Towards a Next-Generation Ocean Model in the GungHo framework: 2D test cases (G-Ocean:2D)

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Project partners: John Thuburn, University of Exeter; Nigel Wood, John Siddorn, UK Met Office; Colin Cotter, David Ham, Imperial College;

Part I: Track record

National Oceanography Centre is a NERC Research Centre that maintains world class oceanographic research. It is situated across two sites, Liverpool (**NOC-L** formerly the Proudman Oceanographic Laboratory) and Southampton (**NOC-S**). **NOC** maintains world-class interdisciplinary research strengths in shelf sea and coastal systems, sea level, global ocean and climate modelling, global-scale hydrographic and satellite observations, air-sea fluxes, ocean biogeochemistry, seafloor geology and geophysics, oceanographic data archiving and dissemination, plus strong capabilities in marine technology and operational oceanography, as a partner in the National Centre for Ocean Forecasting (NCOF). **NOC-L** contributes expertise in shelf scale, ocean-margin, coastal and estuarine modelling of hydrodynamics, coupled ecosystems and surface waves. It has a substantial international reputation and has particularly contributed to the development of operational shelf sea forecast services at the Met Office and to the investigation of the impact of climate change in the marine environment. In Southampton, **NOC-S** specialises in high-resolution global ocean circulation models and physical processes, ecosystems, sea-ice, and uncertainty. The group contributes substantially to the development of UK coupled climate models through a joint initiative with the Met Office under the Joint Weather and Climate Research Programme (JWCRP).

Dr Jason Holt (NERC Band 4) is associate head of the Marine Systems Modelling Group at NOC. With 20+ years experience of physical oceanography, he specialises in the synthesis of model and observations to develop our understanding of shelf-sea physical and coupled physical-biological systems. Particular areas of interest include model capability and accuracy; the impact of large scale variability (e.g. climate change) on shelf-sea physics and ecosystems; and transports and budgets of freshwater, carbon and nutrients across shelf sea basins. As an originator of the POLCOMS-ERSEM model system and more recently through coordinating work on NEMO-shelf, he has worked in close collaboration with the UK Met office for over 10 years on developing and assessing shelf sea models for operational oceanography and climate downscaling (e.g. UKCP09). Currently he chairs the Joint Coastal Ocean Modelling Programme. He leads the modelling component in the NERC FASTNet (ocean-shelf exchange) programme and led the Next Generation Ocean Dynamical Roadmap Project. He sits on the ICES/PICES Strategic Initiative on Climate Change Impacts on Marine Ecosystems, the GungHo executive committee and the NERC High Performance Computing Steering committee. He has published 50+ peer reviewed papers primarily on the modelling of hydrodynamics and ecosystems in shelf seas and ocean margins.

Prof. Adrian New (NERC Band 3) is the head of the Marine systems Modelling Group at NOC. With 30+ years of research experience and 51 peer-reviewed publications, he has wide-ranging interests in most aspects of physical oceanography, covering both numerical ocean models and direct observations at sea. Specific interests include ocean general circulation and coupled climate modelling, decadal to centennial timescale variability of the ocean and climate system, large-scale ocean circulation and dynamics, and internal waves and their associated mixing processes. He was a leading member of the international DYNAMO model intercomparison exercise, which generated new insights into the capabilities of ocean models with different vertical grid structures. More recently, he has been instrumental in forging a key strategic partnership with the UK Met Office for the development and validation of the global NEMO ocean model. This will be the ocean component of the UK's next generation climate model, UKESM1. He also sits on the international NEMO Steering Committee for the coordination of NEMO and the GungHo executive committee.

Dr. Hedong Liu joined the National Oceanography Centre, Liverpool in 2008 as a band 5 research scientist. During the past 14 years, he has worked on the development and application of 3-D structured/unstructured grid ocean models (NEMO, ICOM, FVCOM, POM, ECOM_si) at universities and national laboratories in USA and UK. He is currently a member of the NEMO System's team. He specialises in shelf sea and coastal ocean modeling, especially the development and application of the state-of-the-art numerical methods for computational fluid dynamics and ocean models including structured and unstructured meshes, hydrostatic and non-hydrostatic pressure methods, advanced turbulence models, high order advection schemes, free surface/interface and wetting/drying algorithms.

STFC's Scientific Computing Department (SCD) has around 180 staff focused on the development and optimization of scientific applications across a wide range of scientific disciplines, the application of new and emerging HPC technologies and the provision of compute and data services. SCD provides support for most of the Collaborative Computational Projects and High-End Computing Consortia. Over the last 10+ years NOC and STFC have developed a strong working partnership in ocean model development and optimisation, most recently in the NERC Ocean Roadmap Project.

Dr Mike Ashworth is Head of Application Performance Engineering (APE) in the Scientific Computing Department at STFC's Daresbury Laboratory. He leads on the development and optimization of large-scale applications for high-performance systems across a wide range of scientific disciplines, including evaluation and exploitation of novel architectures and the application of Grid technologies. Mike was one of the team which successfully attracted £56.5 million funding to establish the Hartree Centre at STFC and is involved in a range of projects especially focused on environmental, astrophysical and fluid flow simulations. He was one of the founders of the GungHo project, and leads on many ocean model developments and has been a contributor to NERC's Ocean Roadmap project.

Rupert Ford joined STFC Daresbury Laboratory in 2012, previously he was a founding member of the Centre for Novel Computing, a High Performance Research Group based in the School of Computer Science, at the University of Manchester, where he worked for over 20 years. At STFC, he continues to pursue his interests in performance engineering and flexible frameworks for model coupling. The majority of his research over the past 10 years has been undertaken in the Earth System Modelling and Integrated Assessment domains in which he has co-developed the BFG coupling system. He is currently involved in the EU ISENES-2, EU ERMITAGE and U.K. GungHo projects. He has written over 30 peer reviewed papers.

Graham Riley is a Computational Scientist at STFC/Daresbury (30%) and a senior Research Fellow in the Advanced Processor Technologies Group (APT, apt.cs.manchester.ac.uk) in the School of Computer Science, Manchester University, where he has worked since 1990. His research expertise covers areas related to High Performance Computing, including performance analysis and improvement, performance modelling and, more recently, the software engineering aspects of flexible coupled modelling, primarily in the field of Earth System Modelling. Riley has a long association with the UK Met Office. He currently leads Manchester's involvement in GungHo and the EU-funded IS-ENES-2 and ERMITAGE projects and is a co-developer, with Rupert Ford, of the BFG coupling system. He has published around 30 peer-reviewed papers.

Relevant publications

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Part II: Description of the proposed project

1. Background

The recently completed Next Generation Ocean Dynamical Core Road Map project[1] identified three key drivers for change in ocean hydrodynamic modelling: Improved subgrid scale mixing, ocean-shelf coupling and effective use of next generation computer architectures. While all three are important, the last is unavoidable if the UK is to maintain a world-leading position in ocean science. Increases in computational power are now occurring almost exclusively through increased parallelism, but with concurrent decrease in memory amount and bandwidth per computational core; a trend that is set to continue until there is a radical change in how computers are built. Hence all ocean models will have to adapt to this change, with those that adapt faster having a substantial competitive advantage over those that are slow to adapt.

Meeting this challenge requires introducing as much concurrency as possible into the ocean model, from coarse-grained domain decomposition (with MPI), through multithreading (e.g. with OpenMP), to loop level vectorisation. To achieve this, incremental evolution of existing ocean models (such as NEMO[2], the ocean model system most widely used in Europe, including the UK Met Office and NOC) is an option, but the effort involved would be so extensive and intensive that this would really constitute a complete re-write of the code. Moreover, in the current code structures computational and natural science codes are mixed. So after this optimisation effort, the resulting code would be very difficult to develop by anyone who was not both a numerical modelling and computational science expert (an unreasonable expectation). Hence a new approach is required.

A similar issue has been identified in the atmospheric modelling community and NERC, Met Office and STFC have made a substantial investment (~£7.7M over 5 years) into the GungHo project to design a new atmospheric dynamical core for climate and weather operational and research use, with the specific goal of producing a model that is at least as accurate as the current system, but scales effectively on 10^5-10^6 cores. A central principle behind the GungHo computational framework (Fig. 1; Ford et al., In Review) is the division of the code into layers to separate the natural science and computer science aspects. The identification of these layers enables a separation of concerns between largely independent components which have different requirements and require developers with very different skill sets. The driver layer schedules individual models in a coupled system. For a single model (our concern here), the layers above (algorithm) and below (kernel) are thus isolated from the complexities of the parallelisation process (PSy) layer, which sits between these. The kernel layer provides the building blocks that are assembled by the algorithm layer, which is essentially a set of subroutine calls and control code operating on whole fields. The kernels themselves describe individual dynamical operations (e.g. divergence, gradient, etc), and physical parameterisations either on fields of a flexible size or on individual elements with looping controlled by the PSy layer. Hence the natural scientist works on the Alg. layer, the computer scientist on the PSy layer and they work together on the kernel layer.

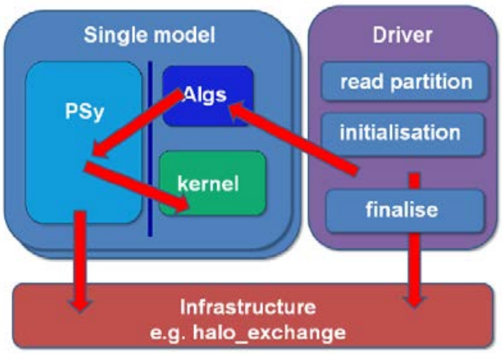

Figure 1 Gung Ho Software components. The arrows represent Application Programming Interfaces (API's) and direction shows the flow control.

Oceans and atmospheres share the same equations of motion and so it is natural to consider developing a new ocean model that builds on the ongoing GungHo work and which addresses the identified issues thereby giving substantial added value to the investments. However, modelling the oceans and the atmosphere each face unique challenges not applicable to the other. The atmosphere has the 'pole problem', whereby singularities in the global coordinates (at the poles) can severely impact the scalability (i.e. the increase in performance as the number of cores used increases), and this leads to either esoteric grid arrangements and/or to alternative solution approaches. This issue is readily avoided in the

[1] www.nerc.ac.uk/research/programmes/ngwcp/findings.asp
[2] www.nemo-ocean.eu

ocean by choosing a coordinate system with poles over land e.g. the tri-polar grid used by NEMO. Moreover, unlike in the atmosphere, oceans are subject to O(1) changes in water depth (*h*) with concurrent changes in dynamical scale (simplistically these tend to vary ~$h^{0.5}$), and they also have complex coastlines, straits and passages, and other regions of restricted exchanges. Hence, a multiscale approach, in which different regions of the ocean are modelled with grids of different resolutions, depending on dynamic/geographic scales and or regions of interest is an important capability for ocean models. This was identified as the coupled ocean-shelf driver for change in the Ocean Road Map project. Much effort has been directed to this over recent years, but progress in the global context has been slow, with only a few examples reaching the published literature (e.g. Ringler et al., 2013; Timmermann et al., 2009). Considerations of multiscale applications are present in GungHo, but are not the primary drivers. However, the GungHo computational framework is specifically designed to support the unstructured meshes and solution approaches needed for multiscale capability, driven by the need for esoteric grids to solve the pole problem. Hence this approach represents an important opportunity to make substantial progress towards a full multiscale capability in a global ocean context.

Therefore, while the approaches chosen for the atmospheric model in GungHo may be perfectly satisfactory (or better) for the ocean, they are not necessarily optimal or natural choices. Specifically, the analysis of GungHo Phase I identified three mixed Finite Element (FE) approaches (Cotter and Shipton, 2012):

1. Primal-only RT1-Q1DG on a quadrilateral mesh (quads) and primal-dual RT0-Q0 on quads;
2. BDFM1-P1DG on triangles;
3. Primal-dual RT0-Q0 on hexagons.

Any of these might be a good choice for an ocean model, but they are not necessarily the natural choice. The use of the FE method, with its extra complexity but without the benefits of an advanced multiscale capability as in quadrilateral (1) and to some extent hexagonal (3) grids would require careful justification to the oceanographic community, noting again that the ocean does not have the pole issue that led to these choices in the atmosphere. Hence two important concepts that need to be proven ahead of designing and building a new ocean model in this context are:

1. That the computational framework under development in GungHo is sufficiently flexible to accommodate the natural choices of grids and solution approaches for ocean models
2. That, when coded within this framework, conventional solution approaches can perform at least as well as the existing models in terms of efficiency and scalability, and also have benefits of ease of use and development when highly optimised.

With these established the ocean modelling community would then be free to choose to follow the solution approaches of GungHo or not, as the scientific understanding dictates. In order to make this decision a set of well defined test cases, within this framework is also required.

Numerical choices for ocean models

There are three broad categories of solution approaches commonly used in dynamical ocean modelling: Finite Difference (FD), Finite Volume (FV), and Finite Element (FE), approximately in order of increasing complexity of code and computational cost. FD is generally used on structured meshes, and FV and FE are used on unstructured meshes (i.e. where the computational data structure does not match the mesh, so indirect addressing of how the mesh is connected is required). Each of these has a variety of ways of arranging the different dynamical variables (particularly velocity and pressure) on the computational grid (e.g. Fig. 2) and has varying degrees of accuracy and flexibility. However, any chosen approach may have computational modes, which can contaminate the solution to a varying degree depending on their nature (e.g. Danilov, 2013). Choosing approaches without computational modes, or controlling those that exist in a way that does not otherwise compromise the solution (e.g. by making it too dissipative) is a crucial element to model design, which can be explored to some extent by theoretical analysis, but generally requires testing in idealised and realistic cases.

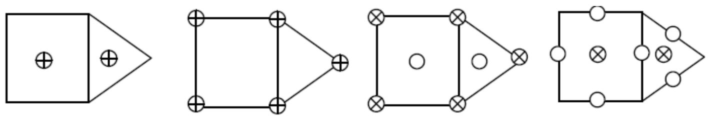

Fig. 2 Example variable arrangement on quad. and triangular elements. From left to right A, A1, B, C Grids. A and A1 are collocated grids, B and C have velocity components at the open circles and velocity at diagonal crosses.

The issue of flexibility here relates to the ability to apply resolution where it is needed, both dynamically and to focus on a region of interest. Multiscale mesh refinement can readily be realised with triangular meshes, which are used in many (generally coastal-ocean) models.

However, these have a tendency to introduce numerical modes; hence finding a good balance between numerical accuracy/stability and multiscale capability is a substantial challenge.

Putting aside multiscale capability, there is a clear winner in terms of grid choice: the C-Grid arrangement on an orthogonal quadrilateral grid. This has the unique property of a 2:1 ratio of velocity to pressure degrees of freedom – a necessary condition for the absence of numerical modes. This works well with FV and FD solution approaches and allows structured meshes. There is a growing consensus that this is the best mesh for global ocean models, particularly those used in coupled climate models, and without the pole problem this would remain an excellent choice for the atmosphere.

Hence a successful application of an FD or FV model with a C-grid, quadrilateral arrangement, within the GungHo computational framework would be an important demonstration of capability. The scientific benefits of this would arise from the exploitation of next generation computer systems in a framework that is straightforward for the natural scientist to develop, a substantial benefit over current models that have suffered from incremental optimisation. It would provide the benchmark against which other approaches (including the GungHo choices above) could be judged.

The choice of grids and approaches that offer a full multiscale capability, and so meet the coupled ocean-shelf driver for change, is far from straightforward. Many options have been tried using triangular and hexagonal meshes with FV and FE approaches. There is no general consensus in the community as to which is optimal (Danilov, 2013), but there is a tendency towards FV methods particularly in the regional to global scales, while FE methods remain popular at coastal scales. Hence, what is needed is a flexible computational test bed that can straightforwardly explore a wide range of options in increasingly sophisticated cases, and that will also form the framework for the full operational/research 3D model. This will allow the identification of the best choice, and the issues associated with it, given a particular set of design criteria dictated by the target scientific applications. Delivering this test suite is the underlying objective of this work; here we focus on the 2D (horizontal) case as an important starting point, on which more sophisticated applications can be developed.

2. Objectives

This project has three key objectives

1. Develop the G-Ocean:2D test bed (WP1). We will code a set of ocean specific kernels and an algorithm layer focusing on a FD and generalised FV approach.

2. Develop the G-Ocean:2D test cases (WP2). A set of test cases covering simple oceanic and shelf seas circulation examples will be configured and tested. These will be applied to the C-grid quad FD and FV cases as the benchmark.

3. Exploiting the system (WP3). We will look to expand the use of the system in the oceanographic community.

3. Technical Work Plan

WP1 Develop the G-Ocean:2D test bed

We will develop the required set of kernel and algorithm routines to solve the 2D shallow water equations in Cartesian coordinates. These routines will be connected via the PSy layer under development in GungHo. Both FD and FV approaches with closed and open lateral boundaries will be implemented. The FD approach will mirror that used in NEMO, but with a single time level i.e. it will use an orthogonal quadrilateral C-Grid, with an energy and enstrophy conserving solution to the momentum and continuity equations, with the momentum advection being treated in a vector invariant form and a quadratic friction term. The NEMO model will be configured in a matching case, to provide a conventionally coded comparison. The FV approach will be coded in a generic form for arbitrary element shapes, and so will be readily extendable to explore multiscale options, although initially a C-grid quadrilateral configuration will be used. A model for this approach has already been coded in a standalone framework.

WP2 Develop the G-Ocean:2D test cases

We will configure a set of test cases for basic 2D oceanic processes. These will draw on tests suggested for other models systems and will include: **i** Stommel Gyre solution for wind driven circulation in an ocean basin (Stommel, 1948); **ii** Equatorial Rossby Wave propagation (Boyd, 1980); **iii** tidal dynamics in an enclosed sea (Davies and Jones, 1996). These will be judged on: accuracy, stability, ease of configuration (qualitatively assessed), a careful assessment of computational efficiency, and scalability. The PSy layer in Gung Ho is still under development, so the level of multiprocessor comparison that can be undertaken is dependent on progress in that project, but we expect at least an MPI decomposition to be available. We will be able to test the performance against NEMO and between the FD and FV methods. This will assess the difference between the methods and the costs (if any) associated with the more sophisticated data structure in GungHo (albeit with the caveat that NEMO is a longstanding well optimised code).

WP3 Exploiting the system

The developments described bring this technology to the software equivalent of TRL4. To take this further requires a detailed exploration of approaches and grid choices that goes beyond this project, e.g., to explore the prospects for a full multiscale capability within the GungHo framework. This will be initiated in the final Ocean Road Map Project workshop on G-Ocean model design planned for early 2014. We will make the code and tools developed in this work available to the wider oceanographic community as they are developed, and hold a workshop at the end of the project to present the outcomes and train other model practitioners on how to use them.

4. Outcomes and scientific application

This work will provide a first view of how an ocean model built and designed in the GungHo framework is likely to perform in terms of accuracy, ease of configuration and what the relative pros and cons are in terms of the computational efficiency of the solution. The tools built here will allow an extensive investigation of ocean model design to be conducted and inform the question: Are the numerical approaches being developed in GungHo for the atmosphere appropriate for the ocean? Or will alternatives be needed to develop a full 3D ocean code? This will provide a vital decision point in developing a full ocean model in this context, informing the level of effort required. This work will also provide evidence for the other partners in the international NEMO consortium to inform the decision as to whether this is the appropriate route for the evolution of the NEMO modelling concept.

The long term impact of this work is potentially very far reaching. The vision is that this is the first step on the route to an ocean model that, by circa 2020, scales on 10^5-10^6 cores with full multiscale capability, and yet is readily developed and used by a full spectrum of oceanographers. Realising this vision would represent a step change in Earth System Modelling and Regional System Modelling capability that would be truly world leading, and impact climate science, weather forecasting, marine impacts assessments, as well as fundamental oceanographic research into (e.g.) the thermohaline circulation, ocean-shelf coupling and global biogeochemical cycles.

5. Connections to and support from other activities

This work aligns strongly with the on-going GungHo project, but note there is no funding for oceanographic model development in that project. PI Holt and CoIs New and Ashworth sit on the GungHo executive committee, Riley and Ford work directly on the GungHo computational science work package and other key players in that project are Project Partners in this: Nigel Wood (Met Office; Head of Dynamics Research), John Thuburn (University of Exeter, GungHo PI), David Ham and Colin Cotter (Imperial College; GungHo data structures and grids). Through these links we will be informed by developments in GungHo, and may in turn influence these. We will also build strong connections between this work and those looking to build the link between the Imperial College Ocean Model and GungHo. As head and associate head of the Marine Systems Modelling Group at NOC, the CoPI (New) and PI (Holt) will ensure very close working across the rest of this group and the cohesion of the project. The early scientific application of this work will be supported by modelling national capability funding at NOC (initially ~3 months effort) to start exploring other grid/solution options. STFC will contribute development time on a range of Hartree Centre computer systems, including novel architectures systems such as Intel Xeon Phi and GPU-based systems.

6. Project management

The project will be managed on a day to day basis by the PI, with 2-weekly teleconferences to monitor progress and deal with issues arising. The work will be divided into tasks scheduled according to Gantt chart below. The code will be managed according to the protocols established in GungHo. Quarterly project meetings will allow for a more in-depth discussion of the work. Progress will also be reported to the GungHo executive and at the plenary meetings of that project, to ensure alignment of the two projects. A small group of ocean dynamics experts will be identified to advise on the details and outcomes of the test cases, and have oversight of the project outcomes. This Advisory Group will also be tasked with looking for opportunities to follow up on this work beyond the end of this first stage, through studentships, Responsive Mode, Research Programme and European projects.

		Lead	Month: from Feb 2014											
WP	Task		1	2	3	4	5	6	7	8	9	10	11	12
1	T1:Familiarisation and Planning	NOC												
1	T2:Kernel development	STFC												
1	T3:Algorithm development	NOC												
1	T4:Connection to PSy layer	STFC												
2	T1:Test case design	NOC												
2	T2:Benchmark tests with NEMO	NOC												
2	T3:Benchmark tests with Gocean:2D	NOC												
2	T4:Scalability tests	STFC												
3	T1:Exploitation/outreach	NOC												

Project Gantt Chart: NOC and STFC will work together on each task - the lead responsibility is indicated.

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