GEOS–Chem User Resources, Code Development Guidelines, and Debugging Tips

Bob Yantosca
Philippe Le Sager
Claire Carouge
Atmospheric Chemistry Modeling Group
School of Engineering & Applied Sciences
Harvard University

geos-chem-support@as.harvard.edu
Contents

GEOS–Chem User Resources
  – Wiki
  – Email lists
  – Website

GEOS–Chem Code Development Guidelines
  – Steering Committee and Working Groups
  – Best Practices
  – Who supports what
  – User responsibilities
  – Documentation

GEOS–Chem Debugging Tips
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 and benchmark simulations
- Monthly informational newsletters
- Bugs, fixes, and machine issues
- Emissions options and chemistry mechanism
- Offline simulations
- Met fields
- Adjoint simulations
- GAMAP

Create a login and password, then you can edit pages
“Recent changes” wiki page has RSS feed option!

RSS Feed Readers
- Google Reader
- Mozilla Thunderbird
- Internet Explorer
- Akregator
- Safari
- Mail
- etc...

SUBSCRIBE for automatic notification
### GEOS–Chem User Resources

#### Subscribe to the GEOS–Chem email lists

<table>
<thead>
<tr>
<th>GEOS-Chem Email List</th>
<th>Intended Audience</th>
</tr>
</thead>
<tbody>
<tr>
<td><a href="mailto:geos-chem@seas.harvard.edu">geos-chem@seas.harvard.edu</a></td>
<td>All GEOS-Chem users</td>
</tr>
<tr>
<td></td>
<td>Version updates and bug fixes will be announced via this list!!</td>
</tr>
<tr>
<td><a href="mailto:geos-chem-adjoint@seas.harvard.edu">geos-chem-adjoint@seas.harvard.edu</a></td>
<td>Adjoint Working Group</td>
</tr>
<tr>
<td><a href="mailto:geos-chem-aerosols@seas.harvard.edu">geos-chem-aerosols@seas.harvard.edu</a></td>
<td>Aerosols Working Group</td>
</tr>
<tr>
<td><a href="mailto:geos-chem-carbon@seas.harvard.edu">geos-chem-carbon@seas.harvard.edu</a></td>
<td>Carbon Gases and Organics Working Group</td>
</tr>
<tr>
<td><a href="mailto:geos-chem-emissions@seas.harvard.edu">geos-chem-emissions@seas.harvard.edu</a></td>
<td>Emissions Working Group</td>
</tr>
<tr>
<td><a href="mailto:geos-chem-oxidants@seas.harvard.edu">geos-chem-oxidants@seas.harvard.edu</a></td>
<td>Oxidants and Chemistry Working Group</td>
</tr>
<tr>
<td><a href="mailto:geos-chem-regional@seas.harvard.edu">geos-chem-regional@seas.harvard.edu</a></td>
<td>Regional Air Quality Working Group</td>
</tr>
</tbody>
</table>

To subscribe to any of these lists, visit: [https://lists.seas.harvard.edu/mailman/listinfo](https://lists.seas.harvard.edu/mailman/listinfo)
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**
The charge of the GEOS–Chem Steering Committee is to:

- Develop long-term strategies for the model and for the functioning of the user community
- Prioritize and enable model development
- Facilitate sharing of information across model users through the GEOS–Chem Working Groups.

GEOS–Chem Steering Committee membership

- Is rotating (fixed-length terms)
- Is international
GEOS–Chem Working Groups

- Each **Working Group** focuses on a particular area of research:
  - Adjoint Model and Data Assimilation
  - Aerosol Processes
  - Carbon Gases and Organics
  - GMAO Liaison
  - Emissions
  - Oxidants and Chemistry
  - Regional Air Quality

- Responsibilities of each Working Group:
  - To foster communication between Working Group members for collaboration and sharing of information
  - To facilitate identification of *model development priorities*. 
GEOS–Chem Best Practices

1. GEOS–Chem is a grass-roots community model that relies on contributions and good practices from all its users for continued successful operation. These practices include:

2. Identifying yourself to model engineer Bob Yantosca and providing a link to your research for the People and Projects web page

3. Subscribing to model and working group email lists, keeping up to speed through the model newsletters and wiki pages

4. Providing credit to recent developers in publications

5. Contributing bug reports and fixes to the GEOS-Chem support team

6. Upgrading regularly to the latest standard version of the model

7. Helping out as you can in response to user requests

8. Contributing mature new developments to the standard model
Criteria for including updates into GEOS–Chem

- Each update to G–C must have an identifiable user base
  - This ensures that all new functionality that is added into GEOS–Chem will benefit the largest possible number of users
  - If an update to GEOS–Chem has no readily identifiable user base, it will be assigned a lower priority and/or left as a research option
  - Code developers should interact with the relevant Working Group(s) to prioritize and coordinate updates for inclusion into GEOS–Chem

- Each update to GEOS–Chem must be mature and stable
  - Ready to be plugged in (i.e. no major rewriting needed)
  - Well-documented source code and data files
  - If necessary, provide results for comparison
    - E.g. for tagged and/or offline simulations
Who supports what?

- Bob, Philippe, and Claire (aka B/P/C) 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 standard code
GEOS–Chem user responsibilities

- GEOS–Chem users are responsible for:
  - Setting up their hardware systems (w/ help of local IT if possible!)
  - 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
  - Joining the Working Group(s) most relevant to their area(s) of research

- 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
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!
Automatic documentation with ProTeX

• Protex is a very useful Perl script (developed @ GSFC) that can strip information from a Fortran document header and save that to a LaTeX file.

• The LaTeX file can then be converted to PDF, PS, HTML formats

• We strongly recommend all new GEOS–Chem code be equipped with ProTeX documentation headers!

• GEOS–Chem v8-01-03 and higher now uses ProTeX

• Please see the following Wiki page for more information:

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?**
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

- **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](http://www.as.harvard.edu/ctm/geos/geos_resources.html)