A Python wrapper for AM and towards an opacity database for the VLA site

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Overview and outline

- Scott Paine's AM atmospheric radiative code.
- Python wrapper "amwrap"
  - Overview and examples.
- Towards a VLA site climatology:
  - IGRA2 radiosonde measurements from Albuquerque.
  - EarthScope/NOTA GNSS stations and wet delays.
  - Validation of GNSS derived PWVs against sondes.
- Work in progress:
  - Process atmospheric opacity spectra for all dates >2010.
  - Empirically derived WVR channel weights (e.g., Sault et al.).
  - Application to phase correction with VLA switched power.

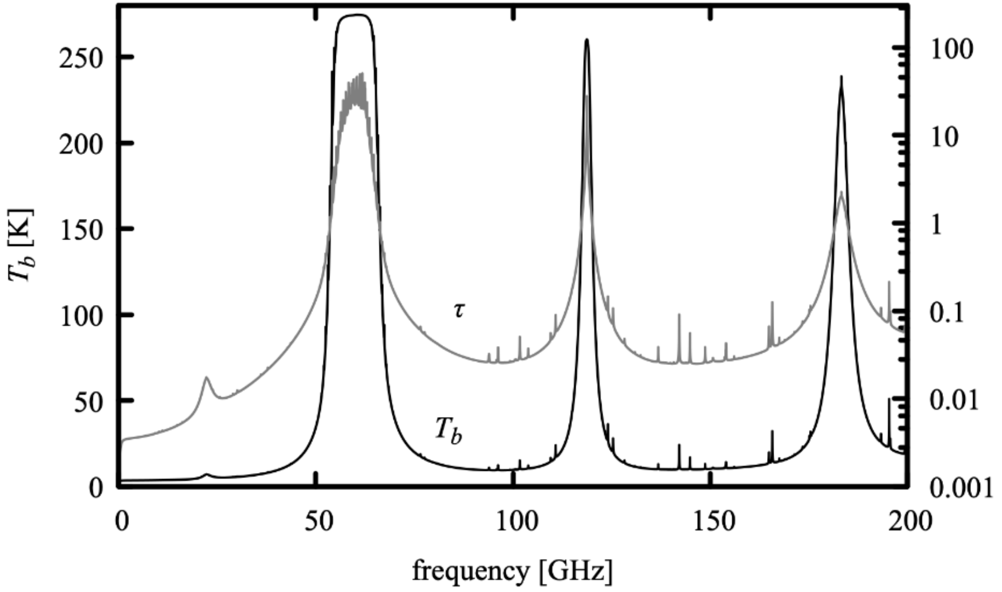
Atmospheric radiative transfer codes

- `ATM`: stand-alone is not publicly accessible, available upon request. Version shipped with CASA through the atmosphere toolkit is limited.
- `pyrtlib`: highly convenient and with good examples, but slow and limitations in accuracy.
- "Serious atmospheric codes" `ARTS`, `CRTM`, `PAMTRA`, `RTTOV`
    - All are C/Fortran based and nominally include Python interfaces, but are very complex to install, understand, and use.
    - In my investigation `PAMTRA` had the best documentation of the bunch, but the recommended install path is to use a virtual machine: virtually guarantees niche use for code intended to be distributed to VLA end-users (i.e., phase calibration from switched power).

Atmospheric Model: AM

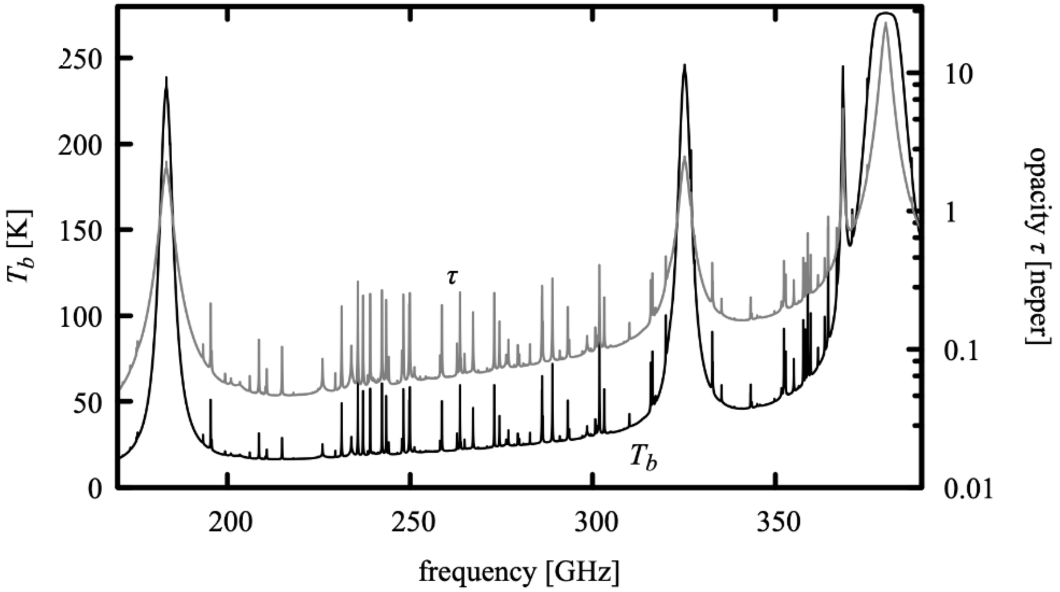
- `AM` is a flexible program by Scott Paine (SAO/SMA) for LTE atmospheric radiative transfer modeling at cm to sub-mm wavelengths.
  - Predict brightness temperature, opacity, delay, transmission.
  - Treatment of major, minor, and trace species (HITRAN); collision-induced absorption, water/ice clouds, non-planar geometry.
- *Advantages:* among "best in class" codes, publicly available, accurate, mature and community tested, and fast. Flexible with nearly arbitrary layer specification. Good documentation/manual.
- *Limitations:* interface is IO based and non-trivial to script. Tied to a detailed configuration format for the model specification.

https://lweb.cfa.harvard.edu/~spaine/am/index.html

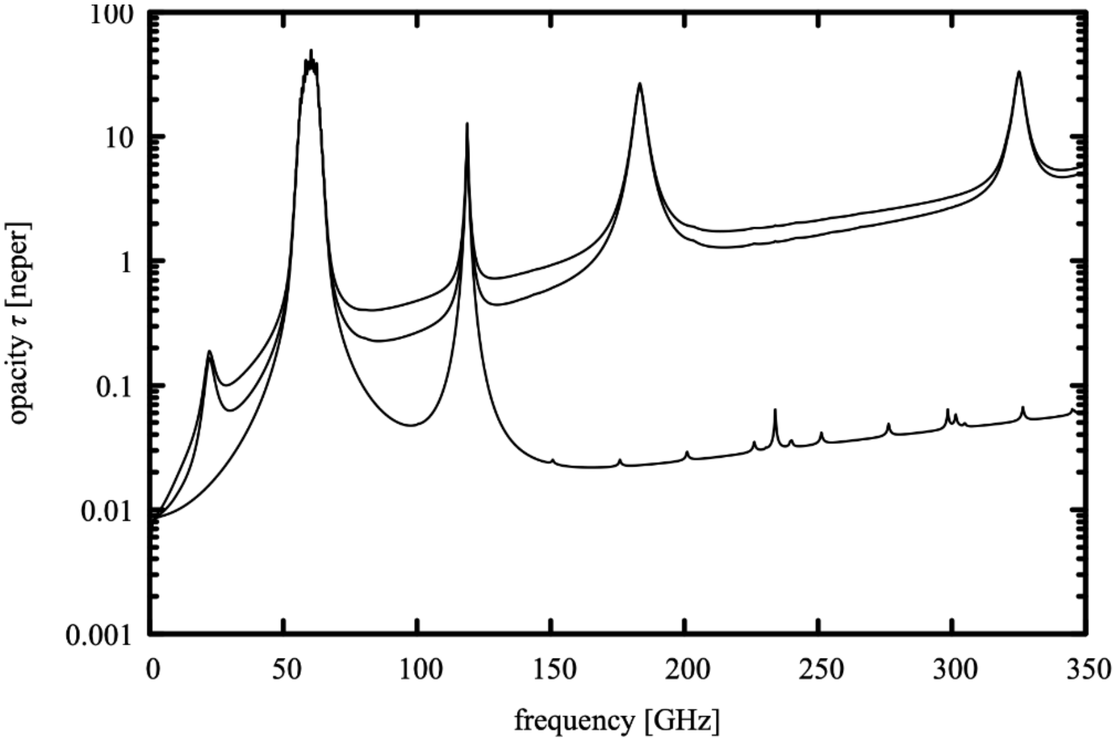


Example "downwelling" (ground-based upward looking) spectrum of sky brightness temperature and opacity from 0 to 200 GHz. Note the 22 GHz water line, 50-60 GHz oxygen band, 120 GHz oxygen line, and 183 GHz water line, plus a few faint ozone lines.

Same but between 170 to 390 GHz. Note the water line at 183 GHz and numerous, brighter ozone lines.



AM Manual, S. Paine; Figs. 2.6, 2.7.



Opacity spectrum for (1) dry atmosphere only, (2) constant 50% RH, and (3) constant 75% RH plus 0.2 kg/m² liquid-phase water from cloud.

AM Manual, S. Paine; Fig. 2.2.

```
f %1 %2  %3 %4  %5 %6
output f GHz  tau  Tb K
za %7 %8
tol 1e-4

Nscale troposphere h2o %11

T0 2.7 K

layer mesosphere
Pbase 0.1 mbar
Tbase 222.3 K
lineshape Voigt-Kielkopf
column dry_air vmr
column h2o vmr 6.46e-06
column o3 vmr 1.77e-06

layer mesosphere
Pbase 0.3 mbar
Tbase 243.3 K
lineshape Voigt-Kielkopf
column dry_air vmr
column h2o vmr 6.60e-06
column o3 vmr 1.65e-06

...

layer troposphere
Pbase 600 mbar
Tbase 275.0 K
column dry_air vmr
column h2o vmr 1.46e-03
column o3 vmr 4.30e-08

layer troposphere
Pbase 625 mbar
Tbase %9  %10
column dry_air vmr
column h2o vmr 1.87e-03
column o3 vmr 4.23e-08
```

All parameters of an execution are specified in a model configuration file (“.amc”) and passed as input to the AM executable.

The format specifies properties per layer in grouped sections. Items with “%” are interpolated from command line arguments.

Left: a detailed example for an empirically derived vertical profile from MERRA-2 re-analysis data of Mauna Kea.

AM Manual, S. Paine; S2.2.5 example.

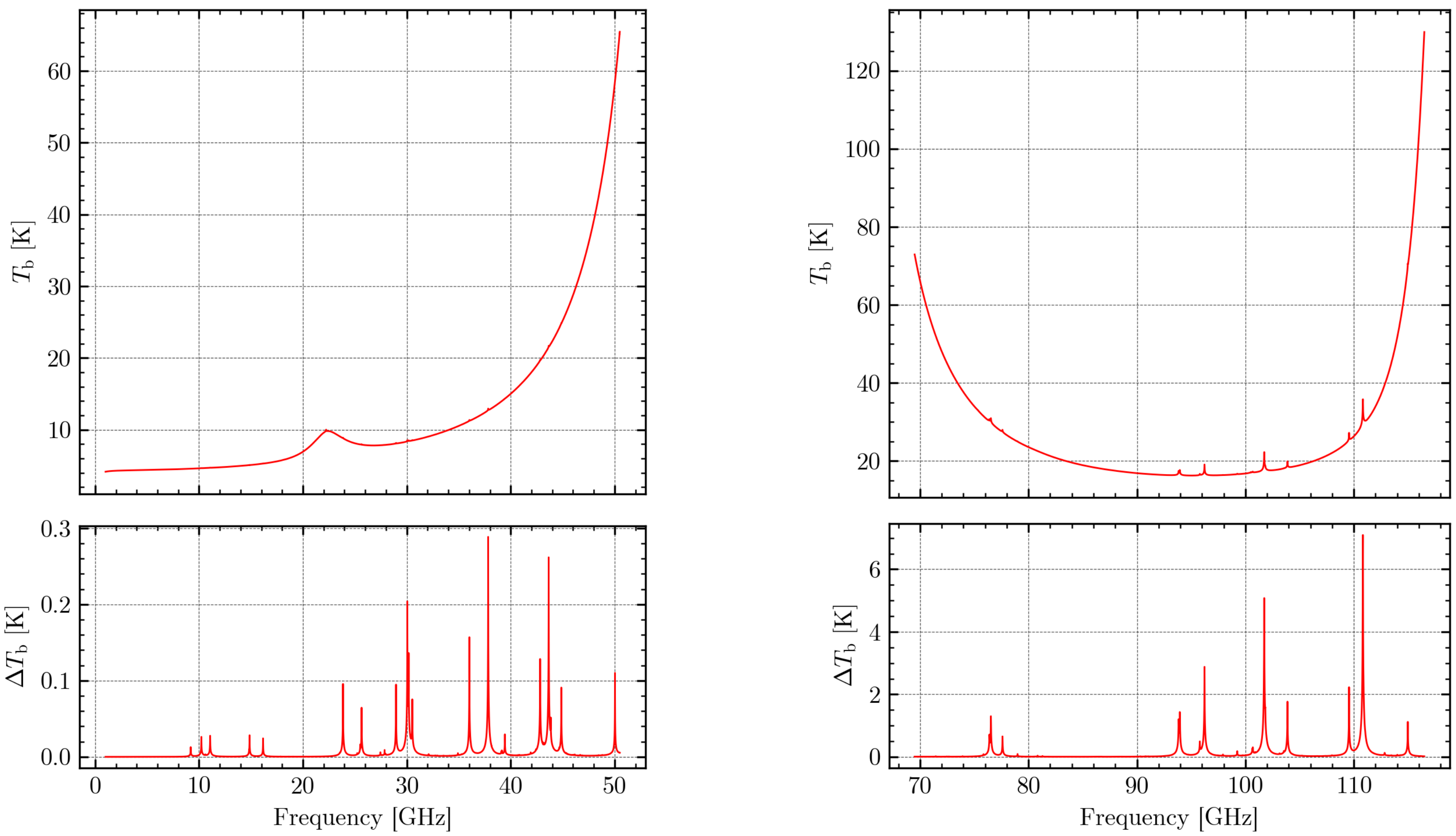
AM Python wrapper: amwrap

- Goals to make it trivial to install, straightforward to use programmatically from Python, and parallelizable across runs.
- Package and dependencies can be installed using `pip`.
- Installation automatically compiles AM and links executables.
- No files written: all input/output handled through pipes.
- Can specify atmospheric parameters in terms of arrays with units. Results are returned in a pandas `DataFrame`.
- Includes standard climatologies for the U.S. (taken from `pyrtlib`).
- Documentation on ReadTheDocs and tests run with GitHub Actions.

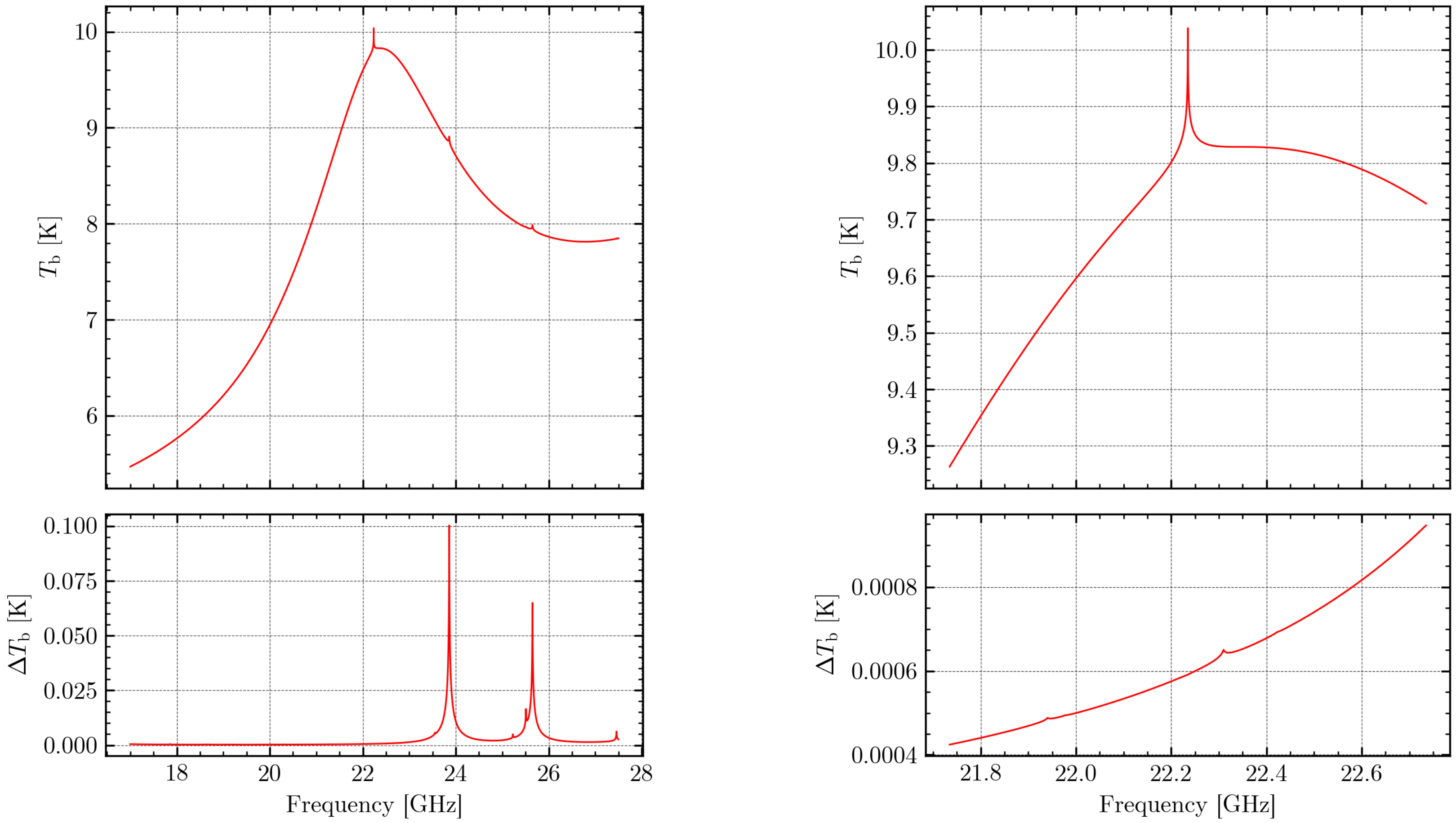
https://github.com/autocorr/amwrap
https://amwrap.readthedocs.io

AM Python wrapper: amwrap

- Prediction with overheads takes about 10 millisec for typical models.
- Absorption coefficient cache files written to RAM (`/dev/shm`).
- AM includes in-built parallelization for a single model using OpenMP. Copies of AM built in either serial-mode or parallel-mode can be called for running a single heavy model with multi-threading or by computing many models concurrently with one model per thread, for e.g., Monte Carlo or calculating parameter grids.
- With 40 cores and 10 ms run-time, can execute approx. 4000 models per second, sufficient for computation of parameter grids for even faster prediction using interpolation (i.e., over PWV, liquid/ice, pressure, temperature).



T_b [K]
ΔT_b [K]
Frequency [GHz]
T_b [K]
ΔT_b [K]
Frequency [GHz]



10
9
8
7
6
T_b [K]
0.100
0.075
0.050
0.025
0.000
ΔT_b [K]
18
20
22
24
26
28
Frequency [GHz]
10.0
9.9
9.8
9.7
9.6
9.5
9.4
9.3
T_b [K]
0.0008
0.0006
0.0004
ΔT_b [K]
21.8
22.0
22.2
22.4
22.6
Frequency [GHz]

Towards a VLA site climatology

- Accurate flux calibration requires a good estimate of the atmospheric opacity to transfer the solution from a flux calibrator to a target at a different elevation angle.
- Current method (`plotweather`) uses a fixed climatology given surface conditions to predict opacity weighted against a seasonal model.
- Sufficient quality for 5-10% absolute accuracy in good weather because the opacity at VLA frequencies are typically low (0.02 to 0.15).
- With precise estimates of PWV/opacity we can potentially reach 1-2% flux calibration accuracy in good weather and satisfactory in poor conditions (e.g., 30mm PWV, light clouds).
- Precise estimate of the predicted sky brightness temperature is likely required for good calibration of the switched power.

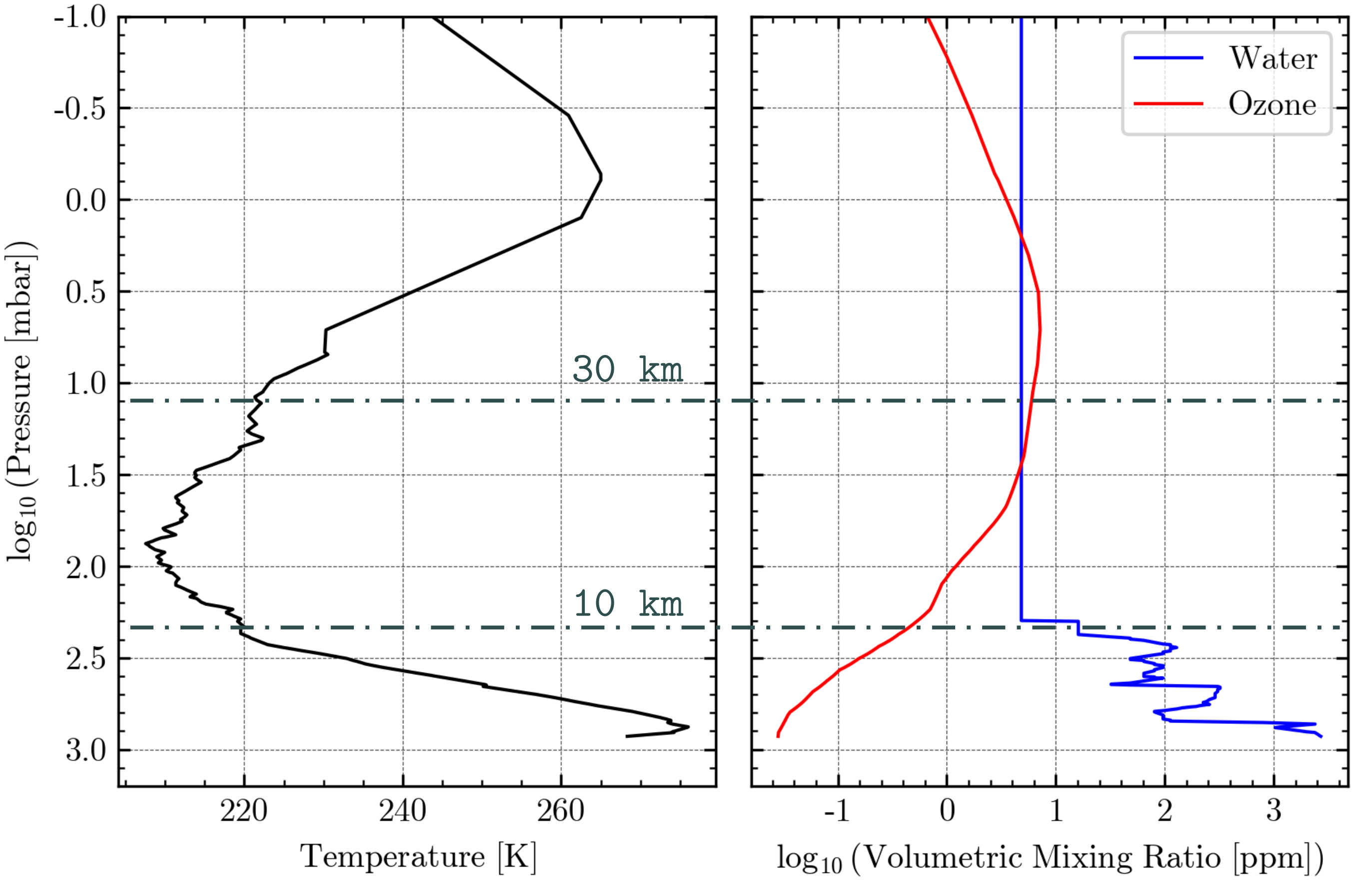
Towards a VLA site climatology

- Creating a VLA site climatology from existing data:
  - IGRA2 radiosondes launched from Albuquerque for validation.
  - EarthScope GNSS/GPS derived wet delays for PWV.
  - ECMWF ERA5 for site pressure, temperature, and moisture profiles. Can be used directly on day for older data ($>$ 1 month), or averaged by day-of-year to create a seasonal climatology that incorporates surface conditions.
- All data $>$2010 downloaded for IGRA2 radiosondes launched from ABQ along with all troposphere-type EarthScope GNSS data.
- EarthScope GNSS data is currently being re-analyzed for improved accuracy with a new release slated for this summer.

Soundings

Twice daily launches (5 AM/PM) from ABQ international airport. Provides "ground truth."

Right: vertical profiles of water from an ABQ radiosonde on a cold winter day with 2.1mm PWV.



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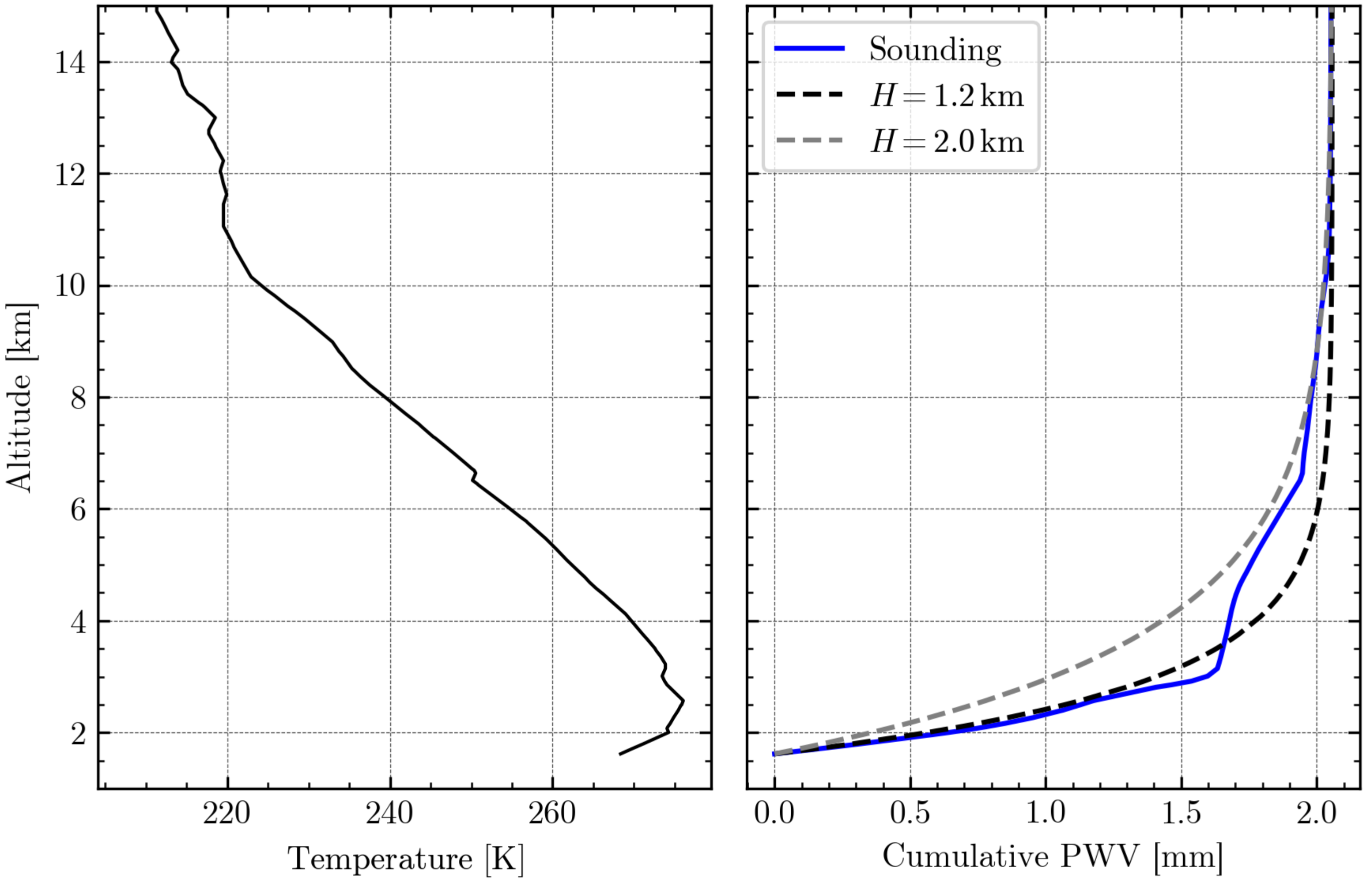
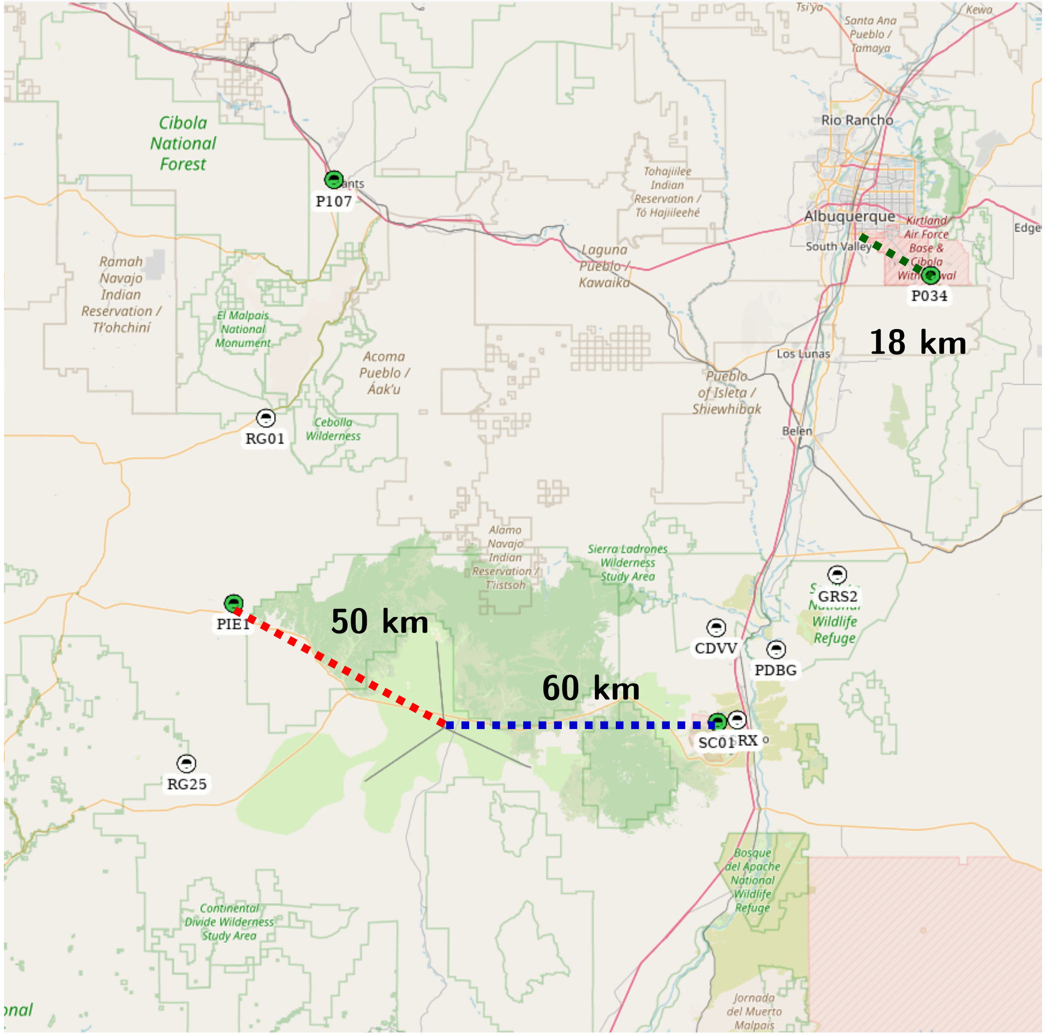
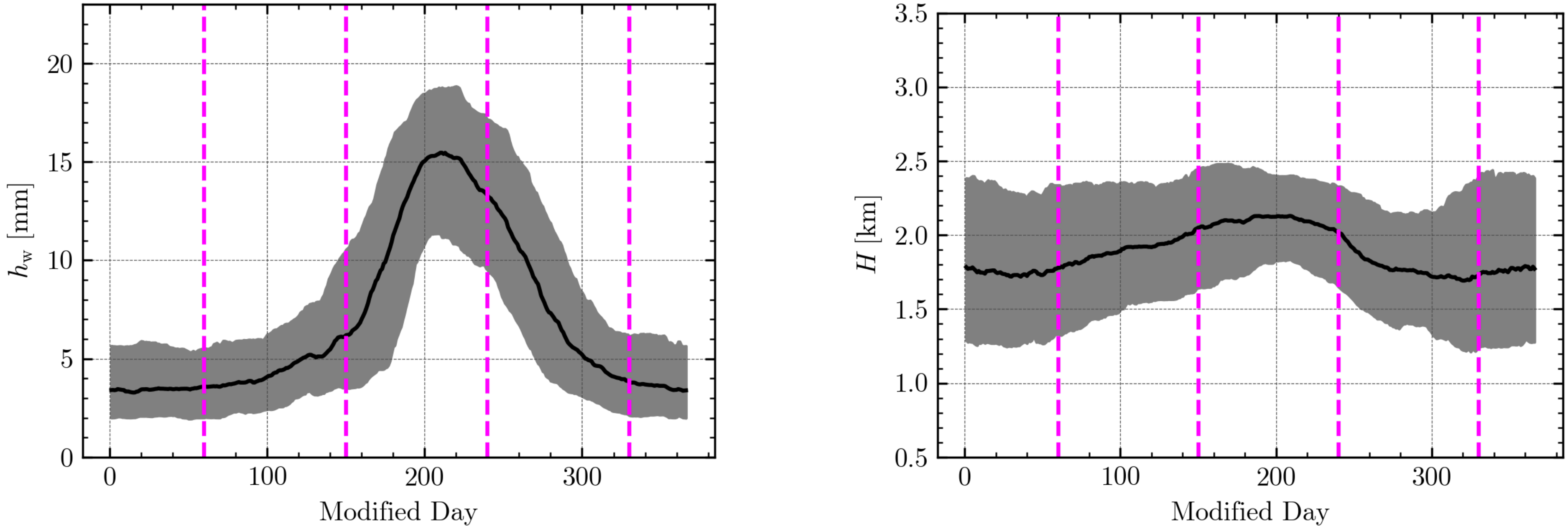


EarthScope/IGS GNSS

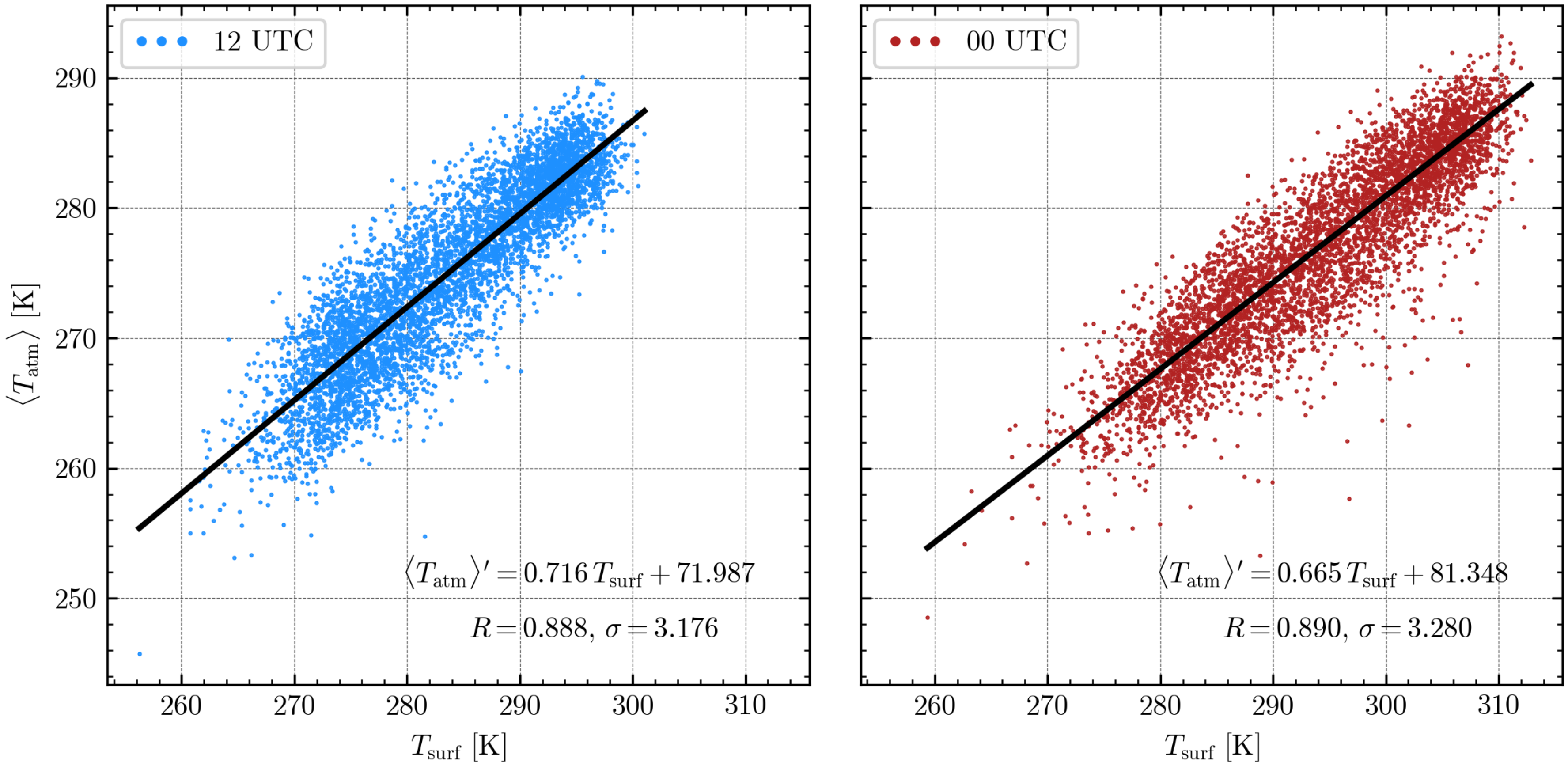
Data sampled at 5 min cadence with reported wet delay, convert to PWV using a weighted atmospheric temperature and transfer to different elevation.

Right: Stations near to the VLA site and Albuquerque. Closest stations are Pie Town (`PIE1`) and Socorro Peak (`SC01`), both about 55 km away but at similar elevations to the Plains.

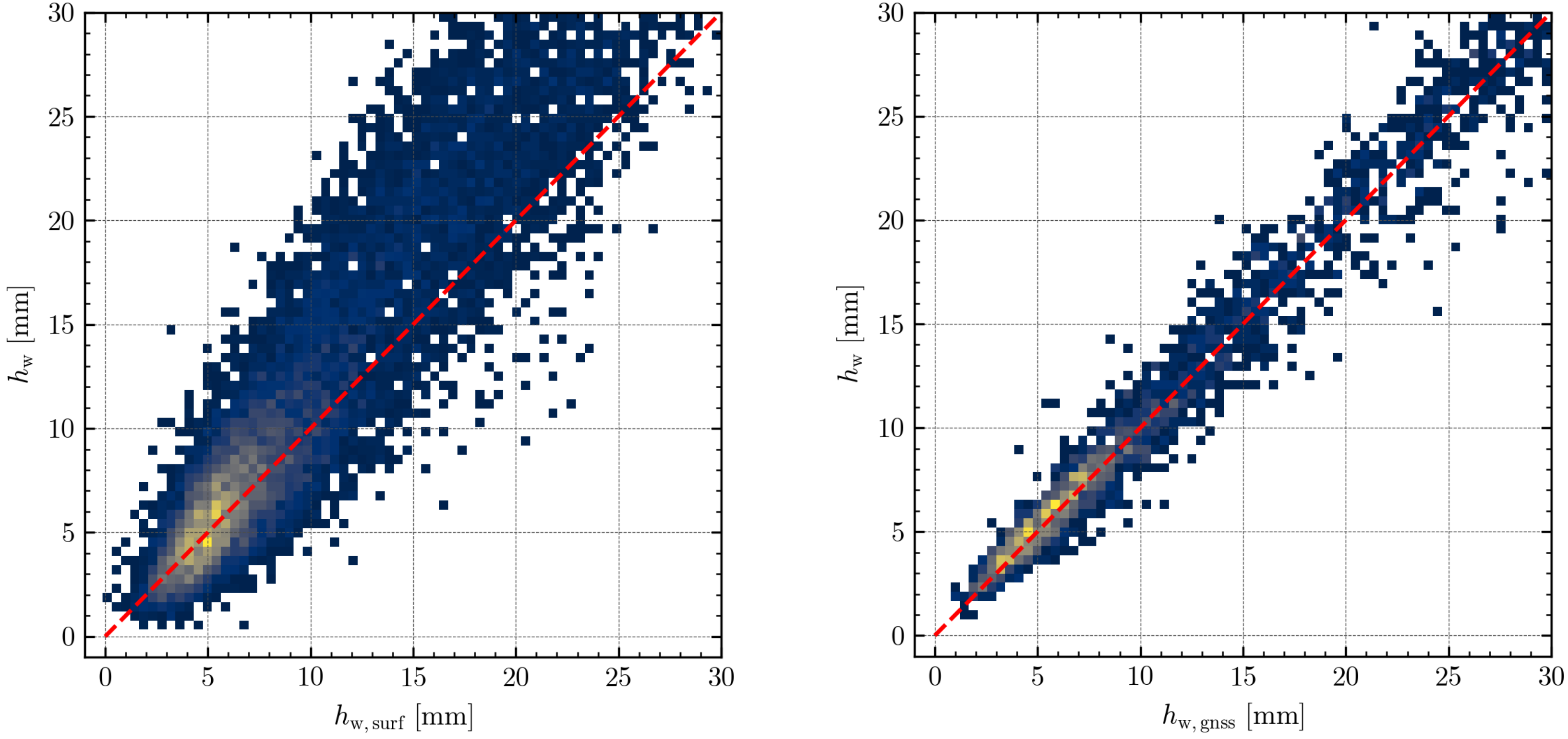




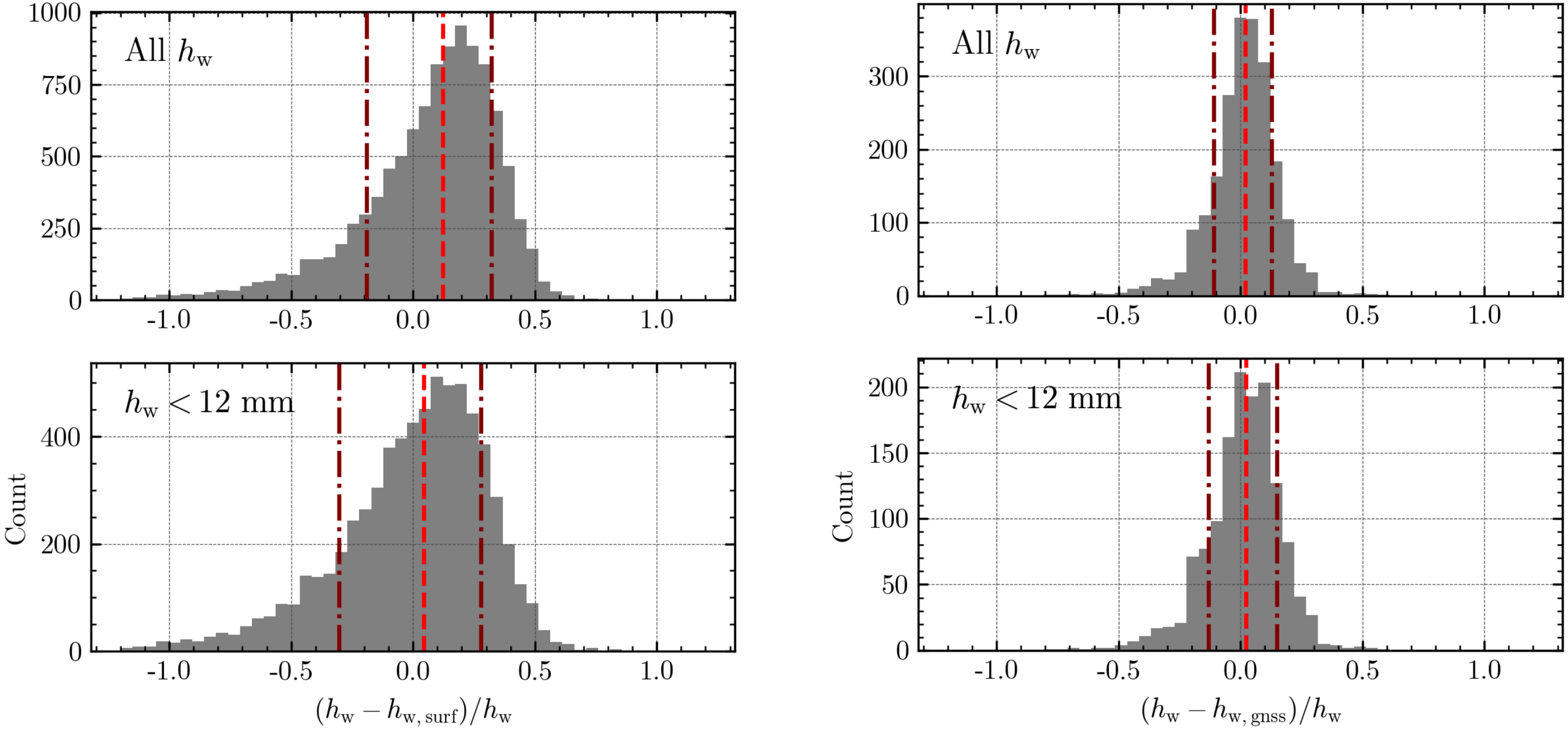
Rolling median and 16 and 84 percent quantiles with a 30 day wide window for PWV and water vapor scale height. Magenta lines show calendar seasonal boundaries (Winter: DJF, Summer: JJA). The "monsoon" season corresponds from early July to mid-to-late September. Median winter PWV of 3.5 mm and scale height of 1.8 km.



Re-derived Bevis et al. surface temperature to weighted-mean mean atmospheric temperature but with morning/evening split.



Radiosonde derived PWV versus (a) surface-derived PWV from surface pressure, dewpoint, and a fixed 2.0 km scale height, and (b) GNSS derived using the surface-to-mean temperature relation. GNSS value is converted to 200m lower altitude using a 1.8 km scale height.



The surface-derived estimate has a 21% relative error and the GNSS-derived estimate has about a 7% standard error. Statistical uncertainty in GNSS wet delay is about 5% and with a typical absolute error of 0.4 to 0.6mm.

Next steps

- Compare difference between PIE1 & SC01 stations and compare leading/lagging estimates from P034 to the radiosondes to simulate the PIE1 & SC01 stations being further away.
- Download all of ECMWF ERA5 pressure, temperature, and relative humidity profiles, create seasonal model. Compare to GNSS.
- Compare predicted opacities to Pedro's collection of 100 or so tipping measurements at same dates and times for ground truth to determine typical accuracy of available flux calibration.
- Forward model all opacity and sky brightness spectra, fit with spline, and store knots in database that users can query (thanks SSA) in lieu of the `plotweather` task.

Summary and outlook

- Atmospheric radiative transfer is essential for modeling radiometric phase correction schemes and flux calibration (opacity).
- Trade-offs in available codes. Paine's AM code is available, fast, and accurate. `amwrap` provides a simple Python interface for easier programmatic usage.
- A wealth of remote sensing and meteorological data exists to inform atmospheric modeling. Possible to use GNSS and global circulation models to improve VLA calibration.
- Ultimate aim is to use AM for model fitting of sky temperature spectra measured with the VLA's switched power for post-hoc tropospheric phase correction.