Evolving HPC and application design
toward a coupled data assimilation system at NASA
suitable for emerging Exascale platforms

Bill Putman
Tom Clune
NASA Global Modeling and Assimilation Office

Dan Duffy
NASA Computational and Information Sciences and Technology Office

Tsengdar Lee
NASA Headquarters
The Goddard Earth Observing System (GEOS)

1. Primary GEOS Modeling & Assimilation Systems
   • GEOS-FP [Forward Processing] – *NWP Analysis + 10-day Forecast*
   • GEOS-CF [Composition Forecasting] – *5-day chemistry & air quality*
   • GEOS-S2S [Sub-seasonal to Seasonal] – *Seasonal prediction*
   • GEOS-CAM [Convection Allowing Model] – *Storm-scale NWP & OSSEs*

2. Our Path to Exascale
   - The evolution of compute at NCCS through FY2025
   - The evolution of GEOS: Coupled-DA
   - The UFS and community development (FV3, DA and physics)
   - Enabling disruptive technologies
     • Artificial Intelligence
     • Domain specific languages
     • Cloud computing & storage
GEOS-FP: Near real-time forward processing for NWP

12-km (c720) 72-Levels 4D Hybrid EnVar GSI (32-mem)

Throughput of GEOS-FP

- GMAO-Ops
- No GOCART

Aerosols (Advection+GOCART) & Cloud Interactions
50+ species/bins add 1.8x to the AGCM Cost

Geos-5 Forecast
02-Apr-2019 00z
GEOS-CF: A near real-time composition forecasting system

- Highest-resolution global near real-time system for chemical composition
- 3416 CPU’s, ~7-hour wall-clock time for 1-day analysis plus 5-day forecast

25-km Global Resolution
250 Reactive Gases
1-day Analysis + 5-day Fcst

GMAO PI: Christoph Keller
GEOS-CF: Artificial Intelligence replacing Chemical Integrator

**GEOS -vs- GEOS-CF runtime**

- **GEOS**
  - Other
  - I/O
  - Dynamics
  - Chemistry

- **GEOS-CF**
  - Other
  - I/O
  - Dynamics
  - Chemistry

**Idea: use machine learning in place of numerical solution**

- **Numerical model**
  - Initialize
  - Transport
  - Emissions
  - Subgrid
  - Photolysis
  - Chemical integrator
  - Deposition
  - Diagnostics

- **Emulator**
  - Initialize
  - Transport
  - Emissions
  - Subgrid
  - Photolysis
  - Chemical integrator
  - Deposition
  - Diagnostics

**Random Forest**

**Training time (GPU):**
15-20 seconds per species

**Chemistry Speedup:**
10-100x

---

**London**

- Ozone [ppbv] vs Simulation days

**Beijing**

- Ozone [ppbv] vs Simulation days

GMAO PI: Christoph Keller
GEOS-S2S: Subseasonal to Seasonal Prediction

"...developing an Integrated Earth System Analysis (IESA) capability, which links simultaneous analyses of Earth system components and captures the necessary interactions between them"

- **Ocean GCM, Sea-Ice and Biogeochemistry**
  - *Evolution to the GEOS S2S and IESA:*
    - MOM5 => MOM6
    - Development of CICE
    - Inclusion of NOBM Biogeochemistry to complete the carbon cycle

- **Wave Model**
  - *Improving air-sea fluxes:*
    - Implementing the Miami Wave Model *(MAP16 funded)*
    - Inclusion of sea-spray effects *(feeding into aerosol model)*
    - Strengthen ocean-atmosphere coupling in the IESA

- **Land Processes**
  - *Catchment Land Surface Model developments:*
    - Dynamic phenology and carbon storage
    - Improved river routing to predict catchment transport of surface water
    - Updated snow model

**Synergistic Collaborations**
- North American Multi-Model Ensemble (NMME)
- NOAA MAPP/CTB Subseasonal Experiment (SubX)

**Areas of focus for future collaboration:**
- Coupling strategies and Data Assimilation
  - *JEDI unification of DA amongst Earth system components:*
    - Easily leverage scientific developments across components
    - Provide a natural pathway to coupled DA

GMAO PI: Andrea Molod
DYAMOND: NH Simulations (August 2016)
Sub-5km Global Domain

Dynamics of the Atmospheric general circulation Modeled On Non-hydrostatic Domains

https://www.esiwace.eu/services/dyamond

9 Models: ICON, NICAM, MPAS, GEOS, FV3, SAM, UM, ARPEGE, IFS

- **GEOS Global Simulations**
  - 3km (c2880) 72-levels [*and 132-levels*]

- **Scale-aware convective parameterization**
  - Grell-Freitas + UW ShallowCu
  - *Additional 3-km cases with DeepCu disabled*

- **Cloud microphysics**
  - Single-moment GEOS microphysics
  - *Alternate convective scale GFDL cloud microphysics*

GEOS 3-km DYAMOND Simulation : August 2016
NASA GEOS Forecast Experiments

These forecast products are purely experimental and not to be used for any predictive or decision making purposes.

6km-132L Research Forecasts

00z, 06z, 12z & 18z:
6-hour Replay

00z & 12z:
10-day Forecast

Replay to near real-time GEOS analysis

Model produces the convective scale processes

7.5-hours on 15,552 Intel Skylake Cores
**NCCS Discover Scalable Unit Hardware Specifications**

<table>
<thead>
<tr>
<th>Scalable Unit 9</th>
<th>Scalable Unit 10</th>
<th>Scalable Unit 11</th>
<th>Scalable Unit 12</th>
<th>Scalable Unit 13</th>
<th>Scalable Unit 14</th>
<th>Scalable Unit 15</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer: IBM</td>
<td>Manufacturer: SGI</td>
<td>Manufacturer: SGI</td>
<td>Manufacturer: SGI</td>
<td>Manufacturer: SGI</td>
<td>Manufacturer: Supermicro</td>
<td>Manufacturer: Supermicro</td>
</tr>
<tr>
<td>91 Tflop/s</td>
<td>1,229 Tflop/s</td>
<td>683 Tflop/s</td>
<td>683 Tflop/s</td>
<td>723 Tflop/s</td>
<td>1,560 Tflop/s</td>
<td>1920 Tflop/s</td>
</tr>
<tr>
<td>4,480 Intel Xeon Sandy Bridge processor cores</td>
<td>30,240 Intel Xeon Haswell processor cores</td>
<td>17,136 Intel Xeon Haswell processor cores</td>
<td>17,136 Intel Xeon Haswell processor cores</td>
<td>18,144 Intel Xeon Haswell processor cores</td>
<td>20,800 Intel Xeon Skylake processor cores</td>
<td>25,600 Intel Xeon Skylake processor cores</td>
</tr>
<tr>
<td>IBM iDataPlex Compute Nodes</td>
<td>SGI C2112 Compute Nodes</td>
<td>SGI C2112 Compute Nodes</td>
<td>SGI C2112 Compute Nodes</td>
<td>SGI C2112 Compute Nodes</td>
<td>520 Supermicro FatTwin nodes</td>
<td>640 Supermicro FatTwin nodes</td>
</tr>
</tbody>
</table>

"Discover" supercomputing cluster: an assembly of multiple Linux scalable units built upon commodity components

- 6.8 PFlops
- 133,536 Cores
GEOS Footprint on NCCS Discover Supercomputer

FY 2019: GEOS-FP 12km 72 levels

Compute Capability:

- # of Cores at NCCS
  - 8,400 Cores (10%)
  - 30,212 Cores (35%)
  - 69,324 Cores (65%)

107,936 Cores
5.1 PF

General Science Dev GMAO Pre-Ops GMAO Ops

5 PFlops
GEOS-FP
12km 72L
4D Hybrid ENVAR

8,400 Haswell Cores

Throughput:
~100 days/day
4 hrs for 10-day fcst

~5.5 days/day
Cycled Ens Analysis

GEOS 12-km 72L
4D-Hybrid-EnvVar
32-Ensemble DA members

2019-05-10 00:00Z
2019 Sep 11
08:00pm EDT Wednesday

Outgoing Longwave Radiation (W/m²)

084 Forecast Hours
INIT: 20190101 00z
GEUS 1522_fp
GEOS Footprint on NCCS Discover Supercomputer

FY 2019: GEOS-FP 12km 72 levels

Compute Capability:

- # of Cores at NCCS:
  - 107,936 Cores
  - 30,212 (~26%)
  - 69,324 (~64%)
  - 8,400 (~8%)

- 5.1 PF

15,552 Skylake Cores

Throughput:

- ~26-days/day
- 7.5 hrs for 10-day forecast

GEOS 6-km 132L
Replay to GEOS-FP
Single Deterministic Forecast

GEOS-FP 12km 72L
4D Hybrid ENVAR

GEOS-FP 9-km 132L
Non-Hydrostatic

GEOS-FP Advanced Physics

GEOS-FP Coupled NWP
JEDI-DA

GEOS-FP 6-km 132L
Ensemble Prediction System
NCCS will fall ~10x short of science demands in 2025

15 PF Peak Capacity

This assumes constant funding levels and best guess at processor capability

## GEOS Footprint on NCCS Discover Supercomputer

**FY 2019: GEOS-FP 12km 72 levels**

<table>
<thead>
<tr>
<th>Compute Capability: # of Cores at NCCS</th>
<th>107,936 Cores</th>
<th>8,400</th>
<th>30,212</th>
<th>69,324</th>
</tr>
</thead>
<tbody>
<tr>
<td>General Science Dev</td>
<td>GMAO Pre-Ops</td>
<td>GMAO Ops</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **107,936 Cores**
- **5.1 PF**
- **30,212 Cores**
- **26%**
- **69,324 Cores**
- **64%**

### Discover Compute Capability By Fiscal Year

- **Peak**
- **Core Count**

#### Peak Capacity at ~15 PF in 2025

- **12km 4D EnVar**
- **3D-Hybrid**
- **50-km 3DVar**
- **25-km (FV3)**

#### Total Peak Capacity (PF)

- **200,000**
- **180,000**
- **160,000**
- **140,000**
- **120,000**
- **100,000**
- **80,000**
- **60,000**
- **40,000**
- **20,000**
- **0**

#### Total Core Count

- **200,000**
- **180,000**
- **160,000**
- **140,000**
- **120,000**
- **100,000**
- **80,000**
- **60,000**
- **40,000**
- **20,000**
- **0**

### PFlops

- **5 PFlops**
  - GEOS-FP 12km 72L
    - 4D Hybrid ENVAR
  - GEOS-FP 9-km 132L
    - Non-Hydrostatic
- **15 PFlops**
  - GEOS-FP Advanced Physics
- **20 PFlops**
  - GEOS-FP Coupled NWP JEDI-DA
- **30 PFlops**
- **50 – 100+ PFlops**
  - GEOS-FP 6-km 132L
    - Ensemble Prediction System
Impact of GEOS-FP Evolution on Expected Compute at NCCS

**FY 2021:** GEOS-FP 9km 132 levels

- Compute Capability: 140,792 Cores 8.6 PF
- 56,741 (~40% General Science Dev)
- 44,629 (~32% GMAO Pre-Ops)
- 39,422 (~28% GMAO Ops)

**FY 2023:** GEOS-FP 9km 132 levels Coupled DA

- Compute Capability: 149,632 Cores 9.8 PF
- 99,296 (~66% General Science Dev)
- 41,897 (~28% GMAO Pre-Ops)
- 8,439 (~6% GMAO Ops)

**FY 2025:** GEOS-FP 6km 132 levels Coupled DA

- Compute Capability: 193,920 Cores 15 PF
- 191,800 (~99% General Science Dev)
- 770 (~99% GMAO Pre-Ops)
- 1,150 (~99% GMAO Ops)

---

5 PFlops
GEOS-FP 12km 72L
4D Hybrid ENVAR

15 PFlops
GEOS-FP 9-km 132L
Non-Hydrostatic

20 PFlops
GEOS-FP Advanced Physics

30 PFlops
GEOS-FP Coupled NWP JEDI-DA

50 – 100+ PFlops
GEOS-FP 6-km 132L
Ensemble Prediction System
Achieving a 10-20x Speedup for GEOS by 2025

It will require a lot of ~2x gains…

- Aerosols & Chemistry
  - Simplified species list for GEOS-FP
  - Asynchronous transport on a reduced grid
  - Offload all aerosol & chemistry to GEOS-CF

- Hybrid multi-core
  - GEOS Physics (GPU enabled with PGI Cuda Fortran)
  - FV3 Dynamics – Domain Specific Language – GridTools or Kokkos or something else…

- Code refactoring
  - Not just refactor, redesign (algorithm development)

- Artificial intelligence
  - Replacing expensive parameterizations (cloud microphysics, chemistry, radiation…)
  - FV3 chemistry transport (corrective approach in PPM)
  - Data assimilation techniques

- Data handling, memory usage and I/O

- Ocean modeling, MOM6 optimization (community)
Active Development of FV3 into the Future

- GFDL and GMAO continue to actively develop FV3 for Exascale and beyond...
Active Development of FV3 into the Future

- GFDL and GMAO continue to actively develop FV3 for Exascale
- Adoption of Git by GMAO, GFDL, and NOAA EMC
  - FV3 as a shared repository (shared development)
  - Possibly further contributions from the wider community
  - Status...
    - GEOS now uses a fork of the communal FV3
Active Development of FV3 into the Future

- GFDL and GMAO continue to actively develop FV3 for Exascale and beyond
- Adoption of Git by GMAO, GFDL, and NOAA EMC
  - FV3 as a shared repository (shared development)
  - Possibly further contributions from the wider community
  - Status...
    - GEOS now uses a fork of the communal FV3

- Deployment on Amazon Web Services (AWS)
  - Provides simplified access to the broader community
  - Facilitates vendor benchmarking and optimization
Active Development of FV3 into the Future

- GFDL and GMAO continue to actively develop FV3 for Exascale and beyond
- Adoption of Git by GMAO, GFDL, and NOAA EMC
  - FV3 as a shared repository (shared development)
  - Possibly further contributions from the wider community
  - Status...
    - GEOS now uses a fork of the communal FV3
- Deployment on Amazon Web Services (AWS)
  - Provides simplified access to the broader community
  - Facilitates vendor benchmarking and optimization
- FV3 with Domain Specific Languages (DSL)
  - One element of major push for GCM as a whole
    - GPGU’s are on the critical path for performance
  - Using DSLs to enable performance portability
    - Exploring multiple options:
      - GridTools, Kokkos, OpenACC, CUDA, ???
    - Most options involve a migration towards C++ from Fortran
  - Planning to hire GPU developers in the near term in conjunction with NASA NCCS and NOAA GFDL developments
GEOS Collaborative Physics Development

Advanced physics development around the FV3 dynamical core
implementing community physics code as connected ESMF/MAPL components

- Scale aware convection parameterization (Grell-Freitas)
- Shallow cumulus parameterization (UW, Park-Bretherton)
- Unified boundary layer schemes (EMDF or SHOC)
- 2-Moment cloud microphysics (Morrison, Gettelman, Barahona)
- Warm cloud microphysics (GFDL, Thompson or MG3)
- Aerosol aware cloud microphysics (MAM)
- High-performance radiation (RRTMGp)
- Gravity Waves & Stratosphere (NWRA: Alexander & Holt & NCAR: Bacmeister)

Common Community Physics Package (CCPP) at NOAA DTC
- The CCPP framework based on ‘suites’ for Unified Forecast System at NOAA
- Close collaboration with the NOAA Earth Prediction Innovation Center (EPIC)

https://ufscommunity.org

Global Modeling and Assimilation Office
gmao.gsfc.nasa.gov
Up to now data assimilation systems have been developed in parallel for the different models, with various levels and approaches for coupling between data assimilation and model components.
A key component of JEDI is the Unified Forward Operator (UFO), which introduces standard interfaces for observation operators that link the model and observation worlds. The UFO accommodates the assimilation of observations for coupled or uncoupled models in an analogous (unified) manner.
Moving toward a JEDI-based GEOS system for coupled DA

- **New Moist Physics**
  - Ocean Interface
  - EnKF SPPT
  - New LSM

- **GMI All-Sky Radiances**
  - Updated Radiation
  - and Convection

- **Hybrid 4D-EnVar**
  - 13-km L72
  - Aerosols
  - AO Skin SST

- **GEOS FP weather**
  - Jan 2017

- **GEOS S2S seasonal**
  - Oct 2017

- **New MoM5**
  - L72
  - CICE4
  - UMD LETKF

- **New S2S v2**
  - MOM5 0.5° L40

- **New S2S v3**
  - MOM 0.25° L50
  - Catchment-CN
  - Salinity

- **S2S v4**
  - July 2019
  - mid 2021
  - O:H4DEnVar (JEDI)

- **GEOS AOGCM**
  - July 2018
  - mid 2020
  - 132 Levels
  - New Microphysics
  - All-Sky MHS, AMSUA

- **S2S v4**
  - Oct 2017

- **MERRA-2 Ocean Product**
  - July 2018
  - mid 2020

- **GEOS CDAS**
  - Jan 2017

- **GEOS S2S**
  - Jul 2018
  - mid 2019

- **GEOS AOGCM**
  - Jul 2018

- **JEDI ODAS**
  - MOM6 L72
  - O:H4DEnVar

- **S2S v4**
  - Jul 2018
  - mid 2019
  - O:H4DEnVar (JEDI)

- **S2S v4**
  - Jul 2018
  - mid 2020
  - A:H4DEnVar (JEDI)

- **GEOS Unified Coupled System (JEDI-based)**
  - **NWP**
  - **Reanalysis**
  - **S2S Prediction**
Questions?

GMAO
https://gmao.gsfc.nasa.gov

NCCS
https://www.nccs.nasa.gov

High-End Computing Program
https://www.hec.nasa.gov