EMPM2.3 Documentation

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Abstract

The explicit mixing parcel model (EMPM) simulates finescale internal processes of cumulus clouds e.g., mixing of environmental air (entrainment) into these clouds using a 1D domain. "The EMPM links the conventional parcel model, which has no internal structure, and multidimensional cloud models, which resolve cloud-scale structure produced by large eddies."[1] After an extension by Su et al. EMPM accounts for condensational droplet growth as well [2]. The physical characteristics within the cloudy domain and the temporal evolution are represented by and can be investigated with EMPM that incorporates the ascent of the parcel through the cloud, droplet growth, entrainment of environmental air, turbulent mixing and molecular diffusion.[3] Environmental profiles, precalculated or measured initial droplet size distribution, ccn size distrubtion as well as incloud vertical velocities can be provided to create realistic conditions.

1. License

2. Literature

The following publications describe the model and its underlying concepts and provide further information.

@ARTICLE{Kerstein91,
author = {Kerstein, A. R. },
title = {Linear-eddy modelling of turbulent transport. Part 6. Microstructure of diffusive scalar mixing fiels},
journal = {Journal of Fluid Mechanics},
volume = {231},
year = {91},
pages = {361-394},
doi = {10.1017/S0022112091003439},
resource = {http://journals.cambridge.org/action/displayAbstract?fromPage=online&aid=397533&fileId=S0022112091003439}, }

@ARTICLE{Krueger93,
author = {Krueger, S. K.},
title = {Linear Eddy Modeling of Entrainment and Mixing in Stratus Clouds},
journal = {Journal of the Atmospheric Sciences},
volume = {50, 18},
year = {93},
pages = {3078-3090},
doi = {10.1175/1520-0469(1993)050%3C3078:LEMOEA%3E2.0.CO;2},
resource = {http://journals.ametsoc.org/doi/abs/10.1175/1520-0469(1993)050%3C3078%3ALEMOEA%3E2.0.CO%3B2},}

@ARTICLE{Krueger97,
author = {Krueger, S. K. and Su, C.-W. and McMurtry, P. A.},
title = {Modeling Entrainment and Finescale Mixing in Cumulus Clouds},
journal = {Journal of the Atmospheric Sciences},
volume = {54},
year = {97},
pages = {2697-2712},
doi = {10.1175/1520-0469(1997)054%3C2697:MEAFMI%3E2.0.CO;2},
resource = {http://journals.ametsoc.org/doi/abs/10.1175/1520-0469%281997%29054%3C2697%3AMEAFMI%3E2.0.CO%3B2}, }

@ARTICLE{Su98,
author = {Su, C.-W. and Krueger, S. K. and McMurtry, P. A. and Austin, P. H.},

title = {Linear eddy modeling of droplet spectral evolution during entrainment and mixing in cumulus clouds},
journal = {Atmospheric Research},
volume = {47-48},
year = {98},
pages = {41-58},
doi = {10.1016/S0169-8095(98)00039-8},
resource = {http://linkinghub.elsevier.com/retrieve/pii/S0169809598000398},
alternate_resource = {http://clouds.eos.ubc.ca/~phil/austinpapers/su98.pdf}, }

@ARTICLE{Krueger08,
author = {Krueger, S. K. },
title = {Fine-Scale Modeling of Entrainment and Mixing of Cloudy and Clear Air},
conference = {IPCC 2008},
location = {Cancun (Mexico)},
date = {July 7-11, 2008},
resource = {http://cabernet.atmosfcu.unam.mx/ICCP-2008/abstracts/Program_on_line/Poster_01/Krueger_extended.pdf}, }

3. EMPM Schematic

Only a short and general oveview of EMPM is provided here since it has been described in several papers [1], [2] and [3]. The original undiluted, but cloudy air parcel rises from cloud base. Its initial updraft speed and its microphysical properties are preset. Discrete entrainment events throughout the ascent of the parcel are simulated by the substitution of a segment of cloudy air with clear, non-cloudy air. The size of the entrained segment and the entrainment rate are to be set in the namelist. The entrained air is then turbulently mixed by the linear eddy model (triplet mapping) and molecular diffused (see figure 1).

Triplet Map[4]
To simulate turbulent mixing the linear eddy model (LEM), developed by Kerstein [4], is implented in EMPM. Turbulent deformation is treated as random rearrangements within a randomly selected segment of length l of the scalar fields. This segment which represents the effect of an eddy of size l is compressed by a factor of three. The original scalar fields within the segment boundaries is then replaced by three copies of this compressed segment with the middle copy mirror-inverted (see figure 2). Using the method the regional gradient within the segment increases while the global gradient stays constant.[5]

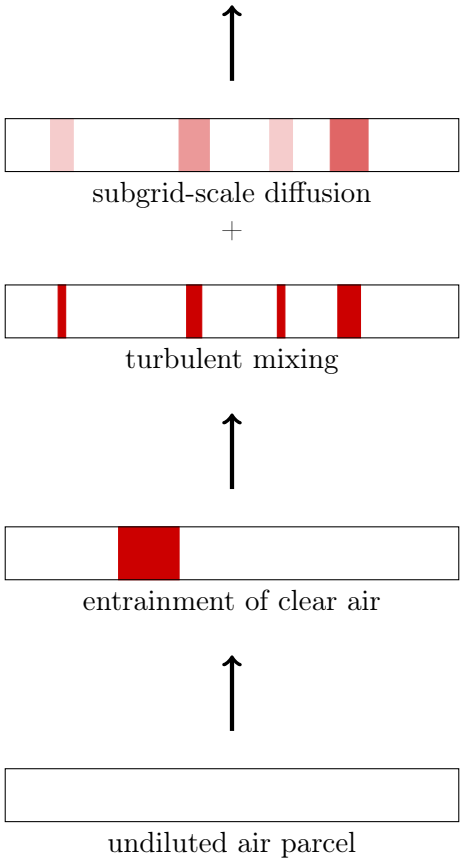


Figure 1: Schematic description of EMPM. See text for description. [2]

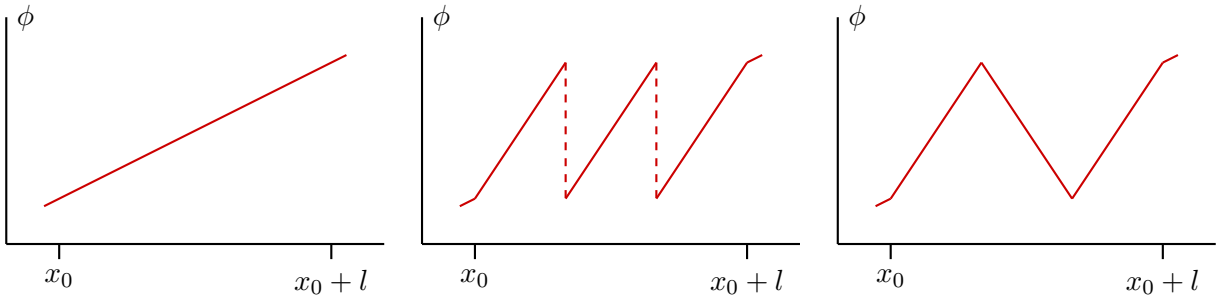


Figure 2: Triplet Mapping: A randomly selected segment of length l is compressed by the factor of three. The original scalar field is replaced by three copies of the compressed segment with the middle copy mirror-inverted. [4]

4. Governing Equations

The governing equations for the turbulent deformation (linear eddy model), molecular diffusion and the condensational droplet growth are shortly presented.

4.1. Turbulent Deformation

The simulation of turbulent eddies is limited to the range $\eta \leqslant l \leqslant L$, where η represents the Kolmogorov length scale and L the integral length scale of the flow. The actual size of the segment (l), which represents the turbulent eddy of size l, is sampled from a distribution $f(l)$ of segment sizes [5]

$$f(l) = \begin{cases} \frac{5}{3}\frac{l^{-8/3}}{\eta^{-5/3}-L^{-5/3}} & \text{if } \eta \leqslant l \leqslant L, \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

The segment-size probability density function satisfies the condition

$$\int_{\eta}^{L} f(l)dl = 1 \tag{2}$$

and leads to

$$l = \left(F(l)\left(L^{-5/3} - \eta^{-5/3}\right) + \eta^{-5/3}\right)^{-3/5} \quad , \tag{3}$$

where $F(l)$ is replaced by random numbers in EMPM.

The convective time step (frequency of rearrangement events) is calculated using

$$t_{\mathrm{c}} = \frac{1}{\lambda D} \tag{4}$$

with domain size D and the frequency of turbulent rearrangement events per unit length

$$\lambda = \frac{54}{5}\frac{D_{\mathrm{T}}}{L^3}\left(\frac{L}{\eta}\right)^{5/3} = \frac{54}{5}\frac{Re^{5/4}}{\tau L} \quad , \tag{5}$$

where D_{T} is the turbulent diffusivity, $Re = (L/\eta)^{4/3}$ the Reynolds number and $\tau = L^2/D_{\mathrm{T}}$ the large-eddy turnover time.[5] The turbulent diffusivity is related to the dissipation rate of the

tubulent kinetic energy ϵ by

$$D_{\mathrm{T}} \approx 0.1 L^{4/3} \epsilon^{1/3} \quad . \tag{6}$$

4.2. Diffusion

The changes of the temperature and water vapor field due to diffusion are calculate following

$$\left.\frac{\partial T}{\partial t}\right|_{\text{molecular diffusion}} = D_{\text{temp}} \frac{\partial^2 T}{\partial x^2} \tag{7}$$

and

$$\left.\frac{\partial q_{\mathrm{v}}}{\partial t}\right|_{\text{molecular diffusion}} = D_{\mathrm{m}} \frac{\partial^2 q_{\mathrm{v}}}{\partial x^2} \quad . \tag{8}$$

It is assumed that D_{temp} and D_{m} are equal. Using the Schmidt number Sc_{s} for simulations, the molecular diffusivity D_{m} can be related to the turbulent diffusivity D_{T}

$$Sc_{\mathrm{s}} = \frac{(D_{\mathrm{T}}/D_{\mathrm{m}})}{Re} \quad , \tag{9}$$

where $Sc_{\mathrm{s}} = 1$ is assumed. In dependence on the molecular diffusivity D_{m} the time step for diffusion t_{d} can be calculate using

$$t_{\mathrm{d}} = 0.2 \frac{(\Delta x)^2}{D_{\mathrm{m}}} \quad , \tag{10}$$

where Δx is the grid size.

4.3. Droplet Growth Equations

The diffusional droplet growth equation by [2] reads like

$$r_j \frac{dr_j}{dt} = \frac{s - A_1 + A_2}{A_3 + A_4} \quad , \tag{11}$$

where r_j is the radius of the jth droplet, s the supersaturation, A_1 and A_2 represent the droplet curvature and solution effect and A_3 and A_4 are the heat conduction and vapor diffusion terms:

$$A_1 = \frac{2\widehat{\sigma}}{R_\mathrm{v} T \rho_\mathrm{l} r_j} \quad , \tag{12}$$

$$A_2 = \frac{(i/M_\mathrm{s}) M_\mathrm{w} m_\mathrm{s}}{(4/3)\pi r_j^3 \rho_\mathrm{l} - m_\mathrm{s}} \quad , \tag{13}$$

$$A_3 = \frac{\rho_\mathrm{l} L_\mathrm{v}^2}{f(\alpha) K_\mathrm{T} R_\mathrm{v} T^2} \quad , \tag{14}$$

$$A_4 = \frac{\rho_\mathrm{l} R_\mathrm{v} T}{f(\beta) D e_\mathrm{s}} \quad , \tag{15}$$

where the symbols represent:

$\widehat{\sigma}$	droplet surface tension
R_v	gas constant for water vapor
T	temperature
ρ_l	liquid solution density
r_j	droplet radius at the jth class
i	the degree of ionic dissociation
m_s	mass of the solute
M_s	molecular weight of the solute
M_w	molecular weight of water
L_v	latent heat
K_T	thermal conductivity of air
$f(\alpha)$	kinetic factor $f(\alpha) = [r_j/(r_j + l_\alpha)]$
	$l_\alpha = K_T(2\pi M_\mathrm{d} R_* T)^{1/2}/[\alpha p(c_\mathrm{v} + R_*/2)]$ [6]
α	thermal accommodation coefficient of air (set to 1)
M_d	molecular weight of air
R_*	universal gas constant
p	atmospheric pressure
c_v	specific heat at constant volume of air
D	molecular diffusion coefficient of water vapor
e_s	saturation pressure over bulk water
$f(\beta)$	kinetic factor $f(\beta) = [r_j/(r_j + l_\beta)]$
	$l_\beta = (2\pi M_\mathrm{w}/R_\mathrm{v} T)^{1/2}(D/\beta)$ [6]
β	condensation coefficient of water vapor (set to 0.04)

The droplet growth (or shrinking) impacts the temperature (T) and water vapor (q_v) field by molecular diffusion (discussed in subsection 4.2) and phase change:

$$\left.\frac{dT}{dt}\right|_{\text{phase change}} = -\frac{L_\mathrm{v}}{c_\mathrm{pm}}\left.\frac{dq_\mathrm{v}}{dt}\right|_{\text{phase change}} - w\frac{g}{c_\mathrm{pm}} \tag{16}$$

and

$$\left.\frac{dq_\mathrm{v}}{dt}\right|_{\text{phase change}} = \sum_j 4\pi\rho_\mathrm{w}V_j^{-1}r_j^2\frac{dr_j}{dt} \quad , \tag{17}$$

where the symbols represent:

t	time
L_v	latent heat
c_pm	heat capacity of the system of air, vapor and liquid water at constant pressure
w	rising velocity
g	gravity
V_j^{-1}	inverse volume of jth grid cell
ρ_w	liquid water density
r_j	droplet radius at the jth class

The change in liquid water (q_l) is equal but opposite to the change in water vapor due to phase change

$$\left.\frac{dq_\mathrm{l}}{dt}\right|_{\text{phase change}} = -\left.\frac{dq_\mathrm{v}}{dt}\right|_{\text{phase change}} \quad . \tag{18}$$

Due to the changes in the water vapor and temperature field the supersaturation changes as well

$$\frac{ds}{dt} = (s+1)\left(\frac{1}{q_\mathrm{v}}\frac{R_\mathrm{d}}{(R_\mathrm{v}q_\mathrm{v}+R_\mathrm{d})}\frac{dq_\mathrm{v}}{dt} - \frac{g\rho_\mathrm{d}w}{p} - \frac{L_\mathrm{v}}{R_\mathrm{v}T^2}\frac{dT}{dt}\right) \quad , \tag{19}$$

where ρ_d is the density of dry air.

The hydrostatic equation is used to calculate the parcel's change in pressure

$$\frac{dp}{dt} = -gw\rho_\mathrm{d} \quad . \tag{20}$$

Equations 11, 16, 17, 19 and 20 "are solved using a fifth-order Runge-Kutta formula with an adaptive time step."[2]

5. Input Files

All information needed for simulations of entrainment events in cumulus clouds can be provided in input files and in the namelist. Up to four different input files with the environmental profiles of temperature and water vapor mixing ratio, the profile of the incloud vertical velocity, the initial droplet size distribution and the size distribution of ccn in the environmental air can be read bu EMPM. While the first mentioned environmental profiles are required, the other three files are optional and are only read if the according flags in the namelist are set.

Environmental Profiles

The format of the input file for the environmental profiles of temperature and water vapor mixing ratio had to be pressure in hPa, height in m, water vapor mixing ratio in $\mathrm{kg\,kg^{-1}}$ and temperature in K:

```
1010   13.1  0.01242  293.93
1000  116.0  0.01499  296.34
990   211.1  0.01411  295.84
980   303.4  0.01414  295.14
970   395.9  0.01429  294.43
```

In addition the length of the profiles (number of lines) has to be set in the namelist (`mi`). The path and name of the file can be set in the namelist. Please be aware that the length of the filename for the environmental profiles is limited to 20 characters.

Incloud Vertical Velocity

If the option `ivp` in namelist is chosen (set to 1), a vertical profile of the in-cloud vertical velocity is read from file. The format of the file has to be (pressure in hPa, height in m and vertical velocity in $\mathrm{m\,s^{-1}}$):

```
9.2010e+02  8.60e+02  8.466e-01
9.1585e+02  9.00e+02  8.607e-01
9.1162e+02  9.40e+02  1.103e+00
9.0740e+02  9.80e+02  1.488e+00
```

The path and name of the file can be set in the namelist. Please be aware that the length of the filename for the incloud vertical velocity profiles is limited to 20 characters.

Initial Droplet Size Distribution

It is possible that the user provides the initial droplet information in a file. To use this option the user has to set the appropriate flag in the namelist (see section 6), set the number of droplet categories in the namelist (`ne`) and provide the file in the following format: the list of all droplet radii in m first,

```
0.393005E-07
0.457181E-07
0.531072E-07
0.615938E-07
```

followed by the the solute mass of the droplets in kg and concentration in number per m^3 for each droplet category:

```
0.177828E-19  0.643783E+06
0.251188E-19  0.101334E+07
0.354813E-19  0.152169E+07
0.501188E-19  0.217999E+07
```

The path and name of the file can be set in the namelist. Please be aware that the length of the filename for the droplet properties is limited to 20 characters.

Size Distribution of CCN

Furthermore, the properties of the ccn in the entrained air can be provided in an additional file. As for cloud droplet, the option has to be chosen in the namelist (see section 6) and the number of ccn categories has to be set in the namelist (`nccn`). The format of this file has to be same as for the cloud droplets.

The path and name of the file can be set in the namelist. Please be aware that the length of the filename for the ccn properties is limited to 20 characters.

6. NAMELIST

In addition to the input files described in section 5 the namelist also contains information and settings to run simulations. All possible namelist parameter and their possible setting / values are described.

```
&inipar
bl              = 20.0,          domain length in x-direction (m) - the height and depth
                                 of the domain are set to be 0.001 m
```

`bl_inte`	`= 20.0,`	largest eddy in the domain (m)
`eta`	`= 0.01,`	smallest eddy (assumed Kolmogorov length scale, m)
`epsilon`	`= 0.001,`	dissipation rate of turbulent kinetic energy ($m^2\,s^{-3}$)
`start_t`	`= 0.75,`	start time for writing out droplet history and field data; must follow `start_t = n*t_interval`, where `n` is an integer (s)
`end_t`	`= 999.75,`	end time for writing out droplet history and field data; must follow `end_t = n*t_interval`, where `n` is an integer (s)
`t_interval`	`= 0.75,`	interval for writing out droplet history and field data; must follow `t_interval = n*time_step`, where `n` is an integer (s)
`time_step`	`= 0.015,`	time step for diffusion (s) if `itd` is set to 1
`idimen`	`= 5000,`	|
`ne`	`= 49,`	| - array size for droplet properties
`ne1`	`= 5000,`	|
`mi`	`= 32,`	environmental profile length
`n_max`	`= 30,`	maximal number of blobs possible
`idp`	`= 1,`	switch to set how initial droplet properties are determined 1 - all droplet have the same properties (`m_i`, `N_i` and `r_i` - set in namelist see below) 2 - droplet size distribution is calculated using gamma function and number concentration (`N_i`) and liquid water content `LWC` (given in namelist) 3 - droplet properties are read from file
`m_i`	`= 1.0E-18,`	initial mass of the droplet solute (kg) - (used if `idp=1`)
`N_i`	`= 100,`	initial droplet number concentration (cm^{-3}) - (used if `idp=1, 2`)
`r_i`	`= 1.0E-06,`	initial droplet radius (m) - (used if `idp=1`)
`LWC`	`= 1.51731E-5,`	initial liquid water content in cloud ($kg\,m^{-3}$) - (used if `idp=2`)
`qv`	`= 1.766e-02,`	cloud base water vapor mixing ratio ($kg\,kg^{-1}$)
`temp`	`= 295.15349,`	cloud base temperature (K)
`press`	`= 95906.05692,`	cloud base pressure (Pa)
`w`	`= 1.26215,`	cloud base vertical velocity ($m\,s^{-1}$) if `icw` is set to 0 and cloud vertical velocity ($m\,s^{-1}$) if `icw` is set to 1

`height`	`= 0.0000E+00,`	height above cloud base (m)
`rho_a`	`= 1.12012,`	air density ($\mathrm{kg\,m^{-3}}$)
`aero`	`= 1,`	type of aerosol (molecular weight, solute composition and constants are chosen within DGM accordingly) 1 - NaCl 2 - $(NH_4)_2SO_4$
`cloudtopheight`	`= 0.0`	cloud top height (m) at which the simulation is stopped (if cloud top height is set to 0.0 in namelist or if the cloud top height cannot be reached within the time of the simulation (`end_t`), the simulation ends by the time `end_t` set in namelist)
`run_info`	`= 'EMPM3.0',`	string with information about current run
`itd`	`= 1,`	switch to set a time step for diffusion in namelist 0/1 (no/yes) if it is set to no (0), the time step will be calculate in the model directly
`ire`	`= 1,`	switch to enable random variation of the calculated time step for entrainment 0/1 (no/yes)
`ent_rate`	`= 0.0014,`	bluk entrainment rate ($\mathrm{m^{-1}}$)
`n_blob`	`= 1,`	number of entrained blobs per entrainment event
`psigma`	`= 0.1,`	size of the entrained parcel in relation to domain size (fraction) - 0.1 is recommended
`iim`	`= 0,`	switch to enable isobaric mixing 0/1 (no/yes)
`icw`	`= 1,`	switch to enable constant vertical velocity 0/1 (no/yes) if 0 is selected, the vertical velocity depends on buoyancy
`ivp`	`= 0,`	switch to enable reading incloud vertical velocity profile from file 0/1 (no/yes) if 1 is selected, `icw` may not be set to 0
`icaw`	`= 0,`	switch to enable ending the simulation if vertical velocity becomes negative 0/1 (no/yes)
`thsw`	`= 0.0,`	threshold value (read from namelist) for vertical velocity at which EMPM is stopped

`iinm`	`= 0,`	switch to enable instant mixing 0/1 (no/yes)
`iccn`	`= 1,`	switch to include ccn in entrained air 0 - no ccn are entrained 1 - all entrained ccn have the same radius and mass 2 - ccn radius and mass distribution are read from file
`nccn`	`= 49,`	number of ccn bins given in file
`m_ccn`	`= 1.0E-18,`	mass of ccn (kg) - (used if `iccn=1`)
`r_ccn`	`= 1.0E-08,`	radius of ccn (m) - (used if `iccn=1`)
`idc`	`= 1,`	switch to enable constant droplet number in domain 0/1 (no/yes) can only be used in combination with `iccn=1`
`cb_ent`	`= 0`	switch to enable entrainment at cloud base (first time step) 0/1 (no/yes)
`r_pdf_nbin`	`= 100,`	bin number for droplet radius pdf
`r_pdf_min`	`= 0.0,`	minimum value for droplet radius pdf
`r_pdf_max`	`= 50.0e-6,`	maximum value for droplet radius pdf
`qt_pdf_nbin`	`= 60,`	bin number for total water mixing ratio pdf
`qt_pdf_min`	`= 0.0,`	minimum value for total water mixing ratio pdf
`qt_pdf_max`	`= 0.12,`	maximum value for total water mixing ratio pdf
`scalar_pdf_nbin`	`= 100,`	bin number for scalar (qv, T and s) pdf
`qv_pdf_min`	`= 0.0,`	minimum value for water vapor mixing ratio pdf
`qv_pdf_max`	`= 0.04,`	maximum value for water vapor mixing ratio pdf
`temp_pdf_min`	`= 270.0,`	minimum value for temperature pdf
`temp_pdf_max`	`= 315.0,`	maximum value for temperature pdf
`SuS_pdf_min`	`= -0.8,`	minimum value for supersaturation pdf
`SuS_pdf_max`	`= 0.1,`	maximum value for supersaturation pdf
`mrealization`	`= 1,`	number of realizations

`/`

`&io_file`

```
output_format   = 1,
```
switch to change output file format
1 - all files are written as formatted text files
2 - files for the variables `r_time, x_time, qvtime` and `temptime` are written as unformatted binary files
3 - files for the variables `r_time, x_time, qvtime` and `temptime` are written as netCDF files

```
i_profile_path  = '../data/',
i_profile_file  = 'environment.txt',

v_profile_path  = '../data/',
v_profile_file  = 'incloud_vel.txt',

drop_path       = '../data/',
drop_file       = 'drop.data.new',

ccn_path        = '../data/',
ccn_file        = 'en_ccn.dat',

output_path     = '../output/',
```

7. How to compile and run EMPM

It has been tested to compile and to run EMPM with two different compiler - intel and gfortran:

- Scientific Linux release 6.6 (Carbon) with ifort (IFORT) 14.0.4 20140805
- Scientific Linux release 6.6 (Carbon) with GNU Fortran (GCC) gfortran 4.4.7

Simulations run slightly faster when the code was compiled with the intel compiler, but no significant differences between simulations with different compilers were found.

The structure of the EMPM directory is by default:

```
drwxr-xr-x  2  sonja  aos    4096  Apr  1  10:37  data
-rw-r-r-    1  sonja  aos  532721  Sep  1  10:37  Documentation.pdf
drwxr-xr-x  2  sonja  aos   86016  Apr  1  13:09  output
drwxr-xr-x  2  sonja  aos    4096  Apr  1  10:10  src
```

Whereas the necessary input to run EMPM simulations are stored in the directory `data`, all output data are saved in the `output` directory. Both directories can be moved or renamed as the user

might need or like to do, in this case the new path has to be given in the namelist. The directory `src` contains all source file, the Makefile, the executable as well as the namelist file and a log file with information about the simulation and the setting chosen.

7.1. Compilation

1. Make appropriate changes (choose hardware available) in Makefile (in `src` directory)
2. Compile the EMPM code by typing (in terminal):

```
$ make
```

3. This creates the executable (in `src` directory):

```
-rwxr-xr-x  1  sonja  aos  120844  Apr  1  11:27  EMPM
```

7.2. Starting Simulation

1. Set up your simulation:
   - make changes in namelist according to your demands
   - initial profiles of environmental temperature and humidity have to be given in a separat file (see section 5)
   - (optional: initial droplet information can be provided in a second files (see section 5))
   - (optional: ccn data of the entrained air in a third file (see section 5))
   - (optional: incloud vertical velocity ca be read from an additional file (see section 5))
2. execute EMPM by typing (in terminal):

```
$ ./EMPM
```

3. This produces the one control file in the local `src` directory:

```
-rw-r-r-  1  sonja  aos  79546  Apr  1  12:04  EMPM.log
```

4. And the following files in the `output` directory if `output_format` options 1 or 2 are selected:

```
-rw-r-r-  1  sonja  aos     646000  Aug  12  12:04  ave_1.dat
-rw-r-r-  1  sonja  aos        468  Aug  12  12:04  entm_1.dat
-rw-r-r-  1  sonja  aos      57568  Aug  12  12:04  findex_1.dat
-rw-r-r-  1  sonja  aos         25  Aug  12  12:04  LWP_1.dat
-rw-r-r-  1  sonja  aoS    1954000  Aug  12  12:04  qt_pdf_time_1.dat
```

```
-rw-r-r-  1  sonja  aos  384248149  Aug  12  12:03  qvtime_1.dat
-rw-r-r-  1  sonja  aos    1154000  Aug  12  12:04  r2_mean_time_1.dat
-rw-r-r-  1  sonja  aos    1154000  Aug  12  12:04  r3_mean_time_1.dat
-rw-r-r-  1  sonja  aos      32683  Aug  12  12:04  r_eff_time_1.dat
-rw-r-r-  1  sonja  aos      88000  Aug  12  12:04  r_mean_stats_1.dat
-rw-r-r-  1  sonja  aos    1154000  Aug  12  12:04  r_mean_time_1.dat
-rw-r-r-  1  sonja  aos    5207202  Aug  12  12:04  r_pdf_time_1.dat
-rw-r-r-  1  sonja  aos  320036000  Aug  12  12:04  rtime_1.dat
-rw-r-r-  1  sonja  aos    5256627  Aug  12  12:04  SA1_pdf_ave_1.dat
-rw-r-r-  1  sonja  aos    5256627  Aug  12  12:04  SA2_pdf_ave_1.dat
-rw-r-r-  1  sonja  aos     158000  Aug  12  12:04  super_max_min_1.dat
-rw-r-r-  1  sonja  aos      92000  Aug  12  12:04  super_mean_1.dat
-rw-r-r-  1  sonja  aos    5256627  Aug  12  12:04  sus_pdf_1.dat
-rw-r-r-  1  sonja  aos     206022  Aug  12  12:04  temp_qv_ave_1.dat
-rw-r-r-  1  sonja  aos  384248149  Aug  12  12:03  temptime_1.dat
-rw-r-r-  1  sonja  aos      26000  Aug  12  12:04  t_index_1.dat
-rw-r-r-  1  sonja  aos  520036000  Aug  12  12:04  xtime_1.dat
```

The files `qvtime_1.dat`, `rtime_1.dat`, `temptime_1.dat` and `xtime_1.dat` will not be created if the `output_format` option 3 is selected. Instead there will be netCDF file called `EMPM_output_1.nc` which contains the four variables.

The file `ave_1.dat` contains the time series of the domain average and the standard deviation of liquid water mixing ratio ($\mathrm{kg\,kg^{-1}}$), total water mixing ratio ($\mathrm{kg\,kg^{-1}}$), liquid water static energy ($\mathrm{J\,kg^{-1}}$), buoyancy ($\mathrm{m\,s^{-1}}$), moist static energy ($\mathrm{J\,kg^{-1}}$), supersaturation (-), water vapor mixing ratio ($\mathrm{kg\,kg^{-1}}$) and temperature (K), the mean droplet radius (μm) and standard deviation of the radii (μm), the total droplet number in the domain, the maximal droplet radius (μm) and its index.

The file `entm_1.dat` contains for each entrainment event the time (s), pressure (Pa), height (m), the environmental water vapor mixing ratio ($\mathrm{kg\,kg^{-1}}$), the environmental temperature (K) and the time interval of entrainment events (s).

The file `findex_1.dat` contains for all droplets in the domain their index and their final radius (μm).

The file `LWP_1.dat` contains the liquid water path for the entire cloud ($\mathrm{kg\,m^{-1}}$).

The file `qt_pdf_time_1.dat` contains the pdf of the total water mixing ratio normalized by the total area every of the pdf every `t_interval/time_step`-th iteration.

The file `qvtime_1.dat` contains the water vapor mixing ratio field ($\mathrm{kg\,kg^{-1}}$) for the whole domain

every `t_interval/time_step`-th iteration.

The file `r2_mean_time_1.dat` contains the spectrum of the droplet radius squared ($(\mu\mathrm{m})^2$) every `t_interval/time_step`-th iteration.

The file `r3_mean_time_1.dat` contains the spectrum of the droplet radius cubed ($(\mu\mathrm{m})^3$) every `t_interval/time_step`-th iteration.

The file `r_eff_time_1.dat` contains the effective radius (μm) every `t_interval/time_step`-th iteration.

The file `r_mean_stats_1.dat` contains a time series of the mean droplet radius (μm), the standard deviation (μm) and the droplet number in the domain.

The file `r_mean_time_1.dat` contains the spectrum of the droplet radius (μm) every `t_interval/time_step`-th iteration.

The file `r_pdf_time_1.dat` contains the pdf of the droplet radius normalized by the total droplet number every `t_interval/time_step`-th iteration.

The file `rtime_1.dat` contains the radius (μm) of each droplet every `t_interval/time_step`-th iteration.

The file `SA1_pdf_time_1.dat` contains the pdf of the water vapor mixing ratio normalized by the total area of the pdf every `t_interval/time_step`-th iteration.

The file `SA2_pdf_time_1.dat` contains the pdf of the temperature normalized by the total area every of the pdf `t_interval/time_step`-th iteration.

The file `super_max_min_1.dat` contains a time series of the lowest and highest supersaturation (-) as well as the difference (-).

The file `super_mean_1.dat` contains a time series of the mean supersaturation (-) and the standard deviation (-).

The file `sus_pdf_1.dat` contains the pdf of the supersaturation normalized by the total area of the pdf every `t_interval/time_step`-th iteration.

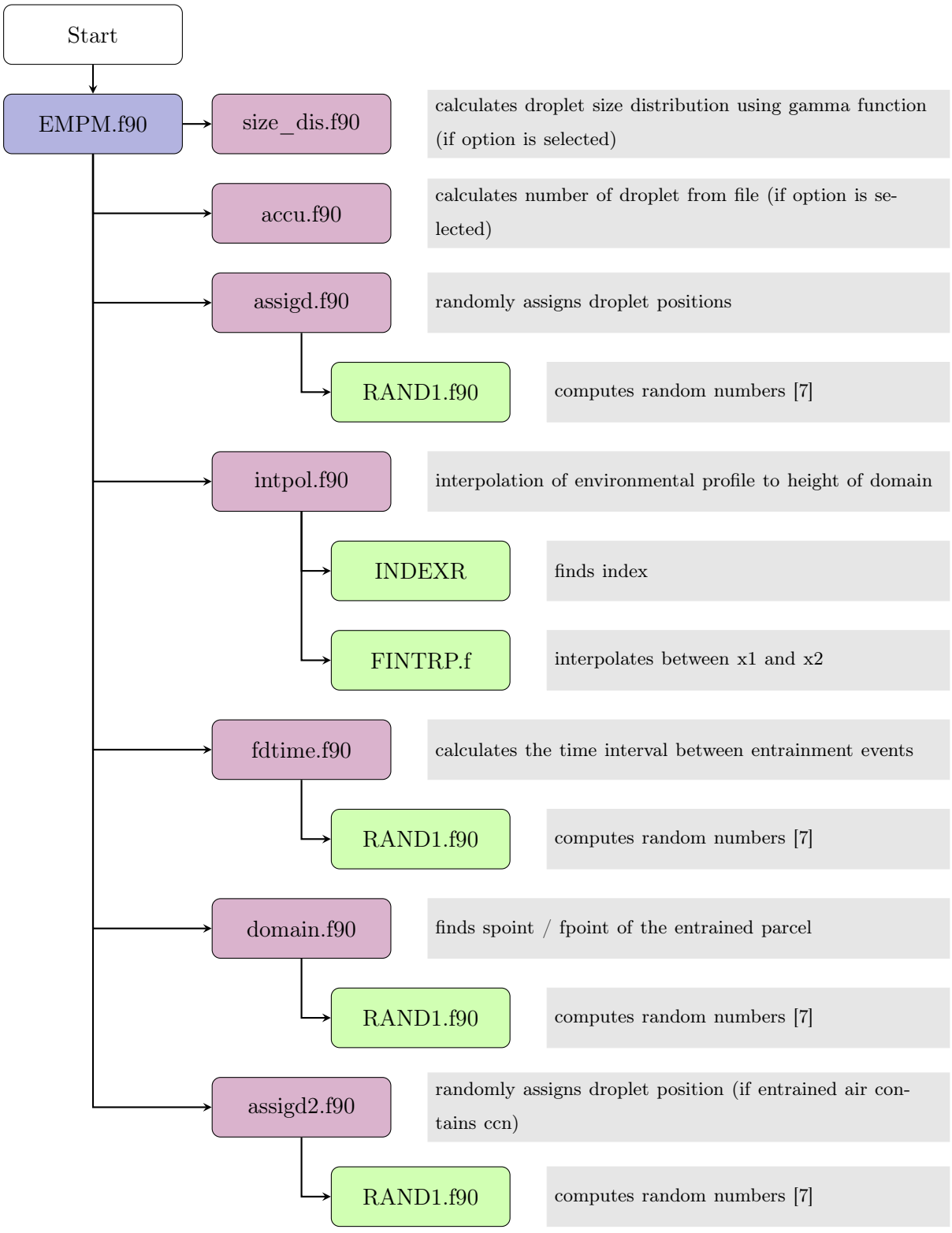
The file `temp_qv_ave_1.dat` contains a time series of the domain averaged water vapor mixing ratio ($\mathrm{kg\,kg^{-1}}$), temperature (K), liquid water mixing ratio ($\mathrm{kg\,kg^{-1}}$) and total water mixing ratio ($\mathrm{kg\,kg^{-1}}$).

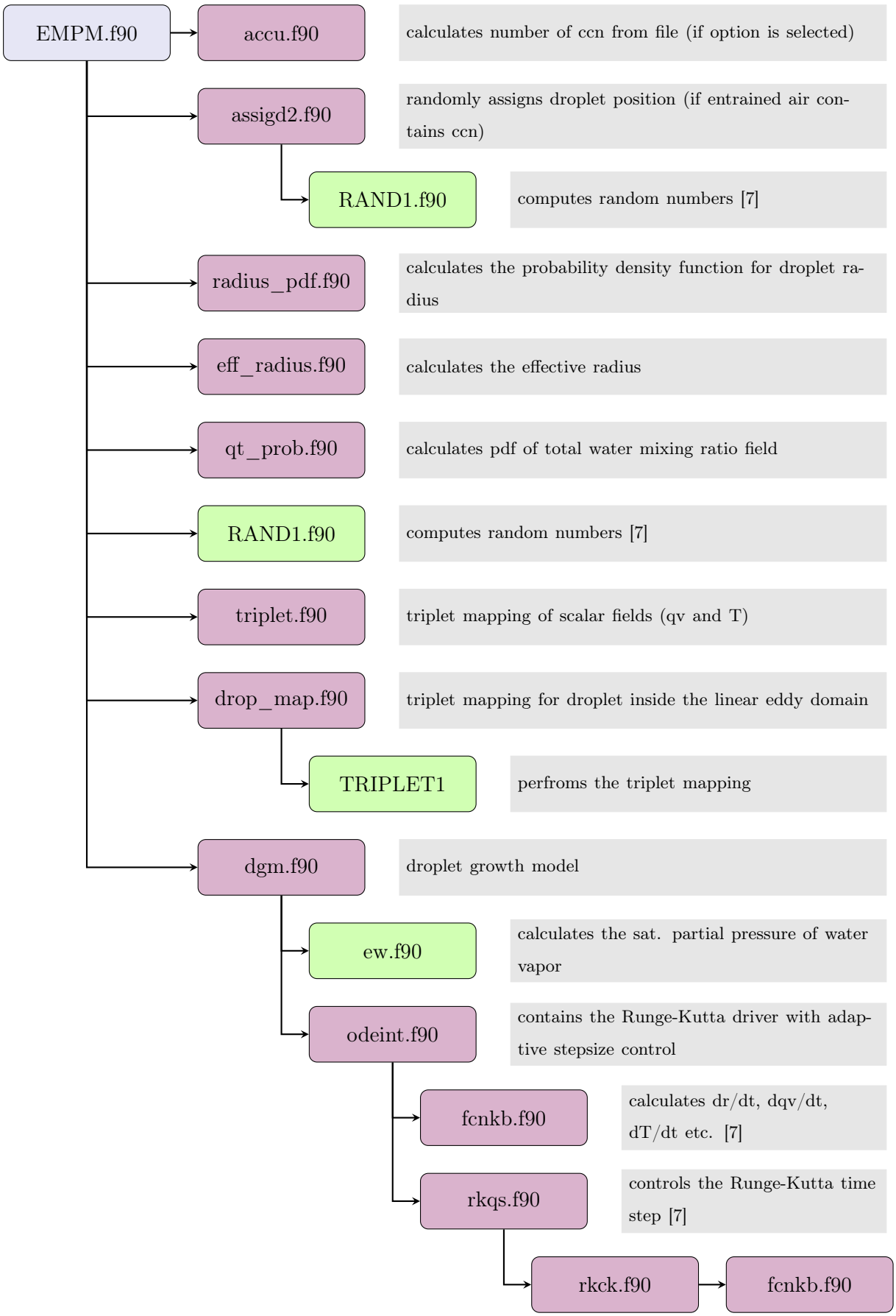
The file `temptime_1.dat` contains the temperature field (K) for the whole domain every `t_interval/time_step`-th iteration.

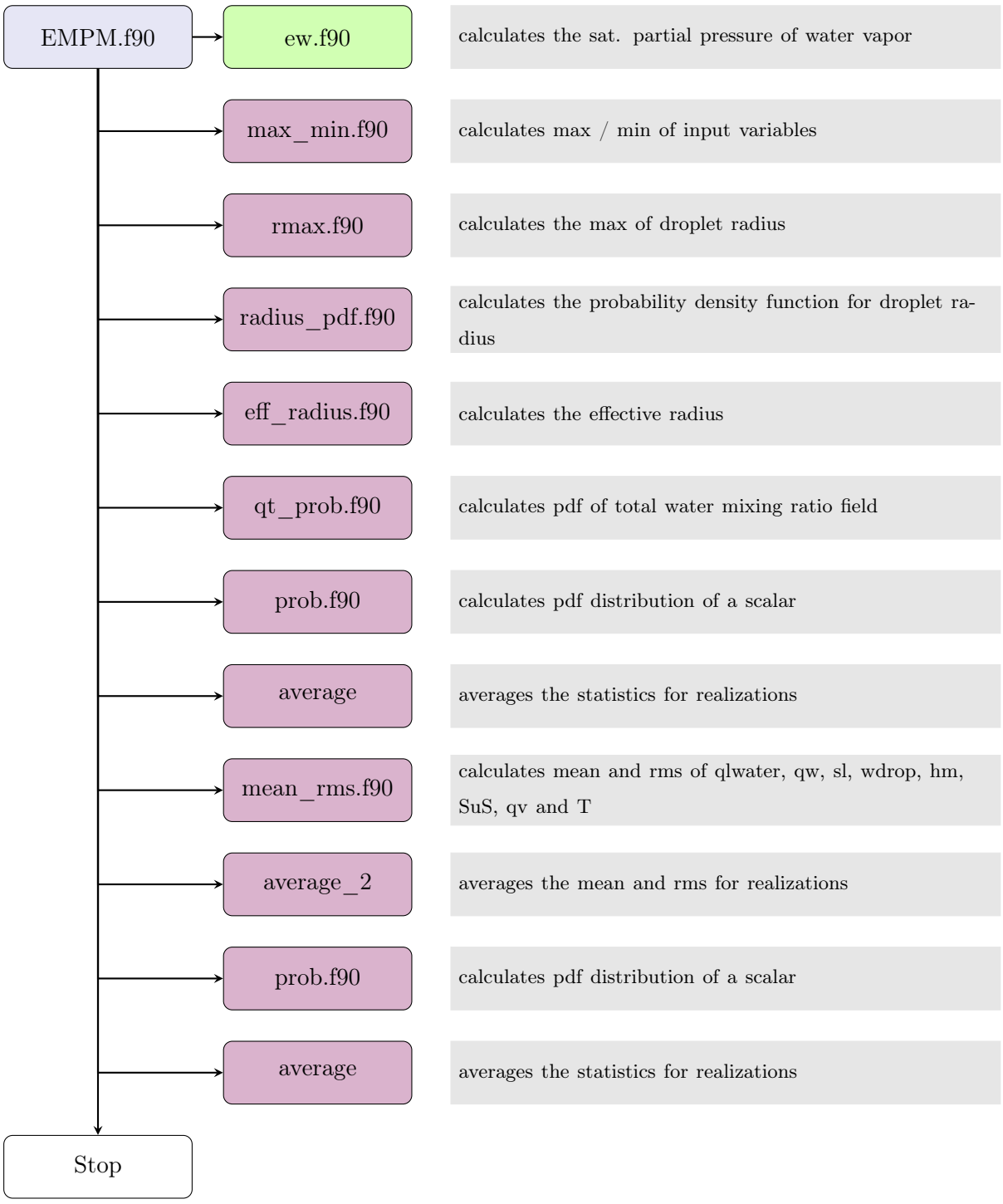
The file `t_index_1.dat` contains a time series of the total droplet number of the domain.

The file `xtime_1.dat` contains the position (-) of each droplet every `t_interval/time_step`-th iteration.

8. Flowchart - Subroutines and Functions




EMPM.f90
accu.f90
calculates number of ccn from file (if option is selected)
assigd2.f90
randomly assigns droplet position (if entrained air contains ccn)
RAND1.f90
computes random numbers [7]
radius_pdf.f90
calculates the probability density function for droplet radius
eff_radius.f90
calculates the effective radius
qt_prob.f90
calculates pdf of total water mixing ratio field
RAND1.f90
computes random numbers [7]
triplet.f90
triplet mapping of scalar fields (qv and T)
drop_map.f90
triplet mapping for droplet inside the linear eddy domain
TRIPLET1
perfroms the triplet mapping
dgm.f90
droplet growth model
ew.f90
calculates the sat. partial pressure of water vapor
odeint.f90
contains the Runge-Kutta driver with adaptive stepsize control
fcnkb.f90
calculates dr/dt, dqv/dt, dT/dt etc. [7]
rkqs.f90
controls the Runge-Kutta time step [7]
rkck.f90
fcnkb.f90



9. First Result

The results shown in this section provide proof that the rewritten EMPM code gives results in near perfect agreement with the original FORTRAN77 code.

9.1. Comparision of F77 and F90

To compare the results of the rewritten FORTRAN90 to the output of the original FORTRAN77 code, the setup given in the original code was used.

domain length	= `20.0`
largest eddy	= `20.0`
assumed Kolmogorov length scale	= `0.01`
TKE dissipation rate	= `0.001`
mass of the droplet solute	= `0.112202E-17`
droplet number concentration	= `103`
droplet radius	= `0.216075E-06`
cloud base water vapor mixing ratio	= `1.57292e-02`
cloud base temperature	= `293.56`
cloud base supersaturation	= `-0.776`
cloud base pressure	= `96395`
cloud base vertical velocity	= `2.0`
height above cloud base	= `0.0`

The environmental profile is taken from a paper by Raga et al. (1990). Furthermore, all droplet start with the same initial properties and entrainment is disabled.

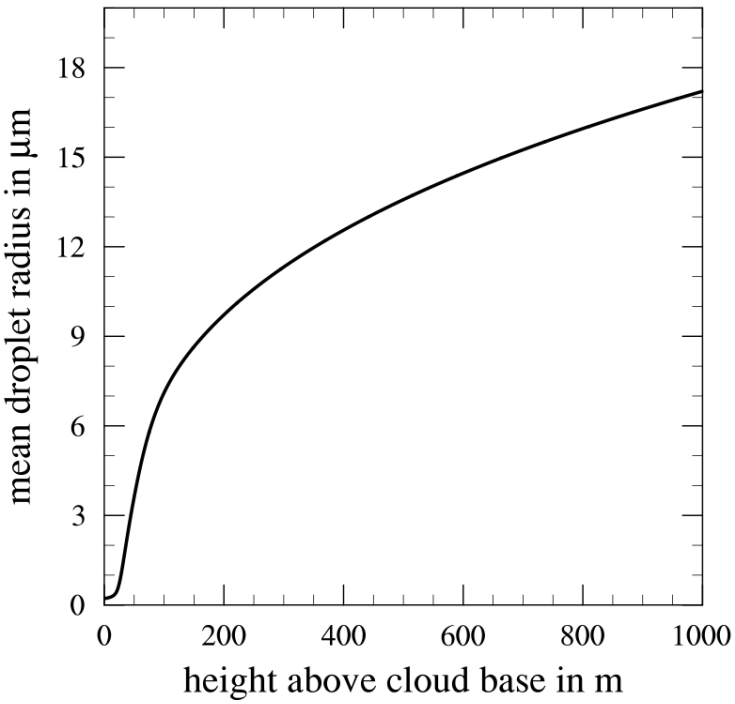


Figure 3: Control simulation of the original F77 code.

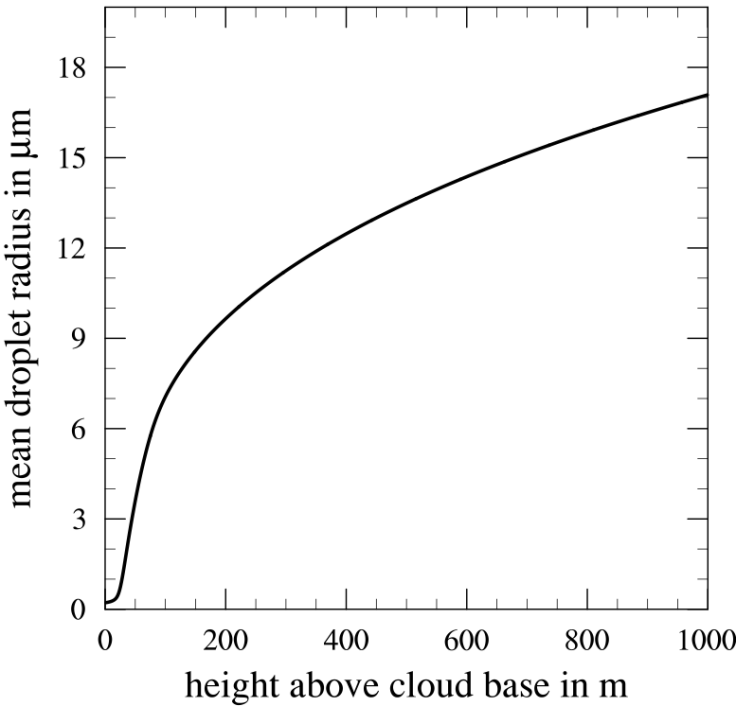


Figure 4: Test of the new F90 code.

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