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TM5-MP: repository, base code and chemistry updates

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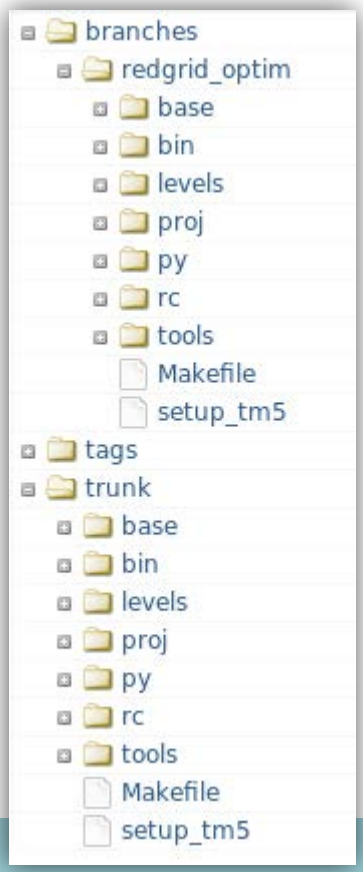
New Repository

New Repository Overview

- same server as TM5 repo ➔ same credentials
- **one** repository for all projects ➔ no unexpected conflicts
- **standard** branches/trunk/tags structure ➔ ease Hg migration
- **familiar** tree



Used since September 2014

- EC-Earth v3.2
- full chemistry
- meteo 1x1 preprocessing

Refactoring (1) User Interface (main rc file)

- **new keys**
  - convective.fluxes.tiedtke : F
  - region.rc : <filename> (from expert.rc)
  - my.meteo.dir : <directory> (from the machine.rc)
  - my.source.proj (subset of my.source.dirs)

- **keys removed** (all moved to expert.rc)
  - my.source.dirs
  - jobstep
  - jobstep.timerange.start
  - jobstep.timerange.end
  - prev.output.dir

- **obsolete macros**: with_pycasso, with_zoom, …

Refactoring (2) Source Code

code has been *displaced, renamed* or *deleted*:

trace1, trace_end, trace_after_read, start_co2, free_emissions, ...

Nothing to worry about...

...nothing drastic, just cleanup!

Refactoring (3)

UI - pycasso

```
[1999] bhw407 ~/TM5/TM5MP $ ./setup_tm5 -h
Usage:
    setup_tm5 [options] rcfile
    setup_tm5 -h|--help

Driver script to com
textfile with sett
should be availabl

Options:
  -h, --help            show
  -v, --verbose         Print extra logging messages to standard output. This
                        option will set rcfile key 'verbose' to 'True'
  -m, --make            Only compilation. All build.* keys are True (except
                        build.new). Run setup is skipped.
  -r, --no-compile      Skip compilation. All build.* keys are False.
```

new options

```
  --steps=STAGES        'stages list' (can contains: init, run, done, all)
                        that overwrites job.steps from expert rc file.
  --time-start=TIME_START
                        'yyyy-mm-dd hh:mn:ss' that overwrites timerange.start
                        of rc file.
  --time-final=TIME_END
                        'yyyy-mm-dd hh:mn:ss' that overwrites timerange.end of
                        rc file.
  --istart=ISTART       overwrite istart of rc file. No effect if empty string
                        ''
```

for EC-Earth

HOW-TO (1)

no install script !!

```
# environment
export rep='https://svn.knmi.nl/svn/TM5-MP'

# start with a branch
svn cp $rep/trunk $rep/branches/XYZ  -m "created XYZ branch"
svn co $rep/branches/XYZ

# setup rc files
cd XYZ
cp rc/main-base.rc.tmpl  my.rc

cp rc/main-chem.rc.tmpl  my.rc
cp rc/chem-input-default.rc.tmpl  chem-input.rc
```

machine, expert, compiler rc files:
"pycasso-" prefix ≡ “need to be adapted”

HOW-TO (2)

 # save your work

```
cd XYZ
svn mkdir DIR            # create and schedule DIR for addition
svn add NEWFILE          # schedule NEWFILE for addition
svn del OLDFILE          # schedule OLDFILE for removal
svn ci -m “message“
svn up
```

 # if you collaborate (several users developing the same branch)

```
cd XYZ
svn up
```

 # incorporating latest from the trunk (no local edit!)

```
cd XYZ
svn merge ^/trunk
```

New Features

https://dev.knmi.nl/projects/tm5/issues

for more details (incl. plots)

http://tm.knmi.nl/index.php/What's_new_in_next_cycle

for overview listing

NEW IN THE BASE CODE

- **grib_api** implemented (cohabits with gribex lib)
- **mmix** output
  - truly a monthly mean mixing ratio
- **restart files**
  - vertical and horizontal remapping (**istart=32**)

    (generalization of start_co2 & istart=6,61 from Andy)
- **savefile** (istart=31)
  - fully usable (ie when running with chunks)
  - useful if netcdf4 not available with parallel IO
- **makefile** : check for “too long” lines of code
- **pycasso** : compilation through job manager (EXPERIMENTAL)

31
32
33

Chemistry Updates (1)

- **Stratospheric boundary**
  - MSR → MSR2 for stratospheric O_3 (*Michiel*)
  - monthly variability in nudging terms (*Jason*)
    - no more erratic jump at month start
- **Timeseries** : output timestep can be < 1 hour
- **Aerosols** (*Twan*)
  - account for nitrate in optical properties
  - AEROCOM output
  - fix M7 deposition budget

Chemistry Updates (2)

Sources & Sinks

- *sources_sinks_apply* runtime cut by 55% [without M7]
  - improve MPI comm in CH_4 nudging
  - smarter workflow in emissions

- consolidated emissions
  - file or sector missing → crash
  - no more pseudo-error mess
  - CB05 only

- CB05 speciation applied to GFED3 emissions (*Jason*)
- scaled up volcanic sulfur emissions (*Twan*)

Chemistry Updates (3)

TROPOMI (Jason)

- HNO3 production during nighttime **DMS chemistry**
  - following *Allen et al.* (1999), conserve mass by
  - adding HNO3 prod. to NO_3 + DMS -> SO_2
  - +10 ppt HNO3
  - remove a NOx sink term
- **gamma(N_2O_5)** variability
  - *Evans and Jacob (2005)*
  - + eff. radius of NO_3-/SO_4= account for swelling (high RH)
  - changes by few percent (eg. O_3)

Chemistry Updates (4)

TROPOMI (Jason)

New tracer HONO

- transported (night lifetime)
- formation and oxidation:

$OH + NO + M$

$HONO + hv \rightarrow OH + NO$; $OH + HONO \rightarrow NO_2$

- motivated by 1x1 (polluted region)
- affect NO2 (+ ~2 Tg N)
- small drydep
- small impact on CO and O_3 (3x2 results)

Chemistry Updates (5)

TROPOMI (Jason)

New tracer $CH_3O_2NO_2$

- ARCTAS measurements (*Browne et al.*, 2011, ACP)
- important for UTLS HOx budget, LiNOx, …

$OH + CH_3O_2NO_2 \rightarrow HNO_3 + ..$

$CH_3O_2 + \mathbf{NO_2} + M \rightarrow CH_3O_2NO_2 + ..$

$CH_3O_2NO_2 \rightarrow CH_3O_2 + \mathbf{NO_2}$

$J(CH_3O_2NO_2) \rightarrow CH_3O_2 + \mathbf{NO_2} \quad \& \quad \mathbf{NO_3} + HCHO + \mathbf{NO_2}$

- introduce T-dependent branching ratio for:

$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$

$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$

Chemistry: Work In Progress (1)

- **ALD2 (C2 & higher aldehydes) photolysis** (*Jason*)
  - switch from

    $ALD2 + hv \rightarrow CH_3O_2 + CO + H_2O$

  - to 3 branching ratios

    $CH_3CHO + hv \rightarrow CH_4 + CO$

    $CH_3CHO + hv \rightarrow CH_3O_2 + CO + HO_2$

    $CH_3CHO + hv \rightarrow CH_3CO_2 + HO_2$

  - increases ALD2 burden by 100%
  - decreases CO in SH by 5%

Chemistry: Work In Progress (2)

Sub-Grid Mixing effect… (*Jason*)

- …on conversion rate of N_2O_5 to HNO_3 in clouds
- account for non-instantaneous mixing of cloud/nocloud in grid cell
- improve CO (lower in SH, high in NH)
- O_3: increase positive bias (comp. w/ EMEP)

NEXT

before release of TM5-MP v1.0

- merge TROPOMI (Jason) and aerosols (Twan) work
- merge EC-Earth 3.2 developments
- MPI decomposition across longitudes with reduced grid

not as urgent

- combine rc.py files into one!
- clean with_prism/oasis3/oasis4 macros (only one is needed)
- LiNox info into budget file instead of log file
- remove gribex lib
- no more long lines (>132)
- KPP
- alternate isoprene scheme (Marly)
- ...