Local scale

Polyphemus Training Session

About

Purpose: Local scale simulations: introduction to the use of Gaussian models with Polyphemus.

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Polyphemus version: 1.7

Location: `http://www.enpc.fr/cerea/polyphemus/sessions.html`

Contents

Installing the Session

You are advised to extract the archive **gaussian.tar.bz2** in your home directory.

```
$ tar -xjvf gaussian.tar.bz2
```

This creates a directory gaussian/ in polyphemus-sessions/, which has also been created if necessary.

Place the source Polyphemus in polyphemus-sessions/ also so that the paths given in configuration files are correct.

During the practical session, we will work in polyphemus-sessions/gaussian/config.

In what follows some command lines might be divided by \, they must be typed as a single line and are only divided for clarity's sake.

Introduction

Gaussian diffusion models are widely used in regulatory applications because they are analytical and conceptually appealing, and computationally cheap to use. Basically, it consists in assuming a Gaussian distribution of mean concentrations in the horizontal and vertical directions at any downwind location from the source. The Gaussian plume model gives the analytical expression of the concentration in the case of a continuous emission from the source at a constant rate, with a stationarity hypothesis. The Gaussian puff model gives the concentration for an instantaneous point source at different times. It can also be used for continuous sources, which are discretized into a series of Gaussian puffs.

The aim of this session is to learn the basic use of Polyphemus Gaussian models, thanks to three test cases. Polyphemus contains two types of Gaussian models: `GaussianPlume` which is a stationary Gaussian plume model, and `GaussianPuff` which is a Gaussian puff model. In addition, `GaussianPlume_aer` and `GaussianPuff_aer` are the corresponding models for aerosol species.

Basically, you only need a few information to run a Gaussian model. If there are no scavenging, deposition, or radioactive decay, the only species data you need is the name of the species. A meteorological data file provides some meteorological information (wind, temperature, stability) that are supposed to be constant and homogeneous. You also need to provide the source data. Sources are supposed to be points emitting either continuously or instantaneously, one or several species. Once you have created all your configuration files, you just have to compile and launch the corresponding program: plume.cpp, for plume model with gaseous species, puff.cpp for puff model with gaseous species, or the corresponding programs for aerosol species plume_aer.cpp and puff_aer.cpp.

Two preprocessing programs are available:

- In case there are scavenging or deposition, gaussian-deposition must be used prior to the simulation to compute scavenging coefficients and deposition velocities.
- In case there is a line source instead of a point source, discretization may be used to discretize it into a series of point sources.

1 Test cases description

The first test case is a simple case using plume with gaseous species emitted by point sources, the second one uses plume_aer with aerosol species, and the third one uses puff with gaseous species emitted by a line source. The test cases are described in Polyphemus guide (part **Polyphemus Gaussian Test-Case**). This training session is based on the same cases, but goes further than

the basic test case description.

The directory polyphemus-sessions/gaussian/ contains:

- A subdirectory config/ which holds all the configuration files used in the preprocessing and the simulation.
- A subdirectory results/ which is meant to hold the results of all simulations. It is also divided in three subdirectories (one for each kind of simulation):

  puff_line/ for the Gaussian puff model and a gaseous line source.

  puff_aer/ for the puff model with point sources of gaseous and aerosol species.

  plume/ for the Gaussian plume model with gaseous species only.

This session is divided into three parts:

1. Using preprocessing programs for Gaussian models.
2. Launching the three simulations.
3. Visualizing results.

2 Deposition preprocessing

2.1 Description

In case loss processes are taken into account, you need to compute scavenging coefficients and deposition velocities for the various species. This is achieved by using gaussian-deposition_aer. This program uses one configuration file, gaussian-deposition_aer.cfg, which contains all necessary information.

- [data] contains paths to other data files containing species data and meteorological data
- [scavenging] is used to choose the parameterization to compute scavenging coefficients for gaseous and aerosol species
- [deposition] is used to choose the parameterization to compute deposition velocities for gaseous and aerosol species
- [output] contains the path to the file where output data will be written.

For a more detailed description, see Polyphemus Guide, part **Preprocessing/Preprocessing for Gaussian models/Programs gaussian-deposition and gaussian-deposition_aer**.

Diameter file. The file diameter.dat contains aerosol diameters. This applies to all aerosol species. For example, if **PM** is an aerosol species, and there are two diameters in the diameter file:

```
[diameter]

# Particle diameter (micrometer)
1.0
5.0
```

the simulation will be run with **PM** particles of the two diameters. Scavenging coefficients, deposition velocities, (as well as concentrations in the main program) will be computed as if there were two different species: **PM_0**, which refers to **PM** with the first diameter in the diameter file, that is, 1 µm, and **PM_1**, which refers to **PM** with the second diameter in the diameter file, that is, 5 µm.

Note that there is no need to define diameters in a special file. It can as well be defined inside a section `[diameter]` in the main configuration file. The reason it is defined in a separated file here is that it is common to the preprocessing program and to the main program.

Species file. The file `gaussian-species_aer.dat` contains data about the species.

- `[species]` and `[aerosol_species]` contain the list of gaseous and aerosol species respectively
- `[scavenging]` and `[deposition]` contain the list of gasous species for which scavenging and deposition occur. For others, coefficients are set to 0. For aerosol species, scavenging and deposition always occur.
- `[scavenging_constant]` and `[deposition_constant]` contain values of scavenging coefficients and deposition velocities for gaseous species when constant values are used. One value is needed for each species.
- `[scavenging_constant_aer]` and `[deposition_constant_aer]` contain values of scavenging coefficients and deposition velocities for aerosol species when constant values are used. One value for each aerosol diameter.

Other data can be added if needed. For a more detailed description, see Polyphemus Guide, part **Preprocessing/Preprocessing for Gaussian models/Programs gaussian-deposition and gaussian-deposition_aer** and also part **Models/GaussianPlume**.

Meteorological data file. The file `meteo.dat` contains meteorological data. For each meteorological situation, temperature, wind angle, wind speed, boundary height and stability class are needed. These information are provided inside a section `[situation]`, and the meteorological data file contains as many sections are there are situations.Note that other information might be provided, depending on the parameterization to compute the standard deviations.

For a more detailed description, see Polyphemus Guide, part **Preprocessing/Preprocessing for Gaussian models/Programs gaussian-deposition and gaussian-deposition_aer**.

2.2 Using the program

First compile the preprocessing program:

```
 cd ../../Polyphemus/preprocessing/dep/
../../Polyphemus/utils/scons  gaussian-deposition_aer
```

Then run it from the configuration files directory ~/polyphemus-sessions/gaussian/config/.

```
 ../../Polyphemus/preprocessing/dep/gaussian-deposition_aer \
gaussian-deposition_aer.cfg
```

The output on screen will be :

```
Reading configuration file... done.
Reading meteorological data... done.
Reading species... done.
Reading diameter... done.
Computation of the scavenging coefficients... done.
Computation of the deposition velocities..done.
Writing data... done.
```

The file gaussian-meteo_aer.dat has been created and placed in the configuration files directory polyphemus-sessions/gaussian/config/. It will be used for all simulations. Open it to see if it has been correctly written: a list of scavenging coefficients and deposition velocities must have been added at the end of each section `[situation]`.

Note: For simulations where only gaseous species are taken into account, the program gaussian-deposition could be used instead of gaussian-deposition_aer.

The scavenging coefficient have been computed with the Belot parameterization for gaseous species, and the Slinn parameterization for aerosol species.
Change the file gaussian-deposition_aer.cfg in order to use now constant values for scavenging of gaseous and aerosol species. Run now the program in order to have constant scavenging coefficients equal to $1. \times 10^{-4}\ \mathrm{s}^{-1}$ *for Iodine and no scavenging for Caesium, and constant deposition velocities equal to* $0.5 \times 10^{-2}\ \mathrm{m\,s}^{-1}$ *for all gaseous species.*
Open the file gaussian-meteo_aer.dat to verify that the correct values are given for all species. This file will be used for all simulations in this session.

3 Discretization

3.1 Description

This step is only necessary for the simulation with a discretized line source. Its aim is to discretize this source into a series of point sources. There are two possible types of line sources:

1. An instantaneous line source is discretized into a given number of point sources that all are emitted at the same time.

2. A moving source (typically an aircraft or a car). Given the source trajectory, its velocity, and its starting time, one can represent it by a series of puffs emitted along the trajectory at different emission times. The number of points on the trajectory is determined by the time step between two puffs Δt.

In addition, the non-moving line source, as point sources, can be a continous source (for example modeling a road traffic) or a puff source. It will then be discretized either into a series of puffs or into a series of plumes.

The program `discretization` uses one configuration file, `discretization.cfg`, which contains all necessary information.

- `[trajectory]` contains the path to a file which gives the trajectory. It also contains N_p (for instantaneous sources) or Δt (for moving sources).
- `[source]` contains basic source data: the type (puff or continuous) and the emitted species.
- `[puff-source]` contains puff data: quantity (divided into the number of points on the trajectory), source velocity, initial release time.
- `[plume-source]` contains plume source rate per unit of length.
- `[output]` contains the path to the file where output data will be written.

Note that when the source velocity is not equal to 0., it is assumed to be a moving source and N_p is not read. Also note that N_p is the number of points to be computed per segment, including the nodes given in the trajectory file. If one node is common to two segments, it is taken into account only once. Thus, one of the two segments contains only $N_p - 1$ points.

The file defining the trajectory looks like this:

```
#X(m) Y(m) Z(m)
0. 10. 0.5
30 10. 0.5
40. 25. 0.5
```

Each line corresponds to the coordinates (abscissa, ordinate, height) of a point on the trajectory. Hence, this contains at least two points, but there can be more (broken line).

For a more detailed description of the files, see Polyphemus Guide, part **Preprocessing/Preprocessing for Gaussian models/Program discretization**.

3.2 Using the program

The first line to be discretized is an instantaneous line source. The trajectory is defined in file `line-emission.dat`.

Compile the preprocessing program `discretization`.

```
cd ../../Polyphemus/preprocessing/emissions/
../../Polyphemus/utils/scons discretization
```

Then run it from the test case directory polyphemus-sessions/gaussian/config/.

```
  ../../Polyphemus/preprocessing/emissions/discretization \
discretization.cfg
```

The output on screen will be:

```
Reading configuration file... done.
Reading trajectory data...  done.
Length of the trajectory: 48.0278
Number of points on the trajectory: 11
Writing source data... done.
```

The file puff-discretized.dat has been created and placed in the configuration files directory ~/polyphemus-sessions/gaussian/config/. It contains a series of puffs representing the discretized line source.

Change the main configuration file to discretize the line source into 27 points instead of 11 (remember that, for this example, the total nomber of points is $2N_p - 1$).

4 Running simulations

4.1 Plume simulation with gaseous species

4.1.1 Simulation

This simulation uses the program plume.cpp along with the configuration file plume.cfg. This file contains the following information:

- [display] contains options about what should be displayed on screen during simulation.
- [domain] contains the cartesian domain where concentrations are to be computed, path to the species file and miscellaneous information.
- [gaussian] contains all options that can be activated: plume rise, decay, scavenging and dry deposition. It also contains paths to meteorological data file and source file.
- [deposition] contains the deposition model.
- [output] contains path to the output configuration file.

The other data files that are used here are:

- gaussian-levels.dat contains vertical levels where concentrations are computed.
- gaussian-species_aer.dat contains species data.

- gaussian-meteo_aer.dat gives all meteorological data, scavenging coefficients and deposition velocities. It was created during preprocessing.
- plume-source.dat contains source data.
- plume-saver.cfg contains paths to results files.

For detailed description, see Polyphemus user's Guide (part **Models/GaussianPlume**).

Compile plume.cpp (in ../../Polyphemus/driver/) and run the plume simulation. Display meteorological data on screen during simulation. Only scavenging is taken into account. There is no plume rise. The output on screen will be:

```
        Temperature     Wind angle      Wind velocity   Stability
Case #0
        15              -100            0.5             D
Case #1
        10              -5              2               D
Case #2
        10              20              5               D
Case #3
        10              60              10              D
```

A quick way to make sure that the simulation has been correctly done is to use the program get_info_float (located in ../../Polyphemus/utils/).

Go in the directory where your results file has been placed. The file Iodine.bin contains concentrations for the species Iodine. The command get_info_float Iodine.bin returns something like:

```
Minimum: 0
Maximum: 0.483831
Mean: 0.0140979
```

For more information about this tool, see Polyphemus user's Guide (part **Using Polyphemus/Useful tools**).

Now run again the program. This time, use also radioactive decay and dry deposition with Overcamp model. Change the results file name so that the previous one won't be overwritten. Then use get_diff_float to compare the two results.

```
 mv ../results/plume/Iodine.bin ../results/plume/Iodine-ref.bin
../../Polyphemus/processing/gaussian/plume plume.cfg
get_diff_float ../results/plume/Iodine.bin ../results/plume/Iodine-ref.bin
```

You should obtain something like:

```
                 File #0         File #1
Minima:          0               0
Maxima:          0.443567        0.483831
Means:           0.0105841       0.0140979
Standard dev.:   0.0411543       0.053437

                 Difference
Minimum:         -0.266971
Maximum:         0
Mean:            -0.00351376
Standard dev.:   0.019425

Correlation between files #0 and #1: 0.948511
```

This shows that radioactive decay and dry deposition are taken into account and induce lower concentrations.

4.1.2 Visualizing results

To easily visualize the results of a simulation, it is recommanded to use the interactive python interpreter IPython (launched with the command `ipython`). For more detailed information about how to launch and use ipython, see Polyphemus user's Guide (part **Postprocessing/Visualizing results**).

Launch IPython from the plume results directory. Then, import the modules that are needed for results visualization with the command:

```
>> import atmopy
>> from atmopy.display import *
```

Then, you need to import the concentration field you want to visualize:

```
>> d = getd(filename = 'Iodine.bin', Nt=4, Nz=2, Ny=200, Nx=200)
```

Nt is normally the number of time steps. Here, as it is a stationary simulation, it should be equal to 1. However, as there are four meteorological situations, we have here $Nt = 4$, as each situation is similar to a time step for an unstationary simulation. It would be the same if it was an unstationary simulation (puff model) with several meteorological situations. If there are 10 time steps, and 4 meteorological situations, you will put $Nt = 40$. The first ten time steps represent the first situation, from 10 to 20 you have the concentration field for the second situation, and so on...
Nz is the number of vertical levels, Ny and Nx the number of points in y and x directions. All numbers must be consistent with the simulation domain. If you are not sure, or if the command

doesn't work, check the size of the binary file you are trying to visualize. It should be of size `Nt` × `Nz` × `Ny` × `Nx` × `4`.

You now have an array named 'd' that contains the concentration field for Iodine. To check it has the right shape, use the command:

```
>> d.shape
(4, 2, 200, 200)
```

This returns `(Nt, Nz, Ny, Nx)`.

Now, visualize domain concentration for the first situation and add a colorbar:

```
>> contourf(d[0,0])
>> colorbar(format='%1.2f')
```

You should obtain the Figure 1.

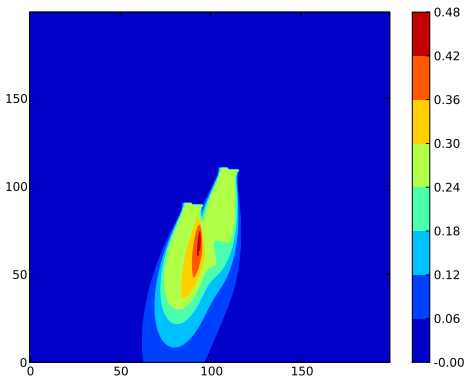


Figure 1: Plume visualization for the first meteorological situation.

Visualize the concentration field for the other meteorological situations. You should see that the wind is turning with increasing speed.

To visualize the plume evolution according to meteorological situations, you can use atmopy function `stat.spatial_distribution`. This function applies a given function to a given field at each time step. Hence, if you type the command:

```
>> s = atmopy.stat.spatial_distribution(d,"max")
>> contourf(s[0])
```

You should see the spatial distribution of maximum concentration at level 0. In our case, it corresponds to the maximum concentration for each meteorological situation. See Figure 2.

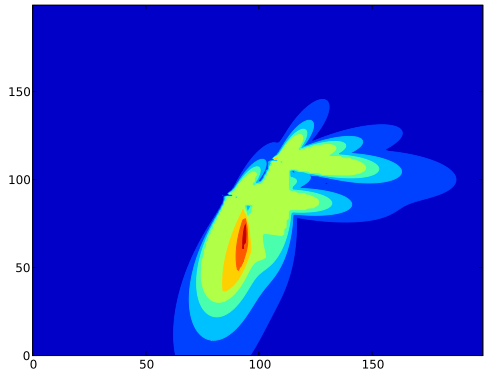


Figure 2: Plume visualization for all meteorological situations.

4.2 Puff simulation with aerosol species

4.2.1 Simulation

This simulation is run with the main configuration file `puff_aer.cfg`. It uses the same files as the plume simulation for vertical levels and species. It uses the meteorological data files created during preprocessing. The saver file, `puff-saver_aer.cfg` is different, because in addition to saving gaseous species, it also has to specify which aerosol species and diameters are saved. For more information about it, see Polyphemus user's Guide, part **Drivers/Output savers/SaverUnitDomain_aer**.

Compile the program `puff_aer` and run the simulation, using scavenging and deposition for all species. Use `get_info_float` to check your results.

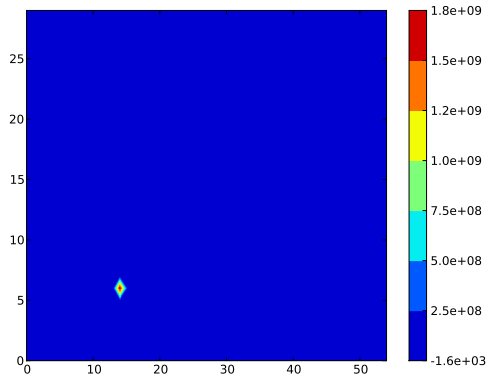
4.2.2 Visualizing results

Without quitting ipython, you can move to the result directory for puff case with aerosol species. Use `getd` to import the concentration field of a given species. Note that there are 4 *meteorological situations and* 80 *time steps for each situation, so you have to put* $Nt = 320$*. If you are not sure, you can also put* $Nt = 0$*, which means that the number of time steps is automatically computed from the other indications (*Nz*,* Ny *and* Nx*, and the total file size). Then, visualize the puff for different time steps with `contourf`.*

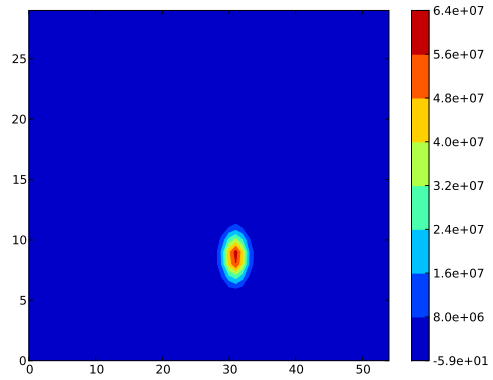
To visualize several time steps on the same figure, just use `contourf` several times. If you want to clear the figure, use the command `clf()`. Figure 3 gives an example of what you can obtain. The commands used to obtain Figure 3(a) are given below.

```
>> d = getd(filename = 'aer1_0.bin', Nt=0, Nz=2, Ny=30, Nx=55)
>> d.shape
>> figure()
```

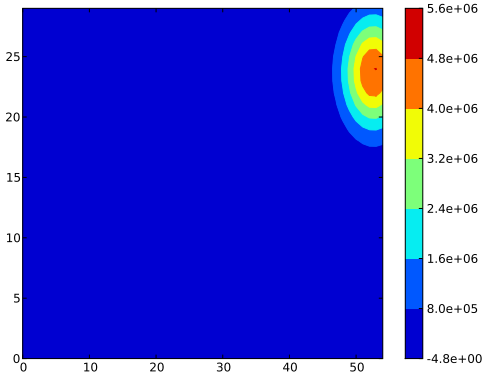
```
>> contourf(d[79,0])
>> xlim(0,54)
>> ylim(0,29)
>> colorbar(format='%1.1e')
>> savefig('puff_79.eps')
```



(a) Time step 79 (first situation)



(b) Time step 159 (second situation)



(c) Time step 239 (third situation)

Figure 3: Puff visualization at several time steps for the 4 meteorological situations, for species aer1 and first diameter.

Add two more diameters for particles: 8 μm *and* 10 μm. *Use the same data for scavenging and deposition as for particles of diameter* 5 μm. *Rerun the simulation. Save concentrations for all species and diameters. Check your results.*

4.3 Puff simulation with line sources

4.3.1 Simulation

This simulation is run with the program `puff` and the main configuration file `puff.cfg`. Note that, except from using a line source, this simulation is simpler: there are no loss processes, hence no need to compute coefficients. The species file is reduced to the section `[species]`, so

it is written directly in the main configuration file. The source file contains the discretized line source created during preprocessing.

In this part, only the first meteorological situation is to be used, so you have to modify the meteorological data file. A useful trick, if you do not want to modify the file too rashly, is to simply add a symbol at the beginning of each section you do not want to be read: for example, `[situation]` becomes `[*situation]`. That way, all information contained in the modified section will not be read, but you can easily come back to the previous file. This works for all configuration files.

Run the simulation.

4.3.2 Visualizing results

Now, go into the directory for puff case with line source. First visualize the concentration field of species CO_2 for 80 time steps.
Figure 4 gives an example of what you can obtain.

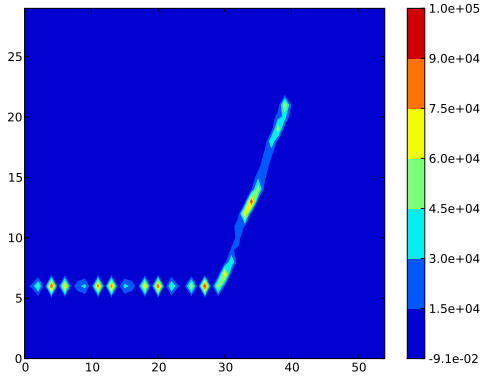


Figure 4: Puff line source for species CO_2 at time step 79.