Turning Lessons Learned Into Guiding Principles: Ideas for Reinventing the Earth System Modeling Enterprise

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Theoretical Division
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The ESM enterprise is ripe for a transformation — a transformation in culture, norms, and best practices.
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Creating the conceptual model of the earth system is a very different activity than producing performant code.

earth scientists — computational scientists

The gap between these two domains of expertise has been widening and will continue to widen.

The era of a typical scientist having sufficient expertise in both domains is long past, but our culture, norms, and best practices have not changed accordingly.

ESM continue to grow in complexity and risk becoming increasingly fragile in ways that impede our productivity and limit the impact of our work.
Different phases of the ESM enterprise:

- **design document**
  Specification: a textual description of the why, what, and how of some aspect of an ESM (physical process, computational algorithm, infrastructure, etc.).

- **prototype algorithm**
  A realization of the design document as software.

- **unit and test cases**
  Demonstrations that the software is doing what is described in the design document (verification) and appropriately represents some physical process (validation).

- **production software**
  A HPC performant version of the prototype algorithm.

- **simulation data**
  Output (usually in the form of netCDF files) produced by executing the software.

At least in concept, most in the community agree that each of these elements are important. The ordering of the elements and emphasis of each element varies significantly across the community.
In 2010, we had a chance to start over with the Model for Prediction Across Scales project.

This is a joint LANL-NCAR model development project to build a suite of unstructured-grid earth system system components based on a shared software framework.

What did we do right?

What would we do differently?
What did we see as problems in 2010?

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What did we do right?

auto-generate nearly all Fortran code from XML, Python, and C
git, Github, and adoption of git feature branch workflow
transparency — model development discussion on Github forum

a project-wide and uniform workflow for model development:
  • design documents
  • software and test case coherency
  • proof of correctness — V&V
  • continuous testing harness under revision control
  • provenance — reproducibility of simulation data
  • project review and fulfilling pull requests
We made dramatic changes in how we develop models ....

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**emphasis**
same scientists
Design documents: Our biggest success.
(And our biggest missed opportunity.)

Chapter 1

Summary

The purpose of this section is to summarize what capability is to be added to the MPAS system through this design process. It should be clear what new code will do that the current code does not. Summarizing the primary challenges with respect to software design and implementation is also appropriate for this section. Finally, this statement should contain a general statement with regard to what is “success.”

Chapter 2

Requirements

2.1 Requirement: XXX

Date last modified: 2011/01/05
Contributors: (add your name to this list if it does not appear)

Each requirement is to be listed under a “section” heading, as there will be a one-to-one correspondence between requirements, design, proposed implementation and testing.

Requirements should not discuss technical software issues, but rather focus on model capability. To the extent possible, requirements should be relatively independent of each other; thus allowing a clean design solution, implementation and testing plan.

Chapter 3

Algorithmic Formulations

3.1 Design Solution: XXX

Date last modified: 2011/01/05
Contributors: (add your name to this list if it does not appear)

For each requirement, there is a design solution that is intended to meet that requirement. Design solutions can include detailed technical discussions of PDEs, algorithms, solvers and similar, as well as technical discussion of performance issues. In general, this section should steer away from a detailed discussion of low-level software issues such as variable declarations, interfaces and sequencing.

Chapter 4

Design and Implementation

4.1 Implementation: XXX

Date last modified: 2011/01/05
Contributors: (add your name to this list if it does not appear)

This section should detail the plan for implementing the design solution for requirement XXX. In general, this section is software-centric with a focus on software implementation. Pseudo code is appropriate in this section. Links to actual source code are appropriate. Project management items, such as svn branches, timelines and staffing are also appropriate.

How do we typeset pseudo code?

verbatim?

Chapter 5

Testing

5.1 Testing and Validation: XXX

Date last modified: 2011/01/05
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How will XXX be tested? i.e. how will we know when we have met requirement XXX. Will these unit tests be included in the ongoing going forward?
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Pull requests should include a design document. On average, the project produced about 10 design documents per year.
Why were design documents such a success?

- Think - Write - Discuss - Code - Test.
- Lots of people will read a text document.
- Good ideas are easy to incorporate.
- Author(s) not yet tied to code.
- Provides an anchor for when things go wrong.
- Turns a cost (documentation) into an investment.
- We now spend very little time “searching for bugs.”
- Empowering.
Our second most successful decision: forcing coherency between model and test cases at every commit

**unit and test cases**
Demonstrations that the software doing what is described in the design document (verification) and appropriately represents some physical process (validation).

**production software**
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test cases auto-configured from XML.
### Where did we come up short?

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Having the design documents in a separate repo made is hard to maintain coherency between design and software. We do not track prototype algorithms.
Risks in front of us.

Disruption in the computing ecosystem ....
- Cori / KNL
- Summit / GPU
- Cloud computing / Xeon
- Aurora / World’s fast machine in 2021 / ??
- Los Alamos / ARM?

How do we get ~1M lines of code to be performant on such a wide diversity of computing architectures?
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Fragility due to being overwhelmed by model complexity ….
If I had it to do over again ….

**earth scientists**

An immersive, self-contained, and complete description of the ESM under revision control.

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**computational scientists**

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**auto-generate**

**simulation data**
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If I had it to do over again ….

Open development from day 1. (“Head” is visible to world.)
Clearly define and maintain a very high bar for the consideration of pull requests.
Entrain the best ideas (and developers) from around the world.
Work with journal editors to connect manuscripts to a hash (DOI).
(Imagine a world where all ESMs were open development ….)

**Elements of a pull request**

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Adopting more professional software practices will improve our productivity and impact.

Changing “how we do business” has the potential to reinvent the ESM enterprise.
Embrace coupled data assimilation from the outset.

Initialization of High-Resolution Earth System Models
Rockville, Maryland
April 9-10, 2018

Jointly produced by DOE and NOAA.
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**same scientists**
Southern Ocean refined 60 to 6km mesh

A variable-resolution mesh with 6 km grid cells in the Southern Ocean

- Effects of eddies are well resolved in Southern Ocean
- Cost of ocean is ~3.5 times less than global high res.
- Domain includes Antarctic ice shelf cavities

<table>
<thead>
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<td>Low: EC60to30</td>
<td>0.2 million</td>
</tr>
<tr>
<td>Refined: SO60to6</td>
<td>1.1 million</td>
</tr>
<tr>
<td>High: RRS18to6</td>
<td>3.7 million</td>
</tr>
</tbody>
</table>

Standard low resolution
30-60km cells

Refined Southern Ocean
6km

Effect of eddies are well resolved in Southern Ocean
Cost of ocean is ~3.5 times less than global high res.
Domain includes Antarctic ice shelf cavities
Ice cavities are included in our coupled simulations.

Overall, the simulation of T and S on ocean floor is improved by including ice shelf cavities.

Note: color bar measures bias.