GEOS-Chem in massively parallel and ESM (GMAO) implementation

1) Include GEOS-Chem chemistry as a coupled component within the GEOS-5 system via the Earth System Modeling Framework (ESMF)

2) Permit the use of MPI parallelization of GEOS-Chem within ESMs and as a stand-alone application

3) Provide an adaptive framework for chemical data assimilation within GEOS-DAS
GEOS-Chem should…

0: Transition without disrupting user community workflow

1: Maintain GEOS-Chem’s current serial functionality

2: be ESMF compliant

3: be Arbitrarily embeddable within GCM’s*

4: be HPC capable as a stand-alone CTM**

* Requires development of GCM-specific interface.
** Current effort will rely on ESMF & MAPL framework.
## GCHP: How far along are we?

<table>
<thead>
<tr>
<th>Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. F77-to-F90 conversion &amp; runtime initialization of horizontal grid.</td>
</tr>
<tr>
<td>2. ESMF I/O Data Socket for GCM Coupling</td>
</tr>
<tr>
<td>3. Chemistry Component</td>
</tr>
<tr>
<td>4. Dry-Deposition Component</td>
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<tr>
<td>5. Emissions Component</td>
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<td>6. Wet Physics Component</td>
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<tr>
<td>7. Dynamics Component</td>
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<tr>
<td>8. Diagnostics</td>
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<tr>
<td>9. GEOS-Chem HP</td>
</tr>
</tbody>
</table>

**Degree of Completion**

- **0%**
- **100%**
| Goal 1: Couple GEOS-Chem within GEOS-5. |
| Goal 2: Enable direct operation within GEOS-DAS |
| Goal 3: Operate GEOS-Chem as stand-alone & HPC |

| 0% | Degree of Completion | 100% |
Coupled GEOS-Chem/GEOS-5 Performance

Surface O$_3$ (nmol mol$^{-1}$)

a) 2° X 2.5°

b) 0.5° X 0.625°
Coupled GEOS-Chem/GEOS-5 Performance
## GEOS-Chem HP Performance Test

### Performance Benchmark

<table>
<thead>
<tr>
<th>PEs</th>
<th>NX</th>
<th>NY</th>
<th>IM (48)</th>
<th>JM (288)</th>
<th>cores</th>
<th>nodes</th>
<th>runlog</th>
<th>Error message</th>
<th>CPUs</th>
<th>CPU time</th>
<th>Wall time</th>
<th>memory(K)</th>
<th>VM(K)</th>
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</thead>
<tbody>
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<td>24</td>
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<td>12</td>
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<td>1</td>
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<td>92144</td>
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<tr>
<td>96</td>
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<td>checkpt file write error</td>
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<td>4:16:03:44</td>
<td>30:01:00</td>
<td>8592</td>
<td>92144</td>
</tr>
</tbody>
</table>

### No. of Processing Elements vs. Execution time

- **Wall time**

No. of chemical tracers: 92
Simulation duration: 1 day
Output frequency / resolution: 3 hourly / 91x144

### Graphical Representation

The graph depicts the relationship between the number of processing elements (PEs) and the execution time. As the number of PEs increases, the execution time decreases, indicating improved efficiency and performance. The data points are plotted on a logarithmic scale for both the x-axis (PEs) and the y-axis (time in minutes and seconds), allowing for a clear visualization of the trend.
GCHP

Ocean Grid

Eulerian, Lat/Lon

Cubed-Sphere
GCHP
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  - Daniel Jacob
  - Jack Yatteau
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  - Meemong Lee

➔GEOS-Chem Users & Developers

S. Eastham: MIT
J. Linford: ParaTools
GEOS-Chem HP Performance Test

Test setup

Compute Server : Discover (NCCS/NASA)
Operating System : Linux
Architecture : x86_64
Environment

Module list:
1) comp/intel-15.0.2.164
2) mpi/sgi-mpt-2.11
3) lib/mkl-15.0.2.164
4) other/comp/gcc-4.6.3-sp1
5) other/SIVO-PyD/spd_1.20.0_gcc-4.6.3-sp1_mkl-15.0.0.090

MPI:
/usr/local/sgi/mpi/mpt-2.11/opt/sgi/mpt/mpt-2.11/bin/mpiexec_mpt.nccs