THE NERC MARINE CENTRES' STRATEGIC RESEARCH PROGRAMME 2007-2012

Theme 9: Next Generation Ocean Prediction Systems

Numerical models are a vital tool for developing our understanding of the Earth system and how it responds to natural and anthropogenic change. Such models must be able to efficiently represent the marine environment from the global ocean to shelf seas and estuaries, linking hydrodynamics and ecosystem processes with the accuracy to provide reliable short and long term predictions. Theme 9 will deliver the state-of-the-art models needed for the next decade of UK marine science.

Theme 9 comprises three Research Units and twelve Work Packages:

Developing and Integrating coastal-ocean modelling systems (Proudman Oceanographic Laboratory). *POL Theme Leader: Jason Holt jholt@pol.ac.uk*

- WP 9.1 Assessing and improving accuracy of shelf sea models
- WP 9.2 Unstructured grid model development: ICOM
- WP 9.3 Structured grid model development: POLCOMS and NEMO
- WP 9.4 Multi-decadal simulations

Quantifying and reducing uncertainty in marine ecosystem models (Plymouth Marine Laboratory). *PML Theme Leader: Icarus Allen jia@pol.ac.uk*

- WP 9.5 Simulation of carbon, nutrients and production of climatically-active gases in the pelagic and benthic marine ecosystem
- WP 9.6 Development and maintenance of the next generation of hydrodynamic-ecosystem models, from estuaries to oceans
- WP 9.7 Reducing uncertainties to improve operational forecasts, climate change simulations and environmental risk assessments
- WP 9.12 Simulation models as integrative and predictive tools relevant to human health risks

Development and maintenance of leading-edge ocean and coupled climate models (National Oceanography Centre, Southampton). *NOCS Theme Leader: Adrian New a.new@noc.soton.ac.uk*

- WP 9.8 Next generation methods for large scale ocean modelling and climate change investigation
- WP 9.9 Development and maintenance of coupled climate models
- WP 9.10 Maintenance and development of global ocean models
- WP 9.11 New methods of analysis and validation: ecosystem model testbeds

The text that follows is based on that submitted to NERC. For details on other Themes and National Facilities, see www.oceans2025.org. This information is made public by the Oceans 2025 Directors to facilitate engagement of the wider community in the programme; permission is required for other uses. This text includes material (WP 9.12) originally part of another; however, it does not include information on resource requirements, and is limited to fully- or partly-funded activities within the Oceans 2025 programme. Since not all the programme is fully-funded, there may be changes to some objectives and deliverables (to be identified in the Implementation Plan).

Theme 9: Next Generation Ocean Prediction Systems

Strategic setting

Oceans 2025 emphasises the need for a strong predictive capability in our understanding of the Earth system, and the delivery of this knowledge and capability to UK stakeholders. This can only be achieved through a concerted and coordinated modelling effort, that is also central to NERC strategic priorities (Global change; Earth's life support system; and Sustainable economies; NERC, 2002. At a recent ocean modelling strategy meeting (at NOC, Jan 2006), the UK ocean modelling community (including NERC Centres, the Met Office, Hadley Centre and the HEI sector) converged on two hydrodynamic ocean models: NEMO (the present-generation community modelling framework of choice, to facilitate concerted interaction by ocean modellers and key users in the UK and Europe) and ICOM (a very promising future generation model). The wider context for ocean modelling was also clearly recognised as delivering into Earth system models, to connect climate, ecosystems and human actions. Some of the most challenging issues and process interactions relate to those wider connections. This approach builds on the AMEMR conference (Plymouth, July 2005[1]), that recognised the need for a new generation of ecosystem models that address the issue of appropriate complexity in a traceable fashion, and that can be verified against observations. This emerging consensus shows that it is now timely to build a coordinated modelling programme, from the global ocean to shelf seas and estuaries - the aim of Theme 9.

Numerical models have a unique ability to integrate our empirical and theoretical understanding of the marine environment. Moreover, modelling provides the only scientific technique to elucidate the workings of the marine system, its coupling with other parts of the Earth system, and predict its short- and long-term evolution. Theme 9 sets out a programme of model development, investigation and maintenance that will substantially improve modelling capability and accuracy, focusing on marine hydrodynamics and ecosystems. The complexity of the systems and interactions being investigated makes model development itself a multidisciplinary scientific challenge of the highest order, drawing on the relevant oceanographic disciplines, and the numerical and computer sciences. Because of the multidisciplinary nature of the work, the considerable resource requirement and the strategic importance, it is appropriate to carry out model development and support at a national and international level, coordinating this effort through the use of community model systems.

In addition to responding to NERC's strategic need for marine modelling within a wider Earth system and climate context, Theme 9 will help meet wider UK requirements: Government bodies, such as Defra/Cefas, SEERAD/FRS, DARDNI, EA, MCA, SEPA and JNCC, have increasing needs for temporally and spatially resolved ocean information, to help protect and manage the marine environment (eg. Renewable Energy Atlas, Cooper *et al* 2006 and Irish Sea Pilot, Vincent *et al* 2004). The underlying modelling technology for operational forecasting, climate change science and environmental risk management is therefore of fundamental importance to the understanding and prediction of change in the marine environment and its consequences. The primary vehicle for this knowledge transfer exercise is the National Centre for Ocean Forecasting – a partnership between the Met. Office, POL, PML, NOC and ESSC, whose mission is to establish ocean forecasting as a part of the national infrastructure, based on world class research and development. In the European context this coordinates with the MERSEA-IP in its delivery of a key component of the Ocean and Marine Services element of GMES by 2008, particularly by harmonising operational and research ocean modelling systems and rapid technology transfer between the two.

The wider marine research community will draw immense benefits from a strong, coordinated modelling effort both through the provision of infrastructure, support and critical mass for myriad curiosity-driven research projects and through its interaction with large directed programmes. Of these programmes, QUEST (2003-09) has the largest emphasis on modelling – with the aim of assimilating information and expertise from many sources within and outside the UK. Its unique

[1] http://www.amemr.info/

focus is on interdisciplinary research that is closely targeted to deliver a substantial improvement in the prediction of global environmental change. QUEST has a joint modelling strategy[2] with NERC centres and the Hadley Centre (Met Office), targeted to provide quantitative understanding of how interactions between all aspects of the Earth system could alter the course of global change. Many aspect of Theme 9 are aligned with this strategy; for example the use of the Hadley Centre coupled atmosphere-ocean models, NEMO and PFT models.

Theme wide science aims

1. To substantially improve our understanding of the causes of model uncertainty (inaccuracy); to improve our ability to quantify this uncertainty; and to reduce it using model development and data assimilation. The focus is on developing a short and long term forecast capability, in both ocean (and shelf sea) only and coupled ocean-atmosphere models.
2. To substantially improve the formal accuracy and capability of our model systems. Through the development of the next generation of hydrodynamic models, using adaptive and unstructured grid methods, we aim to deliver a modelling system capable of seamlessly simulating shelf seas and open oceans that will form the basis of UK community models for subsequent decades.
3. To determine the appropriate levels of complexity required for simulating the cycling of carbon, nutrients and climatically active gases through the pelagic and benthic marine ecosystem of estuaries, shelf seas and open ocean, and use this to develop a new generation of ecosystem models that represent complexity in a objective, systematic and traceable fashion.
4. To provide support for existing modelling systems, including development, maintenance, and large (time/space) scale model simulations to aid analysis in other Themes and for the community as a whole.

Centre contributions

- POL: Development, integration and analysis of shelf sea modelling systems, both current and 'next generation' – particularly physics (hydrodynamics, waves, turbulence) but also working with coupled ecosystem and sediment models
- PML: Better understanding of ecosystem model complexity leading to the next generation plankton functional type models for shelf seas, development of capability for integrated estuarine, coastal and shelf seas ecosystem modelling. Quantification of model uncertainties and improved forecast capability for plankton
- NOC: Next generation modelling methods (including unstructured grid modelling), maintenance and development of coupled atmosphere-ocean and ocean-only models, nested and high-resolution ocean modelling, ecosystem model test-beds.

Substantial added value comes from the Centres' involvement with NERC directed programmes such as RAPID and QUEST (both to 2009); the NERC 'Pain' consortium (see WP 9.8); the NERC EO centre CASIX (to 2008); and funding from the Met Office and EU programmes (eg. MERSEA).

Developing and integrating coastal-ocean modelling systems

Contribution to Theme 9 by Proudman Oceanographic Laboratory

Background

Shelf seas are a disproportionately important component of the marine environment. They are regions of exceptionally high biological productivity fuelled by rapid biogeochemical cycling (Gattuso *et al* 1998). This gives them an important role in the global carbon cycle (eg. Thomas *et al* 2005) and leads to the major fisheries of the world being located in these seas. They mediate the transport and transformation of material (carbon, nutrients, pollutants, freshwater) from the land to the open ocean and hence are the region of the marine environment under most direct human impact, and of which our society has most direct experience. These science issues are addressed by

[2] http://www.nerc.ac.uk/funding/thematics/quest/esms.shtml

Themes 3 and 6, which require substantial modelling capability and effort; the object of Theme 9 is to provide the necessary modelling tools and to help answer key questions concerning the role and behaviour of shelf seas.

Numerical models provide a unique capability for investigating the behaviour of shelf seas and are increasingly used as a management tool to direct environmental policy (eg. Cooper *et al* 2006; Vincent *et al* 2004). The important role of models arises from their ability to provide a complete description of the system (including its fluxes), from their integrating role in investigating how processes from a wide range of disciplines interact simultaneously, and from their ability to make predictions. However, numerical models only ever provide an approximation of reality at some (often limited) level of accuracy. This component of Theme 9 will substantially reduce uncertainties in the shelf sea modelling systems used by POL and stakeholders (particularly NCOF); it will also produce key error-quantified multi-decadal model data sets for use in Themes 3 and 6, and as a resource for the wider community. Since there is a wide diversity of modelling approaches, it is important that we draw from the experience of the full range of models used internationally, whilst focusing our development efforts on a small number of modelling systems.

Specific objectives

i) To identify, quantify and reduce uncertainties in coastal-ocean modelling systems through the inter-comparison of a range of models, model data-synthesis and data assimilation techniques.
ii) To develop the unstructured and structured grid shelf sea modelling capability available to ourselves and the stakeholders
iii) To conduct and validate key model experiments in conjunction with other Themes.

Approach and methodologies

We shall work on a variety of models (described below): developing and testing POLCOMS, ICOM and NEMO, but also include three internationally well established models in the inter-comparison experiments (WP 9.1).

- POLCOMS (Holt & James 2001; structured B-grid, terrain following): A mature multi-disciplinary model of the hydrodynamics-ecosystem-sediment system (here hydrodynamics includes waves and turbulence), based on coupling the POLCOMS, ERSEM (Blackford *et al*, 2004), WAM (Monbaliu *et al*, 2000) and GOTM (Umlauf & Burchard, 2005) models. At high latitudes sea ice is simulated with the CICE model. POLCOMS was developed under POL and PML core science 2001-07, a range of NERC (e.g. MarProd, CASIX, RAPID, GCOMS) and EU (e.g. MERSEA, Ferry Box, ODON) projects, and contracts with the Met Office.
- ICOM (amcg.ese.ic.ac.uk/research/ocean; unstructured finite element 3D adaptive): Based on computational fluid dynamics (CFD) technology substantially more sophisticated than that generally used by the oceanography community, including unstructured and adaptive meshes. This model has the potential to significantly improve our modelling capability over the next decade, but it has not yet been developed for shelf seas.
- NEMO (www.lodyc.jussieu.fr/opa/; structured C-grid, z-star): based on 'traditional' model technology, this deep-ocean model has much improved coupling capability (through the OASIS coupler). It is becoming the primary European model for operational oceanography, and hence can provide rapid knowledge transfer to key stakeholders. It has yet to be developed and extensively tested in shelf sea environments; an area where POL can make a vital contribution.
- ROMS (Haidvogel *et al*, 2000; structured C-grid, terrain following) Rapidly becoming the international standard in terrain following coastal-ocean models
- QUODDY (Lynch, 1996; unstructured finite element, terrain following).
- MIT GCM (Marshall *et al* 1997; structured C-grid, non-hydrostatic, geopotential finite volume).

As time and resources permit other internationally well known models might also be investigated; candidates include FVCOM, HYCOM, TELEMAC, and GETM.

WP 9.1 (POL) Assessing and improving accuracy of shelf sea models

Uncertainties exist in a model's formulation (theoretical, empirical, numerical, and its parameter set) and its forcing (boundary and initial conditions). These uncertainties manifest themselves in a model's ability to reproduce observations, known theoretical and experimental cases where a clear solution exists, and fundamental principles such as conservation laws. The scientific challenge is to relate a given uncertainty to a particular aspect of the model's formulation and/or forcing, and devise an appropriate solution. To achieve this, rigorous and detailed numerical experiments are required along with painstaking analysis. However, because of the complexity of the systems involved and the lack of rigorous constraints, a consensus on a single modelling approach has not been reached in the international modelling community; this has led to a wide diversity of models. WP 9.1 will exploit this diversity to identify the key causes of model uncertainty and use this to direct the model development in WP 9.2 (ICOM) and WP 9.3 (POLCOMS and NEMO).

The work will involve a detailed model inter-comparison experiment starting with the models' ability to reproduce well known test cases and obey fundamental conservation principles, then move on to three test locations, where extensive observational data sets will be used to inform the model inter-comparison. These locations are: eastern Irish Sea (EIS), Malin-Hebrides shelf (MH) and Celtic Sea (CS). Each presents the models with one of the key challenges facing current models: i) representing the horizontal diffusive transport of salinity from coastal sources (EIS), ii) representing the three dimensional (3-D) propagation of internal tides at the shelf edge (MH), and iii) accurately reproducing the thermocline structure and diapycnal mixing in open stratified waters (CS).

Where appropriate, all the models described above (POLCOMS, ICOM, NEMO, QUODDY, MIT, ROMS) will be employed in each test location. The forcing (boundary conditions, atmospheric fluxes, bathymetry) will be consistent between the experiments, and a common set of diagnostics will be used to compare the model results, drawing on the experience of the NOMADS projects[3]. The sensitivity to various oceanic and atmospheric forcing will also be investigated, for example comparing various resolutions of NWP model forcing. The challenge is then to deconstruct the differences in model output to identify key differences in model formulation and forcing that affect its performance. Sophisticated statistical analyses (e.g. Receiver Operator Characteristics, Vayssieres *et al* 2002) will be used to evaluate the models' predictive capability against the available observations, particularly the Liverpool Bay Coastal Observatory in the EIS (SO 11). In addition to accuracy, computational efficiency of the major high performance computer architect-ures will be investigated as this is a significant constraint on our modelling capability. This builds on a strong, long standing, collaboration with CCLRC, Daresbury Laboratory and is also an opportunity for SOFI funding.

Data assimilation techniques will be applied extensively for this work, particularly in the EIS. These provide the formalism for combining model and observations in a systematic fashion to quantify errors and adjust the model state to better represent reality. The application of these techniques has tended to focus at POL on sea surface temperature and sea level (parameters that are comparatively well modelled; Holt *et al* 2005). We shall shift this focus to parameters that are less well modelled: surface currents derived from HF radar, and salinity and SPM from ferry and CTD observations. We shall concentrate on ensemble based assimilation methods, since these provide useful information about the spatial structure and time evolution of the background error of the system, and investigate ways of using this information to develop less expensive methods.

The area of diagnostics to relate model results to theory (e.g. momentum, energy, (potential) vorticity balances) is one that is often neglected in shelf sea modelling. We shall work on general-izing the techniques used in the deep ocean for the high-turbulence regime of shelf seas and aim to produce a tool box of model diagnostic techniques. This is a possible area of SOFI involvement.

[3] www.pol.ac.uk/home/research/nomads2/index.html

While WP 9.1 will focus on the dynamic equations (momentum, continuity and scalar transport), the methodology is readily extendable and we shall collaborate with Theme 3, PML and NCOF, and seek co-funding, to extend the scope to sediment transport and ecosystem modelling.

WP 9.2 (POL) Unstructured-grid model development: ICOM

Resolution is a primary determinant of model accuracy, as demonstrated in the NOMADS II inter-comparison experiment (Delhez *et al* 2004). However, the wide range of space scales acting in marine environments (from coast to ocean) makes uniform resolution models extremely inefficient, significantly limiting our capability and accuracy. Unstructured grid models potentially offer an attractive solution to this. *A priori* knowledge of where increased resolution is required (making a fixed grid appropriate) exists only in cases where it is dictated by bathymetry and/or coastline; otherwise grid adaptivity (whereby the grid is determined dynamically as the flow evolves) is the ideal solution. The ICOM model, currently under development (see WP 9.8), should make it possible to achieve this, through use of techniques developed by the CFD community. However it has yet to be developed and applied for realistic shelf sea cases; hence we shall work in collaboration with Imperial College to develop ICOM for applications such as the cases in WP 9.1.

The aim is to substantially improve the accuracy and capability of the hydrodynamics modelling and work towards developing such systems for multidisciplinary and operational work. We shall start by investigating well defined test cases (e.g. from the COHERENS project[4]) but rapidly progress to realistic domains that have been extensively modelled by more traditional methods and are backed-up by extensive observational data sets (e.g. tides in the Irish Sea, Jones & Davies 1996; seasonal cycle of southern North Sea temperature, Luyten 2003, Holt *et al* 2005; tidal straining in the Southern North Sea, Souza & James, 1996). Our development will focus on aspects of the dynamics of fundamental importance to shelf seas: turbulence/mixing, propagation of coastally trapped waves, oceanic/atmospheric forcing. This topic area is a candidate for SOFI funding.

WP 9.3 (POL) Structured-grid model development: POLCOMS and NEMO

POLCOMS is the primary shelf sea model in use throughout Oceans 2025 (Themes 1, 3, 6 and 10) and provides the backbone of the Met Office's shelf sea operational modelling capability[5]. It is vital therefore that we maintain it at the forefront of structured grid modelling technology through work on all aspects of the code. Development work on the POLCOMS model systems will focus on its use as a multi-disciplinary model capable of simulating interactions between hydrology, circulation, turbulence, waves, ecosystem and sediment systems.

Experience with the operational use of this system at the Met Office (Siddorn *et al* 2006) and extensive error quantification (Holt *et al* 2005) indicate two areas requiring attention. First, the representation of vertical mixing (boundary layers and stable/unstable stratification) and horizontal transport and mixing is crucial to the model's ability to simulate biophysical interactions. This requires assessment and development of (vertical and horizontal) turbulence schemes, internal pressure gradient calculations and advection schemes. Second, the use of a coupled wave-current model (eg. Osuna & Wolf, 2005) to include a new range of processes (eg. Langmuir circulation, wave-current interaction in the benthic boundary layer, radiation stress) has the potential to substantially improve estimates of momentum flux at the surface and sea bed, and hence improve the modelled wind driven circulation and its representation of storm surges (with Theme 3).

These developments will be informed by improved process representations developed in Theme 3 and by the inter-comparison experiments in WP 9.1, and will feed back to further inter-comparison experiments. Developments here will feed into the model simulation used in WP 9.4 and Themes 3 and 6, and operational use in Theme 10.

---

[4] http://www.mumm.ac.be/~patrick/mast/**coherens**.html
[5] see http://www.metoffice.gov.uk/research/ncof/shelf/index.html

In addition to developing POLCOMS, we shall work to develop NEMO for shelf sea use. Based on OPA9 (www.lodyc.jussieu.fr/opa/) and developed by LODYC/ CNRS, NEMO is a deep ocean model that is becoming the main operational oceanographic model in Europe. Thus NEMO underpins the EU MERSEA programme; the UK Met Office is currently transferring to NEMO from FOAM; NEMO forms the ocean component of the NERC QUEST Earth system modelling strategy; and it has a wide range of other international users in research and operational oceanography. Many aspects of NEMO are not yet appropriate for shelf sea modelling (e.g. the vertical coordinates and the treatment of the free surface). Although there has been some effort in developing this system for shelf seas work (at the Met Office and LODYC), this is only planned to reach the level of sophistication of a model such as POLCOMS or ROMS by 2008, and then only with limited testing in hindcast mode.

Exploiting the recent modelling advances made by POL, WP 9.3 will develop NEMO and make it truly a state-of the-art structured grid shelf sea modelling system. To accelerate and extend the scope of this work – and maximise knowledge transfer – we will seek additional funding from the Met Office (eg. for multi-disciplinary coupling and near-coastal applications). While there are limited direct scientific benefits to our modelling capability from this work, there are immense benefits in terms of coordinating the UK shelf sea modelling effort (particularly the increased support that will be available to university stakeholders). These benefits will feed rapidly through to scientific work, for example the GCOMS model (see WP 9.4) could transfer to NEMO, which would mean a consistent marine model is used by QUEST, allowing direct comparison with the oceanic application in regions where they overlap.

WP 9.4 (POL) Multi-decadal simulations

Many shelf sea processes act on multi-year time scales, so investigations of variability arising from atmospheric, oceanic and terrestrial forcing, including distinguishing between climatic and anthropogenic effects, require substantially longer integrations than have generally been carried out. Processes of particular interest are cross shelf (advective and diffusive) transport of water, carbon, nutrients and pollutants, and biogeochemical cycling. It is now appropriate to extend the multi-decadal simulations with POLCOMS (eg. Young & Holt, submitted) in two ways: from physics-only to fully multi-disciplinary, and from hindcast to prediction.

WP 9.4 will provide two key error-quantified data sets, for use in Themes 3 and 6, and that will also be made available for the wider community.

- 1950 to 2050 simulations of the NE Atlantic with the full POLCOMS-ERSEM-WAM-GOTM model. These simulations will use a range of surface forcing both from re-analyses (ERA40, NCAR) and future scenario predictions (HadCM3, HadGEM). Boundary conditions will initially be climatology, but will use data from similar whole North Atlantic simulations carried out by PML (WP 9.6 and Theme 6), as they become available. Model resolution and the number of realisations will depend on the computer resources available, but will be at least 1/10° and 2x50 year hindcast, 2x50 year future scenarios. The physics component of these simulations will be repeated with the NEMO model to provide a direct comparison (with Themes 3 and 6).
- 1960 to 2000 simulations of the global coastal-ocean focusing on the carbon cycle. The GCOM e-science project (2006-09) aims to develop the techniques for running multiple large scale shelf sea domains coupled to global ocean climate simulations. It uses POLCOMS and a reduced complexity (layer integrated) version of ERSEM. This work will follow on from that project to extend the simulation period from 10 to 40 years, and may also include future climate scenarios if the model is deemed to be sufficiently accurate and computer resources are available (with Theme 3).

In both cases the focus will be on large time/space scale model verification, an aspect largely missing from GCOM (sensitivity experiments, analysis and interpretation of the model data sets will primarily be carried out in Themes 3 and 6). We shall utilize the techniques of data mining developed by the e-science community to develop automated model verification procedures, for example by developing a direct interface to data centres and/or the NERC data grid. Our work will focus on verifying the physics models, while we shall collaborate directly with PML on the verification of the biogeochemical model.

Summary research plan and deliverables (WP 9.1 - 9.4)

2007 - 08	• Test cases with data sets (WP 9.1)
2007 - 09	• POLCOMS-ERSEM 50yr hindcasts (WP 9.4)
2007 - 10	• ICOM code appropriate to shelf seas (WP 9.2)
2007 - 12	• Model inter-comparison (WP 9.1)
2008 - 10	• NEMO code appropriate to shelf seas (WP 9.3) • Model verification and diagnostic techniques (WP 9.4) • POLCOMS-ERSEM 50yr forecasts (WP 9.4)
2009 - 12	• Comparison with conventional model systems • GCOMS 40yr hindcasts (WP 9.4)
2010 - 12	• NEMO (shelf) 50yr hindcasts (WP 9.4)
Ongoing	• Periodic POLCOMS upgrades to community (WP9.3)

Quantifying and reducing uncertainty in marine ecosystem models *Contribution to Theme 9 by Plymouth Marine Laboratory*

Background

Modelling is a key scientific technique by which we can elucidate the workings of the marine system and predict its evolution in both the short and long term – including responses to anthropogenic changes. The underlying modelling technology for operational forecast, climate change science and environmental risk assessment is therefore of high strategic importance. The primary role of models in ecosystem science is to provide a simplification of complex reality, yet as our understanding of the marine biogeochemical system increases, more complex models are required. The need is to ascertain appropriate levels of complexity to enable ecosystem models to have predictive skill while also providing scientific insight. The development and enhancement of hydrodynamic-ecosystem models has reached the point where the outputs are of a complexity and volume that require simplification in order to be understood; model evaluation, when attempted, is often qualitative and largely subjective. We intend to make model evaluation the quantitative science it ought to be, to increase understanding and reduce uncertainty in environmental forecast.

Specific objectives

i) To determine the appropriate levels of complexity required for simulating the cycling of carbon, nutrients and climatically active gases through the pelagic and benthic marine ecosystems of estuaries, coastal and shelf seas.
ii) To develop and maintain the next generation of coupled hydrodynamic-ecosystem models for estuaries, shelf seas and contiguous oceans.
iii) To understand and reduce the uncertainties in marine ecosystem models in order to improve our understanding of interactions and feedbacks within the marine system and our capability for operational forecast, climate change simulation and environmental risk assessment.

To meet these objectives we shall address five fundamental scientific questions:

- How can we most efficiently parameterise, in a model, key processes to reproduce the seasonal cycle and interannual variability of planktonic and benthic ecosystems?
- How can we best parameterise the acclimation of ecosystem processes to climate change?
- Can a hierarchical approach to modelling, from 0-D to 3-D, conceptual to analytical, allow us to better understand an ecosystem and formulate models of appropriate complexity?

- What are the uncertainties in our models and how can we reduce them?
- How can we assimilate Earth observation data to reduce uncertainty in our models and hence improve forecast?

Approach and methodologies

PML's overall approach to modelling involves three overlapping areas: the development of the process knowledge and modelling base; the quantification and understanding of models errors; and the nature of emergent properties. This Theme deals with the first two tasks, the last is dealt with in Themes 2, 3, 4 and 6.

PML was instrumental in developing the European Regional Seas Ecosystem Model (ERSEM), and in Oceans 2025 the model will radically evolve. ERSEM was developed to simulate nutrient cycling and ecosystem response in European shelf seas (Baretta *et al* 1995, Blackford *et al* 2004). It is a generic model which incorporates a distributed, 'plankton functional type' (PFT) description of 8 plankton, quantifying the cycling of carbon (C), nitrogen (N), phosphorus (P) and silicon (Si) through the pelagic and benthic ecosystem. It includes dynamic C:N and C:P ratios for each PFT, dynamic C:chlorophyll for each phytoplankton type and carbonate chemistry. A complementary version, ERSEM-BioGas, describes the planktonic production of biogenic sulphur compounds (DMS/DMSP) and their biological modification into climatically active gases (Archer *et al* 2004).

We aim to establish and maintain a shelf-ocean ecosystem model for the N Atlantic and NW European shelf based on ERSEM and NEMO, and to establish and maintain an estuarine-coastal ecosystem model based on ERSEM and POLCOMS.

WP 9.5 (PML) Simulation of carbon, nutrients and production of climatically-active gases in the pelagic and benthic marine ecosystem

In WP 9.5 we shall explore how complex a functional group model must be to represent the shelf seas ecosystem, balancing the need to describe all relevant processes, uncertainty in parameter-isations and the discovery of new processes. Our purpose is to optimise ecosystem representations for shelf seas modelling, with the additional benefit of addressing the issue of model complexity for application in global ocean models. We propose three strands of work: improvement of existing model parameterisations; the addition of new processes; and the evaluation of these developments. This work can be undertaken with existing knowledge and data sets, but will be considerably strengthened by strong interactive links with Themes 2 (biogeochemistry), 3 (shelf seas processes) and 4 (biodiversity). In return, improved simulation models will be delivered to these Themes for use in hypothesis testing. These model developments will benefit from data acquisition by the Oceans 2025 Sustained Observatories, AMT (SO 1), WCO (SO 10) and CPR survey (SO 15)

The aim is to build models to quantify carbon, nutrients and sulphur cycling in European seas including the North Atlantic margins. Building on radiative transfer and inherent optical property models (eg. Lee *et al* 2002) we will improve the parameterisation of the propagation of light through the water column and hence improve short term forecast capability. Advances in our understanding of DMS/DMSP cycling indicate that we should reparameterise both photo-oxidation of DMS (eg. Toole & Siegel 2004) and the photo-protective role of DMSP (Sunda *et al*. 2002) in our parameterisations of the intracellular content and turnover of DMS. Bioturbators and bio-irrigators have been demonstrated to be important in mediating nutrient cycling and benthic pelagic exchange (eg. Howe *et al* 2004); we will revise the benthic model to explicitly describe this. New parameterisations will be developed to describe how viruses short-circuit the flow of carbon and nutrients to higher trophic levels by shunting it to the DOM pool. Emerging work (Flynn & Mitra, 2005) indicates that selective grazing as a consequence of food quality may be an important response of zooplankton populations; improved parameterisation of zooplankton grazing is an opportunity for SOFI involvement.

The impact of climate change may potentially be damped by the ability of plankton to buffer the effects of changes in light, nutrients and pH (eg. Allen *et al*. 2006). We will focus on the following key acclimatory processes. Standard logarithmic parameterisations of temperature response are not substantiated (Montagnes 2003), and we will explore the implications of this for functional type models. To date it has been shown that high CO_2 and acidification affects nitrification, calcification, primary production and the health and fecundity of many higher trophic levels, including benthic recyclers (Raven *et al*, 2005). We will develop ERSEM to simulate these effects and quantify the integrated impact on C and N cycling (with PML Theme 6). There are still large uncertainties in estimates of the balance between photosynthesis and respiration; we will improve parameterisation of photosynthesis (light acclimation) and respiration.

We will investigate model complexity by testing if we can reduce the number of functional groups/ processes in the model without compromising functionality or performance. Model data comparison using our suite of 0-D and 1-D shelf seas ecosystem models (Blackford *et al* 2004) as a test-bed, allows key processes to be identified along with their relative size, error and importance. Parameter estimation techniques (Spitz *et al* 1998; Wirtz & Wiltshire 2005) will be applied to assess parameter sensitivity and to derive model data misfit functions. The best model structures and parameterisations will be evaluated in 3D and delivered as new versions of the PFT model. WP 9.5 will benefit from working closely with the oceanic ecosystem test-bed studies proposed by NOC in this Theme.

WP 9.6 (PML) Development and maintenance of the next generation of hydrodynamic-ecosystem models, from estuaries to oceans

To simulate shelf seas ecosystem function response to climate change we need to model two way exchange across the shelf ocean interface. We will develop an infrastructure of coupled hydrodynamic ecosystem models that link via the same ecosystem model, the estuary to the open ocean (using NEMO, see WP 9.3 and 9.10), thus removing uncertainties in boundary conditions created by nesting biological models of differing structure and complexities. Our existing model infrastructure is POLCOMS-ERSEM (eg. Allen *et al* 2001, Holt *et al* 2004), which resolves shelf seas ecosystem processes at a scale of up to 1.8km. POLCOMS can be run at much finer resolutions (~ 100m) and is highly suitable for coastal and estuarine applications.

Initially we will couple ERSEM to NEMO for the 1/3˚ North Atlantic, to provide boundary conditions for the shelf seas model and to compare model performance between the ocean model and the shelf seas model (in conjunction with POL). The North Atlantic NEMO setup will be provided by the Met Office through NCOF. We will also couple ERSEM-Biogas to NEMO to enable quantification of the North Atlantic DMS budget. This work will provide simulation tools to underpin related work in Themes 2 and 6. The models will later be upgraded to a 1/9˚ resolution. The existing POLCOMS- ERSEM model will be set up to simulate key UK estuaries and their adjacent coastal zones at high resolution (~100m) and the benthic ecology adapted to intertidal environments. The initial focus will be the data-rich Plymouth coastal zone (including the Tamar estuary) and will provide simulation tools to underpin the Western Channel observatory (SO 10) and sediment water interface studies in Theme 3.

WP 9.7 (PML) Reducing uncertainties to improve operational forecasts, climate change simulations & environmental risk assessments

Increasingly marine system models are being used for prediction (eg. Siddorn *et al* 2006); however any mechanistic model can obtain a good fit for the wrong reasons and a model which provides a poor fit clearly may not give an adequate representation of the underlying processes. To develop the next generation of ecosystem models, and thereby make significant progress in reducing model uncertainty, far more attention needs to be paid to model errors, validation, and the abilities of various models to reproduce spatio-temporal dynamics in real ecosystems. Data assimilation is the reanalysis, estimation and prediction of an unknown true state by merging observed information into a model, and is used to improve model forecast capability. The Ensemble Kalman Filter (EnKF; Evensen 2003) has been demonstrated to improve the estimation of both assimilated and non-assimilated variables in ERSEM (Torres & Allen 2006) suggesting these methods could improve our short term ecosystem forecast capability.

We will investigate novel techniques for model validation to understand the spatio-temporal variability of uncertainty. Our focus will be the use of satellite remote sensing data. A suite of error quantified fields of up to 30 years in duration (eg. GHRSST-PP sea surface temperature, chlorophyll, sea surface height, primary production, sea surface fronts and satellite derived PFT) will be used to compare with 3D hydrodynamic ecosystem model output on daily, weekly, monthly and annual time scales. Statistical techniques and analysis tools (e.g. ROC; Vayssieres *et al* 2002), multidimensional scaling (Clarke 1993), EOF analysis and SOMs (Richardson *et al* 2004) will be applied to allow quantification of differences which will then feedback to improve the processes perceived to be the source of the error. Time-series analysis tools and techniques will be used to quantitatively assess model performance against *in situ* data.

To improve short term forecast capability for phytoplankton, we will use data assimilation techniques for satellite-derived inherent optical properties in 3-D regional models (eg. the data rich SW English Channel), including a comparison between a full EnKF and a reduced rank ensemble based algorithm (eg. SEIK and related algorithms; Pham *et al* 1998). SOMS will be used to define biomes and hence restrict the impact of observations to ecologically consistent regions. We will investigate the benefits of combined physical and biological data assimilation in 3D high resolution models using intensive sampling periods. The most appropriate methods will allow implementation of a 3D system with routine assimilation of satellite derived optical properties to be run for the Western Channel Observatory (SO 10). Effort will also be directed at developing methods to use data assimilation to trace and identify error sources in the model dynamics and parameterisation.

WP 9.12 (PML) Simulation models as integrative and predictive tools relevant to human health risks

Specific objectives

i) To use structured complex models to simulate environmental processes that may impact on human health.
ii) To predict environmental risks to human health from pollutants, biogenic toxins and microbial and viral pathogens.
iii) To develop modelling tools as novel research aids to reduce dependence on animal testing and provide pre-operational tools for environmental management related to human health risks.

Rationale and approach

Generic quantitative models will provide solutions to the problem of predicting the risk of natural and man-made stressors, by simulating pollutant pathways in the human food chain, and the behaviour of human pathogens in the environment. Novel models will determine pathological reactions, at the molecular and tissue level, to environmental toxins and nanoparticles. Models, if used under carefully defined conditions, allow a larger number of possible scenarios to be investigated '*in silico*', than could be assessed in laboratory experiments (Hunter *et al*., 2002; Moore & Noble, 2004). Thus, experimental design can be refined and redundant scenarios can be rejected at an early stage (Noble, 2002).

A number of functional models use analytical approaches to simulating chemical and biological systems, setting up differential equations to represent some part of the system, then solving the equations (Hunter *et al*., 2002). Alternative approaches to model chemical-biological interactions involve the use of cellular automata (rule-based approaches) and network theory (Kohler *et al*., 2001; Tyson *et al*., 2001; Watts & Strogatz, 1998; Wolfram, 2002). Each approach has advantages. Holistic automaton-based models are highly versatile and can have rich qualitative characteristics as simulators, and analytical differential equation-based models are more quantitative. Increasingly, large quantities of data are being generated by new molecular analytical procedures. Bioinformatics, coupled with modelling tools, will provide an effective means for integrating and interpreting this wealth of data. Simulation will also be used as an integrative tool that will enhance the ability to make meaningful predictions.

Several modelling methods will be integrated. Network and cellular automata will simulate the toxin behaviour in the human food-web, microbial pathways and processes and toxin-induced pathological reactions in shellfish. These models will be coupled to differential equation-based models to determine fluxes of contaminants and pathogens; differential equations will also be used to model molecular and cellular components of the surrogate target systems (Kohler *et al.*, 2001; McVeigh *et al*., 2004, Tyson *et al*., 2001; Watts & Strogatz, 1998). These models will be integrated with the ecosystem models of Theme 9 to develop pre-operational tools to assess the risk to human health of toxins, contaminants and pathogens in the marine environment.

Summary research plan and deliverables

WP 9.5 - 9.7

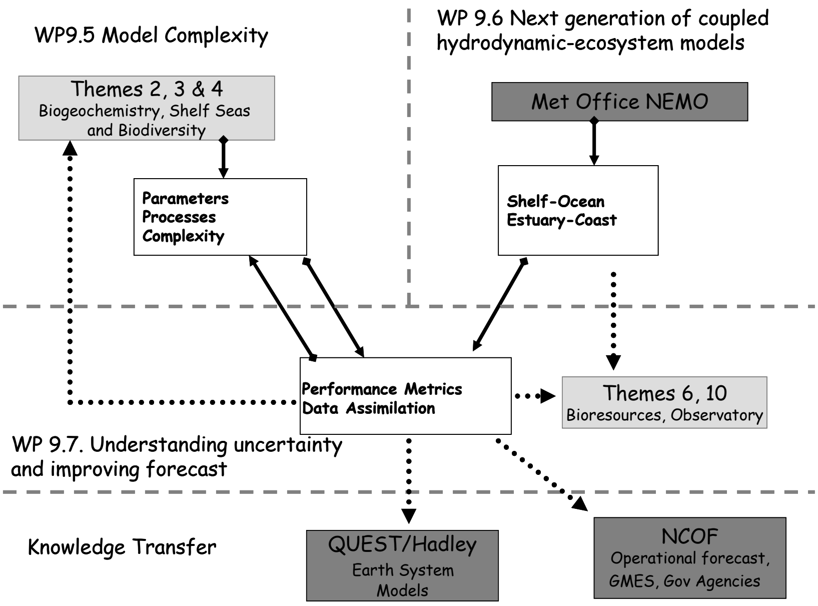

Figure 1 Schematic of contribution of PML WPs 9.5-9.7 to Theme 9. White boxes, work within Theme 9; light grey boxes, other relevant themes at PML; dark grey boxes, external stakeholders. Dotted arrow indicates transfer of knowledge outside the Theme

WPs 9.5, 9.6 and 9.7 are complementary (Fig. 1). They address model complexity and parameter uncertainty; develop the modelling infrastructure for integrated, estuarine; shelf, ocean ecosystem modelling using the best available hydrodynamic models within the UK community; and address the issue of quantifying model uncertainty to improve our short term forecast capability for plankton.

The scheduling of main deliverables for WP 9.5 – 9.7 is as follows:

2007 - 08	• North Atlantic model (ERSEM-NEMO 1/3˚) (WP 9.6)
2007 - 09	• Ecosystem data assimilation system for EO/IOP data (WP 9.7)
2007 - 12	• Improved ecosystem model parameterisations (WP 9.5) • An ability to simulate the acclimation of the ecosystem in response to environmental change (WP 9.5) • Revised PFT models ERSEM and ERSEM-BioGas (WP 9.5) • Library of metrics for analysis and quantification of uncertainty in marine ecosystem models (WP 9.7)
2008 - 09	• North Atlantic Model (ERSEM-BioGas-NEMO 1/3˚) (WP 9.6)
2008 - 12	• Western Channel coastal estuarine model system (WP 9.6)
2010	• Daily forecast capability for phytoplankton using EO data and data assimilation (WP 9.7)
2011 - 12	• N. Atlantic Model (ERSEM-NEMO 1/9˚) (WP 9.6)

WP 9.12

Summary research plan & deliverables

- Designed and parameterisation of different models types.
- Co-evolution of simulations and empirical measurement.
- Hindcast experiments.

- Evaluation of predictive capabilities of the models in collaboration with public health scientists and epidemiologists.

Development and maintenance of leading-edge ocean and coupled climate models

Contribution to Theme 9 by the National Oceanography Centre, Southampton

Background

Ten years ago, cruise-based fieldwork was planned without any reference to model output. Today, almost all seagoers refer to high-resolution model data during their planning process. Model results are also used to put synoptic or space-limited observations into a wider context and are essential for testing hypotheses and making predictions. As such, models have become a necessary technology component of NERC's marine science. This change has occurred because many models now reflect reality to an extent only dreamt of a decade ago. However, this realism comes at high cost: NOC's most realistic global ocean model is too expensive to run for more than a few decades, making it unsuitable for climate prediction purposes. Models are still not easy for the wider community to use, nor is it easy to store and manipulate the many-terabyte datasets produced. The 'joining-up' of models (e.g. coastal and deep ocean) is still under discussion, as is the level of complexity required to represent biogeochemical processes and the carbon cycle in the ocean. Ocean and coupled climate modelling thus faces many challenges. NOC, as the UK centre for deep-sea and global ocean modelling, has both the opportunity and the ability to lead and coordinate ocean components of these activities in the next decade, across NERC Centres and UK universities.

Specific objectives

i) To create new ocean and coupled climate models, either directly or by adapting existing models
ii) To develop and improve existing models in new and innovative ways
iii) To maintain existing ocean, biogeochemical and climate models, e.g. across changes of computing platform, and to ensure their continuing viability
iv) To create new methods of analysing and validating models, including statistical approaches about their uncertainty
v) To facilitate cross-centre interaction and develop closer links with external users, involving movement of codes and modules between centres, sharing of data resources, implementing common standards, and forward planning
vi) To undertake model simulations to support the science in Themes 1, 2 and 5.

Linked to these objectives, we wish to investigate seven questions connected either with climate research or with modelling activities themselves:

- Is there a more suitable ocean model than existing finite-difference models?
- How sensitive are climate models to the structure of the ocean model component?
- How sensitive are climate models to the parameterisations of unresolved oceanic processes?
- How sensitive are climate models to the manner in which sea ice is coupled?
- Can nested models be trusted to give accurate results?
- Can an ocean model be made energetically self-consistent?
- What is the most appropriate level of complexity of biogeochemical models in climate studies?

Approach and methodologies

Four work packages are proposed, in which the aims listed above are integrated into a range of modelling activities that will:

- develop unstructured grid modelling (the ICOM model; WP 9.8).
- develop and maintain coupled climate models, in particular assessing their sensitivity to z-coordinate and isopycnic ocean codes (WP 9.9).

- develop NEMO as the core OGCM for use by the scientific community in the UK, at resolutions of 1°, ¼°and 1/12°, and with nested grids (WP 9.10).
- develop an ocean model testbed permitting objective intercomparison and validation of a range of ecosystem models, with a view to embedding the most promising in OGCMs (WP 9.11).

WP 9.8 (NOC) Next generation modelling methods for large scale ocean modelling and climate change investigation

The finite-difference models currently in use internationally and operationally (eg. at the Met. Office) retain the same structure as those in use 30 years ago (Bryan, 1969), although making use of advanced modern parameterisations and codings. Their ongoing success is due to the increased accuracy provided by finer grids and increased computer power. Nevertheless, a meeting of the international modelling community in 1999 (New Ocean Model Creation Meeting at SOC) concluded that new methods were required to meet future demands of climate science. Future needs include a seamless junction between coastal and deep water models (long sought by POL and NOC) and a physically (and numerically) sensible ‘nesting’ of small detailed areas within larger models. The meeting identified the unstructured grid approach as being the key potential development, and particularly the use of model grids that can self-adapt.

The ‘Pain consortium’ (Imperial College, NOC and Reading University) is funded (2005-09) to deliver a global ocean circulation model of this type, involving the development of fundamental architecture for a next generation ocean model (ICOM). This non-hydrostatic model uses both an unstructured grid (already used in many coastal applications) and, unusually, permits the grid to adapt dynamically over time, steering resolution where it is needed to maximise model accuracy. Within the time frame of the consortium grant, ICOM is unlikely to contain all the sub-models (sub-grid-scale mixing, ecosystems, chemistry and ice) necessary for many practical applications. Furthermore, linking ICOM with other components of the Earth system poses new challenges, not least in the coupling with atmospheric models (NCAS), including the next generation that may themselves be unstructured and /or self-adaptive. Such sub-models and developments are beyond the scope (and skills) of the consortium, but not of the larger NERC community. We therefore propose to engage the NERC Centres (and university groups) at the earliest opportunity in scientific projects which exploit the capabilities of ICOM, while simultaneously helping to improve the consortium’s model. In the final stages of the consortium it is envisaged that the Centres will be using ICOM (outside the scope of the consortium). This will involve:

- constructing a user and model development support base for the community
- continuing development of the fundamental modelling methods and sub-models
- interfacing (eg. with sub-grid-scale parameterisations/models) ecosystem, chemistry, ice and atmospheric models
- creating user friendly interfaces for analysis and problem set up
- development of data assimilation methods so that ICOM can be used as an operational model with increasing confidence.

The ‘Pain’ consortium grant ends in 2009, when there is the opportunity to further develop ICOM as described above, funded via SOFI. This work requires expertise in unstructured adaptive grid modelling, which exists and is being fostered within the UK community external to NOC.

WP 9.9 (NOC) Development and maintenance of coupled climate models

Coupled model framework

While much of our modelling work is aimed at understanding the ocean and its role in the climate system, a full understanding of the latter requires coupling of the atmosphere. A framework for coupled climate models will be imported, developed and maintained at NOC which will allow us to run climate models with different ocean components, whilst also helping other UK groups (Met Office, Hadley Centre, NCAS/CGAM, ECMWF). The initial framework will be based on the

OASIS flux coupler (which follows the European PRISM standard) and the Unified Model Environment from the Met Office. This framework, which will be replaced by FLUME when it is available, provides atmospheric models identical to those used by the Hadley Centre. Thus we will not have to expend effort on the configuration and calibration of atmospheric models. The ocean models that we will provide as part of this framework include the 1° and ¼° NEMO models (WP 9.10), as well as the HYCOM model that is already included in CHIME. Decadal and centennial timescale integrations of the coupled models will be undertaken as required by Theme 1, with both fixed and increasing atmospheric CO_2 levels.

Coupled model sensitivity to the ocean component

We are currently running a coupled ocean-atmosphere model (CHIME) that employs an identical atmospheric component to that used in HadCM3, but with a largely isopycnic representation of the ocean (HYCOM). Current tests show that the long term evolution of the coupled system is sensitive to this alternative to the original z-level ocean representation. The two approaches exhibit markedly differing results when run under conditions of constant atmospheric CO_2, showing a net warming of the climate in CHIME instead of a net cooling in HadCM3. Sea-surface temperature differences reach 5-6° C, with associated air-sea heat flux differences of several hundred Wm^{-2}.

We will investigate the sensitivity of the coupled system to the choice of ocean model configuration in a rigorous framework using the CHIME/HYCOM combination in a 3-year programme. In particular, HYCOM can be configured to run as an isopycnic, z-level, or purely “terrain-following” (sigma-coordinate) model. Runs of the coupled climate system with each of these ocean types will be undertaken with both fixed and increasing atmospheric CO_2 levels. The relative benefits of each configuration will be assessed through inter-comparisons with CHIME (using a mixed vertical description), and with HadCM3 (the z-level version of CHIME being expected to show similar behaviour to that of HadCM3). These simulations will inform the future development of the NEMO ocean model (see WP 9.10; eg. an arbitrary vertical co-ordinate is under discussion), and hence impact on the plans for future coupled models being run at other UK centres such as the Hadley Centre (assisting their model choice for future IPCC assessments of climate change), ECMWF, NCAS/ CGAM, and QUEST, all of which plan to make NEMO their principal ocean model. We shall work with the academic community, via SOFI, for model tuning and for analysis of the atmospheric model data.

WP 9.10 (NOC) Maintenance and development of global ocean models

[50% of this Work Package is considered to be Category 1 in the NERC definitions of different funding modes; Annex 6 of Overview]

A key requirement of climate science is the continued development of existing and new ocean models. NOC has made the strategic decision to discontinue the development of OCCAM and join the NEMO framework, thereby fully supporting a new UK-wide (and partly European) modelling strategy based on NEMO. While OCCAM will still be run in several ongoing projects and thereby require limited strategic support, all NOC model development and simulations for Themes 1, 2 and 5 of Oceans 2025 will be based on NEMO. To ensure a coordinated UK modelling strategy, we will set up global NEMO configurations at 1 and ¼° resolution, so that NOC will provide the central UK repository for global ocean models at these resolutions. This work will be carried out in close collaboration with the Hadley Centre, ECMWF, NCOF and NCAS and will greatly help the development of the next generation HadGEM3 and HiGEM2 climate models (aiming for the next IPCC assessment). We will ensure that these ocean models can be coupled to Hadley Centre and ECMWF atmospheric models via PRISM-compatible flux couplers.

To support the science of Themes 1, 2, and 5, we will carry out ocean-only simulations with the global 1/4° NEMO model with biogeochemical tracers and carbon chemistry under realistic atmospheric forcing (ECMWF, NCEP, and NOC fluxes) over the last 50 years. We will also develop high-resolution (1/12°) North Atlantic and Southern Ocean models nested (2-way) into the global ¼° model. Initial comparison with our completed 1/12° OCCAM results will allow us to establish the accuracy of the nesting approach. NOC model development will also include:

a) Changes in numerics; eg, inclusion of new advection schemes suitable for biogeochemical modelling and QUEST activities.
b) Optimisations of codes for new architectures or computing environments, to ensure that NERC obtains the best return on its HPC investments.
c) Changes to ensure our models fit coupling paradigms such as PRISM. This may involve negotiating changes to the coupling paradigms where existing couplers do not cater for certain features of climate models, eg. ice embedded in the ocean.
d) Additional parameterisations (described below) required to keep our models at the leading edge.
e) Development of NEMO as part of the international NEMO consortium.

Parameterisations

We include parameterisation work in Theme 9 because its necessity goes beyond specific scientific goals - it is important to ensure that our models are as accurate as we can make them for the range of scientific activities being undertaken both by NOC and the wider scientific community. We will therefore continue to develop parameterisations at NOC and to create ways of including them numerically in current and future models, as well as importing the best practice from other groups. Parameterisation work at NOC will involve a variety of process modelling activities:

i) eddies - this is part of a long-term international study into how well climate models represent the turbulent ocean, and how to incorporate these effects in models which cannot include them explicitly, eg. because of coarse resolution (cf. Ferreira *et al* 2005; Canuto & Dubovikov, 2006).
ii) mixing by internal waves, and at the base of the mixed layer - we need to understand both how this mixing occurs in the real ocean, and also how excessively diffusive our existing and future models are; this is vital for both physics and biogeochemistry (cf. Wunsch & Ferrari 2004; Lee *et al* 2002).
iii) ocean throughflow in sills and straits - which even our finest resolution models fail to resolve (part of Theme 5); (cf. Riemenschneider *et al* 2005).

Ice dynamics

NEMO urgently needs the import of an accurate ice model (note that an ice model also forms part of our planned improvements to ICOM). The existing code misrepresents sea ice because in reality sea ice does not simply float on the water surface (which implies an air pressure which varies with ice keel depth), but extends below the surface into the ocean itself (the maximum recorded depth of ice keels in the Arctic is 47m; Wadhams 1998). We will:

i) Import an energy-conserving sea ice model with multi-category ice thickness representation as implemented in the NCAR CSIM5.0 model.
ii) Incorporate embedded sea ice into the ocean boundary layer. This has been recently tested in the coupled OCCAM model and has demonstrated a 20% increase in winter ice volume in the Arctic Ocean. A strategy to solve the problem of the underside of sea ice extending down into several grid boxes is to use the ‘z* coordinate’ which redefines a pseudo-vertical coordinate to be zero at the atmosphere-ocean or ice-ocean interfaces (Adcroft & Campin, 2004). The dynamical coupling is based on incorporating the ice internal stresses into the momentum balances for the sea ice cover and the ocean boundary layer (Heil & Hibler, 2002). However, free-surface elevations under ice shelves, if included in later models, can vary by several hundred meters, and the associated pressure-gradient error will be non-negligible. It may then be necessary to recode the ocean model to permit ice to extend many grid points in the vertical.
iii) Improve the description of the ice melting and formation processes in the model by better parameterisation of bottom and lateral ice melting, and snow-metamorphic ice formation, and including formation of the melt ponds into the ice albedo scheme. Tests performed with 1° and ¼° OCCAM have demonstrated the sensitivity of sea ice volumes to these processes. These changes should overcome the unrealistic skew in the North-South sea ice volume distribution, characteristic of the majority of current climate models.

Nesting and global 1/12° NEMO

The main model configurations we will develop and maintain are the 1° and ¼° global NEMO models, with a progression to a resolution of 1/12° during the latter stages of Theme 9. Access to data generated by our recent 1/12° global OCCAM simulation for the period 1985 to the present day will be provided from the outset. This has been run for about a decade, and by 2007 will be complete (1985-present). This is the only dataset produced in the UK from a fully eddy-resolving global ocean model. Such datasets are vital for cruise planning and model-data intercomparisons, as well as straightforward model analysis.

Several regional studies (including work in Themes 1, 2 and 5) and process studies require spatial grid resolutions finer than the ¼° resolution that we will provide from the outset. Higher resolution will be achieved by using the AGRIF package to couple regional 1/12° sub-models (North Atlantic and Southern Ocean) into the ¼° global model, including biogeochemical tracers. AGRIF is available within the NEMO package and provides a 2-way nesting approach. Results of multi-decadal runs under realistic forcing will be compared with our global 1/12° simulations (those completed in OCCAM, and later to be undertaken in NEMO, see below). Attention will focus in particular on the interannual variability and associated signal transmission across the nesting boundary and also the as yet untested application to sea ice and biogeochemical tracers. This will allow us to study the regions of interest in Themes 1, 2 and 5 at high resolution for a number of scenarios (e.g., windiest winters, warmest summers, global warming) while keeping computational costs manageable. This nesting is not only of direct relevance to the Met Office's FOAM, but also forms immediate links with the shelf sea modelling at POL (WPs 9.1 and 9.3) and PML (WP 9.6).

High-resolution global ocean modelling is a particular strength of the work carried out at NOC. During the latter half of the project, by which time the ¼° NEMO code will be well established and tested, we will configure and run a physics-only 1/12° global version of NEMO that includes the mixing parameterisations developed in this WP (with the possibility of running biogeochemical tracers in off-line mode). The aim will be to produce the best possible hindcast of the oceanic state over a period covered by the NCEP CORE forcing (1977-present). The results of this run will be compared with those of 1/12° OCCAM.

Energetically consistent, mechanistic descriptions of mixing

Present ocean models do not account for the energy required to mix vertically. This is a serious drawback if we want to investigate the sensitivity of mixing to climate-related changes in energy input to the ocean, and to changes in ocean stratification (Huang, 1996). To account for possible feedbacks in the climate system that involve ocean mixing, we aim to develop a mechanistic and energetically consistent description of mixing processes, in parallel with the work described above.

The energy required for mixing in the ocean interior is thought to derive mainly from inputs by wind and by tides (Wunsch & Ferrari, 2004). Internal waves are generated in and at the base of the mixed layer, driven by wind and, at the ocean floor, by interaction between bottom topography and both tidal motions and mean and eddy (ultimately wind driven) flows. They then propagate into the oceanic interior, where they break and drive mixing. These processes are poorly represented in standard OGCMs, that do not include tides or surface wind waves, and resolve only a small portion of the internal wave spectrum that fluxes energy from the source to the dissipation regions. Furthermore, OGCMs do not generally link mixing to internal wave activity.

We will investigate a number of approaches to derive an energetically consistent description of mixing in the ocean, expanding previous work on the impact of eddies on the energy budget at the base of the mixed layer (Nurser & Zhang, 2000; Oschlies, 2002). Our main strategy will involve the explicit representation of the internal wave spectrum and fluxes of internal wave energy and the separation of kinetic energy into resolved and sub-grid scale parts. The standard surface mixed-layer model in NEMO already has a prognostic variable for the sub-grid scale turbulent kinetic energy (TKE), although the present set-up does not conserve TKE below the mixed layer. We will extend the TKE concept to work throughout the water column.

Initially we will use limited-area process models with an equidistant vertical resolution of a few meters and a horizontal resolution of 1 km, to resolve a good part of the internal wave spectrum. Energy inputs at the sea surface will include the coupling of tidal and wave models, eventually considering interactions with sea ice. Particular attention will be paid to the generation of internal waves by the interaction of strong bottom mean and eddy flows over topography, with the aim of linking to funded observational work being carried out at NOC by Naveira-Garabato. Theme 5 is closely linked to WP 9.10 and will provide valuable data for it, as will other planned NOC observational work linked to DIMES.

Building biogeochemistry into NEMO

Realistic representations of biogeochemistry in OGCMs are essential in order to study the impact of ocean feedbacks in climate change. The role of marine biota in this context is a key component of QUEST, as well as proposed work in Themes 1, 2 and 5. An existing core nutrient-phytoplankton-zooplankton-detritus (NPZD) model, currently being run in OCCAM, will be embedded in NEMO at the earliest opportunity, with subsequent implementation of advanced ecosystem models, building incrementally on the NPZD base, as they are developed. We will work closely with the Met Office and PML (WP 9.5) in the design of new ecosystem models, as well as tailoring them to NOC needs within Oceans 2025. Factors that will be included in the new model include the influence of different phytoplankton groups on particle flux, production and export of dissolved organic matter, stoichiometric effects on elemental cycles and the influence of nitrogen fixation on nutrient budgets. Tracers required to model the carbon system (dissolved inorganic C, alkalinity) will be included as part of the modelled biogeochemistry.

Additional complexity gives rise to its own difficulties, including poorly understood ecology and model sensitivity to the parameterisations involved, such that it is unclear precisely what level of complexity is most appropriate for climate studies (Anderson, 2005). Various approaches of representing extra complexity will therefore be explored. For this purpose, a 1-D NEMO-based testbed will be set up to investigate the performance of a range of ecosystem models (WP 9.11). The most promising of these will be used as a basis of global realisations of 3-dimensional NEMO.

We will investigate impacts, in particular with respect to effective diffusion, of the different advection schemes used to ensure positive concentrations of biogeochemical tracers. The results from tracer release experiments, such as DIMES, will be used to assess the appropriateness of the advection scheme. We will also investigate time stepping methods to ensure efficient and accurate coupling of biological source and sink terms that often have fast time scales relative to a more slowly changing physical environment.

Practicalities: model maintenance and operations – manpower and computing

In the past, ocean modelling at NERC marine Centres has been treated in two distinct ways: a) as a scientific endeavour leading to publications, and b) as engineering to permit (a). Direct funding has mainly been aimed at (a). However, moving to new HPC platforms requires many months of highly-skilled work in rewriting code to work efficiently. Such work is essential (defined by NERC as Category 1 research) and provides significant added value and improved integration with NERC stakeholders; nevertheless, its resources are frequently squeezed in favour of direct science (despite the fact that it fits all the criteria identified by OST for Research Council activities; OST, 2002). Whilst Earth observation data can often be easily obtained by researchers, and processed hydrographic data are often available within weeks of a research cruise, much effort is required to achieve a long or high-resolution integration of a complex ocean or climate model: it takes months to years to achieve a sufficiently long simulation period with a large model, even when available computers are pushed to their limits. It is vital that the UK keeps the ability to run and maintain accurate ocean models (which implies high resolution) for analysis by UK Earth system scientists. NOC can provide the facilities and expertise to do this, and will represent the NERC community on the NEMO consortium board, ensuring that model developments are consistent with this aim.

Substantial effort is needed to provide the model runs required for the science to be undertaken in Themes 1, 2 and 5 and elsewhere in the Oceans 2025 programme. Manpower is required to ensure optimal use of HPC resources and to deal efficiently with enormous quantities of output data. Model maintenance is also important for the development of the next generation of ocean and coupled modellers. Many PhD projects (both at NOC and elsewhere) do not necessarily require models at the finest resolution (indeed, the computer requirements for parameter searches in Earth system models often preclude fine resolution). Yet although the CPU requirements are reduced, the complexity of working with such models is not. Thus apart from the models themselves, support packages, advice, and manuals need also to be maintained. Retaining the expertise and skills necessary to provide these services efficiently requires continuity of funding.

We seek to put model maintenance on to a firmer footing, by directly requesting funds for manpower to support this operation. We shall not only support current models (and new ones as they come online) but also ensure that they are straightforward to access and use. Where the direct use of a model is not appropriate, we shall permit easy user acquisition of model results from our most realistic simulations via web interfaces and through a variety of other forms, by drawing upon existing expertise gained through local funding and the GODIVA e-Science project. We shall ensure that both models and model runs are documented in line with NERC data policy.

The model development work proposed in Theme 9 requires continuous and immediate access to adequate computer resources. NOC has a 56-processor itanium cluster but current usage is already high and the job queues rarely drain. In addition to the 40 processors presently on order to meet the current demand by SOES and RAPID investigators, a further upgrade of the NOC cluster by an extra 128 processors is required to enable the proposed development work to proceed. These will be reserved for the model development work of Theme 9. We plan to submit all large-scale production runs (¼° and finer resolution) to the national HPC centres, but we need continuous and immediate access to a local machine for efficient work on model development. Our current estimate is that we can run tests of the ¼° NEMO model, with a modest number of biogeochemical tracers, on 64 processors. With up to 4 people working simultaneously on different model-development aspects, a set of 128 processors is the minimum requirement for a smooth running of the programme.

WP 9.11 (NOC) New methods of analysis and validation: ecosystem model testbeds

NOC will develop new ecosystem models to address the role of marine biology in the carbon cycle and climate in Themes 2 (Marine Biogeochemical Cycles) and 5 (Deep Ocean), linking to WP 9.10. Such work is also supported by QUEST, at NOC and elsewhere, with emphasis on the development of complex plankton functional type models. It is not enough, however, to develop new models. What is needed is a rigorous intercomparison of all new models with data and each other, i.e. to determine the merits of different models within a highly structured framework. Existing model intercomparison, if done at all, tends to be *ad hoc.*

In WP 9.11, we will develop an evaluation and validation system for emerging marine ecosystem models. This will involve a structured approach, based on objective measures of model evaluation. A system of this kind is being developed in the USA, stimulating much interest (Friedrichs *et al*., in press), but does not yet exist in the UK or Europe. The majority of recently published ecosystem models have not even undergone a thorough observation-based model evaluation. To bring (back) together models and observations, we will establish a model validation and benchmarking centre (or virtual centre involving several NERC Centres) which would play a leading role in Europe and closely collaborate with US colleagues. One dimensional testbeds will be set up, with a common physical framework, allowing model comparison at many sites, both for open ocean and in shelf seas (cross-cutting with PML WP 9.7). Approaches to intercomparing full 3-D models will also be developed (with POL WP 9.1). Modularity in approach will be key, permitting smooth switching between different ecosystem models, and ensuring consistency in forcing.

Each of the various ecosystem models will be objectively optimised for a range of sites. Their performances will be quantitatively compared to assess how well different model processes represent biogeochemical cycling in the real world. Due attention will be given to the 'model-data misfit function'. The real ocean is full of sub-mesoscale behaviour, poorly observed.. In order to best judge the success of each of a set of models purporting to describe that ocean in an objective fashion, we shall use statistical and other tools to define a set of descriptors (with WP 9.7). These will be of great interest to other NERC Centres and the Met Office, for climate-related purposes.

Summary research plan and deliverables (WP 9.8 – 9.11)

2007 – 10	• An assessment of the sensitivity of coupled climate models to the type of ocean model used (WP 9.9) • An energetically consistent description of mixing within the ocean (WP 9.10) • Accurate coupling of a fully functional biogeochemical submodel into NEMO (WP 9.10)
2007 – 12	• Parameterisations of poorly treated physical processes for existing and new codes (WP 9.10) • Methodologies and critical tests for nesting submodels (WP 9.10) • Physical and computational test-bed environments in which emerging ecosystem models can easily be evaluated (WP 9.11) • Development of a widely accepted model-data misfit function as a main tool for ecosystem model benchmarking (WP 9.11) • Development of statistical tools to extract maximal information from model-data misfits and guide further improvement of the individual ecosystem models (WP 9.11)
2009 – 12	• Global ca. 50 year ¼° and 1/12° runs of NEMO (WP 9.10)
2010 – 12	• Development of additional modules for ICOM (WP9.8) • Multi-century integrations of coupled climate models (WP 9.9)
Ongoing	• Code repositories for coupled climate models to extend the diversity of such models in the UK (WP 9.9) • Code repositories for maintained ocean model codes and global configurations (WP 9.10)

Theme 9 Synthesis and Concluding Material

Oceans 2025 synergies and wider links

Since Theme 9 will develop underlying technologies to allow other Themes to address key science issues, it necessarily has major cross-Theme links. The need for systematic observational programmes to comprehensively verify the model systems provides a strong link with the sustained observations of Theme 10, particularly the coastal observatories (SO 10, 11, 12), AMT (SO 1), Ellet Line (SO 4), CPR (SO 15) and ships of opportunities (SO 8). These SOs, (augmented by EO products) are the primary source of data for data-assimilation and re-analysis, required to provide best estimates of the state of the marine environment and its evolution. The model development carried out in this Theme will benefit directly from improved process representation and understanding arising from Themes 1-5. In turn, the model products will feed back into aspects of these Themes (particularly 1 and 3) and the marine bioresources and renewable energy aspects of Theme 6 – providing the ability to integrate ('upscale') small-scale processes and provide balanced budgets and fluxes. The model improvements carried out in this Theme will also directly benefit the development of operational model systems in the context of coastal observatories (Theme 10).

The coordination of modelling effort between the three Centres in this programme represents a substantial added value element. There are a wide range of specific linkages: common verification and inter-comparison techniques and data sets in ecosystem model testbeds will allow traceability and objectivity in the investigation of ecosystem model structure and parameters sets. The convergence on a common physics model code (NEMO) for some applications will facilitate rapid sharing of knowledge and the straightforward exchange of boundary condition data, and multi-resolution inter-comparisons (for example between shelf and oceanic application). The multidisciplinary nature of the programme, encompassing hydrodynamics (including waves and turbulence), ecosystems (pelagic and benthic) and model systems, will result in a rapid transfer of disciplinespecific advancements into the coupled context of Earth system modelling. This will build on existing relationships that have successfully delivered coordinated, multidisciplinary science; for example in previous NERC core strategic funding, also MarProd, MERSEA and CASIX.

Synergies with other Themes in Oceans 2025 and existing collaborations with other UK and international research groups are summarised in Tables 1 and 2.

Table 1. Main links between Theme 9 and other parts of Oceans 2025

Theme 1	Next generation global ocean models. Improved process understanding for implementation in models.
Theme 2	Next generation of global ocean ecosystem models including biogases. Improved understanding of biogeochemical processes for implementation in models.
Theme 3	Provision of coastal and shelf model infrastructure. Improved parameterisation of process models. Multi-decadal simulations of the global coastal-ocean.
Theme 4	Improved understanding of ecological processes for implementation in models. .
Theme 5	Down slope flow modelling; Improved process understanding for implementation in models
Theme 6	Provide POLCOMS multi-decadal runs for analysis of climate change impacts on coastal-ocean ecosystem
Theme 10	All the SOs will provide data for model validation. Pre-operational forecast models will be evalauted in the Western Channel and Liverpool Bay Coastal Observatories.
NF1	Theme 9 will use BODC-archived data, and will supply simulation data for archival

Table 2. Main existing science collaborations between Theme 9 and other research groups (UK and international) not part of Oceans 2025.

UK

BAS	Antarctic Shelf Sea Modelling
BGS	Sea bed stress modelling
CASIX	North Atlantic and European Shelf carbon fluxes and budgets
CCLRC	High performance computing
Cefas	In-situ monitoring e.g. SMART buoy, ecosytem modelling
DARC	Data assimilation
ESSC	E-science
Hadley Centre	Climate modeling
Imperial College	Unstructured/adaptive grid models
JNCC	Marine spatial planning/habitat mapping
NCOF	Operational Oceanography
QUEST/MarQUEST	Global and coastal-ocean coupled hydrodynamic-PFT models
RAPID	Modelling Arctic shelves + THC modelling
NCAS/CGAM	Coupled climate modelling.
UK SOLAS	Process models for planktonic production of DMSP and halocarbons
Univ of East Anglia	Plankton functional type models; ocean modeling
Univ of Essex	Phytoplankton light acclimation
Univ of Liverpool	Temperature response of protozoa, shelf sea dynamics
Univ of Reading	Data assimilation, coupled atmosphere-ocean models
Univ of Strathclyde	*In situ* marine optics
Univ of Swansea	Plankton physiology, zooplankton grazing
Univ of Wales, Bangor	Sediment transport, modelling

International

CARBO-OCEAN	Air-sea CO2 fluxes
DRAKKAR consortium	High resolution global modeling
MERSEA/GMES	Operational Oceanography, Data assimilation, model error assessment
NEMO consortium	European ocean modelling
Old Dominion Univ. and Univ. of Maryland	Ecosystem modelling testbeds

EUROCEANS	EC network of excellence for marine ecology
U. Bologna Italy	Bacteria/DOM models, operational oceanography
Dartmouth College,USA	QUODDY model
IOW Warnemünde	Turbulence modeling
NRL, USA	Sea Ice modeling (CICE), HYCOM model

Theme-wide stakeholder relevance and Knowledge Transfer

The nature of Theme 9 makes stakeholder interaction and corresponding knowledge transfer a vital component of the work. There are four main stakeholder groups:

- *Operational oceanography:* particularly the Met. Office through the prevision of model codes for use in ocean forecasting. For example, POL and the Met. Office have a close relationship through a history of contract research dating back to the 1970's, that has facilitate a rapid transfer of modelling technology to operational use at the Met. Office[6]. This started with the Storm Surge Model and has progressed to baroclinic and multi-disciplinary models, with PML, via the MERSEA programme and the formation of NCOF. These roles will be expanded in Oceans 2025, for example through the use of a common modelling framework (NEMO).
- *Government bodies*: close links with agencies such as the Hadley Centre, Defra, JNCC, EA and 'fisheries laboratories' allow a rapid transfer of policy relevant model products and advice on modelling strategies (for example choice of ocean model in IPCC assessments of climate change). The focus on error quantification throughout this theme means the confidence levels associated with these products will be well established. Moreover, work on model diagnostics and interpretation means that appropriately synthesized information can be provided.
- *The wider scientific community:* HEIs and directed programmes (e.g. QUEST) can benefit immensely from a coordinated modelling effort through the provision of support, maintenance, large scale simulations, infrastructure and training. The mechanisms for delivering this will be more formal in oceans 2025, including 6-monthly workshops, improved documentation and training, and the use of e-science techniques such as live access servers to distribute model data (e.g. GODIVA) and the Access Grid to facilitate meetings.
- *The general public:* model output in the form of graphics and animations can provide a readily accessible window on the marine environment that can be taken up by schools, the media and the interested public at large. We shall work to improve access to these out reach elements and increase their visibility through an improve web presence.

Table 3. Examples of policy/application issues and stakeholders in relation to Theme 9 science

Policy/application issues	Main stakeholders with interests	Relevant Theme 9 science
EU Water Framework Directive, the Marine Bill, aggregate extraction/dredging, flood warning systems, tsunami threat and instrumental warning systems, coastal defence and managed retreat schemes	Defra, SE, EA, SEPA, CCW, EN	Dispersion and mixing; sediment transport; improved forecasts of coastal flooding
Improved operational models (Storm Surge Forecasting Service, HAB prediction, diver visibility, search and rescue, NWP) ensemble forecasts, reducing uncertainty	GMES, Met Office and NCOF	Integrated hydrodynamic-wave-ecosystem shelf seas models
Forecasting Climate Change in response to increasing levels of greenhouse gasses.	Defra, Hadley Centre, EU, DTI.	Coupled atmospheric ocean models, ecosystem models
Threat to and changes in coastal and estuarine environ-ments; development of indices to identify change; maintaining healthy ecosystems; marine conservation policy; marine spatial planning and surveying renewable energy capacity	EN, SNH, CCW, JNCC, NGOs, local authorities and other coastal zone managers	Ecosystem and hydrodynamic models
Pollution dispersal; environmental impacts of CO_2 leaks from geological storage sites	Oil industry, Defra, DTI	Hydrodynamic and acidification models

[6] see http://www.metoffice.gov.uk/research/ncof/shelf/index.html

Developing ecosystem approach for fisheries;	Defra/Cefas and SEERAD/FRS, EU	Water quality and ecosystem models

Strategic Ocean Funding Initiative (SOFI)

Up to 10% of the research funding for Oceans 2025 will be made available to UK universities and other academic institutions eligible to receive NERC support. Such funding will be awarded for research that is complementary to the Oceans 2025 science Themes, in defined topic areas in a series of funding calls (first call to be announced in 2007). For Theme 9, the following SOFI opportunities have been identified:

- Coupled ocean atmosphere modelling
- Improved parameterisation of the role of food quality in zooplankton grazing.
- Hydrodynamic model diagnostics
- Improved process models for shelf seas physics (turbulence and internal waves)
- Unstructured grid models
- Model optimization on HPC
- Modelling support for the HEI community
- Using cellular ecosystem models to drive whole ecosystem models (e.g. ECOPATH).

Summary of theme-wide outcomes

- Model systems with well-understood error properties
- The next generation of UK hydrodynamic models utilizing the technology of adaptive and unstructured grids
- The next generation of ecosystem models that addresses the issue of model complexity
- Key model data sets (A4)
- A support system for the UK modelling community**.**

References

Adcroft A & Campin JM (2004) Rescaled height coordinates for accurate representation of free-surface flows in ocean circulation models. *Ocean Model*., 7, 269-84.

Allen *et al.* (2001) A highly spatially resolved ecosystem model for the North West European continental shelf. *Sarsia* 86, 423-40

Anderson TR (2005) Plankton functional type modelling: running before we can walk? *J Plankton Res*. 27, 1073-81

Allen JI, Archer S, Gilbert F, Taylor AH and Blackford JC (2006) Changes in DMS production and flux in relation to decadal shifts in ocean circulation. Tellus B, in press

Archer SD *et al* (2004) Modelling of the seasonal patterns of dimethyl sulphide production and fate during 1989 at a site in the North Sea. *Can J Fish Res,* 61, 765-87

Baretta *et al* (1995) The European regional seas ecosystem model, a complex marine ecosystem model. *Neth J Sea Res*, 33, 233–46

Blackford JC *et al* (2004). Ecosystem dynamics at six contrasting sites; a generic model study. *J Mar Sys*, 52, 191-215.

Bryan K (1969) A numerical method for study of the circulation of the world ocean. *J Comput Phys*, 4(3), 347-76.

Canuto V & Dubovikov MS (2006) Dynamical model of meso-scales in z-coordinates. *Ocean Model*, 11, 123-66.

Clarke KR (1993) Nonparameteric multivariate analyses of changes in community structure. *Aust J Ecol* 18, 117-43.

Cooper WS, Hinton CL, Ashton N, Saulter A, Morgan C, Proctor R**,** Bell C, Holt J, Young E & Huggett Q (2005) UK Marine Renewable Atlas. *ICE J Maritime Engineering*, in press.

Delhez ÉJM and 11 others (2004) Variability of shelf-seas hydro-dynamic models: lessons from the NOMADS2 Project. *J Mar Syst*, 45: 39-53.

Evensen G (2003) The ensemble Kalman filter: theoretical formula-tion and practical implementation. *Ocean Dynamics 53*, 343–67

Ferreira D, Marshall J & Heimbach P (2005) Estimating eddy stresses by fitting dynamics to observations using a residual mean ocean circulation model and its adjoint. *J Phys Oceanogr* 35, 1891-10.

Flynn K & Mitra A (2005) Predator–prey interactions: is 'ecological stoichiometry' sufficient when good food goes bad? *J Plankton Res.* 27, 393-9.

Friedrichs MAM, Hood RR & Wiggert JD (2006) Ecosystem model complexity versus physical forcing: quantification of their relative impact with assimilated Arabian Sea data. *Deep-Sea Res. II*, in press.

Gattuso JP, Frankignoulle M & Wollast R (1998) Carbon and carbonate metabolism in coastal aquatic ecosystems. *Ann Rev Ecol Systematics,* 29, 405-34.

Haidvogel DB, Arango HG, Hedstrom K, Beckmann A, Malanotte-Rizzoli P & Shchepetkin AF (2000) Model evaluation experi-ments in the North Atlantic Basin: simulations in nonlinear terrain-following coordinates *Dyn. Atmos. Oceans* 32, 239-81

Heil,P & Hibler WD III (2002) Modelling the high-frequency component of arctic sea ice drift and deformation. *J Phys Oceanogr*, 32, 3039-57.

Holt JT & James ID (2001) An s-coordinate model of the North West European continental shelf. Part 1: Model description and density structure. *J Geophys Res*, 106(C7): 14015-34.

Holt JT *et al* (2004) Advective controls on primary production in the stratified western Irish Sea: An eddy-resolving model study. *J Geophys Res-Oceans* 109, C05024 doi:10.1029/2003JC001951

Holt JT *et al* (2005) Error quantification of a high resolution coupled hydrodynamic-ecosystem coastal-ocean model. Part 1: model overview and assessment of the hydrodynamics. *J Mar Syst*, 57, 167-88.

Howe RL *et al* (2004) The impact of two species of bioturbating shrimp (*Callianassa subterranea* and *Upogebia deltaura*) on sediment denitrification *J Mar Biol Assoc UK* 84(3): 629-32.

Huang RX (1999) Mixing and energetics of the oceanic thermo-haline circulation. *J Phys Oceanogr*., 29, 727-46.

Jones JE & Davies AM (1996) A high resolution three dimensional model of the M2, M4, M6, S2, N2, K1 and O1 tides in the eastern Irish Sea. *Est Coastal Shelf Sci,* 42, 311-46

Lee MM *et al* (2002) Spurious diapycnal mixing of the deep waters in an eddy- permitting global ocean model. *J. Phys. Oceanogr*, 32, 1522-35.

Lee Z *et al* (2002) Deriving inherent optical properties from water color: a multiband quasi-analytical algorithm for optically deep waters. *Appl Optics* 41, 5755-72.

Luyten PJ, Jones JE & Proctor R (2003). A numerical study of long- and short-term temperature variability and thermal circulation in the North Sea. *J Phys Oceanogr*, 33(1): 37-56.

Lynch D, Ip JTC, Naime CE & Erner FE (1996) Comprehensive coastal circulation model with application to the Gulf of Maine. *Cont Shelf Res*, 16, 248-55.

Marshall J, Adcroft A, Hill C, Perelman L & Heisey C (1997) A finite-volume, incompressible Navier Stokes model for studies of the ocean on parallel computers, *J Geophys Res*, 102(C3), 5753-66.

Monbaliu J, Padilla-Hernandez R, Hargreaves JC, Carretero-Albiach JC, Luo, Sclavo M & Gunther H (2000) The spectral wave model, WAM, adapted for applications with high spatial resolution. *Coastal Eng*. 41: 41-62.

Montagnes D *et al* (2003) Using Q(10): Can growth rates increase linearly with temperature? *Aquatic Microb Ecol* 32 (3): 307-13

NERC (2002). *Science for a Sustainable Future 2002-2007*. NERC Swindon

Nurser AJG & Zhang JW (2000) Eddy-induced mixed layer shallowing and mixed layer/thermocline exchange, *J Geophys Res,* 105, 21851-68.

Oschlies A (2002) Improved representation of upper ocean dynamics and mixed layer depths in a model of the North Atlantic on switching from eddy-permitting to eddy-resolving grid resolution. *J Phys Oceanogr*, 32, 2277-98.

Osuna P & Wolf J (2005) A numerical study on the effect of wave-current interaction processes in the hydrodynamics of the Irish Sea. In: *Proc 5th Int Conf on Ocean Wave Measurement and Analysis:* WAVES2005, 3-7 July, 2005, Madrid, Spain.

OST (2002) *Quinquennial Review of the Research Councils*. Stage 2 report.

Pham *et al* (1998) Singular evolutive Kalman filters for data assimilation in oceanography. *Academie des Science, Paris* 326, 255-60.

RavenJ *et al*. (2005) *Ocean acidification due to increasing atmospheric carbon dioxide*, Royal Society Policy Document 12/05 60 pp ISBN 0854036172.

Richardson A J *et al* (2003) Using self-organising maps to identify patterns in satellite imagery. *Prog. Oceanogr*. 59, 223-39.

Riemenschneider U, Smeed DA & Killworth PD (2005) Theory of two-layer hydraulic exchange flows with rotation. *J Fluid Mech*, 545, 373-95.

Siddorn *et al* (2006) Modelling the hydrodynamics and ecosystem of the North-West European continental shelf for operational oceanography *J. Mar. Sys* (in press)

Spitz YH *et al* (1998) Data assimilation and a pelagic ecosystem: parameterisation using time series observations. *J Mar Sys*. 16, 51-68.

Souza & James (1996) A two-dimensional (x−z) model of tidal straining in the Rhine ROFI, *Cont. Shelf. Res*.,Sunda *et al* (2002) An antioxidant function for DMSP and DMS in marine algae, *Nature*, 418: 317-20.

Thomas H, Bozec Y, de Baar HJW, Elkalay K, Frankignoulle M, Schiettecatte L-S & Borges AV (2005) The carbon budget of the North Sea. *Biogeosciences*, 2(1), 87-96

Toole DA & Siegel DA (2004) Light-driven cycling of dimethyl-sulfide (DMS) in the Sargasso Sea: Closing the loop. *Geophys Res Lett* 31 (11): L11307

Torres & Allen (2006) Sequential data assimilation in an upwelling influenced estuary *J. Mar. Sys* (in press)

Umlauf L & Burchard H (2005), Second-order turbulence closure models for geophysical boundary layers. a review of recent work, *Cont. Shelf. Res*., 25, 795-827.

Vayssières MP *et al* (2002). Classification of trees: An alternative non parameteric approach for predicting species distributions. *J. Veg. Sci*.11: 679-94.

Vincent MA, Atkins SM, Lumb CM, Golding N, Lieberknecht LM & Webster M (2004) *Marine nature conservation and sustainable development – the Irish Sea Pilot*. Report to Defra by JNCC, Peterborough.

Wadhams P (1998) Sea ice morphology. In: *Physics of Ice Covered Seas*, ed: M Lepparanta, Helsinki Univ, 231-87.

Wirtz KE & Wiltshire K (2005). Long-term shifts in marine ecosystem functioning detected by inverse modelling of the Helgoland Roads time-series. *J Mar Sys* 56, 262-82

Wunsch C & Ferrari R (2004) Vertical mixing, energy and the general circulation of the oceans. *Ann Rev Fluid Mech*, 36, 281-314

Young and Holt (2006) Long term temperature and salinity variation in the Irish Sea. J Geophys Res (submitted).

Acronyms

AGRIF	Adaptive Grid Refinement in Fortran
AMT	Atlantic Meridional Transect
AMEMR	Advances in Marine Ecosystem Modelling Research
BAS	British Antarctic Survey
BGS	British Geological Survey
CARBOCEAN	Marine carbon sources and sinks assessment
CASIX	Centre for Observation of Air-Sea Interaction and Fluxes
CCLRC	Council for the Central Laboratory of the Research Councils
Cefas	Centre of Environmental, Fisheries & Aquaculture Scienc
CFD	Computational Fluid Dynamics
COHERNS	Coupled Hydrodynamical Ecological model for Regional Shelf seas
CS	Celtic Seas
CTD	Conductivity Temperature Depth
CGAM	Centre for Global Atmospheric Modelling
CHIME	Coupled Hadley-Isopycnic Model Experiment
CICE	Los Alamos Sea Ice model
CNRS	Centre National de la Research Scientifique
CORE	Common Ocean Reference Experiments
CPR	Continuous Plankton Recorder
DARC	Data assimilation Research Centre
DARDNI	Department of Agriculture and Rural Development, Northern Ireland
Defra	Department for Environment, Food and Rural Affairs.
DIMES	Diapycnal and Isopycnal Mixing Experiment in the Southern Ocean
DMS	Dimethylsulphide
DMSP	Dimethylsulfoniopropionate
DOM	Dissolved Organic Material
DRAKKAR	An international ocvean modelling project
DTI	Department of Trade and Industry
EA	Environment Agency
ECMWF	European Centre for Medium-Range Weather Forecasts
ECOPATH	Ecosystem pathways modelling software
EIS	Eastern Irish Sea
EnKF	Ensemble Kalman Filter
EO	Earth Observation
EOF	Empirical Orthogonal Function
ERA40	ECMWF reanalysis
ERSEM	European Regional Seas Ecosystem Model
ESSC	Environmental Systems Sciences Centre
Euroceans	EU network for Ocean Ecosystems Analysis
FLUME	Flexible Unified Model Environment
FOAM	Forecast Ocean-Atmosphere Model
FRS	Fisheries Research Services
FTE	Full Time Equivalent
GENIE	Grid Enabled Integrated Earth System Model
GETM	General Estuarine Transport Model
GMES	Global Monitoring for Environment and Security
GCOMS	Global Coastal-Ocean Modelling System
GODIVA	Grid for Ocean Diagnostics, Interactive Visualisation and Analysis
GOTM	General Ocean Turbulence Model

GHRSST-PP Global High Resolution Sea Surface Temperature Pilot Project
HAB Harmful algal bloom
HadGEM3 Hadley Centre Global Environmental Model
HadCM3 Hadley Centre Climate Model 3
HECToR High End Computing Terascale ResourceNPZD Nutrient-phytoplankton-zooplankton-detritus
HEI Higher Education Institute
HiGEM High Resolution Global Environmental Modelling
HF High Frequency
HPC High Performance Computing
HYCOM Hybrid Coordinate Ocean Model
ICOM Imperial College Ocean Model
IOW Baltic Sea Research Institute, Warnemünde
IP Integrated Programme
IPCC: Intergovernmental Panel on Climate Change
JNCC Joint Nature conservation Committee
LODYC Laboratoire d'Océanographie Dynamique et de Climatologie
MarQUEST Marine Biogeochemistry and Ecosystem Modelling Initiative in QUEST
MarProd Marine Productivity (NERC directed programme)
MCA Maritime and Coastguard Agency
MERSEA Marine Environment and Security for the European Area
MH Malin-Hebrides shelf
MITGCM Massachusetts Institute of Technology General Circulation Model
MOC Meridional overturning circulation
NCAR National Centre for Atmospheric Research, USA
NCAS National Centre for Atmospheric Science
NCOF National Centre for Ocean Forecasting
NEMO Nucleus for European Modelling of the Ocean
NOC National Oceanography Centre, Southampton
NOMADS North Sea Model Advection Dispersion Study
NRL Naval Research Laboratory
NWP Numerical Weather Prediction
OASIS Ocean Atmosphere Sea Ice Soil
OCCAM Ocean Circulation and Climate Advanced Modelling
ODON Optimal Design of Observational Networks
OGCM Ocean General Circulation Model
OPA Océan PAralléllisé
OST Office of Science and Technology
PFT Plankton Functional Type
PML Plymouth Marine Laboratory
POL Proudman Oceanographic Laboratory
POLCOMS POL Coastal Ocean Model System
PRISM PRogram for Integrated Earth System Modelling
QUEST Quantifying and Understanding the Earth System
QUODDY Dartmouth College Circulation Model
RAPID NERC Rapid Climate Change directed programme
ROMS Regional Ocean Model System
ROC: Receiver Operator Characteristics
SAMS Scottish Association of Marine Science
SEERAD Scottish Executive Environment & Rural Affairs Dept
SEPA Scottish Environmental Protection agency
SEIK Singular evolutive interpolative Kalman filter
SEPA Scottish Environmental Protection Agency
SOES School of Ocean and Earth Science, NOC
SOFI Strategic Ocean Funding Initiative
SOLAS Surface Ocean Lower Atmosphere Study
SOM Self Organising Map
SPM Suspended Particulate Matter
TKE Turbulent kinetic energy
TELEMAC Hydrodynamic modelling system
WAM A Wave model
WCO Western Channel Observatory