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An Integration and Evaluation Framework for ESPC Coupled Models

PI: Ben Kirtman
University of Miami – RSMAS
Atmospheric Sciences
4600 Rickenbacker Causeway
Miami, FL 33149
Phone: (305) 421-4046 Fax: (305) 421-4696 email: bkirtman@rsmas.miami.edu

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LONG-TERM GOALS

To realize its potential, a U.S. Earth system modeling and prediction capability must encompass a network of agencies and organizations that contribute model components, infrastructure, and scientific and technical expertise. The model component contributions must be integrated using coupling software, the coupled systems optimized for emerging computing platforms, and the predictive skill of the resulting models assessed using standard metrics. We propose to provide these integrative functions for the Earth System Prediction Capability (ESPC), using as a reference application a version of the Community Earth System Model (CESM) running an optimized version of the HYbrid Coordinate Ocean Model (HYCOM).

OBJECTIVES

The objectives of our work are:

- To establish an ESPC Coupling Testbed that allows for collaborative research into coupling technologies, and use it to prototype multi-model optimization techniques focused on computing systems with accelerator technologies.
- To support migration of optimization strategies from the ESPC Coupling Testbed to infrastructure packages and coupled model applications, and provide support for coupling of optimized components in the ESPC program.
- To update a newly coupled CESM-HYCOM model configuration with an optimized version of HYCOM and assess the coupled system performance.
- To evaluate the CESM-HYCOM model using standard measures of predictive skill, and promote the usage of standard metrics by other models in the program.
- To extend ESPC-related computational committees to address new requirements driven by changes in computing architectures and program needs, and to initiate scientific committees.

APPROACH

A one-year seed project entitled *Optimized Infrastructure for the Earth System Prediction Capability* (*OI for ESPC*) initiated several technical elements of this project: updating numerical libraries in the Earth System Modeling Framework (ESMF) to use the DOE-supported MOAB finite element mesh; exploring how to optimize a component architecture like ESMF for accelerators; and coupling the

HYbrid Coordinate Ocean Model (HYCOM) to the Community Earth System Model (CESM). The *OI for ESPC* project ended on on October 31, 2014.

The team's technical approach relies on making incremental changes and validating work frequently against established versions and known quantities. This is applicable to tasks associated with the integration of MOAB into ESMF (where MOAB is compared to the existing finite element mesh in ESMF), the integration of ESMF-based software into CESM (where the ESMF-based code is compared to native CESM and its resident MCT - Model Coupling Toolkit code), and the coupling of HYCOM to CESM (where HYCOM in CESM is compared to HYCOM standalone versions and will be compared to the Parallel Ocean Program – POP model in CESM). Where the work is more research oriented, the team has explored ideas using prototypes and toy codes. This is the approach being used for the exploration of accelerators in a modeling framework.

WORK COMPLETED

Year 2 milestones and their current status are shown below.

CESM-HYCOM

(Carried over from FY14) Complete the CESM-HYCOM coupled system under the OI for ESPC award.

First updates of the coupled CICE-HYCOM code with optimizations from the linked Accelerated Prediction of Polar Ice and Global Ocean (APPIGO) award. Test performance against baseline in coupled code.

At the end of the *OI for ESPC* project in October 2014, the CESM system with NUOPC interfaces was able to run a HYCOM and CICE coupled components (with no other active components). In FY15, the CU team worked closely with NCAR and FSU to complete an all-active CESM-HYCOM system, including the Community Atmosphere Model (CAM) and the Community Land Model (CLM) as active components. During summer 2015, the River Transport Model (RTM) in CESM was also added as an active component. With the HYCOM ocean replaced with POP, the fully coupled CESM system with NUOPC interfaces validated bit-for-bit against the original CESM code. A record of the development, with linked test reports, is here:

https://www.earthsystemcog.org/projects/espc-infrastructure/nuopc_in_cesm

An optimized version of CICE-HYCOM from APPIGO is not yet available to run.

Model evaluation

CESM-HYCOM simulations at low and high resolution (coupled system under the OI for ESPC); science application evaluation and comparisons with existing CCSM4 and CESM simulations – focus on Indian Ocean variability and MJO initiation and demise.

The CESM-HYCOM code was used to run several simulations, described in the Results section. The initial HYCOM configuration tested was low resolution (1 degree); a 0.72 degree configuration was recently added. The high resolution configuration has not yet been set up. A record of development is here:

https://www.earthsystemcog.org/projects/espc-infrastructure/hycom_in_cesm_science

Model evaluation

Develop initial conditions (atmosphere-land-ocean-ice) for prediction experiments following NMME protocol. Test initial condition with first prototype and updated infrastructure and code from the linked Navy Atmosphere-Ocean Coupled Models on Many-Core Computer Architectures award.

We have developed, tested and evaluated initialization strategies for a version of a fully active coupling compset of CESM that uses a very high-resolution (10 km x 10 km ocean component. A set of evaluation metrics have been developed and implemented. In particular, we find seasonal-to-decadal variability climate phenomenon that are otherwise not represented in current coupled models that use a 1 degree ocean component. For instance, on seasonal-to-intraannual timescales, we find that a retreated Loop Current within the Gulf of Mexico is related to reduced precipitation over southern continental US but enhanced precipitation over the Intra-Americas Seas (IAS) and Caribbean islands. This may be due to better resolved Caribbean Current bringing warm tropical waters into the IAS and supporting convective precipitation. On interannual timescales, we identify a tropical-subtropical oceanic teleconnection between SST over the Agulhas leakage and wind stress curl over tropical Indian Ocean associated with ENSO. This suggests the use of ENSO as a predictor for Agulhas leakage interannual variability and possibly the Atlantic meridional overturning circulation. On decadal timescales, we find the atmospheric jet responding to shifts in western boundary currents over the North Pacific and North Atlantic, with downstream implications on precipitation over continental US and Europe.

This results are going to be evaluated in similar simulations using a configuration HYCOM-CICE-CAM (BHY compset) with the tripolar 1/10º POP grid and 0.5º atmosphere and 2) a configuration HYCOM-CICE-CAM (BHY compset) with the tripolar 1/12º HYCOM grid and 0.5º atmosphere.

ESPC Testbed: Basic Optimization

Implement data reference for component exchange. Implement driver creation of interleaved resource lists, and prototypes for resource negotiation and optimized mediator. Migrate ESPC Coupling Testbed findings into production application and infrastructure codes.

In FY14, nine prototype codes were developed by ANL in collaboration with CU partners to explore how the ESMF and NUOPC infrastructure could help modelers optimize coupled codes using accelerators. In FY15, work focused on developing the ESMF methods needed for the implementation of resource lists that include heterogeneous computing resources, including accelerators. These methods included query functions to determine the resources available.

Three new prototype codes demonstrated a set of new ESMF interfaces:

- An ESMF application with two components - an MPI non-accelerated components, an OpenCL accelerated component - and a coupler that uses the newly added support in ESMF to query the number of accelerator devices. The application allocates all devices attached to a node to the lowest ranked MPI process running on the node.
- An ESMF application with two components - an MPI non-accelerated components, an OpenACC accelerated component - and a coupler that uses the newly added support in ESMF to query the number of accelerator devices. The application allocates all devices attached to a node to the lowest ranked MPI process running on the node.
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This work is a prerequisite for resource negotiation and mediator optimization. The data reference for component exchange is not yet completed, and no optimizations for accelerators have been migrated into production codes.

https://www.earthsystemcog.org/projects/couplingtestbed/acceleratorplans

ESPC Testbed: Technical Evaluation

(Carried over from FY14) Begin performance comparison tests of Testbed infrastructure with CPL7 dead and data models.

Continue performance comparison tests of Testbed infrastructure using simple configurations of CPL7 and CESM-HYCOM (e.g. ocean driven by surface winds).

The performance of the CESM code modified for NUOPC interfaces was evaluated relative to the performance of the original CESM, using the POP ocean so that the components in both cases were the same. Initial tests of an all-active component configuration showed a 20-25% slowdown for the NUOPC-based CESM code, much higher than expected. Typically ESMF component interfaces impose negligible (2-3%) overhead (Collins et al. 2005).

An intensive investigation of CESM-HYCOM code performance took place in April and May 2015. Simpler versions of the CESM system (e.g. single-processor set up, dead model configuration) were used as needed to identify the issues. An early optimization included a change to the field dictionary lookup, and a fix to the control flow, in which the ocean was called more frequently in the NUOPC case than in the original code. This first set of changes took the overhead down to about 15%, still higher than expected. The second round of optimizations focused on the NUOPC Layer itself. The character string comparisons that are used in NUOPC to examine metadata describing the components were a primary culprit. Optimizations to minimize the need for such comparisons reduced the overhead to 5% in the runs performed. Additional optimizations may be needed.

ESPC Testbed: Adaptive Grids

First prototype of coupling to an adaptive grid with updated infrastructure and code from the linked Navy Atmosphere-Ocean Coupled Models on Many-Core Computer Architectures award.

Prototype code is not yet available from the Atmosphere-Ocean Coupled Models on Many-Core Computer Architectures project.

ESPC Testbed: Adaptive Grids

Mediator to receive meshes from components and dynamically compute interpolation weights.

The nature of this task has changed, for the following reason.

The CESM-HYCOM system completed under this award contains both the original (MCT-based) component interfaces, and NUOPC interfaces. This "hybrid framework" leads to complexity in the CESM code. The CESM project intends to focus future development of their coupled system on only NUOPC interfaces. The plan is to have two starting points: a simplification of the CESM-HYCOM code that removes the restriction that MCT must be supported, and the mediator developed for the NOAA Environmental Modeling System (NEMS) with CESM components. To support the latter, a FY16 pilot project has been proposed to the NOAA Next Generation Global Prediction System (NGGPS) that will move the NEMS mediator into the Common Infrastructure for Modeling the Earth (CIME) community repository created by the CESM project. The new CESM mediator will likely merge elements of these two starting codes.

The changes required to dynamically compute interpolation weights in the hybrid CESM-HYCOM framework are substantial. The NEMS mediator already supports dynamic computation of interpolation weights. The idea is therefore to postpone implementation of this dynamic grid remapping task until FY16 and development of a prototype of the CESM-HYCOM code with only NUOPC Layer interfaces.

ESPC Testbed: Interactive Ensemble

Replacement of a few multi-model interactive ensemble components with actual components and preliminary testing.

The interactive ensemble implementation developed for the NCAR family of models (CCSM3, CCSM4 and CESM1) uses multiple realizations of the atmospheric model (CAM) coupled to a single realization of the ocean model (POP), a single realization of the sea-ice model and a single realization of the land-surface model. The coupling of the multiple realizations of CAM to the single realizations of the other component models is accomplished through the CCSM coupler. The purpose of this coupling strategy is to significantly reduce the stochastic forcing of the ocean due to internal atmospheric dynamics. Ensemble averaging of fluxes of heat, momentum and fresh water produced by the individual CAM ensemble members before they are passed to POP effectively filters the noise in the fluxes due to internal atmospheric dynamics.

Over the ocean this approach works well since the coupling is entirely through the fluxes and the ensemble averaging of the fluxes is found to due little damage to the mean state of the coupled system. However, over the ice and land the coupling includes fluxes and state variables that are used by the component models to calculate fluxes. The ensemble averaging, therefore, has a disproportionately large effect on state variables compared to flux fields, which ultimately leads to differences in the climatology of ice and land that are too large. For instance, over ice and land wind-dependent fluxes are calculated using the ensemble mean *state* (as opposed to flux) variables leading to strong biases over land and ice.

The above implementation of the interactive ensemble that only allows a single land and ice component model not only has bias issue noted above but is also a major difficulty in the development trans-Atlantic super-model. The problem for the trans-Atlantic super model is that we need the flexiblity to include additional atmospheric component models that may not include their own land or ice component models or may use fluxes and state variabiles as noted above. *To solve this problem, we enhanced the interactive ensemble so that multiple atmosphere, land and ice component models can be simultaneously coupled to a single ocean component model.*

The second major code divelopment was to implement a "coupling wrapper" so that any AGCM (whether or not it includes an independent land or ice component model) can be encorporated into the interactive ensemble in a multi-model sense. This coupling wrapper has been fully tested with a data model and will be implemented the US Navy NAVGEM model. The NAVGEM software agreement is under negociation between UMiami and NRL.

MOAB Mesh **Initial updates to MOAB to accommodate requirements of ESPC codes; changes may be needed for nonconformal NUMA grids. Release updated MOAB.**

Full use of the MOAB library requires the creation of an ESMF Mesh with a MOAB Mesh underneath. At the end of FY14, this capability was not complete. The code could only create the vertices of a MOAB mesh from the ESMF specification. In FY15, the capability was completed and conservative grid remapping in ESMF can now be implemented using either the native ESMF finite element mesh framework, or MOAB. Performance measurements are not yet finished. No additional requirements for nonconformal grids have come up.

RESULTS

CESM-HYCOM. In the last year, the focus of the work has been the technical set-up of HYCOM into the CESM. Starting with version 2.2.35 of HYCOM, the first part of the year has been dedicated to the proper implementation of the routine responsible for the exchange of fluxes between HYCOM, the ice and the atmospheric component. In the second part of the year, HYCOM has been updated to the latest version available (2.2.98) and the river transport component has been connected to HYCOM. Also, since no more computer hours were available on the NCAR machine, Yellowstone, this version of CESM along with the latest version of ESMF (7.0.0beta) was installed on the NAVY DSRC machines, Kilrain (IBM iDataPlex) and Shepard (Cray XC30). During the implementation of the model and after the installation of the model on the NAVY machines, a series of 10 years experiments were performed to ensure the technical and scientific good behavior of HYCOM when coupled with only CICE (G compset) and when coupled with both CICE and CAM (B compset).
Using the same bathymetry, grid and as close as possible diffusion and viscosity parameters, results of G compset experiments showed similar behavior in the ocean but differed over the Polar Regions. To investigate, we extended the simulations to 20 years: 1- HYCOM in CESM coupled with CICE (CESM-HYCOM), 2- POP in CESM coupled with CICE (CESM-POP). A third experiment using the stand-alone HYCOM coupled with CICE was also performed for comparison purposes (HYCOM-CICE).

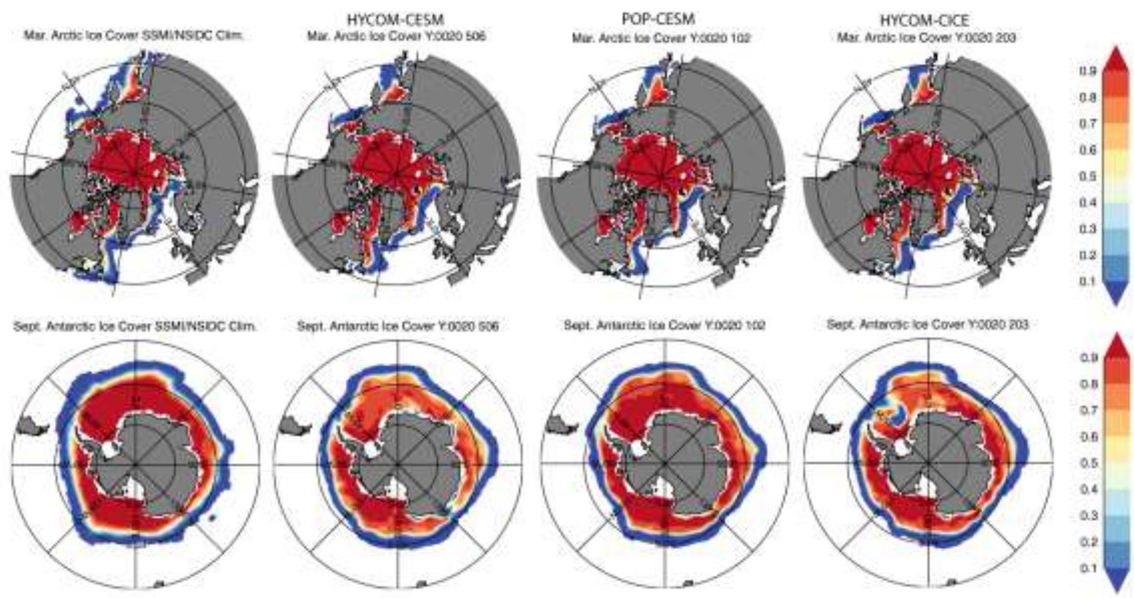

Fig. 1: (Top) Ice cover in March (left to right) from NSIDC/SSMI climatology, CESM-HYCOM, CESM-POP and HYCOM-CICE at year 20 of the simulation. (Bottom) same as above for September.

All three experiments showed reasonable ice extent compared with the climatological SSMI ice extent produced by the NSIDC in the Arctic region (Fig. 1) and an improvement of the CESM-HYCOM ice extent during the summer when compared with HYCOM-CICE (not shown). In the southern hemisphere, CESM-HYCOM again shows improvement with a Weddell Sea fully covered in September while the HYCOM-CICE Weddell Sea is partially uncovered. This problem had been linked to the use of sigma-2 coordinate creating local density instabilities. Despite a better coverage, the ice cover of CESM-HYCOM remains, however, weaker than in CESM-POP or the SSMI climatology.

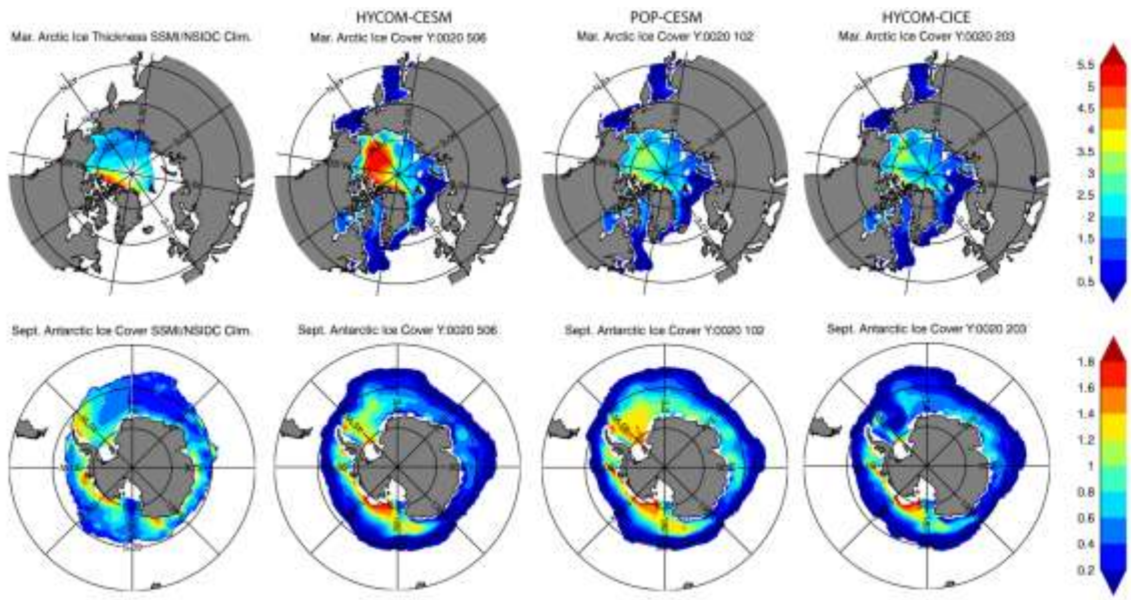

Fig. 2: (Top) Ice Thickness in m in March (left to right) from NSIDC/IceSat climatology, CESM-HYCOM, CESM-POP and HYCOM-CICE at year 20 of the simulation. (Bottom) same as above for September.

The main difference between the experiments is found when comparing the ice thickness. While the region of maximum ice thickness is limited to the northern coasts of the Canadian Archipelago in the NSIDC/IceSat climatology, the region of maximum ice thickness extends to cover the Beaufort gyre region in CESM-HYCOM (Fig. 2). A similar feature is found in CESM-POP but while the ice thickness over the region goes beyond 5m in CESM-HYCOM, it is limited to 3m in CESM-POP. In HYCOM-CICE, only the western part of the Beaufort gyre developed an ice thickness of ~3m.

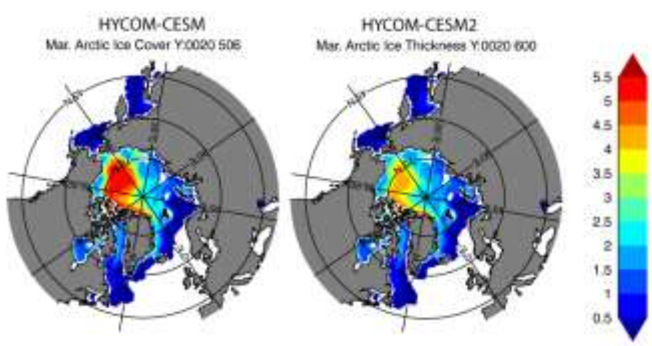

Fig. 3: (Top) Ice Thickness in m in March (left to right) from CESM-HYCOM and CESM-HYCOM2 at year 20 of the simulation.

The time evolution of the total volume of ice over the Arctic region seems to increase over the 20 years with a seasonal cycle between 1.9×10^{13} m^3 and 3.5×10^{13} m^3 in CESM-HYCOM while it is stabilized in CESM-POP and HYCOM-CICE with a range of 1.0×10^{13} m^3 to 2.7×10^{13} m^3 and of 0.7×10^{13} m^3 to 2.6×10^{13} m^3, respectively (Fig. 4). To test the sensitivity of the ice to the ocean diffusion and viscosity parameters, a fourth experiment (CESM-HYCOM2) is performed. Using a set of parameters optimally tuned during the CORE-II project, CESM-HYCOM2 still presents a high ice thickness over the Beaufort Gyre (Fig. 3). However, the maximum thickness is limited to 4m instead of more than 5m in CESM-HYCOM. The time evolution of the total ice volume in CESM-HYCOM2 is also stabilized after 20 years with a weaker range than CESM-HYCOM. This result indicates a strong sensitivity of the ice thickness to the ocean circulation. In the southern ocean, CESM-POP has an overall higher ice thickness than in the HYCOM simulations, with maximum in the Weddell and Ross Seas (Fig. 2). We notice a slight increase of the ice thickness in CESM-HYCOM compared with the ice thickness in HYCOM-CICE, but mostly in Weddell Sea, which is covered in CESM-HYCOM and mostly uncovered in HYCOM-CICE. These differences found between the CESM-HYCOM and HYCOM-CICE can be attributed to the different way fluxes are applied over the ice in CESM and the stand-alone.

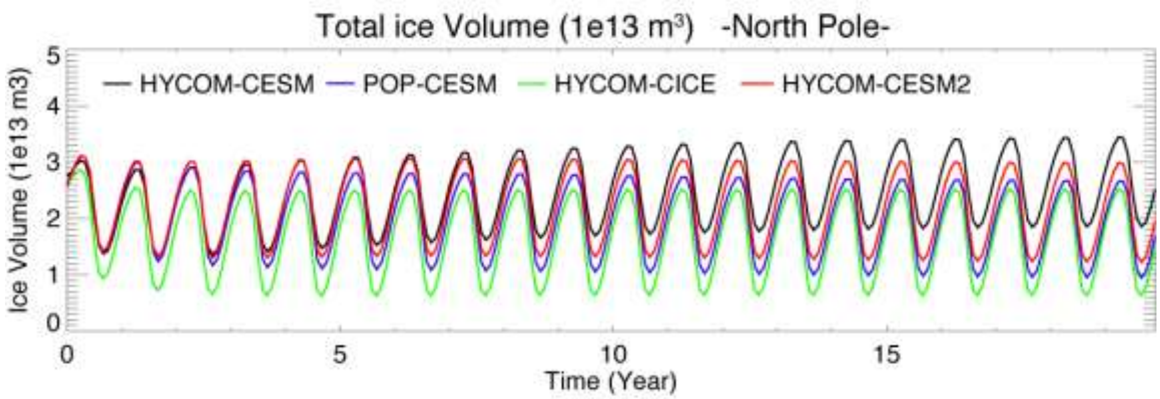

Fig. 4: Evolution of the total ice volume in the Arctic Region for CESM-HYCOM (black), CESM-POP (blue) and HYCOM-CICE (green).

Concurrently to the G compsets experiments and in order to make sure that the technical set-up was done properly, two test experiments of 10 years were performed with the B compset framework: 1- HYCOM in CESM coupled with CICE and CAM, 2- POP in CESM coupled with CICE and CAM. Again, results, between the two configurations, were comparable in terms of fluxes and ocean response (not shown). However, longer simulations and further diagnostics are required to make a full evaluation of the HYCOM behavior in CESM. These first experiments were only designed to get an idea of how comparable were the fluxes between the components.
Finally, a global 0.72º HYCOM tripolar grid has been introduced in CESM. Tests are currently underway to assess the behavior of this new configuration within CESM. As with the gx1v6 global POP grid and bathymetry, this 0.72º CESM configuration will be compared with a stand-alone HYCOM coupled with CICE.

Accelerator Optimizations for Coupled Systems.
Jayesh Krishna of the ANL team developed ESMF interfaces that enable users to query for available resources and then create resource lists that include bth CPUs and accelerator devices. ESMF data objects and their associated computations are mapped to these resource lists. This approach enables heterogeneous resources to be introduced into ESMF-based applications in a non-intrusive way, following the existing paradigm for resource mapping.

Prototype applications were developed to demonstrate these capabilities when using four accelerator software stacks - OpenACC, OpenCL, OpenMP4, and the Intel MIC – and also a no accelerator option. The applications run the accelerated code on the persistent execution threads (PETs) with accelerator devices allocated to them and run the non-accelerated (MPI-only) code on the rest of the PETs. ESMF unit tests were added for the new interfaces. Methods were tested on the Fusion cluster and Jenny Supermicro SuperServer platform at ANL.

The interfaces that enable users to create PET lists for heterogeneous resources can be used either in the ESMF library or by model developers. They are based on several iterators, which enable buffers to be split into different categories or "colors." Recent development includes a parallel version of the splitting algorithm. Below is an outline of the process required to create a heterogeneous list.

1. (VM Global) Divide the global PET list, global_pet_list, to
    - List of PETs with access to accelerator devices, acc_global_pet_list
    - List of PETs without access to accelerator devices, noacc_global_pet_list
2. (VM Global) Divide the list of PETs with access to accelerator devices, acc_global_pet_list to
    - List of node local PETs with access to accelerator devices, local_acc_pet_list
    - Rest of the PETs, nonlocal_acc_pet_list
3. (PET Local) Divide the local PETs with access to accelerator devices, local_acc_pet_list based on a local node allocation policy to get policy_based_local_acc_pet_list
4. (VM Global) Join (Allgather) the local PETs created based on the local node allocation policy, policy_based_local_acc_pet_list to get the global PET list that has (allowed to) access to accelerator devices, policy_based_global_acc_pet_list
5. (PET Local) Subtract the policy based global pet list that accesses the accelerator devices, policy_based_global_acc_pet_list from the global PET list, global_pet_list to get the list of PETs, policy_based_global_noacc_pet_list, that can be allocated to non-accelerated components.

With the current set of utilities, the code required to create heterogenous, ordered PET lists is fairly complex. It would be useful to build shortcuts to create the PET lists constrained by user policies (at least cover the common cases in an easy way) and a new section "Simplified User Interface" explores the alternatives:
https://www.earthsystemcog.org/projects/couplingtestbed/simplify_petlist_creation

However, the interfaces are functional and can be used to proceed with other tasks in the project, including prototypes of resource negotiation in a multi-component setting.

Coupling Testbed. The Coupling Testbed proposed as part of this project was intended as a repository and collaborative in which examples and information could be found about research problems in model coupling. The initial problems posed included optimization of multi-component systems on computing platforms with accelerators, coupling components with adaptive grids, and coupling involving interactive and multi-model ensembles. So far, the original concept of the Coupling Testbed has been limited to incorporating awareness of accelerators into ESMF, and the team has used ESMF repositories (see: https://www.earthsystemcog.org/projects/couplingtestbed/)

The CIME repository created by the NCAR CESM group shares many of the characteristics desired for a Coupling Testbed. Currently, a user can check out a coupler (the original CESM coupler) that can be used for experimentation, with a full set of synthetic test models and an associated test framework. In the coming year ESPC project members will explore how CIME, NUOPC-based prototypes generated by ESPC application projects, and the migration of the NEMS mediator into CIME might evolve to create a more multi-agency test platform anchored by CIME.

IMPACT/APPLICATIONS

Through the actions of a succession of infrastructure projects in the Earth sciences over the last two decades, a common model architecture (CMA) has emerged in the U.S. modeling community. This has enabled coupled models to wrap high level model components in community-developed ESMF and NUOPC interfaces. The Earth System Prediction Suite (ESPS), a collection of multi-agency coupled weather and climate systems that complies with these interfaces and can more easily exchange components, is a tangible outcome of this coordination. A publication describing the ESPS, led by Navy contractor Gerhard Theurich, was accepted in BAMS during FY15.

A follow-on whitepaper, "Building on Technical Interoperability to Achieve a More Effective U.S. Earth System Modeling Community," has been initiated and an early draft is available here: https://docs.google.com/document/d/1r2hjIzVJ0QU-x168jGcCBl_Gj0B_LnZoMoCEJugIhnE/edit#heading=h.mw7pjma2bak8

The ESPS is a direct response to the recommendations of a series of National Research Council and other reports recommending common modeling infrastructure. Integration of the HYCOM model with CESM contributes to development of the ESPS, and prototyping of interactive and interactive multi-model ensembles looks to a future where experimental model configurations are more readily assembled.

RELATED PROJECTS

Optimized Infrastructure for ESPC, funded by ONR, was a one-year seed project for this effort. Partners also include projects under the program *Advancing Atmosphere-Ocean-Land-Ice Global Coupled Prediction on Emerging Computational Architectures*, described here: http://coaps.fsu.edu/aoli/projects

PUBLICATIONS

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CIME: https://www2.cgd.ucar.edu/sites/default/files/events/related/cime-background.pdf
CoG: http://earthsystemcog.org/
ESMF: http://www.earthsystemmodeling.org/
HYCOM: http://hycom.org/
MCT: http://www.mcs.anl.gov/research/projects/mct/
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NUOPC Layer: http://earthsystemcog.org/projects/nuopc/