Modularizing TM5 4DVAR

A pythonic approach

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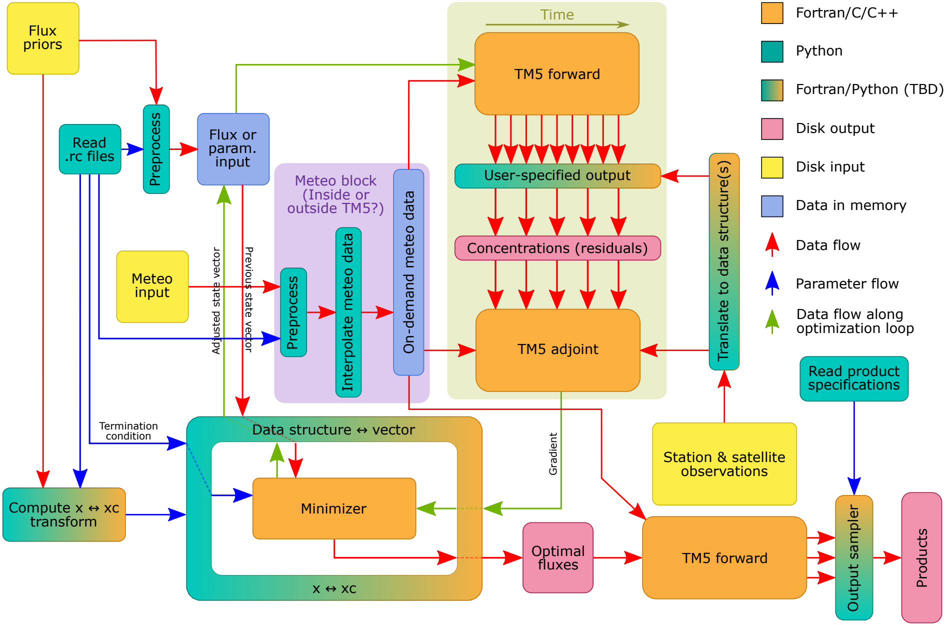
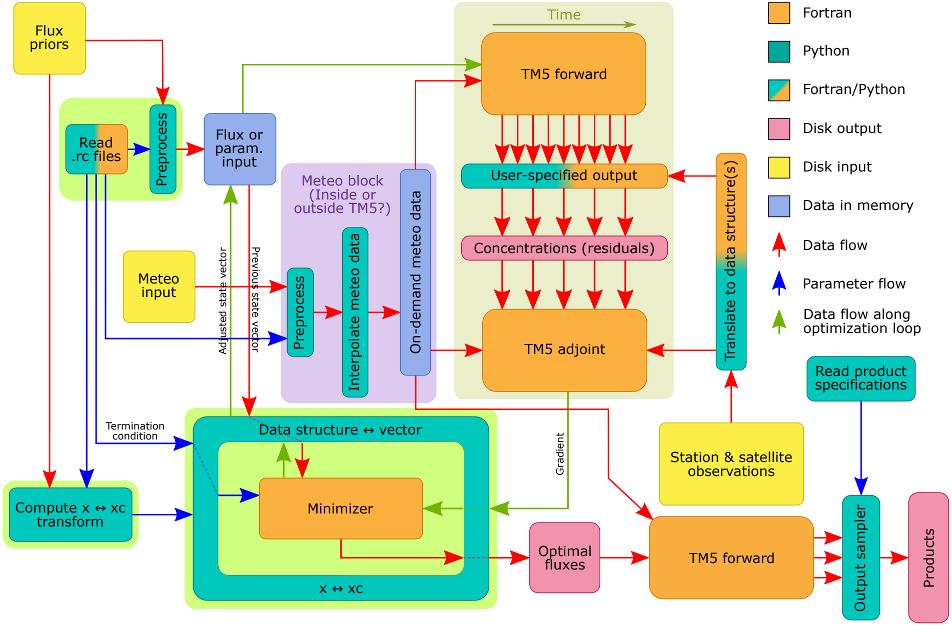
- Parts of 4D-VAR were hard-coded for specific purposes
- Structure is complicated to read for a new user
- Cumbersome to change something (optimization algorithm, meteo format, etc.)
- Difficult to develop code together by working on different parts separately

- More modular structure:
  - Forward model, adjoint model *specific to atmospheric dynamics*
  - Process observations, sample output *specific to instrument*
  - Process meteo *specific to meteo source*
  - Optimization algorithm *specific to application (4DVAR)*

- Computationally intensive parts : Fortran

- Organizational parts (the glue) : Python


Flux priors
Read .rc files
Preprocess
Flux or param. input
Meteo input
Adjusted state vector
Previous state vector
Meteo block (Inside or outside TM5?)
Preprocess
Interpolate meteo data
On-demand meteo data
Time
TM5 forward
User-specified output
Concentrations (residuals)
TM5 adjoint
Translate to data structure(s)
Termination condition
Data structure ↔ vector
Minimizer
x ↔ xc
Compute x ↔ xc transform
Gradient
Optimal fluxes
TM5 forward
Station & satellite observations
Read product specifications
Output sampler
Products
Fortran/C/C++
Python
Fortran/Python (TBD)
Disk output
Disk input
Data in memory
Data flow
Parameter flow
Data flow along optimization loop



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Compute x ↔ xc transform

Data structure ↔ vector

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x ↔ xc

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TM5 forward

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Products

- 🟧 Fortran
- 🟩 Python
- ◩ Fortran/Python
- 🟥 Disk output
- 🟨 Disk input
- 🟦 Data in memory
- ↑ Data flow
- ↑ Parameter flow
- ↑ Data flow along optimization loop

The class hierarchy

```
class ParseConfig                                          # to parse and modify config files
    def SetStartTime()
⋮
class Emissions                                 # general routines for writing emission files
    def WriteEmissions()
    class CO_Emissions                                             # tracer-specific routines
        def Anthropogenic()
    class CH4_Emissions
⋮
class Observations                                       # create OBS files from observations
    def WriteOBSFiles()
    class Aircraft
    class Satellite                                            # instrument-specific routines
        def ParseGOSAT()
⋮
class Precon                                               # pre-conditioner for optimization
    def ReadHorizontalCorrelation()
⋮
class RunTM5                                   # routines for running forward, backward, etc.
    def GradientTest()
```

CO emissions: Fortran

```
select case (emission_dims)
    case (SURFACE)
        call readhdf(‘emissions.hdf’, emis(region)%surf, region)
! not exact F90 code, just an example
! ‘emissions.hdf’ contains monthly emissions in ‘n_region’ arrays:
!     categories × months × latitude divisions × longitude divisions
! kg/sec/gridbox at model resolution
```

CO emissions: Python

```
class Emissions                                   # general routines for processing emissions
    def LoopThroughMonths()
    def AssembleEmissions()
    def WriteEmissions()                                             # writes ‘emissions.hdf’
    class CO_Emissions                                                 # CO-specific routines
        def AssembleEmissions()                # replaces AssembleEmissions() of parent class
        def Anthropogenic()
        def Natural()
        def BiomassBurning()
```

A forward run

```
[1]: %run ParseInit.py
[2]: r = RunTM5((2004,2,27,0),(2004,3,3,0))
[3]: r.SetupEmissions(‘CO’, emisFile=‘input/emissions_CO.hdf’)
[4]: r.RunForward(‘tm5.rc’)
```

A forward run

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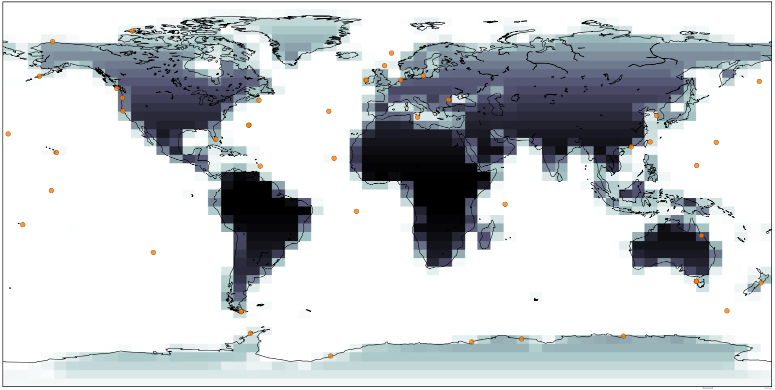
A 4D-VAR run

```
r = RunTM5((2004,2,27,0),(2004,3,3,0))
r.CleanUp()
r.SetupEmissions(‘CO’, emisFile=‘input/emissions_CO.hdf’)
r.RunForward(‘tm5.rc’)
r.StoreModelReprErrors()
r.preco = Precon(r.StartTime, r.EndTime)
for i in range(r.max_iter):
    r.RunForward(‘tm5.rc’)
    r.RestoreModelReprErrors()
    r.RunBackward(‘tm5.rc’)
    r.OptimizerLoop()
```

- Emission in a grid-box $\propto$ land area
- "Measure" at 47 NOAA stations
- 27-2-2004 to 3-3-2004 (5 days)
- Prior emission in a grid-box $\propto$ surface area
- Prior total = "True" total
- Emissions close to stations constrained



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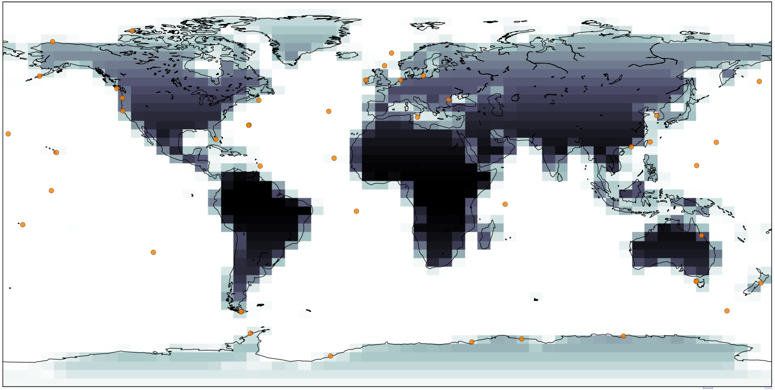

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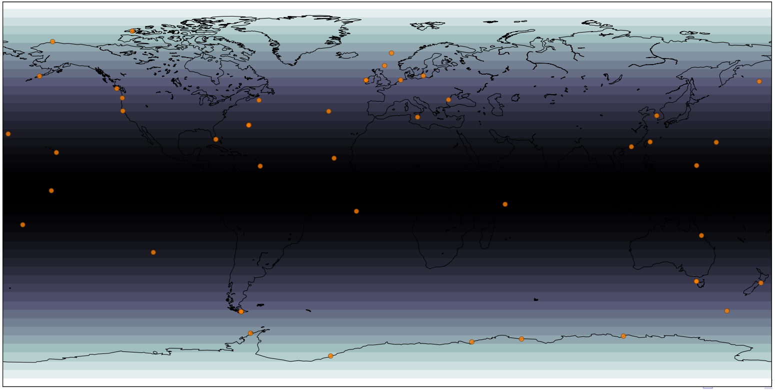

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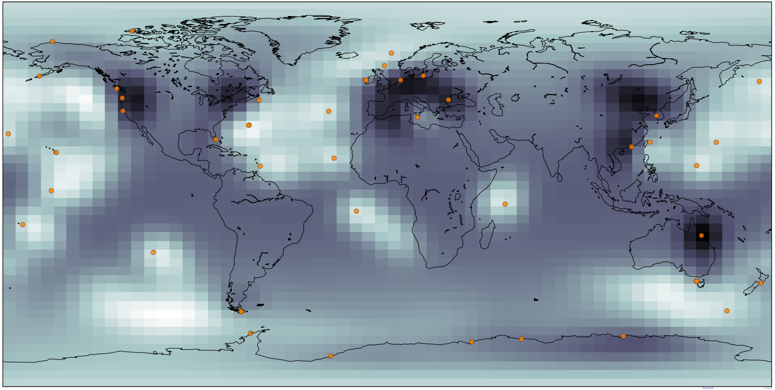
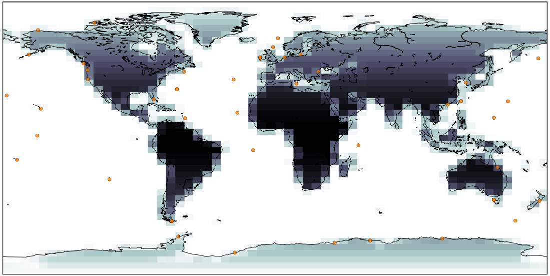
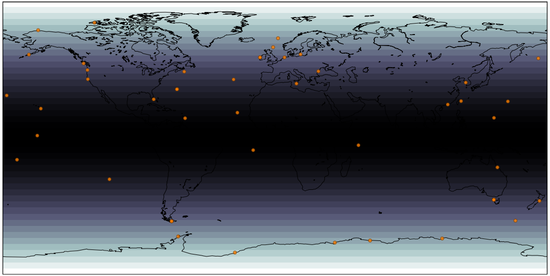
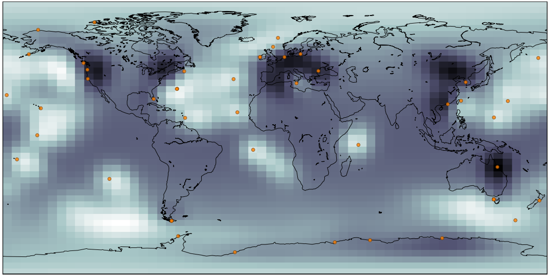
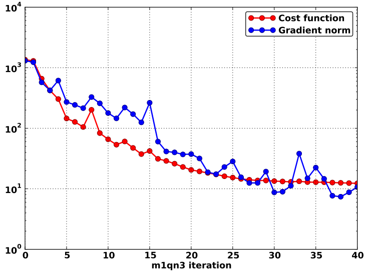




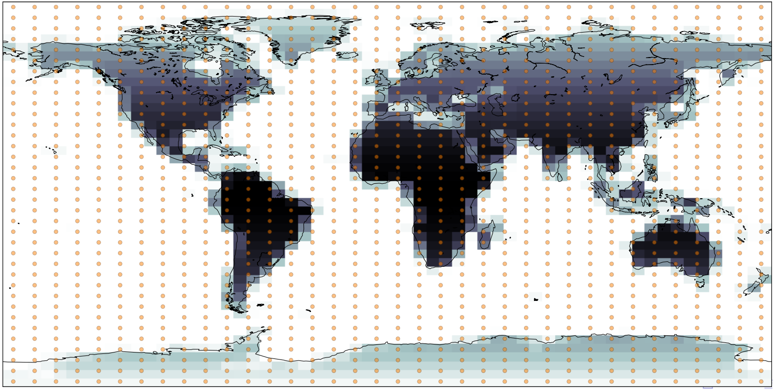






Let’s put stations everywhere!

- Emission in a grid-box ∝ land area
- “Measure” at 1296 stations
- 27-2-2004 to 3-3-2004 (5 days)
- Prior emission in a grid-box ∝ surface area
- Prior total = “True” total
- Enough observations to constrain emissions



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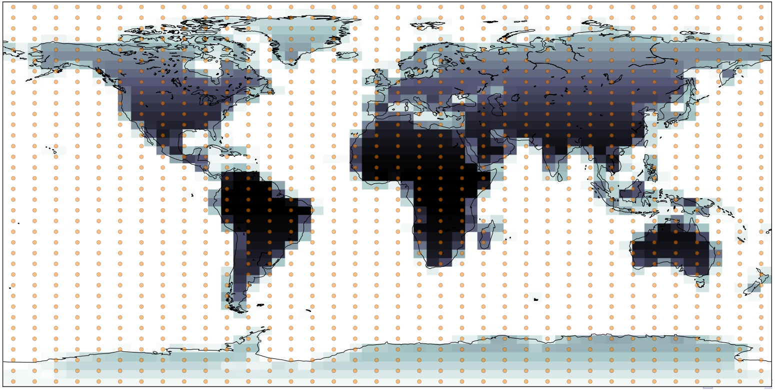

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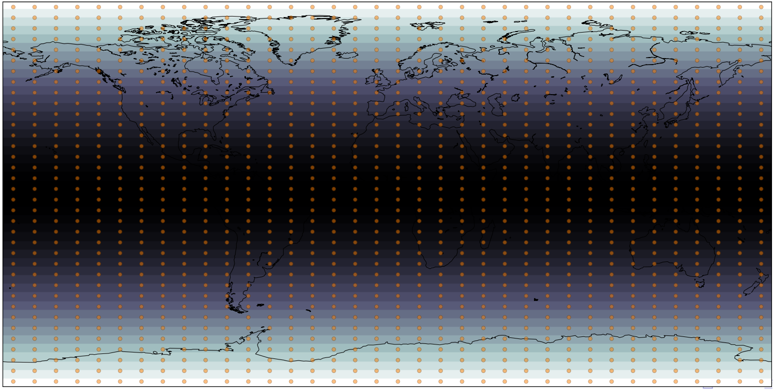

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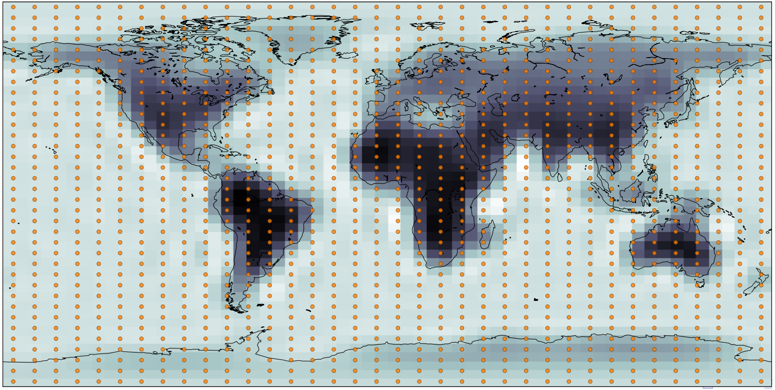
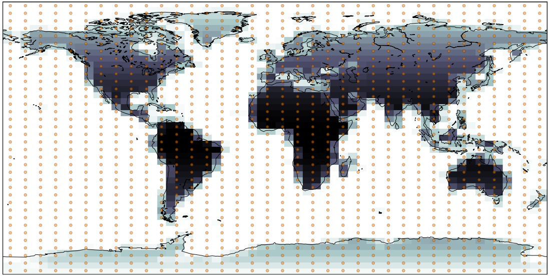
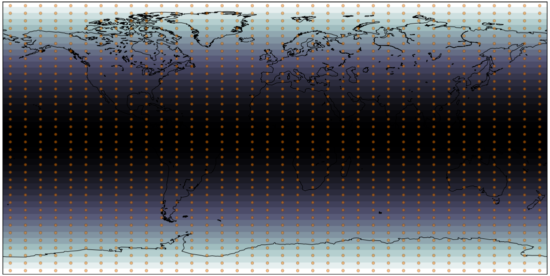
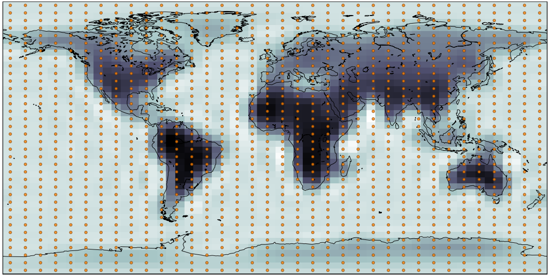
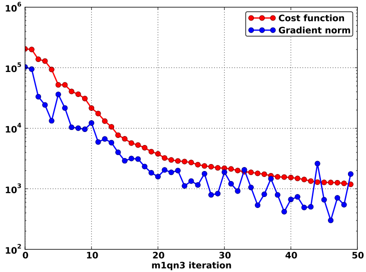




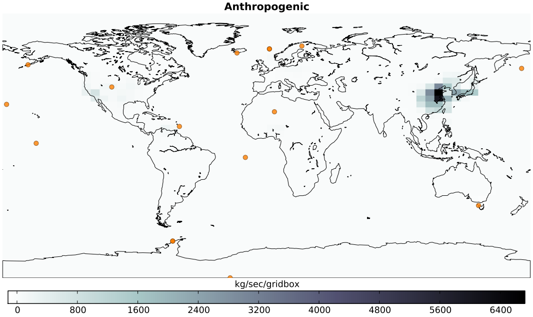


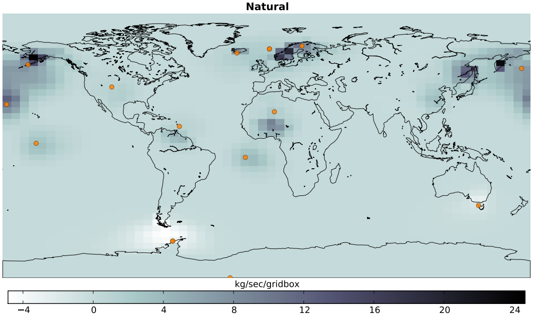


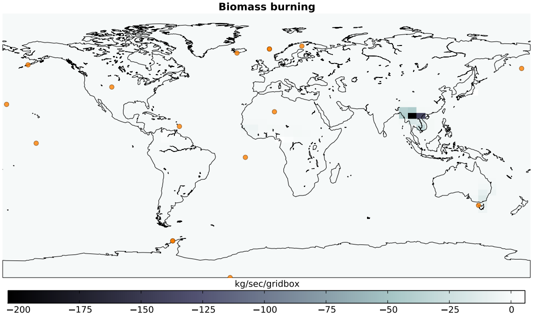


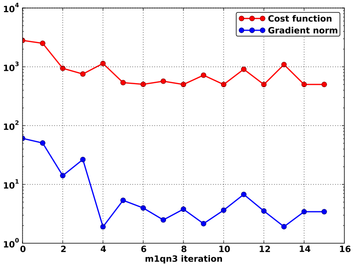
Proof of concept, not a realistic inversion

- Pim Hooghiemstra's inversion using NOAA station data
- 27-2-2004 to 3-3-2004 (5 days)
- Prior emissions from GFED, EDGAR
- Total of 16 observations









Optimized emission – prior

- Add vertical distribution of emissions (e.g., CO)
- Separate the meteo processing, settle on input meteo format for TM5
- Complete parser for config files
- Move observations outside TM5
  - Add satellite module (GOSAT)
  - Interpolation scheme for stations
- Add initial field and arbitrary parameters to preconditioner
- Settle on I/O format for optimizer
- Implement zoom regions