS radio occultation measurements are subject to various sources of errors (e.g., residual ionospheric effects, tracking errors, super refraction, use of climatology at the upper boundary,. . .)

Assimilating occultation data into NWP

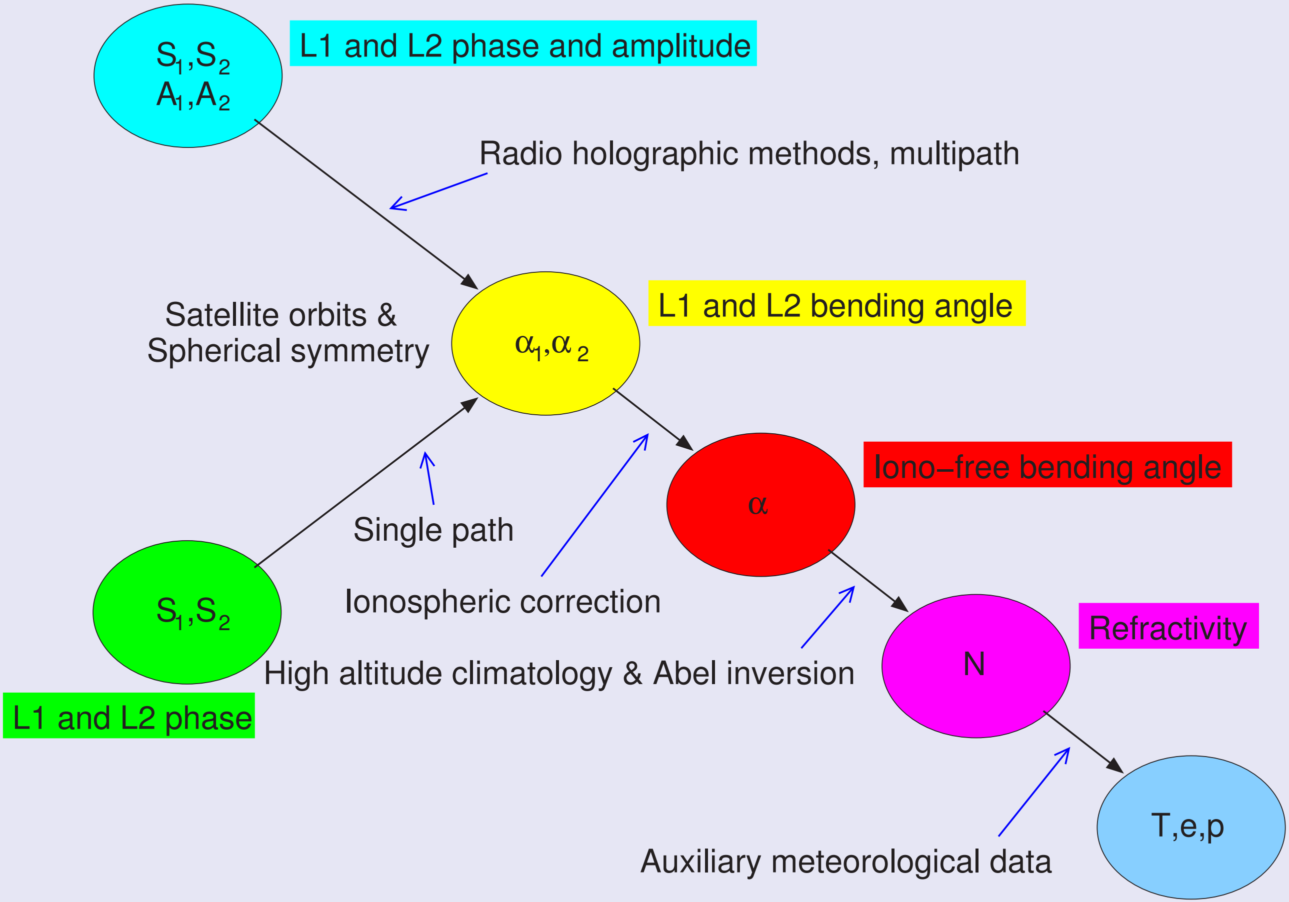
The purpose of data assimilation is to extract the maximum information content of the data, and to use this information to improve analysis of model state variables (u, v, T, q, p,$\ldots$).

Minimization of a cost function (objective function):

$$J(\mathbf{x}) = (\mathbf{x}-\mathbf{x}_{\mathrm{b}})^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_{\mathrm{b}})+(\mathbf{y}-\mathbf{H}(\mathbf{x}))^{\mathrm{T}}(\mathbf{O}+\mathbf{F})^{-1}(\mathbf{y}-\mathbf{H}(\mathbf{x}))$$

- Here we concentrate on the red part, in particular the observation operator $\mathbf{H}$

GPS RO measurements & processing



S_1,S_2 A_1,A_2

L1 and L2 phase and amplitude

Radio holographic methods, multipath

α_1,α_2

L1 and L2 bending angle

Satellite orbits & Spherical symmetry

α

Iono–free bending angle

Single path

S_1,S_2

L1 and L2 phase

Ionospheric correction

N

Refractivity

High altitude climatology & Abel inversion

T,e,p

Auxiliary meteorological data

Choice of Assimilation Variable

Should consider the following factors:

- Use the raw form of the data to the extent possible (based on the philosophy that the less processing the better; let your NWP model provide the a priori that is needed via the observation operator)
- Ease to model the observables (and the adjoint)
- The need for auxiliary information (before the assimilation of the data)
- Ease to characterize observation (measurement) errors
- Ease to characterize observation operator (representativeness) errors
- Computational cost

Representativeness errors

Errors of representativeness arise from two sources (Schlatter 2000):

1. The limited resolution of the NWP model
2. The inability of the observation operator to derive a perfect measurement from a perfect model state

- When I talk about representativeness errors, I (most often) mean the latter (also referred to as forward modeling errors by some)
- Depending on the observation operator and the resolution of the NWP model, (1) may be more important than (2), but if we have a high enough model resolution (perhaps better than $\sim$100 km horizontally) then (2) may be more important than (1)
- For less sophisticated data assimilation than 4DVar, there may also be a temporal misrepresentation of the data which I will not address

Assimilation of phases and amplitudes

Pros

- (Al)most "raw" form of the data
- No assumptions are used
- Easy to characterize measurement errors

Not practical

Cons

- Observation operator needs to be able to model wave propagation (diffraction and multipath) inside weather models
- Require precise GPS and LEO satellite orbit information
- Require ionospheric model to account for ionospheric delays (we do not have very accurate ionospheric models)
- Computationally very expensive

Assimilation of L1 and L2 bending angles

Pros

- Second most "raw" form of the data
- Does not require precise orbit information
- Relatively easy to characterize measurement errors (may be challenging for lower troposphere)

Not practical

Cons

- Assumption of spherical symmetry introduced in the processing
- Need to consider uncertainty in the "independent" variable (impact parameter) which is derived from observations
- Require ionospheric model to account for ionospheric bending
- Computationally expensive

Assimilation of iono-free bending angles

Pros

- Still quite close to the "raw" form of the data
- Does not require precise orbit information
- Does not require ionospheric model, but still extrapolation above the uppermost NWP level
- Reasonably easy to characterize measurement errors (may be challenging for lower troposphere)

A possible choice

Cons

- Assumption of spherical symmetry introduced in the processing
- Need to consider uncertainty in the "independent" variable (impact parameter) which is derived from observations
- Residual ionospheric observation error
- May be computationally expensive (ray tracing)

Assimilation of atmospheric refractivity

Pros

- Simple observation operator (local operator on model variables)
- Does not require precise orbit information
- Does not require extrapolation above the uppermost NWP level
- Less sensitive to uncertainty in independent variable (height)
- Computationally inexpensive (operationally feasible)

A possible choice

Cons

- Interpreting retrieved profile as model local refractivity
- Residual ionospheric observation error
- Requires initialization by climatology for upper boundary
- Representativeness errors include effects of horizontal refractivity gradients
- Bias in lower troposphere due to super refraction

Assimilation of retrieved T, q, and/or p

Pros

- Requires little or no work in the development of observation operator (as T, q, and p are model state variables)
- The retrieved data can be assimilated by simple analysis or assimilation methods (e.g., nudging)
- Computationally inexpensive

Not an optimal choice

Cons

- Far from the “raw” data
- Auxiliary information is needed for retrieval (e.g., 1DVar), and additional errors are introduced
- Representativeness errors must include effects of horizontal refractivity gradients
- Errors in retrieved T, q, and p are correlated
- Bias in lower troposphere due to super refraction

Local refractivity observation operator

Observation operator based on the refractivity equation:

$$N \approx 77.6\frac{p}{T} + 3.73 \times 10^{5}\frac{e}{T^{2}}$$

- Refractivity is obtained from model state variables interpolated to the location of the retrieved profile
- May also include hydrostatic integration and conversion to geometrical height levels
- The observation operator does not represent very well how the data are collected and how they are processed using the spherical symmetry assumption
- Errors of representativeness dominate below 25–30 km by not taking into account the horizontal gradients
- Assimilation using CHAMP data show positive impact (Healy 2005)

Local bending angle observation operator

Assuming spherical symmetry:

$$\alpha(a) = -2a \int_{r_0}^{\infty} \frac{\mathrm{d}\ln n/\mathrm{d}r}{\sqrt{n^2 r^2 - a^2}} \mathrm{d}r$$

- Operator consists of the same steps as included in a local refractivity observation operator + the *forward* Abel transform
- One may have to extrapolate the NWP above it's highest level
- The observation operator may become significantly non-linear in the lower troposphere via the relation $a = r_0 n(r_0)$ (because the independent variable a becomes a function of the model state)
- Errors of representativeness dominate below 25–30 km by not taking into account the horizontal gradients (same problem as with local refractivity)
- Main advantage: avoids the introduction of climatology at high altitudes in the retrieval

2D ray tracing bending angle operators

Observation operator based on ray tracing (e.g., Zou et al. 1999, Gorbunov 2003):

$$\frac{\mathrm{d}\vec{r}}{\mathrm{d}\tau} = \vec{n}\,, \qquad \frac{\mathrm{d}\vec{n}}{\mathrm{d}\tau} = n\nabla n$$

- Calculation of the ray path through the atmosphere (a good representation of how the data are collected)
- Across-ray horizontal gradients are neglected
- Non-linear because the ray path depend on the model state
- Observation operator includes interpolation of the NWP model variables into the 2D occultation plane
- Main advantage: takes into account most of the influence from horizontal gradients (although limited by the horizontal resolution of the NWP model)
- Main disadvantage: ray tracing is computationally expensive

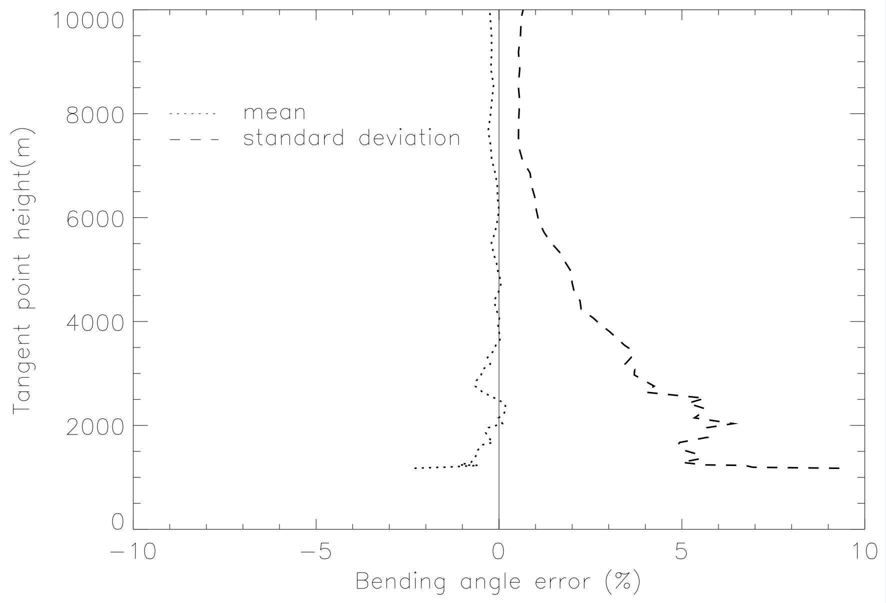
Alternatives to ray tracing

Bending angle integration (2D operator):

$$\mathrm{d}\alpha = -\frac{1}{n}\left(\frac{\partial n}{\partial r}\right)_{\theta} r\,\mathrm{d}\theta + \frac{1}{n}\left(\frac{\partial n}{\partial \theta}\right)_{r} \frac{\mathrm{d}r}{r}$$

- Can be derived from the ray tracing equations
- Suggested by Eyre (1994)
- Second term is small and can be ignored (Healy 2001)
- Impact parameter and tangent point height related via $a = r_0 n(r_0)$
- Observation operator still includes interpolation of the NWP model variables into the 2D occultation plane
- Main advantage: faster and simpler than ray tracing
- Main disadvantage: uncertainty in the estimated impact parameter

Error of bending angle integration operator



(Healy et al. 2003)

- Be aware: fractional errors in bending angle are significantly larger than corresponding errors in refractivity (perhaps a factor of 5 or so near the surface)
- Does not mean that assimilation of refractivity would be 5 times better

Alternatives to ray tracing

Fast Atmospheric Refractivity Gradient Operator (FARGO) (Poli 2005)

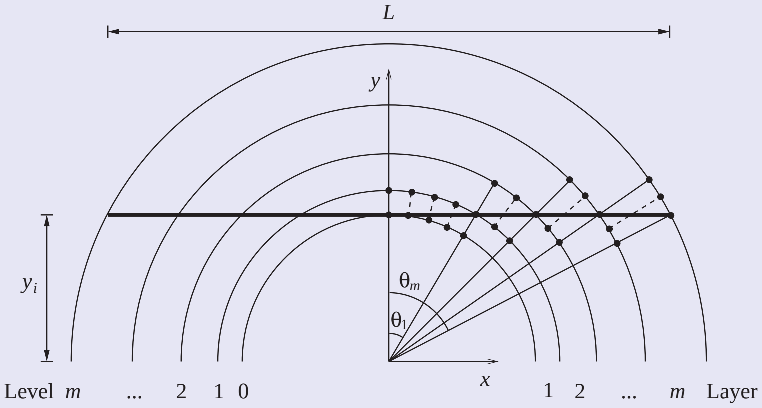
- FARGO-α: $\alpha_{\mathrm{FARGO}} = \alpha_{\mathrm{local}} - \Delta\alpha_{\mathrm{FARGO}}$
  - α_{local} is the forward Abel transform of N_{local}
  - $\Delta\alpha_{\mathrm{FARGO}}$ is a small correction term:

$$\Delta\alpha_{\mathrm{FARGO}} = \int_{\mathrm{path}} \cos\theta \left[\frac{\mathrm{d}n}{\mathrm{d}r}(r,\theta) - \frac{\mathrm{d}n}{\mathrm{d}r}(r,\theta=0)\right]\mathrm{d}s$$

  - path is determined by spherically symmetrical ray tracing restricted to ± 600 km centered at the tangent point
- FARGO-α is quite similar to bending angle integration
- FARGO-N: $N_{\mathrm{FARGO}} = N_{\mathrm{local}} - \mathrm{Abel}_{\mathrm{inverse}}(\Delta\alpha_{\mathrm{FARGO}})$

Forward-inverse refractivity mapping

(Syndergaard et al. 2003, 2005)



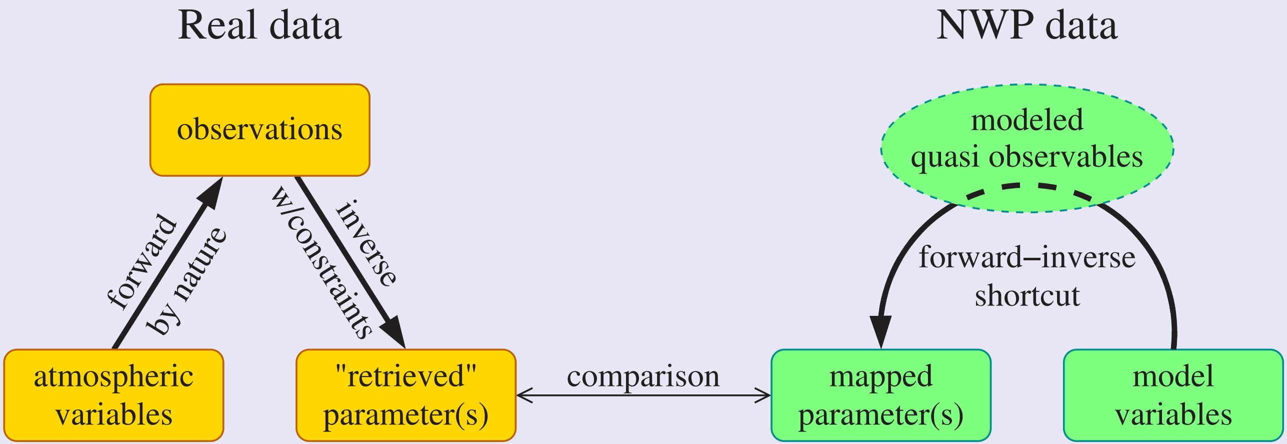
Mimicking the observations and the Abel inversion using finite straight lines

Somewhat similar to a 2D weighting function (Ahmad and Tyler 1998)

Basic requirement: $$\int_{-L/2}^{L/2} N(x,y)\mathrm{d}x = \int_{-L/2}^{L/2} \bar{N}(r)\mathrm{d}x$$

- Discretized and solved for $\bar{N}(r)$ → $\bar{\mathbf{N}} = \mathbf{AVN}$
- $N(x,y)$ evaluated at (pressure) levels of NWP model

Forward-inverse refractivity mapping


Real data

NWP data

observations

forward

by nature

inverse

w/constraints

atmospheric variables

"retrieved" parameter(s)

comparison

modeled quasi observables

forward–inverse shortcut

mapped parameter(s)

model variables

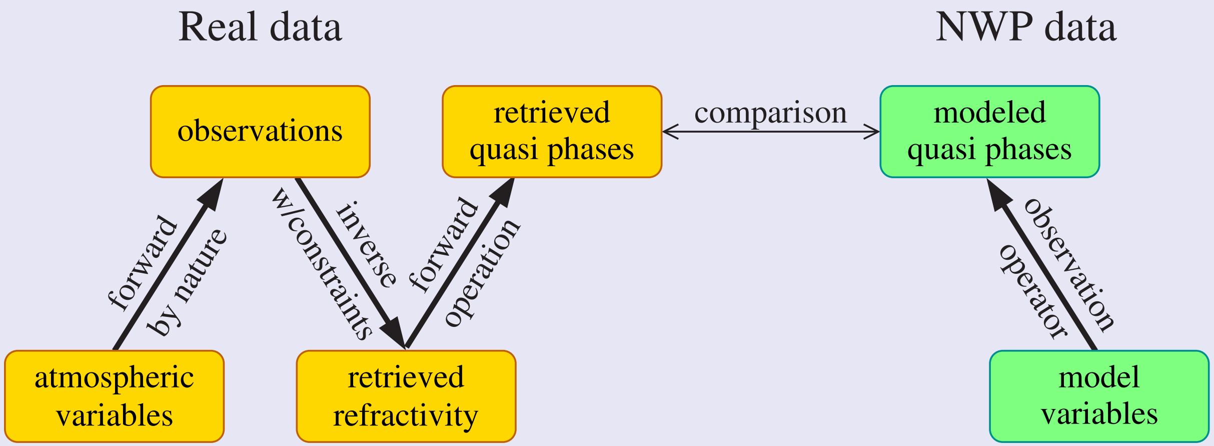
- Because of the forward-inverse shortcut: near cancellation of otherwise crude approximations (e.g., use of straight lines)
- Because of the forward-inverse shortcut: fast, but still quite accurate
- Useful for all kinds of occultation measurements (absorption too)

Example of observation operator

1. Horizontal interpolation (along pressure surfaces) of the temperature and specific humidity to the points used in the mapping
2. Evaluation of the refractivity at these points
3. Mapping the refractivity into a profile at the tangent points using the mapping operator
4. Integration of the hydrostatic equation to obtain a precise relation between pressure and geometric height at grid points near the tangent points
5. Horizontal interpolation of the geometric height to the tangent point locations
6. Vertical interpolation of the mapped refractivity to the observation points (observed tangent points)

Quasi-phase observation operator

Introduced by (Sokolovskiy et al. 2005)



Real data

NWP data

observations

retrieved quasi phases

comparison

modeled quasi phases

forward by nature

w/constraints inverse

forward operation

observation operator

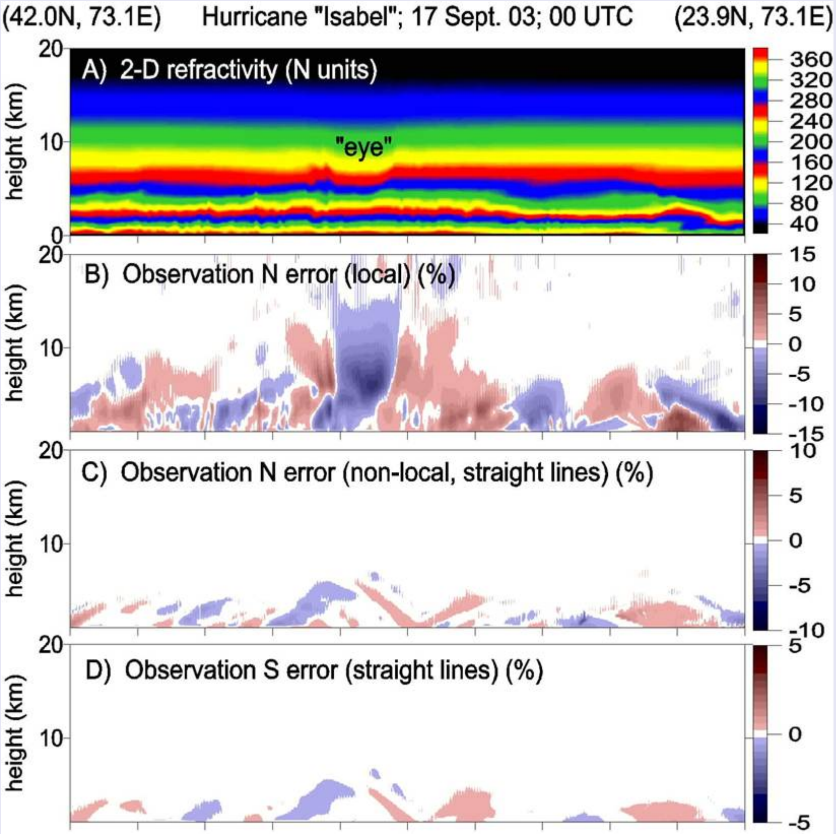
atmospheric variables

retrieved refractivity

model variables

- Same advantages as refractivity mapping
- Simpler implementation of observation operator
- Extra step on the retrieval side
- Different representativeness and observation error covariances

Simulation of representativeness errors

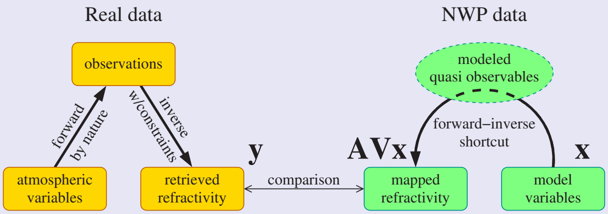


(Sokolovskiy et al. 2005)

Mapping operator vs. phase operator

$$\nabla_{\mathrm{x}} J = \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_{\mathrm{b}}) + \mathbf{H}^{\mathrm{T}}(\mathbf{O}+\mathbf{F})^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y})$$

refractivity mapping operator



Real data

NWP data

observations

modeled quasi observables

forward by nature

w/constraints inverse

$\mathbf{y}$

$\mathbf{AVx}$

forward–inverse shortcut

$\mathbf{x}$

atmospheric variables

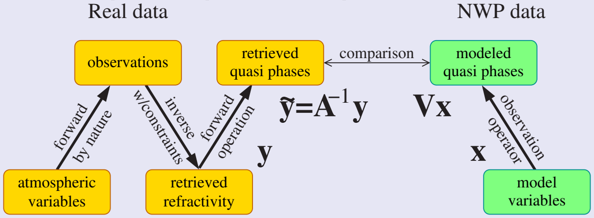
retrieved refractivity

comparison

mapped refractivity

model variables

quasi-phase operator



Real data

NWP data

observations

retrieved quasi phases

comparison

modeled quasi phases

forward by nature

w/constraints inverse

forward operation

$\tilde{\mathbf{y}}=\mathbf{A}^{-1}\mathbf{y}$

$\mathbf{Vx}$

observation operator

$\mathbf{y}$

$\mathbf{x}$

atmospheric variables

retrieved refractivity

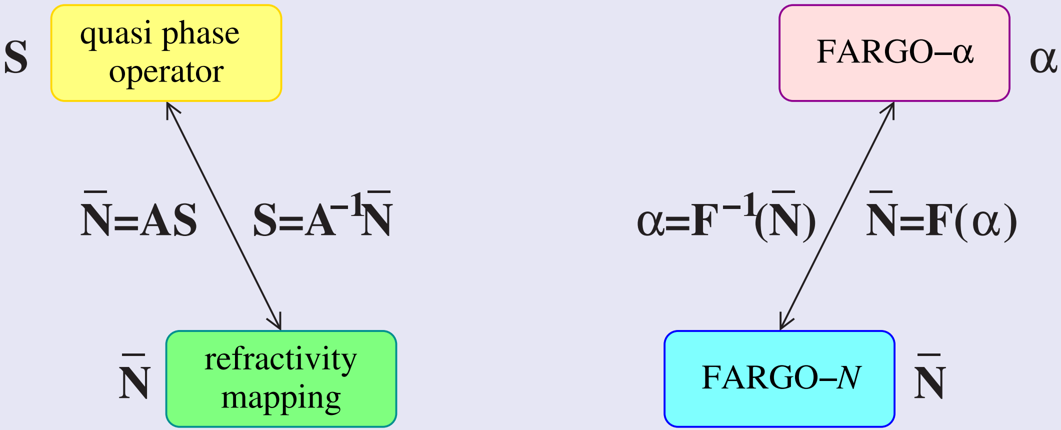
model variables

$$\mathbf{V}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}(\mathbf{O}+\mathbf{F})^{-1}(\mathbf{AVx}-\mathbf{y}) \quad = \quad \mathbf{V}^{\mathrm{T}}(\tilde{\mathbf{O}}+\tilde{\mathbf{F}})^{-1}(\mathbf{Vx}-\mathbf{A}^{-1}\mathbf{y})$$

$$(\tilde{\mathbf{O}}+\tilde{\mathbf{F}})^{-1} = (\mathbf{A}^{-1}\mathbf{O}\mathbf{A}^{-\mathrm{T}}+\mathbf{A}^{-1}\mathbf{F}\mathbf{A}^{-\mathrm{T}})^{-1} = \mathbf{A}^{\mathrm{T}}(\mathbf{O}+\mathbf{F})^{-1}\mathbf{A}$$

- If error covariances are consistent between the two operators, they should lead to exactly the same assimilation result
- Question: which one of the two has the simplest (easy to describe) representativeness error covariances?

Relations between observation operators



$\mathbf{S}$

quasi phase operator

$\bar{\mathbf{N}}$=AS

$\mathbf{S}=\mathbf{A}^{-1}\bar{\mathbf{N}}$

$\bar{\mathbf{N}}$

refractivity mapping

FARGO–α

α

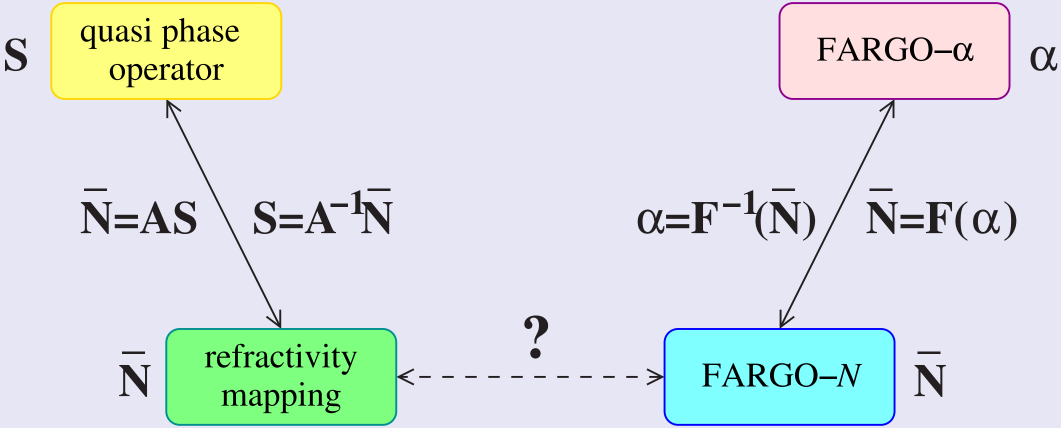
$\alpha=\mathbf{F}^{-1}(\bar{\mathbf{N}})$

$\bar{\mathbf{N}}=\mathbf{F}(\alpha)$

FARGO–*N*

$\bar{\mathbf{N}}$

Relations between observation operators



$\mathbf{S}$ quasi phase operator

FARGO–α α

$\bar{\mathbf{N}}$=$\mathbf{AS}$ $\mathbf{S}$=$\mathbf{A}^{-1}\bar{\mathbf{N}}$

α=$\mathbf{F}^{-1}(\bar{\mathbf{N}})$ $\bar{\mathbf{N}}$=$\mathbf{F}(\alpha)$

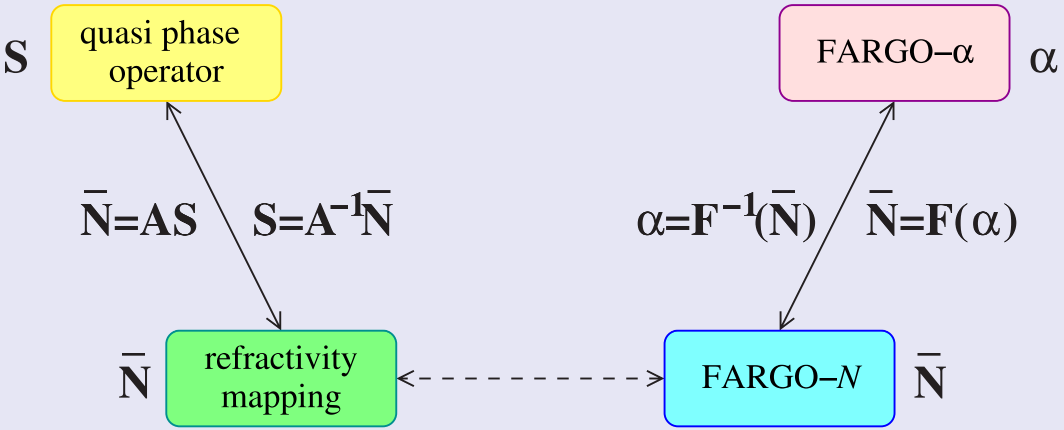
?

$\bar{\mathbf{N}}$ refractivity mapping

FARGO–N $\bar{\mathbf{N}}$

$$\bar{\mathbf{N}} = \mathbf{N}_{\mathrm{local}} + \mathbf{AV}(\mathbf{N} - \mathbf{N}_{\mathrm{local}}) \qquad \bar{\mathbf{N}} = \mathbf{N}_{\mathrm{local}} + \mathbf{F}(\Delta\alpha_{\mathrm{FARGO}})$$

Relations between observation operators



$\mathbf{S}$ quasi phase operator

FARGO–α α

$\bar{\mathbf{N}}=\mathbf{AS}$ $\mathbf{S}=\mathbf{A}^{-1}\bar{\mathbf{N}}$

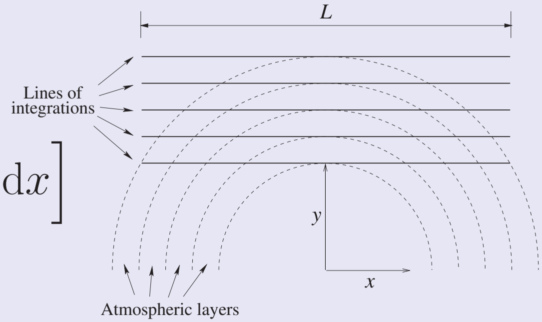
$\alpha=\mathbf{F}^{-1}(\bar{\mathbf{N}})$ $\bar{\mathbf{N}}=\mathbf{F}(\alpha)$

$\bar{\mathbf{N}}$ refractivity mapping

FARGO–N $\bar{\mathbf{N}}$

$$\bar{\mathbf{N}} = \mathbf{N}_{\text{local}} + \mathbf{AV}(\mathbf{N} - \mathbf{N}_{\text{local}}) \qquad \bar{\mathbf{N}} = \mathbf{N}_{\text{local}} + \mathbf{F}(\Delta\alpha_{\text{FARGO}})$$

$$\mathbf{F}(\Delta\alpha_{\text{FARGO}}) \approx \int_{r}^{r_{\text{top}}} \frac{\mathrm{d}y}{\sqrt{y^2 - r^2}} \frac{\mathrm{d}}{\mathrm{d}y}\left[\int_{-L/2}^{L/2} (N - N_{\text{local}})\mathrm{d}x\right]$$



Summary and prospects

- Lots of effort over the past 10 years have been made to develop observation operators taking into account horizontal gradients
- Recently a simple local refractivity operator has shown positive impact
- Ray tracing is potentially very accurate but also very time consuming
- Looking for trade-off between accuracy and speed has lead to alternatives
- Recently developed operators have small representativeness error and reduce computational cost significantly
- How fast are these new operators actually? Extraction of 2D refractivity field from the NWP model may be the limiting factor (certainly will be for refractivity mapping)
- A better understanding/knowledge about the representativeness errors is needed (including vertical error correlations)
- Have we found the optimum trade-off between accuracy and speed?

References and suggested reading

Ahmad, B. and G. L. Tyler, 1998: The two-dimensional resolution kernel associated with retrieval of ionospheric and atmospheric refractivity profiles by Abelian inversion of radio occultation phase data. *Radio Sci.*, **33**, 129–142.

Eyre, J. R., 1994: Assimilation of radio occultation measurements into a numerical weather prediction system. Technical Memorandum No. 199, European Centre for Medium-Range Weather Forecasts.

Gorbunov, M. E. and L. Kornblueh, 2003: Principles of variational assimilation of GNSS radio occultation data. Report No. 350, Max-Planck-Institute for Meteorology, Hamburg, Germany.

Healy, S., A. Jupp, D. Offiler, and J. Eyre, 2003: The assimilation of radio occultation measurements. *First CHAMP Mission Results for Gravity, Magnetic and Atmospheric Studies*, C. Reigber, H. Lühr, and P. Schwintzer, eds., 453–461, Springer.

Healy, S. B., 2001: Radio occultation bending angle and impact parameter errors caused by horizontal refractive index gradients in the troposphere: A simulation study. *J. Geophys. Res.*, **106**, 11 875–11 889.

Healy, S. B., A. M. Jupp, and C. Marquardt, 2005: Forecast impact experiment with GPS radio occultation measurements. *Geophys. Res. Lett.*, **32**, L03 804, doi:10.1029/2004GL020806.

Kuo, Y. H., S. V. Sokolovskiy, R. A. Anthes, and F. Vandenberghe, 2000: Assimilation of GPS radio occultation data for numerical weather prediction. *Terrestrial, Atmospheric and Oceanic Sciences*, **11**, 157–186.

Kuo, Y.-H., X. Zou, and W. Huang, 1997: The impact of Global Positioning System data on the prediction of an extratropical cyclone: an observing system simulation experiment. *Dynam. Atmos. Oceans*, **27**, 439–470.

References and suggested reading

Marquardt, C., J. R. Eyre, S. B. Healy, A. Jupp, and D. Offiler, 2003: Use of GPS radio occultation data in meteorological services. *OIST-4 Proceedings, 4'th Oersted International Science Team Conference*, P. Stauning, H. Lühr, P. Ultré-Guérard, J. LaBrecque, M. Purucker, F. Primdahl, J. L. Jørgensen, F. Christiansen, P. Høeg, and K. B. Lauritsen, eds., 261–268, narayana press, Copenhagen, Denmark.

Palmer, P. I., J. J. Barnett, J. R. Eyre, and S. B. Healy, 2000: A nonlinear optimal, estimation inverse method for radio occultation measurements of temperature, humidity, and surface pressure. *J. Geophys. Res.*, **105**, 17 513–17 526.

Poli, P., 2004: Effects of horizontal gradients on GPS radio occultation observation operators. II: A Fast Atmospheric Refractivity Gradient Operator (FARGO). *Quart. J. Roy. Meteorol. Soc.*, **130**, 2807–2825.

Poli, P. and J. Joiner, 2004: Effects of horizontal gradients on GPS radio occultation observation operators. I: Ray tracing. *Quart. J. Roy. Meteorol. Soc.*, **130**, 2787–2805.

Schlatter, T. W., 2000: Variational assimilation of meteorological observations in the lower atmosphere: a tutorial on how it works. *J. Atmos. Solar-Terr. Phys.*, **62**, 1057–1070.

Sokolovskiy, S., Y.-H. Kuo, and W. Wang, 2004: Evaluation of a linear phase observation operator with CHAMP radio occultation data and high-resolution regional analysis. *Mon. Weather Rev.*, in press.

Sokolovskiy, S., Y.-H. Kuo, and W. Wang, 2005: Assessing the accuracy of a linearized observation operator for assimilation of radio occultation data: case simulations with a high-resolution weather model. *Mon. Weather Rev.*, in press.

References and suggested reading

Syndergaard, S., D. Flittner, R. Kursinski, and B. Herman, 2003: Simulating the influence of horizontal gradients on refractivity profiles from radio occultations. *OIST-4 Proceedings, 4'th Oersted International Science Team Conference*, P. Stauning, H. Lühr, P. Ultré-Guérard, J. LaBrecque, M. Purucker, F. Primdahl, J. L. Jørgensen, F. Christiansen, P. Høeg, and K. B. Lauritsen, eds., 245–250, narayana press, Copenhagen, Denmark.

Syndergaard, S., D. E. Flittner, E. R. Kursinski, D. D. Feng, B. M. Herman, and D. M. Ward, 2004: Simulating the influence of horizontal gradients on retrieved profiles from ATOMS occultation measurements—a promising approach for data assimilation. *Occultations for Probing Atmosphere and Climate*, G. Kirchengast, U. Foelsche, and A. K. Steiner, eds., 221–232, Springer.

Syndergaard, S., Y.-H. Kuo, and M. S. Lohmann, 2005: Observation operators for the assimilation of occultation data into atmospheric models: A review. *Occultations for Probing Atmosphere and Climate: II*, U. Foelsche, A. K. Steiner, and G. Kirchengast, eds., Springer, submitted.

Syndergaard, S., E. R. Kursinski, B. M. Herman, E. M. Lane, and D. E. Flittner, 2005: A refractive index mapping operator for assimilation of occultation data. *Mon. Weather Rev.*, in press.

Zou, X., Y.-H. Kuo, and Y.-R. Guo, 1995: Assimilation of atmospheric radio refractivity using a nonhydrostatic adjoint model. *Mon. Weather Rev.*, **123**, 2229–2249.

Zou, X., H. Liu, R. A. Anthes, H. Shao, J. C. Chang, and Y.-J. Zhu, 2004: Impact of CHAMP radio occultation observations on global analysis and forecasts in the absence of AMSU radiance data. *J. Meteorol. Soc. Japan*, **82**, 533–549.

Zou, X., et al., 1999: A raytracing operator and its adjoint for the use of GPS/MET refraction angle measurements. *J. Geophys. Res.*, **104**, 22 301–22 318.