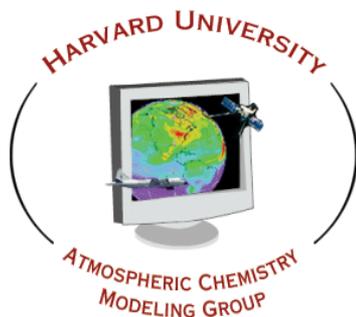
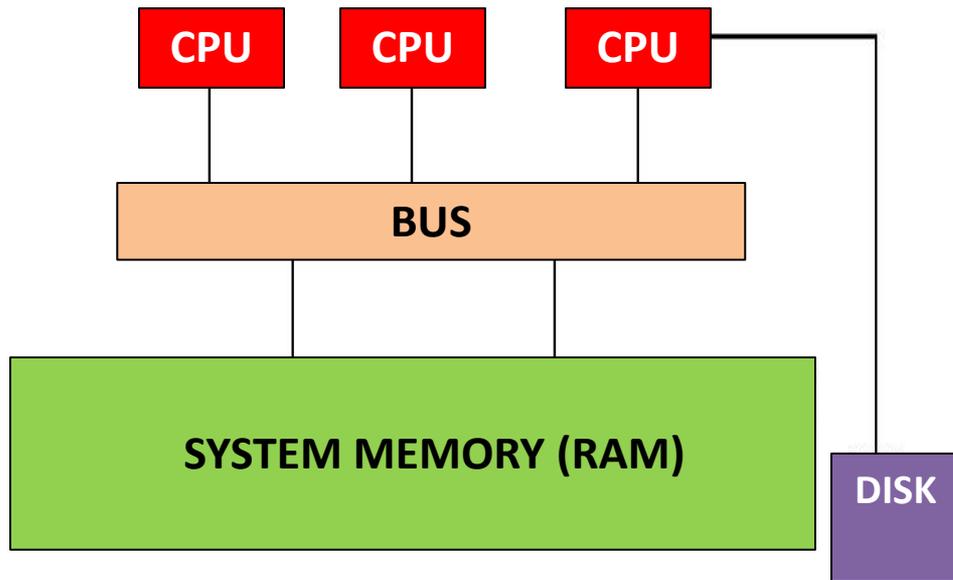


GEOS-Chem Model Engineer's Report

Bob Yantosca
Senior Software Engineer
GEOS-Chem Support Team

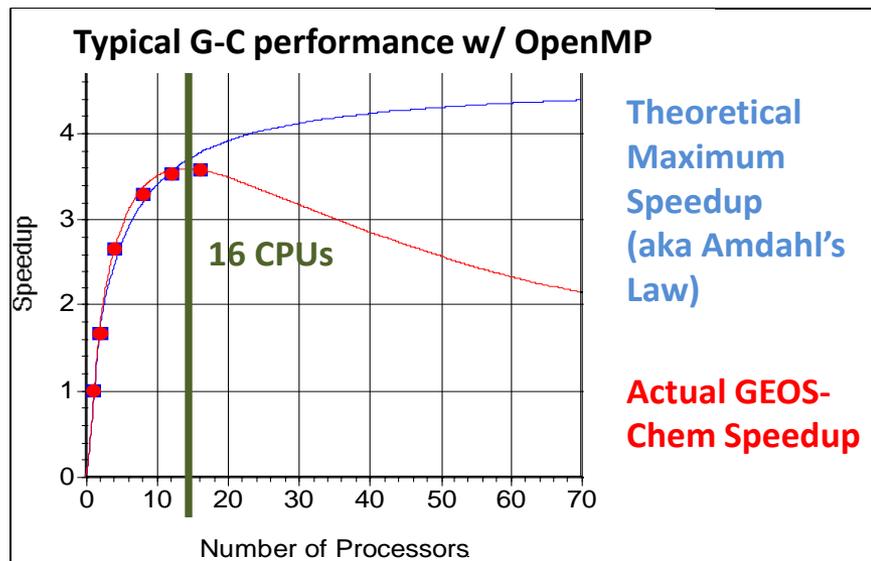
The 6th International GEOS-Chem Meeting
06 May 2013 @ Cambridge, MA





GEOS-Chem was originally created by the **merger of source code from two different CTMs** more than 15 years ago. It was originally intended to run on **shared memory architecture (SMA) computer**.

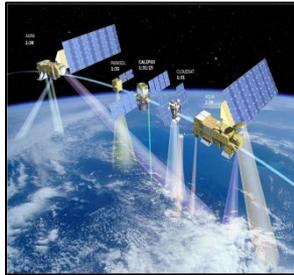
A SMA computer is one where all of the CPUs can “see” all of the memory on the machine. SMA machines usually have **small #'s of CPUs (~8-16)**.



GEOS-Chem simulations utilize **OpenMP parallelization** to split up the work flow among all of the CPUs on a SMA computer.

But due to **overhead**, after some point adding more CPUs does not make GEOS-Chem run any faster.

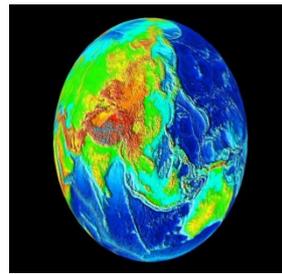
We would like to be able to do “Big Science” simulations



with Satellite Observations



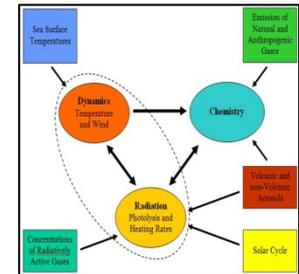
with Aerosol Microphysics



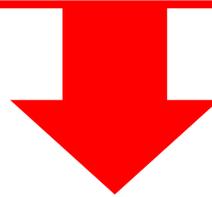
with 1/4 Degree Resolution



with Dynamic Land Models



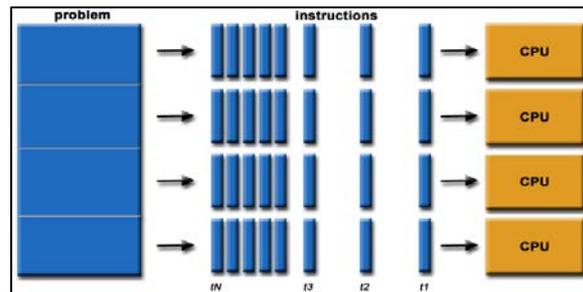
with Climate and Chemistry Feedbacks



But we need “Big Computing” to do “Big Science”



Using 100's or 1000's of CPUs on HPC clusters or supercomputer systems

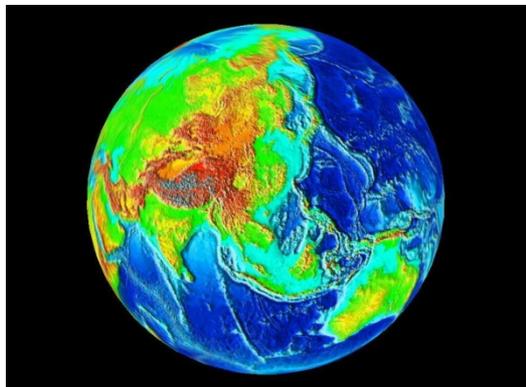


Using Message Passing Interface (MPI) parallelization



Utilizing Earth System Model Framework (ESMF) Library

Ongoing Projects



Pushing GEOS-Chem to higher resolution

- Grid-Independent GEOS-Chem (aka GIGC)
 - Embed G-C within the NASA GEOS-5 GCM
 - Make G-C be able to use 100's or 1000's of CPUs
- $\frac{1}{4}$ degree nested-grid capability
 - Using newest NASA/GMAO met field product



Replacing legacy code in GEOS-Chem

- FLEXCHEM: New chemical solver package
 - Replace inefficient SMVGEAR w/ new KPP build
- GIGC Emissions Component
 - Replace legacy emissions code w/ new data structure, netCDF I/O, consistent units, and regridding capability



Reducing memory usage in GEOS-Chem

- Introducing a flexible precision definition
 - Changing REAL*8 variables to REAL*4
 - Memory usage will be halved!



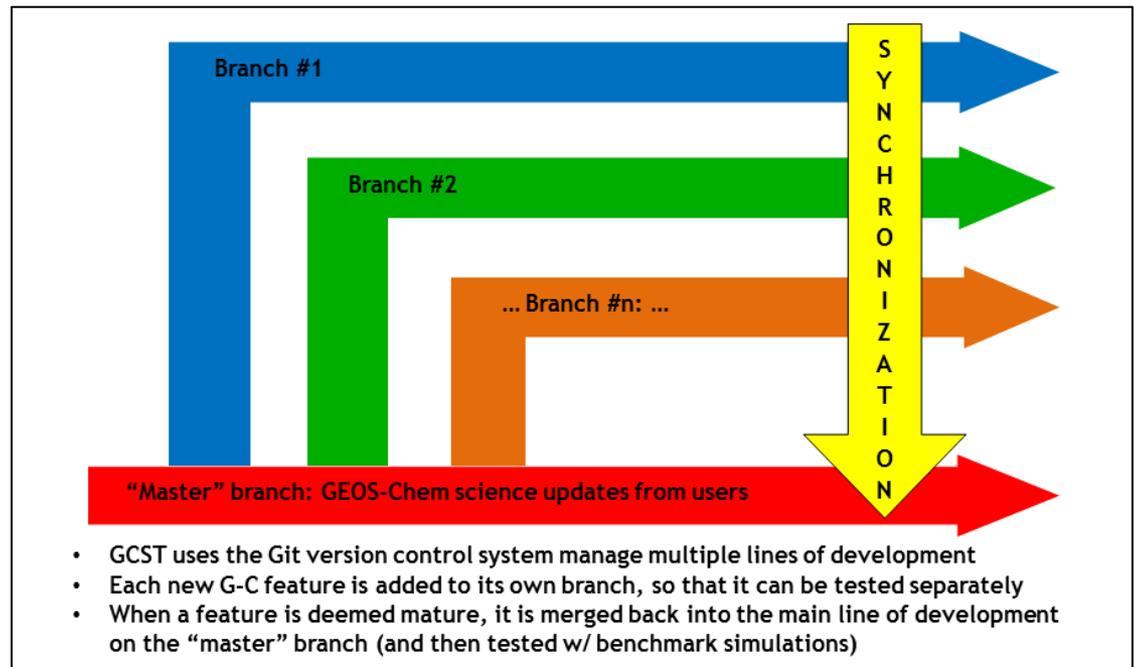
In order to **avoid disrupting the existing GEOS-Chem workflow**, we add structural modifications in parallel to the ongoing scientific updates.

Think of this process as **building a new bridge next to the old bridge**. At some point the new bridge is opened to traffic and the old bridge is taken down.

We use the **Git version control system** to keep track of several parallel lines of software development.

Code updates made in one branch don't affect the other branches.

Branches can later be merged back into the “main line” of development.





GEOS-Chem Support Team

- Current GCST members
 - **Bob Yantosca** (Model development, GIGC)
 - **Melissa Payer** (Model development, benchmarking)
 - **Mike Long** (GIGC, Flexchem)
 - **Sajeev Philip** (Met fields, nested-grid simulations)
 - **Nicolas Boussez** (Adjoint model)
- GCST functions
 - Fundamental G-C software development
 - Support G-C users in research (doc, tech support)
 - Link G-C innovations to NASA modeling efforts



For more info ...

- IGC6, Monday Evening
 - GEOS-Chem model clinic
 - GEOS-Chem adjoint clinic
 - Q &A session about NASA/GMAO and GIGC
- IGC6, Wednesday Evening
 - Software engineering breakout session
- Anytime
 - GEOS-Chem wiki (wiki.geos-chem.org)
 - GEOS-chem website (www.geos-chem.org)