PuffR

An integrated system
for dispersion modelling
with CALPUFF


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Dispersion Modelling as a Means to Characterize Regional Air Quality

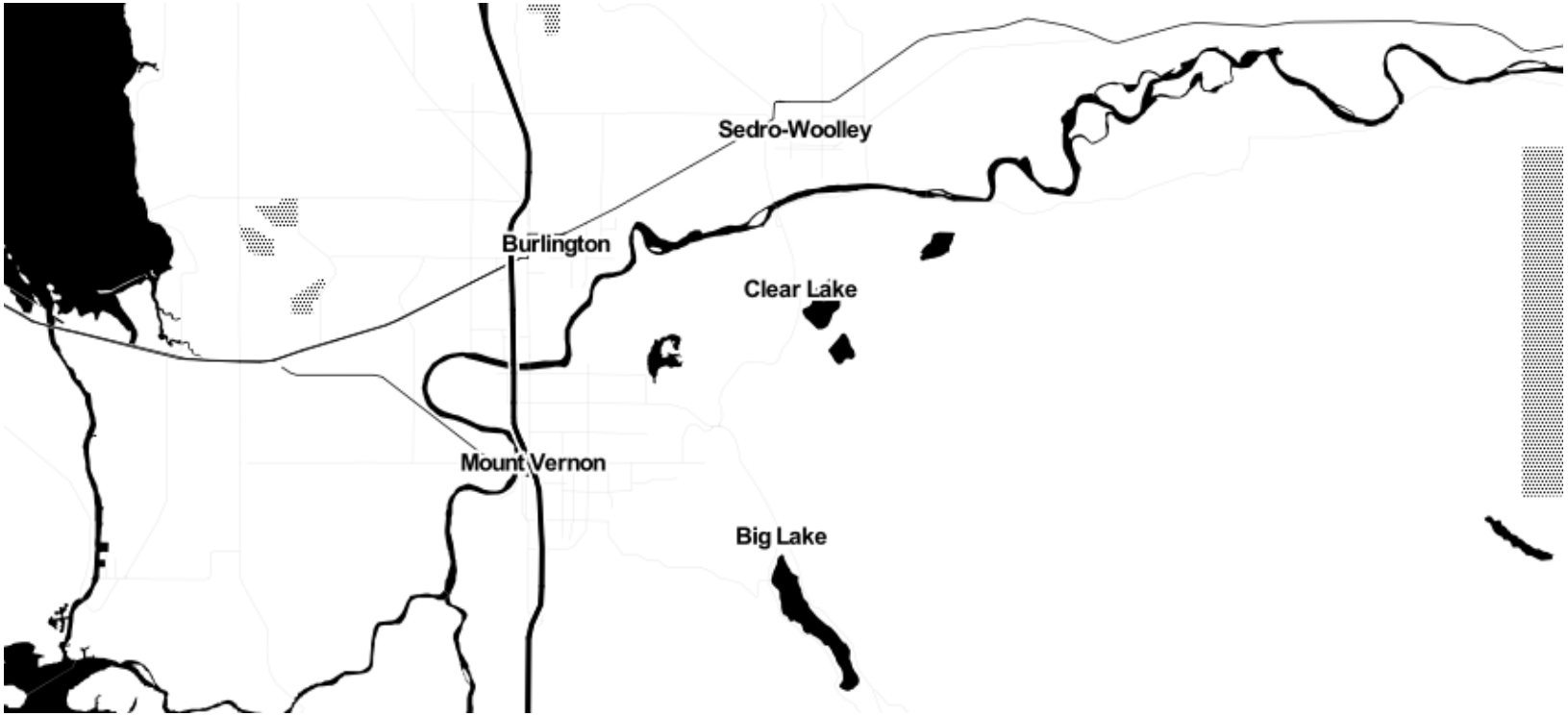
Dispersion modelling is a great tool for understanding how pollutants disperse from sources to receptors.

Air quality modelling is a great tool for describing the causal relationship between emissions, meteorology, atmospheric concentrations, deposition, and other factors. Air pollution measurements give useful quantitative information about ambient concentrations and deposition, however, such measurements can only describe air quality at specific locations and times.

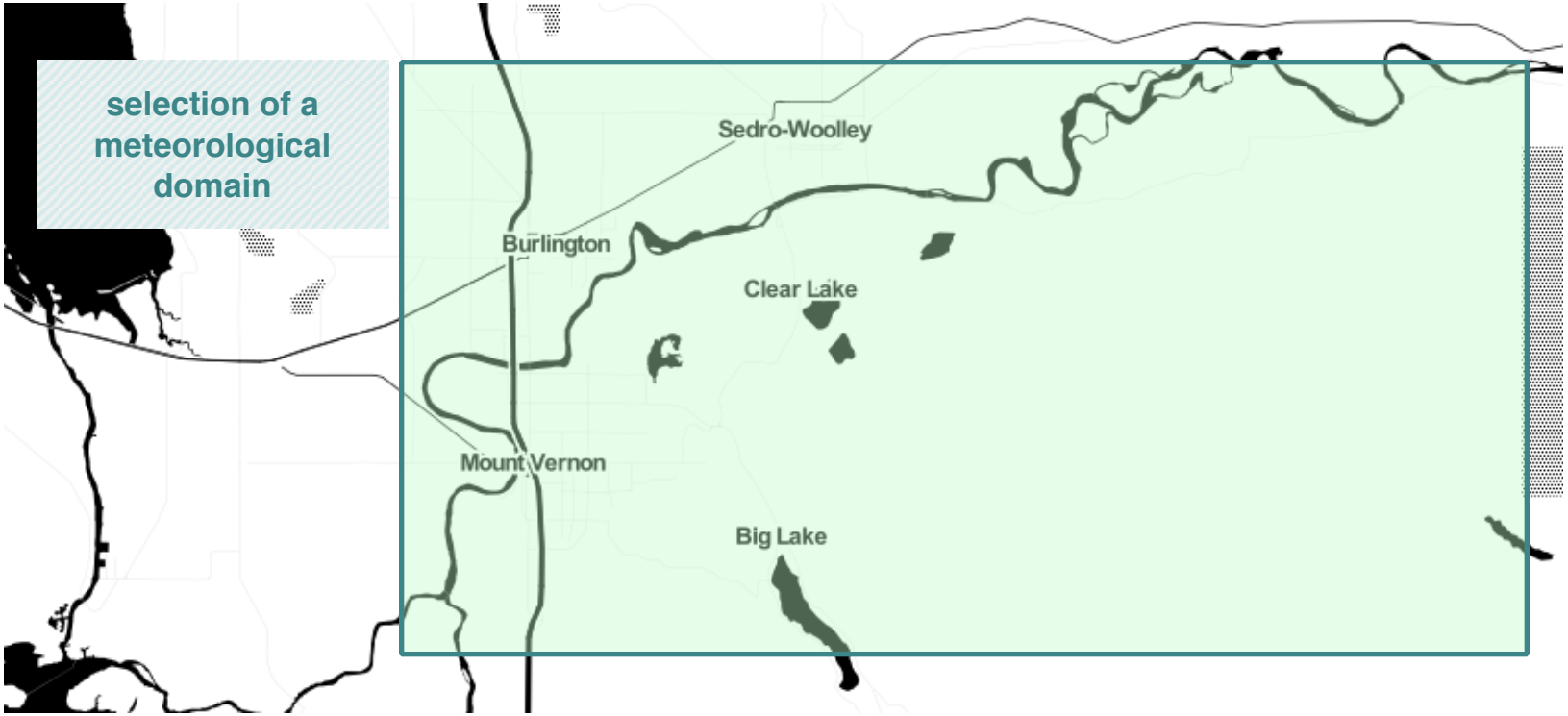
Moreover, monitoring usually doesn't provide very good information concerning the causes of the air quality problem.

Dispersion modelling can instead provide a more complete deterministic description of the air quality problem, including an analysis of factors and causes (e.g., emission sources, meteorological processes, physical changes, and chemistry). Air quality models play an important role in science and in policy, because of their capability to assess the relative importance of the relevant processes and to provide an assessment of potential human exposure.

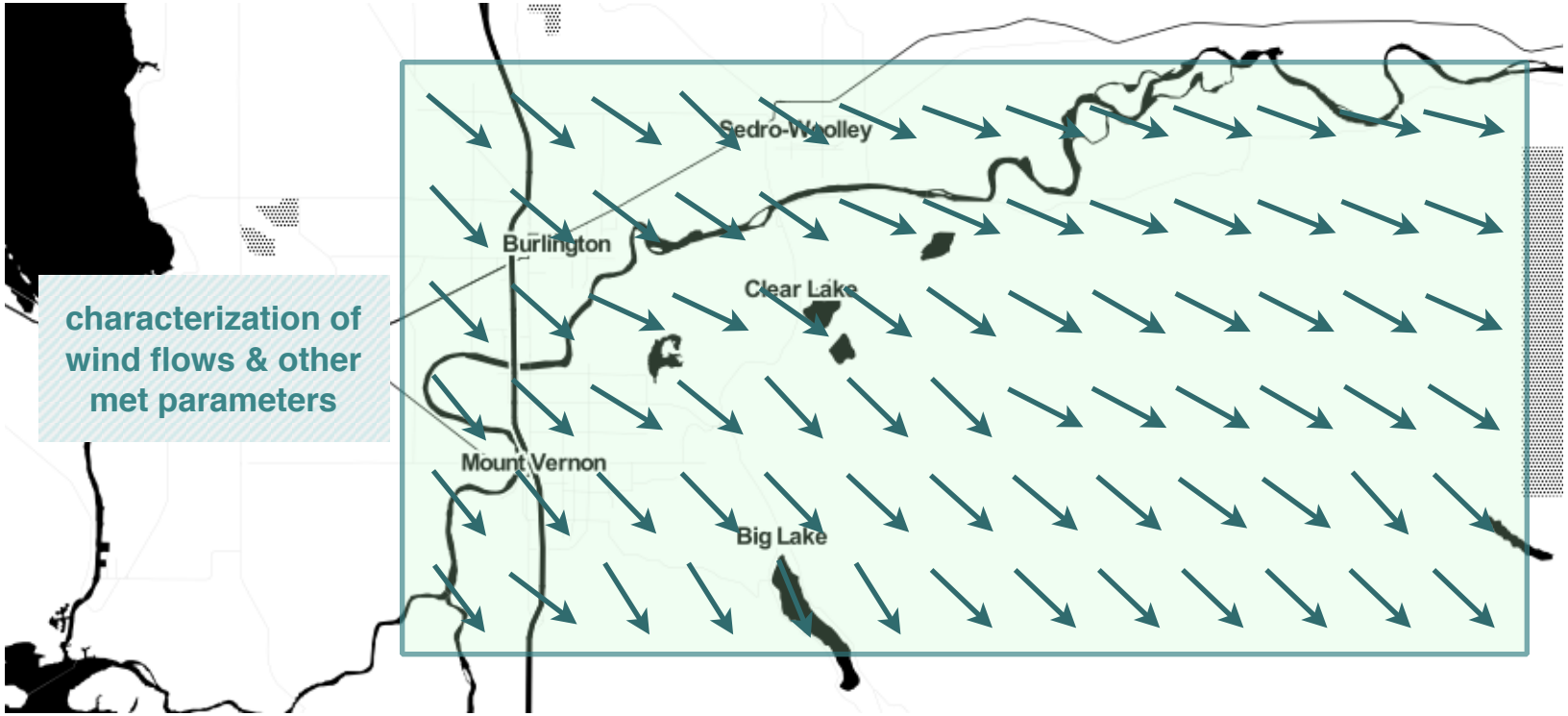
Basic Scheme for How Dispersion Models Work



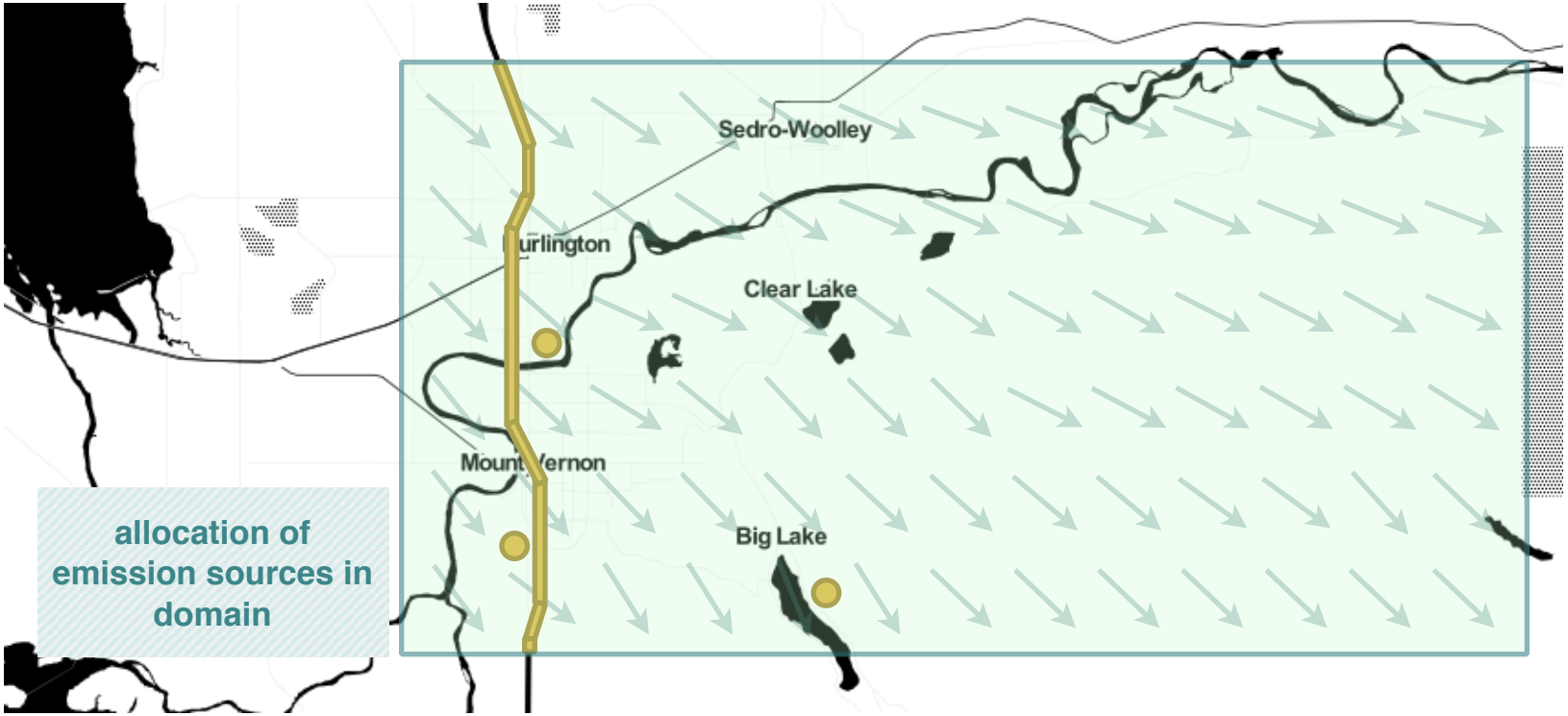
Basic Scheme for How Dispersion Models Work



Basic Scheme for How Dispersion Models Work



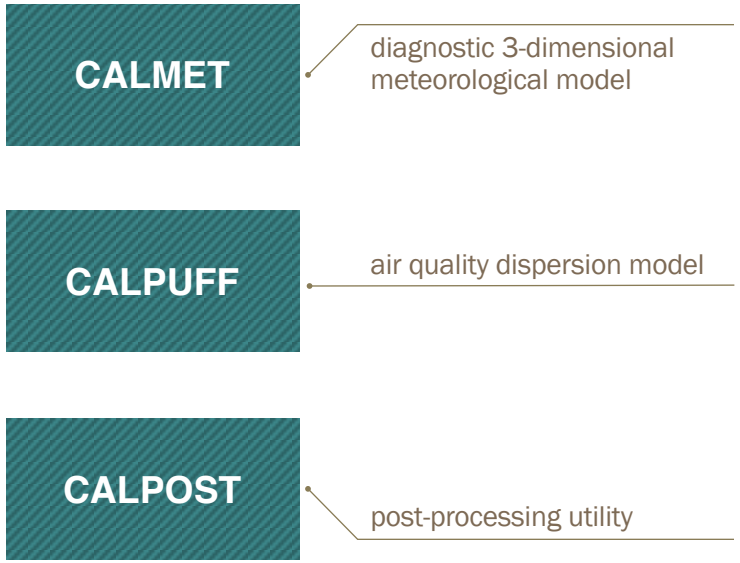
Basic Scheme for How Dispersion Models Work



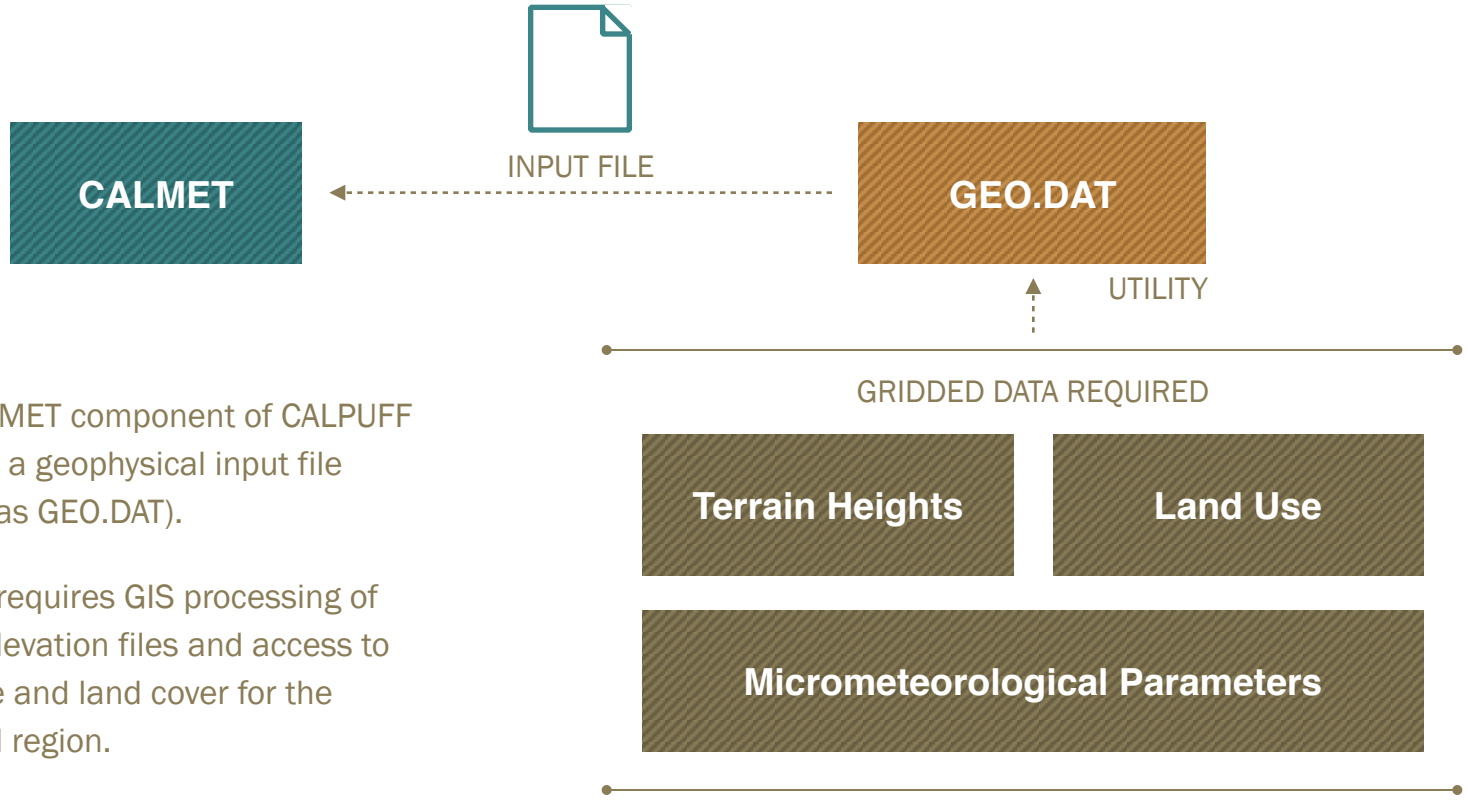
The CALPUFF Modelling System

The CALPUFF modelling system consists of a collection of formatted input files and binary executables.

The CALPUFF modelling system consists of three main components and a set of preprocessing and postprocessing programs. The main components of the modelling system are CALMET, CALPUFF, and CALPOST (typically used in that order). A number of utility programs aid in the production of the necessary input files.



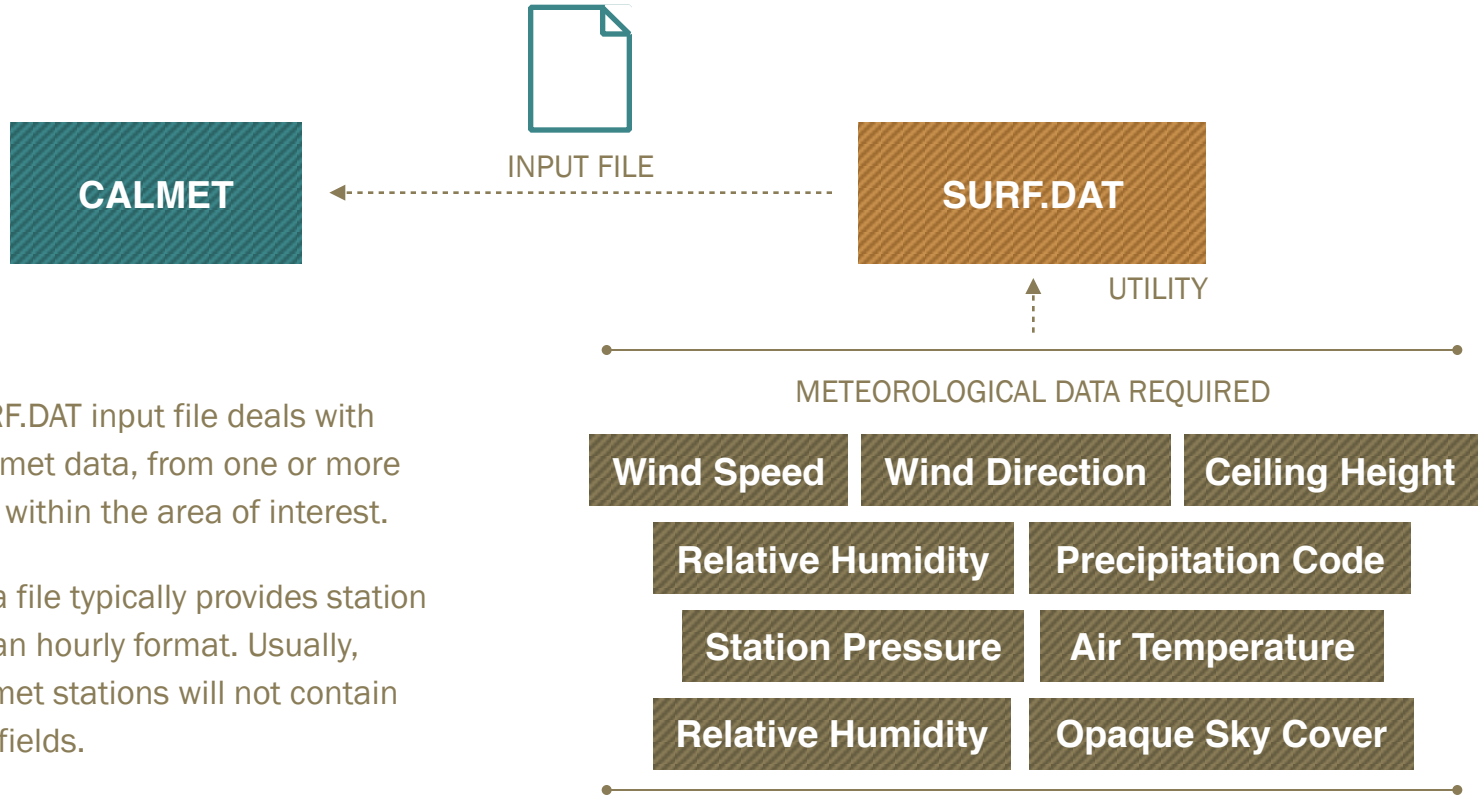
CALMET Primer: Geophysical Data



The CALMET component of CALPUFF requires a geophysical input file (known as GEO.DAT).

The file requires GIS processing of digital elevation files and access to land use and land cover for the selected region.

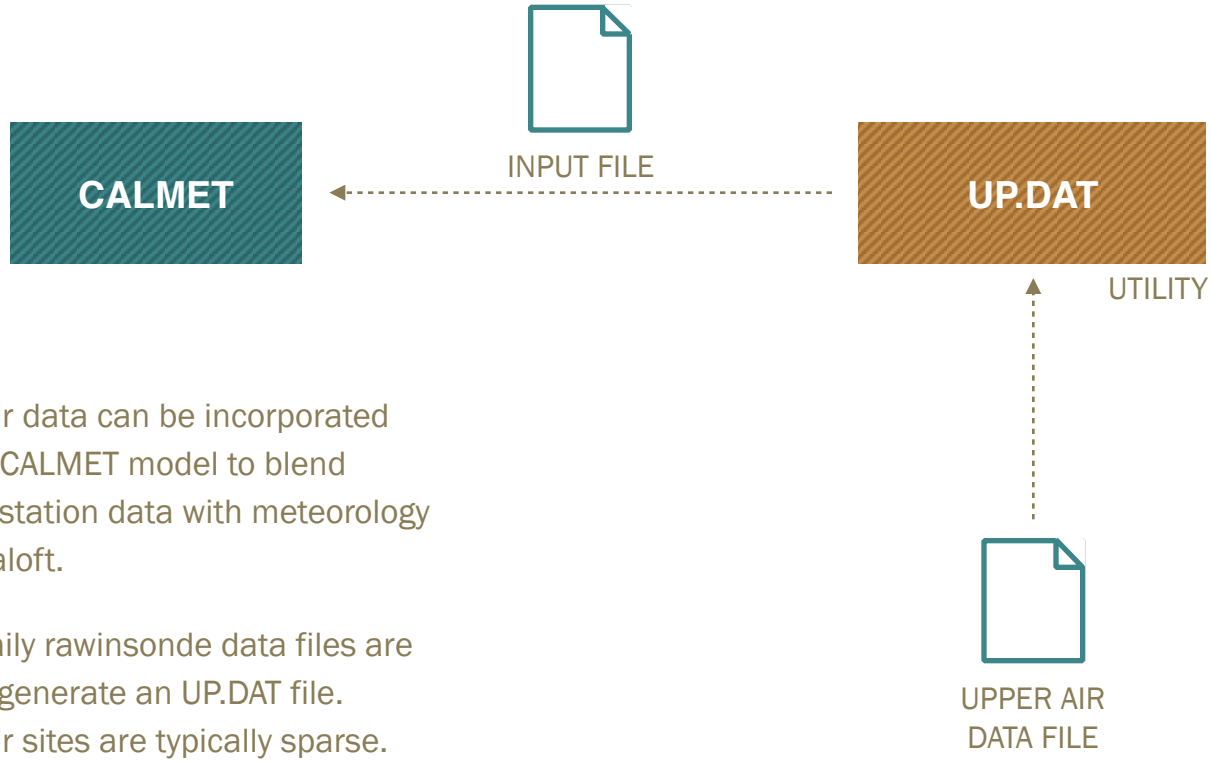
CALMET Primer: Surface Met Data



The SURF.DAT input file deals with surface met data, from one or more stations within the area of interest.

The data file typically provides station data in an hourly format. Usually, nearby met stations will not contain all data fields.

CALMET Primer: Upper Air Data



Upper air data can be incorporated into the CALMET model to blend surface station data with meteorology further aloft.

Twice-daily rawinsonde data files are used to generate an UP.DAT file. Upper air sites are typically sparse.

CALMET Primer: Control File

The CALMET input file contains a large variety of model option, parameters, and I/O settings.

These controls are split across several input groups:

- 1 / Temporal Parameters
- 2 / Grid & Levels
- 3 / Output Options
- 4 / Met Data Options
- 5 / Wind Field Options & Parameters
- 6 / Mixing Height, Temperature, Precipitation Parameters
- 7 / Station Parameters

CALMET Primer: Model Execution

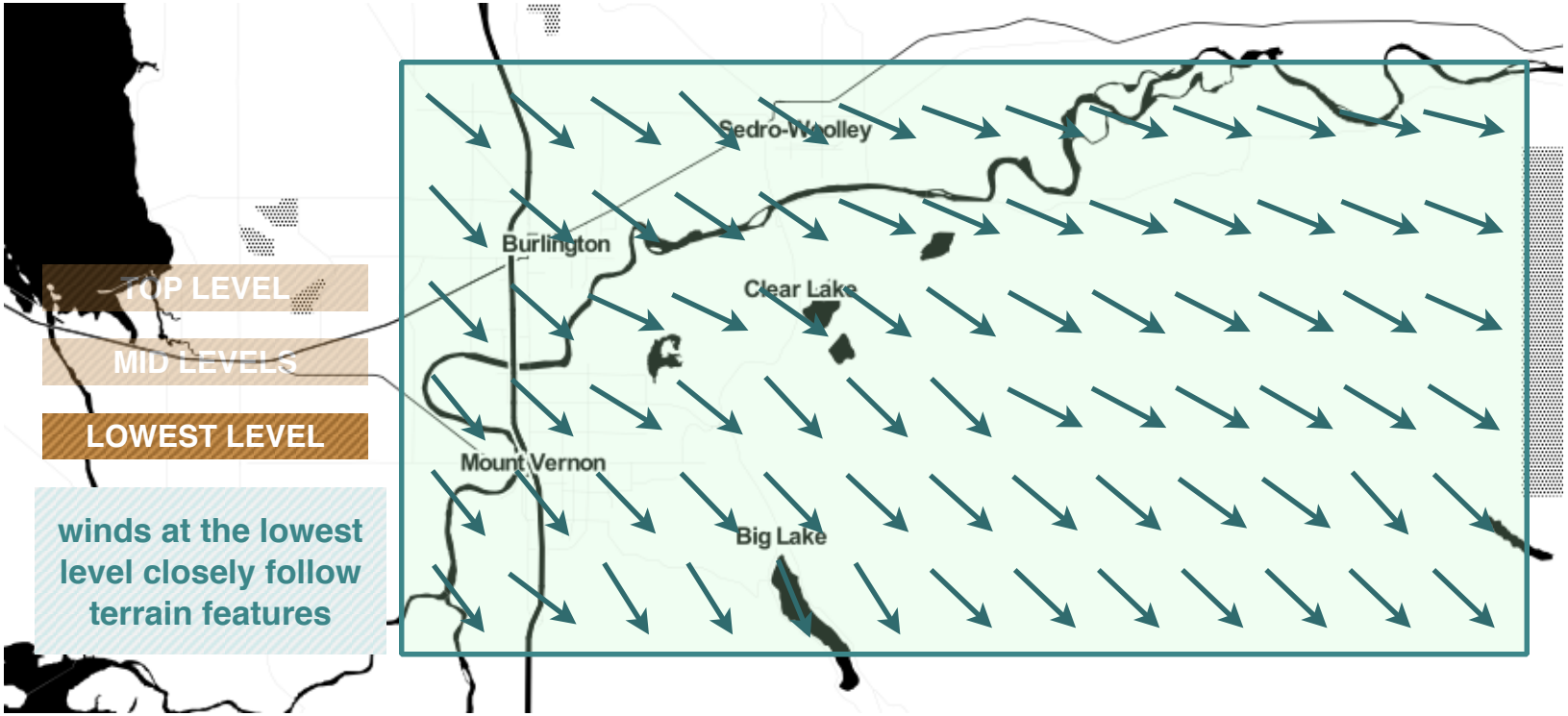
CALMET binary output file; it's for CALPUFF

The CALMET model is to be run with the input file and the associated input data files.

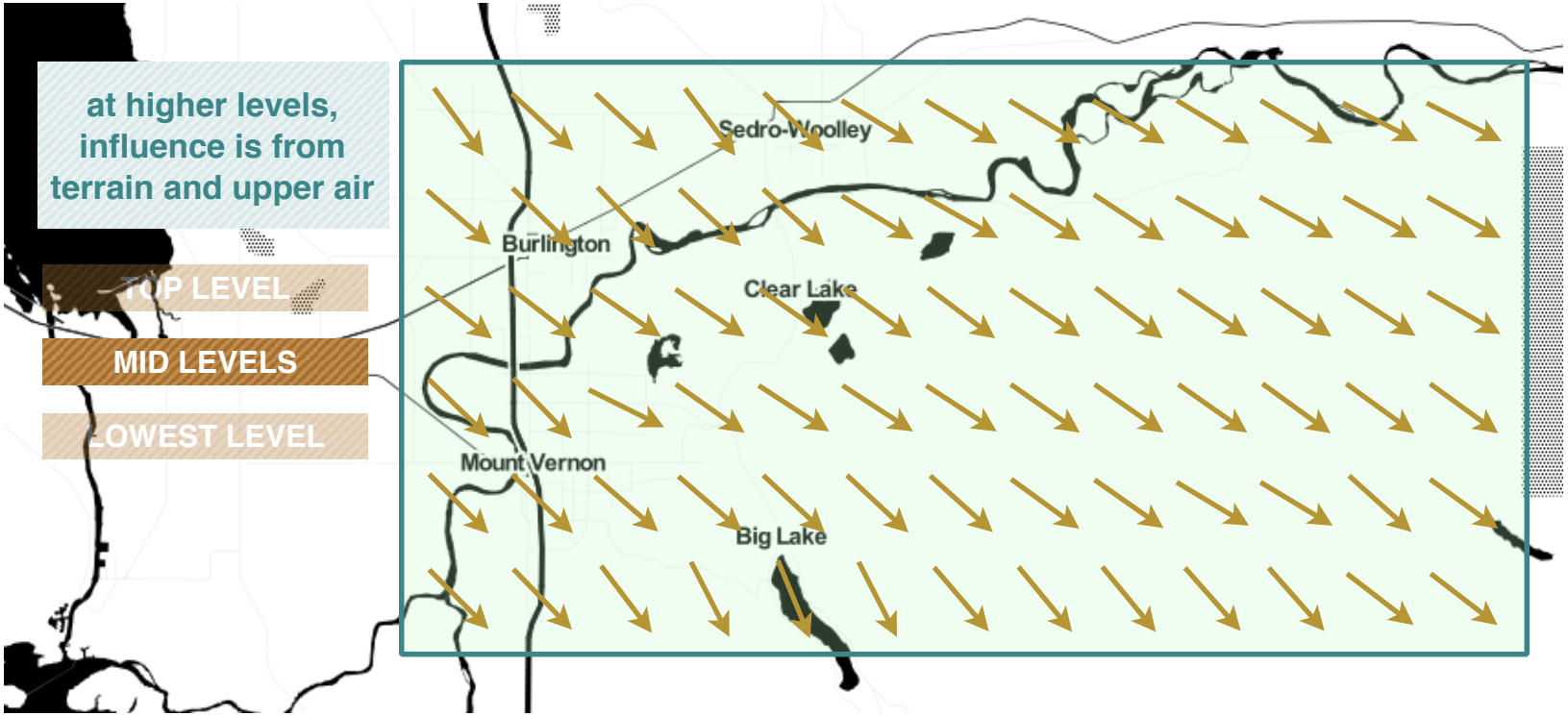
There are several other types of input data files that could be used, depending on model settings:

- **Precipitation Data File**
- **Overwater Station Files**
- **Gridded Cloud Field File**
- **Preprocessed Met Data for Diagnostic Wind Module**
- **Hourly Gridded Wind Fields**

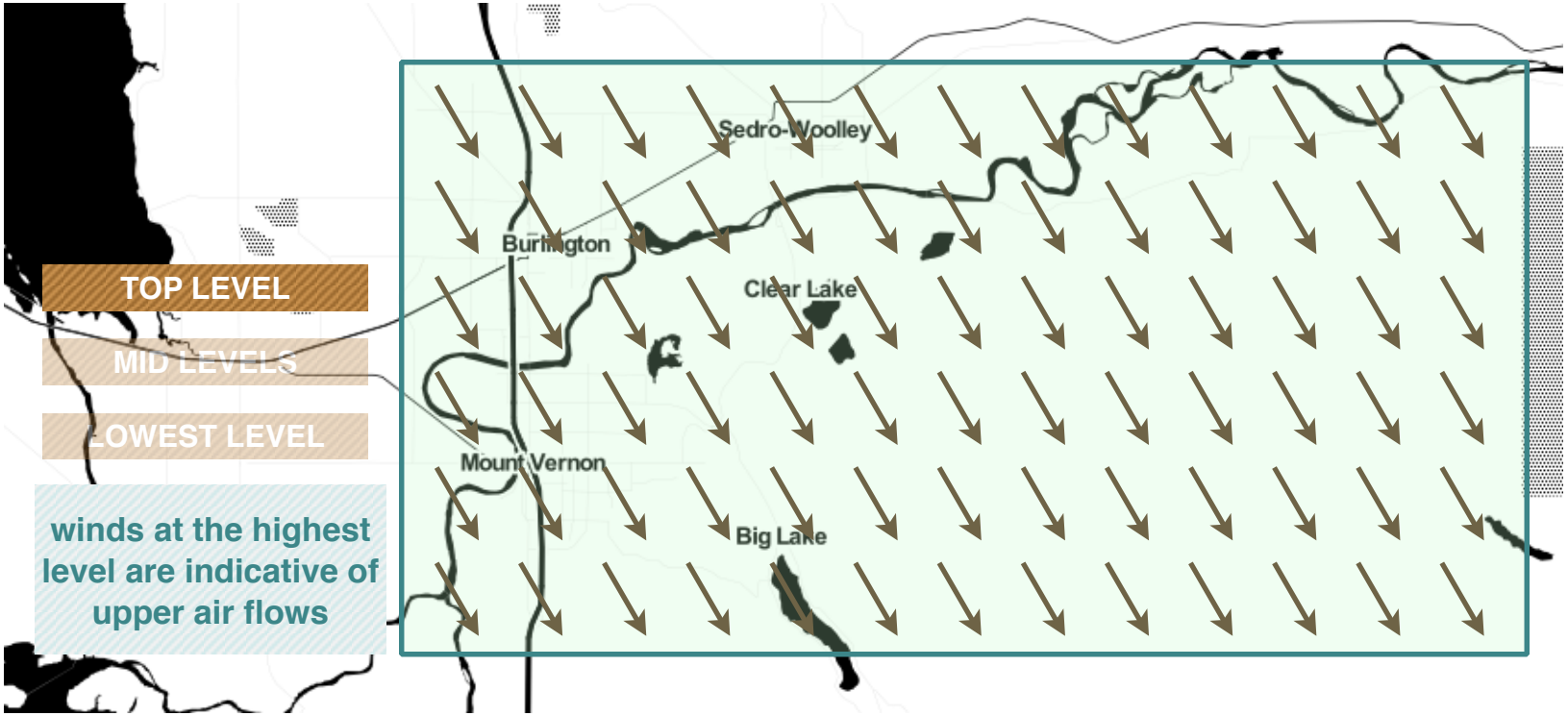
CALMET Primer: Model Wind Fields



CALMET Primer: Model Wind Fields



CALMET Primer: Model Wind Fields

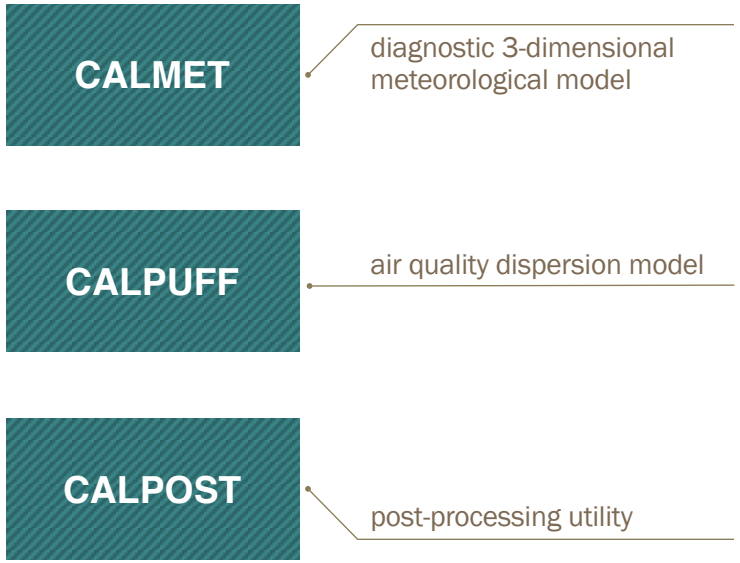


The CALPUFF Modelling System

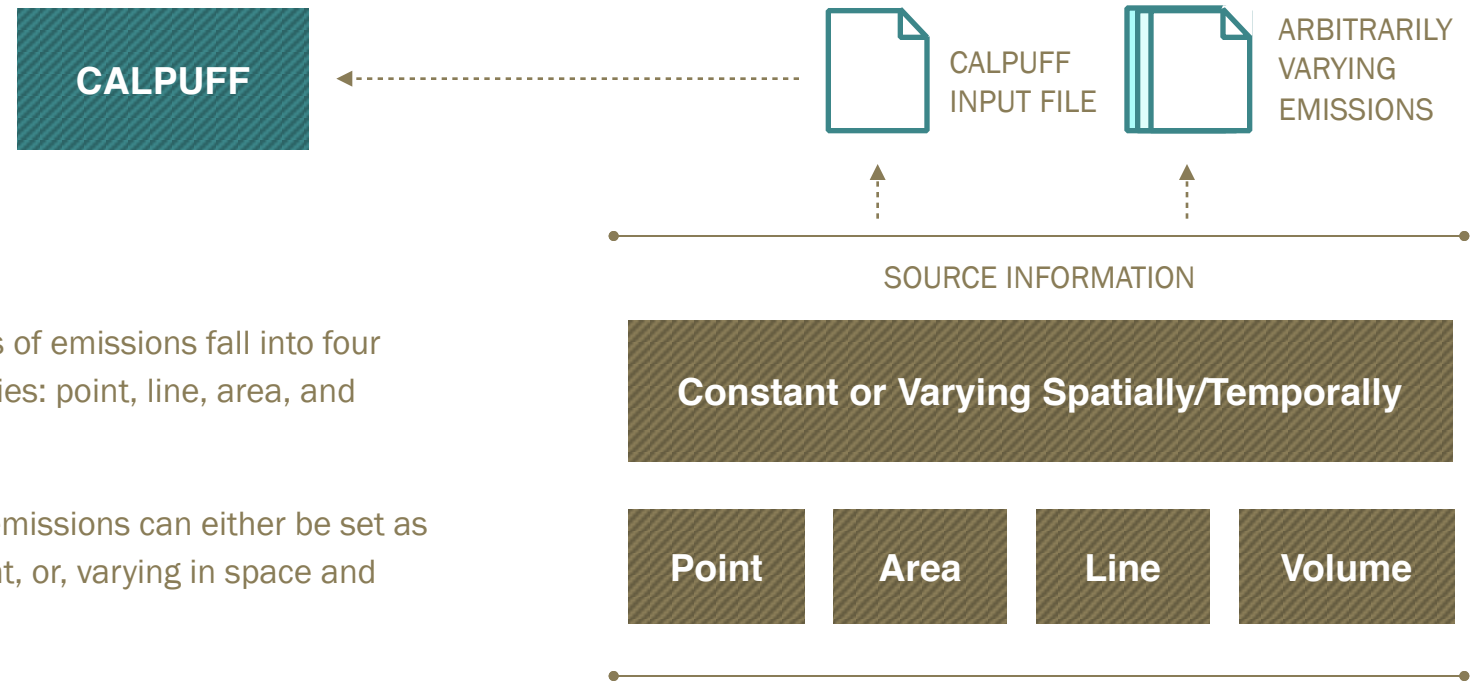
After running the CALMET model, inputs to CALPUFF must be prepared.

The CALPUFF air quality dispersion model requires CALMET model output and a properly formatted CALPUFF input control file.

The CALPUFF input control file contains a vast array of options for defining a dispersion model.



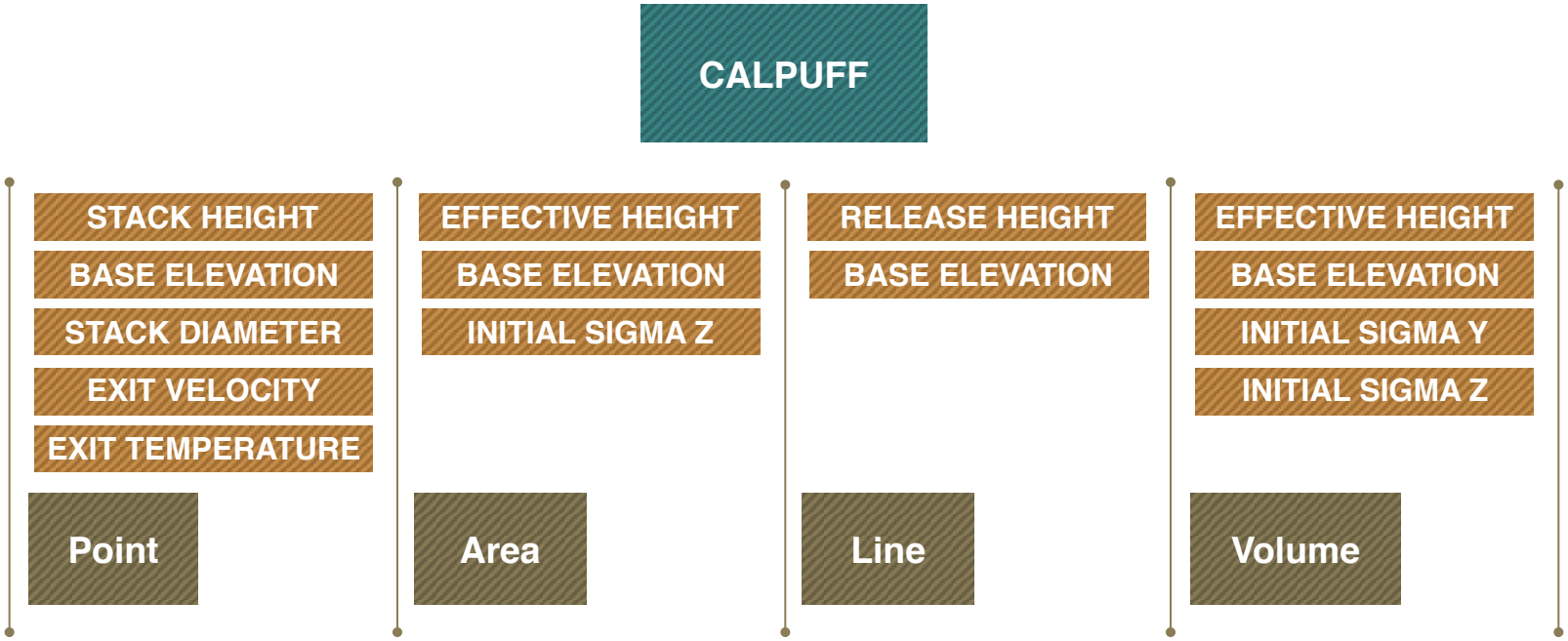
CALPUFF Primer: Sources



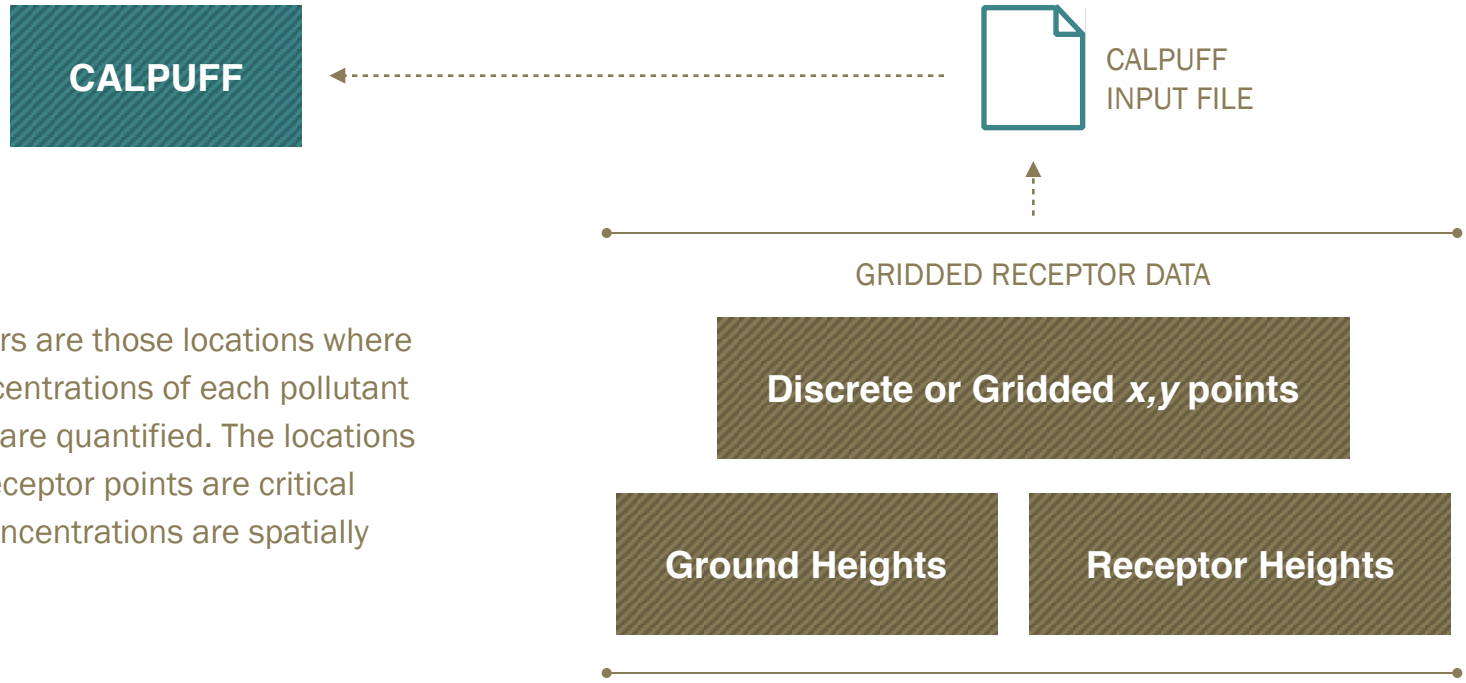
Sources of emissions fall into four categories: point, line, area, and volume.

These emissions can either be set as constant, or, varying in space and time.

CALPUFF Primer: Source Parameters



CALPUFF Primer: Receptors



Receptors are those locations where the concentrations of each pollutant species are quantified. The locations of the receptor points are critical since concentrations are spatially varied.

CALPUFF Primer: Model Execution

CALPUFF binary output file; it's for CALPOST

The CALPUFF model is to be run with the input file and the associated input data files.

There are several other types of input data files that could be used, depending on model settings:

- **Coastline Data File**
- **Hydrogen Peroxide Data**
- **Ozone Data**
- **Ammonia Data**
- **Background Conditions**
- **Arbitrarily Changing Point, Area, Line, or Volume Sources**

Contents

Main Goals

The workflow for atmospheric dispersion modelling with CALPUFF needs to be reconsidered—both in the interest of saving time and ensuring that the quality of the input data is high

There are many goals for the PuffR package. Here are some of the ways PuffR can provide some value.

data visualizations generated at each step of the process

rely on sensible defaults and DRY principles to automate mundane data collection tasks

useful help system and example library to aid in the understanding of every model setting

automatically collect and process the best data available

Data Visualization

CALPUFF requires (and generates!) a lot of data. It would be nice to visualize that.

If it's not visualized, how can we make sense of the data? Visuals confirm what we might know and they allow us to explore the data and more easily find connections and patterns.

The ocular nerve should be used for more than looking at pages of plaintext data tables.

data visualizations generated at each step of the process

- TERRAIN MAPS
- WIND VECTORS
- STABILITY CLASSES
- SOURCES
- RECEPTORS
- CONCENTRATIONS
- VERTICAL PROFILES
- ANIMATIONS

Sensible Defaults

Much of the time, atmospheric dispersion modelling follows a predictable workflow.

Reducing the need to repeat information across different tasks can reduce the possibility for user error.

Reducing the need to specify commonly-used settings and parameters is also great. If you need to drill down and modify things, that's possible (but won't be often required).

rely on sensible defaults and DRY principles to automate mundane data collection tasks

Documentation and Examples

It cannot be understated how important a good documentation system is for complex tasks.

To aid in understanding of what is actually going on when you conduct model runs, a help system is vital. You'll learn more.

I'm a big believer in using examples to learn about why certain things are done. To that end, full-featured examples will be provided as part of the PuffR package.

useful help system and example library to aid in the understanding of every model setting

- THEORY
- SETTINGS
- PARAMETERS
- CASE STUDIES
- EXAMPLES
- DEFINITIONS
- SEARCHABLE INDEX

Automation of Data Collection

There is an staggering quantity of publicly-available data. PuffR will collect some of that on your behalf.

A model is nothing without good input data. Fortunately there is plenty of no-cost source data, and, PuffR will obtain the best data and prepare the appropriate input data files.

The aim is to allow for the automated preparation of CALMET input data for the widest range possible of global locations.

automatically collect and process the best data available

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Summary of Data Sources

Type of Data	Name and Description	Provider
Surface Station Meteorology	1-Hourly Datasets for Global Meteorological Stations	National Climatic Data Center (NCDC)
Upper Air Data	RAOB Radiosonde Database	Earth System Research Laboratory (ESRL) and National Oceanographic and Atmospheric Administration (NOAA)
Surface Elevation	1 // U.S. National Elevation Data (NED) 2 // Canadian Digital Elevation Data (CDED) 3 // Global SRTM V4 GeoTIFF Archive	1 & 3 // U.S. Geological Survey (USGS) 2 // GeoBase.ca
Land Use and Land Cover	1 // U.S. National Land Cover Data (NLCD) 2011 2 // GeoBase Land Cover Product (Canada) 3 // GlobCover 2009 (Global Land Cover Map) 4 // MODIS Gridded Land Cover Data	1 // U.S. Geological Survey (USGS) / Multi-Resolution Land Characteristics Consortium (MRLC) 2 // GeoBase.ca 3 // European Space Agency (ESA) data user element (due) 4 // MODIS

Hourly Surface Met Station Data

The National Climatic Data Center (NCDC) has an archive of hourly (and sub-hourly) surface station data. It's coverage is global.

Surface station data is essential if you're not running CALPUFF solely with prognostic meteorological fields (e.g., WRF, RUCS, etc.).

Even if you do have modelled met fields, the surface station station can be blended together with that (i.e., running a hybrid model).

```
027071785099999200601010000 4+49017-122783SY-SA+0013CWWK
007071785099999200601010100 4+49017-122783SAO  +0013CWWK
007071785099999200601010200 4+49017-122783SAO  +0013CWWK
007071785099999200601010300 4+49017-122783SAO  +0013CWWK
007071785099999200601010400 4+49017-122783SAO  +0013CWWK
007071785099999200601010500 4+49017-122783SAO  +0013CWWK
027071785099999200601010600 4+49017-122783SY-SA+0013CWWK
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007071785099999200601010800 4+49017-122783SAO  +0013CWWK
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007071785099999200601011000 4+49017-122783SAO  +0013CWWK
007071785099999200601011100 4+49017-122783SAO  +0013CWWK
026071785099999200601011200 4+49017-122783SY-SA+0013CWWK
007071785099999200601011300 4+49017-122783SAO  +0013CWWK
007071785099999200601011400 4+49017-122783SAO  +0013CWWK
007071785099999200601011500 4+49017-122783SAO  +0013CWWK
007071785099999200601011600 4+49017-122783SAO  +0013CWWK
007071785099999200601011700 4+49017-122783SAO  +0013CWWK
007071785099999200601011900 4+49017-122783SAO  +0013CWWK
007071785099999200601012000 4+49017-122783SAO  +0013CWWK
```

Upper Air Rawinsonde Data

Upper air data: because the met observations are not the same at the surface as they are further aloft.

CALMET generates meteorological data fields within the *x*,*y* grid of cells for every *z* level specified. Upper air soundings provide vital data for wind, temperatures, and pressure values well above the surface.

The RAOBS archive contains twice-daily global soundings. UP.DAT files can be made from them.

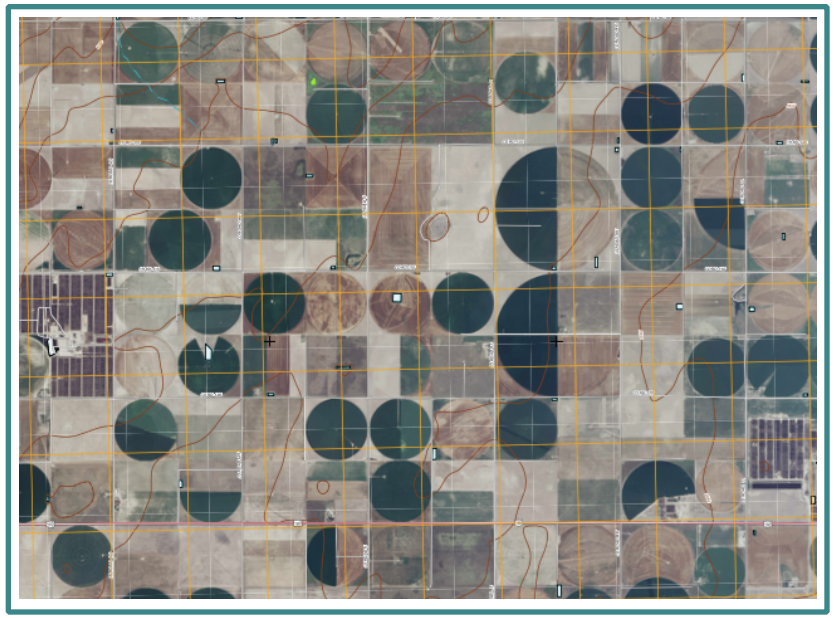
```
   254      0      7      NOV    2014
     1   3990  72249  32.80N 97.30W   196    2307
     2     70    122   1350    151  99999       3
     3           FWD                99999      kt
     9  10020    196    202     32     20       7
     4  10000    212    200     30     20       8
     6   9545    609  99999  99999     20      14
     4   9250    877    146    -54     20      18
     6   9209    914  99999  99999     25      20
     5   9120    996    138    -82  99999   99999
     5   9030   1079    132   -118  99999   99999
     6   8880   1219  99999  99999     25      22
     5   8800   1294    120    -60  99999   99999
     5   8510   1572    102    -78  99999   99999
     4   8500   1585    102    -68     10      21
     6   8253   1828  99999  99999     20      30
     5   8190   1891     82    -48  99999   99999
     5   8010   2073     72    -68  99999   99999
     6   7952   2133  99999  99999     25      23
     5   7860   2228     74   -116  99999   99999
```

Surface Elevation Data

The knowledge of surface elevation and presence of coastlines has a great effect on near-surface wind flow.

There are many high-resolution terrain datasets that PuffR can use to generate gridded surface elevation fields for the CALMET GEO.DAT file.

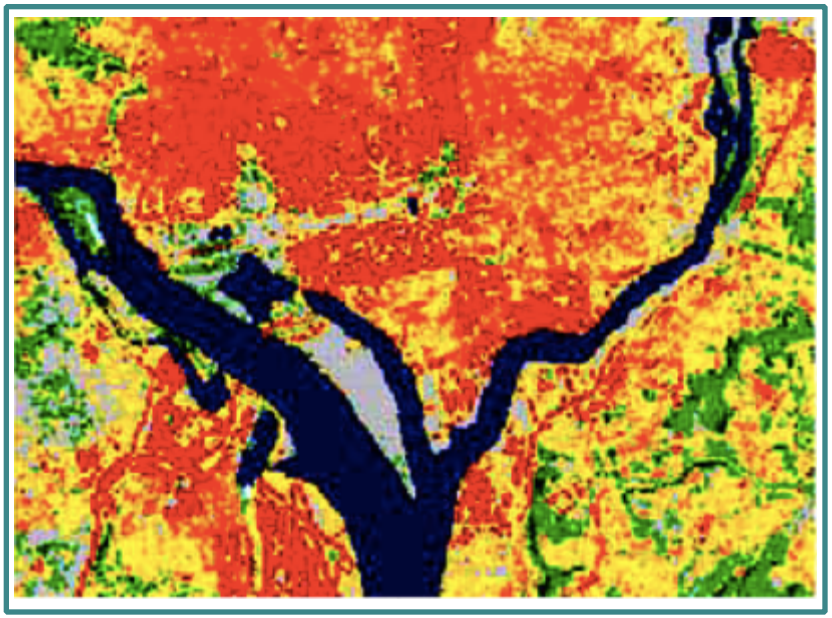
In the U.S., the National Elevation Data (NED) product is best. In Canada, it's Canadian Digital Elevation Data (CDED). Globally, the SRTM V4 GeoTIFF Archive is suitable.



Land Use and Land Cover

The characteristics of the land have a marked effect on the wind flow and a host of micrometeorological parameters.

Different world jurisdictions have their own land use and land cover databases. The GlobCover Global Land Cover Map provides a standardized dataset for land cover. While the data sources are diverse, a goal off the PuffR project is to incorporate as many of these datasets as possible. This data is essential.



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Where to Get the Installers

There are two places where you must go to get software installed. It'll be worth it.

r-project.org

What's R? It's a free software environment for statistical computing and graphics. It compiles and runs on a wide variety of UNIX platforms, Mac OS X, and Windows.

rstudio.com

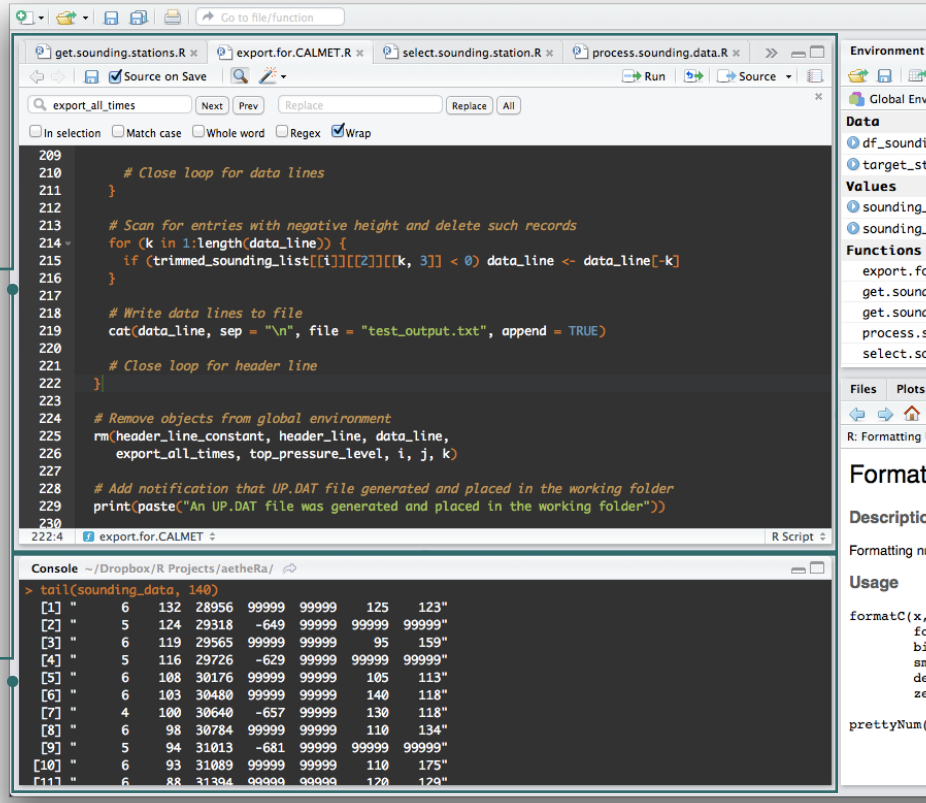
RStudio is an IDE that provides a great set of tools for working in R. You get a code editor, a console, and a customizable panes for package management, navigating local files, source control, etc.

Some Information on RStudio: that Excellent IDE for R

Basic overview on where stuff is.

source

console



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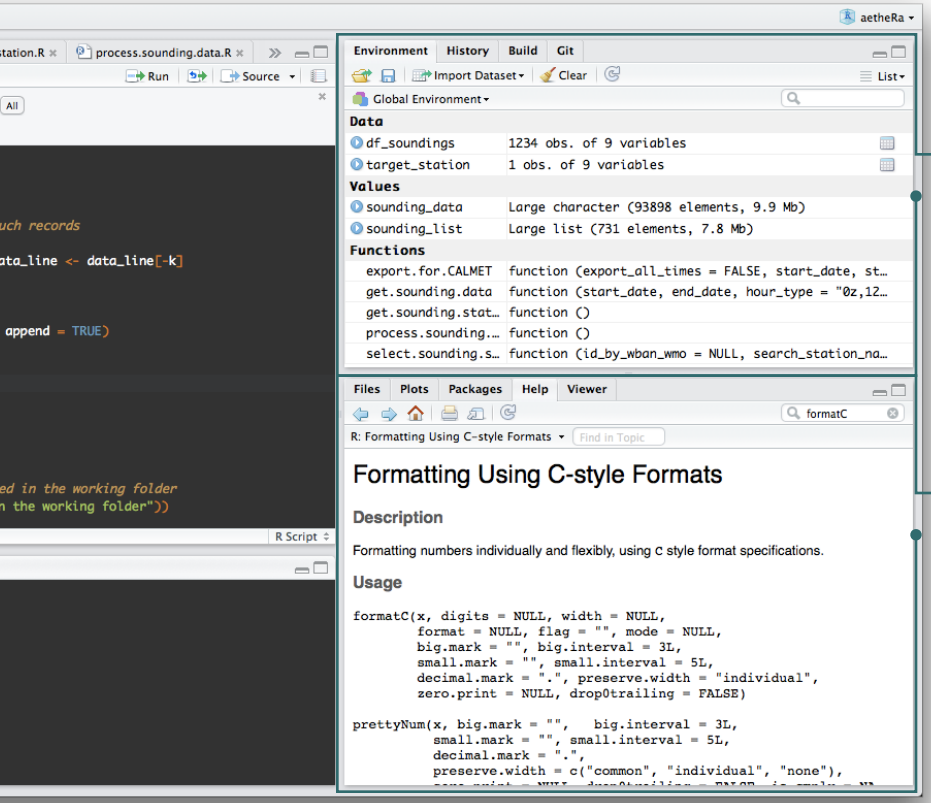


environment
history
build (optional)
version control (optional)

files
plots
packages
help
viewer

How to get the development version of PuffR

Getting the development version of PuffR is not very complicated. Just follow these steps.

You have R and possibly RStudio? Great! The next thing to do is make certain that you have the 'devtools' package installed. It's a package that makes it easy to install R packages that are not on CRAN (the Comprehensive R Archive Network). Just type this into the R console:

```
install.packages(devtools)
```

The PuffR package source code is hosted on GitHub. However, you don't need to visit the repository to get the package installed. Simply use the following command in the R console:

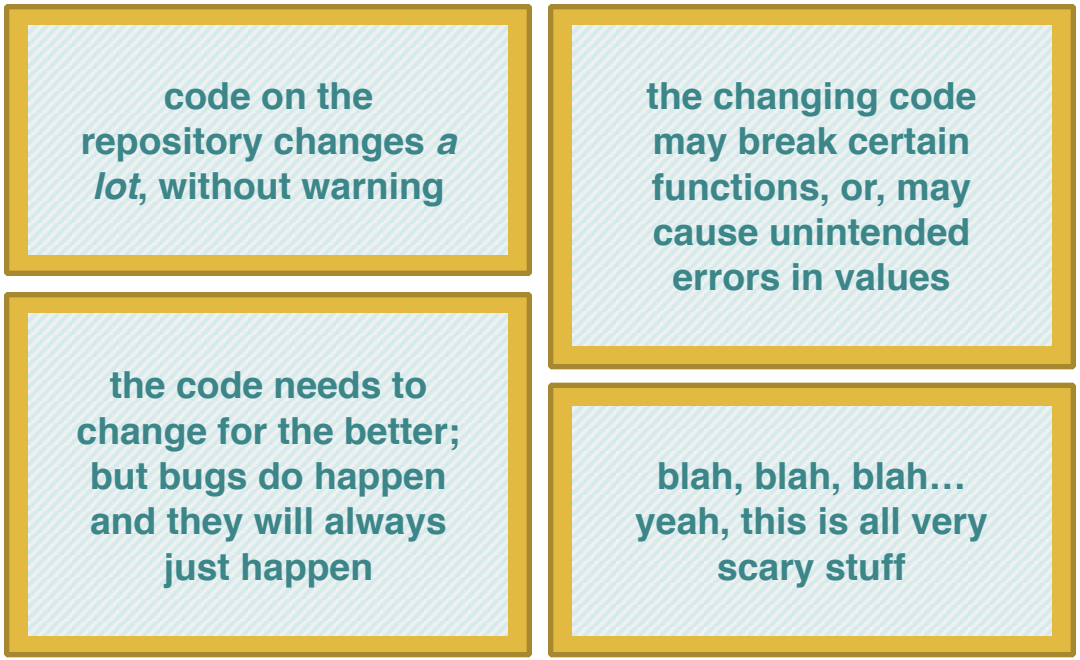
```
install_github('PuffR', 'rich-iannone')
```

Then you should have it. Between sessions, you may have to use the following command to load the package:

```
require(PuffR)
```

Otherwise, the PuffR functions will not be available for use.

General Warnings about Packages in Active Development



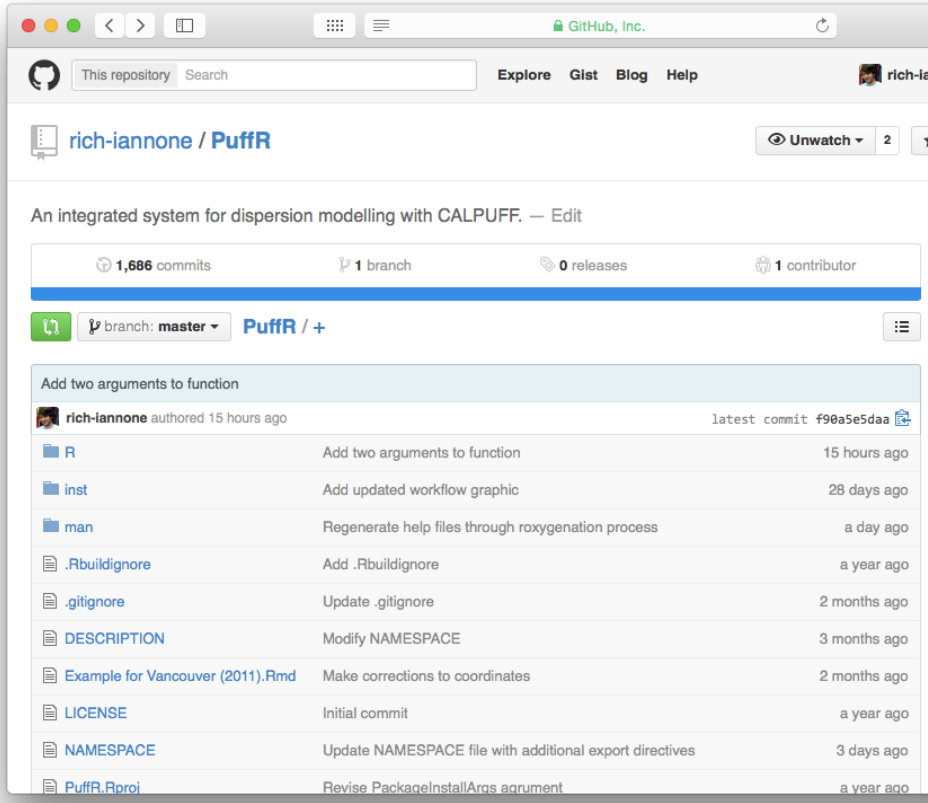
The PuffR Source Repository on GitHub

The source for the PuffR package lives on GitHub. Have a peek at the code or the README, if you're so inclined.

Point your browser to this address:

https://github.com/rich-iannone/PuffR

If you're a member of GitHub and you like what you see. Give me a ⭐— I really appreciate my stargazers.



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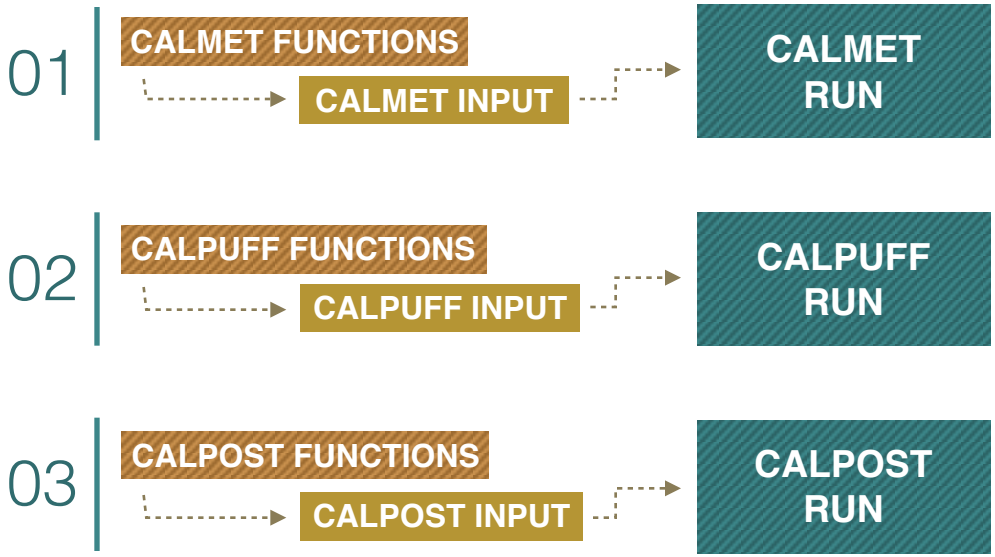
From CALMET to CALPOST— It's Functions All the Way Down

The PuffR workflow proceeds in the expected order.

The basic method for use of PuffR is to call its functions for building the model inputs. You are to supply the basic info and get specific only when you need to.

There is a specified order, since later function calls will depend on output generated from earlier-called functions.



Using the PuffR Function to Define Receptor Locations for CALPUFF

In this example, the geophysical input file (GEO.DAT) is produced with a single function call.

First, some preliminaries! Create a folder with the name of the location. Create an R script and place it in that folder. In that new script, add a require statement for PuffR and set the working directory:

```
require(PuffR)

setwd('~/PuffR/vancouver')
```

Use the following function call:

```
calmet_define_geophys(
   location name = 'vancouver',
   lat_dec_deg = 49.196116,
   lon_dec_deg = -122.505866,
   domain_width_m = 117000,
   domain_height_m = 43250,
   cell_resolution_m = 500,
   download_SRTM = TRUE)
```

This will consist of a grid centered on 49.196116°N and 122.505866°W. The width (E–W distance) of the grid will be 117000 m, and the height (N–S distance) will be 43250 m. We will download SRTM terrain height data are store it locally.

Using PuffR to Generate Surface Met and Upper Air Data Files

The surface met input file—commonly known as SURF.DAT—can be easily made.

Here is the function call:

```
calmet_surface_met(
   location name = 'vancouver',
   year = 2011,
   lat_dec_deg = 49.196116,
   lon_dec_deg = -122.505866,
   domain_width_m = 117000,
   domain_height_m = 43250,
   cell_resolution_m = 500,
   time_offset = -8)
```

It relies on the location's domain to obtain hourly met data for 2011 from the NCDC archive.

Same goes for the upper air data file: UP.DAT.

This will look familiar:

```
calmet_upper_air(
   location name = 'vancouver',
   year = 2011,
   lat_dec_deg = 49.196116,
   lon_dec_deg = -122.505866,
   domain_width_m = 117000,
   domain_height_m = 43250,
   cell_resolution_m = 500,
   time_offset = -8)
```

This collects upper air data from two nearby sounding sites and generates the required files.

Putting Together the CALMET Input Control File

CALMET input control files (CALMET.INP) are created right before executing the CALMET model.

Start with a template:

```
calmet_inp_generate_template()
```

This creates an effectively empty CALMET input file in the working directory. While this file is readable plaintext, it really shouldn't be modified by hand.

We will use a group of functions to populate input files with parameter values. In this way, validation of inputs can be performed at every step.

The CALMET input file can be built up using a series of functions that address each of the input file's main sections.

```
calmet_01_temporal_params()
calmet_02_grid_levels()
calmet_03_output_opts()
calmet_04_met_data_opts()
calmet_05_wind_field_opts_params()
calmet_06_mixhgt_temp_precip_params()
calmet_07_station_params()
calmet_inp_finalize()
```

These call build up and complete the creation of the CALMET.INP file(s), checking the working directory for created input files. The presence of those files signals inclusion in CALMET model execution.

The Generated CALMET Input Files

'GEO.DAT' INPUT FILES

geo--vancouver-234x86x500--1-winter.txt
geo--vancouver-234x86x500--2-spring.txt
geo--vancouver-234x86x500--3-summer.txt
geo--vancouver-234x86x500--4-fall.txt
geo--vancouver-234x86x500--5-winter.txt

'UP.DAT' INPUT FILE

up--vancouver-234x86x500--2011.txt

'SURF.DAT' INPUT FILE

surf--vancouver-234x86x500--2011.txt

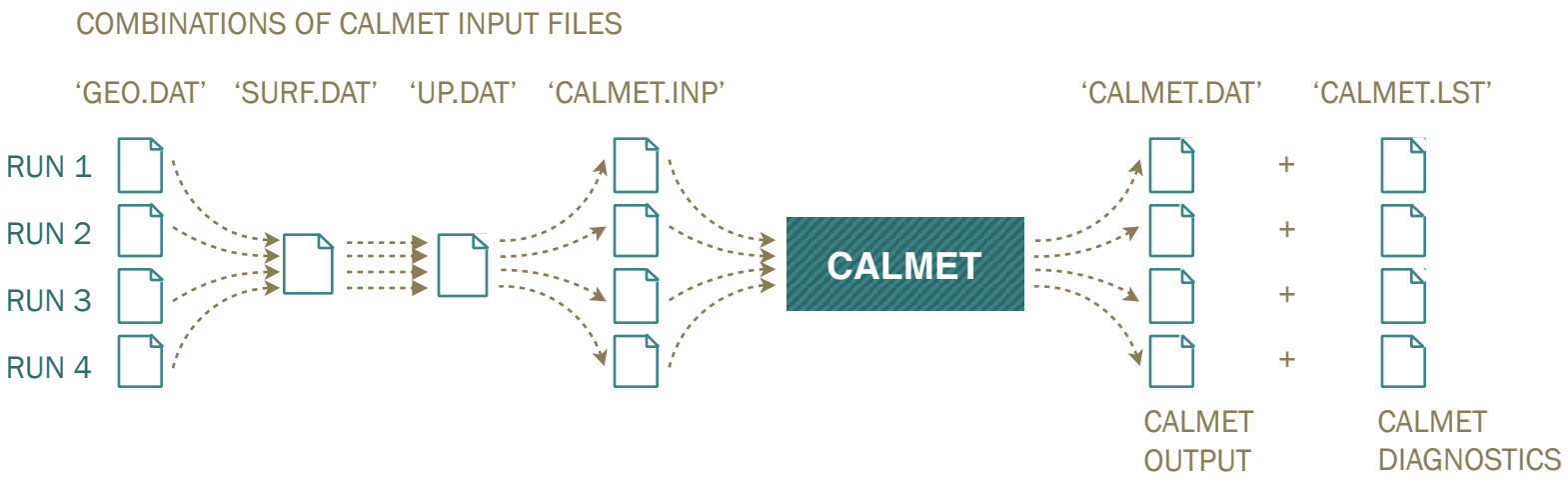
'CALMET.INP' INPUT FILES

calmet_in--vancouver-234x86x500--2011-1-winter.txt
calmet_in--vancouver-234x86x500--2011-2-spring.txt
calmet_in--vancouver-234x86x500--2011-3-summer.txt
calmet_in--vancouver-234x86x500--2011-4-fall.txt
calmet_in--vancouver-234x86x500--2011-5-winter.txt

Those function calls created quite a few input files!

Those functions used sensible defaults that assumed quite a lot. For instance, there were seasonal splits (making separate geophysical input files in different seasons). Also, the functions automatically chose which public datasets to use. Of course, you can have granular control of this but, oftentimes, you don't need to.

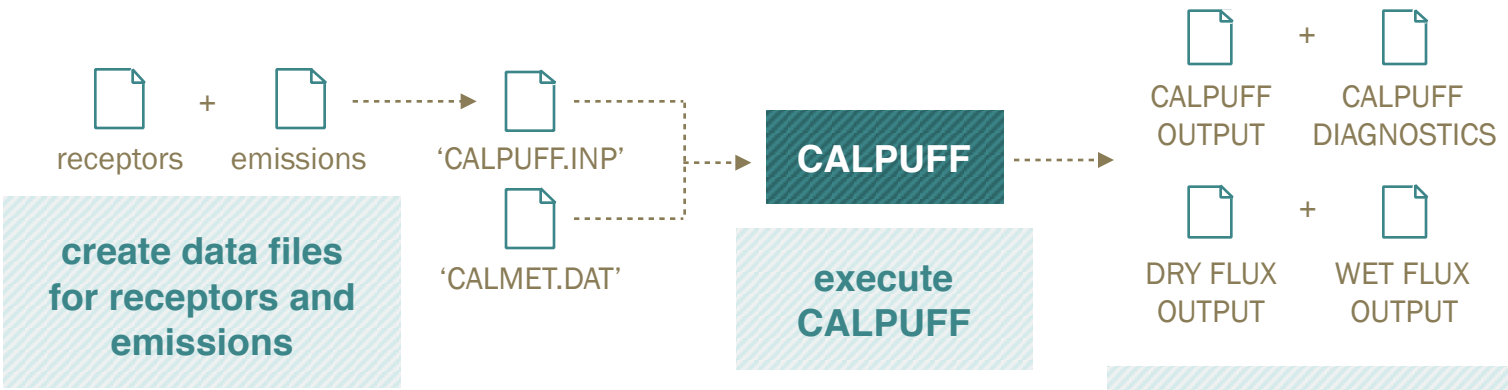
The Generated CALMET Output Files



Combinations of CALMET input files generate the appropriate output files.

A function call executes the CALMET runs from the input files.Once each CALMET model run is executed, binary CALMET output files (and associated diagnostics files) are created with a strict naming convention.

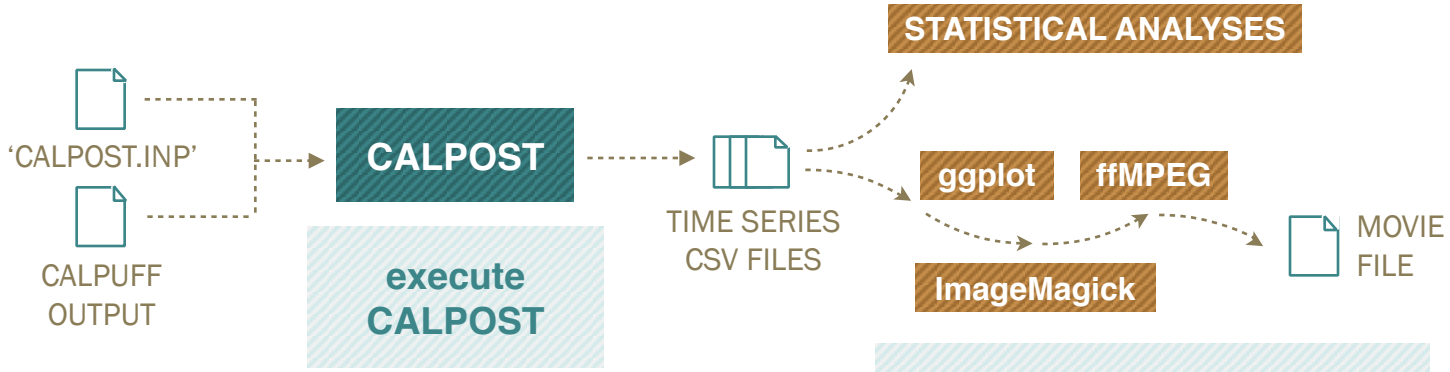
The Analogous CALPUFF Process



The workflow for CALPUFF is also quite simple.

Functions are available to generate receptor grids, define emission sources, build the CALPUFF input control file, and initiate the CALPUFF runs. Self-describing filenames are given to all CALPUFF output.

Analyzing the CALPUFF Output with CALPOST



CALPOST interfaces with the binary CALPUFF output data files.

PuffR includes functions to generate data summaries from binary CALPUFF output data by using the CALPOST utility. For example, time series data for all receptors can be extracted and used in statistical analyses of pollutant exposure.

Contents

There is a lot planned for this

greater selection of data sources

method to import and validate MM4/MM5 files

output/visualization of concentrations at receptors

data imputation methods for upper air soundings

method to create a precipitation input file for CALMET

method for computing building downwash for point sources near large structures

The intent of PuffR is to greatly simplify the process of running an advanced air quality dispersion model. I think it's important to understand how emissions of pollutants affect populations' exposure to those pollutants.

Aside from simplicity, there will be power. We can take advantage of many high-quality R packages to conduct statistical analyses and gain additional insights from the modelling data. This is all quite exciting and I can't wait to take this further.

method to create an overwater meteorological data file for CALMET

documentation library for understanding model options and parameters

methods for specifying emissions sources and creating time-and-space-varying emissions

PuffR

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for dispersion modelling
with CALPUFF


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