



# CTM's, ESMF, and Shared Software (Oh my!)

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GMI



# Outline

- New study/project commissioned by NASA HQ to determine feasibility and cost of creating a framework tailored for CTM collaboration via ESMF.
- Core team software initiatives for GMI
  - Redesign of chemical mechanism
  - Emphasis on unit and system testing
  - New directory structure



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# CTM Framework Project

- Motivation - exploit advances in technology, esp. ESMF.
  - Facilitate collaboration among various CTM investigators
  - Rapidly propagate innovations between models
  - Reduce collective long-term cost of software development and stewardship
  - Support GMI's mission to understand consequences of varying implementations and data sets.
  - Enhance software flexibility, maintenance, performance, blah, blah ...



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# Road Map

- Identify resources to perform survey
  - Software Architect - Brice Womack (SIVO/NGC)
  - Rough estimate of 2 months to perform survey and preliminary analysis. Starting *now*.
- Interview investigators, developers, and users from designated CTM activities:
  - GMI, GEOS-CHEM, GOCART, “the model” ...
  - Subject to HQ priorities and time constraints
- Identify common functionalities/components as well as fundamental differences among models. E.g.

Meteorological Field  
Transport  
Convection  
Wet/Dry Scavenging  
Boundary layer

Chemistry Mechanism  
ODE Solver  
Microphysics, Aerosols  
Diagnostics  
Lightning



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# Road Map (cont'd)

- Propose a CTM framework (i.e. request \$\$)
  - Standard suite of CTM components and couplers
  - Conventions for interfaces
  - Reference implementations
  - Estimate cost and level-of-effort to deliver
  - Also quantify long-term benefits to NASA/community
- Establish community software repository for sharing components.
  - MAP requirement for SIVO
  - CTM efforts can focus on aspects that make them unique.
  - SIVO will only provide *direct* software management for GMI



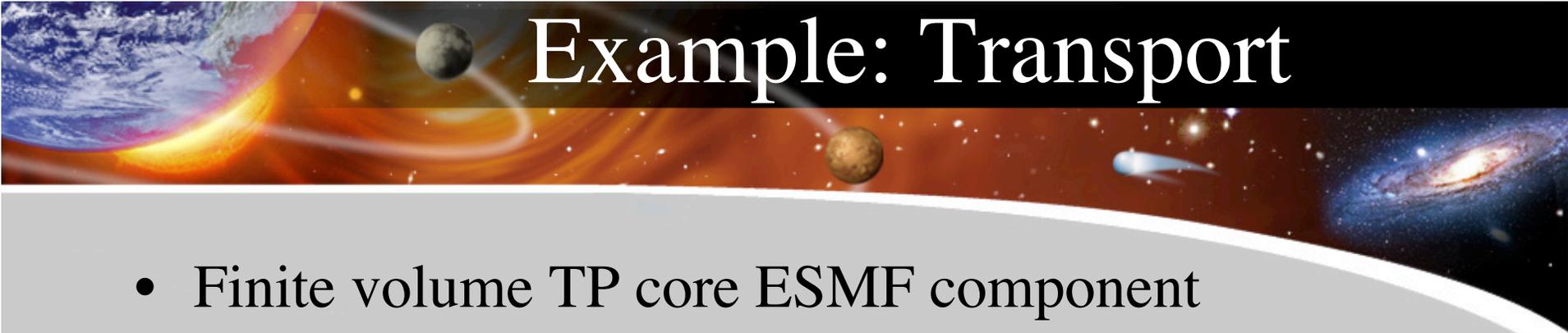
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# Enabling Technology: ESMF

- ESMF provides level of abstraction to couple multiple components in a manner independent of detailed implementation.
  - “Gridded” components specify
    - “import” and “export” states for exchanging data
    - “init”, “run” and “finalize” methods
  - Coupler components specify how to translate data between components.
- ESMF enables creation of simple couplers
  - Regridding services with various interpolation schemes including flux conservation.
  - Does not directly assist with units, but at least provides mechanism to assign physical units to data.





# Example: Transport

- Finite volume TP core ESMF component
  - Under development within GMAO, with long-term support from multi-agency project.
  - After initial investment to couple given CTM to FV component, subsequent FV updates can be incorporated with no modifications to other components.
    - Couplers may need to be modified for nontrivial FV changes such as “cubed sphere” implementation under development.
  - CTM’s can inherit FV parallelism and performance
    - Unfortunately incompatible with current GMI decomposition.



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# Example: Met Fields

- Leverage ESMF grid capabilities to obtain data interpolated to the relevant grid and units.
- Serve meteorological fields via abstract mechanism
  - Significantly reduce the dependency of other CTM components on the specific met fields.
- Reduce cost for CTM models to handle various met fields: *implement once, share often.*



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# Chemistry and ESMF

- Create an ESMF component for exporting GMI Chemistry into GMAO GEOS-5
  - Create standalone driver. (J. Kouatchou)
    - Identify import and export data
    - Bootstrap via data files that capture state info
    - Use driver to establish canonical verification tests of chemistry functionality.
  - With confidence based upon these tests, *refactor* chemistry produce modular component
    - All data exchanges must be via explicit argument lists
    - I.e. common blocks must go ...
  - Create ESMF wrapper (the easy step)



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# While we're looking ...

- Other desirable enhancements to GMI chemistry
  - Allow a single build/executable to handle any specific mechanism: trop, strat, combined
  - Perhaps even use multiple mechanisms in distinct portions of the domain during a single experiment.
  - Isolate SMVGEAR solver from mechanism
    - SMVGEAR is primarily a generic solver for stiff ODE's, but has some hardwired aspects to support chemistry.
    - Solver will become a component unto itself - possibly ESMF
    - Enable investigation of alternative solvers
  - Potentially performance improvement
    - Existing implementation optimized for vectors
    - Possibly not ideal for cache based memory systems
    - Fringe benefit - better control of “strong” reproducibility



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# New Implementation

- Ground-up redesign base on OO
  - Strong encapsulation - F90 modules, derived types
  - I.e. no common blocks or even module variables
- Using recently developed SIVO tool: Funit
  - Fortran based unit-testing framework analagous to Java's Junit
  - Test-driven development (TDD) yields better predictability and cleaner, more robust implementation.
  - Yes - this is a blatant plug for TDD and Funit.
- Absorbing KMG capabilities within Fortran base
  - Unfortunate consequence of requirement for run-time flexibility
  - Will support same file format for specifying mechanism.
  - Parser is 80% complete (*really!*)



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# New Implementation (cont'd)

- Most of the detailed lower-level code can be reused as-is or with little modification.
  - Numerical expressions and inner loops not targeted
  - Probably will convert to free format in any event
  - Access to data structures will be very different
- Test based verification
  - As with ESMF aspect, tests will be constructed which capture existing behavior of chemistry.
  - Tests will grow to become new verification suite for GMI.



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# New Directory Structure

- Current GMI source directory tree reflects LLNL heritage that is not optimal for GMI
  - Important GMI components relegated to deep corners of the tree
  - Needs to be modified to support modular components.
- New tree patterned after GMAO GEOS-5 (A. da Silva)
  - Should help facilitate sharing of components with GMAO
    - GMI Chemistry
    - FV TP core
- Will not affect official GMI releases until GMI 3.0



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