Python-based Atmospheric Transport Model for Spruce Budworm (SBW-pyATM) v1 Technical Document, last updated 24 January 2022

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in cooperation with

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NASA Application Readiness Level: 2

Maximum for stand-alone model: 3

1. Principal Sources (see References for full citations)

Greenbank et al. (1980, *Mem. Ent. Soc. Can.*) Sturtevant et al. (2013, *Ag. For. Meteor.*)

Boulanger et al. (2017, Ag. For. Meteor.)

Régnière et al. (2019a, Forests)

Régnière et al. (2019b, Forests)

Garcia et al. (2022, Ag. For. Meteor.)

2. Overview

Sturtevant et al. (2013) introduced an individual-based model of spruce budworm (SBW) moth migration that was driven by WRF-based meteorological fields. That model examined the likelihood that an area of known SBW outbreak populations in northern Minnesota could have produced the moths that were caught in pheromone traps along the northwestern shoreline of Lake Superior, where it was known that the native SBW population was not yet ready for flight at the time of the simulated dispersal events. In this sense, the model examined "ill-timed flights" where immigrant and native SBW populations were phenologically distinct.

The Sturtevant et al. (2013) flight model was based on the movement of individual moths based on early work in aerobiology by Scott and Achtemeier (1987) and later modeling by Isard et al. (2005), who considered the insect dispersal/migration flight in three phases: liftoff, cruising, and landing. Figure 1 of that paper shows this phased process:

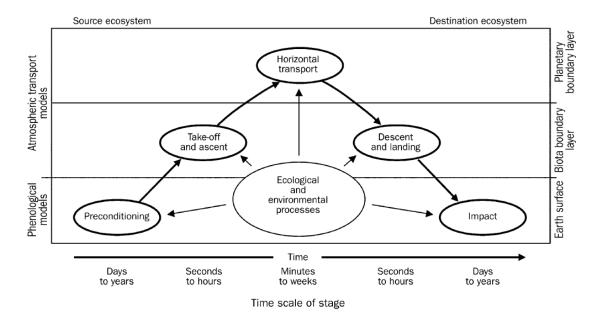


Figure 1. Aerobiology process model. Developed during the 1970s, this model provides a unifying approach to synthesize knowledge of processes associated with the aerial movement of biota. It was intended to focus research on ecological and environmental factors that affect aerobiota and to facilitate the study of organisms that use the atmospheric pathway as an integral part of dynamic ecological systems (Edmonds 1979). The time scales associated with these processes typically range from days to years for preconditioning and impact, minutes to weeks for horizontal transport, and seconds to hours for takeoff and ascent as well as descent and landing. Preconditioning and impact stages occur in ecosystems to which the aerobiota are functionally adapted. Takeoff and ascent as well as descent and landing occur within the biota boundary layer, which varies in depth with organism, weather conditions, time, and space. Winds encountered during the horizontal transport stage govern aerial pathways and consequently geographic destinations of aerobiota. Quantification of the atmospheric pathway requires the integration of phenological models that characterize aerobiota and their hosts in source and destination ecosystems with multiscale atmospheric transport models.

Figure 1 from Isard et al. (2005, BioScience).

This three-phase model of insect flight was elaborated for the simulation of many moths over a large geographical area. The object-oriented model structure developed for the 2013 paper treated each moth as an individual in an "agent-based" simulation environment, with individuals having their own identity and morphology (body size, flight speed, etc.) and all individuals subject to a common set of flight rules in the shared environment. The model structure in Sturtevant et al. (2013) was illustrated in Figure 1 of that paper:

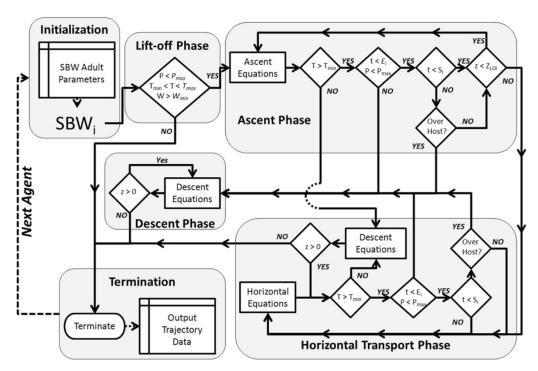


Fig. 1. Model flow diagram illustrating the logic of the spruce budworm flight behavior model. See Table 1 for parameter descriptions and values. Ascent, horizontal, and descent equations are delineated in Eqs. (1–3).

Figure 1 from Sturtevant et al. (2013, Agricultural and Forest Meteorology).

In addition to ill-timed flight events, the individual-based model of moth flight could be applied to any migration flight event to judge the likely landing locations of SBW moths from a known outbreak area, closing a major methodological gap in understanding the spatiotemporal dynamics of SBW outbreaks. Models of the SBW life cycle were well-established. However, the behavior of the adult SBW as a moth, subject to wind and weather and known to travel in large numbers, in coherent directions, and over long distances in a single night had been observed by several methods but had not been modeled. Prior models generally considered local dispersal, but none had been able to develop a way to anticipate and track long-distance migration as observed in SBW (and several other species).

The three-phase flight model developed by Sturtevant et al. (2013) was rewritten by Régnière and Saint-Amant as part of the Canadian Forest Service BioSIM modeling framework in C++ and known as the Atmospheric Transport Model (BioSIM–ATM). In that setting, the growth phases of the SBW larva as determined by weather conditions (esp. temperature) are estimated stochastically for an area of known outbreak right up to the adult phase, at which point each individual in the BioSIM model is allowed to fly according to the rules of the ATM and subject to the weather conditions applied to the flight portion of the model. That selection of weather conditions has varied according to the interests of the developers but is generally a medium-resolution numerical model analysis, such as the North American Model (NAM) or similar products, covering the area of interest in eastern Canada.

This Python-based Atmospheric Transport Model for Spruce Budworm (SBW–pyATM) is a counterpart to the original flight model (Sturtevant et al., 2013) and the BioSIM–ATM modeling frameworks. The most important parts related to SBW moth flight behavior, primarily the empirical descriptions of moth physiology and circadian rhythm, have been collected in a limited number of the components described below. Physiology and flight calculations for SBW are updated to the statistical-empirical formulations developed by Jacques Régnière of the Canadian Forest Service (Régnière et al., 2019a, b). Moth migration is determined in large part by atmospheric conditions, for which SBW–pyATM takes in WRF model output grids (based primarily on NARR large-scale input datasets) at a user-defined interval for the area and time of investigation. These are not raw WRF output files, but specific variables that have been preprocessed to a specific geographic configuration for pyATM use. This preprocessing also reduces the volume of data required for testing on an individual computer or transferred through a computing cluster when distributed simulations are performed. WRF preprocessing scripts are also available as part of this software package.

Version 1 of SBW-pyATM is oriented on single-night simulations of SBW flight activity, as documented by Garcia et al. (2022). The following pages contain component listings, descriptions, and flowcharts that outline the three major phases of a simulation: startup, temporal loop procedures, and rule-based decisions to determine individual moth flight behavior. The behavioral ruleset is broken into parts for ease of illustration. Additional flowcharts representing pre- and post-processing steps, parameter calibration (including comparison with radar), and multi-night simulations will be added upon completion.

3. Design

The overall approach to moth phenology and migration in BioSIM-ATM is an individual- or agent-based process. Accordingly, I developed SBW-pyATM in an object-oriented manner. Each moth is represented as a single instance (object) carrying its own morphological and environmental information but subject to a common set of flight rules (behaviors) that apply to every moth in the simulation. In this formulation, the agents are non-interactive (agents are influenced only by their environment) and are not intelligent; that is, the moths do not "learn" and adjust their behavioral rules over the course of the simulation. The user can specify any number of moths in a simulation but will likely notice a decline in model performance at large numbers because of the need to interpolate meteorological variables to each moth's individual location at every time step. Given the nature of the simulation with no interactions between the agents, simulations are linearly separable: the results of several smaller simulations over the same domain and times can be combined to give the effect of a large simulation, but with those results obtained with far less computing time. I typically run simulations with 1000 moths for speed and ease of post-processing and have run as many as 2500 such simulations simultaneously on UW-CHTC and OSG distributed computing resources, bringing their results together afterward with post-processing routines to gather flight statistics and maps of outcomes.

A high-level schematic of the SBW-pyATM model infrastructure and data processing stream, including necessary inputs, was given by Garcia et al. (2022, Figure 2):

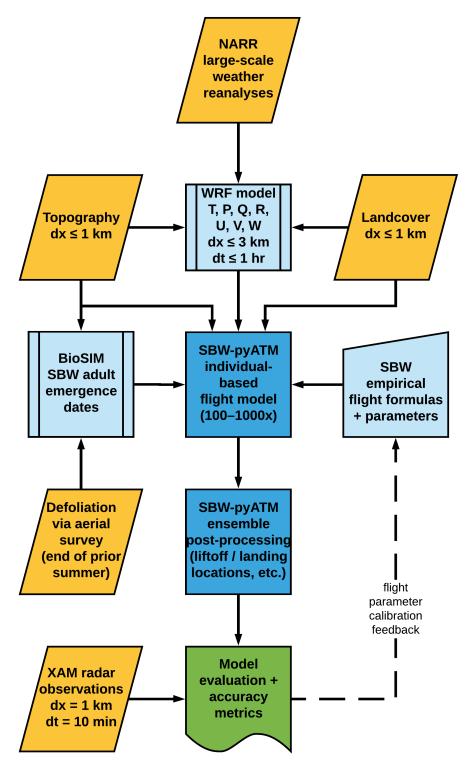


Figure 1: SBW-pyATM modeling procedure and data processing stream.

SBW-pyATM is a stand-alone model for use on any system that can support Python v3.8, such as Linux and MacOS (both tested) as well as Windows (though not yet specifically tested). In only the loosest sense is pyATM a "translation" (a.k.a. "port") of the original C++ components of BioSIM: I didn't use any pre-programmed translators or tools to convert C++ code to Python, and I didn't develop any wrappers to embed C++ code in a Python programming structure. Portions of the BioSIM-ATM modeling procedures, specifically the flight decision-making processes, are replicated in SBW-pyATM but the infrastructure and calculations necessary to drive the simulation were written entirely from scratch in Python. *Any errors in SBW-pyATM are my own*.

4. External requirements (each with their own dependencies)

```
copy, datetime, warnings, os, sys (Python standard libraries)
iso8601
matplotlib
mpl_toolkits.basemap (NOTE: to be replaced with cartopy)
netCDF4
numpy
GDAL (called via "osgeo") (NOTE: to be replaced with geotiff)
pandas
pyproj
scipy.interpolate
wrf-python (called as "wrf")
```

5. Components (by file name, in alphabetical order)

```
Notation
Courier = persistent data structure or variable name
Courier italics = file name
Courier bold = class (object) name
Courier_bold_italics = class method name
Times New Roman italics = standard or external Python library
Times New Roman bold = pyATM component as a Python module
Times New Roman bold italics = function name
Clock.py
      Description:
             Initialize and update the simulation time clock.
      External module requirements:
             datetime
      Internal module dependencies:
             (none)
      Classes defined:
             Clock
      Class methods defined:
```

```
init
                    classes used: Simulation
             advance clock
      Functions defined:
             (none)
Circadian calculations.py
      Description:
             Initialize an individual moth's circadian temporal function and pre-calculate
             necessary parameters using formulations in Régnière et al. (2019b).
      External module requirements:
             datetime, numpy
      Internal module dependencies:
             Interpolation, WRFgrids class
      Classes defined:
             (none)
      Class methods defined:
             (none)
      Functions defined:
             assign circadian
                    classes used: Simulation, SBW, Flier
             calc circadian deltas
                    classes used: SBW
             calc circadian from WRF T
                    classes used: Simulation, SBW, Flier
```

classes used: Clock, Flier

classes used: Simulation, WRFgrids

classes used: Simulation, SBW, Flier

Flier_class.py

Description:

Each moth is initialized as an individual of the **Flier** class, with variable declarations for moth identification, status, location, morphology, flight characteristics, and environment. Contains methods for updating these variables on a time-step basis, for recording those values throughout the moth's activity and flight period, and for reporting that record as JSON output. Moth locations are updated in Cartesian (UTM) coordinates on a time-step basis and converted back to geographic coordinates for other uses, e.g., mapping, post-processing, etc.

External module requirements:

calc circadian p

get flier environments

initialize circadian attributes

numpy, pandas

Internal module dependencies:

Flier summary, Geography, Map class, Plots gen

Classes defined:

```
Flier
Class methods defined:
     init
           classes used: Simulation, SBW
     calc AM ratio
     flight_status_info
           classes used: Clock
     inside_grid
           classes used: Simulation
     landing loc info
     liftoff conditions
           classes used: Simulation, SBW
     liftoff loc info
           classes used: Clock
     report status
           classes used: Simulation, Clock
     state decisions
           classes used: Simulation, Clock, SBW, Map, Radar
     update_empirical_values
           classes used: Simulation, SBW
     update environment
     update location
           classes used: Clock
     update motion
           classes used: Simulation, SBW, Radar
     update nu
           classes used: Simulation, SBW
     update state
     update state motion
           classes used: Simulation, SBW, Radar
     update status
           classes used: Clock
     update v h components
     zero motion
           classes used: Simulation
Functions defined:
     (none)
```

Flier grids.py

Description:

Create and populate grids of flier/liftoff/landing/egg density during simulation. (NOTE: this module may be deprecated as most of these fields are now mapped on an ensemble basis, not for individual simulations. In addition, post-processing of liftoff/landing/egg density now uses actual lat—lon locations for hexbin-based mapping. –MG, 12 Jul 2021)

External module requirements: *numpy*, *pandas*, *pyproj*

```
Internal module dependencies:
              (none)
       Classes defined:
              (none)
       Class methods defined:
              (none)
       Functions defined:
              create fill grids
                     classes used: Simulation, Proj (via pyproj)
             grid flier dvels
                     classes used: Simulation, Clock, Radar
             grid flier locations
                     classes used: Simulation, Clock, Radar
              grid liftoff locations
                     classes used: Simulation
             grid_landing locations
                     classes used: Simulation
              grid egg deposition
                     classes used: Simulation, Proj (via pyproj)
Flier setup.py
       Description:
              Moth location is initialized in geographic coordinates and converted immediately
              to UTM coordinates. Starting locations and morphological characteristics of the
              simulated moths can be provided in a BioSIM output file (CSV format) or
              determined by a random selection of locations on a map of defoliation severity
              (GeoTIFF format). If a BioSIM output file is provided, the moth morphology
              given in that file are used, with a random selection of the provided moths
              depending on the user's specification. If a defoliation map is provided, moth
              morphology for each random location is determined from the supplied empirical
              distributions.
       External module requirements:
              datetime, numpy, pandas
       Internal module dependencies:
              Interpolation, Geography, Map class
       Classes defined:
              (none)
       Class methods defined:
              (none)
       Functions defined:
             generate flier attributes
                     classes used: SBW
             generate flier locations
                     classes used: Map, WRFgrids
              read flier locations attributes
                     classes used: Simulation, Clock
```

```
Flier summary.py
       Description:
              Summarize various statistics and histograms of moth flight characteristics,
             including full-flight trajectories.
       External module requirements:
             datetime, iso8601, numpy, pandas
       Internal module dependencies:
              Flier grids, Plots gen
       Classes defined:
             (none)
       Class methods defined:
             (none)
       Functions defined:
             get alt histogram
             get dist histogram
             get horizontal speed histogram
             get liftoff speed histogram
             get speed stats histogram
             get time histogram
             get time mean stdv
             get time stats histogram
             flight status columns
             plot trajectories
                    classes used: Simulation, WRFgrids
             report_flier locations
                    classes used: Simulation, Clock, Radar
             report flier statistics
             report liftoff stats
             report mean
             report mean stdv
             report mean stdv pooled
             report stats
             report time stats
             summarize activity
                    classes used: Clock, Flier
             summarize locations
                    classes used: Clock, Flier
             summarize motion
                    classes used: Flier
Geography.py
       Description:
              Functions for geography-based calculations and conversions.
       External module requirements:
             numpy, pyproj
```

```
Internal module dependencies:
              (none)
       Classes defined:
              (none)
       Class methods defined:
              (none)
       Functions defined:
              calc GpH
             get utm zone
              inside grid
                     classes used: Simulation
              inside init box
                     classes used: Simulation
              lat lon to utm
                     classes used: Proj (via pyproj)
              utm to lat lon
                     classes used: Proj (via pyproj)
Interpolation.py
       Description:
              Functions for interpolation of WRF environment information in space and time.
       External module requirements:
              numpy, scipy.interpolate
       Internal module dependencies:
              (none)
       Classes defined:
              (none)
       Class methods defined:
              (none)
       Functions defined:
             get interp vals 2D
              get nearest columns
             get nearest vals 2D
             get vals 1D
              interpolate time
Map class.py
       Description:
```

Methods for reading GeoTIFF files of topography, landcover, and defoliation intensity. Each GeoTIFF is initialized as an object of the **Map** class with a method for querying map values by location during the simulation. Maps of topography and landcover are cropped to the specified simulation domain. The landcover map query function uses IGBP/MODIS landcover class values, translated to the forest/non-forest categories needed for moth status determination: water or non-host forest landing, host forest landing and thus egg-laying event, etc. For topography and/or landcover the user may also use the fields provided in

preprocessed WRF output files. The provided defoliation map is not required to cover the entire simulation domain.

```
External module requirements:
      numpy, gdal (via "osgeo"), sys
Internal module dependencies:
      (none)
Classes defined:
      Map
Class methods defined:
      __init
            classes used: Simulation
      check map boundaries
            classes used: Simulation
      get value
      get values (static method)
      subset_grid
Functions defined:
      lc categories
      lc category
      setup defoliation map
            classes used: Simulation
      setup_lc map
            classes used: Simulation
      setup_topo map
            classes used: Simulation
```

Model_control.py Description:

Central initialization and loop-based execution of the simulation. Initialization includes invoking the **Simulation**, **Clock**, and **SBW** classes, loading the topography and landcover **Map** objects, loading the defoliation **Map** object (if provided) and generating **Flier** locations and attributes, assigning the collection of **Flier** objects, loading the initial **WRFgrid** objects, and determination of the initial **Flier** environments. The temporal (outer) loop then proceeds from the designated start to end times, at the designated time step, with directives for updating **WRFgrid** objects at their own designated times. Inner loops cover the collection of moth **Flier** objects with steps for updating individual moth location, environment, decision-making (described in greater detail below), and resulting motion. For efficiency in the required interpolation routines, the environments of all moths are updated together. Also included are end-of-simulation directives to write any remaining active **Flier** records and egg deposition mapping information.

External module requirements:

SV

Internal module dependencies:

```
Clock, Flier summary, Model initialization, Model wrapup,
             Oviposition calculations, SBW empirical, Simulation specifications,
             Temporal operations
      Classes defined:
             (none)
      Class methods defined:
             (none)
      Functions defined:
             ATM main
                    classes used: Simulation, Clock, SBW, WRFgrids, Radar
Model initialization.py
      Description:
             Functions for initialization of simulation classes and persistent data structures.
             Includes processing of command-line arguments to change some model
             parameters.
      External module requirements:
             numpy
      Internal module dependencies:
             Circadian calculations, Flier class, Flier setup, Flier summary, Map class,
             Radar class, Solar calculations, WRFgrids class
      Classes defined:
             (none)
      Class methods defined:
             (none)
      Functions defined:
             command line args
                    classes used: Simulation
             load initial WRF grids
                    classes used: Simulation, Clock, WRFgrids
             setup fliers
                    classes used: Simulation, Clock, SBW, WRFgrids
             setup maps
                    classes used: Simulation, Map
             setup radar
                    classes used: Simulation, Radar
Model wrapup.py
      Description:
             Delegates generation of summary reports and plots at end of simulation.
      External module requirements:
             (none)
      Internal module dependencies:
             Flier grids, Flier summary
      Classes defined:
             (none)
```

```
Class methods defined:
             (none)
       Functions defined:
             report remaining fliers
                    classes used: Simulation, Clock, Flier
             report statistics
                    classes used: Simulation, Clock
             report summary grids
                    classes used: Simulation
             report trajectories
                    classes used: Simulation
Oviposition calculations.py
       Description:
             Simple oviposition function, in the absence of BioSIM-type daily calculations.
       External module requirements:
             (none)
       Internal module dependencies:
             (none)
       Classes defined:
             (none)
       Class methods defined:
             (none)
       Functions defined:
             oviposition
                    classes used: SBW, Flier
             update flier morphology
                    classes used: Simulation, SBW, Flier
Plots gen.py
      Description:
              Mapping moth trajectories at end of flight or simulation. (NOTE: this module may
             be relegated to post-simulation processing to reduce python time and memory
             overhead incurred in matplotlib and basemap usage. –MG, 12 Jul 2021)
       External module requirements:
             iso8601, matplotlib, mpl toolkits.basemap, numpy, warnings
       Internal module dependencies:
             (none)
       Classes defined:
             (none)
       Class methods defined:
             (none)
       Functions defined:
             plot all flights
                    classes used: Simulation, WRFgrids
             plot single flight
```

```
setup basemap
                   classes used: Simulation, Basemap (via mpl toolkits)
Radar class.py
      Description:
             Initialize a radar location and define its coverage area for mapping of moth flight
             locations and Doppler velocity.
      External module requirements:
             numpy, pyproj, warnings
      Internal module dependencies:
             Geography
      Classes defined:
             Radar
      Class methods defined:
             init
                   classes used: Proj (via pyproj)
             accumulate grid
             average grid
             count grid
             doppler vel
                   classes used: Proj (via pyproj)
      Functions defined:
             (none)
SBW empirical.py
      Description:
             Variable declarations and methods for eastern spruce budworm (Choristoneura
             fumiferana) adult moth morphology and flight parameterization, based primarily
             on Greenbank et al. (1980) and Régnière et al. (2019a, b).
      External module requirements:
             numpy
      Internal module dependencies:
             (none)
      Classes defined:
             SBW
      Class methods defined:
              init
             calc fecundity
             calc fecundity 0
             calc mass from gravidity
             calc_mass_from_wing_area
             calc nu L
             calc_nu_L_Ts
             calc nu T
             calc_{	extsf{TL}}
             calc Ts
```

classes used: Simulation

```
Functions defined:
             (none)
Simulation_specifications.py
      Description:
             Variable declarations for simulation: geographic domain, start/end times, time
             step, external data files (defoliation maps, WRF grids, etc.), flier (agent) numbers,
             and any parameterized variables that are subject to calibration. This file is the
             main interface for the user to change model simulation parameters.
      External module requirements:
             (none)
      Internal module dependencies:
             (none)
      Classes defined:
             Simulation
      Class methods defined:
              init
      Functions defined:
             (none)
Solar calculations.py
      Description:
             Calculates sunrise and sunset times for a provided location and date.
      External module requirements:
             datetime, numpy
      Internal module dependencies:
             (none)
      Classes defined:
             Sun
      Class methods defined:
             \_init
             __calc
             __preptime
              timefromdecimalday (static method)
             solarnoon
             sunrise
             sunset
      Functions defined:
             update suntimes
                    classes used: Clock, Flier
Temporal operations.py
      Description:
             Functions used in the main temporal loop of the model.
      External module requirements:
             copy, datetime
```

Internal module dependencies:

```
Circadian calculations, Interpolation, Solar calculations, WRFgrids class
Classes defined:
      (none)
Class methods defined:
      (none)
Functions defined:
      count active fliers
            classes used: Simulation, Clock, Flier
      end sim no fliers (poss. deprecated)
            classes used: Clock, Flier
      end sim no flights
            classes used: Simulation, Clock, Flier
      interpolate flier environments
            classes used: Clock, Flier
      load_next_WRF_grids
            classes used: Simulation, Clock
      query flier environments
            classes used: Simulation, Clock, WRFgrids
      remove fliers
            classes used: Simulation, Clock, Flier
      shuffle WRF grids
            classes used: Simulation, Clock, WRFgrids
      update flier environments
            classes used: Clock, Flier
      update flier locations
            classes used: Clock, Flier
      update flier states
            classes used: Simulation, Clock, SBW, WRFgrids, Flier
      update flier status
            classes used: Clock, Flier
```

WRFgrids class.py

Description:

Methods for reading pre-processed WRF output files on a user-defined interval, storing variables for use on a time-step basis, interpolating 3D WRF variable cubes from sigma coordinates to vertical coordinates based on geopotential height, and 2D interpolation to a moth location to obtain surface environmental variables (using 2D WRF surface variable grids) or a 1D column of values that vary with geopotential height (using 3D WRF upper-air variable cubes), from which variable values at the moth's calculated geopotential height are then interpolated. The 2D interpolation uses a nearest neighbor selection method and 1D vertical columns use a linear interpolation method to obtain the **Flier** environment. A single preprocessed WRF output file at one time-point is initialized as a **WRFgrid** object containing all available surface variable grids and upper air variable cubes for that time, and the use of these grids and

interpolation methods is determined by the moth altitude (above ground level, AGL) at each time step in the simulation.

```
External module requirements:
```

netCDF4, numpy, os, sys, wrf-python (called as "wrf")

Internal module dependencies:

Interpolation

Classes defined:

WRFgrids

Class methods defined:

```
___init__
```

classes used: **Dataset** (via *netCDF4*)

get_col_3D

classes used: **Simulation**

get_flier_environments

classes used: Simulation, Map

 ${\tt get_interp_columns}$

get_nearest_locs

get_vals_2D

classes used: Simulation

get_WRF_grid_by_name

interpolate_space

classes used: **Simulation**

Functions defined:

check for WRF file

6. Usage

First, edit the file Simulation_specifications.py for your desired simulation domain and time period, simulation time step, WRF file path and interval, number of fliers (max 100K), BioSIM file path, landcover and topography GeoTIFF file path(s), experimental variable values, etc. Then, for a simulation using all default values, at the command prompt ("\$") type

For an experiment in which the sensitivity of the model to different parameter values is used, type something like

The first integer value after the program name is a simple numerical label, as for a sensitivity experiment, and has no effect on the model performance. If a flight parameter name and value are also given, the given value overrides the default value for that parameter in the simulation.

7. Model Internal Operations

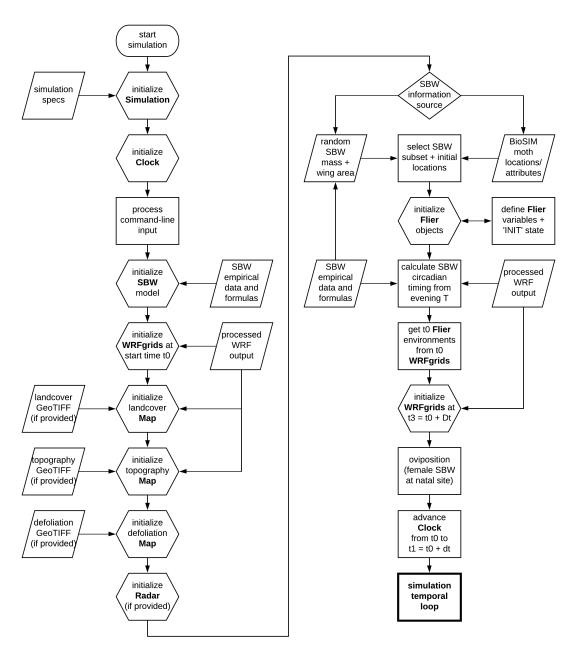


Figure 2: SBW–pyATM v1 simulation startup procedure. Note: Dt = WRF input interval, dt = model time step.

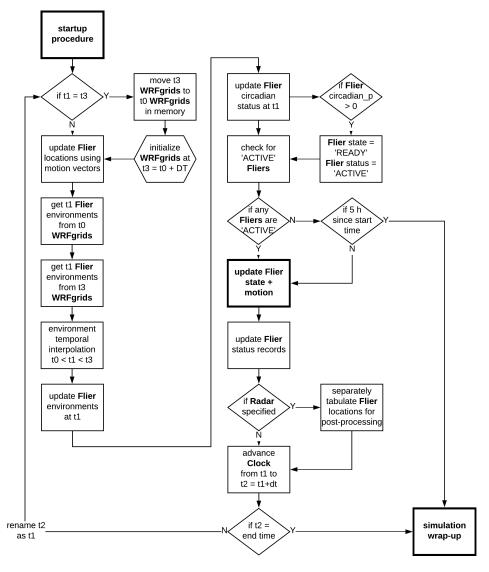


Figure 3: SBW-pyATM v1 simulation temporal loop procedure. Note: Dt = WRF input interval, dt = model time step.

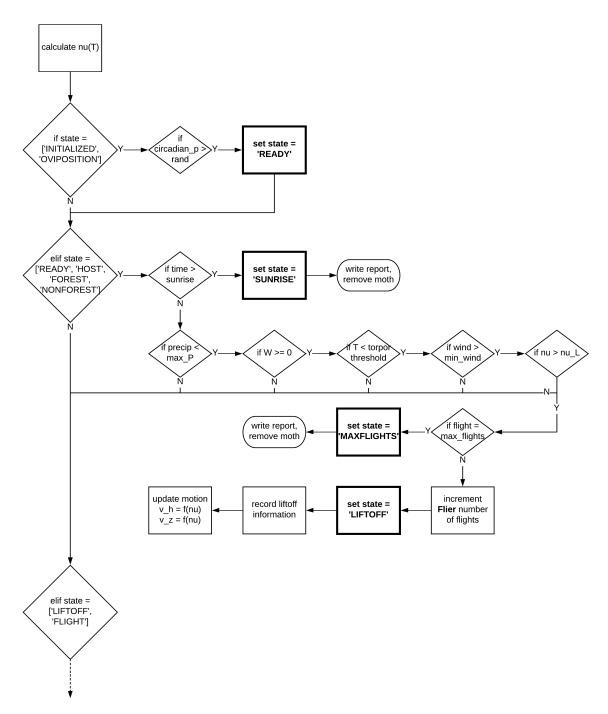


Figure 4: SBW-pyATM v1 rule-based moth behavior, part 1.

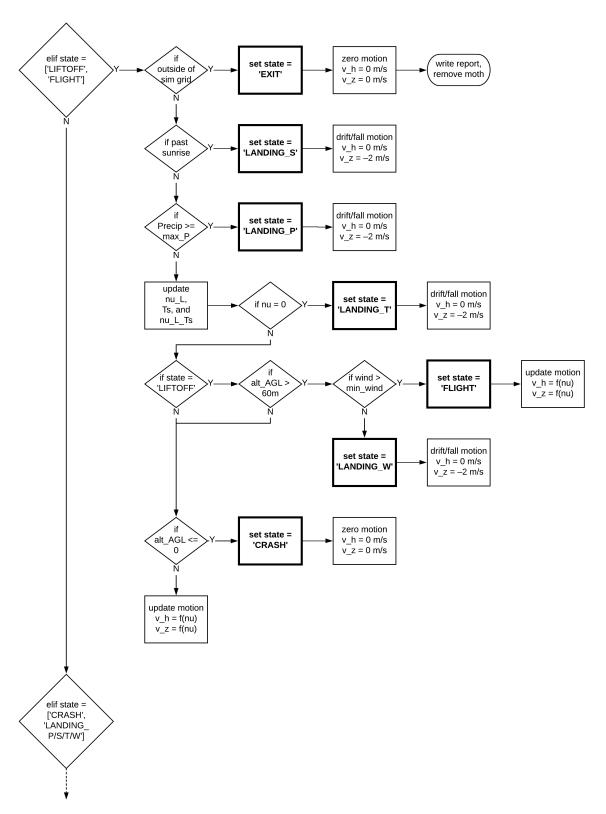


Figure 5: SBW-pyATM v1 rule-based moth behavior, part 2.

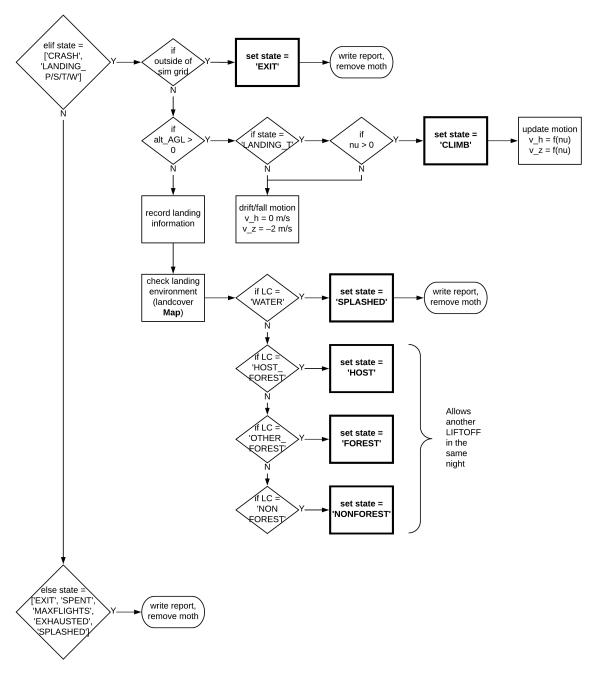


Figure 6: SBW-pyATM v1 rule-based moth behavior, part 3.

References

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