Preliminary Information Collection and Analysis for Earth System Model Framework

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Outline

- Current climate models
- Existing frameworks
- Prototyping of strawman
- Unsolved questions
- Summary

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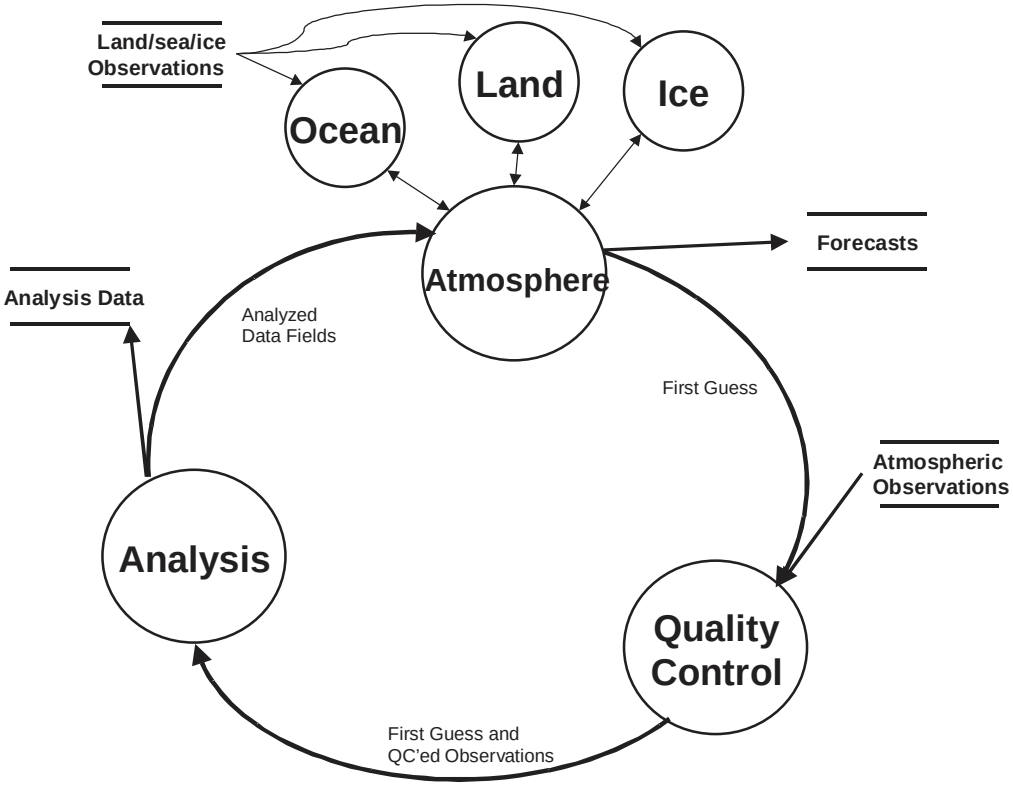
Review Current Climate Models

- Broad review of Earth Science numerical modeling and data analysis activities
  - Data Assimilation Office (DAO)
  - National Centers for Environmental Prediction (NCEP)
  - NASA Seasonal to Interannual Prediction Project (NSIPP)
  - Geophysical Fluid Dynamics Laboratory (GFDL)
  - National Center for Atmospheric Research (NCAR)
- Examine the most recent operational/production software versions of the global data circulation models and data analysis schemes and summarize:
  - Major modules and data flows
  - Major data structures and interface methods
  - Regions of parallelization
  - Programming languages and device dependencies
  - Functional overlap with other products
  - ESMF framework Issues

Climate Model and Data Assimilation Cycle



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Climate Model Summary

- In general *communication* is not good across five organizations. Their application models are considerably different , especially in the code structure. There is little or no documentation for codes and algorithms.
- Organizations are reusing application models through *reprogramming*.
- All codes are written in *FORTRAN*: A large amount of legacy FORTRAN 77 with subsequent development in FORTRAN 90
  - Current re-writes of DAO and NSIPP software heavily modified to take advantage of many FORTRAN 90 capabilities
- *MPI* and domain decomposition are used in most of the application models.

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Review Existing Frameworks

- **Detailed survey and analysis**
  - Overture
  - POOMA
  - GEMS
  - NCAR Flux Coupler
  - Cactus
  - UCLA Data Broker (DDB)
- **Limited Survey:** ALICE, PAWS, PETsc, ROOT, Grace, …
- **Very Limited Survey:** CAT,CCAT, DAHG, Globus, GlobalArrays, ISIS++, Kelp, PADRE, PAWS, PETsc, SAMRAI, Java, CC++, Charm++, CINT,HPC++, HPF, Java, Mentat, MPC++, Python, SILOON, Tcl/Tk, Titanium, ZPL, and others (links provided in web-site) …..

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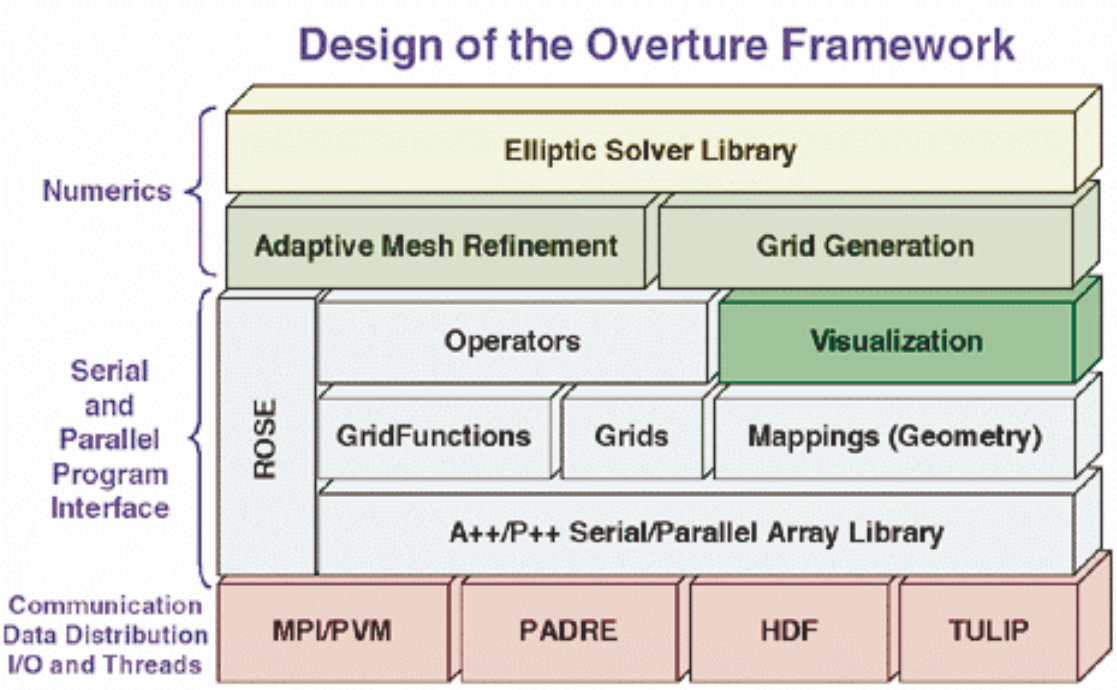
Overture (LLNL and LANL)



Overture provides an object-oriented framework for solving partial differential equations in serial and parallel computing environments.

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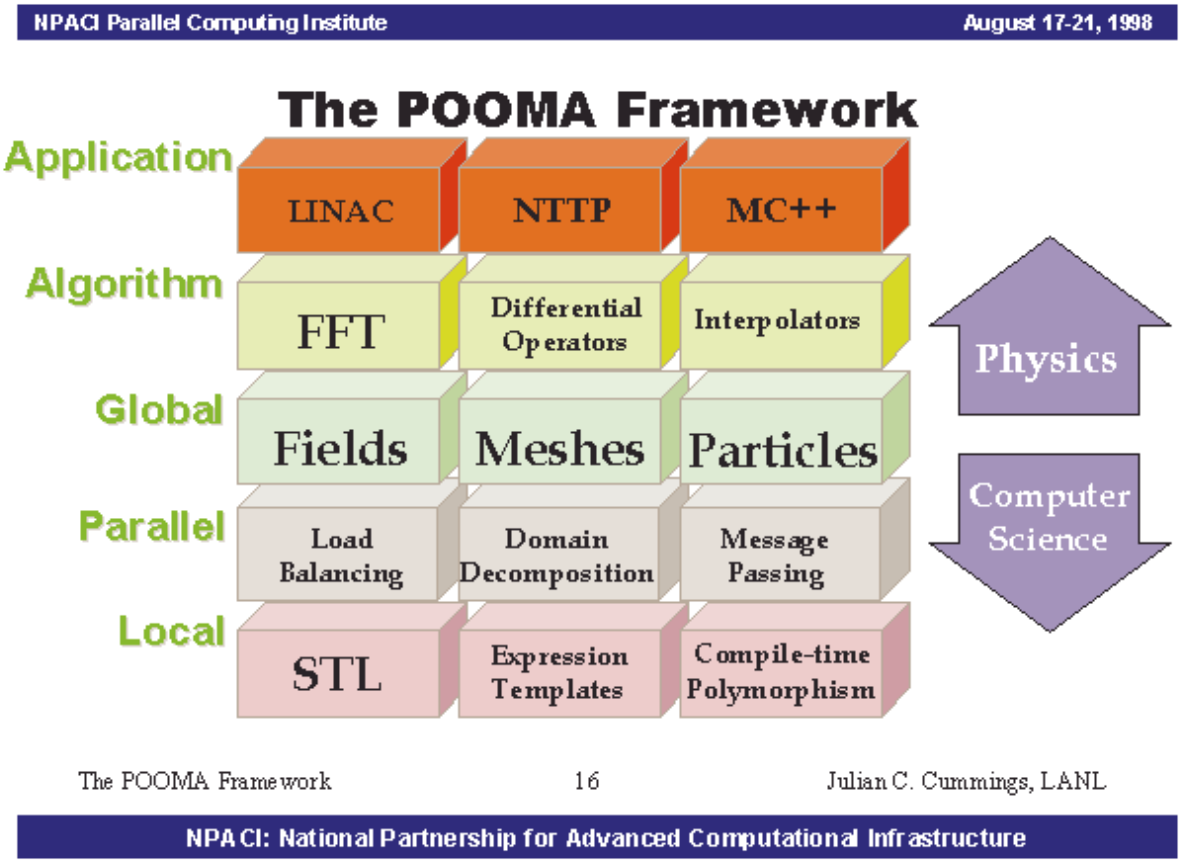
POOMA (LANL)



POOMA provides an object-oriented framework for applications in computational science requiring high-performance parallel computers

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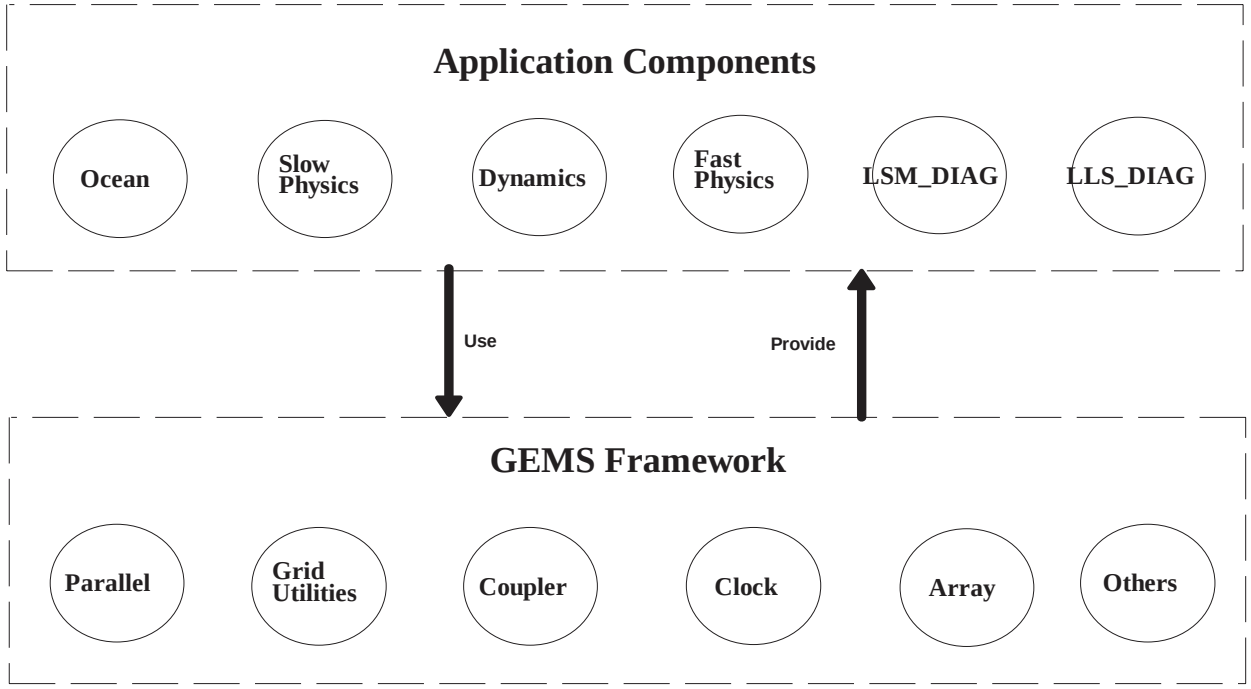
GEMS (NSIPP)



GEMS provides tools for climate modeling components, which are modularized with F90

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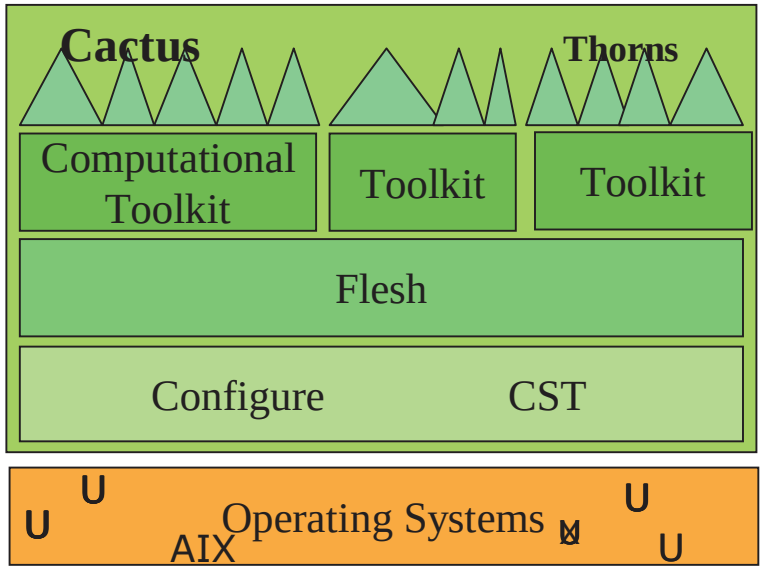
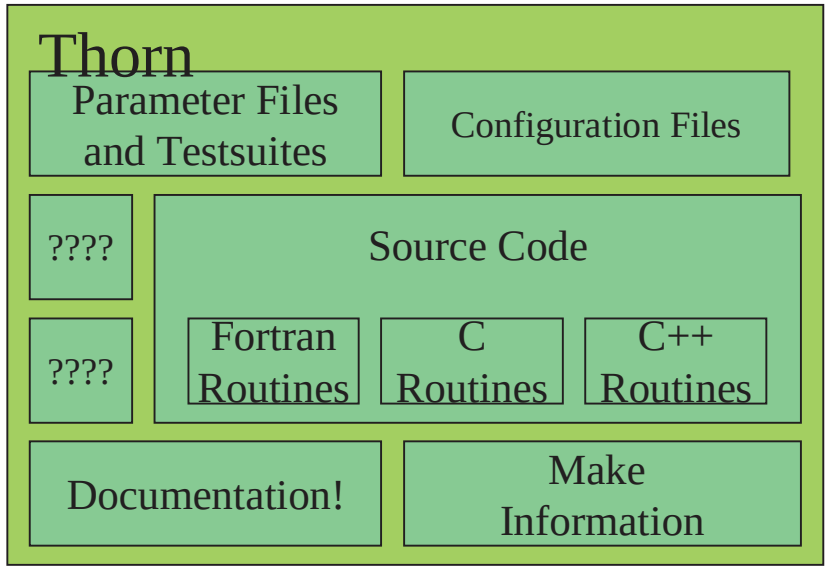
Cactus: (Max Plank Institute, NCSA)

System Architecture

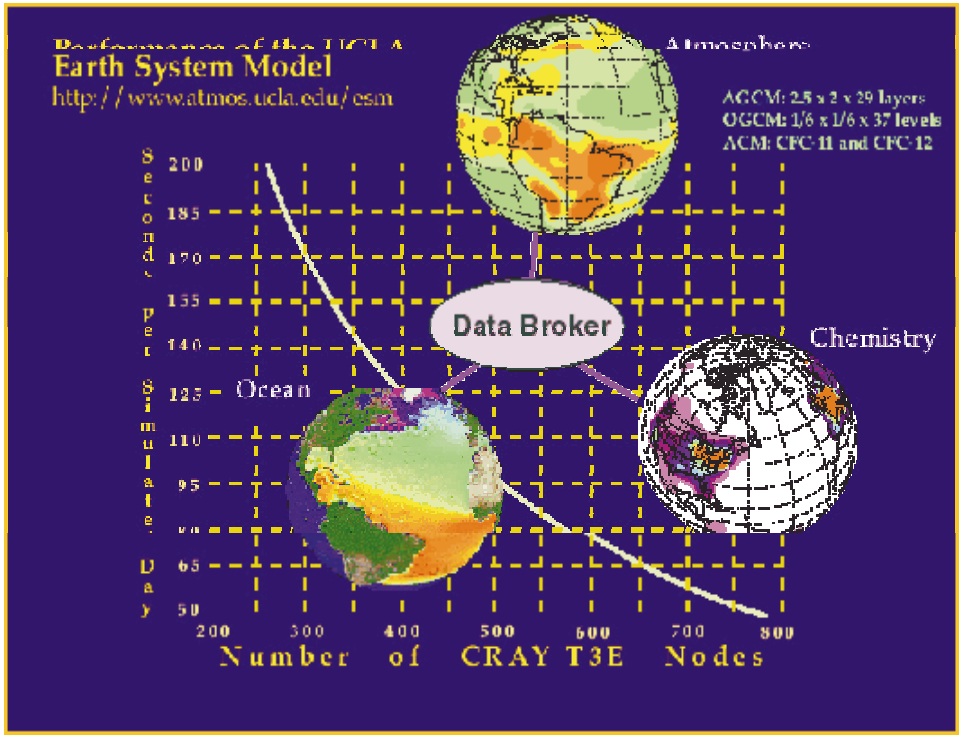


Thorn Architecture



Cactus is a component-level framework, written in C, C++, and Perl. It can support the thorn written in Fortran, C, and C++. Its parallel communication toolkit enables the code portable from single-processor to multi-processor computers.

DDB – Distributed Data Broker (UCLA)



DDB provides data interchange services between multiple climate-related models.

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Motivation for ESMF (from the CAN)

- Reduce the *time* required to develop and modify application codes for research and production
- Structure systems for better *management* of evolving and increasingly complex codes
- Enable software exchange and *interoperation* between major research centers
- Foster *reusability* among software components and *portability* among high-end computing architectures

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Earth Science Community Needs

- Develop *data-exchange* libraries to couple existing ESM components (e.g. ocean, land, ice, atmosphere)
  - Similar to UCLA/Distributed Data Broker and NCAR/Flux Coupler but more flexible interface and extensible capabilities
- Develop *tools/utilities* to facilitate developing new ESM components and sub-components (e.g. radiation, cloud)
  - Similar to GEMS, Overture, POOMA
    - Parallel communication
    - I/O
    - Grid generation, transformation utilities
    - Calendar and timer
    - Performance optimization

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Constraints for ESMF

- ESMF needs to serve the missions of five Federal agencies (NASA, DOE, NSF, NOAA, DOD)
- Poor communication among various research groups
- Considerable legacy *FORTRAN* code
- Ability to continue to apply expertise to write new FORTRAN code
- Object oriented concepts and languages are not familiar to researchers

Correlation of Frameworks with Community Needs: Each framework has both desirable and undesirable characteristics.

CACTUS

Desirable: Next best example of comprehensive community framework, more easily adapted to climate modeling in FORTRAN than ROOT.

Undesirable: Coupling function may need adaptation, awkward scheduling**.**

Overture

Desirable: Powerful framework shows that the combination of PDE solver and visualization is possible with OOD.

Undesirable: Lacks utilities for earth system modeling, team support is limited.

POOMA

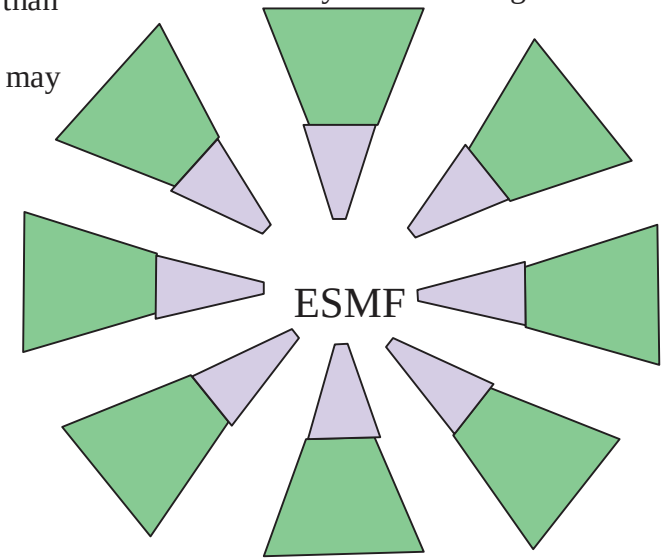
Desirable: Portable across parallel, non-parallel platforms with OOD.

Undesirable: Too complex, team support uncertain.

ROOT

Desirable: Best overall example of community-level framework

Undesirable: C++, not specifically adapted to earth system modeling.



DDB

Desirable: Excellent coupler architecture

Undesirable: Maturity, documentation, number of users, organizational support

FMS

Desirable: Basic utilities for climate modeling

Undesirable: Maturity, documentation, number of users, organizational support

GEMS

Desirable: Basic utilities for climate modeling

Undesirable: Maturity, documentation, number of users, organizational support

Flux Coupler

Desirable: Basic coupling utilities, documentation, organizational support, number of users

Undesirable: Poor coupler architecture

Framework Summary: Observations

- No single existing framework can be used without change to construct the ESMF
  - All incorporate *some* desirable features
  - All lack *some* desirable features
- Most of frameworks intend to encapsulate parallel programming and isolate machine-dependent parts.
- Majority of Climate community code written in FORTRAN 77/90
  - Most researchers do not want to migrate to other languages (e.g., C++)
  - C++ performance relative to FORTRAN questioned
  - FORTRAN is not extensively used outside the research community

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Framework Summary: Observations (Cont'd)

- The most powerful frameworks identified (ROOT and Overture) are written in C++
  - No equivalently powerful frameworks written in FORTRAN
  - There are, however, many useful FORTRAN libraries
- FORTRAN is missing two key OO features available in C++ and Java: inheritance and polymorphism
  - FORTRAN 2000 is scheduled to have these features in a few years
- C++ can be combined with FORTRAN in a limited way
  - No standard way of having a C++ program read dynamically allocated FORTRAN 90 data structures
  - Problem will still exist with FORTRAN 2000

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Framework Summary: Beliefs and Opinions

- OO design and algorithmic design are **complements** to one another, not competitors
  - Some system components are better expressed with algorithms
  - Some system components are better expressed with objects
- Most complex systems incorporate complementary components:
  - Microsoft EXCEL: Data visible (spreadsheet) and algorithms visible (Visual Basic Macros)
  - Overture framework: OO high-level structure. Some of the linear solvers for PDEs are written in FORTRAN and are legacy codes.

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Frameworks Summary: Beliefs and Opinions (Cont'd)

- Physics focuses on algorithmic expressions, which may be best represented by a functional language such as FORTRAN.
- Frameworks focus on relationships between participating objects (models), which are best represented by an object-oriented language such as C++, Java, or Smalltalk.
- It may be that in the climate community, the issue of language, instead of evolving properly into a question regarding the proper blend of complements (OO and algorithmic expression, Java and FORTRAN, etc.) has evolved into a competition between complements (FORTRAN or C++, etc.)
- The issue of language is absolutely central to the design of the ESMF.

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Framework Summary: Beliefs and Opinions (Cont'd)

- OO design is critical for building a flexible and extensible ESMF meeting CAN requirements
  - Inheritance and polymorphism are the important OO features that are building blocks of a comprehensive framework
  - Inheritance is a way of distributing capabilities to models that minimizes the programming burden on the researchers.
  - Polymorphism provides a simple mechanism for researchers to modify models for various situations.
  - Together, inheritance and polymorphism reduce cost and error. They provide clear hierarchical structure for a complex problem

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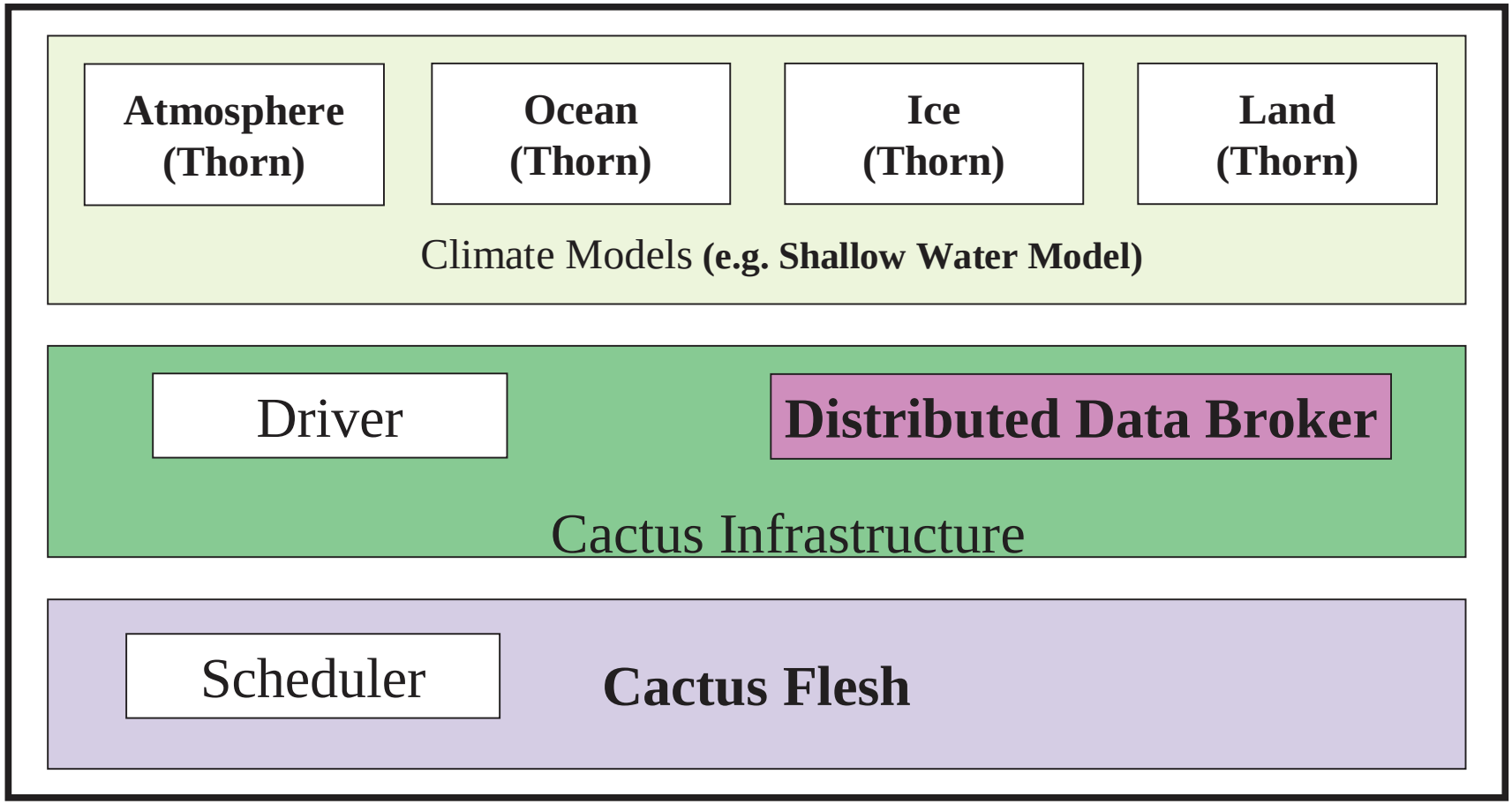
Strawman Design For ESMF

Language, Infrastructure, and Reuse



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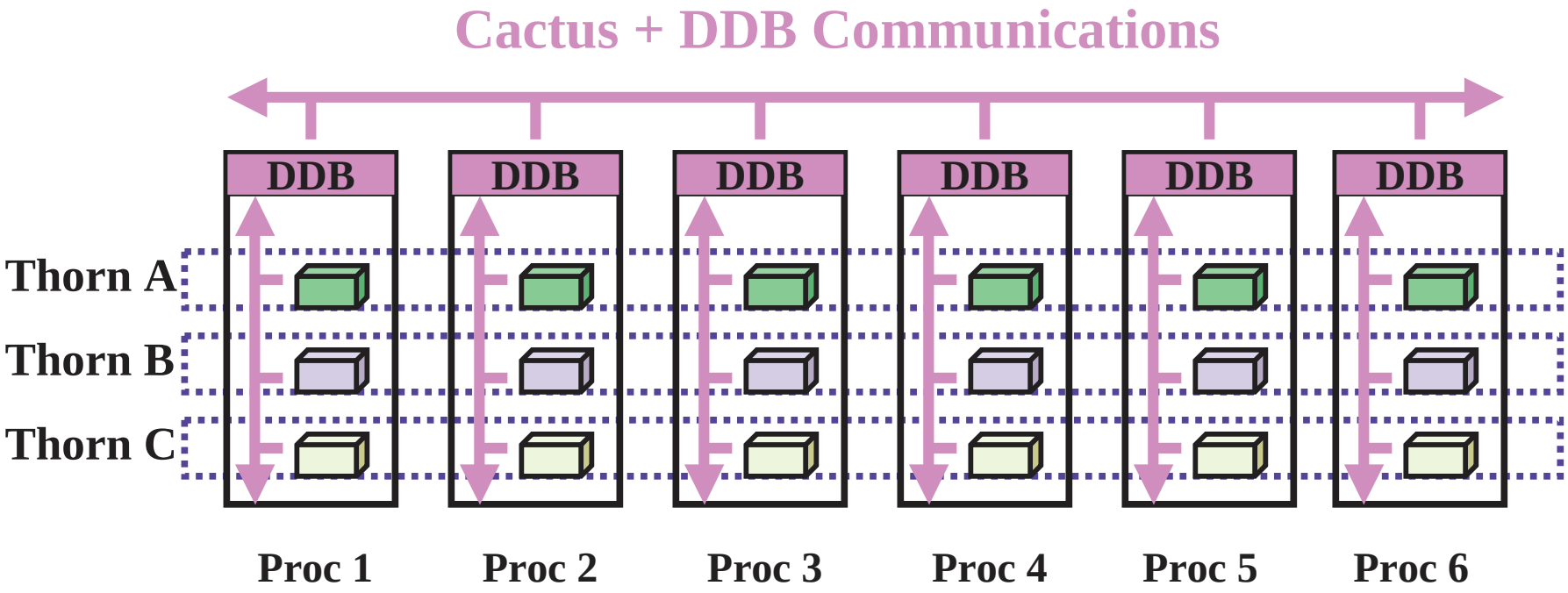
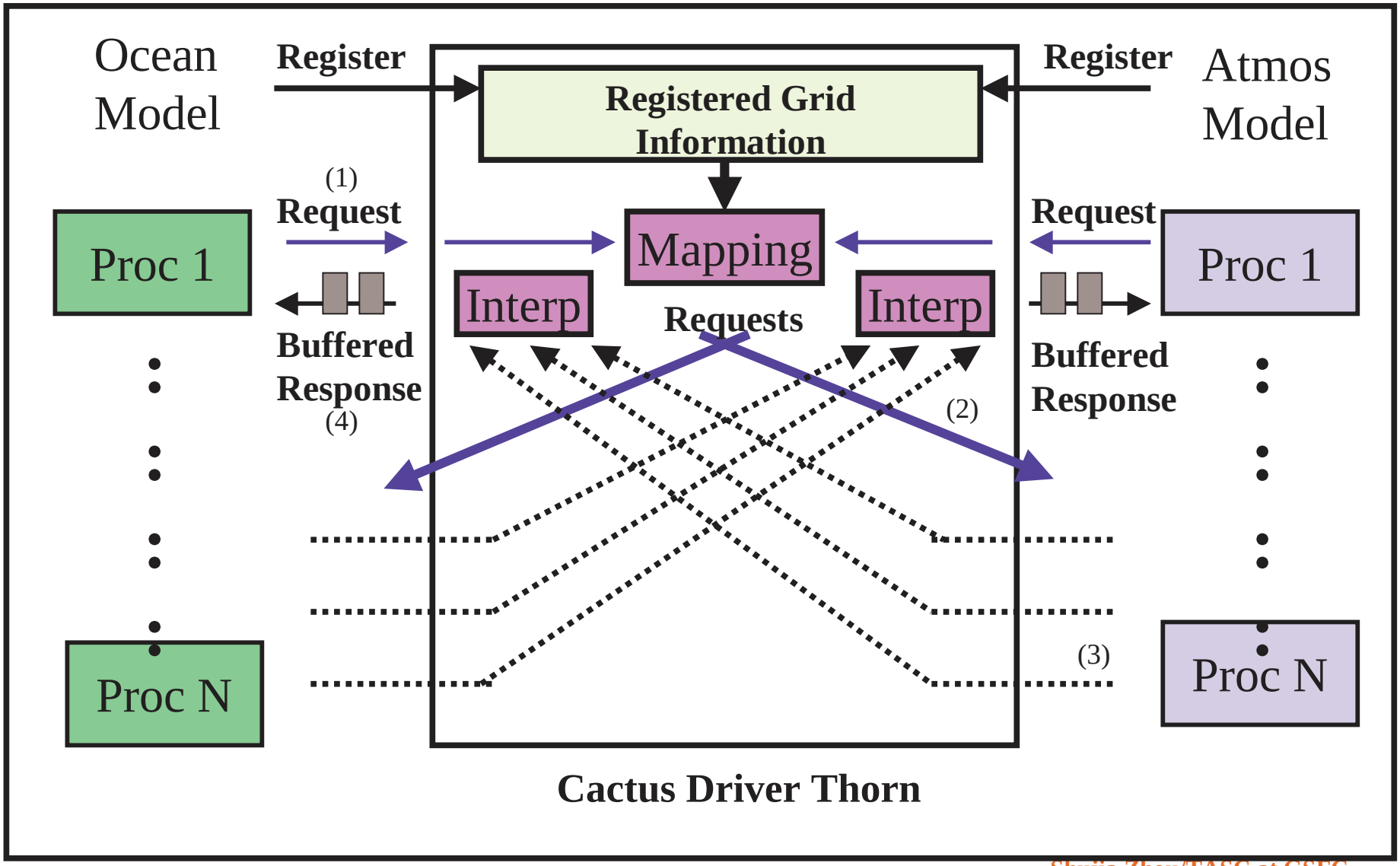
Integrate DDB with Cactus to Support Data Exchange



Integrate DDB with Cactus to Support Data Exchange (Cont'd)



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Unsolved Questions

- How to develop a flexible interface for the community framework to support various current and future applications/models?
- How to deal with legacy Fortran codes while introducing new languages and paradigms such as object-oriented programming?
- ESMF is a framework for scientific research, which is constantly evolving. Industrial products are based on relatively mature technology. How much "software engineering principle" shall be applied?

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Summary

- Developing ESMF will be very interesting and challenging (the sociology more than the technology)
- Welcome ideas and suggestions
- More information on our survey and analyses can be found at http://esdcd.gsfc.nasa.gov/ESS/esmf_tasc/index.html

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List of Potential Collaborations

- Expert support for Investigator Team Design Reviews
- Propose to ESS “Plug-in” and “Open Source” solicitations
- Some ESS Round-3 Investigators should participate in the next Frameworks Workshop