

I. Update on CH₄ Inverse Modeling at JRC

Arjo Segers
Peter Bergamaschi

European Commission Joint Research Centre, Institute for Environment and Sustainability, Climate Change Unit, I-21027 Ispra (VA), Italy

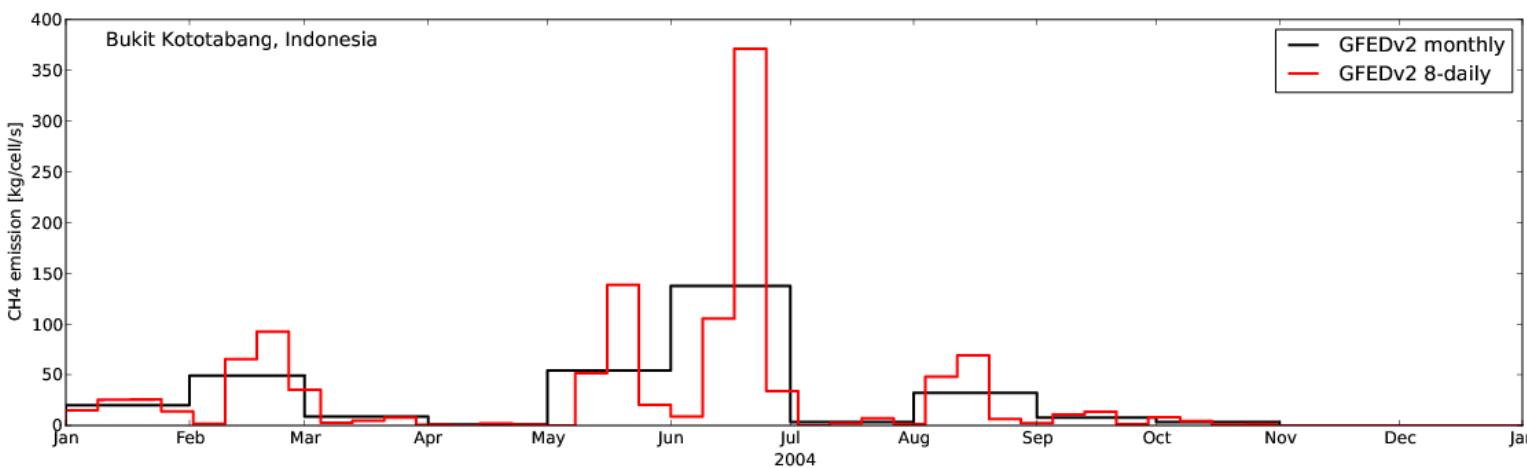
upgrade of the 4D-var CH4 system

- new scripting ('pycasso')
 - easier running same code on different platforms
 - decreases number of scripts (input.sc, output.sc)
 - less (!) settings visible for users
- brought back to live : TIPP
 - TM Input Pre-Processor (Jan Fokke Meirink)
 - converts raw emissions into single format
 - extended with various Edgar 4.0 formats
 - support GFED 8-daily biomass burning emissions

CH4 inversions - 8-daily fire emissions

extended 4D-var system

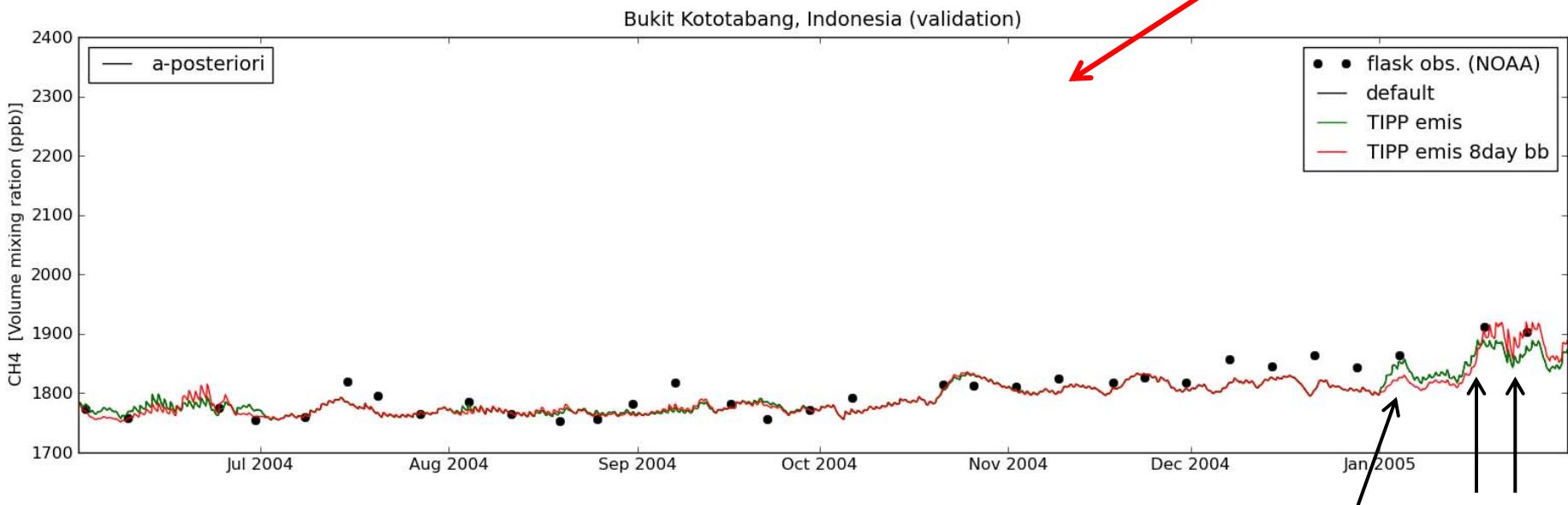
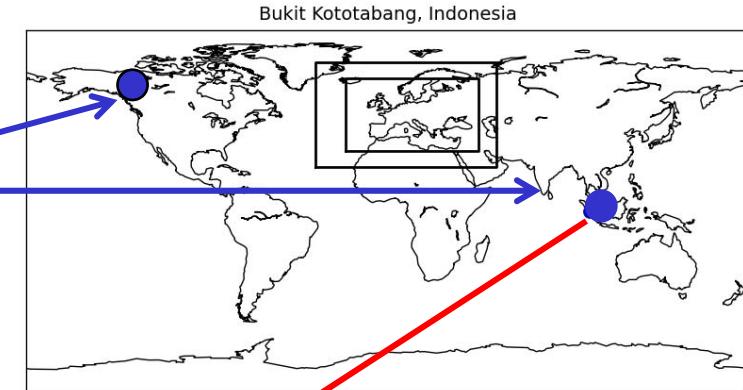
- Default optimization on monthly averages
- Added 8-daily profile on top of monthly average



- results after inversion should be not too different!

CH4 inversions - 8-daily fire emissions

- Tested for year 2004
- Difference 'monthly' vs 'monthly+8daily' visible at 2 NOAA stations only



- optimization of monthly averages only !
- ** coming soon ** 4D-var with time scales other than monthly

worse better

II. Update on meteo format

Arjo Segers

European Commission Joint Research Centre, Institute for Environment and Sustainability, Climate Change Unit, I-21027 Ispra (VA), Italy

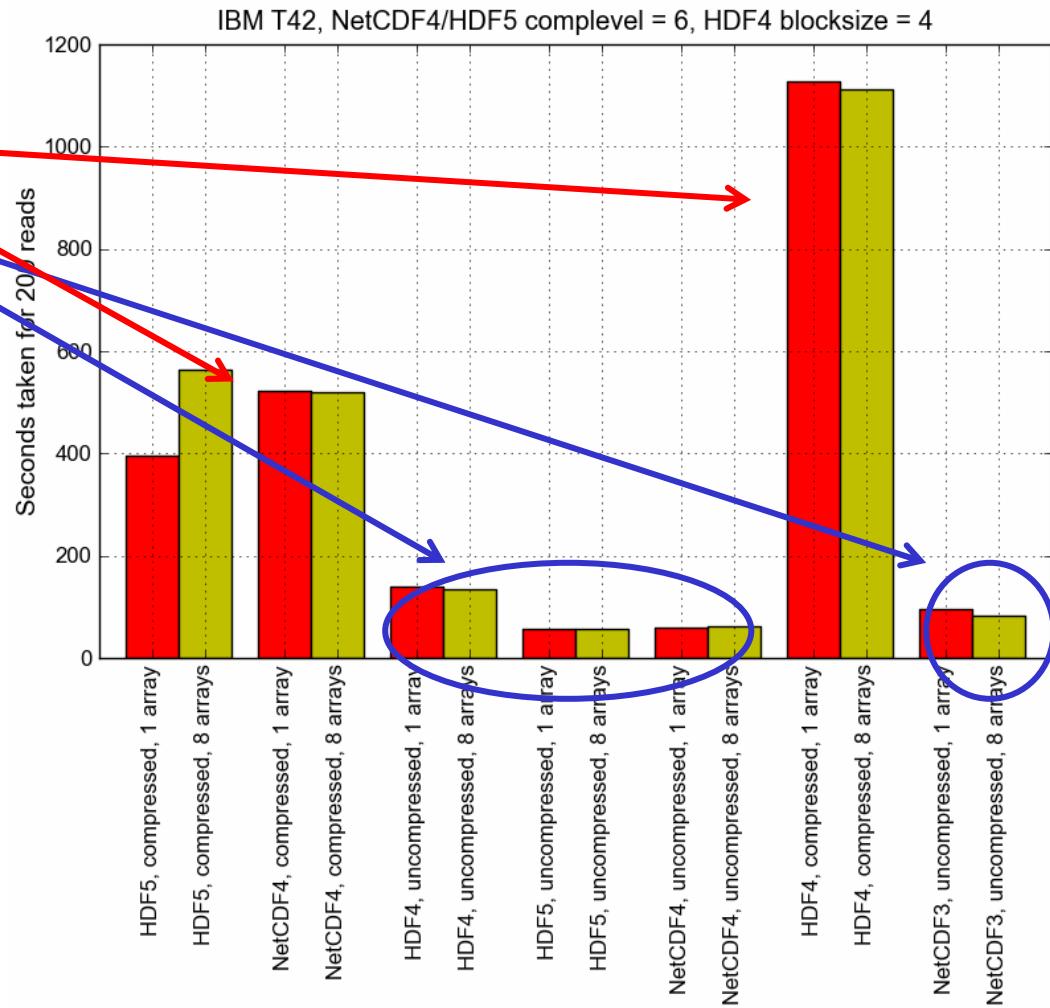
- from previous TM meeting:

timer	system_clock	(%)
root	2566.69	
field2d	37.36	(1.5 %)
field3d	1392.87	(54.3 %)
other	1136.46	(44.3 %)
field3d	1392.87	
field3d read	1322.58	(95.0 %)
field3d transform hori	66.50	(4.8 %)
field3d transform vert	3.57	(0.3 %)
other	0.22	(0.0 %)

- In some applications, reading meteo files took about 50% of total time!

- Experiments by Sourish:
 - compressed
 - uncompressed

- reading files is slow due to:
 - hdf
 - compression
- is this a problem ?
depends on:
 - application
 - 1 tracer 4D-var
 - full chemistry
 - file system (access time)
 - installed hdf libraries ?



- **current format:**
 - hdf
 - internal compression
 - saves 25% of disk space
 - useful when we only used workstations with small disks
 - multiple 3D records in a file
 - 8-10 years old ?
- **testing a new format:**
 - NetCDF4
 - = based on HDF5
 - ! bug in HDF5 for IBM AIX machines (ecmwf ...);
therefore tests with 'classic' NetCDF
 - 4D records
 - uncompressed

- test:

- TM5 from trunk (version `last week`)
- L60, glb6x4 / eur3x2 / eur1x1
- test ‘chemistry’ (5 transported tracers)
- 12 hour simulation
- ecmwf/c1a, single cpu

timer	HDF		NC	
	system_clock	(%)	system_clock	(%)
root	102.42		87.46	
init	2.18 (2.1 %)		2.21 (2.5 %)	
step start	13.32 (13.0 %)		9.44 (10.8 %)	
step init	41.27 (40.3 %)		30.20 (34.5 %)	
step run	45.12 (44.1 %)		45.12 (51.6 %)	
other	0.53 (0.5 %)		0.49 (0.6 %)	

→ about 12% reduction of time

- test:
 - v3.0 chemistry benchmark
 - ecmwf/c1a, 4 mpi tasks, 2 openmp threads

	HDF		NC	
timer	system_clock	(%)	system_clock	(%)
root	2276.34		2018.85	
init	2.86 (0.1 %)		2.76 (0.1 %)	
done	1.30 (0.1 %)		1.23 (0.1 %)	
step start	25.19 (1.1 %)		18.98 (0.9 %)	
step init	918.70 (40.4 %)		682.77 (33.8 %)	
step run	1325.78 (58.2 %)		1310.80 (64.9 %)	
step done	0.02 (0.0 %)			
other	2.49 (0.1 %)		2.31 (0.1 %)	

→ about 12% reduction of time

- test:
 - 4D-var CH4
 - JRC cluster (**fast local disk, one user**)
 - not tested with NC files yet

	HDF		NC	
	system_clock	(%)	system_clock	(%)
timer				
tracer model	208.87			
model init	5.00	(2.4 %)		
timestep init	32.17	(15.4 %)		
timestep run	169.96	(81.4 %)		
timestep done	1.70	(0.8 %)		
other	0.05	(0.0 %)		

→ reduction of time max. 15%

Proposal for coming months:

- wait for upgrade of HDF5/NetCDF4 libs at ECMWF
 - large scale test of run times:
 - different applications
 - different machines
- could volunteers be identified by meeting ?**
(support for coding and configuration is available...)
- next meeting:
 - decide if improvement is worthwhile the investment
 - if so, decide on switch/conversion to new format

III. Scripting

Arjo Segers

European Commission Joint Research Centre, Institute for Environment and Sustainability, Climate Change Unit, I-21027 Ispra (VA), Italy



Evolution of the TM5 scripting ...

- 'run-tm5'
 - 2002-2010
 - bourne shell (/bin/sh)
 - to build source code from base/proj directories
 - many settings hard coded in many files:
 - run-tm5, run-tm5.jb, config.compiler, configure, ...
- 'runtm5.py'
 - 2009-...
 - python
 - translation of 'run-tm5'
 - many configurations now controlled by rcfie settings
- 'pycasso' branch
 - based on 'runtm5.py'
 - *all* settings now controlled by rcfie settings
 - get rid of runtime files 'times.in', 'runtime.rc', etc



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pycasso - setup/submit scripts

Split between 'building' and 'running' an executable

- Before: one script to do all:
`./runtm5.py tm5.rc`
- Now first build:
`./setup_tm5 tm5.rc`
- and then from run directory:
`/scratch/run> ./submit_tm5 tm5.rc`
- ... but for the impatient those could be combined again:
`./setup_tm5 tm5.rc --submit --queue`
- Advantage: to reproduce a run it is sufficient to store:
 - executable
 - rcf file
 - submit script

without the need to re-build the executable again

- building a code : pycasso scripts
 - 'python compile and setup script organizer'
 - set of scripts to compile a code and setup a run directory without any reference to TM5
 - ... but with all tasks necessary for TM5 included
- All configuration done through rcfile settings:
 - code directories (base,proj,...)
 - which files to copy and which not (source.rc)
 - compiler flags
 - libraries
- special TM5 configurations in module 'user_scripts_tm5'
(dims_grid.h, TracerOrder, ...)



Revised job chain

- job scripts are written by submit script
 - as small as possible!
 - queue options
 - specified in rcf file! facilitates many platforms
 - run a single script or executable
 - submit a new job if necessary
 - ... thus no long 'run-tm5.jb' template script anymore ...
 - each job in the chain has its own rcf file:
 - tm5_001.jb tm5_001.rc
 - tm5_002.jb tm5_002.rc
 - ...
- with different values inserted for time range, istart, ...
→ easier to re-run a job

- **(extra) MDF module**

- "multiple data formats"
- single interface to both HDF and NetCDF(4)
- interface similar to NetCDF F90 interface:

```
call MDF_Create( 'test.hdf', MDF_HDF      , MDF_NEW, hid, status )
call MDF_Create( 'test.nc' , MDF_NETCDF4, MDF_NEW, ncid, status )
```

- could replace 'file_hdf'
- single (large) source file
- created using python scripts
- available from 'tools' directory



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pycasso - macros



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- **(extra) Macro definitions not via compiler flags:**
`f90 -c tm5.F90 -DMPI -Dwith_zoom -Dwithout_anything ...`
- **... but defined in include file "tm5.h", written by setup script:**
`! this is tm5.h
#define MPI
#define with_zoom
#define withoutAnything`
- **Include this file in the top of every TM5 source file:**
`#include "tm5.h"`
- **Advantage:**
 - macro definitions now part of source, thus shipped together: always clear which macros where defined to compile a code
 - if macro definitions change, code is re-compiled automatically thanks to makedep.f90

- **(extra) grid definition in rcf file, including reduced grid:**

- ```
! global 6x4
region.glb600x400.xcyc : 1
region.glb600x400.touch_np : 1
region.glb600x400.touch_sp : 1
region.glb600x400.xbeg : -180
region.glb600x400.xend : 180
region.glb600x400.ybeg : -90
region.glb600x400.yend : 90
region.glb600x400.im : 60
region.glb600x400.jm : 45
region.glb600x400.redgrid.nh.n : 4
region.glb600x400.redgrid.nh.comb: 60 20 10 5
region.glb600x400.redgrid.sh.n : 4
region.glb600x400.redgrid.sh.comb: 60 20 10 5
```

- **specify a list of regions to be used:**

```
regions : glb600x400 eur300x200 eur100x100
```

- **no need for ‘proj/grid’ and ‘RedGrid’ files anymore**

- **(extra) timing routines**
  - added lines to the code:

```
integer :: itim
call GO_Timer_Def(itim, 'main')
...
call GO_Timer_Start(itim)
... ! this is the main task
call GO_Timer_Done(itim)
```

- at end of the run a profile is written:

| timer         | system_clock     | (%) |
|---------------|------------------|-----|
| tracer model  | 208.87           |     |
| model init    | 5.00 ( 2.4 %)    |     |
| timestep init | 32.17 ( 15.4 %)  |     |
| timestep run  | 169.96 ( 81.4 %) |     |
| timestep done | 1.70 ( 0.8 %)    |     |
| other         | 0.05 ( 0.0 %)    |     |
| .....         |                  |     |



- Where used ?
  - JRC 4D-var CH4 code
  - TM5/base/branches/pycasso
- Recently tested:
  - trunk source with pycasso scripts : ok
  - pycasso source with trunk scripts : ok
  - pycasso source with pycasso scripts : ok
- If no objections: merged into the trunk soon ...