Using GitHub and Other Computational Tools to Enhance Research in Aerosol Optics

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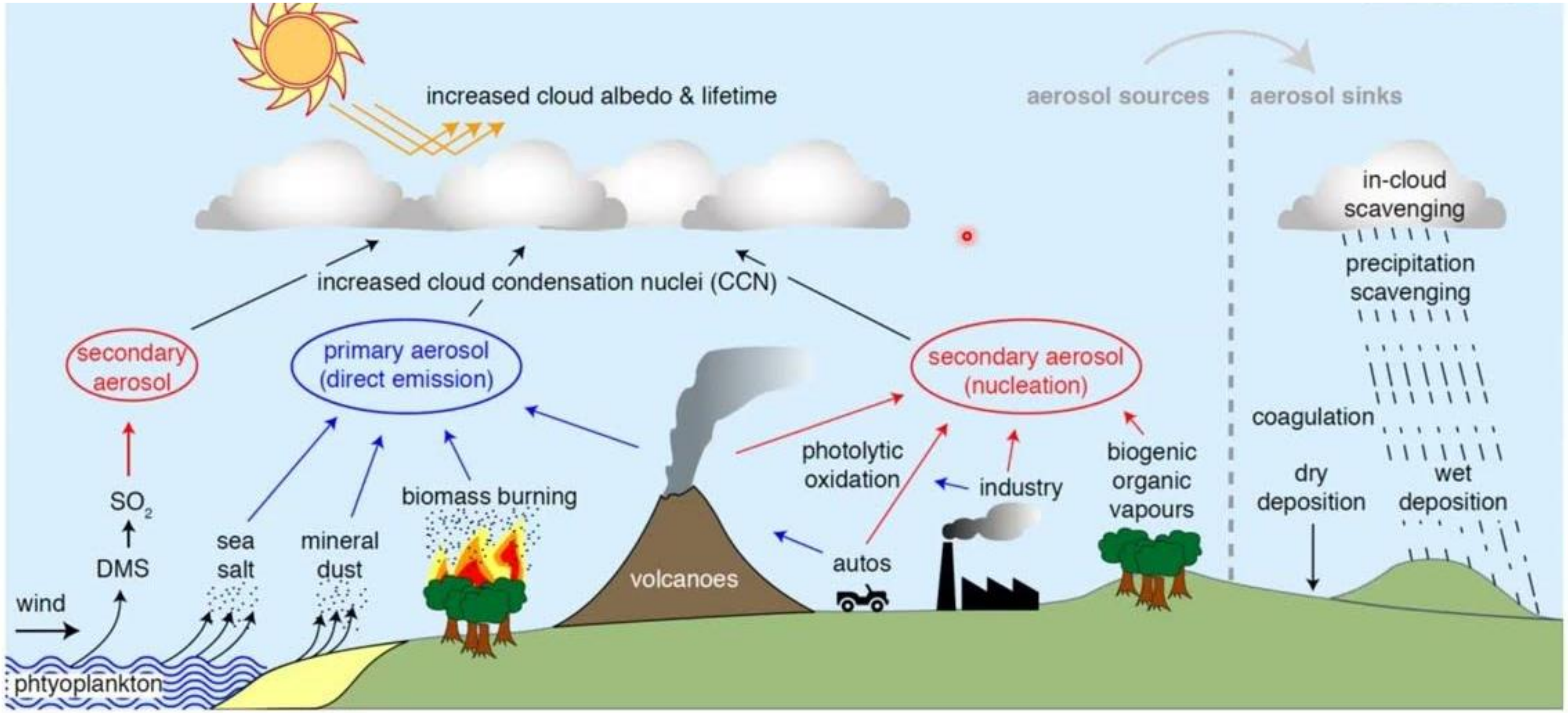
What is Roots for Resilience (R4R)?

The Roots for Resilience Program provides training and support to select graduate students on open, reproducible science and computational infrastructure to enhance research focused on resiliency in the environment.

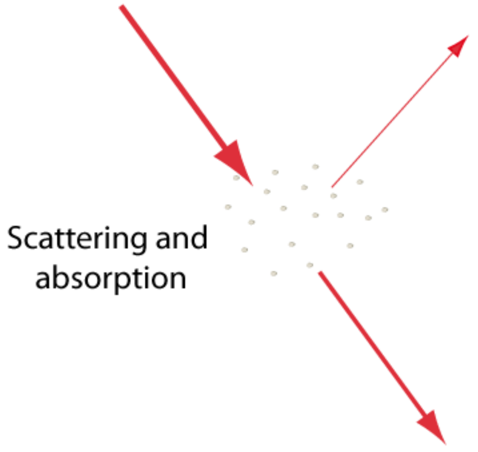
- Data science fellowship program targeting departments that support **environment/resilience-focused research**.
- Hosted by the Arizona Institute of Resilience (AIR), CyVerse, and the Data Science Institute (DSI).
- How to participate: one graduate student who has passed his/her qualifying exam or is an exceptional Master's student **is nominated by department head.**
- **$7,000 stipend disbursed in two installments.**
    - Second installment awarded upon completion of Foundational Open Science Skills course, capstone project, and final presentation to home department.

What are aerosol particles?

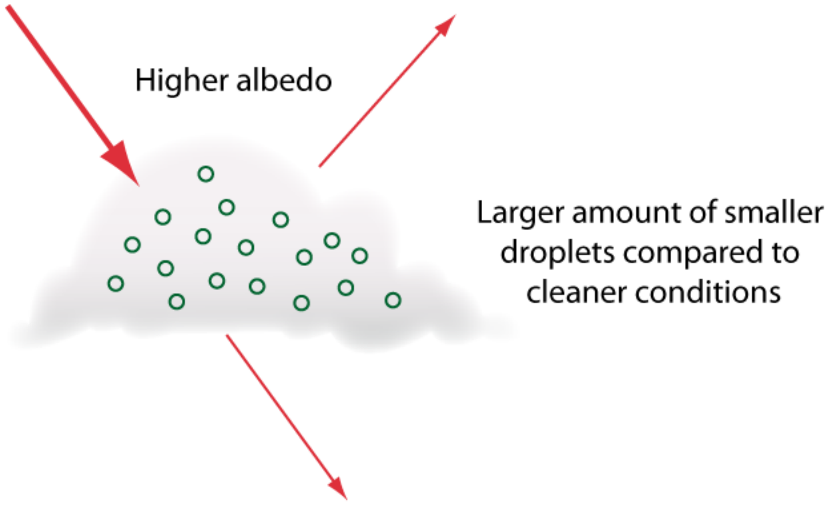
Suspensions of liquid droplets or solid particles in air.



Why are aerosol particles important?



Direct effects

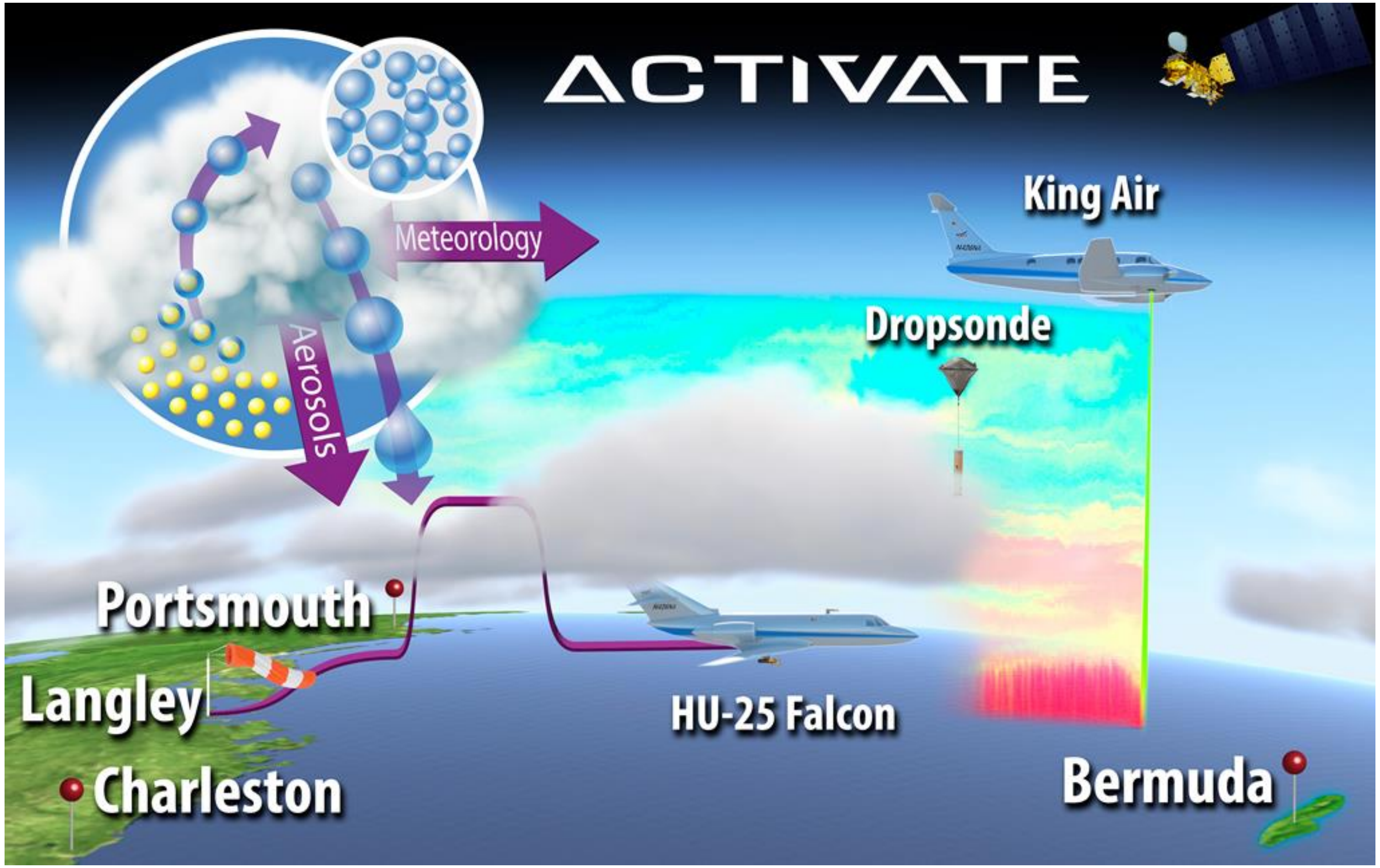


First indirect effect: cloud-albedo effect

How do we measure them?

- Different agencies conduct airborne field campaigns in various parts of the world to measure aerosol particles.
- Instruments housed on field aircraft (e.g., spectrometers, lidar, polarimeters) measure aerosol optical, chemical, and microphysical properties.

Example: NASA Aerosol Cloud meTeorology Interactions oVer the western ATlantic Experiment (ACTIVATE)



HU-25 Falcon

- Flies in coordinated legs below, in, and above clouds in the boundary layer.
- Instruments measure aerosol particles, clouds, trace gases, and various meteorological parameters in situ.
- TSI-3563 Integrating Nephelometer and Radiance Research Particle Soot Absorption Photometer **measure aerosol particle scattering and absorption.**

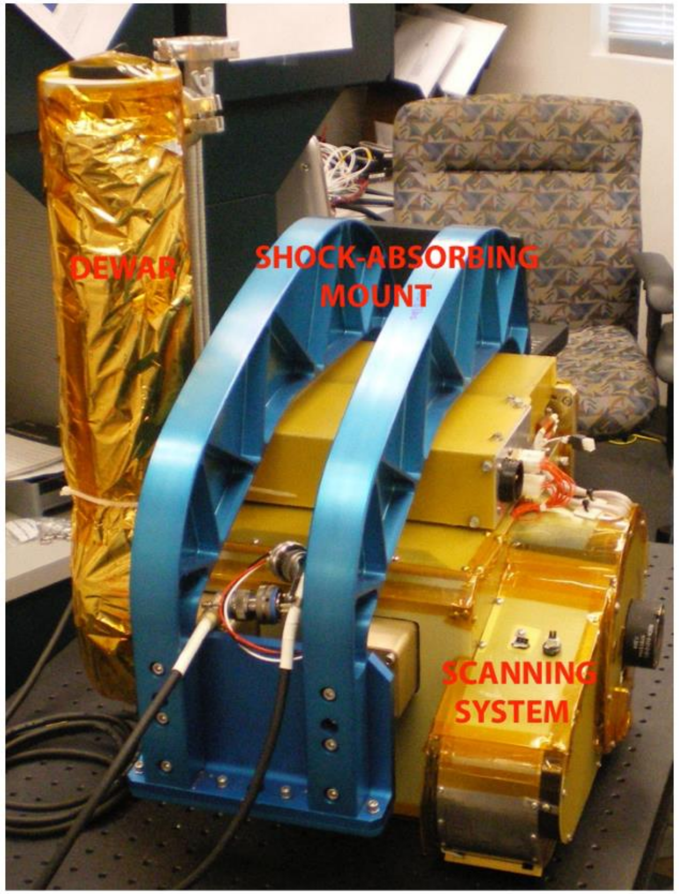
B-200/UC-12 King Air

- Flies high above the Falcon (at ~9 km) to serve as remote sensing platform.
- Instruments
  - HSRL-2: High Spectral Resolution Lidar - generation 2
  - RSP: Research Scanning Polarimeter
  - Dropsondes (not discussed)

HSRL-2 Overview

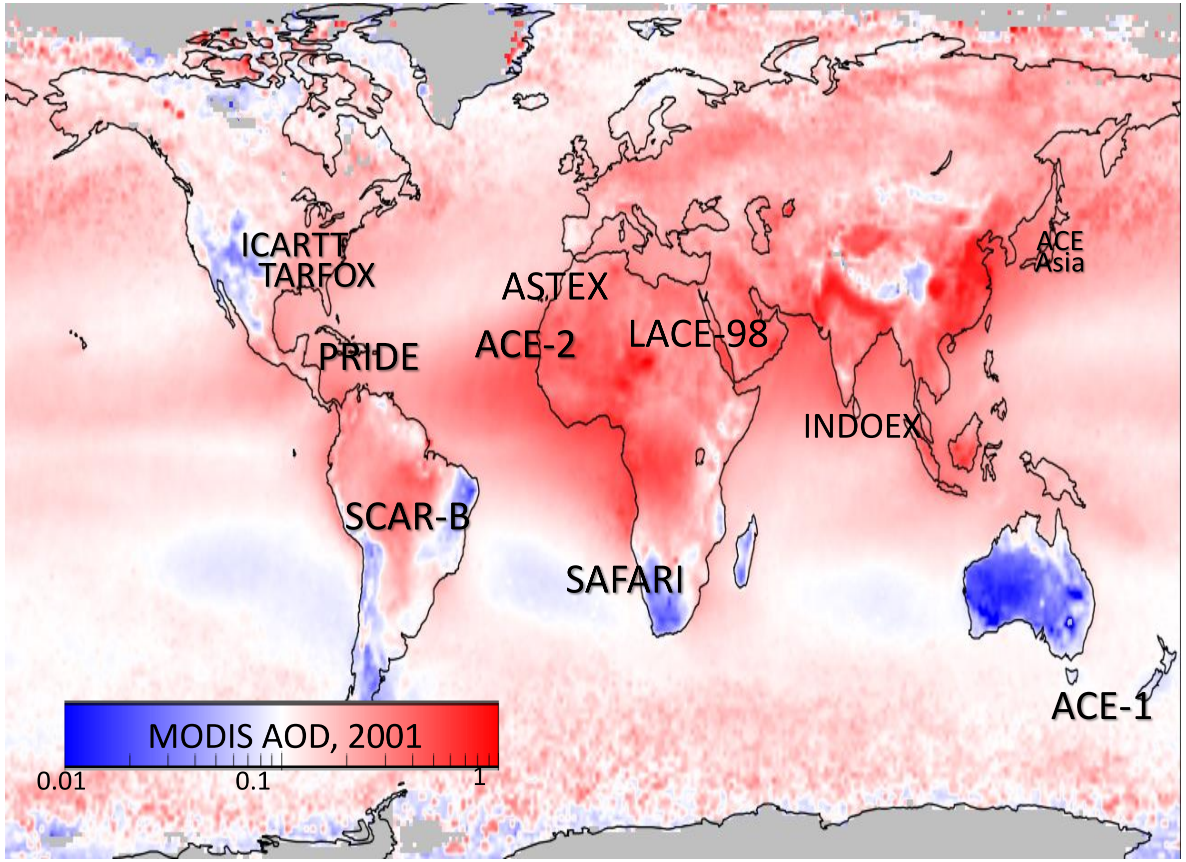
- Uses 3α + 2β method that measures aerosol backscatter and extinction **independently**.
  - Backscatter coefficients measured at 355, 532, and 1064 nm.
  - Extinction coefficients measured at 355 and 532 nm.
- Provides vertical profiles of various aerosol and cloud optical and microphysical properties.
- Uses field-widened Michelson interferometer to distinguish molecular scattering from aerosol/cloud particle scattering.

RSP Overview



- Nine spectral channels (410 – 2250 nm), 7 of which retrieve aerosol and cloud properties.
- Paired sets of telescopes provide radiance and linear polarization measurements of observed scene within a 105° along-track swath.
- **Result**: Spectral/angular snapshot that provides information on aerosol and cloud properties with high-angular resolution and polarimetric accuracy.
  - 152+ viewing angles in a single pixel swath
  - Pixel observation time: 1.875 ms

How do we verify measurements?



- To perform verification analysis (i.e., closure), field scientists compare data between instruments within field campaigns and/or global models.
- However, difficult because
  - Diverse sets of field campaign instruments use differing calibration standards.
  - In situ aircraft instruments tend to **dry aerosol particles before measurement**, significantly changing their shape, size, and composition.
    - Remote sensors measure aerosol particles in “ambient” without altering them, making comparison with in situ data difficult.

How ISARA can help with closure analysis

- In coordination with Office of Naval Research (ONR) and NASA Langley Research Center (LaRC), I am helping develop an open-source Python codebase called the **In Situ Aerosol Retrieval Algorithm (ISARA).**
  - Based on Modelled optical properties of ensembles of aerosol particles (MOPSMAP) Fortran package.
- ISARA models **ambient in situ** aerosol optical and microphysical properties at the relative humidity (RH) level(s) and wavelength(s) of choice using real in situ field data.

ISARA Retrieval Methodology

1) Retrieve dry imaginary refractive index (IRI) using dry size-resolved aerosol number concentration (n^o) and in situ scattering and absorption measurements.

↓

2) Retrieve hygroscopicity (κ) using n^o, Diode Laser Hygrometer relative humidity (RH) measurements, and in situ scattering measurements.

↓

3) Apply cloud filtering and calculate ambient optical and microphysical properties.

↓

4) Apply collocation algorithm to ensure spatiotemporal proximity between in situ and remote sensing data (data filtered within 15 km spatially and 6 min temporally).

↓

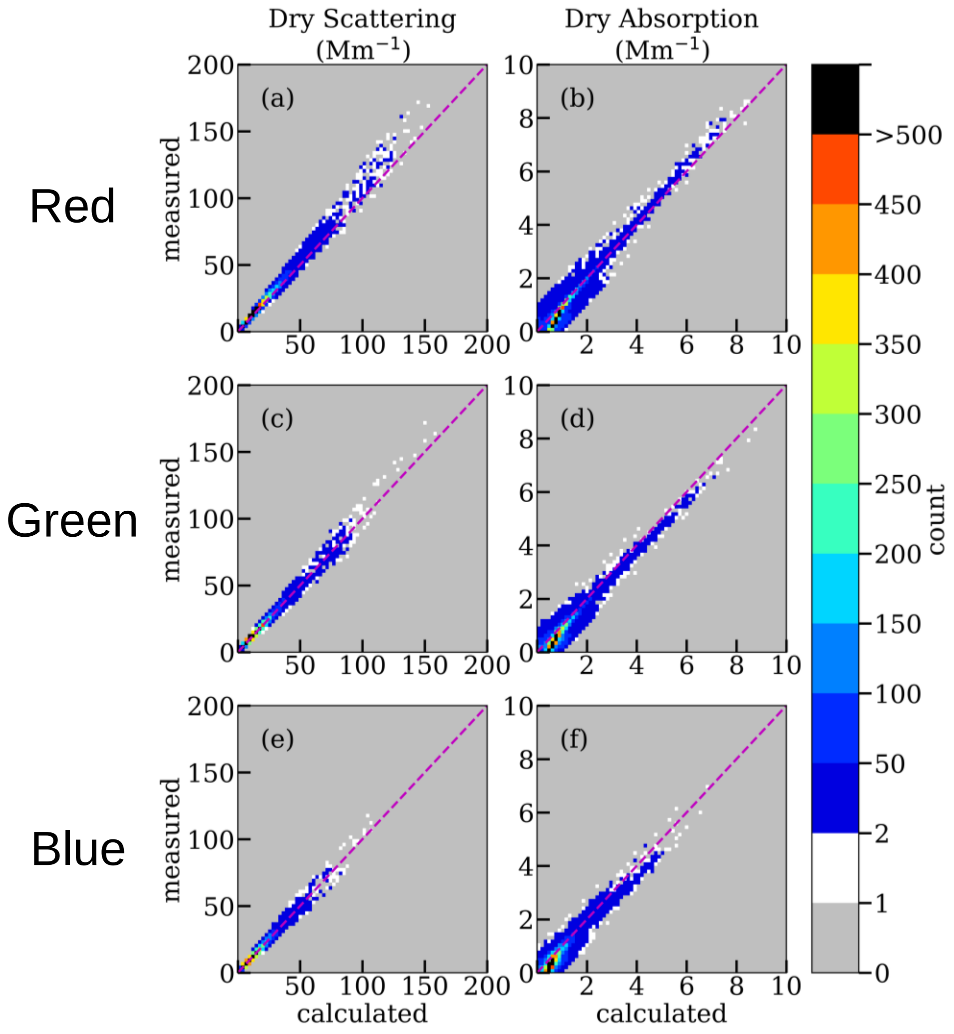
5) Determine agreement between in situ and remote sensing values with normalized-range mean absolute deviation (NMAD):

$$\sum_{j=1}^{n} \frac{|Y_j - X_j|}{n} \cdot \frac{100\%}{\max(X) - \min(X)}$$

where Y_j is set of ISARA-modelled in situ data, X_j is set of remote sensing data, and n is the total number of points.

- ISARA uses Mie theory to compute humidified optical and microphysical properties at user-specified wavelength(s).
- Mie theory: Aerosol particle is a single, homogeneous sphere of radius r, whose material is dielectric with a complex refractive index m.
- Other forward optical models available for more complex-shaped particles (e.g., T-matrix method, discrete dipole approximation).

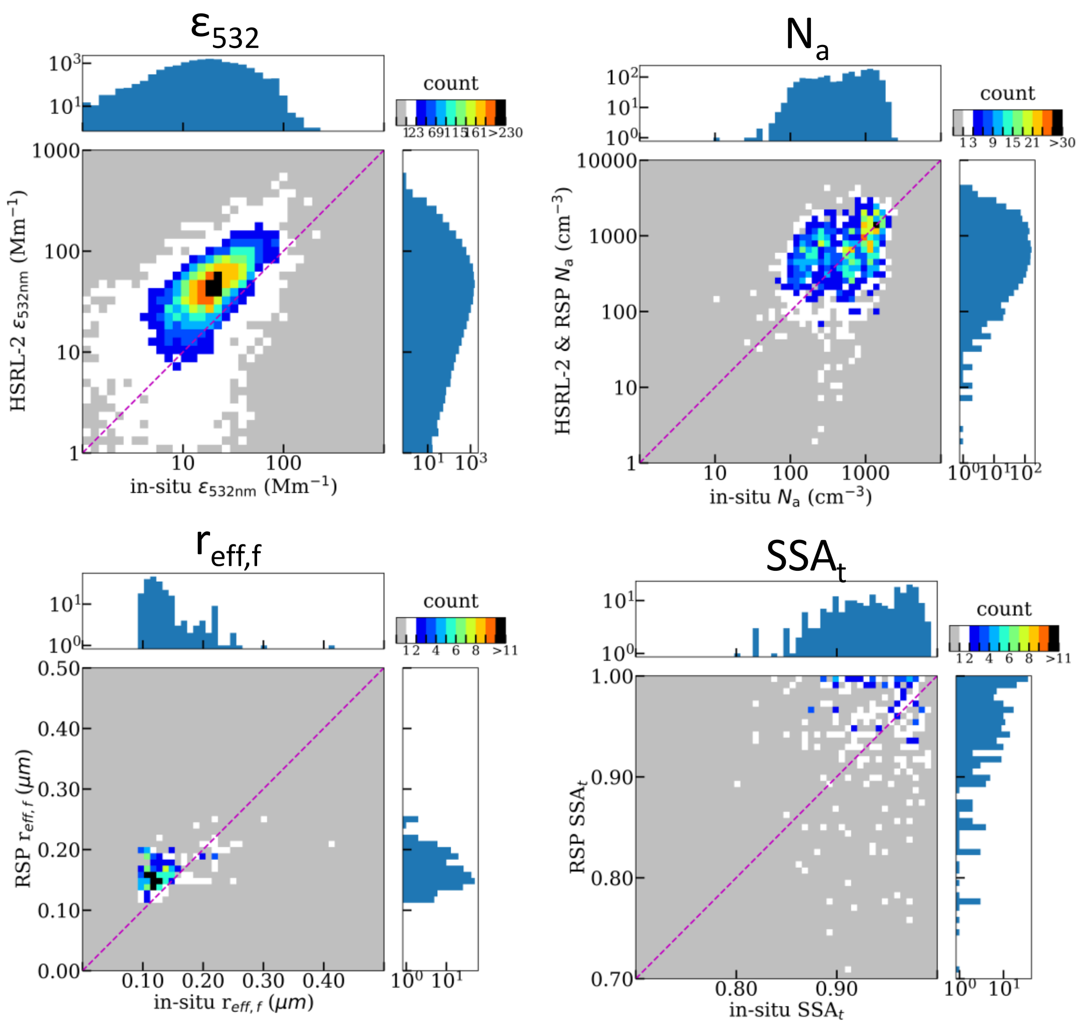
Initial Testing Results



- Dry scattering coefficients agree within 1%.
- Dry absorption coefficients agree within 5%.

	Scattering			Absorption		
Wavelength (nm)	450	550	700	470	532	660
NMAD (%)	0.5	0.5	0.3	2.3	2.6	3.7

External Closure Results



- External closure: Comparison of in situ measurements to remote sensing retrievals.
- Four parameters:
  - HSRL-2 extinction at 532 nm (ε_{532})
  - HSRL-2 + RSP aerosol number concentration (N_a) (Joseph Schlosser)
  - RSP aerosol fine-mode effective radius ($r_{eff,f}$)
  - RSP total effective single-scattering albedo (SSA_t)

	ε_{532nm}	N_a	$r_{eff,f}$	SSA_t
NMAD (%)	4.5	8.5	16	24

Next Steps

- Investigate discrepancies in RSP r_{eff} and SSA comparisons.
- Introduce flexibility in user-inputted particle size distribution data to extend software to other field campaigns.
- Provide detailed instructions on software installation and use on website.
- Use Docker containerization to create easy-to-use application for ISARA.

Thank you!