MUNICH model test case: a Paris suburb Le Perreux-sur-Marne

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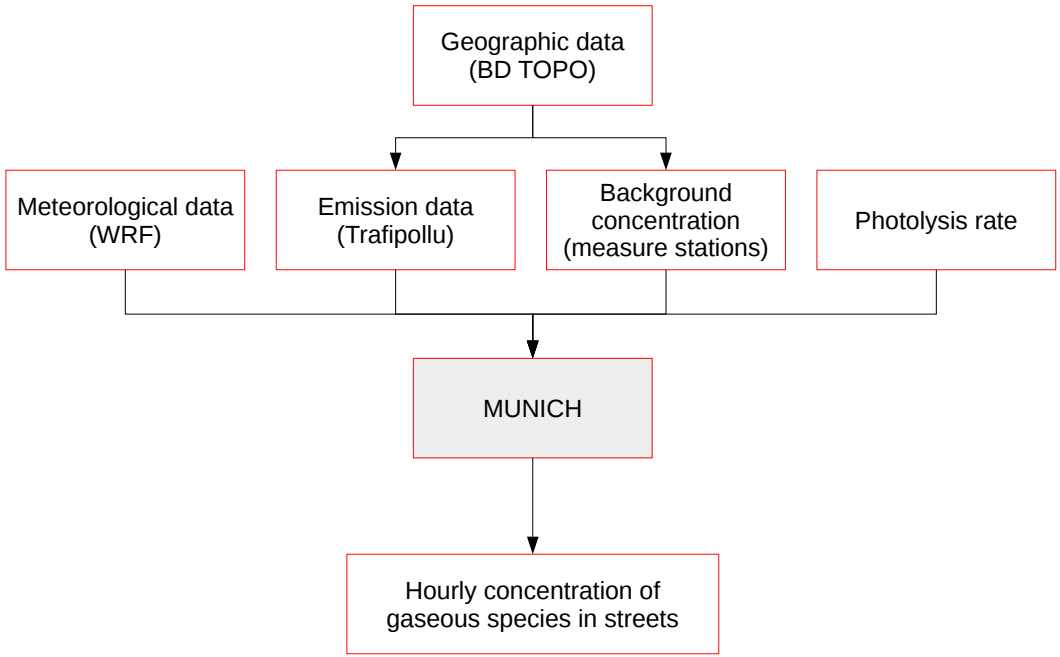
Contents

Introduction

- Model of Urban Network of Intersecting Canyons and Highways (MUNICH)
- Street-canyon component
- Intersection component



Studied area

- Le Perreux-sur-Marne - Paris suburb - 13km east of Paris
- 557 streets
- 433 intersections
- Boulevard Alsace-Lorraine - Air monitory stations

Boulevard Alsace-Lorraine

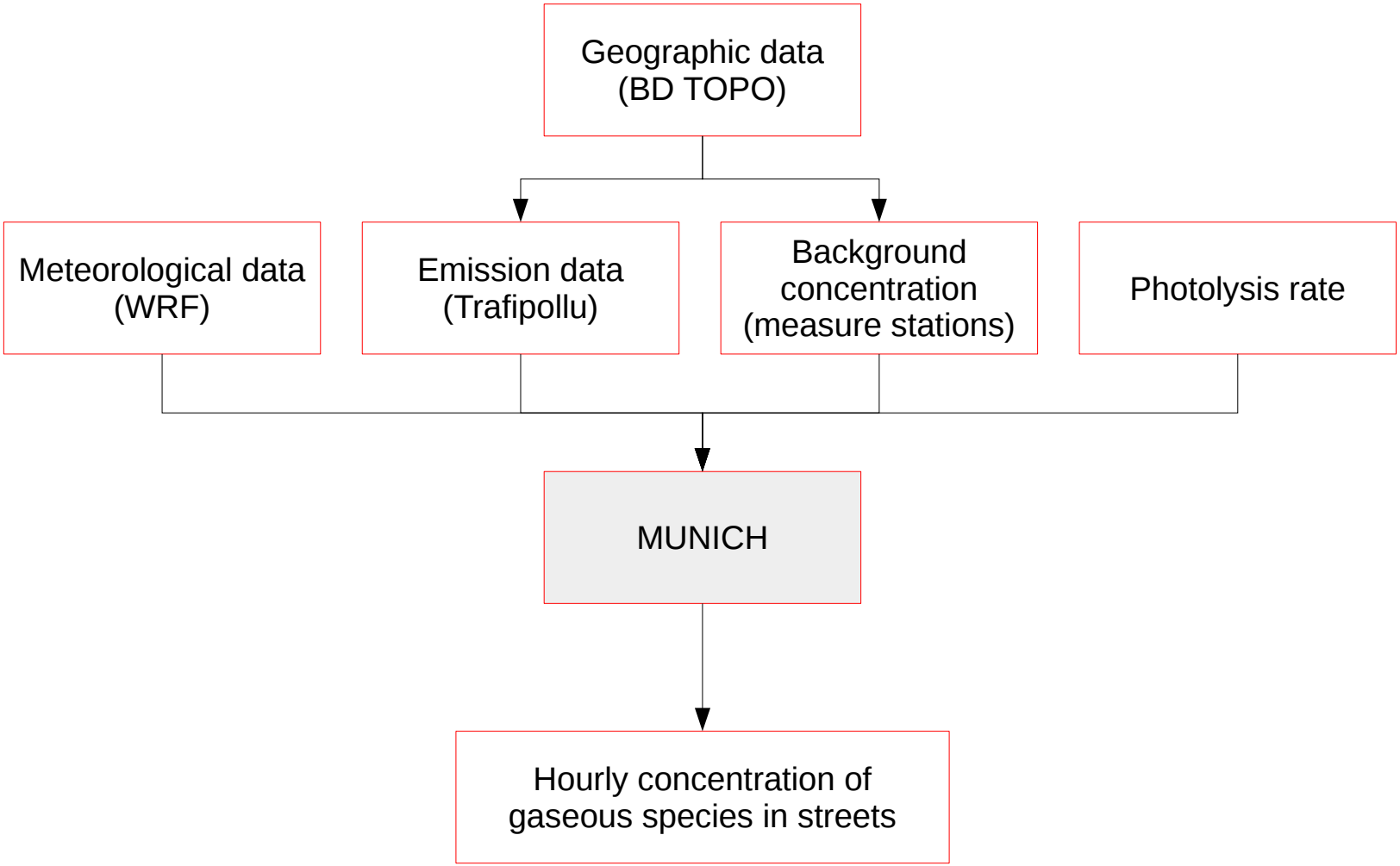
Île de France - Le-Perreux-sur-Marne highlighted

Configuration applied

- Domain: Le Perreux-sur-Marne
- Simulated period: March 24^{th} to March 30^{th}
- Simulation of gas-phase species (including NO_x, and O_3)
- Chemical reactions: CB05 chemical kinetic mechanism (Yarwood et *al.*, 2005)

Measured data - Trafipollu campaing

- **Emission and concentration data at Boulevard Alsace-Lorraine**
- ANR Project - Agence nationale de la recherche
- Multi-scale modeling of traffic pollution in an urban environment
- Main objective: Development of modeling tools to dynamically determine the location of pollutants generated by road traffic in an urban environment


Geographic data
(BD TOPO)
Meteorological data
(WRF)
Emission data
(Trafipollu)
Background
concentration
(measure stations)
Photolysis rate
MUNICH
Hourly concentration of
gaseous species in streets

Geographical data

- Traffic lane widths and building heights → BD TOPO
- Street widths and building heights of the 15 major streets were explicitly estimated;
- For minor surfaces roads → width = 3m;
- Average street → width = 7.5m and building height = 6.9m (default);

http://professionnels.ign.fr/bdtopo

Geographical data

- Street data are available in "*street.dat*" file;
- For each street we obtain:
  - Column 1: Street ID
  - Column 2: Initial intersection
  - Column 3: End intersection
  - Column 4: Street length
  - Column 5: Street width
  - Column 6: Street height

```
1;1;2;122.686160495;7.5;6.9
3;1;6;107.94798805;7.5;6.9
4;7;8;155.856467313;7.5;6.9
5;8;10;124.490042998;7.5;6.9
6;11;12;196.113095869;41.0;10.2
7;13;10;99.5930099431;7.5;6.9
8;1;13;169.563212564;7.5;6.9
9;17;18;156.567562811;7.5;6.9
10;17;8;145.452588007;7.5;6.9
11;1;22;198.442274833;7.5;6.9
12;22;24;189.386592243;7.5;6.9
14;27;28;129.283403254;7.5;6.9
15;29;27;28.243530365;7.5;6.9
17;33;34;88.3260073982;7.5;6.9
19;8;38;110.337649;7.5;6.9
```

Geographical data

- Intersection data are available in "*intersection.dat*" file;
- For each intersection we obtain:
  - Column 1: Intersection ID
  - Column 2: Longitude
  - Column 3: Latitude
  - Column 4: Number of streets that generate interception
  - Others columns: List of streets that generate interception

Meteorological data

- WRF (*Weather Research and Forecasting Model*) results were applied to calculate meteo data in each street and intersection;
- Grid resolution: 1.5×1.5 km^2;

- Attenuation;
- Monin–Obukhov length;
- Planetary boundary layer height;
- Specific Humidity;
- Pressure;
- Temperature;
- Friction velocity;
- Wind direction;
- Wind speed;

Traffic model and emissions

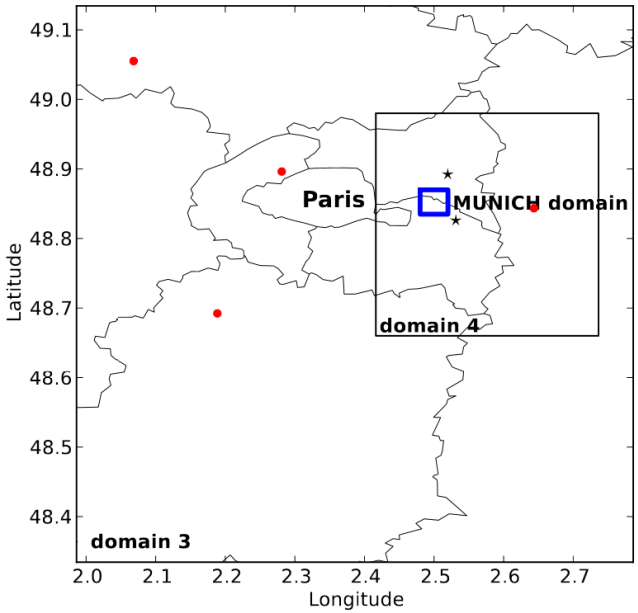
- Hourly traffic emissions for NO, NO_2 and VOC
- COPERT4
  - Total vehicle number;
  - Hourly average speed for each street;
  - Optional fleet in circulation data: carburant, vehicles category (heavy or light), etc...
  - Four categories to calculate EF: NO_x and VOC's $\rightarrow$ Group 1
  - Pollutants for which a detailed methodology exists, based on specific emission factors and covering different traffic situations (i.e. urban, rural, highway) and engine conditions

Traffic model and emissions

- In Trafipollu project: HEAVEN model was applied based in COPERT4
- Two typical days were simulated: 25/03/2014 (working day) and 30/03/2014 (weekend day)
- Hourly emission data for several atmospheric pollutants, including: NO, NO_2, NMHC, CH_4, PM_{10}...
- For CB05 gas-phase chemical mechanism $\rightarrow$ NMHC specifiation;

Boundary conditions

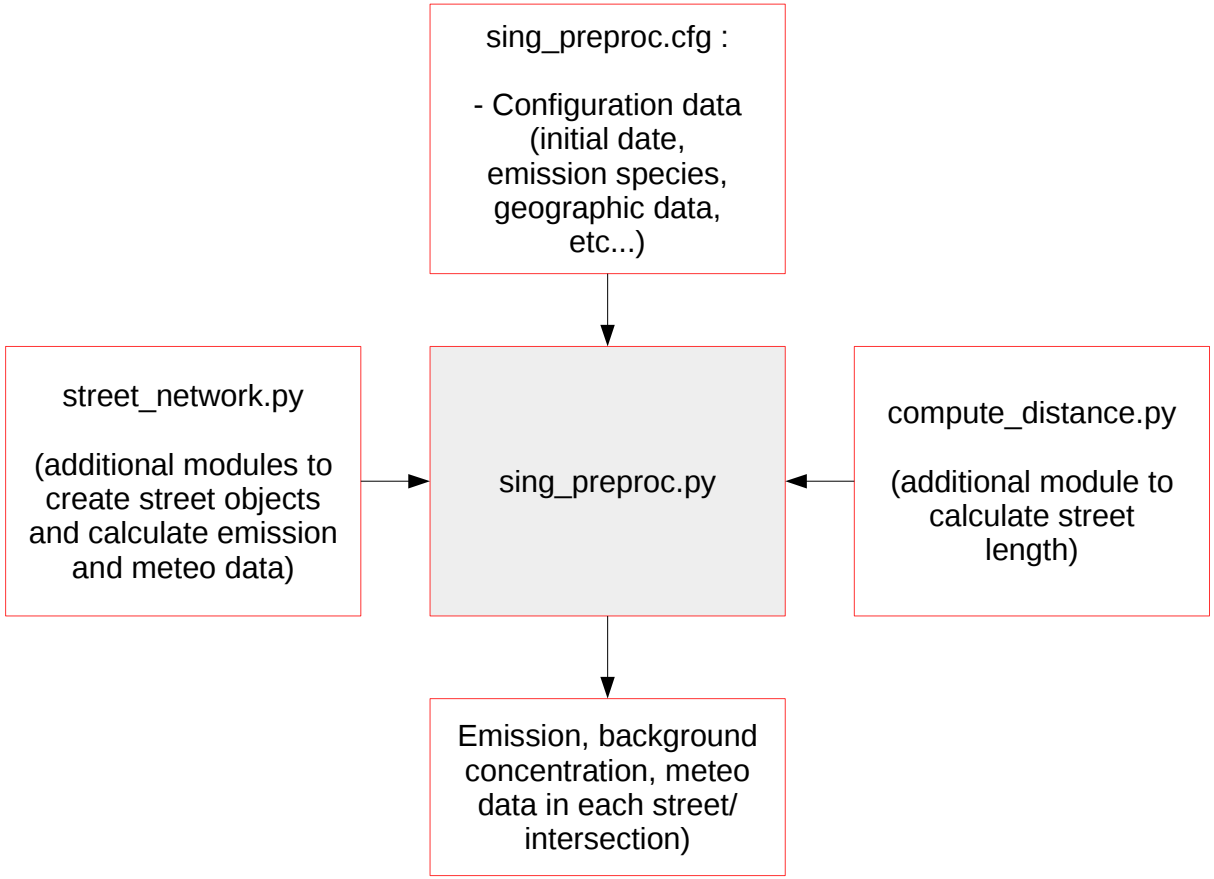
- Mean value → Mass concentration measured in near air quality stations for O_3, NO and NO_2;
- Distance of 5 to 7km from the area;



Photolysis Rate

- Photolytic reactions play a critical role in controlling the abundance of many atmospheric pollutants $\rightarrow NO_2$;
- FAST-J algorithm $\rightarrow$ (Wild et al., 2000) - UC Irvine
  - Date min; Delta t, Ndays;
  - Time angle min, Delta time angle, Ntime angle;
  - Latitude min, Delta latitude, Nlatitude;
  - Altitudes;
  - Chemical species;

Preprocessing code



Preprocessing code - sing_preproc.py

1. Read current date and associate to emission file (weekend or weekday);
2. *read_traffic_data*: Reads total number of streets and emission of selected chemical species;
3. *get_street_geog*: Get street geographical informations: length, width, builiding height;
4. Merging streets:
   - Automatic merging → "street-merging-lookup-table.txt"
   - Manual merging → "street-merging.txt"
5. Merging nodes:
   - Removing the same nodes;
   - Removing the nearest nodes (Distance inferior to 10m);

Preprocessing code - sing_preproc.py

6. *get_meteo_data*:
   - Reads meteorological data for each street and intersection;
   - Compute wind direction
   - Compute heights;
   - Compute attenuation;
   - Compute LMO;
7. *get_background_concentration*: Measurements data for NO, NO_2 and O_3;
8. *write_output*: ASCII files $\rightarrow$ Intersection and street data;
9. Output meteo, emission and background files in binary format;

Preprocessing code - sing_preproc.cfg

```
[input]

t_min: 20140324_00
Delta_t: 1 # in hr
Nt: 168 # for 7 days until 30/03/2014

emission_dir_weekday: input/data-newref/20140325-TrafiPollu-REF/ # Tuesday

emission_dir_weekend: input/data-newref/20140330-TrafiPollu-REF/ # Sunday

emission_species: CH4 NMHC CO NOx

input_dir: input/

geog_info: <input_dir>/street-geog-info.dat

background_concentration: <input_dir>/airparif_background_concentration.dat

meteo_dir: <input_dir>/meteo/
wrfout_prefix: wrfout_d04

[output]

Output_dir: output/
```

Preprocessing code

python sing_preproc.py sing_preproc.cfg

Preprocessing code - speciation_aggregation.py

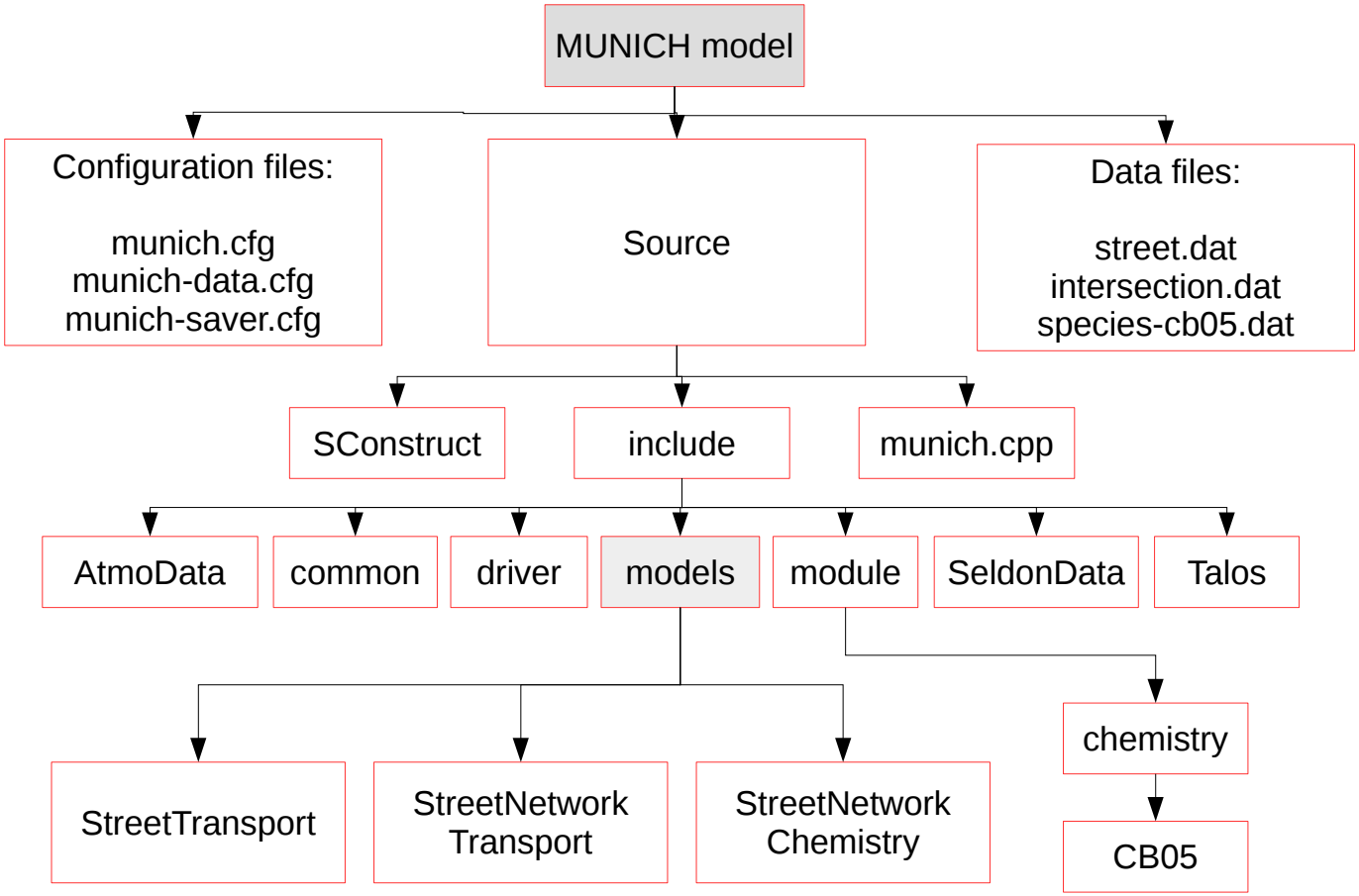
Script used to organic speciation from NMHC emission data → CB05 chemical kinetic mechanism ;

1. COVNM.dat
2. aggregation_cb05-siream.dat

Preprocessing code - speciation_aggregation.py

python speciation_aggregation.py

General model view



General model view - munich.cpp

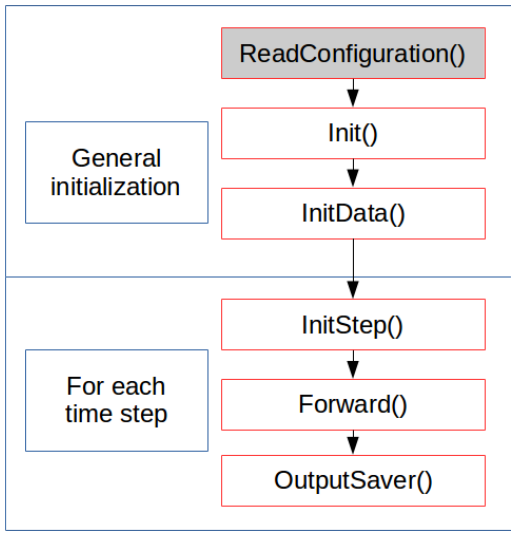
```
//////////////
// INCLUDES //

#define SELDONDATA_DEBUG_LEVEL_4

#include "AtmoData.hxx"
#include "StreetDriver.cxx"
#include "BaseOutputSaver.cxx"
#include "StreetNetworkChemistry.cxx"
#include "PhotochemistrySinG.cxx"

using namespace Polyphemus;

// INCLUDES //
//////////////

int main(int argc, char** argv)
{

  TRY;

  if (argc != 2)
    {
      string mesg  = "Usage:\n";
      mesg += string("  ") + argv[0] + " [configuration file]";
      cout << mesg << endl;
      return 1;
    }

  typedef double real;
  typedef StreetNetworkChemistry<real, Photochemistry<real> > ClassModel;

  StreetDriver<real, ClassModel, BaseOutputSaver<real, ClassModel> >
    Driver(argv[1]);

  Driver.Run();

  END;

  return 0;

}
```

General model view - StreetDriver.cxx

```
//! Performs the simulation.
/*! Initializes the model and the output saver, and then performs the loop
  over all meteorological conditions with calls to the model (over all time
  steps) and to the output saver.
*/
template<class T, class ClassModel, class ClassOutputSaver>
void StreetDriver<T, ClassModel, ClassOutputSaver>::Run()
{
  string line;

  /*** Initializations ***/

  Model.ReadConfiguration();
  Model.Init();
  Model.InitData();
  OutputSaver.Init(Model);
  Model.InitOutputSaver();

  for (int i = 0; i < Model.GetNt(); i++)
    {
      if (option_display["show_iterations"])
        cout << "Performing iteration #" << i << endl;

      if (option_display["show_date"])
        cout << "Current date: "
             << Model.GetCurrentDate().GetDate("%y-%m-%d %h:%i") << endl;

      Model.InitStep();
      OutputSaver.InitStep(Model);

      Model.Forward();

      OutputSaver.Save(Model);
      Model.OutputSaver();
    }
}

} // namespace Polyphemus.
```

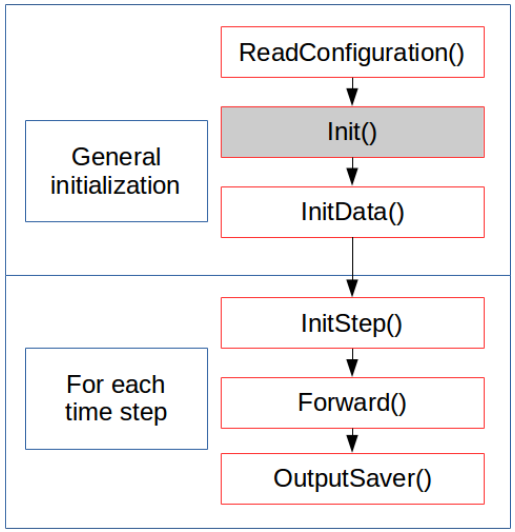
ReadConfiguration()

- Initial date;
- Simulation time;
- Species list → CB05: 56 gaseous species;
- Transfert parameterization: "Sirane" or "Schulte";
- Mean wind speed parameterization: "Sirane or Lemonsu";
- With horizontal fluctuation;
- Minimum street sind speed → 0.1m/s;
- Inlet files: meteo, emission, background;
- Chemistry and photolysis option;



Init()

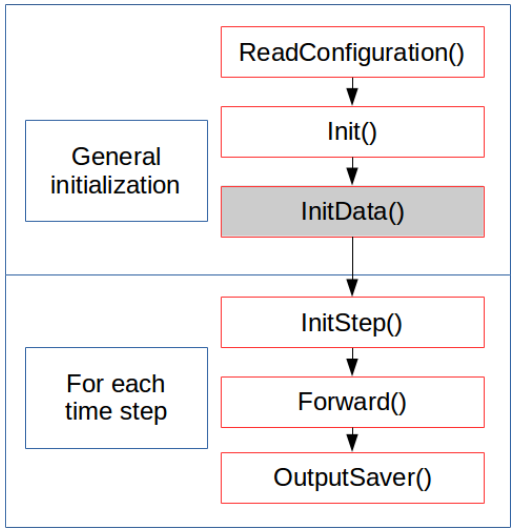
- Create street objects;
- Create intersection objects;
- Compute the street angle which is defined as the angle bewteen the street intersections (begin intersection to end intersection);
- Init chemistry module;



InitData()

- Input data initialization:

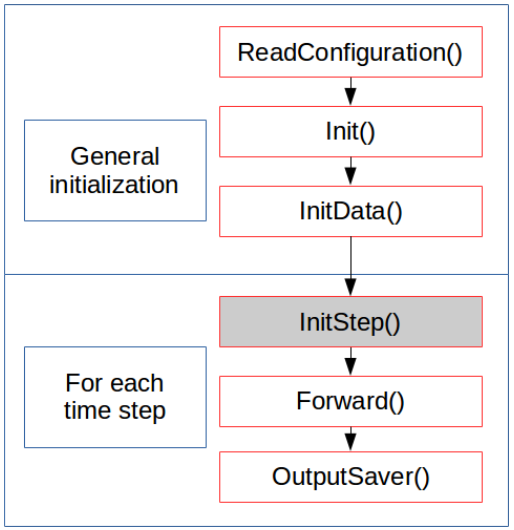
- Read meteo files;
- Read atmospheric emissions for each emitted specie;
- Read concentrations for each background specie;



InitStep()

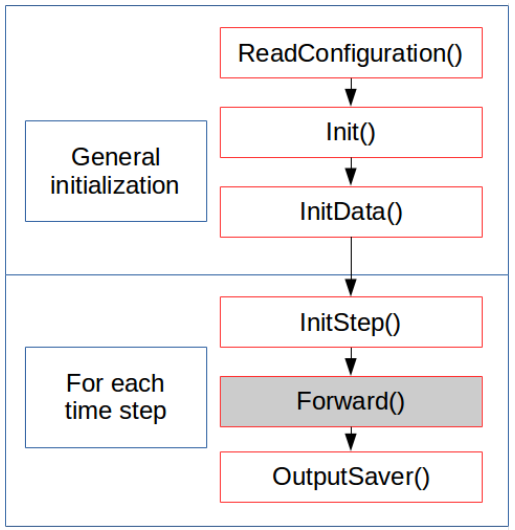
- Method called at each time step to initialize the model:

- Read meteo data for each street and intersections;
- Read emission data in each street;
- Read background data in each street;



Forward()

- Transport section:
  - Compute street mean velocity;
  - Compute the standard deviation of the vertical wind speed at a roof;
  - Compute the transfer velocity at roof level;
  - Compute the horizontal fluctuation of the wind direction;
  - Compute inflow and outflow in each street;



Forward()

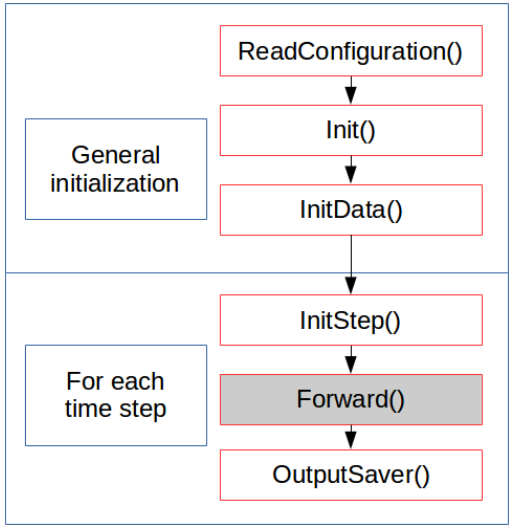
- Transport section:
  - Compute street concentration $\rightarrow$ Stationnary state assumption;

$$Q_{emis} + Q_{inflow} + Q_{chem} = Q_{vert} + Q_{outflow} + Q_{dep}$$

$$C = \frac{Q_{emis} + Q_{inflow} + (transfer_{velocity} \times W \times L) \times C_{background}}{Q_{outflow} + transfer_{velocity} \times W \times L}$$

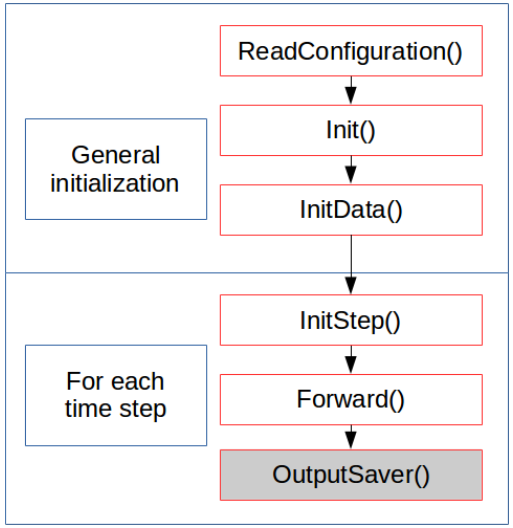
Forward()

- Chemistry section:
  - Calls the chemistry module to calculate the gain or loss of each chemical specie;
  - CB05 gas-phase chemical mechanism (Yarwood et al., 2005)
    - 52 species
    - 155 reactions (23 photolysis);



OutputSaver()

- Option of write the results in the output files in the text format (O_3, NO and NO_2);
- Street's hourly concentration in binary files for each one of the 52 species;



Configuration files - munich.cfg

```
[display]

Show_iterations: yes
Show_date: yes

[domain]

# Domain where species concentrations are computed.
Date_min = 2014-03-24-00»       Delta_t = 3600.0  Nt = 168

# File containing the species data.
Species: species-cb05.dat

[options]

# With chemistry module (yes or no)
With_chemistry: yes

# Which chemistry model (RACM, RACM2 or CB05, Leighton)?
Option_chemistry: CB05

# With adaptive time stepping for gaseous chemistry?
With_adaptive_time_step_for_gas_chemistry: yes
Adaptive_time_step_tolerance: 0.001
# Minimum time step that can be used.
Min_adaptive_time_step: 10.0
# Maximum time step that can be used.
Max_adaptive_time_step: 600.0

With_photolysis: yes

# Photolysis tabulation option compute from tabulations (1) or read from binary
# files (2).
Photolysis_option: 2
```

Configuration files - munich.cfg

```
[street]

# Parameterization to compute turbulent transfert velocity: "Sirane" or "Schulte".
Transfert_parameterization: Schulte

# Parameterization to compute mean wind speed within the street-canyon: "Sirane" or "Lemonsu".
Mean_wind_speed_parameterization: Lemonsu

# If the horizontal fluctuation is taken into account.
With_horizontal_fluctuation: yes # yes or no

# File containing the input data for intersections.
Intersection: intersection.dat

# File containing the input data for streets.
Street: street.dat

# Minimum wind speed within the streets.
Minimum_Street_Wind_Speed: 0.1 # in m/s

# If meteo data and background concentrations are available for each street.
With_local_data: yes

[data]

# File describing the input data.
Data_description: munich-data.cfg

[output]

# File describing which concentrations are saved.
Configuration_file:  munich-saver.cfg
```

Configuration files - munich-data.cfg

```
Directory: /net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/data-munich/

[emission]

Date_min: 20140316_00
Delta_t = 3600.
Nt = 2568

Fields: ALD2 ALDX API CH4 CO ETH ETHA ETOH FORM IOLE ISOP LIM MEOH OLE PAR TERP TOL XYL NO NO2
Filename: <Directory>/emission/&f.bin

[meteo]

Date_min: 20140316_00
Delta_t = 3600.
Nt = 2568

Fields: WindDirection WindSpeed PBLH UST LMO WindDirectionInter WindSpeedInter PBLHInter USTInter LMOInter Attenuation SpecificHumidity SurfacePressure
SurfaceTemperature
Filename: <Directory>/meteo/&f.bin


[background_concentration]

Date_min: 20140316_00
Delta_t = 3600.
Nt = 2568

Fields: O3 NO NO2
Filename: /net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/data-munich-background/background/&f.bin
```

Configuration files - munich-data.cfg

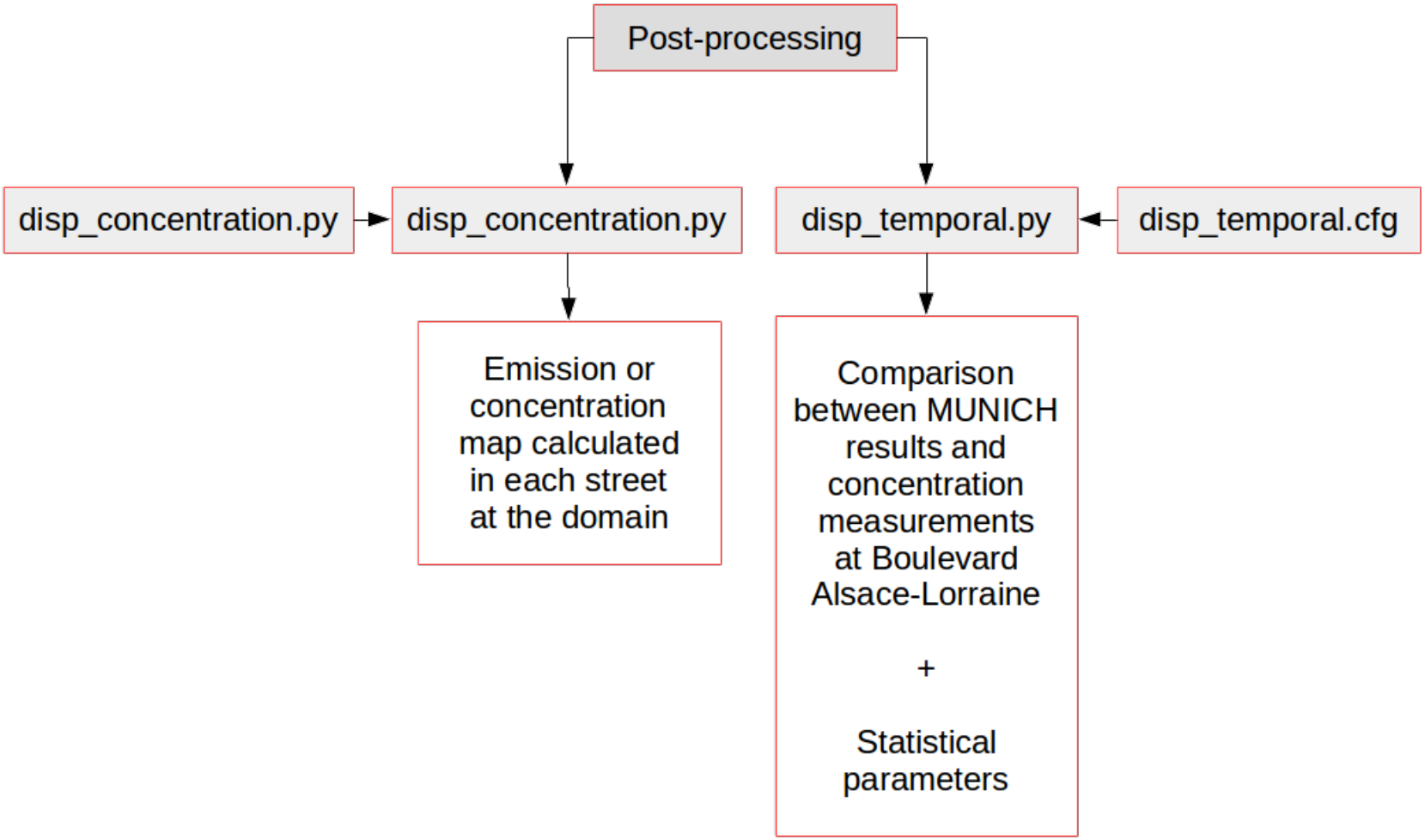
```
[photolysis_rates]

Date_min: 2014-01-01_12

# In days:
Delta_t = 1
Ndays = 365

# In hours:
Time_angle_min = 0.
# In hours:
Delta_time_angle: 1.
Ntime_angle = 9

# In degrees:
Latitude_min = 0.
# In degrees:
Delta_latitude = 10.
Nlatitude = 10

# In meters:

Altitudes: 0. 1000. 2000. 3000. 4000. 5000. 10000. 15000. 20000.

Fields: NO2 O3O3P O3O1D NO3NO2 NO3NO HONO H2O2 HNO4 HNO3 N2O5 ORGNIT HOP MHP HCHOrad HCHOmol ALD PAN C2CHO MGLY OPEN ISPD PANX PACD
Filename: /net/libre/yomi/kimy/StreetInGrid/Trafipollu/data_photolysis/&f.bin
```

Configuration files - munich-saver.cfg

```
[save]

# Put "all" to output all species.
Species: all

Date_beg: -1 # Put -1 to start from the simulation initial date.
Date_end: -1 # Put -1 to end at the simulation final date.
Interval_length: 1 # 1 for all steps.
Averaged: no
# Save initial concentrations in case concentrations are not averaged?
Initial_concentration: no

# Choices: streeet
Type: street

Levels: 0

Output_dir: /net/libre/halong/kimy/munich/test-case/results/

Output_file: <Output_dir>/&f.bin

Text_file: yes # yes
```

Processing...

- Compilation: compile
- munich munich.cfg


Post-processing
disp_concentration.py
disp_concentration.py
disp_temporal.py
disp_temporal.cfg
Emission or concentration map calculated in each street at the domain
Comparison between MUNICH results and concentration measurements at Boulevard Alsace-Lorraine
+
Statistical parameters

Post-processing: disp_concentration.py

This script calculates the hot emissions of gasoline passenger car for each arc during after-work rush hours.

1. Pre-setting figures for articles $\rightarrow$ size;
2. Display streets map $\rightarrow$ "node-trafipollu-eff.txt"
3. Input visualisation data $\rightarrow$ "emission-trafipollu-eff.txt"
4. If we analyze NO_x data:

$$emis_{NO_x} = emis_{NO_2} + \frac{46}{30} emis_{NO}$$

5. Plot data

Post-processing: disp_concentration.cfg

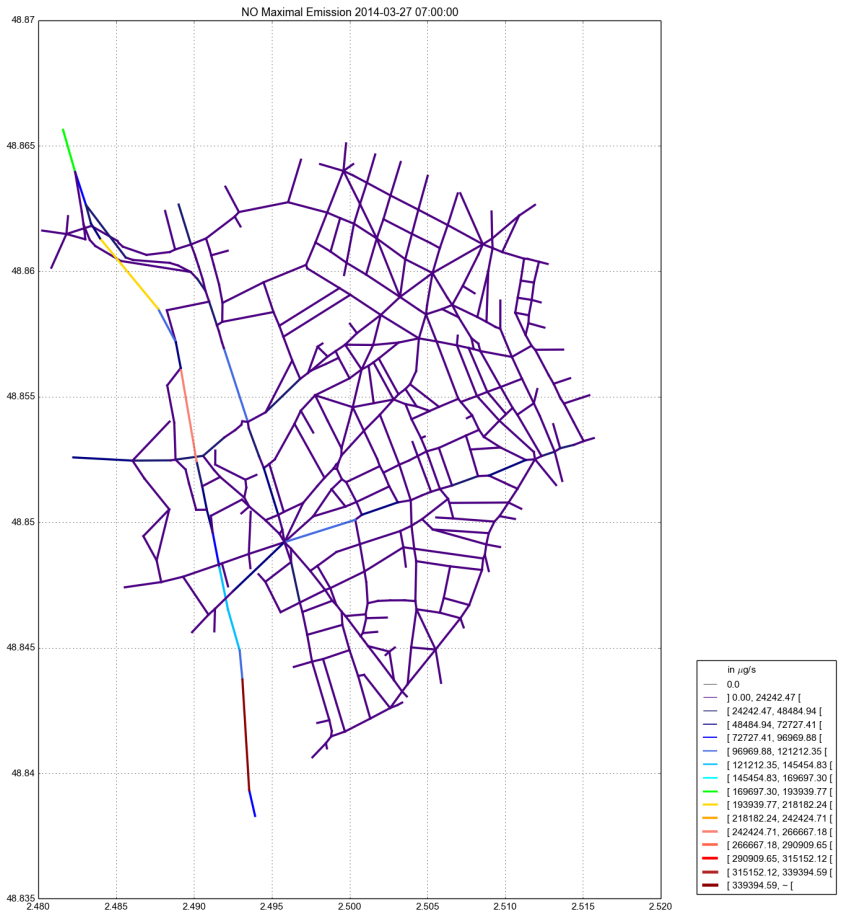
```
[input]

Species: NO2

Directory: /net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/munich/reference/results/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/munich/noxcorr/results/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/results_sing/street/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/sing/test/results/street/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/results_sing/street/

Nx = 1
Ny = 1

# Be careful with Nz and Nt, they can differ from the values
# given in general.cfg.


Nz = 577
Nt = 2016 # 336 # for all time step
```

Post-processing: disp_concentration.cfg

python disp_concentration.py disp_concentration.cfg

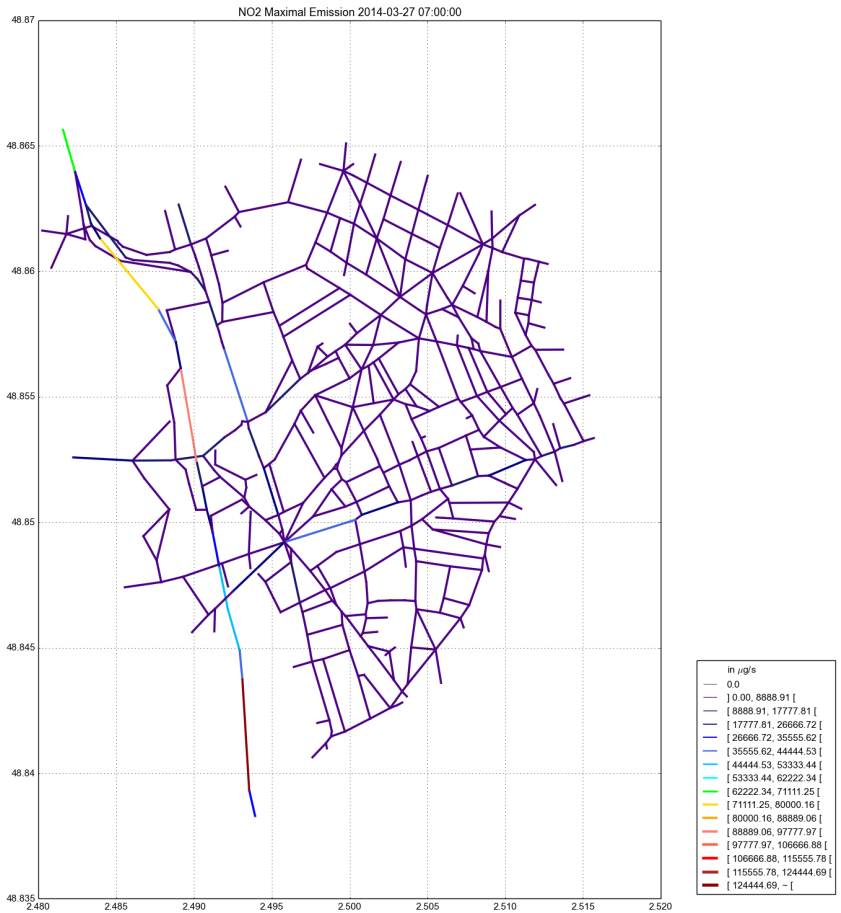
Post-processing: NO emissions

March 27^{th} - 7h00 am: Max emission = 363,637.06 $\mu g/s$



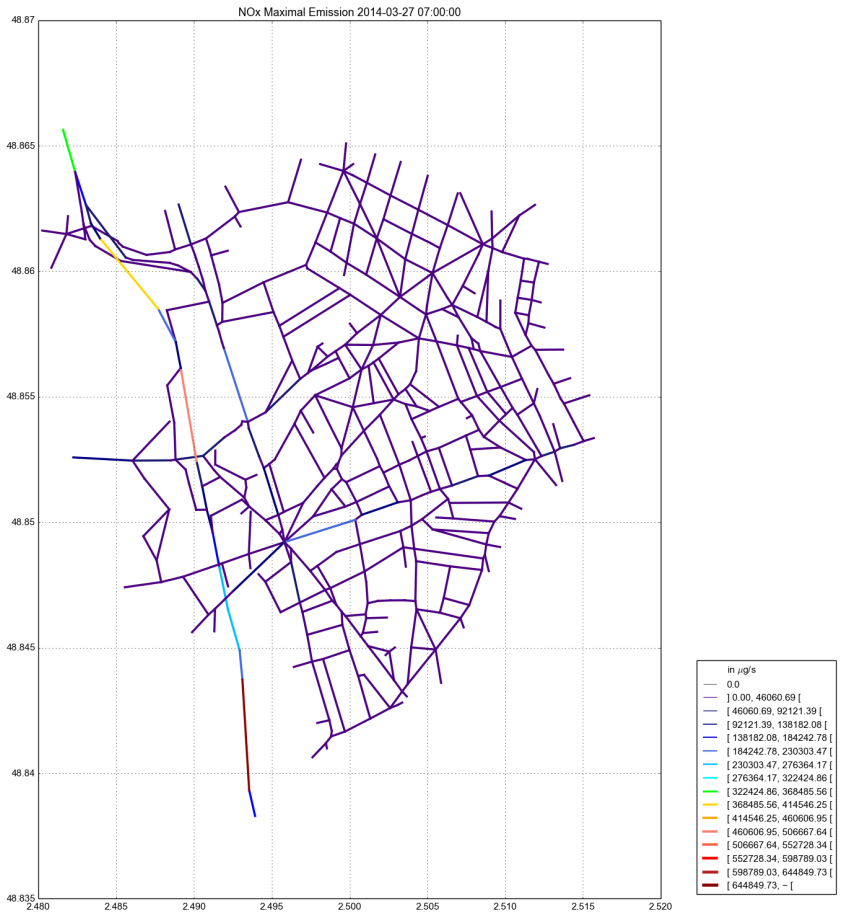
Post-processing: NO_2 emissions

March 27^{th} - 7h00 am: Max emission = 133,333.59 $\mu g/s$



Post-processing: NO_x emissions

March 27^{th} - 7h00 am: Max emission = 690,910.42 $\mu g/s$



Post-processing: disp_concentration.cfg

```
[input]

Species: NO2

Directory: /net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/munich/reference/results/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/munich/noxcorr/results/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/results_sing/street/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/sing/test/results/street/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/results_sing/street/

Nx = 1
Ny = 1

# Be careful with Nz and Nt, they can differ from the values
# given in general.cfg.


Nz = 577
Nt = 2016 # 336 # for all time step
```

Post-processing: disp_concentration.cfg

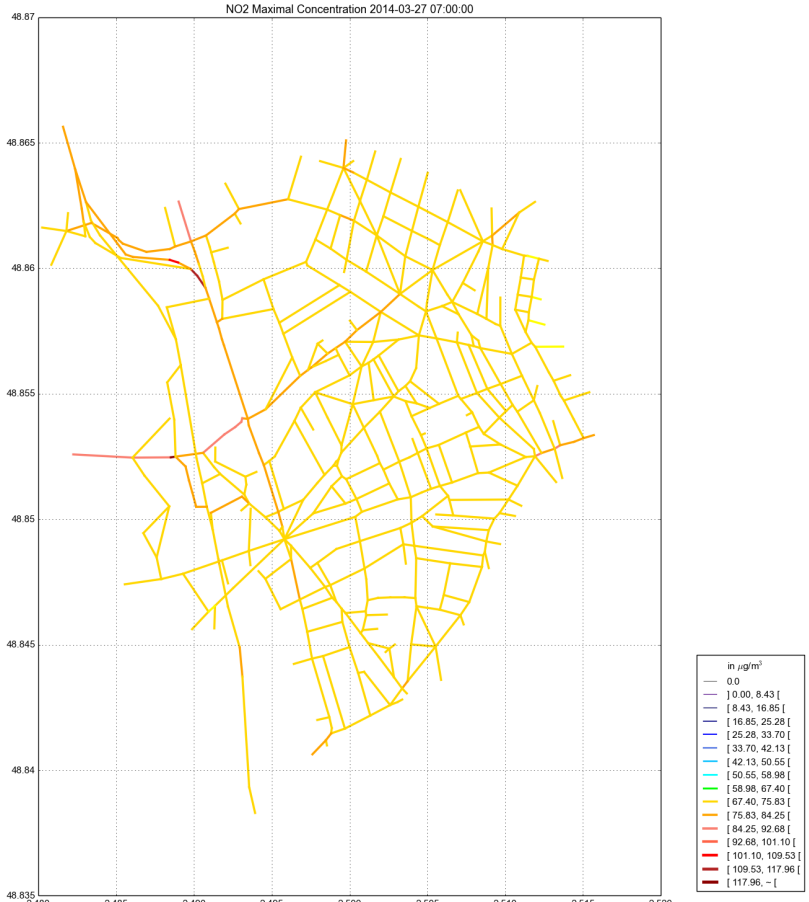
python disp_concentration.py disp_concentration.cfg

Post-processing: NO concentration

March 27^{th} - 7h00 am: Max concentration = 262.84 $\mu g/m^3$

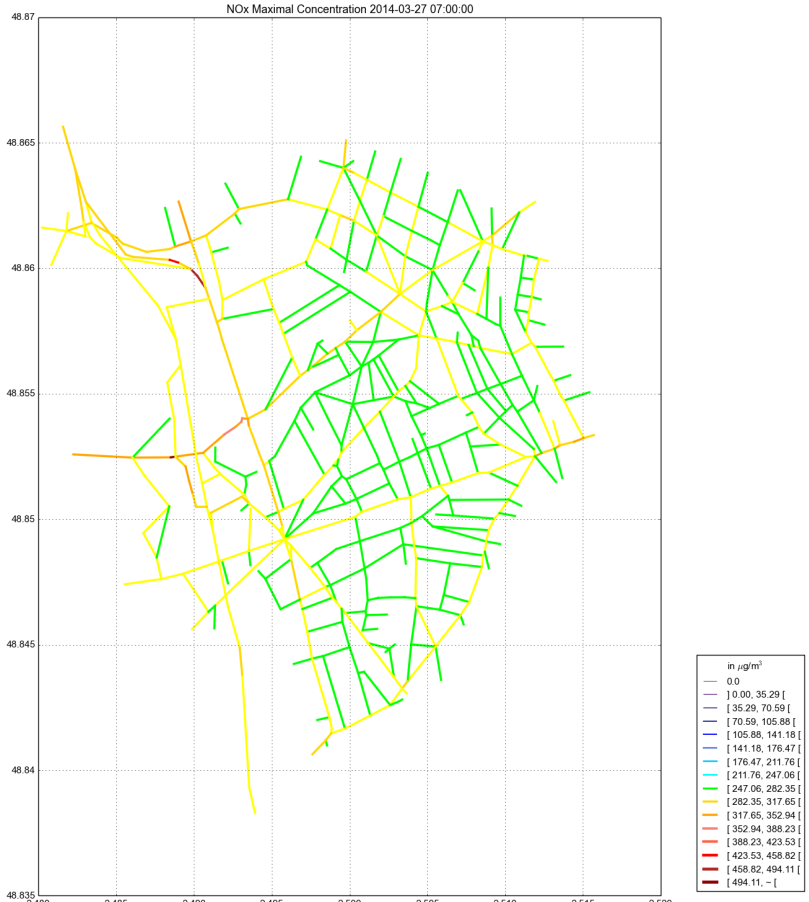
Post-processing: NO_2 concentration

March 27^{th} - 7h00 am: Max concentration = 126.38 $\mu g/m^3$



Post-processing: NO_x concentration

March 27^{th} - 7h00 am: Max concentration = 529.40 $\mu g/m^3$



Post-processing: disp_temporal.py

This script calculates the hot emissions of gasoline passenger car for each arc during after-work rush hours.

1. Reads pollutant concentration in each street in Boulevard Alsace Lorraine;
2. Calculates the average concentration;
3. Reads measurement data;
4. Plot simulated and measured concentrations
5. Calculates statistical parameters $\rightarrow$ statistics.py

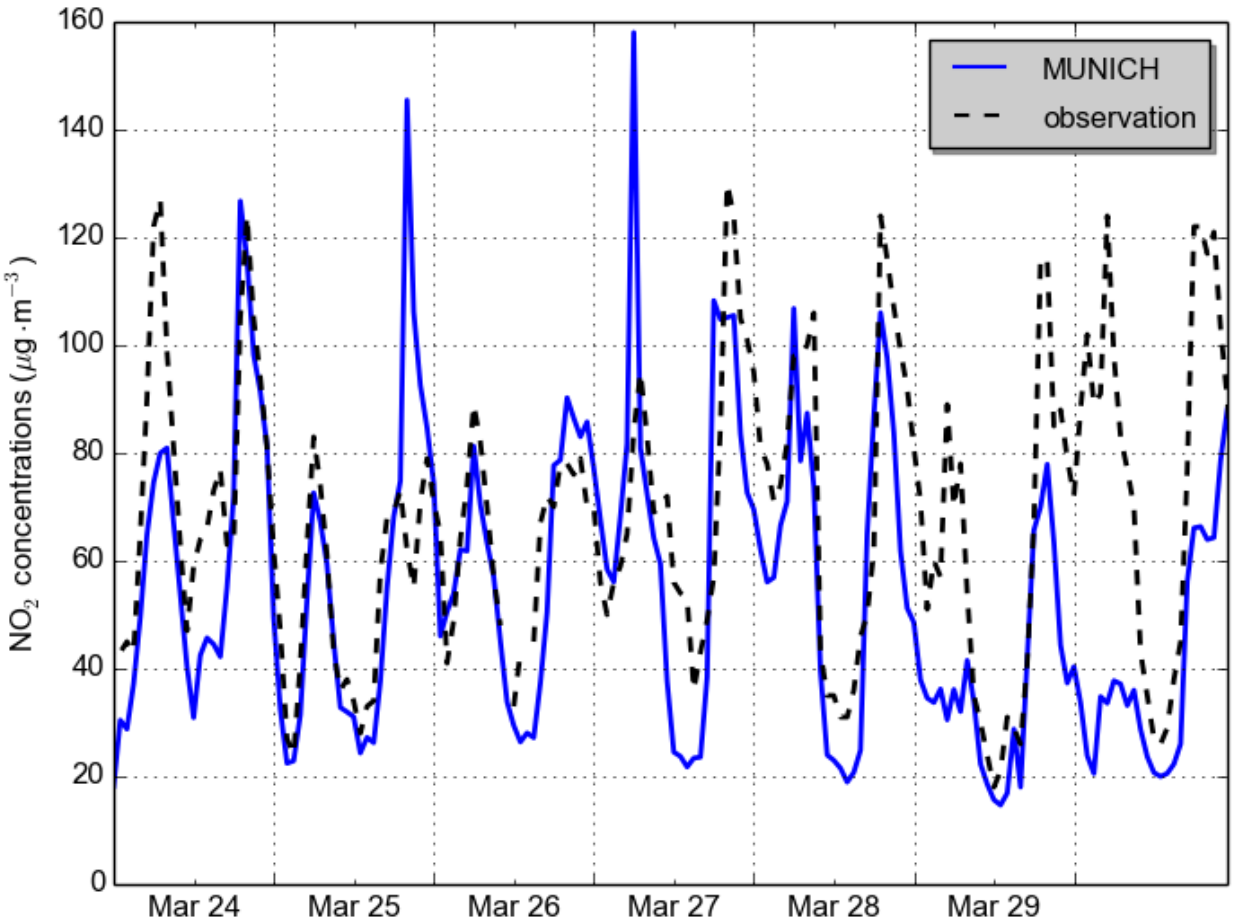
Post-processing: disp_temporal.cfg

```
[input]

Species: NO2

Directory: /net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/munich/reference/results/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing-voc/munich/noxcorr/results/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/results_sing/street/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/sing/test/results/street/
#/net/libre/yomi/kimy/StreetInGrid/Trafipollu/sing/leperreux/results_sing/street/

Nx = 1
Ny = 1

# Be careful with Nz and Nt, they can differ from the values
# given in general.cfg.


Nz = 577
Nt = 2016 # 336 # for all time step
```

Post-processing: disp_temporal.cfg

python disp_temporal.py disp_temporal.cfg

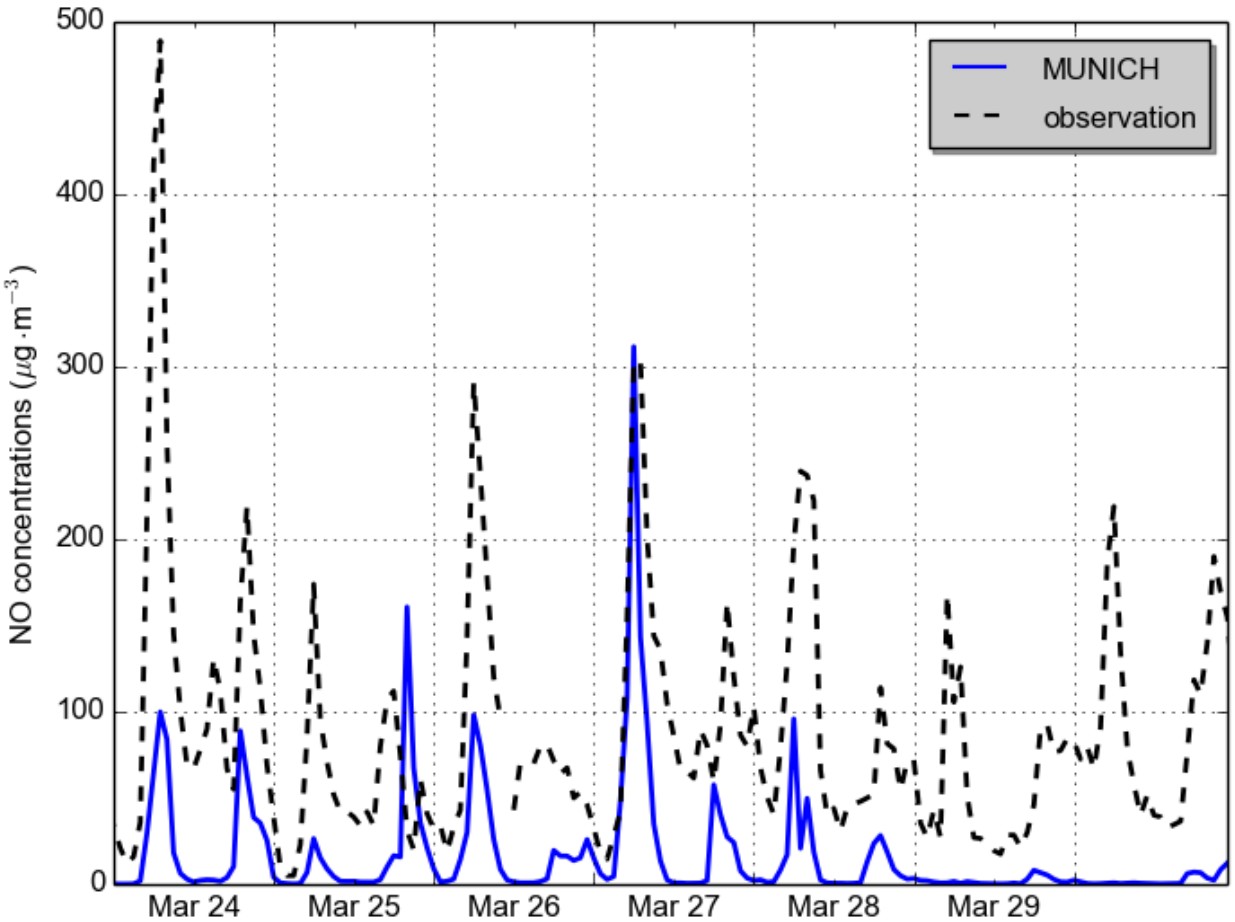
NO_2 concentrations



NO_2 concentrations - Statistical indicators

- **sim mean: 54.53**
- **obs mean: 68.33**
- RMSE: 26.93
- MFB: -0.26
- MFE: 0.33
- NMB: -0.20
- NME: 0.29
- MNGE: 0.28
- MNB: -0.18
- FB: -0.22
- VG: 1.22
- MG: 0.76
- FAC2: 0.90
- **correlation: 0.64**

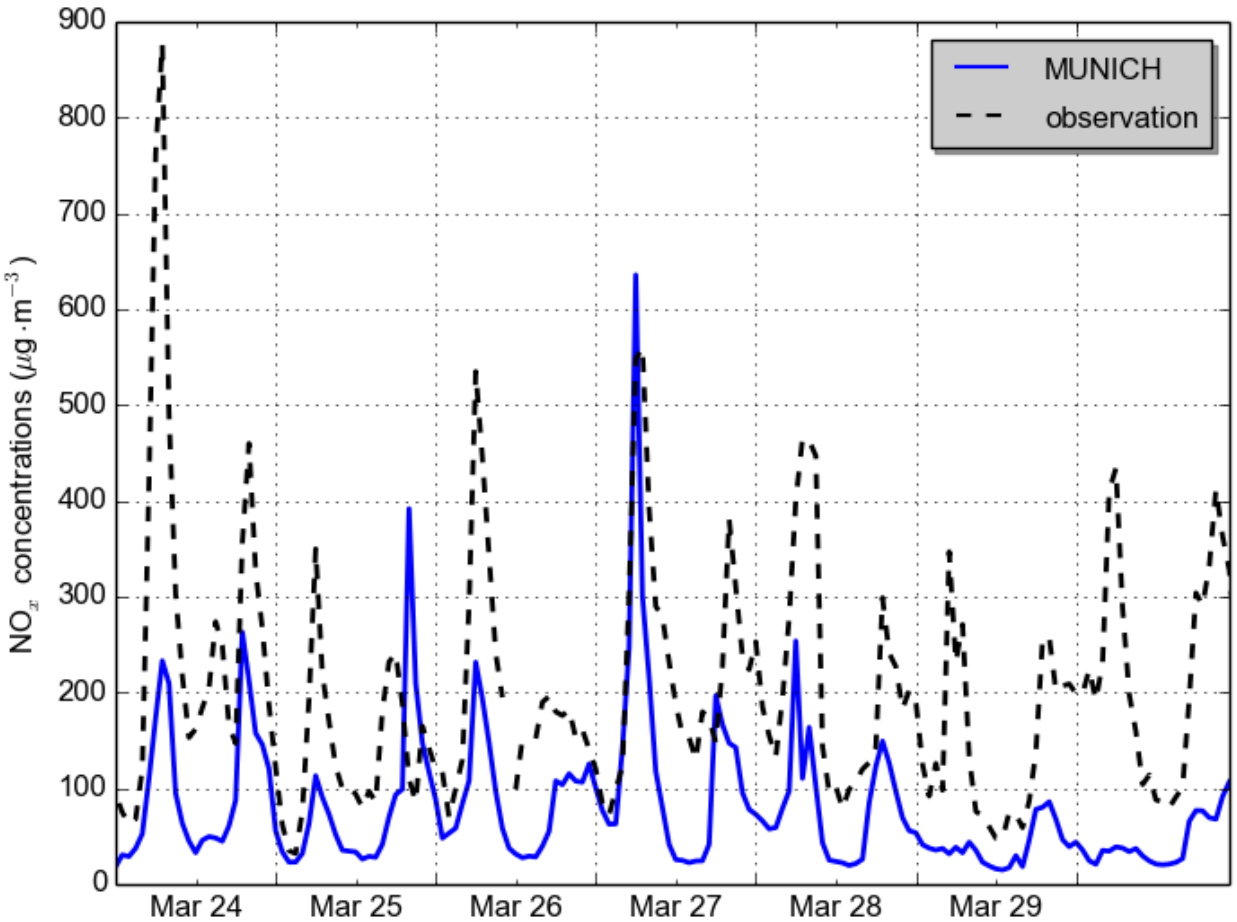
NO concentrations



NO concentrations - Statistical indicators

- **sim mean: 16.91**
- **obs mean: 88.75**
- RMSE: 93.98
- MFB: -1.57
- MFE: 1.60
- NMB: -0.81
- NME: 0.83
- MNGE: 0.89
- MNB: -0.81
- FB: -1.35
- VG: 46907.78
- MG: 0.05
- FAC2: 0.04
- **correlation: 0.58**

NO_x concentrations



NO_x concentrations - Statistical indicators

- **sim mean: 80.47**
- **obs mean: 204.44**
- RMSE: 164.06
- MFB: -0.91
- MFE: 0.94
- NMB: -0.60
- NME: 0.64
- MNGE: 0.63
- MNB: -0.57
- FB: -0.87
- VG: 4.23
- MG: 0.35
- FAC2: 0.22
- **correlation: 0.58**

Conclusions

- A street-network model MUNICH was applied to simulate NO_x concentrations in a suburb Paris area;
- The simulated period was 24/03/2014 to 30/03/2014;
- All steps of preprocessing, processing and post-processing were presented and applied;
- We observed a reasonable NO_2 estimation (mean negative biais of 20.2%);
- We have a considerable understimation of NO and consequentily NO_3 prediction;
- Great importance of background data;

Thank you for your attention !!