Optimized Infrastructure for the Earth System Prediction Capability

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Award Number: N00014-13-1-0508
http://www.earthsystemcog.org/projects/espc-infrastructure/

LONG-TERM GOALS

The Earth System Prediction Capability (ESPC) interagency program was established in 2010 as an effort to improve collaboration across the federally sponsored environmental research and operational prediction communities. The ESPC goal is to coordinate scientific development and operational implementation of improved global prediction at the weather to climate interface. Part of the ESPC role is to advocate for and support the basic foundations of modeling and data systems, such as the computational efficiency of models and common coupled system architectures.

The *Optimized Infrastructure for ESPC* (*OI for ESPC*) project is working to advance the computational foundations of ESPC through three integrative activities. These activities are designed to leverage numerical libraries across agencies; to explore the impacts of emerging computing platforms on coupled model infrastructure; and to reconcile conventions across different model architectures. The activities are serving as a starting point for a broader effort funded through the 2013 NOPP program *Advancing Air-Ocean-Land-Ice Global Coupled Prediction on Emerging Computational Architectures* (AOLI).

OBJECTIVES

1. **Update Numerical Libraries in ESMF**. The Earth System Modeling Framework (ESMF) is widely used in the ESPC community for building and coupling models. We will adapt MOAB, a finite element mesh package in active development at the University of Wisconsin and Argonne National Laboratory, for use as an ESMF computational kernel. The intent is to evaluate MOAB as a replacement for the native ESMF implementation of finite element mesh software. The framework uses this mesh software to create a unified representation of structured and unstructured grids, and define operations that work across grid types. The desired outcome is an immediate boost of new features in ESMF, and in the longer term, an opportunity to leverage the work that goes into ongoing functions and optimizations in MOAB and associated DOE libraries.

2. **Optimize Component Architecture for GPUs**. We will prototype a set of mechanisms that enable a component framework to optimize for accelerators, and explore how accelerators may affect mapping of components to resources. The product will be a code consisting of sample or toy components with representative operations. The intent of this research is to inform both infrastructure development and optimizations undertaken by ESPC modeling teams.

3. **Couple HYCOM to CESM**. We will work with developers of the HYbrid Coordinate Ocean Model (HYCOM) to couple it to the Community Earth System Model (CESM). This will enable HYCOM to be evaluated in many new coupled configurations. The activity will also define a mapping between the different coupling rules and conventions implemented in HYCOM and CESM. HYCOM uses a standard ESMF-based interface developed by a NOAA and DoD consortium (the National Unified Operational Prediction Capability, or NUOPC conventions), while CESM has its own native format based on the Model Coupling Toolkit (MCT). This is an important exercise because that mapping will apply not just to this coupling, but will provide insight into how any components that use the NOAA/DoD interface can be coupled into a CESM-based system, and vice versa.

APPROACH

Team members hold weekly telecons to discuss plans and progress. Participants include both technical and scientific team members, below:

Argonne National Laboratory/University of Chicago/University of Wisconsin: Rob Jacob, Jayesh Krishna, Tim Tautges

Florida State University: Alexandra Bozec, Eric Chassignet

NCAR: Jim Edwards, Mariana Vertenstein, Tony Craig

NASA Jet Propulsion Laboratory: Peggy Li

Naval Research Laboratory: Alan.Wallcraft

University of CA San Diego: Caroline Papadopoulos, Julie McClean

University of Colorado/NOAA: Cecelia DeLuca, Kathy Saint, Gerhard Theurich, Fei Liu, Bob Oehmke, Walter Spector

University of Miami: Ben Kirtman

Above are subscribed to an espc_tech@list.woc.noaa.gov mailing list used for organizing the calls.

A website for the *OI for ESPC* project was created on the CoG collaboration environment: http://www.earthsystemcog.org/projects/espc-infrastructure/

Some of the *OI for ESPC* project activities are closely associated with a Coupling Testbed, which is a collaborative area for groups working on research problems involving model coupling. The Coupling Testbed was funded under the larger *Integration and Evaluation Framework* NOPP award. A site for the Coupling Testbed was also initiated and is here: http://www.earthsystemcog.org/projects/couplingtestbed/

Initial roadmaps were created for each of the three objectives, and are linked under the Roadmap tabs on the two sites above. The roadmaps include status at start, team members, desired outcomes, and a sequence of tasks.

1. **Update Numerical Libraries in ESMF**
   http://www.earthsystemcog.org/projects/espc-infrastructure/moab_in_esmf

2. **Optimize Component Architectures for GPUs**
   http://www.earthsystemcog.org/projects/couplingtestbed/acceleratorplans

3. **Couple HYCOM to CESM**
   (Part 1) Introducing NUOPC conventions into CESM
   http://www.earthsystemcog.org/projects/espc-infrastructure/nuopc_in_cesm
   (Part 2) HYCOM in CESM scientific validation
   http://www.earthsystemcog.org/projects/espc-infrastructure/hycom_in_cesm_science

The roadmaps are being updated by team members prior to the weekly telecons, and progress and issues are discussed during the calls. Where appropriate, test reports describing how a code base was validated are linked to the roadmaps. These test reports include information that supports the reproducibility of results.

Work to date has focused mainly on the third item, coupling HYCOM to CESM.

WORK COMPLETED

The Roadmap pages listed under **Approach** contain detailed descriptions of the work completed. See summaries below.

1. **Update Numerical Libraries in ESMF**

   Walter Spector integrated the MOAB software into the ESMF build and tested it on about 14 different platform/compiler combinations. He wrote a unit test so that checking the correct operation of MOAB is part of standard ESMF regression testing.

2. **Optimize Component Architectures for GPUs**

   This part of the project has not been started yet.

3. **Couple HYCOM to CESM**

   Work began with introducing the NUOPC conventions into the "dead" model configuration of CESM. The dead configuration does not generate valid data, but exercises the coupler internals and is used for testing. The dead NUOPC CESM configuration will serve as a starting point for an active ocean-only configuration. HYCOM will be the ocean and all other components will be run in a "data" mode where they provide only data inputs. This ocean-only CESM configuration will be tested for correctness against a HYCOM code running outside of the CESM. Additional active components will be introduced incrementally, beginning with the ice model.

   There are two distinct parts to this effort: introducing NUOPC conventions into CESM and setting up baselines (and later, experiments) for scientific validation of HYCOM.

   (Part 1) Introducing NUOPC conventions into CESM

   Kathy Saint modified the CESM driver so that it implements the NUOPC driver, wrapped all the CESM dead components with NUOPC wrappers, confirmed correct operation, and generated a test report. Next, Kathy put NUOPC wrappers on each of the data and active components. She then added the CESM exchange fields to the NUOPC field dictionary, which is used to check that fields passed between components match properly. Next steps will likely include filling out the NUOPC CESM configuration with NUOPC generic connector and mediator components, and validating the NUOPC version of CESM in the data mode.

A synergistic activity (not funded under *OI for ESPC)* is being undertaken by the NCAR CESM team. It involves restructuring the CESM driver based on an abstraction representing the component type. This abstraction subsumes both the physical domain of the component and the framework that the component is written in. It allows the calling sequence in the driver to be simple and clear, and enables options for MCT-based component types and ESMF-based component types to be handled in a concise fashion. In addition, the CESM team developed a strategy for referencing memory between its native coupling datatype (MCT Attribute Vectors) and ESMF Arrays. This will reduce the copies required and will enable ESMF and MCT to be used together in the coupler.

(Part 2) HYCOM in CESM scientific validation

Alexandra Bozec has been working on setting up baseline runs of HYCOM with data ice. The current challenge is in setting up the ice inputs correctly, so that expected forms of quantities match.

RESULTS

The most tangible results to date are two test reports that show successful completion of interim milestones.

The first is a test report for the MOAB build within ESMF, summarized here:
http://www.earthsystemcog.org/projects/nuopc/moab_build_in_esmf
This step is a prerequisite for further integration of MOAB within ESMF.

The second is a test report for the CESM dead configuration with a NUOPC driver, summarized here:
http://www.earthsystemcog.org/projects/espc-infrastructure/nuopc_in_cesm_deadcomp_test_rpt
This step represents proof of concept that CESM can operate as a NUOPC-based system, and is a first step toward integration of HYCOM into CESM using NUOPC infrastructure.

There are important advances not reflected in these test reports. In the few months since the project started (funds became available in July 2013) there has been excellent progress on improving the compatibility of NUOPC and CESM code. The NCAR team's redesign of the CESM coupler and driver has meant that NUOPC can be introduced in a natural and clean manner within CESM, while preserving the capability to support established NCAR and DOE infrastructure. Further, the newly introduced ability within CESM to share memory between ESMF and MCT datatypes makes using both tools together much easier. Using both is appealing because there are functions in each package that the other does not contain. This ability to reference memory will support future work in which MCT and ESMF anticipate sharing a MOAB mesh-based data representation.

IMPACT/APPLICATIONS

The results obtained here can be viewed as a head start for the linked proposals funded under the 2013 NOPP AOLI awards. There is a direct correspondence between this preliminary work and the AOLI project *An Integration and Evaluation Framework for ESPC Coupled Models* (PI: Ben Kirtman). The Kirtman-led project also focuses on a coupled CESM-HYCOM configuration and builds on joint technical work involving NCAR, NRL, DOE laboratories, and ESMF/NUOPC developers.

The work presented here is likely to inform the technical strategies adopted by other NOPP projects as well. For example, streamlining the CESM coupler while introducing NUOPC code is enabling ESMF data structures and methods that support in-memory, during-run grid remapping to be introduced into CESM in an efficient way, preserving existing infrastructure where it makes sense. This capability is likely to be a first step in coupling components with adaptive grids, an objective of the NPS-NRL-Rice-UIUC NOPP AOLI project.

RELATED PROJECTS

The *OI for ESPC* project is most closely related to the projects supported under the 2013 NOPP AOLI awards, listed on this page: http://coaps.fsu.edu/aoli/projects

The current work is particularly relevant to the AOLI project *An Integration and Evaluation Framework for ESPC Coupled Models* (PI: Ben Kirtman), which also focuses on a CESM-HYCOM configuration and includes joint technical work involving NCAR, DOE laboratories, and ESMF/NUOPC developers.

REFERENCES

AOLI: http://coaps.fsu.edu/aoli

CESM: http://www2.cesm.ucar.edu/

CoG: http://earthsystemcog.org/

ESMF: http://www.earthsystemmodeling.org/

HYCOM: http://hycom.org/

MCT: http://www.mcs.anl.gov/research/projects/mct/

MOAB: https://trac.mcs.anl.gov/projects/ITAPS/wiki/MOAB

NUOPC Layer: http://earthsystemcog.org/projects/nuopc/