WRF-STILT Transport Modeling: An Introduction to the ASC Source-Receptor ("footprint") Library

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# **Purpose of Talk**

- Advertise existing footprint and WRF libraries to broader ABoVE community
- Describe how to read and apply footprints to your research
- Receive feedback from ABoVE science team members
  - Audience is encouraged to think about how these products can help with your current and future research
- Framework for testing models (flux estimates) being put in place
  - Help us tailor the scripts to your needs
- Outline of talk:
  - Introduction to footprints; how they are generated; their availability and application
  - Less focus on theoretical concepts and details of WRF-STILT model
  - Provide sample high-resolution WRF fields



# Footprints – basic concept

# Inferring fluxes from atmospheric data

• Path and CH<sub>4</sub> mixing ratio of an air parcel:



Friedemann Reum Methane Emissions from the East Siberian Arctic Shelf 2016 Fall AGU 20 /25

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# **Footprints - basics**

- Footprints describe "source-receptor" relationship
  - Often used to identify biogenic/biomass burning contributions
  - Receptor=observed concentration of GHG at x, y, z and t
  - Source=upstream location on Earth's surface that may have contributed GHG fluxes
- Time-dependent, two-dimensional grid on Earth's Surface
   Typically 0.5x0.5-deg grid, but can be finer
- Effective adjoint of the transport model
- Computed using STILT Lagrangian Particle Dispersion Model
   follow 500 tracer particles backward in time for each receptor
- Often applied to observations obtained from aircraft and towers

   need x,y,z and t only -> species independent



### **STILT Transport Model: Standard footprint**

- Footprints equivalent to adjoint of transport field of NWP model
- Species independent sourcereceptor relationship
- Release 500 particles at each receptor location
- Movement dictated by mean wind and turbulent motions
- Footprints are function of residence time of those trajectories in lower part of PBL and are inversely proportional to mixing height
- Continental-scale 0.5 deg x 0.5 deg footprint+0.1 deg nearfield
- Units: ppm/(umol/m<sup>2</sup>s)

Aggregate footprint: t - 12 h





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STILT influence at Toolik Lake, 100m agl



0.5-deg lat-lon grid for multiple receptors at Toolik Lake



# **Comparison with flux footprint**

#### STILT concentration footprint:

- Appropriate for regional and larger studies
- Cumulative effect of multiple upstream surface contributions
- Strongly influenced by regionalscale advection, plus stochastic component

#### • Flux footprint:

- Eddy covariance: high-frequency vertical wind and gas concentration measurements
- Source is immediately upstream (meters)
- Scale of turbulent eddies; subgrid scale wrt WRF grid; requires LES





#### **Reconstruction of flow toward obs location**





# Footprints – How they are generated

- Two-step process using WRF-STILT:
  - Step 1): Simulate high-resolution meteorological fields using WRF (numerical weather prediction model)
  - Step 2) Apply WRF fields to Stochastic Time-Inverted Lagrangian Transport (STILT) dispersion model



## **Step 1 - CARVE WRF domain placement**

Polar stereographic grid

D1: 30-km 418x418

D2: 10-km 799x649

D3: 3.3-km 550x550

41 vertical levels





## **Step 1 - CARVE-CAN domain placement**

Polar stereographic grid

D1: 30-km 418x418

D2: 10-km 799x649

D3: 3.3-km 550x550

41 vertical levels





#### **Particles move with WRF winds and terrain**





# 2012 flight tracks on domain 3 of WRF





# **Step 2- STILT overview**

- Based on NOAA/ARL HYSPLIT code
- Lagrangian Particle Dispersion Model coupled offline with WRF
  - WRF 3D fields advect particles backward in time in STILT
  - Turbulence and dispersion represented as stochastic technique
  - AER enhancements for WRF: customized time-averaged mass, and convective mass, flux mass fields for mass conservation, a critical consideration for inversion work.
- Optimized implementation on HPC for 100,000+ receptors
- Major STILT features not currently in HYSPLIT:
  - Mass conservation
  - Convection scheme that utilizes WRF convective fluxes (Grell-Devenyi; see AER for Grell-Freitas support in v38)
  - More complex turbulence module with reflection/transmission scheme for Gaussian turbulence. This preserves well-mixed distributions of particles moving across interfaces between step changes in turbulence parameters.
  - Account for transport errors by incorporating uncertainties in winds into the motion of air parcels

(Chris Loughner NOAA :  $CO_2$ -Urban Synthesis and Analysis (" $CO_2$ -USA") Workshop, NIST, 6-7 Nov 2017)



# **Footprint Library**

- Location: NASA Ames Lou and ORNL DAAC; ASC in near future
- Period of record:
  - CARVE domains (mainland Alaska): 20120101 to 20160830
  - CARVE-CAN domains (Mackenzie river delta, NWT): 20140501 to 20170330
- Two products in netcdf4 format for each receptor:
  - footprint files (prefix: foot)
    - 0.5-deg north of 30N and receptor-centered nearfield 0.1-deg grid 3x5 deg in size
  - transport files (prefix: stilt)
    - "thinned" particle file describes location of particles as they move backward in time
    - · times and locations where contribution to footprint is zero have been removed
    - Also contains footprint field
- Footprint library and processing code will be made available on ASC
  - Transport files available upon request
- ABoVE email subgroup will enable communication



# **Footprint file**

• Nomenclature for one footprint file:

foot2013x12x10x16x00x64.9863Nx147.5980Wx00300.nc

#### • File sizes for 10-day back trajectory:

foot2013x07x15x00x21x71.2602Nx156.7502Wx00415.nc**280K**foot2013x07x15x00x21x71.2602Nx156.7502Wx00415.nc.gz**68K**CARVE-AIRMETH-2013-convect-footprints.tar (4322 f\*nc)**1.3GB**CARVE-AIRMETH-2013-convect-particle-files.tar (4322 s\*nc)**9.6GB** 



netcdf4 format

#### **Footprint file – Most important contents**

ncdump -h foot2013x07x15x00x21x71.2602Nx156.7502Wx00415.nc:

dimensions: **foot1lon=**720, **foot1lat=**120, **foot1date=**240 **footnearfield1lon=**50, **footnearfield1lat=**30 **footnearfield1date=**24

variables:

float origagl [m AGL], float origlat, float origlon, char origutctime

float foot1(foot1date, foot1lat, foot1lon) [ppm per (micromol m-2 s-1)]

double foot1lon(foot1lon), double foot1lat(foot1lat) double foot1date(foot1date) [days since 2000-01-01 00:00:00 UTC] float foot1hr(foot1date) [stilt footprint hours back from stilt start time]

float footnearfield1(footnearfield1date, footnearfield1lat, footnearfield1lon) [ppm per (micromol m-2 s-1)]



# **Footprint applications - Validation**

- Validate estimates of flux field from a model (empirical or process-based)
- Evaluate different assumptions and datasets that are input to the flux model



model input calculation

**PVPRM-SIF**: Polar Vegetation Photosynthesis and Respiration Model-Solar-Induced Fluorescence



# **Convolving footprint files – simplified steps**

footprint.file='foot2013x05x10x15x00x64.9863Nx147.5980Wx00300.nc'

#only one footprint file in this example

| <pre>#outline of script 'crv.tower.convolve.src':<br/>fp = nc_open(footprint.file)<br/>m=ncvar_get(fp,"foot1")<br/>flat=ncvar_get(fp,"foot1lat"); flon=ncvar_get(fp,"foot1lon")<br/>fp.time = ncvar_get(fp,"foot1date")</pre> | #open ncdf4 footprint file using library(ncdf4)<br>#read the 0.5x0.5-deg STILT footprint<br>#read lat/lon of footprint grid<br>#read dates of footprint grids; 5-day footprints= 120 h |  |  |  |  |  |  |
|---|--|--|--|--|--|--|--|
| name=load("nee.pvprm.sif.2013.RData")<br>nee=get(name)  | #load process model NEE; assume times match  |  |  |  |  |  |  |
| lat.extent = c(50,75); lon.extent = c(-169,-120)<br>flat.index = flat>=lat.extent[1] & flat< lat.extent[2]<br>flon.index = flon>=lon.extent[1] & flon< lon.extent[2]  | #define spatial extent of grid for convolution<br>#create mask for lat/lon extent<br>#can also use land mask   |  |  |  |  |  |  |
| conv.tower = matrix(NA,nrow = 1,ncol=7)<br>colnames(conv.tower)=c("JD","Lat","Lon","Alt","Time","STILT","STIL   | #define output matrix<br>TxPVPRMSIF") #output matrix column names  |  |  |  |  |  |  |
| conv.tower[1,"STILT"] = sum(apply(m[flon.index,flat.index,1:120],c(   | 1,2),sum,na.rm=T)) #write out cumulative footprint field   |  |  |  |  |  |  |
| #convolve footprints with fluxes: multiply time-dependent 2D matrices:<br>mm = m[flon.index,flat.index,]*nee #apply spatial mask to NEE input from PVPRM  |  |  |  |  |  |  |  |
| #write out footprints convolved with model fluxes<br>conv.tower[1,paste("STILTxPVPRMSIF")] = sum(apply(mm[,,1:120],c(1,2),sum,na.rm=T))   |  |  |  |  |  |  |  |
| #Write out R data object:<br>save(conv.tower,file="carve.towerconvolved.pvprm.sif.Data")  |  |  |  |  |  |  |  |



## **Convolving footprint files – simplified steps**

#Run script: source('crv.tower.convolve.r') #creates: carve.tower.convolved.pvprm.sif.Data

##Read in R data object: convolved.data.name <- load('carve.tower.convolved.pvprm.sif.Data') #returns 'conv.tower' string convolved.data <- get(convolved.data.name')</pre>

#display output matrix of STILT footprint and footprint convolved with flux estimate from physical model: convolved.data:

|     |         |        |        |     | I                   | [ppm/(umol/m²s)] | [ppm]          |
|-----|---------|--------|--------|-----|---------------------|------------------|----------------|
| rec | JD      | Lat    | Lon    | Alt | Time                | STILT            | STILTxPVPRMSIF |
| 1   | 129.625 | 64.986 | -147.6 | 301 | 2013-05-10T15:00:00 | 6.993728         | 3.916888       |

#convolved field represents change in concentration due to the influence of upstream fluxes



# **Footprint applications - Inversions**

- Top-down estimate studies (Inversions)
  - Refine regional estimates of GHG surface fluxes
  - Can involve complex variational data assimilation
- Example: NOAA/GMD CarbonTracker-Lagrange
  - Minimize:  $\hat{s} = s_p + (HQ)^T * (HQH^T + R)^{-1} * (z Hs_p)$
  - Python code at: https://www.esrl.noaa.gov/gmd/ ccgg/carbontracker-lagrange/doc/index.html



# Papers using CARVE footprints

- Chang, R. Y.-W., et al., 2014: Methane emissions from Alaska in 2012 from CARVE airborne observations. *Proceed. National Academy Sci.*, doi:10.1073/pnas.1412953111.
- Henderson, J. M., et al., 2015: Atmospheric transport simulations in support of the Carbon in Arctic Reservoirs Vulnerability Experiment (CARVE). *Atmos. Chem. Phys.*, 15, 4093-4116, doi:10.5194/ acp-15-4093-2015.
- Zona, D., B. et al., 2016: Cold season emissions dominate the Arctic tundra methane budget. *Proceed. National Academy Sci.*, doi:10.1073/pnas.1516017113.
- Miller, S. M. et al., 2016: A multiyear estimate of methane fluxes in Alaska from CARVE atmospheric observations. *Global Biogeochem. Cycles*, 30, doi:10.1002/2016GB005419.
- Xu, et al. 2016: A multi-scale comparison of modeled and observed seasonal methane emissions in northern wetlands. *Bio. Geo. Sc.*,13, 5043–5056, doi: 10.5194/bg-13-5043-2016.
- Luus, K. A., et al., 2017: Tundra photosynthesis captured by satellite-observed solar-induced chlorophyll fluorescence, *Geophys. Res. Lett.*, *44*, doi:10.1002/2016GL070842.
- Commane, R. et al., 2017: Carbon dioxide sources from Alaska driven by increasing early winter respiration from Arctic tundra budget. *Proceed. National Academy Sci.*, doi: 10.1073/pnas. 1618567114.
- Hartery, S. et al., 2018: Estimating regional-scale methane flux and budgets using CARVE aircraft measurements over Alaska, Atmos. Chem. Phys., 18, 185-202, doi: 10.5194/acp-18-185-2018.



#### Stepping back: WRF High-Resolution meteorological fields

- High-resolution meteorological fields used to drive STILT are available

   Fields: http://www2.mmm.ucar.edu/wrf/users/docs/user\_guide\_V3.9/ users\_guide\_chap5.htm#fields
- Period of record (same as footprints):
  - CARVE WRF domains (mainland Alaska): 20120101 to 20160830
  - CARVE-CAN WRF domains (Mackenzie river delta): 20140501 to 20170330
- Spatial grid: 30, 10 and 3.3 km, 41 vertical levels
- Temporal availability: d01 and d02: hourly; d03: 30 minutes
- Reanalysis products (e.g., NARR, MERRA(2), ERA-5) are on ~30-km grid at best



### **Step 1 - CARVE WRF domain placement**

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41 vertical levels





### **Step 1 - CARVE-CAN domain placement**

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41 vertical levels





#### Sample WRF fields – terrain height







#### **Sample WRF fields – terrain height**

#### 151.5°W 151°W 150.5°W 150°W 149.5°W 149°W 148.5°W 148°W 147.5°W 147°W 146.5°W 146°W 145.5°W 145°W 144.5°W



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#### **Sample WRF fields – Soil temperature**

151.5°W 151°W 150.5°W 150°W 149.5°W 149.5°W 148.5°W 148.5°W 147.5°W 147.5°W 146.5°W 146.5°W 145.5°W 145.5°W 145.5°W 144.5°W



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# **Sample WRF fields - SWDOWN**





# Value of high-res WRF over reanalyses



- Tanacross, AK, windstorm event of 17 September 2012
- Domain 1 30-km grid spacing (panel b) does not support downslope windstorm that is present in innermost domain 3 (3.3-km grid; panel a)



# **Bias during 2012 aircraft campaign**

| Surface Variable                     | May   | June  | July  | August | September | 2012<br>Campaign |
|--------------------------------------|-------|-------|-------|--------|-----------|------------------|
| 2-m Temperature (K)                  | -2.24 | -1.81 | -1.60 | -1.08  | -0.70     | -1.44            |
| 2-m Dewpoint temperature (K)         | 1.11  | 0.11  | -0.74 | -0.63  | -0.04     | -0.10            |
| 10-m Wind speed (m s <sup>-1</sup> ) | -0.67 | -0.47 | -0.30 | -0.32  | 0.25      | -0.29            |
| 10-m Wind direction (deg)            | 4.7   | 3.3   | 1.6   | 4.6    | 4.1       | 3.7              |

- Trends in surface temperature and moisture evident
- Overall error values compare well with literature



# **Temperature bias plots for 2012**











- Location of largest negative temperature bias mirrors northward progression of thaw
- Potentially related to inadequate representation of soil moisture/state



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# PBL Height Validation: Daily 0000 UTC



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#### **Future Work**

- Update WRF-STILT to Polar WRF v3.9: Improved land use (21-cat IGBP MODIS) and terrain height (30-arc-second USGS GMTED2010) datasets
- Design new unified WRF domain for ABoVE and its aircraft campaigns

#### **ArctiCAP Airborne Measurements**







- Generate footprints for 2017 Arctic Carbon Atmospheric Profiles (ArctiCAP) campaign and NOAA/ECCC towers
- Rerun CARVE-era receptors using WRF v3.9



# Summary

- Multi-year library of footprints on ASC
- Simple netcdf format enables use by all ABoVE community
- Code/scripts available for processing:
  - reading/writing, convolving, inclusion in formal inversions
- High-spatial and temporal WRF fields can be requested
- We are here to help apply these datasets to your current and future research:
  - Mailing list will soon be available
  - Biophysical model experts are part of ABoVE
  - AER: transport modeling for ABoVE (jhenders@aer.com)

