drops 1.0 - manual

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Abstract

This manual describes the usage and some technical aspects of the C++ implementation of the CCN activation model described in Arabas and Pawlowska (2010). Both the source code and this manual are supplements to the paper. The user is encouraged to google for any newer version of this manual and the source code, though. The implementation is named *drops* (name of a candy in Polish) and is free software released under the GNU GPL. Bug reports and contributions are highly welcome!

Contents

0.1 Dependencies

C++ compiler

Drops is written in C++ utilizing the Boost.Units library, the latter being "fairly demanding of compiler compliance to ISO standards". The code was tested with **GCC** 4.3 and 4.0 on Linux and OS X, respectively.

External libraries

Drops requires the following libraries to be available during compilation/runtime:

- **Boost** (for Boost.Units) available at http://www.boost.org/
- **SUNDIALS** (for CVODE and NVECTOR_SERIAL) available at http://computation.llnl.gov/casc/sundials/
- **GSL** available at http://www.gnu.org/software/gsl/ (tested with v4.4, will not work with v4.0 or older)

External programs/services

Both the CLI and GUI rely on **gnuplot** (http://www.gnuplot.info/). SVG support in gnuplot is required for the GUI. The GUI requires an **HTTP server** equipped with a recent version of **PHP** at server-side (tested with Apache and PHP5) and an **SVG-aware browser** at client-side (tested with Firefox and Safari). The PHP scripts rely on the exec() and proc_open() calls, and the nice shell command.

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0.2 Tarball contents

The drops tarball contains the following directories and files referenced hereinafter:

```
drops/ ..........
|-- COPYING ..... the text of GPL v3
|-- configure ..... autoconf-generated configuration shell script
|-- doc ..........
|   |-- drops.bib ..... BibTeX records used in paper.tex and manual.tex
|   |-- manual ..........
|   |   |-- Makefile ..... compilation rules for LaTeX/BibTeX
|   |   |-- manual.tex ..... LaTeX source of this document
|   |   `-- ... ..........
|   `-- paper ..........
|       |-- Makefile ..... compilation rules for LaTeX/BibTeX
|       |-- figs ..........
|       |   |-- */fig.svg ..... Inkscape-generated figure source files
|       |   |-- */fig.pdf ..... PDF versions of the above used in paper.tex
|       |   `-- */plot*.svg ..... source files of all figures as generated by gnuplot
|       |-- paper.tex ..... LaTeX source of the paper
|       `-- ... ..........
|-- src ..........
|   |-- drops.hpp ..... definitions of abstract classes
|   |-- *.hpp ..... implementations of the above (mostly one class per file)
|   |-- drops.cpp ..... the only .cpp file here, contains main(), includes all of the headers above
|   `-- ... ..........
|-- webgui ..........
|   |-- index.php ..... the main web-GUI file (contains <frameset>)
|   `-- *.php ..... other web-GUI files
`-- ... ..........
```

0.3 Configuration and compilation

Drops uses the GNU build system, hence the configuration and compilation (of the src/drops executable) should go as follows:

```
$ tar xvjf drops.tar.bz2
$ cd drops
$ ./configure
$ make
```

There are also makefiles for the documentation that call pdflatex and bibtex in the right order and the needed number of times, hence one can compile the doc/manual/manual.tex and the doc/paper/paper.tex files by invoking:

```
$ cd doc/manual
$ make
$ cd ../paper
$ make
$ cd ../..
```

The PHP files of the web interface are placed in the webgui directory hence one needs to point the web server to this directory. The webgui, in turn, calls the drops executable assuming it is located in ../src/drops with relation to the PHP script location. One option is to make a symlink to the webgui directory within the server's docroot, for example (on OS X with Web Sharing enabled) by invoking:

```
$ ln -s `pwd`/webgui ~/Sites/drops
```

The webgui should than be available at http://localhost/~USERNAME/drops/

1 User's guide

1.1 Command line interface (CLI)

The drops executable accepts UNIX-like command line options for defining model input and parameters. The list of options is discussed in section 1.3, and is available after typing:

```
$ ./src/drops --help
```

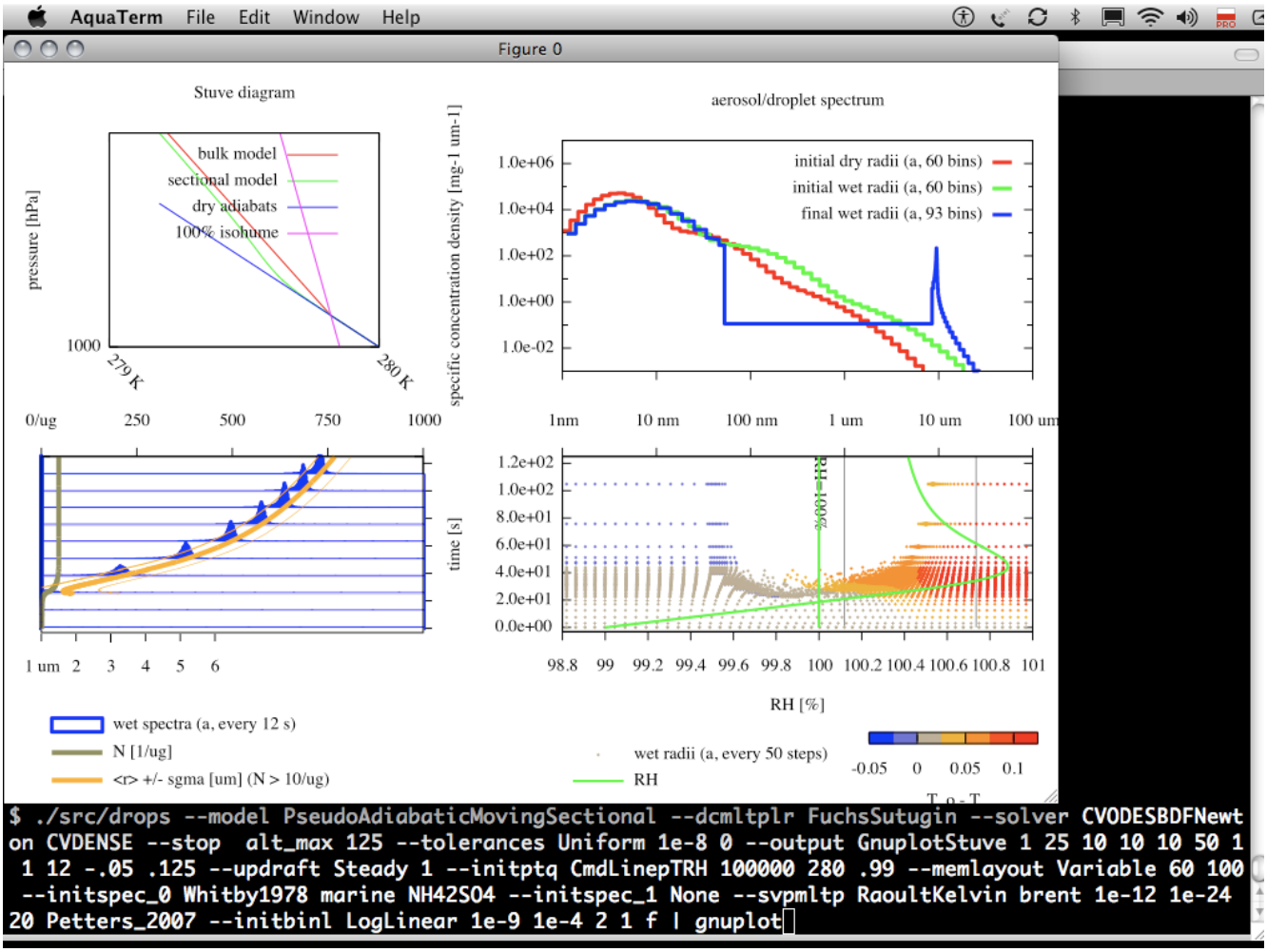
Drops communicates with the user via standard error, and by default sends gnuplot commands to standard output, hence a typical a typical invocation sequence is:

```
$ ./src/drops OPTIONS | gnuplot
```

or if the user wants to save the model output or alter the plot parameters:

```
$ ./src/drops OPTIONS > drops_output.gpi
$ gnuplot drops_output.gpi
```

A screenshot showing an example simulation run using the CLI with the drops output redirected to gnuplot, which in turn used AquaTerm for drawing the plot, is show below:

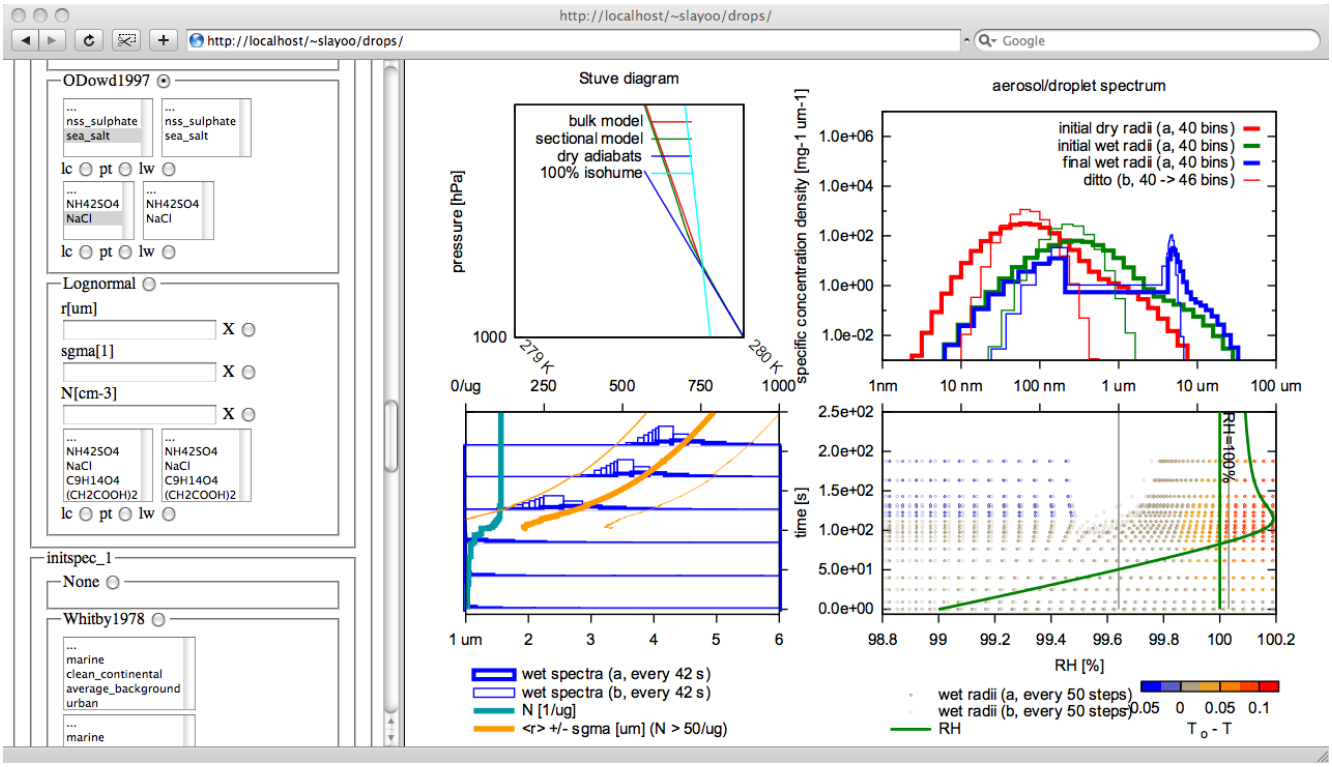


1.2 Web-based graphical user interface (web GUI)

The web GUI consists of two frames. The left-hand side frame contains an HTML form in which simulation parameters are set. The right-hand side frame is used to display the model output in the form of an SVG plot in case of success, or the messages sent by drops to standard error in case of failure. The web GUI has two modes of operation:

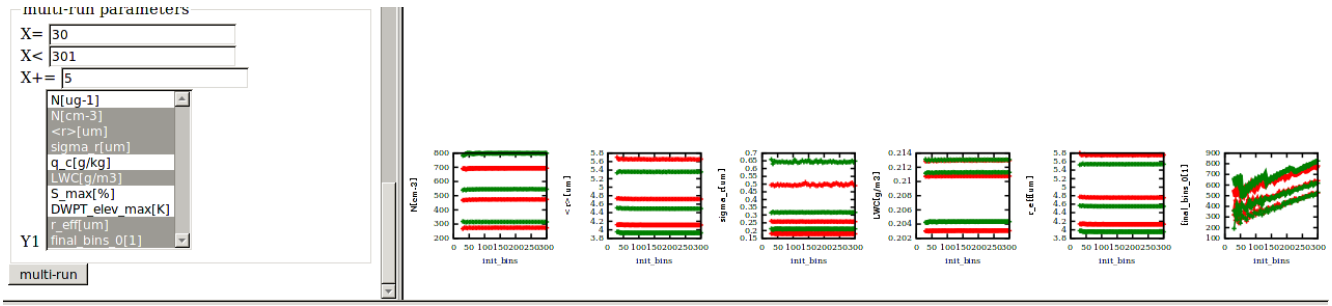
Single-simulation mode

This mode is chosen by clicking on the *single-run* button. One simulation at a time is run and its output is shown in the right-hand side frame. The default values filled in the form constitute the set-up used in section 3.1 of the article but with adaptivity.



Multiple-simulation mode

This mode is chosen by clicking on the *multi-run* button and is intended for running multiple simulations with one, two, free or four parameters of the model being altered between the simulations. The results are summarised in the plots displayed in the right-hand side frame. The number of plots correspond to the number of parameters chosen in the box just above the *multi-run* button (see picture below). The x-axes of the plots represent the parameter marked as X in the form (see picture above). The range over which X is varied is defined by filling in the $X=$, $X<$ and the $X+=$ form fileds (see picture below). The width of the lines on the plot, the type of symbols, and their color may be chosen to correspond to other parameters being varied in the multi-run mode by marking a parameter as lw, pt and lc, respectively (see picture above). The corresponding set of values of the lw- pt- or lc-marked parameter has to be than supplied in a right-hand side select box in the form (see picture above).



1.3 Model options

The following options of the model are available for setting in both the CLI and GUI. The default values can be obtained by invoking drops with the `--help` option, and are visible in the GUI.

dcmltplr multiplier of the diffusion constants, one of:

- **FuchsSutugin** the Fuchs-Sutugin formula (enabling transition régime corrections)
- **Unity** unity (disabling the transition régime corrections)

solver ODE solver, one of:

- **CVODESAdamsFunctional** the Adams-Moulton method with functional iteration (suitable for non-stiff systems)
- **CVODESBDFNewton** the BDF formula with Newton iteration (suitable for stiff systems), needs one argument:
  - Jacobian matrix representation, one of:
    - **CVDIAG** diagonal approximation
    - **CVDENSE** dense matrix using difference quotients
    - **CVDENSE-JAC** dense matrix using analytical Jacobian
    - **CVSPGMR** scaled preconditioned GMRES method
    - **CVSPBCG** scaled preconditioned Bi-CGStab method
    - **CVSPTFQMR** scaled preconditioned TFQMR method

stop stopping condition, one of:

- **t_max** stop at a given time, needs one argument:
  - **t** the time in seconds
- **alt_max** stop at a given altitude, needs one argument:
  - **h** the altitude in meters

tolerances ODE solver tolerances, one of:

- **Uniform** same tolerances for all variables, needs two arguments:
  - **relative_tolerance** the relative tolerance
  - **noise_level** the absolute tolerance

output Output format:

- **GnuplotStuve** gnuplot script with four plots including a Stuve diagram, needs 11 arguments:
  - **cloud_min** r_{min} in μm (consult the paper)
  - **cloud_max** r_{max} in μm (consult the paper)
  - **N_min** minimum concentration for which spectral parameters are plotted, in μg^{-1}
  - **n_spec** numer of spectra drawn in the bottom-right plot
  - **div_spec** scaling factor for the above spectra
  - **dot_step** dots are plotted in the bottom-right plot every dot_step records
  - **rec_step** records are output every rec_step ODE solver time-steps
  - **range_r_min** lower range of the x-axis in the bottom-left plot (in μm)
  - **range_r_max** upper range of the x-axis in the bottom-left plot (in μm)
  - **range_delta_t_min** lower range of the colour-scale (in K)
  - **range_delta_t_max** upper range of the colour-scale (in K)

updraft profile of vertical velocity with time, one of:

- **Steady** constant, needs one parameter:
  - **U** vertical velocity in m/s
- **SteadyPredefined** constant, needs one parameter:
  - vertical velocity in m/s, one of:
    - **.1,.25,.5,1,4,5,10**
- **Bells** bell-shaped profile defined by $w(t) = U_{max} sin(2\pi t/T) \cdot |sin(2\pi t/T)|$, needs two parameters:
  - **U_max** U_{max} in the above formula (in m/s)
  - **period** T in the above formula (in s)

initptq initial pressure, temperature, specific humidity; one of:

- **CmdLine** needs three parameters:
  - **p** pressure in Pa
  - **T** temperature in K
  - **q_v** specific humidity in kg/kg
- **CmdLinepTRH** **p** pressure in Pa
  - **T** temperature in K
  - **RH** relative humidity, dimensionless (not per cent)

memlayout ODE state-vector memory layout, one of:

Variable variable (needed for adaptivity), needs two parameters:
init_bins initial number of bins (per spectrum)
max_bins maximum number of bins (approximately per spectrum)

Constant constant, needs one parameter:
n_bins number of bins (per spectrum)

initspec_0 dry aerosol size spectrum (for the first chemical component), one of:

Whitby1978 tri-modal log-normal distributions from Whitby (1978), needs two parameters:
- air-mass type, one of:
  marine, clean_continental, average_background, urban
- chemical component, one of:
  NH42SO4, NaCl, C9H14O4, (CH2COOH)2

Jaenicke1993 tri-modal log-normal distributions from Jaenicke (1993), needs two parameters:
- air-mass type, one of:
  polar, background, maritime, remote_continental, desert_dust_storm, rural, urban
- chemical component, one of:
  NH42SO4, NaCl, C9H14O4, (CH2COOH)2

ODowd1997 log-normal distributions from O'Dowd et al. (1997), needs two parameters:
- size-spectrum:
  nss_sulphate (single-mode distribution)
  sea_salt (tri-modal distribution)
- chemical component, one of:
  NH42SO4, NaCl, C9H14O4, (CH2COOH)2

Lognormal single-mode log-normal distribution, needs four parameters:
r mode radius in μm
sgma geometric standard deviation (dimensionless)
N total concentration in the mode in cm^{-1}
- chemical component, one of:
  NH42SO4, NaCl, C9H14O4, (CH2COOH)2

initspec_1 dry aerosol size spectrum (for the second chemical component), one of:

None
... (the same set of values as for initspec_0)

svpmltp vapour pressure over solution droplet, one of:

Raoult Raoult term only
RaoultKelvin Raoult and Kelvin terms, needs five arguments:
- root-bracketing method, one of:
  brent
  falsepos
  bisection

relative_tolerance relative tolerance for root-bracketing
noise_level absolute tolerance for root-bracketing
max_iter maximum number of iterations for root-bracketing
- chemical composition parameterization, one of:
  Konopka_1996 using density, van't Hoff factor etc... (see e.g. Konopka, 1996)
  Petters_2007 using single parameter κ (Petters and Kreidenweis, 2007)

initbinl initial layout of bins, one of:

Linear linear in radius, needs two parameters:
min minimum radius in m
max maximum radius in m

LogLinear linear in log radius, needs four parameters (last two are related with the adaptivity)
min minimum radius in m
max maximum radius in m
max_mult maximum ratio of log radius to the initial value (cf. the article)
noise_spec_conc the tolerance (cf. the article)

2 Developer's guide (a stub of it . . .)

2.1 Program structure, error handling

The drops.cpp file contains the main() function and is the only non-header file. The drops.hpp file defines numerous abstract classes which have their implementations in other header files (mostly one class per file). Error handling is carried out using the standard *exception* class. The exceptions are caught in main() and triggering an error is done with the following sequence:

```
cerr << "message" << endl;
throw exception();
```

2.2 Class hierarchy

All classes inherit from class root which is an abstract class with a virtual destructor. This enforces execution of child-class destructors. The hierarchy of classes is as follows (the file in which a class is defined is indicated on the right):

- **root** ..... drops.hpp
  - **constants** ..... constants.hpp
  - **ModelParams** ..... drops.hpp
    - **ModelPseudoAdiabaticBulk::params** ..... ModelPseudoAdiabaticBulk.hpp
    - **ModelPseudoAdiabaticMovingSectional::params** ..... ModelPseudoAdiabaticMovingSectional.hpp
  - **Updraft** ..... drops.hpp
  - **UpdraftBells** ..... UpdraftBells.hpp
  - **UpdraftSteady** ..... UpdraftSteady.hpp
  - **SpectraMemLayout** ..... drops.hpp
  - **SpectraMemLayoutVariable** ..... SpectraMemLayoutVariable.hpp
  - **Solute** ..... drops.hpp
  - **SoluteAmmoniumSulphate** ..... Solutes.hpp
  - **SoluteKappaKohlerOnly** ..... Solutes.hpp
    - **SolutePinicAcid** ..... Solutes.hpp
    - **SoluteSuccinicAcid** ..... Solutes.hpp
    - **SoluteSodiumChloride** ..... Solutes.hpp
  - **InitpTq** ..... drops.hpp
  - **InitpTqCmdLine** ..... InitpTqCmdLine.hpp
  - **InitpTqCmdLinepTRH** ..... InitpTqCmdLinepTRH.hpp
  - **InitSpectrum** ..... drops.hpp
  - **InitSpectrumLognormal** ..... InitSpectrumLognormal.hpp
    - **InitSpectrumJaenicke1993** InitSpectrumJaenicke1993.hpp
    - **InitSpectrumODowd1997** InitSpectrumODowd1997.hpp
    - **InitSpectrumWhitby1978** InitSpectrumWhitby1978.hpp
  - **InitBinLayout** ..... drops.hpp
  - **InitBinLayoutLinear** ..... InitBinLayoutLinear.hpp
  - **InitBinLayoutLogLinear** ..... InitBinLayoutLogLinear.hpp
  - **Solver** ..... drops.hpp
  - **SolverCVODESAdamsFunctional** ..... SolverCVODESAdamsFunctional.hpp
  - **SolverCVODESBDFNewton** ..... SolverCVODESBDFNewton.hpp
  - **Tolerances** ..... drops.hpp
  - **TolerancesUniform** ..... TolerancesUniform.hpp
  - **InBinSpectrum** ..... drops.hpp
  - **InBinSpectrumConstNr** ..... InBinSpectrumConstNr.hpp
  - **SatVapPresMltplr** ..... drops.hpp
  - **SatVapPresMltplrKelvin** ..... SatVapPresMltplrKelvin.hpp
  - **SatVapPresMltplrRaoult** ..... SatVapPresMltplrRaoult.hpp
  - **SatVapPresMltplrRaoultKelvin** ..... SatVapPresMltplrRaoultKelvin.hpp
  - **SatVapPresMltplrRaoultPetters_2007** ..... SatVapPresMltplrRaoultPetters_2007.hpp
  - **SatVapPresMltplrUnity** ..... SatVapPresMltplrUnity.hpp
  - **DiffCoeffMltplr** ..... drops.hpp
  - **DiffCoeffMltpltFuchsSutugin** ..... DiffCoeffMltpltFuchsSutugin.hpp
  - **DiffCoeffMltpltUnity** ..... DiffCoeffMltpltUnity.hpp
  - **Model** ..... drops.hpp
  - **ModelPseudoAdiabaticBulk** ..... ModelPseudoAdiabaticBulk.hpp
  - **ModelPseudoAdiabaticMovingSectional** ..... ModelPseudoAdiabaticMovingSectional.hpp
  - **Output** ..... drops.hpp
  - **OutputGnuplotOneLine** ..... OutputGnuplotOneLine.hpp
  - **OutputGnuplotStuve** ..... OutputGnuplotStuve.hpp

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