Software Engineering, Code Development, User Support Issues

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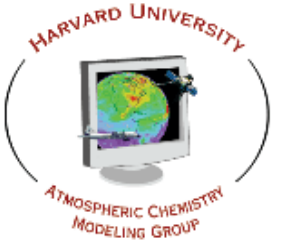
GEOS–Chem Meeting
Thursday, April 9th, 2009



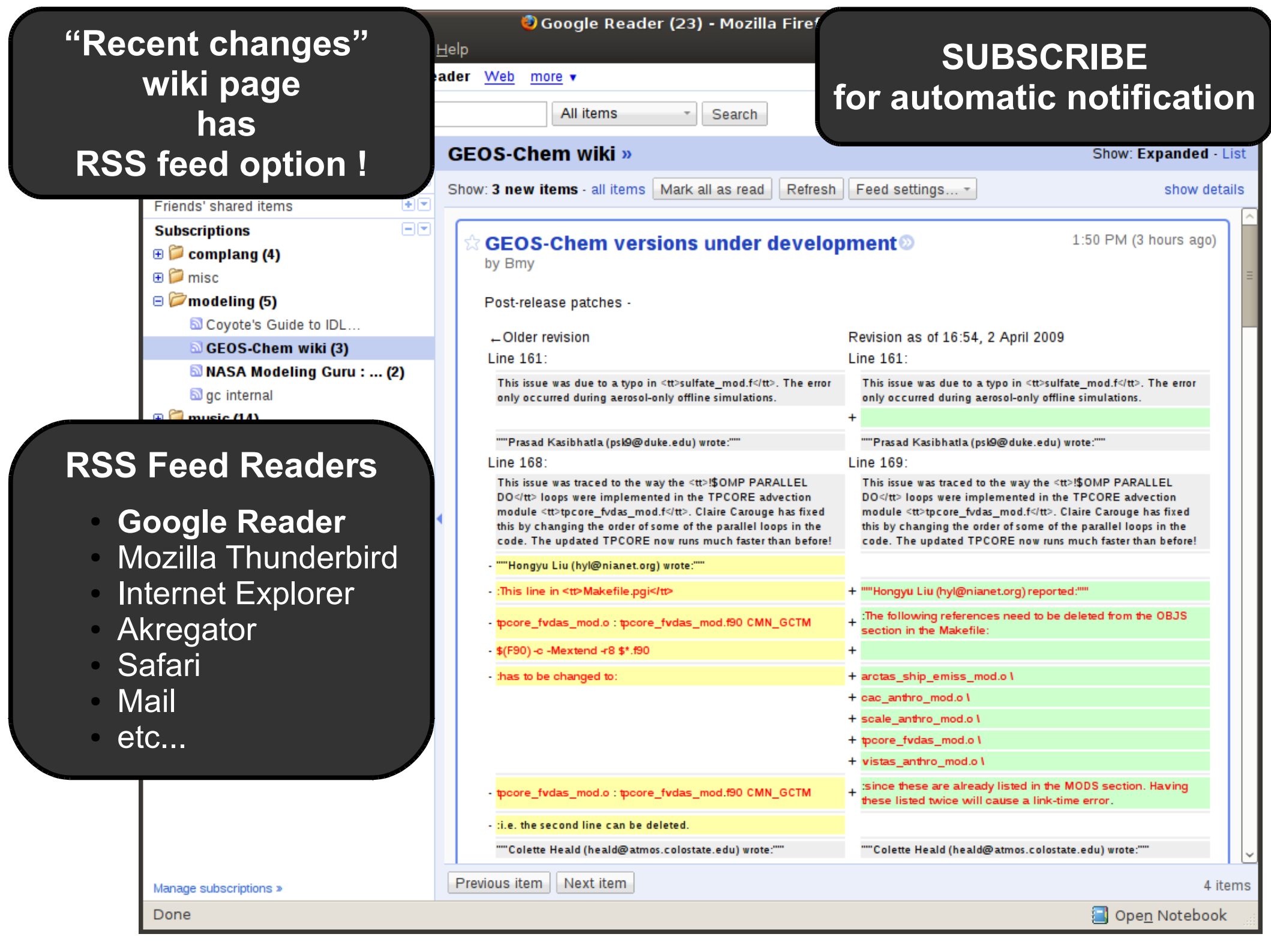
Outline

- User Resources:
  - Where to find information?
- Code development:
  - Who does what?
  - And how to do it?
- Debugging
  - Tips and tricks
- Next ?
  - Moving towards netCDF?

GEOS–Chem User Resources

Subscribe to the GEOS–Chem wiki

- The wiki facilitates communication among GEOS–Chem users and developers. ***It is the first place you should look for info!***
- The wiki contains information about
  - GEOS–Chem versions
  - Benchmark simulations
  - Bugs, fixes, and machine issues
  - Emissions options
  - Chemistry mechanism
  - Offline simulations
  - Met fields
  - Adjoint simulations
  - GAMAP
- Create a login and password, then you can edit pages
  - Wiki URL: ***http://wiki.seas.harvard.edu/geos-chem/***


"Recent changes" wiki page has RSS feed option !
SUBSCRIBE for automatic notification
RSS Feed Readers
Google Reader
Mozilla Thunderbird
Internet Explorer
Akregator
Safari
Mail
etc...
Google Reader (23) - Mozilla Fire
Help
eader Web more
All items
Search
GEOS-Chem wiki »
Show: Expanded - List
Show: 3 new items - all items
Mark all as read
Refresh
Feed settings...
show details
Friends' shared items
Subscriptions
complang (4)
misc
modeling (5)
Coyote's Guide to IDL...
GEOS-Chem wiki (3)
NASA Modeling Guru : ... (2)
gc internal
GEOS-Chem versions under development
by Bmy
1:50 PM (3 hours ago)
Post-release patches -
←Older revision
Revision as of 16:54, 2 April 2009
Line 161:
Line 161:
This issue was due to a typo in <tt>sulfate_mod.f</tt>. The error only occurred during aerosol-only offline simulations.
"""Prasad Kasibhatla (psk9@duke.edu) wrote:"""
Line 168:
Line 169:
This issue was traced to the way the <tt>!$OMP PARALLEL DO</tt> loops were implemented in the TPCORE advection module <tt>tpcore_fvdas_mod.f</tt>. Claire Carouge has fixed this by changing the order of some of the parallel loops in the code. The updated TPCORE now runs much faster than before!
"""Hongyu Liu (hyl@nianet.org) wrote:"""
:This line in <tt>Makefile.pgi</tt>
tpcore_fvdas_mod.o : tpcore_fvdas_mod.f90 CMN_GCTM
$(F90) -c -Mextend -r8 $*.f90
:has to be changed to:
"""Hongyu Liu (hyl@nianet.org) reported:"""
:The following references need to be deleted from the OBJS section in the Makefile:
arctas_ship_emiss_mod.o \
cac_anthro_mod.o \
scale_anthro_mod.o \
tpcore_fvdas_mod.o \
vistas_anthro_mod.o \
tpcore_fvdas_mod.o : tpcore_fvdas_mod.f90 CMN_GCTM
:since these are already listed in the MODS section. Having these listed twice will cause a link-time error.
:i.e. the second line can be deleted.
"""Colette Heald (heald@atmos.colostate.edu) wrote:"""
Manage subscriptions »
Previous item
Next item
4 items
Done
Open Notebook

GEOS–Chem User Resources

Subscribe to GEOS–Chem email lists

- GEOS–Chem general
  - geos-chem@seas.harvard.edu
  - Intended for ALL geos chem users!
  - Version updates & other info will be sent to this list
- GEOS–Chem aerosols
  - geos-chem-aerosols@seas.harvard.edu
  - Intended for developers of aerosol simulations
- GEOS–Chem adjoint
  - geos-chem-adjoint@seas.harvard.edu
  - Intended for users of the adjoint model

For info about how to subscribe, please see this wiki page:

GEOS-Chem_welcome_letter_for_new_users#Subscribing_to_the_GEOS-Chem_email_lists

GEOS–Chem User Resources

GEOS–Chem web page and user manuals

- GEOS–Chem web page, contains
  - Recent publications and presentations
  - Information about GEOS–Chem user groups
  - Information about parallelization and coding style
  - Links to programming resources (e.g. F90 tutorials, HDF info, etc.)
  - Links to various types of GEOS–Chem output
  - And more...
- User manuals
  - GEOS–Chem Users' Guide
  - GAMAP Users' Guide
  - GEOS–Chem Style Guide
  - TESTRUN

GEOS–Chem Code Development

Who supports what?

- Bob, Philippe, and Claire support GEOS–Chem's "full-chemistry" simulation (NOx – Ox – HC's – Aerosols)
  - 1 month & 1 year benchmark simulations
  - User manual on the GEOS–Chem website … etc
- The GEOS–Chem user community is responsible for the upkeep and validation of other simulations, including:
  - Offline tagged Ox
  - Offline tagged CO
  - Offline tagged aerosols
  - Offline CH4
  - Mercury
  - Nested grid simulations, … etc.
- Users should provide B/P/C with updates for offline simulations, for inclusion into the GEOS–Chem std code

GEOS–Chem Code Development

GEOS–Chem user responsibilities

- GEOS–Chem users are responsible for:
  - Setting up their systems
  - Learning F90, IDL, shell scripts, etc...
  - Periodically updating to the latest version of G–C
    - i.e. at the start of a new project
  - Debugging code
- Promptly report any bug fixes you have made to B/P/C
  - Other users may be struggling w/ the same problem and could benefit from the fix that you have made
- Code submission guidelines
  - When any code you have written is mature, submit it to B/P/C for inclusion into the GEOS–Chem std code.
  - Also provide the appropriate documentation

GEOS–Chem Code Development

Documentation: Do's

- Please provide copious comments in your code
  - List the name and purpose of each module, subroutine, and function
  - Label each input/output argument and its units
  - Provide citations to journal references where appropriate
  - Use descriptive names for variables, subroutines, functions
  - Clearly identify your modifications in the code using your initials
- For data that is meant as input to GEOS–Chem, provide:
  - A README file describing:
    - Individual data files and their contents (and units!!)
    - Source of the data and any journal references
    - The FTP/web site from which the data was obtained
  - Plots, tables and/or sums of emissions data
  - IDL/F90 etc. code that was used to create individual data files
- Feel free to post documentation for code & data on the wiki!

Documentation: Don'ts

- Don't use a language other than English
- Avoid partial citations such as:
  - “see Smith & Jones, 2001”
  - “see Smith's paper”
  - “see Amanda's slide”
  - List the full citation first, then abbreviate thereafter...
- Avoid cryptic comments
  - e.g. “NOx 1.2, Ox 2.0”
- Don't assume that the person reading your documentation will have any prior knowledge about this code and/or data
  - Leave nothing unexplained!

Debugging / Testing Tips

Use GEOS-Chem utilities

- **CHECK_STT** if NaN or a negative tracer appears
- **SAFE_DIV** to avoid potential overflow (division by zero)
- **IS_SAFE_DIV** to check both overflow & underflow in division
- **CHECK_VALUE** to check for NaN or INFINITY

Look for numerical traps

- "**catastrophic cancellation**" when subtracting huge and small
- use **F90 utilities**

  TINY to get a small positive number
- compile with **warnings** on

  check bounds, check uninit, check pointers (ifort)

Debugging / Testing Tips (2)

Use a Debugger

- F90 -> Totalview, dbx, GDB
- IDL, Matlab -> included

Report a bug

- Use this address: geos-chem-support@as.harvard.edu
- Please provide this information:
  - GEOS-Chem version number & Type of Simulation
  - Met field type & horizontal resolution (e.g. 4 x 5 GEOS–5)
  - Platform, Compiler, Number of Processors
  - Description of problem
  - Log file output from the simulation w/ the error message
  - ***Important! Have you made any changes to the standard code?***

Debugging / Testing Tips (3)

Some Useful Resources:

- *Floating-point math issues* page on the GEOS-Chem wiki
  - Brief description of how floating-point math works
  - How to avoid some common numerical pitfalls
  - ***http://wiki.seas.harvard.edu/geos-chem/index.php/Floating_point_math_issues***
- *Programming resources* page on GEOS–Chem website
  - Links to tutorials, compiler sites & manuals, and other information
  - ***http://www.as.harvard.edu/ctm/geos/geos_resources.html***

Pros and Cons of netCDF

PROS:

- Binary format with header
- Easy access to the data from command line
- Easy to share with other teams

CONS:

- Every user has to install the netCDF library by himself
- Do not give more information than .bpch files
- Reading netCDF files w/ Fortran is relatively easy
- Writing netCDF files w/ Fortran is more involved
- A substantial amount of work to implement in G-C

It's not a priority for us. But feel free to begin the work if you want to

Next ?

Questions?