GEOS-Chem: looking ahead

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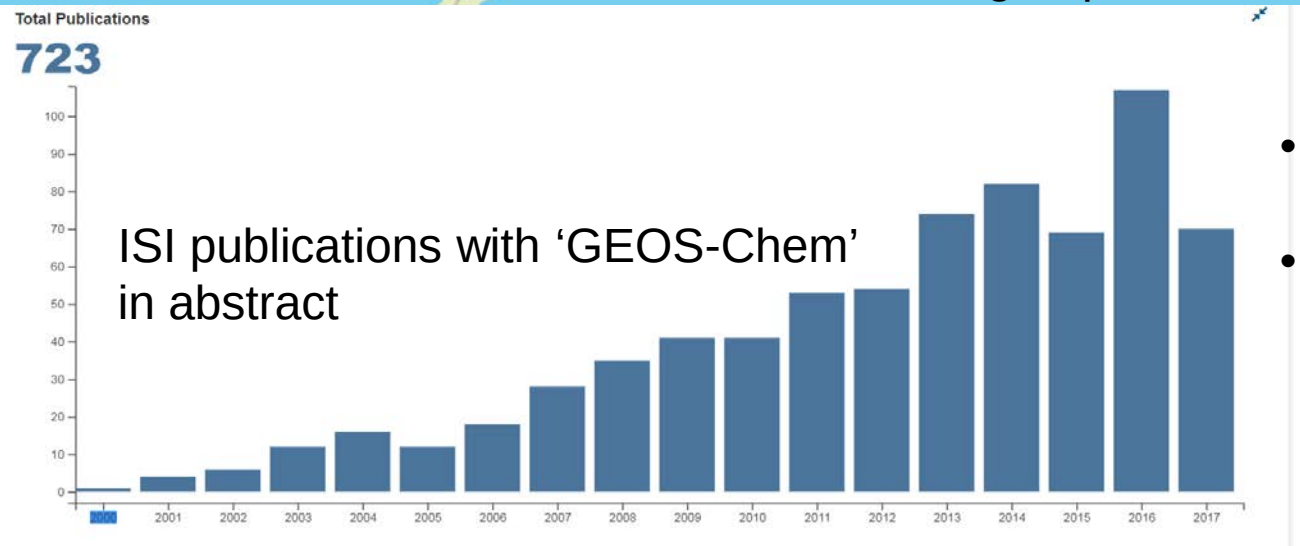
GEOS-Chem: a large worldwide grass-roots community

http://www.geos-chem.org/geos_people.html

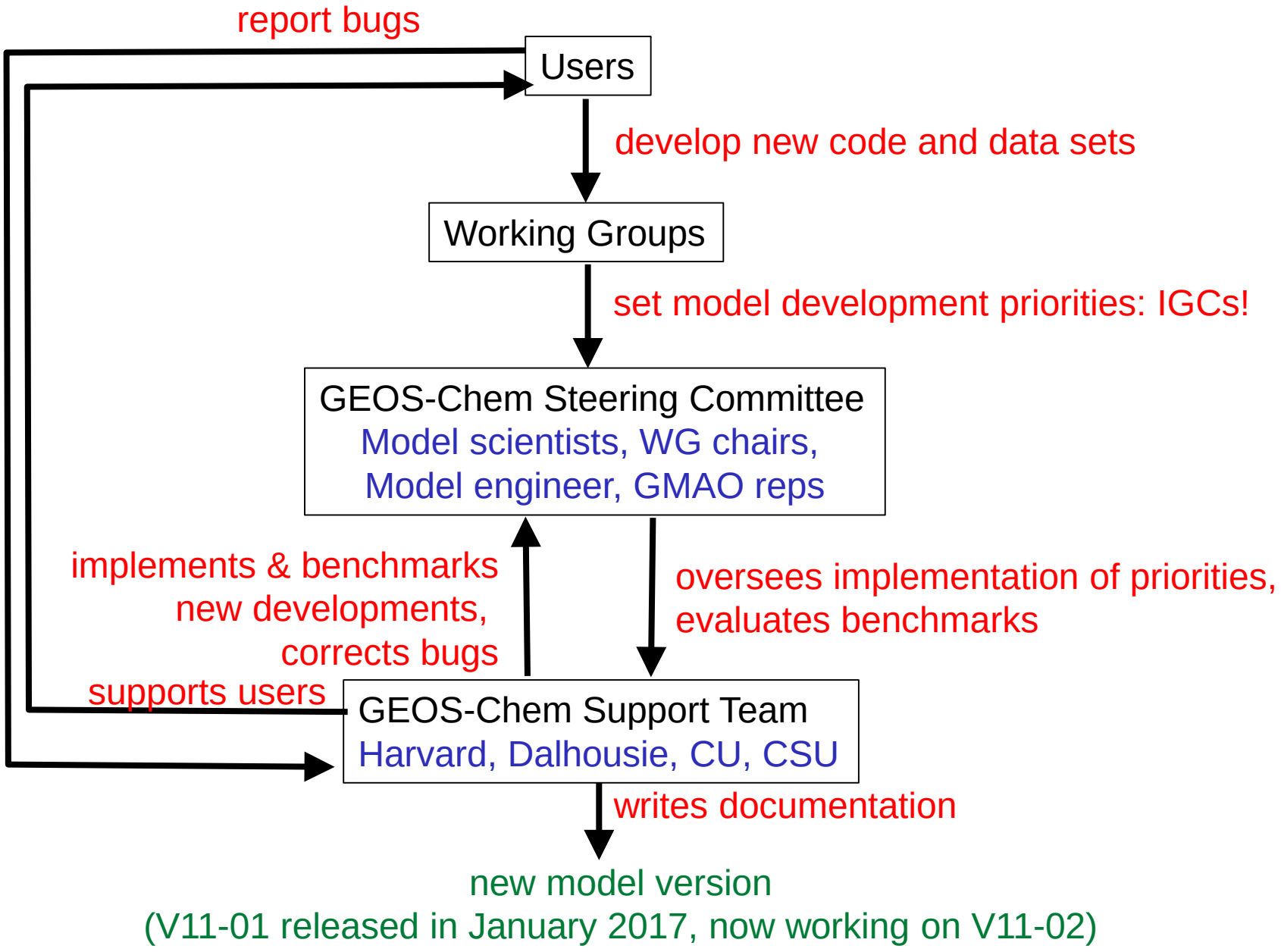


ISI publications with ‘GEOS-Chem’ in abstract

- IGCs at Harvard every 2 years
- First GC Asia,GC Europe meetings to be held in 2018 – alternate years with IGCs?

GEOS-Chem Community Mission: *to advance understanding of human and natural influences on the environment through a comprehensive, state-of-the-science, readily accessible global model of atmospheric composition*

GEOS-Chem scientific development is driven by its users



Major effort in software engineering in recent years:
necessary to bring GEOS-Chem into the 2020s

- HEMCO emissions pre-processor [Keller et al., 2014]
  - emissions and other data now added, combined, scaled without editing source code
- GEOS-Chem operation on 1-D columns for any grid selected at runtime [Long et al., 2015]
  - enables use of meteorological fields produced on any grid
  - facilitates distributed-memory parallelization
- Reconfiguration of chemical module (FlexChem) (Mike Long and GCST)
  - Facilitates changes in chemical mechanism
  - Makes GEOS-Chem compatible with its adjoint
  - Choice of chemical solvers
- ESMF compatibility [Long et al., 2015]
  - enables use of GEOS-Chem as chemical module for Earth System Models (ESMs)
  - enables MPI parallelization
- NetCDF I/O (GCST)
  - self-describing, selective-read format for input/output files, essential for GCHP
- GCHP [Eastham et al., 2017]
  - massively parallel hi-res simulations using cubed-sphere GEOS data and ESMF
  - more accurate transport
  - gateway to stretched-grid capability
- Compatibility with open-access software gfort and Python (GCST, Dan Rothenberg…)
  - no need to purchase expensive Intel Fortran and IDL licenses
  - enables cloud-based GEOS-Chem computing
- Running GEOS-Chem on the cloud [Zhuang et al., 2018]
  - Opens GEOS-Chem access to a wide user base
  - Provides cheap easy access to occasional users
  - Establishes standard version of model

GEOS-Chem is open-source, licensed software

- Having an open-source code is essential for
  - Academic publications
  - Use in policy-relevant documents
  - Creation of a large user community

- Code is licensed as of September 2017 (Seb Eastham and GCST)
  - Identifies the model developers (a long list!) as owners of the model
  - States freedom of use and distribution
  - Establishes that all code in GEOS-Chem is free to use
  - Protects us against nightmare scenarios
  - Provides tangible credit to code development

- Attribute a DOI to new versions (in the works; Jenny Fisher and GCST)
  - Provides a reference to that version
  - Needed to satisfy ‘code availability’ requirement in publications

Looking ahead to GEOS-Chem v11-02

In development; expect public release in early 2018

- V11-02a: chemical updates, emission updates, bug fixes *(US EPA, U. York, CSU, UW, Duke, Dalhousie…)*
- V11-02b: GCHP capability *(GEOS-Chem Support Team)*
- V11-02c: isoprene chemistry and SOA updates *(Harvard, U. Wollongong, U. Birmingham, Caltech, CSU)*
- V11-02d: comprehensive halogen chemistry (*U. York, U. Copenhagen, MIT, Harvard)*

In the pipeline: flux diagnostics, NetCDF diagnostics (GCST), new emission inventories, scale-independent emissions (Dalhousie, PKU, U. Rochester, MIT), flexible nesting capability (Jiawei Zhuang),…

Looking to the future: GCHP

- GCHP is mature – so how do we get users to use it?
  - Improve diagnostics: current work to update diagnostics to NetCDF
  - Get GMAO to provide operational cubed-sphere archive: soon, we are told!
  - At that point lat-lon data will not be produced at native resolution anymore (we will still have lat-lon for MERRA-2)
  - Produce journal publication documenting GCHP
  - Getting the adjoint and specialty simulations to work with GCHP

- There is absolutely no plan to pull the plug on GEOS-Chem Classic (GCC)
  - GCC and GCHP will continue to be developed together for foreseeable future
  - The reliance of the GEOS-Chem community on GCC is fully recognized
  - GCHP may become eventually more scientifically attractive because of better transport, stretched-grid options…
  - One can imagine a distant future where the GEOS-Chem community has gravitated to GCHP and GCC becomes obsolete, but that future is distant.

Looking to the future: GEOS-Chem on the cloud

- Great work by Jiawei Zhuang in demonstrating the capability
  - Lots of excitement in GEOS-Chem community
  - Enabled by Gnu fortran, GCPy diagnostics
  - Could greatly expand usage
  - Could facilitate model fidelity
- Current bottleneck: making GEOS data available through the cloud
  - Wish to have data posted/downloadable for free, users pay for CPU cycles
  - Currently in negotiation between Amazon and Harvard

Looking to the future: GEOS-Chem as ESM component

- GEOS-Chem "chemistry-at-large module" is in place in GEOS ESM (Keller, Long)
  - All local operations $dC/dt = P - L$ are performed by GEOS-Chem module
  - Currently applied to AQ forecasts
  - Ongoing comparisons of strat chem with GMI
  - Need to establish quality of aerosol simulation
  - Need to apply it to chemical data assimilation – will require improvement in computational performance: faster chemical solvers, coarser chemical grid?
- GEOS-Chem incorporated in BCC model (Xiao Lu, Lin Zhang)
  - Enthusiasm at BCC
  - Next step is to evaluate simulation
  - First application priority: S2S AQ predictions
  - Second application priority: CMIP6 simulations
- GEOS-Chem chemistry module to go into ECMWF Copernicus (Seb Eastham)
  - Chemistry separate from emissions, deposition, radiation – not ideal!
- Plan to implement GEOS-Chem as module into CESM2
  - Interest of Seb Eastham and Mike Long, still in take-off mode
- Plan to implement GEOS-Chem as module in WRF-Chem
  - Interest of May Fu, still in take-off mode

Looking to the future: dealing with increasing resolution

- As resolution of the model increases, the off-line CTM approach becomes more challenging [Yu et al., 2017]
  - Need to increase both spatial and temporal resolution of met archive
  - As ESM moves to cloud-resolving scales, convection is increasingly resolved as transient advection missing from the met archive – needs to be added to CTM
  - As resolution increases, chemical simulations will eventually need to be done on-line – but what is the threshold?
  - In any case, there will be sustained demand for off-line simulations at coarser resolution – but this will require adjusted met fields
  - Envision a future where user-initiated developments will be done in the coarse-resolution CTM, to serve high-performance applications on-line

Looking to the future: balancing community needs for innovation and stability

GEOS-Chem Community Mission: *to advance understanding of human and natural influences on the environment through a comprehensive, state-of-the-science, readily accessible global model of atmospheric composition*

- GEOS-Chem is **unique** among atmchem models in its ease of use; allows atm chemists with low computing resources to contribute scientific innovation
- But they wouldn't use it if it didn't stay at the cutting edge of science – meaning that we have to continuously innovate in both the science and the software engineering needed for that science
- But somebody's "cutting edge" is someone else's "unnecessary update" and users are stressed when the model keeps changing
- This is particularly the case for specialty simulations that get broken in model updates
- Also need to be careful before retiring existing capabilities (for example, we plan to keep old non-NetCDF diagnostics in v11-2)
- On the other hand, continued support for older versions unduly stresses the GCST, and GEOS-Chem is intended to be a research model with no backward compatibility commitment
- Counting on GCSC and Working Groups to provide guidance in striking a balance between innovation and stability