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Three-dimensional unstructured mesh ocean modelling

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Abstract

In this article the advantages and current status of unstructured mesh ocean modelling are reviewed. Future challenges are discussed along with the potential of resulting methods to make a significant impact on ocean modelling over the next decade. These methods are important because they are the only techniques that can simultaneously resolve both small and large scale ocean flows while smoothly varying resolution and conforming to complex coastlines and bathymetry. Realising the full potential of such methods will necessitate the use of dynamic mesh adaptivity. A number of techniques need to be combined and developed from different numerical modelling and geophysical fluid dynamics disciplines in order to create a powerful unstructured mesh ocean model. These are: accurate and robust methods for the discretisation and advection of tracers, density and momentum; the choice of element/cell and satisfaction of the LBB stability condition; representation of hydrostatic and geostrophic balance; the ability to deal with sigma coordinate-like errors associated with the use of unstructured meshes; initial mesh generation to follow complex bathymetry and coastlines; sub-grid scale modelling on unstructured and possibly solution adaptive meshes; scalable solvers and parallel computing. A good solution to each problem is required, and thus

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the resulting model may be argued to be considerably more complex than traditionally used structured mesh models. It is these topics that are addressed here.

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1. Introduction

Traditional ocean models (for background material, see Haidvogel and Beckmann, 1999; Griffies et al., 2000) are extremely sophisticated with hundreds of person-years invested in all aspects of their development. However, the fundamental techniques used to solve the momentum and continuity equations have remained largely unchanged since their original development (Bryan, 1969; Bryan and Cox, 1967). They have typically evolved to a high degree of sophistication (e.g. the MIT model; Marshall et al., 1997), with a range of methods for parameterising the various unresolved physical processes, as well as the use of hybrid meshes (although still structured) for example. However, evolution does not always result in optimality since current models only reflect the methods and computing resources that used to be available. Thus it seems timely to investigate the possibility of changing some of the fundamental aspects of these models; the use of an unstructured mesh with the option for dynamically changing resolution seems a natural next step.

The first work on the use of finite elements and unstructured meshes in the field of ocean modelling was probably by Fix (1975). Examples of other important early work may be found in Lynch and Gray (1979), Haidvogel et al. (1980), Platzman (1981), Dumas et al. (1982) and Le Provost and Vincent (1986). Subsequent work concentrated mainly on diagnostic models (e.g. Myers and Weaver, 1995; Greenberg et al., 1998; Nechaev et al., 2003), and models based upon shallow water systems (e.g. Lynch and Werner, 1987; Ma, 1993; Iskandarani et al., 1995). More recently models which compute solutions with three-dimensional (3-D) hydrostatic (Lynch et al., 1996; Iskandarani et al., 2003; Danilov et al., 2004) and non-hydrostatic (Ford et al., in press-a; Labeur and Pietrzak, 2004), dynamics have been developed.

There is currently a fairly wide range of approaches and techniques employed by the 'unstructured-mesh' community. For example, the Spectral Element Ocean Model (SEOM) of Iskandarani et al. (1995) uses an unstructured mesh of rectangles in the horizontal, sigma coordinates in the vertical, and is very accurate with the typical use of sixth degree or higher Legendre polynomials. The model of Lynch et al. (1996) uses an unstructured mesh of triangles in the horizontal, with sigma coordinates in the vertical. Buoyancy forces are evaluated by interpolating density onto a structured background mesh. The FEOM model (Danilov et al., 2004) uses a Galerkin least squares approach to stabilise and remove spurious modes, as well as a finite difference treatment of buoyancy forces on nodes stacked one on top of another in the vertical. The MIT model, although using a structured mesh, can use shaved cells (Adcroft et al., 1997) to conform to bathymetry, and can use modified z coordinates to adjust the coordinate system to follow a free surface (Adcroft and Campin, 2004).

New to unstructured mesh models is the need to obtain a suitable coastline and bathymetry conforming mesh (Legrand et al., 2000; Gorman et al., submitted for publication). Another important aspect of an unstructured mesh ocean model is the choice of element, i.e. how the various solution variables are represented on the mesh. This can be viewed as the analogue of

Arakawa grid staggering in structured mesh models. Work on analysing these choices with regards their impact on spurious computational modes and the representation of states close to geostrophic balance in shallow water models may be found in Le Roux et al. (1998), Hanert et al. (2002) and Le Roux et al. (2004).

The potential advantages of an unstructured mesh ocean model are significant. For example, there are issues relating to boundary conditions when bathymetry and coastlines are represented by a 'staircase' regular structured mesh. The result can be an inadvertent application of no-slip boundary conditions, and consequent problems with the transport of dense fluids along slopes. This process must be parameterised for staircase topography, for example using enhanced diffusion in the cells adjacent to the ocean floor. Having the mesh aligned with the bathymetry avoids many of these problems (Adcroft and Marshall, 1998) and allows the fluid to slide over bathymetry, as described by a frictional model for example. Unstructured meshes also enable the use of greater mesh resolution in the direction normal to the coastline than tangential to it where typically boundary layers develop (e.g. western and frictional). Resolving developing flow features (e.g. fronts, eddies, overflows) whose positions are not necessarily known *a priori* requires the use of adaptive mesh resolution. Thus ideally mesh adaptivity techniques would be employed which can dynamically change model resolution to optimally resolve such flows.

The aims of future unstructured mesh ocean models are to:

- be accurate and robust in ocean flow conditions (e.g. accurate noise-free representation of hydrostatic and geostrophic balance);
- be non-hydrostatic but without the additional computational overhead when the flow is close to hydrostatic;
- exploit nonlinear advection methods on unstructured meshes so that both accuracy and robustness may be combined;
- use sub-grid scale modelling designed for unstructured (inhomogeneous and anisotropic meshes) and possibly dynamically changing meshes;
- be conservative:
- possess a free surface and accurately resolve barotropic and baroclinic modes;
- be implicit, or semi-implicit, so that time-step sizes are not necessarily restricted by grid size (i.e. allow large Courant numbers associated with the various physical processes present);
- have an unstructured mesh in the vertical as well as the horizontal to optimise efficiency gains;
- use anisotropic mesh adaptivity with resolution controlled through error measures, or to better resolve areas of socio-economic importance, and also to include mesh movement to allow the model to follow isopycnal layers or coherent structures;
- make use of parallel computing with load-balanced domain decompositions methods;
- be able to assimilate data into a predictive model and exploit natural grid hierarchies to accelerate inversion and obtain sensitivity information.

The remainder of this article addresses these issues with a number of modelling demonstrations using the model under development as part of this work (Ford et al., in press-a). The next section describes numerical advection methods, and highlights the relative merits of a wide range of approaches. In Section 3 the closely related topic of sub-grid scale modelling on unstructured evolving meshes is discussed. In Section 4 the important issue of element choice and its links with

Arakwawa grid staggering is reviewed. Section 5 covers the topics of mesh adaptivity, mesh movement and error measures, which are crucial in many ways for reaping the full benefits of unstructured mesh modelling. This is followed in Section 6 by a discussion on the links between adaptivity and the choice of vertical coordinate which has proved to be so important for traditional ocean models. Section 7 covers initial mesh generation and draws heavily on the previous two sections. Finally, in Section 8 the importance of the accurate representation of balance, solvers and scientific computing issues are discussed.

2. Advection

This section presents numerical methods for resolving on unstructured meshes the transport of density, tracers, momentum, free surface height, and sets of coupled advection equations.

The accurate numerical modelling of advection (or transport) remains a central problem in many areas of fluid dynamics such as oceanography (Pietrzak, 1998; Smolarkiewicz and Margolin, 1998; Hanert et al., 2004; Iskandarani et al., 2004). This is mainly due to the conflicting demands of accuracy and the requirement for stability and boundedness of the numerical discretisation scheme (Darwish, 1993). First-order discretisation schemes, although stable, are highly numerically diffusive. Conversely high-order schemes, although accurate, tend to give rise to numerical oscillations in regions where there are large solution gradients. In the field of fluid dynamics it was realised quite early on (for background see Hirsch, 1990), that the only way to achieve a high-order bounded scheme free from numerical oscillations was to introduce nonlinearity into the discretised equations, even if the original differential equations are linear. This is a consequence of Gudonov's theorem (Toro, 1997) which states that there are no linear monotone high-order schemes for hyperbolic systems of equations.

2.1. Petrov-Galerkin methods

While Bubnov–Galerkin (using the same weighting/test functions as expansion functions) discretisations of transport equations are dispersive, generalised least squares discretisations (Ackroyd, 1997) represent an alternative approach which tend in general to be quite dissipative. If the least squares error is minimised using finite elements as basis functions, a discrete system with a symmetric-positive-definite matrix results. To overcome the problems related to each approach for advection processes, it is popular to combine the dissipative least squares methods with non-dissipative Galerkin methods to produce an attractive compromise in the Galerkin-least-squares (GLS) method (Hughes et al., 1989). These methods are all Petrov–Galerkin in nature (a weighted residual method) and typically applied using finite elements. They have the advantage that they attempt to reduce explicitly the residuals of the governing equations. The consistency of the approach (being a residual based formulation) leads to robustness and accuracy advantages. For example, usually (depending on the element choice) all mass matrices have the property that they are distributed (i.e. non-diagonal).

Similar to GLS is the typical Petrov–Galerkin (PG) weighting; that is, using a weighting function which puts more emphasis on what is happening in the upstream direction. It is a popular choice and the weighting is almost universally chosen for scalar equations as $N_i + \frac{1}{2} \frac{h}{|\mathbf{u}|} \mathbf{u} \cdot \nabla N_i$,

in which N_i is the finite element basis function associated with node i and u is the transport velocity for the scalar being solved for. The element width h depends on the element choice, e.g. h is the width of an element for linear interpolants and half that width for quadratic interpolants. However, these methods are still prone to oscillate in the direction normal to the flow as their dissipation is streamline based. The common cure is to introduce additional nonlinearity (Hughes et al., 1986; Oñate et al., 1997; Almeida and Silva, 1997). This usually takes the form of diffusing away large equation residuals, often in the direction of largest spatial gradients (Masud and Hughes, 1997; Hughes and Mallet, 1986b; Codina, 1993). Although these methods can be shown to be non-oscillatory and satisfy a maximum principle (the maximum and minimum values of the solution variable are on the boundaries of the space—time domain for a scalar advection/diffusion equation with a divergence free advecting velocity field), they tend to be more dissipative than nonlinear finite volume (FV) or control volume (CV) methods. Nonlinear CV methods are well developed and certainly the most widely used transport methods and thus this advantage does not seem surprising.

More recently, discontinuous finite element methods (DFEM) in both the space and time domains have been applied to the time-dependent transport equation (Wareing et al., 1999). Although linear discontinuous representations are more robust than other time-stepping schemes such as Crank-Nicolson, they still lack sufficient numerical stability. Also, variational principles for the time-dependent form of the transport equation have been derived (Donea and Huerta, 2003; Ackroyd, 1997). These variational finite element schemes use continuous finite elements for both the space and time domains. The variational principle can also be recast as a weighted residual formulation with an appropriate spacetime PG weighting. The advantages of these schemes are that their stability properties are potentially better than the linear discontinuous formulations employing Bubnov–Galerkin weightings due to the dissipation introduced from the PG weighting. However, due to the linearity of the scheme it does not preclude the possibility that oscillations may occur in the space–time solution (since this can only be achieved using methods which introduce nonlinearity).

Space–time Petrov–Galerkin methods have found widespread application for solving advection–diffusion-type problems. Space–time finite element methods use either continuous or discontinuous finite elements for both the space and time domains; the time domain is simply treated as another dimension over which transport takes place. The most crucial issue in most space–time formulations is the distance over which numerical dissipation is applied. For linear space–time formulations, typically this has meant a choice between using either the spatial or temporal meshes to determine these distances, or alternatively, using the distance across the space–time elements. If the spatial mesh is used to determine the element length scales, this introduces the correct amount of numerical dissipation for steady-state cases (Eriksson et al., 1996). If the temporal mesh is used to determine the element length scales, this assumes that the spatial dimension is largely invariant. Examples of this approach include the Lax–Wendroff (Lax and Wendroff, 1960) and Taylor–Galerkin (Donea, 1984) methods. A disadvantage of this approach is that the time-step size needs to be tuned in order to represent a typical element length scale associated with a spatial mesh. Thus this approach can become computationally inefficient as steady-state is approached.

None of these methods used to calculate representative distances are entirely satisfactory. A more appropriate way of calculating the distance is to use the variation of the solution in

space—time. Therefore the space—time methods must in general introduce nonlinearity and use the local solution gradients in order to calculate representative distances. For instance, if the steepest gradients in the solution are in the time dimension then the time-step size (or a multiple of it) should act as the representative distance over which numerical dissipation is introduced, see Pain et al. (in press-a).

In addition to the calculation of the representative distance over which numerical dissipation is introduced, the angle between the gradient of the solution and the streamline direction is important and is used in most nonlinear Petrov–Galerkin methods.

2.2. Control volume methods

Control volume (CV) methods involve integrating the transport terms over surfaces of CVs in order to gauge the quantity of incoming and outgoing information. Thus the accuracy of this approach is limited by the accuracy of the information evaluated at the CV boundaries. High-order schemes are typically realised by placing polynomials through local CV values in order that accurate values on the CV boundaries can be established. These high-order polynomials can put more emphasis on interpolating upstream CV cell values such as in the QUICK (Leonard, 1979, 1991) scheme for example. Other possible methods involve constructing a local Taylor series expansion through nearby CV values (Ackroyd, 1997), fitting a plane (which defines a gradient) through nearby CV values in a least squares fashion, or using finite element/spectral element interpolation (Karniadakis and Sherwin, 1999).

These CV methods can easily switch to a non-oscillatory method when a solution extrema is detected, and thus preserve the non-oscillatory (in N-dimensions), and even the Total Variation Diminishing (TVD) property in 1-D. The Sweby diagram approach (Sweby, 1984), is particularly successful at this and typically switches between a number of schemes such as QUICK and a central method as defined by a curve on the Sweby diagram. This curve can be changed to optimise the compressive properties of the scheme (e.g. sharp interface preserving properties) as in the superbee approach (Roe, 1985), or a compromise which does not act to make sine waves square such as in the van Leer approach (van Leer, 1974, 1977).

The Normalised Variable Diagram (NVD) (Leonard, 1988) approach to flux limiting produces equivalent schemes to the Sweby diagram approach, at least in 1-D. However, it acts on more fundamental extrema detecting variables and as such is the approach adopted in the multi-dimensional unstructured mesh formulations employed here. It is the method used to obtain the high fidelity density solutions in the gravity current simulation presented in Fig. 1. The domain here is 20 km long and 5 km wide, with a linearly varying bathymetry of maximum depth 1 km and minimum depth 0.2 km. A column of dense water 5 °C cooler than the surrounding water is released in the shallower part of the domain (cf. Özgökmen and Chassignet, 2002). The Kelvin–Helmholtz instability resulting in vertical mixing and entrainment, and the lobe and cleft structure of the gravity current head can clearly be seen. See Pain et al. (in press) for a full description of the advection method that uses an implicit approach with temporal limiting as well as spatial limiting to avoid oscillations introduced by high-order interpolants used in the time domain, especially when large time-steps are used (the maximum local Courant number for this simulation was 15). The Barton scheme (Centrella and Wilson, 1984) is an effective alternative to other

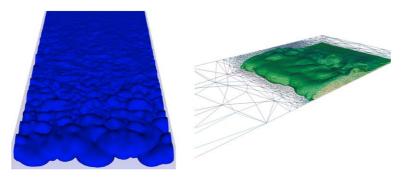


Fig. 1. Density field in a gravity current simulation as described in Section 2.2. Left: an isosurface of density obtained on a fixed hexahedral mesh of approximately 1.5 M nodes, and utilising control volume based high-resolution advection of density. Right: result obtained with standard discontinuity capturing SUPG for the advection of density (an isosurface of which is shown) on an adaptive unstructured mesh of approximately 80 000 nodes and 200 000 elements.

approaches for unstructured meshes and uses a combination of a number of schemes to evaluate fluxes on CV boundaries.

The DFEM is a combination of CV and FEM methods and typically (as in the Discontinuous Galerkin (DG) method) uses a Galerkin discretisation within each element and CV-like fluxes for incoming/outgoing element information. Attempts have been made to suppress oscillations occurring in DFEM solutions. For example in Kershaw et al. (1998) linear and quadratic elements were used, as well as a nonlinear programming approach, to suppress the oscillations and alter the solution in a minimal way. Since it is a hybrid approach it is especially complex to design a DFEM scheme that satisfies the maximum principle.

2.3. Coupled systems of equations

For coupled systems of hyperbolic equations, such as the shallow water equations, it is possible to determine the incoming/outgoing information to each control volume by looking at eigenstructure of the resulting equations (Brunner and Holloway, 2001a,b). The eigenstructure is spatially variant in many fluid flow problems (e.g. in the compressible inviscid and shallow water systems), but fortunately analytical expressions for the eigenvalues and eigenvectors exist (Toro, 1997, 2001). Multi-dimensional Riemann methods typically form a 1-D Riemann decomposition normal to each face of a control volume. The most accurate approach (also used to form the basis of a residual formulation) is to use the same upwind bias used to discretise the fluxes to discretise the sources in the equations normal to a face. In addition, since this approach allows one to determine the quantity of incoming and outgoing information for coupled systems of hyperbolic equations, it allows the easy application of limiting methods (limiting the fluxes on the control volume boundaries to avoid oscillations). The limiting functions should ideally take into account sources in the differential equations when calculating extrema detecting functions (Hubbard and Garcia-Navarro, 2000).

Least squares methods are also an effective means of dealing with coupled systems of equations. When dealing with equation sets with different dimensions (e.g. momentum and continuity equations) it can be advisable to multiply one of these equation sets by a certain dimensional number,

or equivalently solve the equations in non-dimensional form. However, one of the main problems with this approach is that it is not always clear what number to multiply one or more of the equation sets by, and this can vastly affect the performance of the least squares discretisation. In addition, practitioners are often disturbed to find the discretised momentum equation within the discretised continuity equation and vice-versa. On the positive side this approach can eliminate spurious modes (e.g. pressure modes), making it possible to use shared pressure–velocity-free surface meshes. It will also suppress spurious numerical oscillations near sharp gradients. However, as with other dissipative discretisation schemes, care must be taken when combining it with subgrid scale models such as Large Eddy Simulation (LES) methods, since the dissipative discretisation method is in effect providing much of the sub-grid scale modelling (Hughes et al., 2000). Similarly, least squares methods and coupled equation PG methods share all the above attributes with GLS methods.

A diffusion based approach of introducing nonlinearity into PG methods for solving strongly coupled systems of equations is reported by Shakib et al. (1991), the magnitude of the diffusion is proportional to the magnitude of the equation residuals. Thus the method acts to diffuse out equation residuals. Nonlinear discontinuity capturing PG schemes applied to coupled systems use a rank-one weighting matrix for the application of isotropic diffusion (Hughes and Mallet, 1986a,b; Shakib et al., 1991). The streamline up-wind Petrov–Galerkin (SUPG) method of Pain et al. (in press-b) uses a nonlinear PG formulation with diffusion introduced only in the streamline direction, and for time-dependent problems this diffusion acts in space–time using DFEM in time, see Pain et al. (in press-a).

To avoid equation coupling issues the momentum and continuity equations are most often treated separately. Moreover, this approach can guarantee to result in bounded densities and tracers when solving the coupled momentum and incompressible continuity equations using a piecewise constant basis function for the density, and the same basis functions for pressure and for the weighting of the continuity equations. For a bounded scheme the fact that the discretised continuity equation is embedded in the discretised advection equation presents additional issues that can be addressed with CV methods. Unless the discretised continuity equation is actually the discretised continuity equation satisfied by the solution to the momentum/continuity equations, then sources/sinks of the advected quantity will result affecting the boundedness and accuracy of the solution. This consistency was achieved in the high-resolution method results shown in Fig. 1, and is the main reason why control volume methods are applied in situations where the solution must be bounded.

3. Sub-grid scale modelling on unstructured meshes

Sub-grid scale (SGS) modelling has many links with, and is strongly related to, the topic of accurate and robust advection methods. This is because much of the sub-grid scale processes requiring modelling (e.g. various turbulent effects) are processes described by transport, but usually on a scale much smaller than the mesh size (Sagaut, 1998). Thus it is not surprising that transport methods themselves have often been used as turbulence models (e.g. Denbo and Skyllingstad, 1996; Hoffman and Johnson, 2004). See also Hughes et al. (2000) for a discussion of the links between the Smagorinsky LES and the variational multiscale approach to numerical stabilisation

when modelling turbulent flows. In fact sub-grid scale modelling techniques have been shown in many ways to be equivalent to some of the stabilisation techniques discussed in the previous section (Hughes, 1995; Brezzi et al., 1997).

Since the error (deviation of the numerical solution from the exact solution) satisfies a transport equation set similar to the original (Donea and Huerta, 2003), it is not surprising that sub-grid scale processes often involve the use of transported variables e.g. turbulent kinetic energies in dynamic Large Eddy Simulation (LES) models. As far as this work is concerned the main issues are the design of sub-grid scale models on variable resolution unstructured meshes, and how they interact with dynamically changing anisotropic resolution (Figs. 1 and 2), right up to the point where the processes become explicitly resolved by the mesh. Bearing in mind that the sub-grid scale model typically depends strongly on resolution, the interaction of sub-grid scale modelling with dynamically changing meshes provides additional nonlinearities that need to be understood. In fact this may provide an entirely new field of endeavour. For example, there is a requirement to include both the discretisation and the modelling errors, e.g. model errors from LES (Hoffman and Johnson, 2004). Goal based mesh optimisation methods, in which the mesh is adapted to optimally represent the goal, e.g. the drag past an obstruction or a measure of the dynamics of the flow, may be constructed to take into account the additional nonlinearities associated with these SGS models, see Hoffman and Johnson (2004) for further discussion on goal based mesh adaptivity. See Bentham et al. (in press) for a discussion on how anisotropic and inhomogenous mesh resolution may be reflected in the sub-grid scale model.

An alternative modelling approach can be derived by averaging the fluid quantities along fluid particle trajectories, i.e. Lagrangian averaging. The advantage is that fluid structures, such as

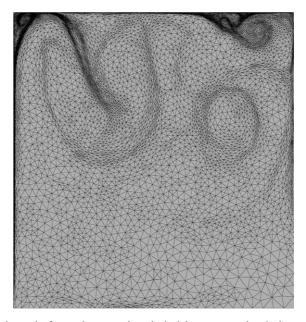


Fig. 2. Adapted unstructured mesh for a barotropic wind driven gyre circulation on a beta-plane. Anisotropic resolution has automatically been focused in the western boundary current region and subsequent nonlinear eddies, and changes in response to the evolving flow fields.

overturning billows and vortices, remain more coherent and are not smoothed to such an extent. One such model, the LANS-alpha model (Foias et al., 2001), changes the momentum equations so that the fluid is advected by a smoothed velocity field (the smoothing may be designed to match the variable numerical resolution). This filtering has been demonstrated to yield very attractive results including, for isotropic turbulence, an improved adherance to Kolmogorov's –5/3 energy-wavenumber scaling-law, up to the length scale set by the filter. For an oceanographic application see (Holm and Nadiga, 2003).

Another example of sub-grid scale modelling is that given by the wind forcing which generates waves and imparts momentum into the ocean depending on the wave amplitude and whether they break (Cavaleri and Bertotti, 2003). This type of sub-grid scale model typically discretises the probability density function of the waves into their frequency (wavelength) and direction, resulting in a large set of coupled differential equations—the coupling is via nonlinear wave interactions. The discretisation of wave direction (as well as frequency) is strongly related to mesh resolution. Not taking into account the spatial resolution can lead to ray effects (spurious numerical rays due to the truncation of direction discretisation). Similar models must also be developed for the interaction with the atmosphere through heat fluxes, and in an analogous way internal waves and diapycnal mixing. Ice modelling also provides additional sub-grid scale challenges.

Various further phenomena, such as overturning and mixing, need parameterisation. They typically range from the use of infinite diffusion in the vertical when an inversion of the stratification occurs, to 2.5 equation approaches to vertical mixing (Mellor and Yamada, 1982). Whereas with attempts at resolving the turbulent 2-D (horizontal) structures via simple eddy parameterisation, e.g. bi-harmonic dissipation (which is difficult to treat implicitly because of large stencils) and LES methods, often no attempt is made at modelling the turbulent fluctuations in the vertical and second moment closure methods are thus frequently used (Mellor and Yamada, 1982). See also Gent and McWilliams (1990) for a popular and successful approach to parameterising isopycnic mixing by geostrophic eddies. Additional parameterisations are required for vertical mixing and entrainment due to fluid moving over inclined bathymetry; effects due to the roughness of the bathymetry and coastlines are typically modelled in the form of Rayleigh friction or viscosity models. For example the friction required in coastal shallow water models is typically a vertical average of the bottom Rayleigh friction.

Numerous other sub-grid scale processes need parameterising, and the models employed need amendment to work on unstructured meshes with potentially fine mesh resolution, right up to the point where the processes become explicitly resolved by the mesh.

4. Mixed finite elements

In an analogous manner to structured A, B, C, D, and E grids (Arakawa and Lamb, 1977) (which respectively consist of a shared velocity/pressure mesh; velocity nodes at the corners and pressure nodes at the centre of elements; velocity normal to a face at the element faces and pressure at the element centre; velocity tangential to a face at the element faces and pressure at the element centre; and the velocity at the faces and pressures at the element centre), there exist many possible finite element pairs which have varying capabilities in resolving inertia-gravity

and Rossby waves for example. For background related to standard structured mesh methods see Haidvogel and Beckmann (1999) and Griffies et al. (2000) and the references therein, and for unstructured meshes see Le Roux et al. (1998), Hanert et al. (2002) and Le Roux et al. (2004), and see also Section 8.4. Some of the simplest and most popular choices are now briefly discussed.

Using the notation of Gresho and Sani (1998), the hexahedral (Q_1P_0) element with tri-linear velocity and piecewise-constant pressure is equivalent to the B-grid and thus has the property of representing well internal waves when the Rossby deformation radius is large in comparison to the local mesh resolution. It is however plagued by singular pressure modes which seem largely not to affect the accuracy of velocity, especially with the limited use of Dirichlet velocity boundary conditions. It is stabilised typically with piecewise-constant shock functions (Gresho and Sani, 1998; Norburn and Silvester, 1998).

The hexahedral (O_1O_1) and tetrahedral (P_1P_1) elements employ a shared mesh and have similarities with the A-grid. Again this choice needs stabilising which typically takes the form of a second or fourth-order dissipation term introduced into the right-hand side of the continuity equation. When a pressure equation is formed in its continuous representation a fourth-order stabilisation term is effectively introduced into the continuity equation (Sotiropoulos and Abdallah, 1991) which explains in part its success. However, this approach is plagued by difficulties in achieving continuity satisfaction locally or globally. Introducing bubble functions to the approximation of velocity (the result is often termed the MINI element) can also cure the stability issues (e.g. Fortin and Fortin, 1985) and has been shown to produce identical discretisations to certain Petrov-Galerkin weightings—vet another form of stabilisation (Hughes, 1995). Recently there has been the realisation that subtracting a more accurate first-order operator from a less accurate representation of the first-order operator has very nice dissipative properties that can eliminate spurious pressure or free surface modes (Codina and Blasco, 2000). This is also true of second-order operators and has been used in ocean modelling for many years by subtracting out one rotated (less accurate) discretisation using a five point stencil from a second five point stencil discretisation of diffusion to eliminate spurious free surface height modes.

The hexahedral (Q_2Q_1) Taylor-Hood element with a linear variation in pressure, a quadratic variation in velocity, and simple continuity between elements is LBB (Ladyzhenskaya, 1969; Babuška, 1971; Brezzi, 1974) stable but has many more velocity nodes than continuity equations. The result can be surprisingly poor accuracy with forcing of the momentum equations, as in, for example, buoyancy-driven flows. The cure seems to be to project the forcing onto the pressure basis functions. The introduction of an additional piecewise-constant pressure component can also be an effective cure. The closely related 20 node serendipity element does not have such problems, but it is considerably less accurate and the resulting mass matrices are not easily lumped (which can be important for solvers). The tetrahedral (P_2P_1) Taylor-Hood element has similar properties to the corresponding hexahedral element.

The lowest-order Raviart-Thomas element $(P_1^{\perp}Q_0)$ consists of a piecewise-linear basis function centred on element edges and used to represent the normal component of velocity, along with a piecewise-constant pressure. It is the analogue of the C-grid and seems particularly useful, for example in Legrand et al. (2000) it was shown not to exhibit spurious free surface pressure modes.

The lowest order Crouzeix-Raviart element $(P_1^{NC}Q_0)$ consists of a piecewise-linear basis function centred on element edges and used to represent velocity components, and a piecewise-constant pressure. It may be considered to be the analogue of the E-grid. It was shown by Le

Roux et al. (1998), along with many other low-order pairs, to have problems representing geostrophic balance accurately.

Other possibilities include using a piecewise-linear discontinuous velocity within each element and a continuous piecewise-quadratic pressure. This has the advantage that the mass matrices are block diagonal (each block being associated with an individual element) and is LBB stable, but its lack of inter-element continuity requires careful treatment of second-order terms generally resulting in large stencils. The choice of quadratic velocity and quadratic pressure can be stabilised with a pressure dissipation term in the continuity equation. Often this term is matched by a corresponding alteration to the discretisation of the pressure in the momentum equations. An alternative form of dissipation is to add a term which penalises the deviation of the pressure from a linear variation. This will manifest itself as supplementary edge equations in quadratic elements; when the value of dissipation is large the result is a linear variation of pressure through each element. Again, introducing a cubic bubble function for velocity can make quadratic elements LBB stable. To allow for the use of equal order interpolants for the representation of velocity and pressure in incompressible Navier-Stokes solvers the constraint may be modified through the inclusion of a 'filter term'. The pressure gradient projection technique constructs this term by introducing a new unknown — the projection of the pressure gradient onto the velocity space, the term added to incompressibility is then the divergence of the difference between the pressure gradient and its projection, multiplied by a suitable parameter ideally defined element-wise (Codina and Blasco, 2000).

For further discussions on the crucial matter of element choice, see Fortin and Fortin (1985), Gunzburger (1989), Brezzi and Fortin (1991), Girault and Raviart (1986), Gresho and Sani (1998), Le Roux et al. (1998) and the references therein.

5. Mesh adaptivity/node movement

A common problem encountered by model users is that the computational grid or mesh used in a numerical simulation has to be generated a priori to the solution procedure. It is therefore difficult to resolve adequately the local physical features at a first attempt, and the mesh often needs to be adapted to enable the solution procedure to satisfy resolution requirements. Importantly, this also allows for a reduction in computational effort which is crucial for complex applications. As an example see Fig. 2 where an adapted mesh from a simulation of wind driven barotropic circulation in a box is presented. Further discussions on the application of adaptive methods in ocean modelling, including mesh movement techniques, is given in (Piggott et al., 2004).

Many adaptivity techniques make use of a hierarchy of meshes where de-refinement involves rolling back a hierarchy of elements in the mesh (e.g. Jimack, 1998; Oliker et al., 2000). While hierarchical adaptive methods are anisotropic to a degree, it is not possible to form long thin elements aligned with the solution as elements are restricted by their *ancestors* in the hierarchy. An alternative anisotropic mesh optimisation technique is used in the authors' ocean model and was developed by Pain et al. (2001). A tetrahedral mesh is improved through edge collapsing and splitting, edge swapping, face to edge swapping, and smoothing in a fashion similar to Freitag and Ollivier-Gooch (1997) and Buscaglia and Dari (1997).

5.1. Error measures for mesh adaptivity

Mesh adaptivity or optimisation relies on the derivation of appropriate error measures which dictate how the mesh is to be modified. Several error measures which serve as a criterion for mesh modification have been proposed. These range from interpolation-based a priori error measures (Löhner et al., 1985; Peraire et al., 1987; Wu et al., 1990), to a posteriori error measures (Strouboulis and Oden, 1990; Ainsworth and Oden, 1997) which can take into account the physics of the problem by, for example, applying an implicit equation residual technique and often involve the solution of an associated dual problem. A priori error measures tend only to give an indication of the solution complexity at the current time. Conversely, since they take more account of the underlying problem being solved, a posteriori error measures are able to quantify the accumulation and propagation of the error through the mesh. Another approach is to optimise the mesh so as to optimally resolve a quantity or goal of interest. This goal could be configured to be an oceanographically relevant quantity, see Power et al. (2004) and the references therein. An additional consideration when adapting the mesh is that not only node density, but also the alignment of the mesh relative to the solution is important. For example, in boundary layers or fronts the mesh may need to be refined in one direction only e.g. normal to a western boundary current. Hessian-based error measures (derived from interpolation theory) are capable of fulfilling this requirement (Piggott et al., 2004). They have additional attractive features, such as simplicity and ease of evaluation, they also enable the use of a non-Euclidean metric allowing the meshes to be anisotropically adapted truly automatically.

5.2. Methods of adapting a mesh

Once an error measure has been derived the nodes may be re-distributed according to this measure. This step in an adaptive procedure is quite complex algorithmically, and is intrinsically dependent on the initial mesh generation method and geometrical and material boundary conforming requirements (e.g. kinetic energy absorbing sponge layers near domain boundaries). Unstructured tessellation methods can deal with geometries of arbitrary complexity and they lend themselves naturally to adaptivity. There are three main approaches to the generation of unstructured tetrahedral meshes: the Delaunay triangulation scheme (George, 1998); the Advancing Front technique (Löhner and Parikh, 1988; Moller and Hansbo, 1995); and the Quadtree/Octree approach (Kallinderis and Vijaya, 1993). Delaunay tessellation is a procedure for forming optimal tessellations using an appropriate metric for measuring distances. It leads to robust algorithms which can easily incorporate adaptivity. Region-wise coarsening/refinement can be achieved with the Advancing Front technique in which both new nodes and triangles are regenerated in the region (Kallinderis and Vijaya, 1993). The main drawback of this technique is the fact that the mesh has to be regenerated at every mesh adaptation, which can be computationally expensive for large problems. Octree methods by nature do not offer scope for aligning the mesh anisotropically with the solution.

In general 2-D Delaunay meshes are of good quality and can lead to useful mesh adapting schemes for triangular (Xu et al., 1998) and quadrilateral (Borouchaki and Frey, 1998) elements. However, in 3-D when nodes are evenly distributed, the element aspect ratio can

become very large (George, 1998), despite all the edge lengths of an element being approximately equal with respect to the desired metric. Local mesh connectivity transformations have been used by Joe (1989) to obtain a mesh that satisfies the Delaunay property, along with a modification to optimise the interior dihedral angle of the resulting tetrahedral elements and discourage thin 'slivers'. Further work on 3-D Delaunay meshing can be found in Borouchaki and Lo (1995), Borouchaki and George (1996), Castro-Diaz et al. (1997) and Weatherill (1994).

The fact that the Delaunay kernel permits element 'slivers' has provided the motivation to discard it in favour of mesh optimisation methods here. Such optimisation methods are guaranteed to converge and have proved relatively insensitive to computational roundoff error which can be an issue with Delaunay methods (Xu et al., 1998). For example, Freitag and Ollivier-Gooch (1997) demonstrated successful mesh optimisation involving swapping (mesh connectivity adjustments) and smoothing (node position adjustments) of a mesh, and also showed that using either of these independently leads to severely reduced mesh quality. In particular, interior element angles are highly sub-optimal with node movement alone. Also, it was demonstrated that purely optimisation-based node movement is CPU-expensive when compared with simpler methods such as Laplacian-based smoothing, and with little gain in mesh quality over the latter. This has motivated the use of approximate optimisation techniques for mesh smoothing (node movement) based on minimising an energy norm. The quality of the poorest element (as defined by some objective functional) is used as a measure of the overall mesh quality. This quantity is calculated via a Riemannian metric based here on the combination of solution field Hessian matrices. Appropriate scaling of the metric (Castro-Diaz et al., 1997) enables the resolution of multi-scale phenomena as encountered in oceanic flows.

5.3. Mesh movement

Whilst the methods described above represents a major increase in power for numerical models, further important developments are possible. In fluids applications the ability of the mesh to move in a quasi-Lagrangian manner is a considerable benefit. For example, if mesh points were moving approximately with the flow velocity this would effectively result in a much reduced transport velocity (relative to the moving mesh), and hence the possibility of accurately using larger time-steps, cf. the properties of semi-Lagrangian methods (Staniforth and Côté, 1991). A major disadvantage of Lagrangian-like schemes is that mesh tangling may occur. This may be mitigated, and robustness restored, through the combined use of mesh movement and mesh adaptivity or optimisation as introduced in previous sections. This combined approach offers the advantages of each method, without many of the drawbacks, it may be viewed as a generalization of the popular arbitrary Lagrangian-Eulerian (ALE) methods (Donea and Huerta, 2003). Additional advantages of using a moving mesh to account for a large proportion of the mesh resolution change is that the use of mesh-to-mesh interpolation may be minimized (indeed this requirement could be included in the definition of a controlling error measure), and load-imbalances (see Section 8.6) in parallel computations will occur at a reduced rate. Current research is revolving around the issue of using moving variable resolution in the vertical to mimic the properties of isopycnal models in the ocean interior. See Piggott et al. (2004) for further details and discussions.

5.4. Wetting and drying

The 3-D modelling of flood propagation in river and floodplain systems can use existing numerical formulations, but significant developments are needed to include wetting and drying processes and appropriate mesh adaptivity criteria for a moving waterline. An irregular waterline and land geometry, and the appearance and disappearance of isolated dry areas, makes the modelling of wetting and drying a significant challenge. There exists no purely Lagrangian method that can deal with this situation. However the volume of fluid (VOF) approach (as is often used in highly convoluted free surface problems), in which a volume fraction function is used to represent the fraction of each mixed cell occupied by fluid, can represent arbitrarily complex wetting and drying geometries. The wetting/drying interface can be tracked with a volume tracking method with a geometric evaluation of the volume fluxes across the interface. For example, in the new mixed marker and VOF method (Aulisa et al., 2003) the reconstruction and advection of the waterline during wetting and drying processes is modelled. Among numerous algorithms, Aulisa's method combines mass conservation and an accurate representation of the coastline curvature. In order to best represent the movement in the wetting and drying process, meshes near the waterline can be refined and/or mesh adaptivity used as suggested by Tchamen and Kawahita (1998), Horritt (2002) and Bates (2000). Some of the accuracy of Lagrangian wetting and drying methods can be regained with the VOF approach when it is combined with mesh adaptivity and node movement.

6. Coordinate systems and comparison with unstructured mesh methods

In many respects the coordinate system is the most fundamental choice for any ocean model (Haidvogel and Beckmann, 1999; Griffies et al., 2000). It defines the way that the discretisation is performed in the vertical. The three most commonly used choices are: z coordinates (regularly spaced cells/elements in the vertical with cells on the same horizontal level); sigma coordinates which follow the bathymetry and stretch the mesh in the vertical linearly up to the free surface; and isopycnal coordinates which follow surfaces of constant density. Each has its own advantages and disadvantages, the only current certainty being that no single approach is ideal for general wide-ranging oceanic application. z coordinates have the advantages of simplicity and the ability to resolve pressure gradients accurately, however they are poor at representing bathymetry in a smooth and accurate manner (Adcroft et al., 1997). Isopycnal methods, which in effect align the mesh in the vertical with isopycnals and move with them in a Lagrangian manner (see previous section), may result in improved levels of diapycnal mixing which can be very poorly resolved with other methods, although problems may arise when layer thickness vanishes (Bleck, 1998). Sigma coordinates are well suited to accurately follow bathymetry and allow the application of appropriate boundary conditions on the sea floor, but they are prone to large pressure gradients errors in the presence of steep bathymetry (Haney, 1991).

Hybrid methods are used to combine the advantages of more than one approach. For example, isopycnal coordinates may be used in the interior of stratified ocean basins, with z coordinates in the surface mixed layer and on the shelf, and sigma coordinates near the ocean floor (Griffies et al., 2000). There are obviously interfacing issues where the coordinate systems or mesh changes.

In Bleck (2002), isopycnal coordinates are used which relax to Cartesian coordinates as the thickness of cells in the vertical vanishes—one of the major disadvantages of purely isopycnal methods.

However, there is a growing realisation that a 3-D unstructured mesh method can provide an alternative hybrid approach, with a combination of mesh optimisation and node movement in the vertical in a Lagrangian-like manner to follow the free surface and isopycnals, and to improve levels of diapycnal mixing, for example. Mesh adaptive techniques may also be used to re-distribute the mesh resolution locally or more globally, for example in response to the convergence of isopycnal layers, or to optimally represent sections of the bathymetry of most importance to the resulting solution dynamics. The use of an unstructured mesh in the vertical can yield problems analogous to the pressure gradient errors encountered with the use of sigma coordinates. A possible solution to this is described in Ford et al. (in press-a, in press-b).

As previously discussed, an unstructured mesh in the horizontal has the advantage of being able to focus resolution in order to resolve what is of interest, and not be restricted to the resolution dictated by any singular points (e.g. spherical poles) present in the coordinate system used in the horizontal. Although it may seem that finite elements have no problems with singularities (perhaps with the underlying coordinate being arbitrarily chosen as Cartesian coordinates), there may be issues when there is a need to resolve turbulent mixing with anisotropic diffusion/viscosity tensors (e.g. small diffusion in the vertical whilst relatively large in the horizontal). There is still a need to define this and singularities seem unavoidable in its definition (although they are perhaps easier to deal with).

7. Bathymetry and coastline conforming mesh generation

The accurate simulation of various oceanic processes requires not only an appropriate model of the physical forces that drive the system, but also a sufficiently accurate representation of the domain of interest, i.e. here a domain defined by the bathymetry and coastline. Inadequate representation of the coastline may lead to problems such as spurious stresses (e.g. Adcroft and Marshall, 1998), while poor representation of bathymetry can lead to problems modelling internal waves or separation of boundary currents (e.g. Özgökmen et al., 1997; Stern, 1998; Tansley and Marshall, 2000; Munday and Marshall, submitted for publication). In practice there is a trade off between how close the discretised domain is to reality and how appropriate it is for numerical modelling with finite computational resources. Therefore, a computational mesh representing the geometry should be optimised everywhere with respect to this trade off by representing the geometry to a specified error, with a minimum number of mesh elements or nodes.

The majority of ocean models, whether they use regular cell spacing or curvilinear grids, represent the domain with a structured mesh. The curvilinear grid lines yield a mesh of quadrilateral computational cells in the horizontal which may be fitted to the coastal geometry. Typically, this horizontal structure is then maintained throughout the vertical levels. Unstructured mesh models offer an alternative approach. Their flexibility means that a far more accurate and efficient representation of domain geometries is possible. The number of nodes/elements used to represent the boundary will limit the minimum cost of the entire simulation. It is suggested that this representation should not be altered during the course of a simulation; that is, the original surface should not be coarsened during a mesh adaptive simulation to avoid changing the integrity of the domain and associated conservation issues. In an adaptive simulation the mesh may of course be refined

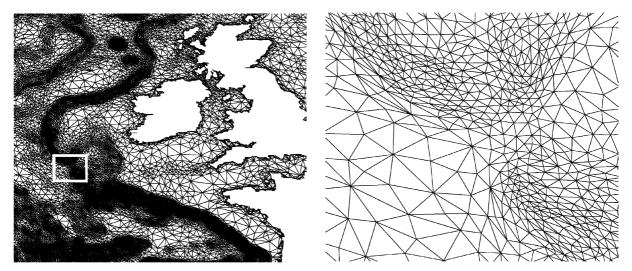


Fig. 3. Section of a mesh constructed for the North Atlantic. The panel on the right is a blow-up of a region of the Celtic Shelf break given by the white box in the left panel.

without changing the bathymetry representation where/when necessary to follow the flow. Thus it is desirable to represent a given geometry to a prescribed accuracy with the minimal number of nodes/elements to avoid excessive resolution in the eventual simulations.

Unstructured grid generators are typically based upon a Delaunay algorithm, for example as used by codes such as TriGrid (Henry and Walters, 1993) and Triangle (Shewchuk, 2003). This approach has been used in oceanographic applications on the sphere by Legrand et al. (2000). Many of these methods provide techniques for inserting extra nodes in regions where there is a steep gradient or curvature. In addition to this, since a Delaunay mesh is the aim, the quality of an element in the mesh is judged more on its geometrical quality in the Euclidean sense, rather than on its accuracy at representing bathymetry.

A typical bathymetry conforming unstructured mesh is presented in Fig. 3. This (sea floor) surface is a section of a mesh constructed for the North Atlantic, and a blow-up is shown to demonstrate the ability to construct a mesh which aligns itself, for efficiency, with bathymetry variations. The mesh generation approach taken here for robustness employs similar anisotropic mesh adaptivity methods as described in Section 5. To conform to the bathymetry the field whose accuracy is being optimised is the depth of the ocean. Thus the quality of elements is measured with respect to a metric constructed from the curvature of the bathymetry. This, combined with appropriate coastline recovery, results in a 3-D anisotropic mesh which focuses resolution where it is required to optimally represent the bathymetry of the domain. For further details and examples, see Gorman et al. (submitted for publication).

8. Solving the linear equations

The main issue in this section is the solution of the coupled momentum and continuity equations, with the incompressibility constraint being enforced through pressure in a similar manner

to a Lagrange multiplier. Due to problems with scalability, direct solvers are not generally used for large scale ocean modelling and so only iterative solution methods are considered in this section. Other important issues include coupling with the free surface through perhaps a supplementary free surface equation, and internal waves through the evolution of the density field. Ultimately, this requires the solution of a large matrix equation which couples velocity, pressure and density, and is formed after linearisation of the equations. Usually Picard iteration is used to linearise the system of equations; Quasi-Newton-type methods are generally not used as their radius of convergence is smaller, resulting in less stable schemes. Most often the coupled pressure/velocity equations are solved together implicitly or semi-implicitly; this allows for the use of larger time-steps than those permitted with explicit methods. Using large time steps (as measured by the local Courant number) may be especially important when an adaptive algorithm provides a wide variation in element sizes.

8.1. Coupled solvers

Standard techniques for solving the coupled systems either solve the equations as they are (Brezzi and Fortin, 1991; Girault and Raviart, 1986; Gresho and Sani, 1998), typically with GMRES (Saad and Schultz, 1986) and a suitable preconditioner (these preconditioners often mimic the actions of projection based methods, see below), or they eliminate velocity and solve for pressure separately. This requires matrix inner and outer iterations. The outer iteration may be of gradient type e.g. FGMRES (Frayssé et al., 1998) and solves the system for pressure. For Stokes flow the result is a symmetric positive definite matrix for pressure, and the method is referred to as the Uzawa method. The inner iteration is required to perform a matrix vector multiplication, as this requires the solution of the discretised momentum matrix. When Coriolis forcing is dominant this provides a good representation of balance not polluted by time truncation operator splitting errors associated with segregated velocity-pressure solution methods.

8.2. Projection methods

Many current ocean models opt for a semi-implicit approach which involves the segregated solution for velocity and pressure, but is still implicit in each individually. These are derived from the SIMPLE family of methods (Patanaker and Spalding, 1970) for obtaining pressure, in which one typically solves the momentum equations with a best guess for pressure, and then projects the resulting velocity field into a continuity satisfying space such that the vorticity remains invariant, see also Gresho (1990) and Ford et al. (in press-a). These systems of equations are repeatedly solved until convergence. Often in time-stepping methods one or two steps of this procedure are used. This approach can also be used with an inconsistent method of solving for pressure, for example solving a second-order equation for pressure. Care must be taken when using mass lumping inconsistently for the scheme to remain stable. This results in a mixed mass method (i.e. lumped mass for pressure and consistent mass for momentum), see Gresho and Sani (1998).

Typically the CFL condition is not violated by orders of magnitude (fluid particles do not travel right across the domain) and thus the resulting matrices that are solved for momentum and tracers are well-conditioned (although mesh quality can play an important role here, see Piggott et al. (2004)) and can easily be solved. However, the elliptic 'pressure' equation that is solved in incom-

pressible flows is not as well-conditioned, since this reflects the global spread of information right across the domain to ensure continuity satisfaction. This is the most difficult case, whereas for compressible flows the matrices become better conditioned. With free surface flows much of the pressure changes can be absorbed by the free surface and so the information is not spread so far in a single time-step.

8.3. Operator splitting to resolve waves

The momentum equation can be depth averaged, either algebraically or by integration, and the result combined with the kinematic free surface equation to obtain a wave equation for the free surface height. Care must be taken to achieve a level of consistency between this approach and the full 3-D equations, particularly when the barotropic and baroclinic modes are solved for separately. For example, the barotropic mode with a free surface may have a much smaller time-step (to resolve the fast surface gravity waves) than the 3-D baroclinic mode which is far more expensive. Uncoupling these can vastly improve computational efficiency, but presents issues when bringing these modes back together, see for example Killworth et al. (1991). How to effectively do this remains an unsolved problem with an unstructured mesh model; for some work towards this goal in a restricted case, see Danilov et al. (2004).

8.4. Balance

As well as relying on the element type to allow the accurate representation of states close to hydrostatic and geostrophic balance (cf. Section 4), there are methods of subtracting out these effects from the governing equations. Released from the constraints of representing balance well, far greater flexibility in the choice of element results. For example, the choice may be made on the grounds of efficiency and accuracy, or in the elements ability to represent other solution characteristics.

LBB stable element choices generally have problems accurately approximating hydrostatic balance $\partial p/\partial z = -\rho g$ on unstructured meshes. Thus it is convenient to split the pressure p into hydrostatic $p_{\rm h}$ and non-hydrostatic parts $p_{\rm nh}$ and solve for these separately. In Lynch et al. (1996) ρ is interpolated onto a regular background mesh and from this p_h is calculated by integration. In the finite element model FEOM (Danilov et al., 2004) the mesh is constructed such that nodes are aligned one on top of the other in the vertical, and p_h is solved for using a 1-D finite difference method. Alternatively, in the non-hydrostatic code of Ford et al. (in press-a) $p_{\rm nh}$ is dealt with in the same manner as the pressure is in standard Navier-Stokes solvers (cf. Sections 8.1 and 8.2), whilst the effects of the hydrostatic pressure gradient are calculated by differentiating the expression $\partial p_h/\partial z = -\rho g$ in the horizontal, and then integrating down from the free surface to obtain $\partial p_h/\partial x$ and $\partial p_h/\partial y$. These are then placed directly into the horizontal momentum equations as additional source terms. This is one of the most accurate ways of dealing with hydrostatic balance for a given polynomial expansion. On a non-uniform unstructured mesh this procedure is not straightforward and discontinuous linear elements are used to represent these derivatives in Ford et al. (in press-a) which allows for an arbitrary mesh structure in the vertical, see Fig. 4 (centre) for the resulting pressure field following the special treatment of buoyancy. In addition, the gravity currents in Fig. 1 were modelled using this approach.

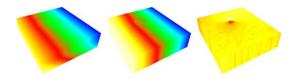


Fig. 4. Pressure field in simulation of stratified flow past a Gaussian seamount on an f-plane. Left: the computed 'full' pressure without any special treatment of the 'hydrostatic' and 'geostrophic' terms. Centre: remaining pressure following the subtraction of the 'hydrostatic' term, as explained in Section 8.4. Right: remaining pressure following the subtraction of both the 'hydrostatic' and 'geostrophic' terms, as explained in Section 8.4.

In an analogous manner, states close to geostrophic balance cause problems for finite element discretisations on unstructured meshes. Again, the appropriate choice of element pair can reduce this issue (Le Roux et al., 1998). See also Adcroft et al. (1999) where a combination of Arakawa staggered grids is suggested for use in grid point schemes. Alternatively, geostrophic balance may be dealt with by forming an elliptic equation for the effect of Coriolis acceleration by first forming a Helmholtz decomposition of the Coriolis term into divergence-free and curl-free components. It is worth mentioning that this can also be done for hydrostatic balance. Since there are no restrictions in the choice of elements used to resolve this expression, for example linear elements can be used with a Q1 (or P1) representation of velocity, it may be solved to a high accuracy to minimise spurious noise effects. Also, since the resulting discretisation matrix is formed in the continuum, the stencil for a given order of pressure approximation is reduced. This makes it cheaper to solve, and since it removes the largest parts of pressure from the governing equations the non-geostrophic/non-hydrostatic parts of pressure can be quickly solved for, using an elliptic equation solver. This combination also enables local continuity satisfaction and in principle, a higher-order polynomial expansion can be used to achieve balance far more accurately. See Fig. 4 (right) for the resulting pressure field following the special treatment of the Coriolis (or 'geostrophic') term.

8.5. Elliptic equation solvers

Solving for pressure or free surface height can often be done by solving a symmetric-positive definite system of equations. The most natural solver is Preconditioned Conjugate Gradients (PCG) and thus the choice of preconditioner is critical (Golub and van Loan, 1989). Incomplete Cholesky factorisation, Symmetric Successive Over Relaxation (SSOR) or Parameterised Forward Backward Gauss-Siedel (FBGS) (Adams, 1983) have often been used, but as the system of equations becomes large, multi-grid type methods or hierarchical preconditioners can become more effective (Stüben, 2000). These have optimal convergence properties but require a series of increasingly finer meshes or solutions. For an unstructured mesh often the only practical choice is an algebraically formed series of coarser problems. These are typically realised by a suitable mapping from a nodal to hierarchical basis, and a corresponding mapping of the matrix to form a coarser representation of it. In practice a series of increasingly coarse matrices are used; this rapidly spreads solution information across the domain and is particularly important for large problems with great horizontal resolution, although perhaps not such a large number of cells/elements in the vertical. When the flow is nearly hydrostatic this method can be encouraged to rapidly coarsen the mesh in the vertical, and then move on to perform coarsening in the horizontal where most

of the work needs to be done. See Stüben (2000) where preferential coarsening in different directions is used based upon graph colouring techniques. Parallel implementations of these methods in an oceanographic context are currently under investigation.

8.6. Parallel computing

Regardless of gains in computational efficiency from advanced numerical methods, there is always going to be a need for parallel computing when a solution cannot be obtained within a reasonable timescale on a serial computer, and/or where there is a limit on local resources such as memory. This is certainly true of ocean modelling, where the desired level of detail and sophistication in the model required for realism will generally far exceed the computational resources available, even when parallelism has been achieved. Because of this, efficient parallel algorithms for ocean modelling are of the utmost importance to reduce the serial bottle-neck. In the case of computational grids, whether they be structured or unstructured, parallelism is achieved through domain decomposition methods (DDM). Fundamental to DDM is the requirement to solve a graph-partitioning problem, the graph being derived from the computational mesh. The graph partitioning problem involves an equal partitioning of the graph nodes into sub-domains which are distributed among processors, thus balancing the computational load across the processors.

The graph partitioning solution is constrained by the need to minimise the number of graph edges dividing the partitions (sub-domains) because the cost of interprocessor communication in a parallel simulation increases with the edge-cut. The most successful methods developed for obtaining good quality graph partitions are k-way multi-level techniques. These techniques typically generate a hierarchy of coarsened graphs where the coarsest level is readily partitioned into k subdomains. This partitioning is then projected up through the hierarchy of meshes where a refinement step is carried out at each step. Partition refinement can be done using neutral network optimisation methods (Pain et al., 1999a) or Fiduccia-Mattheyses type heuristics (Fiduccia and Mattheyses, 1982), as implemented in codes such as Metis (Karypis, 2003) and Jostle (Walshaw, 2003). These methods are themselves parallelised so graph re-partitioning can be calculated in parallel, which is necessary for improving existing graph partitions or addressing the computational load-imbalances which may occur. For parallel machines with heterogeneous communication between processors, the cost of interprocess communication arising from the domain decomposition may be further minimised by mapping domains to processors in some optimal way (Pain et al., 1999b). In the case of a Beowulf cluster using dual processor nodes for example, this would seek to maximise the amount of interprocess communication within the dual node while minimising that over the network.

For solving a set of equations in parallel on a partitioned mesh, a multi-block explicit procedure is commonly used as a preconditioner combined with a gradient based method e.g. PCG or FGM-RES. Relaxation methods such as SSOR within each subdo-main may form the basis of the preconditioner. So-called chaotic preconditioners (see Dertsekas and Tsitsiklis, 1991; Tai and Tseng, 2002) use these same methods but have no-synchronisation step and collect information from neighbouring subdomains when and where they are available to speed up the parallel solution. Again parallel hierarchical preconditioners (Stüben, 2000) provide a way of rapidly spreading solver information across the domain. However, typical multi-grid or hierarchical solvers can be

communication intensive and consequently may be less attractive on slow communicating parallel machines.

The application of mesh adaptivity or optimisation to partitioned meshes (for parallel solutions using DDM) presents a new set of challenges. The central issues with parallel mesh adaptivity are mesh conformity across subdomain boundaries and the treatment of load-imbalances. There are important differences between the mesh adaptivity method applied in this work (cf. Fig. 2) and hierarchical mesh adaptivity methods (e.g. Jimack, 1998) when it comes to parallelisation. Perhaps the most important of these differences is how the elements are adapted to a given error norm. Hierarchical based adaptivity methods use a two-stage process where first elements are coarsened or refined within a single ancestral tree, in effective isolation from neighbouring elements, followed by a sweep over all elements to identify element edges which must be split to obtain a conformal mesh. This allows the mesh adaption process to be carried out in parallel with little communication. Load-balancing is addressed by partitioning the mesh at the coarsest level (Jimack, 1998; Touheed et al., 1998).

In contrast to this, the anisotropic mesh optimisation technique employed here is iterative in nature. This requires each element to change its size and shape in response to local changes in the mesh and solution as the procedure progresses, which could lead to a high number of short communications between domains when adapting elements on or near domain boundaries. To overcome this problem, elements on boundaries between sub-domains are first locked in place. The serial mesh optimisation method is then applied to each domain, disallowing any change to these locked elements. Mesh conformity is maintained because the elements shared between domains are not allowed to change. When the serial optimisation method is finished there may be elements on or near the domain boundary which are still suboptimal. In addition to this a load-imbalance will have invariably occurred due to coarsening and refinement of the mesh in different domains. Both of these issues are addressed simultaneously by re-partitioning the mesh, constraining the graph-partition using edge-weights inversely proportional to the quality of elements connected to the edge. This application of edge-weights discourages the graph partition from cutting across poor quality elements. Once the mesh has been re-distributed to processors according to the new partitioning, the mesh optimisation method can be reapplied to finish adapting the mesh.

Special consideration must be given to mixed element formulations (cf. Section 4) with typically a different polynomial expansion for different variables. The method used here for solving incompressible fluid flow requires a larger stencil size for pressure than for velocity. Thus a second layer of halo (or ghost) nodes is required for the pressure solution; essentially this is an extended halo which includes all elements that share a node with any element cut by the graph partition. Fig. 5 shows how the subdomains dynamically adjust to balance the load in a simulation of incompressible flow past a cylinder at a moderate Reynolds number using the ocean model. In this simulation a diffusive re-partitioning method was predominantly used to reduce the amount of information migrating between processors (Schloegel et al., 1997), however it was found that a re-partition–re-map operation (Karypis et al., 2002) was required periodically to counter degradation in the edge-cut. In this simulation the subdomains may actually be seen to move downstream with the produced von Karman vortex street.

The success of parallel computation in ocean modelling brings its own challenges. Once a large simulation has been performed it then becomes a non-trivial problem to visualise and analyse the

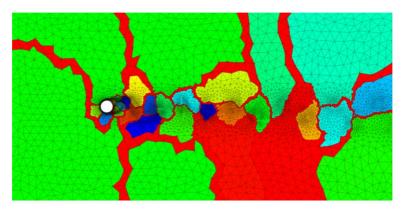


Fig. 5. A demonstration of parallel mesh adaptivity—32 subdomains shown which dynamically adjust to balance the load in the adapting mesh. The mesh here is resolving the von Karman vortex street in a simulation of flow past a cylinder.

results. This in itself requires distributed computing resources for both parallel visualisation and the application of diagnostic tools, for example see GODIVA (2003).

9. Concluding remarks

In this paper the advantages of unstructured mesh ocean models have been discussed. These include the ability to accurately represent coastlines and bathymetry, and the application of appropriate boundary conditions; the ability to choose arbitrarily the mesh resolution (not depending on the coordinate system used), and make this highly non-uniform to match modelling requirements. Also, the use of meshes which dynamically adapt to the solution fields has been discussed. There however remain a number of issues to be addressed in this relatively new field. For example the conservation of key variables; sub-grid scale modelling on changing anisotropic meshes; the optimal representation of balance; and optimal exploitation of node movement and mesh adaptivity. However, the benefits over traditionally used ocean models are immense and justify the substantial amount of work necessary to construct such a model over and above that necessary to produce a traditional model. With more appropriately focused numerical resolution ocean dynamics may be better predicted, as can be events such as climate change. The result would be a single model that can be used efficiently for both coastal and global ocean modelling. It remains to be seen the extent to which such a model will supersede traditional models, but clearly this approach will play an important role in the future of ocean modelling.

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