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The numerics of hydrostatic structured-grid coastal ocean models: state of the art and future perspectives

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Abstract

The state of the art of the numerics of hydrodynamic non-hydrostatic structured-grid coastal ocean models is reviewed here. First, some fundamental differences in the hydrodynamics of the coastal ocean, such as the large surface elevation variation compared to the mean water depth, are contrasted against large scale ocean dynamics. Then the hydrodynamic equations as they are used in coastal ocean models as well as in large scale ocean models are presented, including parameterisations for turbulent transports. As steps towards discretisation, coordinate transformations and vertical and horizontal discretisations based on a finite-volume approach are discussed with focus on the specific requirements for coastal ocean models. As in large scale ocean models, splitting of internal and external modes is essential also for coastal ocean models, but specific care is needed when wetting an drying of intertidal flats is included. As one obvious characteristics of coastal ocean models, open boundaries occur and need to be treated in a way that correct model forcing from outside is transmitted to the model domain without reflecting waves from the inside. Here, also new developments in two-way nesting are presented. Single processes such as internal inertia-gravity waves, advection and turbulence closure models are discussed with focus on the coastal scales. Some overview on existing hydrostatic structured-grid coastal ocean models is given, including their extensions towards non-hydrostatic models. Finally, an outlook on future perspectives is made.

Keywords: coastal ocean models, hydrostatic models, adaptive coordinates, mode splitting, wetting and drying, two-way nesting

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1 1. Introduction

This review paper presents the state of the art of hydrodynamic coastal ocean modelling, with focus on structured-grid hydrostatic models. Here, we define the coastal ocean as ranging from estuaries and shallow coastal areas to the shelf break region. On the small scale end, near-shore and coastal engineering scales are not resolved, but parameterised, if needed. On the large scale end, the dynamics of the ocean basins will not be explicitly treated, since their effects are introduced by means of lateral boundary conditions.

The coastal ocean as defined here, is strongly affected by the superposition g of direct human impacts and climate change and variability. Direct human 10 impacts include for example eutrophication, fishery, large scale constructions 11 (such as offshore wind farms), dredging and dumping of material, discharges 12 (e.g., of cooling water) and pollution. Aspect of natural and anthropogenic 13 climate change and variability impacting on the coastal ocean are relative 14 sea level rise (global and local), global warming, changes of the water cycle 15 (precipitation, evaporation, run-off), and changed wind forcing. These local, 16 regional and global forcings may lead to severe changes in the coastal envi-17 ronment, such as regime shifts in biogeochemistry, coastal erosion, flooding 18 of low-laying coastal regions, increase of oxygen minimum zones, invasion of 19 alien species, and many more. Changes are strong in many coastal regions 20 around the world, but specifically serious in the Arctic where the warming is 21 strongly accelerated. 22

To understand the changing coastal oceans, numerical modelling is one of the most effective tools, allowing for reconstructions of historic states, hindcasts and analysis of the dynamics in the last decades, short term forecasts of coastal ocean states, as well as for coastal climate projections and possible future scenarios. One core requirement for the predictability of such model exercises is the way how basic hydrodynamic processes are reproduced.

Main aspects which need to be resolved are exchanges of matter (such 29 as salt, heat, oxygen, nutrients and particulate matter) in vertical and lat-30 eral directions. In the lateral direction, the coast-to-ocean exchange is medi-31 ated by estuarine dynamics, tidal dispersion, tidal fronts, and meso-scale and 32 submeso-scale dynamics. In the vertical, critical interfaces play a crucial role, 33 such as the sediment-water interface, the *clines* (lutocline, halocline, thermo-34 cline, redoxcline), the surface and bottom wave-affected layers as well as the 35 air-sea interface. Internal waves play a special role for linking horizontal and 36 vertical scales. All these features need to be properly resolved. 37

In this paper, we discuss specific requirements for the hydrodynamic cores 38 of coastal ocean models in terms of driving biogeochemical and suspended 39 sediment models. This will include consequences for interfacing with models 40 for other compartments such as atmospheric models, surface wave models, 41 sea ice models, hydrological models and bottom sediment models, without 42 explicitly discussing such models itself. Also issues of data assimilation will 43 be excluded here. Scales where resolution of non-hydrostatic pressure con-44 tributions become relevant will be parameterised such that we restrict the 45 discussions on hydrostatic models. Furthermore, we restrict ourselves to the 46 class of structured-grid models, since the numerical methods in unstructured-47 grid modelling differ significantly from the structured-grid methods. Due to 48 their flexible grids, unstructured-grid models are known to be specifically 49 suitable for investigating multi-scale dynamics in the ocean. We will here 50 discuss how also structured-grid models combined with nesting strategies are 51 able to resolve multiple scales. 52

⁵³ 2. Characteristics of coastal ocean dynamics

The coastal ocean has a number of characteristics which discriminate it from the global ocean in a way that specific physical and numerical treatment is required. In the following, these characteristics are expressed in terms of characteristic horizontal and vertical length scales H and L, respectively, and the time scale T.

⁵⁹ 2.1. Relatively thick mixed layers

In temperate shelf seas, the surface and bottom mixed layers may occupy 60 a considerable fraction of the water depth. In summer, when stratification 61 shows a maximum, they may still cover 60%-80% of the water column, while 62 in autumn and winter they may completely merge into a vertically homoge-63 neous water column (Bolding et al., 2002). In contrast to this, surface and 64 bottom mixed layers in ocean basins, which may have a comparable absolute 65 thickness to shelf seas may cover only a small portion of the total depth of 66 several thousands of metres (Martin (1985)). 67

⁶⁸ With H being the local time-averaged water depth, and D_s and D_b de-⁶⁹ noting surface and bottom mixed layer thickness, respectively, this charac-⁷⁰ teristics of coastal seas can be expressed as

$$\frac{D_s + D_b}{H} = \mathcal{O}(1) \tag{1}$$

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The major consequence of this is that turbulence closure models are 72 needed which resolve the vertical structure of the mixed layers including the 73 interaction of vertical stratification and mixing. For the relatively thick bot-74 tom boundary layers, another implication is that the bed friction generates 75 relatively strong dissipation of kinetic energy in the water column. The latter 76 may be enhanced in shallow water, when the surface wave length becomes 77 comparable to the water depth, such that the orbital wave motion adds to 78 the bed stress. Due to the dynamic importance of the bottom boundary layer 79 it is required that it is vertically well-resolved everywhere. This means for 80 the generally strongly variable bottom bathymetry of the coastal ocean that 81 bottom-following vertical coordinates are mandatory (see section 4.2). 82

⁸³ 2.2. Relatively high surface elevation amplitude

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The sea surface elevation variability due to tides and storm surges is strongly enhanced in the shallow coastal ocean, adding an important nonlinearity to the dynamics. When denoting the standard deviation of the surface elevation as $\sigma(\eta)$, this characteristics of the coastal ocean could be formulated as

$$\frac{\sigma(\eta)}{H} = \mathcal{O}(1). \tag{2}$$

⁹⁰ First of all, coastal ocean models need to predict the temporally and spatially ⁹¹ varying free surface elevation η , rather than applying the rigid-lid approxi-⁹² mation which large scale ocean models originally used in order to allow for ⁹³ large time steps (Bryan, 1969). Furthermore, the relatively high surface el-⁹⁴ evation variation requires the use of *surface-following vertical coordinates* to ⁹⁵ ensure sufficient vertical resolution of the near surface region.

An extreme case occurs when the surface elevation variability is larger than the mean water depth, such that the sea bed is falling dry at times:

$$\frac{\sigma(\eta)}{H} > 1. \tag{3}$$

In such cases, wetting and drying algorithms must be implemented to prevent
unphysical negative water depths (see e.g., Burchard et al., 2004; Warner
et al., 2013, and section 5).

¹⁰² 2.3. Relatively strong horizontal and vertical gradients

¹⁰³ By definition, all global riverine input is discharged into coastal seas. ¹⁰⁴ Since the exchange between the coasts and the interior of the adjacent shelf

seas is limited, strong gradients build up in the coastal ocean. Salinity may 105 vary from river concentration (almost zero) to ocean concentration within 106 a few kilometres in the horizontal. Strong stratification may be generated 107 in the vicinity of freshwater discharge such that also vertical gradients may 108 be strong. In addition to the salinity, also other tracers such a nutrients 109 or suspended matter discharged by rivers may show strong gradients. Let c110 be a relevant tracer (e.g., salinity), then the fact that horizontal or vertical 111 gradients may be relative strong in coastal seas can be expressed as 112

$$\frac{\Delta c}{|\partial_{[x,y]}c|} \ll L, \quad \frac{\Delta c}{|\partial_z c|} \ll H, \tag{4}$$

¹¹⁴ with $\partial_{[x,y]}$ denoting horizontal gradients and ∂_z denoting vertical gradients.

115 2.4. Relatively short time scale

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The relevant time scale T in the coastal ocean is typically much shorter 116 than in the global ocean. The key time scales in the coastal ocean are tidal. 117 inertial, diurnal or synoptic, i.e. $\mathcal{O}(1 \text{ day})$, whereas large scale ocean stud-118 ies generally concentrate on time scales reaching from seasonal to millenial 119 or beyond. The latter can be achieved by parameterising effects of tides, 120 inertial oscillations or storms (see, e.g., Eden et al. (2014)). In estuaries 121 and coastal regions, complex dynamical changes will occur during a tidal 122 cycle with strong tidal asymmetries in mixing and secondary circulation, 123 and substantial impact on transport e.g. of salt and suspended matter (see, 124 MacCready and Gever (2010)). One example for this is the strain-induced 125 periodic stratification (SIPS, see Simpson et al. (1990)) due to horizontal den-126 sity gradients as often observed in regions of freshwater influence (see, e.g., 127 Rippeth et al., 2001). Interior mixing in shelf seas is often caused by inertial 128 shear caused by episodic storm events combined with coastal coupling (Craig 129 (1989); van Haren et al. (1999); Knight et al. (2002)), a process which cannot 130 be parameterised in the coastal ocean due to its complex bathymetry and 131 coastline. Therefore, different model physics e.g. in terms of turbulence clo-132 sure models (see the discussion at the end of section 3.2.1) requiring different 133 numerical schemes are needed for coastal ocean models. 134

135 2.5. Relatively small spatial scales

Probably the most obvious characteristics of the coastal ocean is its lim ited spatial extent:

$$L \ll r_{Earth},$$
 (5)

with the Earth's radius r_{Earth} . Even if the entire coastal ocean is considered 139 as one single global object (see concepts by Holt et al. (2009)), large scale 140 global or regional drivers need to be transferred to the coastal ocean. For 141 the remote meteorological forcing (weather systems) this is typically done 142 by one-way or two-way nesting to a regional atmospheric model which itself 143 is coupled to a global model. For the remote oceanic impact (tides, surges, 144 planetary waves, etc.) this has to be done via lateral boundary conditions 145 coming from external models. Therefore, the problem of open boundary con-146 ditions (OBCs) and model nesting is characteristic for coastal ocean models 147 (as well as for the basin-scale ocean models), see the discussions in Section 148 6. 149

150 3. Basic equations

151 3.1. Momentum and tracer equations

Coastal and large scale ocean models typically use a common set of dynamic equations, which is based on the Reynolds-averaged primitive equations including hydrostatic and Boussinesq approximations. Detailed derivations of these equations are e.g. found in Griffies and Adcroft (2008).

These equations are derived from the Navier-Stokes equations on the ro-156 tating Earth by first adopting the Boussinesq approximation which includes 157 the use of a constant reference density ρ_0 (instead of the potential density ρ) 158 in all terms except in the gravity term. This has the consequence that mass 159 conservation is replaced by volume conservation. In a next step, the effects 160 of small-scale turbulent fluctuations on the larger scales are considered in a 161 parameterised way without the necessity to numerically resolve them. This 162 procedure assumes an ensemble averaging of the Navier-Stokes equations re-163 sulting in the Reynolds-averaged Navier-Stokes equations which now include 164 unknown turbulent stresses which need to be parameterised (see section 3.2). 165 Finally, a scaling analysis assuming a small aspect ratio (vertical scales are 166 much smaller than horizontal scales) results in the degeneration of the vertical 167 component of the momentum equation to the hydrostatic balance, neglect-168 ing vertical acceleration, the non-linear and the stress divergence terms and 169 the effects of Earth rotation (see the discussion in Kanarska et al., 2007; 170 Klingbeil and Burchard, 2013). The hydrostatic approximation includes the 171 traditional approximation for the Coriolis terms, neglecting the horizontal 172 contributions of Earth rotation in the horizontal momentum equations. The 173

dynamic equations are here for simplicity expressed in local Cartesian coordinates (see section 4 for spherical and curvilinear coordinates). After inserting the Boussinesq approximation into the mass conservation equation, the incompressibility condition remains:

$$\partial_x u + \partial_y v + \partial_z w = 0, \tag{6}$$

with the space coordinate vector (x, y, z) (eastwards, northwards, upwards), and the three-dimensional velocity vector (u, v, w).

Applying the incompressibility condition (6) and the hydrostatic condition (with pressure p and gravitational acceleration $g = 9.81 \,\mathrm{m \, s^{-2}}$),

$$\partial_z p = -g\rho,\tag{7}$$

(remainder of the vertical component of the Navier-Stokes equations) into
the horizontal momentum equations, the resulting dynamic equations are of
the following form:

$$\partial_t u + \partial_x \left(u^2 \right) + \partial_y \left(uv \right) + \partial_z \left(uw \right) + \partial_{\tilde{x}} J^{\mathrm{u}}_{\tilde{x}} + \partial_{\tilde{y}} J^{\mathrm{u}}_{\tilde{y}} + \partial_z J^{\mathrm{u}}_z - fv$$

$$= -\frac{1}{\rho_0} \partial_x p_a - \frac{g}{\rho_0} \partial_x \int_z^{\eta} \rho \,\mathrm{d}\xi$$

$$= -\frac{1}{\rho_0} \partial_x p_a - g \partial_x \eta + \int_z^{\eta} \partial_x b \,\mathrm{d}\xi$$
(8)

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$$\partial_t v + \partial_x \left(vu \right) + \partial_y \left(v^2 \right) + \partial_z \left(vw \right) + \partial_{\tilde{x}} J_{\tilde{x}}^{\mathsf{v}}(u, v) + \partial_{\tilde{y}} J_{\tilde{y}}^{\mathsf{v}}(u, v) + \partial_z J_z^{\mathsf{v}} + fu$$

$$= -\frac{1}{\rho_0} \partial_y p_a - \frac{g}{\rho_0} \partial_y \int_z^{\eta} \rho \, \mathrm{d}\xi$$

$$= -\frac{1}{\rho_0} \partial_y p_a - g \partial_y \eta + \int_z^{\eta} \partial_y b \, \mathrm{d}\xi,$$
(9)

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with time t, the local Coriolis frequency $f = 2\Omega \sin(\phi)$ (with the angular speed of Earth rotation $\Omega = 7.29 \cdot 10^{-5} \mathrm{s}^{-1}$ and the latitude ϕ), the surface elevation η , and the surface pressure p_a . $J^{\mathrm{u}}_{[\tilde{x},\tilde{y},z]}$ and $J^{\mathrm{v}}_{[\tilde{x},\tilde{y},z]}$ are shear stress vectors along the local plain spanned by the vector (\tilde{x}, \tilde{y}) which might be

along geopotentials ($\tilde{x} = x, \tilde{y} = y$), or along general vertical coordinates 194 or along isopycnals. This simplifying notation is used to avoid the intro-195 duction of rotated diffusion tensors and to facilitate the practical numerical 196 implementation. The terms on the left hand sides of (8) and (9) are the 197 tendency term, the three components of the advection terms (written in so-198 called integral form), the stress divergence terms, and the Coriolis term. The 199 terms on the right hand side form the horizontal pressure gradient compo-200 nents $\partial_x p / \rho_0$ and $\partial_y p / \rho_0$. The formulation in the last line splits the pressure 201 gradient into the external pressure gradient (composed of the atmospheric 202 pressure gradient and the surface slope) and the internal pressure gradient, 203 where $b = -(g/\rho_0)(\rho - \rho_0)$ is the buoyancy. The last lines of (8) and (9) 204 result from assuming $\rho(\eta)/\rho_0 \approx 1$ which is consistent with the Boussinesq 205 approximation. In (8) and (9), the flux form for the advective terms is used, 206 which results for any quantity q from the incompressibility condition (6): 207

$$u\partial_x q + v\partial_y q + w\partial_z q = \partial_x(uq) + \partial_y(vq) + \partial_z(wq), \tag{10}$$

which is the preferred form for coastal models in contrast to large-scale models sometimes based on the vector-invariant form for nonlinear terms, which allow an integral conservation of potential enstrophy and/or total energy (e.g. Arakawa and Lamb, 1977) (see section 7.1).

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Equations (8) and (9) are valid for $-H(x,y) < z < \eta(x,y,t)$ (with the bottom coordinate z = -H). Dynamic boundary conditions at the free surface are

$$J_{z}^{[\mathbf{u},\mathbf{v}]}\Big|_{z=\eta} = \frac{\tau_{[\mathbf{x},\mathbf{y}]}^{\mathbf{s}}}{\rho_{0}},\tag{11}$$

with the surface stress vector (τ_x^s, τ_y^s) , which is calculated from meteorological data using bulk formulae (e.g., Kondo (1975); Fairall et al. (1996)). At the bottom, the dynamic boundary conditions are the no-slip conditions

$$[u, v]\big|_{z=-H} = 0.$$
(12)

For numerical reasons, however, generally an equivalent flux boundary condition is applied,

$$J_{z}^{[\mathbf{u},\mathbf{v}]}\big|_{z=-H} = \frac{\tau_{[\mathbf{x},\mathbf{y}]}^{\mathbf{b}}}{\rho_{0}},$$
(13)

with the bed stress vector (τ_x^b, τ_y^b) reconstructed from a logarithmic velocity profile (see Section 7.5). ²²⁶ Kinematic surface and bottom boundary conditions are:

$$w\big|_{z=\eta} = \partial_t \eta + u\big|_{z=\eta} \partial_x \eta + v\big|_{z=\eta} \partial_y \eta + (E - P),$$
(14a)

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$$w\big|_{z=-H} = -u\big|_{z=-H}\partial_x H - v\big|_{z=-H}\partial_y H,\tag{14b}$$

with the evaporation rate E and the precipitation rate P. River run-off can be treated in various ways, e.g. as lateral boundary condition.

There is a large variety of lateral boundary conditions, which will be further discussed in section 6.

Within the Boussinesq approximation, the budget equation for internal energy reduces to a conservation equation for potential temperature θ :

$$\partial_t \theta + \partial_x \left(u\theta \right) + \partial_y \left(v\theta \right) + \partial_z \left(w\theta \right) + \partial_{\tilde{x}} J^{\theta}_{\tilde{x}} + \partial_{\tilde{y}} J^{\theta}_{\tilde{y}} + \partial_z J^{\theta}_z = \frac{1}{C_p \rho_0} \partial_z I, \quad (15)$$

with the horizontal and vertical turbulent fluxes of θ given by $J^{\theta}_{[\tilde{x},\tilde{y},z]}$, the 237 specific heat capacity of water at constant pressure, C_p , and irradiance in 238 water, I. The positive vertical gradient of irradiance depends on the light 239 absorption model applied. A classical model would be the model by Paulson 240 and Simpson (1977), but often more complex models taking into account 241 water colour, suspended matter and biogeochemical components are used. 242 In (15), the heating due to viscous dissipation of turbulent kinetic energy is 243 neglected, since in comparison to other terms in the local heat budget of the 244 ocean this is a very small term (in contrast to conditions in the higher atmo-245 sphere). The surface boundary condition for the turbulent flux of potential 246 temperature is formulated as 247

$$J_z^\theta\big|_{z=\eta} = \frac{Q_s + Q_l + Q_b}{C_p \rho_0},\tag{16}$$

with the sensitive heat flux Q_s (due to the air-sea temperature difference), the latent heat flux Q_l (due to evaporation), and the long-wave back radiation Q_b . Note that upward (positive) fluxes of potential temperature lead to cooling at the surface. For the parameterisation of these heat fluxes various models are available, with the bulk formulae by Kondo (1975) and Fairall et al. (1996) being the most common ones for coastal applications.

The conservation equation for the salinity S is of similar form as the temperature conservation equation, but without source term:

$$\partial_t S + \partial_x \left(uS \right) + \partial_y \left(vS \right) + \partial_z \left(wS \right) + \partial_{\tilde{x}} J^{\rm S}_{\tilde{x}} + \partial_{\tilde{y}} J^{\rm S}_{\tilde{y}} + \partial_z J^{\rm S}_{z} = 0.$$
(17)

²⁵⁸ The diffusive salinity flux at the surface is given as

$$J_z^{\rm S}\big|_{z=\eta} = -(E-P)S,\tag{18}$$

see Beron-Vera et al. (1999) for details. The salinity unit which should be used in all ocean models is the absolute salinity which indicates the mass fraction of salt in seawater in [g/kg], defined according to the TEOS-10 standard (IOC, SCOR and IAPSO (2010)). The potential density is calculated by means of an empirical equation of state as function of potential temperature θ , absolute salinity S and pressure p:

$$\rho = \rho(\theta, S, p). \tag{19}$$

A recent and accurate formulation for Boussinesq models has been provided by Roquet et al. (2015).

269 3.2. Turbulence closure modelling

Turbulence closure modelling involves complex theories which cannot be discussed here. For an overview, the reader is referred to text books (Kantha and Clayson, 2000b; Griffies, 2004; Cushman-Roisin and Beckers, 2011; Olbers et al., 2012). In most ocean models, vertical and horizontal turbulent fluxes of scalars are parameterised by a down-gradient approximation of the form

$$J^c_{[\tilde{x},\tilde{y}]} = -A_c \partial_{[\tilde{x},\tilde{y}]}c, \qquad (20)$$

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$$J_z^c = -K_c \partial_z c, \tag{21}$$

using horizontal and vertical eddy diffusivities A_c and K_c for any scalar c. With this, the turbulent fluxes are directed towards the lower concentrations, as postulated for molecular fluxes in ideal gases.

For the vertical turbulent momentum fluxes, an equivalent formulation is generally used:

$$J_z^{[\mathbf{u},\mathbf{v}]} = -K_{\mathbf{M}}\partial_z[u,v], \qquad (22)$$

with the vertical eddy viscosity $K_{\rm M}$. For the parameterisation of the horizontal turbulent momentum fluxes, additional invariance to vector rotation ²⁸⁷ needs to be taken into account (Blumberg and Mellor, 1987):

$$J_{\tilde{x}}^{u}(u) = -2A_{M}\partial_{\tilde{x}}u,$$

$$J_{\tilde{y}}^{u}(u,v) = -A_{M}\left(\partial_{\tilde{y}}u + \partial_{\tilde{x}}v\right),$$

$$J_{\tilde{x}}^{v}(u,v) = -A_{M}\left(\partial_{\tilde{y}}u + \partial_{\tilde{x}}v\right),$$

$$J_{\tilde{y}}^{v}(v) = -2A_{M}\partial_{\tilde{y}}v,$$
(23)

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with the horizontal eddy viscosity $A_{\rm M}$.

290 3.2.1. Small-scale closure models

For the parameterisation of vertical eddy viscosity and diffusivity, two basic approaches are commonly used in ocean models.

One of them is based on direct algebraic computation of the eddy parame-293 ters from bulk properties (boundary fluxes, mixed layer depth, bulk Richard-294 son number) of the surface and bottom mixed layers, the so-called K-profile 295 parameterisation (KPP) which has been originally proposed for large-scale 296 ocean models by Large et al. (1994). In addition to the down-gradient fluxes, 297 also counter-gradient flux components (for example for convectively unstable 298 boundary layers) are included in the KPP model. Many extensions of the 299 original KPP model have been proposed (see, e.g., Smyth et al., 2002; Durski 300 et al., 2004; Uchiyama et al., 2010) to extend its applicability also to coastal 301 ocean applications (see, e.g., Blaas et al., 2007). The KPP model assumes 302 that the boundary layer turbulence is in equilibrium with the surface or bot-303 tom fluxes, respectively. For large scale ocean models, this might often be 304 an adequate approximation. In many coastal model applications however, 305 the deviation from this equilibrium is a first-order process which cannot be 306 neglected. 307

The other closure approach, which in contrast to the KPP model considers high temporal and spatial variability in boundary layers, is based on a dynamic equation for the turbulent kinetic energy (TKE), k, which can be derived from the Navier-Stokes equations by means of Reynolds-averaging (Wilcox, 1998; Burchard, 2002a):

$$\partial_{t}k + \partial_{x}\left(uk\right) + \partial_{y}\left(vk\right) + \partial_{z}\left(wk\right) - \partial_{z}\left(\frac{K_{\mathrm{M}}}{Sc_{k}}\frac{\partial k}{\partial z}\right) = P + B - \varepsilon, \qquad (24)$$

with the shear production, $P = K_{\rm M} M^2$ including the vertical shear squared, 314 M^2 , and the buoyancy production, $B = -K_c N^2$, with the buoyancy fre-315 quency (or Brunt-Väisälä frequency) squared, N^2 , and the dissipation rate, 316 ε . The shear production P transfers kinetic energy lost from the mean flow 317 due to vertical stress divergence to the turbulent kinetic energy, whereas the 318 buoyancy production B exchanges energy between the mean potential en-319 ergy to the turbulent kinetic energy. Note, that in (24) the down-gradient 320 approximation has been adopted with the turbulent Schmidt number Sc_k , 321 which is of order unity. Horizontal turbulent fluxes are generally neglected 322 for the TKE budget (Delhez et al., 1999). This may also be the case for the 323 advective terms, but in tidally energetic regimes, such a neglect might lead 324 to significant errors or instabilities. In addition to the TKE, also the length 325 scale of the energy containing eddies, l, needs to be approximated to obtain 326 an estimate for the vertical eddy viscosity and eddy diffusivity. Once k and 327 *l* are known, the vertical eddy coefficients can be calculated as 328

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$$K_{\rm M} = S_{\rm M} k^{1/2} l, \qquad K_c = S_c k^{1/2} l,$$
 (25)

with the non-dimensional stability functions $S_{\rm M}$ and S_c . These stability functions can be parameterised by means of second-moment closures based on Reynolds-averaging the Navier-Stokes equations (Mellor and Yamada, 1982; Canuto et al., 2001) or based on simpler empirical relations (Rodi, 1987; Burchard and Baumert, 1995). The dissipation rate ε can be calculated from l via the cascading relation

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$$\varepsilon = c_{\varepsilon} \frac{k^{3/2}}{l} \tag{26}$$

with the empirical constant c_{ϵ} .

Surface and bottom boundary conditions are typically derived from the 338 law of the wall, resulting in k being proportional to the surface or bed stress, 339 respectively, and the length sale to be proportional to the respective rough-340 ness length. Equivalent flux conditions, which proved to be numerically more 341 stable have been proposed (Burchard and Petersen, 1999). To parameterise 342 effects of breaking surface waves, injection of TKE at the surface is applied 343 (Burchard, 2001). Effects of Langmuir Circulation on the dynamics of the 344 surface mixed layer may be parameterised as well (see, e.g., Harcourt, 2014). 345 Additional frictional effects of surface waves on wave drag in shallow water 346 can also be considered in the bottom boundary condition (Mellor, 2002). 347

Various methods are used in ocean modelling to calculate the length scale *l*. In one-equation turbulence closure models (the one equation is for the

computation of the TKE), l is calculated from combinations of geometric 350 length scales (such as the distance from the surface or the bottom) or from 351 hydrodynamic length scales (such as the Ozmidov scale), see e.g., Mellor and 352 Yamada (1982); Gaspar et al. (1990). More common in coastal ocean models 353 are however two-equation turbulence closure models which in addition to the 354 TKE equation calculate a budget equation for a length-scale related quantity 355 such as for the dissipation rate ε (k- ε models, see Rodi, 1987; Burchard 356 and Baumert, 1995), for the turbulent frequency $\omega = \varepsilon/k$ (k- ω models, see 357 Wilcox, 1998; Umlauf et al., 2003), the quantity kl (k-kl models, see Mellor 358 and Yamada, 1982), or the generic length-scale related property $k^m l^n$ with 359 real numbers m and n (the generalised length-scale model, see Umlauf and 360 Burchard, 2003). When properly calibrated, all these two-equation models 361 perform similarly (Burchard et al., 1998; Umlauf and Burchard, 2003; Warner 362 et al., 2005). 363

Two-equation turbulence closure models including algebraic second-moment closures as outlined here (see also the review by Umlauf and Burchard, 2005) have proven in many applications as a good compromise between computational efficiency and realistic representation of relevant processes in the coastal ocean.

There is a number of reasons, why such second-moment turbulence closure 369 models are a necessary feature of coastal ocean models. First of all, as 370 discussed in section 2.1, a large portion of water columns in the coastal 371 ocean (if not the entire water column) are covered by surface or bottom 372 boundary layers. These boundary layers have a vertical structure which 373 locally influences the mixing coefficients. Therefore, boundary layer models 374 reacting on local forcing instead of surface or bottom fluxes only are required. 375 Secondly, relevant times scale in the coastal ocean are much shorter than in 376 the global ocean (see section 2.4). Therefore, the turbulence closure models 377 need to react on correct time scales to rapid time changes in surface or bottom 378 stress instead of instantaneouly adjusting the eddy coefficients in the entire 379 mixed layers such as in the KPP model. Such requirements are only fulfilled 380 by carefully calibrated second-moment turbulence closure models. 381

There are a few global ocean models using low-level second-moment closures (see, e.g., Oschlies (2002); Danabasoglu et al. (2014)), which typically are based on the Gaspar et al. (1990) one-equation model, where the turbulent length scale l is algebraically computed. Two-equation turbulence closure models are generally too complex for global ocean models. This is mainly due to the large baroclinic time steps of global models (about 1 hour) and the coarse resolution in boundary layers. Increasing spatial and temporal resolution of large-scale ocean models in order to allow for the inclusion of two-equation turbulence closure models would result in addionally high computational costs which probably might not pay off on the temporal and spatial scales relevant for global ocean simulations. Therefore, in large-scale ocean models, the KPP model (see above) or other models with reduced dynamics (see, e.g., Jackson et al. (2008)) are used.

395 3.2.2. Meso-scale and submeso-scale closure models

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Whereas in ocean models a consistent theoretical framework for the ver-396 tical turbulent fluxes exists, such a rigorous closure for the horizontal tur-397 bulent fluxes due to meso-scale and submeso-scale eddies is still missing. In 398 the stratified ocean, the physically most relevant direction of horizontal mix-399 ing is along isopycnal surfaces. Since this is however numerically demanding 400 in non-isopycnal models (see the discussion by Griffies et al., 1998; Beckers 401 et al., 1998), in many model applications horizontal mixing is simply carried 402 out along coordinate surfaces. 403

Two simplistic common approaches used in the coastal ocean modelling 404 community are to either neglect horizontal turbulent fluxes (and then rely on 405 the numerical fluxes due to monotone, upstream-biased advection schemes, 406 see section 7) or to set $A_{\rm M}$ and A_c to constant values. In the latter case, the 407 proper choice of the horizontal exchange coefficients is then determined by 408 sensitivity studies. A physically more sound, resolution-dependent parame-409 terisation of horizontal momentum fluxes has been proposed by Smagorinsky 410 (1963). For incompressible fluids under the (quasi)hydrostatic pressure ap-411 proximation the horizontal eddy viscosity can be derived as 412

$$A_{\rm M} = C_{\rm M}(\Delta x \,\Delta y) \sqrt{(\partial_{\tilde{x}} u)^2 + \frac{1}{2} \left(\partial_{\tilde{y}} u + \partial_{\tilde{x}} v\right)^2 + \left(\partial_{\tilde{y}} v\right)^2},\tag{27}$$

with the horizontal grid sizes Δx and Δy , and with the empirical parameter $C_{\rm M}$. The latter has been estimated by Holt and James (2006) in a shelf sea application as $C_{\rm M} \approx 0.2$. The same approach as (27) can also be applied for horizontal tracer diffusivities (see, e.g., Gräwe et al., 2015), using a different value for the empirical parameter.

For large scale ocean models which do not resolve meso-scale eddies, other closures have been proposed, such as the Gent and McWilliams (1990) closure for isopycnal mixing or the dynamic meso-scale eddy closure by Eden and Greatbatch (2008). However, in coastal ocean models eddies are at least ⁴²³ partially resolved, such that these closures cannot directly be used in such
⁴²⁴ models. On the other hand, theories for submeso-scale dynamics are not yet
⁴²⁵ mature and general enough to derive applicable eddy closures.

426 4. Coordinate transformations and spatial discretisation

The set of governing equations, consisting of the continuity equation (6), the hydrostatic momentum equations (8) and (9), and the prognostic equations for temperature (15) and salinity (17), so far has been formulated in a local Cartesian reference frame at the Earth surface for simplicity. However, the transformation to coordinate systems that align with the geometry of the domain is often advantageous.

Most coastal ocean models support orthogonal curvilinear coordinates in 433 the horizontal to offer to some extent the alignment with coastlines and an 434 increased horizontal resolution towards the coast as required by the typically 435 strong near-coastal horizontal gradients, see (4). The corresponding basis 436 transformation introduces additional metric coefficients and terms that also 437 offer the formulation in spherical coordinates, see Sec. 4.3 for details. For 438 clarity, the governing equations in the remainder of this review will be kept 439 in horizontal Cartesian coordinates. 440

In the vertical the alignment with the boundaries (free surface and bottom 441 topography) and proper resolution (of e.g. the boundary layers and pycno-442 clines) is even more critical than in the horizontal. A general description that 443 supports various types of vertical coordinates is given by the s-coordinates 444 of Kasahara (1974). The general vertical coordinate s(x, y, z, t) must be 445 strictly monotone in z in order to guarantee a unique inverse transformation 446 z(x, y, s, t) and a well-defined Jacobian $\partial_s z = (\partial_z s)^{-1}$ for the transformation 447 of the governing equations. For isopycnal coordinates $s = \rho$ this precludes 448 the representation of unstable stratification. The horizontal coordinates and 449 time do not change under the transformation and, if necessary for the purpose 450 of clarity, derivatives with respect to constant s and z will be distinguished 451 by $(\cdot)_s$ and $(\cdot)_z$, respectively. With the Lagrangian derivative D/Dt it can 452 easily be shown, that the grid-related vertical velocity, defined as the differ-453 ence of the fluid's vertical velocity and the vertical velocity of the coordinate 454

surfaces w^{grid} , is given by 455

s

$$w^{s} = w - w^{\text{grid}}$$

$$= \left[\frac{D}{Dt} - \left(\frac{D}{Dt}\right)_{s}\right] z(x, y, s, t) = \partial_{s} z \left[\frac{D}{Dt} - \left(\frac{D}{Dt}\right)_{s}\right] s = \partial_{s} z \frac{Ds}{Dt}.$$

$$(28)$$

4.1. Layer-integrated equations 459

The vertical discretisation of the transformed space into k_{max} layers with 460 interfaces at fixed levels $s_{k+1/2}$ (independent of x, y, t and with $k \in [0, k_{\max}]$) 461 is equivalent to a discretisation of the physical space into k_{\max} layers with 462 interfaces at variable levels $z_{k+1/2}(x, y, t) = z(x, y, s_{k+1/2}, t)$ and $z_{k+1/2} > z_{k+1/2}(x, y, t) = z(x, y, s_{k+1/2}, t)$ 463 464

Therefore substantiable for $z_{k+1/2}(z, y, t) = (z, y, t)$ $z_{k-1/2}$, see Burchard and Petersen (1997). With layer heights $h_k(x, y, t) = \int_{s_{k-1/2}}^{s_{k+1/2}} \partial_s z ds = z_{k+1/2} - z_{k-1/2}$, layer-averaged prognostic quantities $\varphi_k(x, y, t) = h_k^{-1} \int_{z_{k-1/2}}^{z_{k+1/2}} \varphi dz$, for $k \in [1, k_{\max}]$ 465 466 and $\varphi \in \{u, v, \theta, S\}$, and $w_{k+1/2}^{s}(x, y, t) = w^{s}(x, y, z_{k+1/2}, t)$, the layer-integration 467 of (6), (8), (9), (15) and (17) yields: 468

$$\frac{\partial_{t}h_{k} + \partial_{x}(h_{k}u_{k}) + \partial_{y}(h_{k}v_{k}) + \left(w_{k+1/2}^{s} - w_{k-1/2}^{s}\right) = 0,$$
(29)
$$\frac{\partial_{t}(h_{k}u_{k}) + \partial_{x}(h_{k}u_{k}u_{k}) + \partial_{y}(h_{k}v_{k}u_{k}) + \left(w_{k+1/2}^{s}\widetilde{u}_{k+1/2} - w_{k-1/2}^{s}\widetilde{u}_{k-1/2}\right)$$
$$= fh_{k}v_{k} - gh_{k}\partial_{x}\eta - h_{k}\frac{1}{\rho_{0}}\partial_{x}p_{a} + \left(\tau_{x,k+1/2} - \tau_{x,k-1/2}\right)$$
$$+ h_{k}\widetilde{F}_{x}^{h}(h_{k}, u_{k}, v_{k}) + h_{k}F_{x,k}^{IP},$$

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$$(30)$$

$$\partial_t (h_k v_k) + \partial_x (h_k u_k v_k) + \partial_y (h_k v_k v_k) + \left(w_{k+1/2}^{\mathrm{s}} \widetilde{v}_{k+1/2} - w_{k-1/2}^{\mathrm{s}} \widetilde{v}_{k-1/2} \right)$$

(31)

(32)

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474

$$+h_k \widetilde{F}_y^{\rm h}(h_k, u_k, v_k) + h_k F_{y,k}^{\rm IP},$$

$$\partial_t (h_k \theta_k) + \partial_x (h_k u_k \theta_k) + \partial_y (h_k v_k \theta_k) + \left(w_{k+1/2}^{\rm s} \widetilde{\theta}_{k+1/2} - w_{k-1/2}^{\rm s} \widetilde{\theta}_{k-1/2} \right)$$

 $= -fh_k u_k - gh_k \partial_y \eta - h_k \frac{1}{\rho_0} \partial_y p_a + \left(\tau_{\mathbf{y},k+1/2} - \tau_{\mathbf{y},k-1/2}\right)$

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$$= -\partial_x \left(h_k J_{\tilde{x},k}^{\theta} \right) - \partial_y \left(h_k J_{\tilde{y},k}^{\theta} \right) - \left(J_{z,k+1/2}^{\theta} - J_{z,k-1/2}^{\theta} \right)$$
$$+ \frac{1}{C_p \rho_0} \left(I_{k+1/2} - I_{k-1/2} \right),$$

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$$\partial_{t} (h_{k}S_{k}) + \partial_{x} (h_{k}u_{k}S_{k}) + \partial_{y} (h_{k}v_{k}S_{k}) + \left(w_{k+1/2}^{S}\widetilde{S}_{k+1/2} - w_{k-1/2}^{S}\widetilde{S}_{k-1/2}\right)$$

$$= -\partial_{x} (h_{k}J_{\tilde{x},k}^{S}) - \partial_{y} (h_{k}J_{\tilde{y},k}^{S}) - \left(J_{z,k+1/2}^{S} - J_{z,k-1/2}^{S}\right).$$
(33)

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In (29)-(33) the interfacial values $\tilde{\varphi}_{k+1/2}$ with $\varphi \in \{u, v, \theta, S\}$ are approximated by the vertical advection scheme, see Sec. 7.1. The salinity of freshwater fluxes is zero, i.e. $\tilde{S}_{k_{\max}+1/2} = \tilde{S}_{1/2} = 0$. According to (28) the kinematic boundary conditions (14a) and (14b) transform to $w_{k_{\max}+1/2}^{\rm s} = E - P$ and $w_{1/2}^{\rm s} = 0$.

 I_{483} In (30) and (31) the internal pressure gradient force is given by

$$F_{[x,y],k}^{\rm IP} = \frac{1}{h_k} \int_{z_{k-1/2}}^{z_{k+1/2}} \left(\partial_{[x,y]}\right)_z \int_z^{\eta} b \mathrm{d}\xi \mathrm{d}z,\tag{34}$$

and is approximated in terms of the layer-averaged buoyancies b_k (see, e.g. Shchepetkin and McWilliams, 2003 and Sec. 7.2).

Considering the dynamic boundary conditions (11) and (13), the vertical shear stresses are defined as

$$\tau_{[\mathbf{x},\mathbf{y}],k+1/2} = \begin{cases} \tau_{[\mathbf{x},\mathbf{y}]}^{\mathbf{s}}(u_{k_{\max}}, v_{k_{\max}}), & k = k_{\max} \\ K_{\mathbf{M},k+1/2} \frac{[u, v]_{k+1} - [u, v]_k}{z_{k+1} - z_k}, & k \in [1, k_{\max} - 1] , \\ \tau_{[\mathbf{x},\mathbf{y}]}^{\mathbf{b}}(h_1, u_1, v_1), & k = 0 \end{cases}$$
(35)

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492 with centre positions $z_k = \frac{1}{2} (z_{k-1/2} + z_{k+1/2}).$

The lateral contributions of the stress tensor are approximated according to Mellor and Blumberg (1985) and Kantha and Clayson (2000a):

$$\widetilde{F}^{\mathbf{h}}_{[\mathbf{x},\mathbf{y}]}(h,u,v) = -\frac{1}{h} \left(\partial_x \left(h J^{[\mathbf{u},\mathbf{v}]}_{\tilde{x}}(u,v) \right) + \partial_y \left(h J^{[\mathbf{u},\mathbf{v}]}_{\tilde{y}}(u,v) \right) \right), \quad (36)$$

with the diffusive fluxes $J_{[\tilde{x},\tilde{y}]}^{[u,v]}$ given by (23) and all gradients calculated along layer k. In case of diffusion along directions not aligned with constant s, additional terms due to non-diagonal elements of the diffusion tensor would occur (Griffies (2004)).

In (32) and (33) $J^c_{[\tilde{x},\tilde{y}],k}$ denotes the lateral turbulent fluxes (again with all gradients calculated along layer k), $J^c_{z,k\pm 1/2}$ the vertical turbulent fluxes at the layer interfaces, with $J^{\rm S}_{k_{\max}+1/2} = 0$ and $I_{k\pm 1/2}$ the interfacial irradiance.



Figure 1: Sketch showing a vertical transect through a coastal ocean model domain including four different vertical coordinates. The blue lines indicate two selected isopycnals representing a tidal front with a stratified shelf sea region to the right and a well-mixed coastal region to the left. The vertical black lines indicate the horizontal discretisation, the red lines show the vertical coordinate surfaces and the bold black lines show the bottom and surface representation of the coordinates. a: σ -coordinates with zooming towards the surface and the bottom; b: S-coordinates with high near-surface resolution; c: Adaptive coordinates with increased resolution in the stratified region; d: Geopotential coordinates without partial cells at the bottom.

504 4.2. Examples for vertical coordinates

The almost arbitrary choice of the transformation function s = s(x, y, z, t)or equivalently of the moving layer interfaces $z_{k+1/2}(x, y, t)$ allows for a high degree of freedom for the vertical layout which can be exploited to improve the model performance.

509 4.2.1. Geopotential coordinates

Geopotential (or z-) coordinates (see Figure 1d) are based on globally 510 defined z-levels $z_{k+1/2}$ which do not depend on location or time, except for 511 the uppermost coordinate level $z_{k_{\max}+1/2}$ = η which is identical to the free 512 surface. Vertical resolution is typically increased near the surface to properly 513 reproduce the dynamics of the surface mixed layer. Since for too fine near-514 surface vertical resolution the moving and sloping free surface might intersect 515 with one or more coordinate levels, the uppermost geopotential coordinate 516 level $z_{k_{\max}-1/2}$ is chosen such that it is below the minimum surface elevation. 517 For models of shelf seas with a large maximum tidal range (see Sec. 2.2) 518 this would result in a large mean thickness of the upper layer of $\mathcal{O}(10\text{m})$, 519 such that near-surface processes are not well-resolved (see, e.g., Mathis et al. 520 (2015)). For simulations of shallow coastal regions including drying and 521 flooding this would mean that all areas with intertidal flats are not vertically 522 resolved. One solution to this problem has been proposed by Casulli and 523 Cheng (1992) and Burchard and Baumert (1998): Layers at the surface are 524 locally added or removed when the surface layer becomes too thick or too 525 thin, respectively. This problem can also be solved by applying so-called z^* -526 coordinates (Adcroft and Campin (2004)), where geopotential coordinates 527 are obtained for $\eta = 0$ everywhere, and all layer thicknesses are then locally 528 multiplied by $(\eta + H)/H$, such that the layers are squeezed or expanded with 529 the changing water depth. Another disadvantage of geopotential models near 530 the surface (which is not solved by the above mentioned treatment) is that 531 the tidal elevation triggers a large oscillating vertical velocity relative to the 532 fixed coordinate levels which generates strong numerical mixing due to the 533 vertical advection schemes, see Sec. 7.1. 534

At the bottom geopotential layers will be intersecting with the sloping bottom. This leads to a stair-case type of discretisation of bottom slopes which leads to low accuracy in resolving bottom parallel currents such as dense bottom currents (Ezer and Mellor (2004)). A partial solution to this problem has been proposed by Beckmann and Döscher (1997) by coupling an empirical terrain-following bottom boundary layer model to the geopotential

model grid, allowing for bottom-parallel down-slope flow. Another approach 541 to improve representation of along-bottom flow has been proposed by Ad-542 croft et al. (1997): to introduce shaved cells at the bottom to better fit the 543 bottom topography. Geopotential coordinates over sloping topography have 544 one other inherent problem: they do not allow a high vertical resolution near 545 the bottom. A resolution of the bottom layer of 1 m would require equidis-546 tant geopotential coordinates over the entire water column, which is often 547 computationally not affordable. 548

Given all these disadvantages of geopotential coordinates they can generally not be recommended for coastal ocean simulations. There is however one potential problem of vertical coordinates which is not relevant for geopotential coordinates: the internal pressure gradient problem, see Sec. 7.2. Therefore, models with geopotential coordinates are still applied for problems with strong stratification such as the Baltic Sea (Wang et al. (2015)).

The numerical treatment of geopotential coordinates fits into the concept of general vertical coordinates by formally allowing layers of zero thickness at the bottom and, in the case of removable surface layers, also at the surface.

558 4.2.2. Terrain-following coordinates

A transformation function of the form $z(s) - \eta = S(x, y, s, t)D(x, y, t)$ 559 with the local water depth $D = \eta + H$, the stretching function S being 560 strictly monotone in s, $S(s_{1/2}) = -1$ and $S(s_{k_{\max}+1/2}) = 0$ generates terrain-561 following coordinates with $z_{1/2} = -H$ and $z_{k_{\max}+1/2} = \eta$. In addition to the 562 free surface being a coordinate surface (as for the z^* -coordinates), also the 563 bottom is a coordinate surface. Thus, in every watercolumn k_{max} layers are 564 active and masking of layers is not necessary. A classical option for coastal 565 ocean model simulations are σ -coordinates defined by $S = s = \sigma$ (Nihoul 566 et al. (1986); Blumberg and Mellor (1987)), see Figure 1a. They result in 567 layer thicknesses proportional only to the local water depth, which is a dis-568 advantage especially in deeper waters (where layers may become too thick 569 and thus resolution in critical parts of the water column too coarse) or above 570 steep bottom slopes (where coordinate slopes are relatively steep throughout 571 the water column, see Deleersnijder and Beckers (1992)). One other prob-572 lem of terrain-following coordinates is the intersection of sloping coordinate 573 surfaces with isopycnals. For the calculation of the internal pressure gradi-574 ent, this results in a balance of two large terms which typically results in 575 large truncation errors and thus artificial currents (see Sec. 7.2 for a detailed 576 discussion. 577

Some of these problems can be reduced by using non-equidistant σ levels $\sigma_{k+1/2}$ (equivalent to non-linear stretching functions S(s)) and modified stretching functions S(x, y, s) that rescale the near-surface layer heights proportional to a fixed critical water depth instead of to the local water depth (Song and Haidvogel, 1994; Shchepetkin and McWilliams, 2009), see Figure 1b.

An alternative transformation function that maintains high resolution at the surface or at the bottom independently of the local water depth has been developed by Burchard and Petersen (1997) and Burchard and Bolding (2002).

On order to obtain higher accuracy, hybridisations between s- and zcoordinates have been proposed, leading to less steep coordinate slopes than for s coordinates and smaller bottom steps than for z-coordinates, see Gerdes (1993); Burchard and Petersen (1997) for details.

592 4.2.3. Arbitrary Lagrangian-Eulerian (ALE) coordinates

For geopotential and terrain-following coordinates the transformation func-593 tion z(s) is explicitly prescribed. The temporal evolution of the correspond-594 ing interface positions $z_{k+1/2}(x, y, t)$ and layer heights $h_k(x, y, t)$ is fully deter-595 mined by a prognostic equation for the sea surface elevation $\eta(x, y, t)$ (see Sec. 596 5.1). In this case the continuity equation (29) does not serve as a prognos-597 tic equation for h_k , but as a diagnostic equation for the grid-related vertical 598 velocity $w_{k+1/2}^{s}$. Following Adcroft and Hallberg (2006), this is the Eulerian 599 treatment of the vertical direction (EVD). 600

In contrast, the Lagrangian treatment of the vertical direction (LVD) is based on a Lagrangian vertical coordinate, formally defined by $\frac{Ds}{Dt} = 0$ (Starr, 1945). In this case the grid-related vertical velocity vanishes $w^{s} = 0$, see (28), and the continuity equation (29) serves as a prognostic equation for the layer heights h_{k} .

Numerical mixing (induced by truncation errors of discrete advective fluxes; see e.g. Klingbeil et al., 2014) is significantly reduced in Lagrangian vertical coordinates because of the missing advective transport through the coordinate surfaces. However, a pure Lagrangian movement of the layers is prone to grid distortion and possibly vanishing layers, which complicates the numerical treatment.

Therefore, a combination of LVD and EVD gains increasingly popularity. Originally Hirt et al. (1974) defined the Arbitrary Lagrangian-Eulerian (ALE) method by a Lagrangian mesh movement (LVD step) followed by an optional readjustment of the mesh associated with grid-related advective transports (EVD step). The advection during the EVD step can be replaced by instantaneous "remapping" (monotone and conservative interpolation, see e.g. White and Adcroft, 2008) which relaxes the strict CFL constraint to a less severe Lipschitz condition.

Another approach is to consider Lagrangian tendencies in the calcu-620 lation of the layer heights used in EVD algorithms. Separable terrain-621 following coordinates of the form $z - \eta = S(s)D(x, y, t)$ inherently im-622 ply a Lagrangian treatment of merely barotropic motions (Shchepetkin and 623 McWilliams, 2009). Non-separable terrain-following coordinates with time-624 independent stretching functions S(x, y, s) do not exactly treat barotropic 625 motions in a Lagrangian way, but also significantly reduce the correspond-626 ing grid-related vertical transports by scaling the layer heights according to 627 $h_k = \frac{D}{H} h_k^{(\eta=0)}$. The same holds for the z^{*}-coordinates of Adcroft and Campin 628 (2004).629

Recently, Leclair and Madec (2011) proposed to also treat fast oscillating baroclinic currents in a Lagrangian way by introducing the so-called \tilde{z} -coordinate.

633 4.2.4. Adaptive coordinates

In order to further optimise the vertical grid layout in 3D models, Hofmeister et al. (2010) presented adaptive coordinates, see Figure 1c. These do not only consider Lagrangian tendencies, but also a zooming of layers towards boundaries, stratification and shear. This zooming is based on a vertical diffusion equation for the interface positions,

$$\partial_{t} z_{k+1/2} - \left(D_{k+1}^{\text{grid}}(z_{k+3/2} - z_{k+1/2}) - D_{k}^{\text{grid}}(z_{k+1/2} - z_{k-1/2}) \right) = 0, \quad (37)$$

with boundary conditions $z_{1/2} = -H$ and $z_{k_{\max}+1/2} = \eta$ (Burchard and Beck-641 ers, 2004). A vertically constant layer "diffusion" coefficient D^{grid} (unit s⁻¹) 642 tends to generate equidistant layers, whereas locally increased coefficients 643 (e.g. proportional to stratification and shear) increase the local concentra-644 tion of layer interfaces and thus the vertical resolution. Improved vertical 645 resolution decreases the truncation errors of vertical advective fluxes and 646 thus reduces vertical numerical mixing. The layer distribution in adjacent 647 water columns is coupled by lateral adjustment of layer heights and inter-648 face positions. In addition, an optional isopycnal tendency aligns the layers 649 with isopycnals and thus avoids the spurious diapycnal mixing of tracers due 650

to explicit and numerical along-layer mixing in the model. Furthermore, an 651 isopycnal alignment of the layers reduces internal pressure gradient errors (see 652 Sec. 7.2). It should be noted, that pure isopycnal coordinates are not appro-653 priate for coastal ocean models, because of the relatively large mixed layers 654 according to (1). Gräwe et al. (2015) demonstrated the clear advantages 655 of adaptive coordinates compared to σ -coordinates in a realistic state-of-656 the-art model application with different dynamical regimes (tidal/non-tidal 657 parts, seasonal thermocline / permanent halocline). 658

659 4.3. Horizontal discretisation

The layer-integrated equations (29) - (33) include horizontal divergence 660 terms for advection and diffusion which still need to be discretised. Inde-661 pendently from the vertical coordinate specification, a horizontal coordinate 662 transformation is carried out. For the simplest case, no coordinate transfor-663 mation is needed, such that horizontal coordinates remain Cartesian, with 664 typically x denoting the coordinate to the right and y denoting the coordinate 665 orthogonally to it in a right-hand system. Such Cartesian coordinates are 666 consistent with UTM coordinates. This however limits model applications 667 to domains being very small compared to the Earth's radius, since the model 668 domain is assumed to be planar. For larger domains (such as shelf seas), a 669 transformation into spherical coordinates is carried out, with coordinates λ 670 (pointing eastwards) and ϕ (pointing northwards), which is consistent with 671 geographical coordinates. The transformation to spherical coordinates re-672 sults in geometric coefficients by which terms in the dynamic equations are 673 weighted (see, e.g., the text book by Kantha and Clayson (2000a)). To sup-674 port multi-scale applications also with regular coordinates (and not only with 675 unstructured-grid models), orthogonal curvi-linear coordinates have been in-676 troduced (Haidvogel et al. (1991)), having enough flexibility to focus into 677 certain parts of the domain such as estuaries or coastal regions. Curvi-linear 678 coordinates may be referenced to Cartesian or to spherical coordinates, de-679 pending on the scale of the problem, but the resulting grids (after discretisa-680 tion) are of the same type. It should be noted that Cartesian and spherical 681 coordinates can be regarded as special cases of orthogonal curvi-linear coor-682 dinates, such that models which include the latter do automatically offer the 683 numerics for the other two types. Note that also non-orthogonal curvilinear 684 coordinates are in use, to further increase flexibility in spatial resolution, 685 but those have not become common in coastal ocean modelling (Kantha and 686 Clayson (2000a)). 687

After the horizontal transformation, a horizontal discretisation is carried 688 out, by dividing the two coordinates of the Cartesian, spherical or orthogonal 689 curvi-linear coordinates into not necessarily equidistant spatial increments. 690 This leads to a tiling of the horizontal model domain by grid cells which may 691 be rectangles (Cartesian coordinates), trapezoids (spherical coordinates) or 692 general quadruples (orthogonal curvi-linear coordinates). Note that angles 693 between edges are orthogonal only for Cartesian coordinates. Each grid cell 694 has thus four corners and four edges. Grid cells which include mainly land 695 areas are then masked out. 696

The layer-integrated equations (29) - (33) are then area-integrated over 697 these cells, such that in combination with the vertical layer-integration an 698 integration over so-called finite volumes is obtained. By means of this vol-699 ume integration, divergence terms are transformed to differences of interface-700 integrated advective and diffusive fluxes, such that advection and diffusion 701 are discretised in a conservative way. Non-conservative source and sink terms 702 appear as volume-integrals. These finite volumes have 8 corners, 12 edges and 703 6 interfaces, see Fig. 2. With $\Delta x_{i,j}$ and $\Delta y_{i,j}$ denoting mean length and width 704 of the volumes and $h_{i,j,k}$ denoting the mean height, these volumes are defined 705 as $\mathcal{V}_{i,j,k} = \Delta x_{i,j} \Delta y_{i,j} h_{i,j,k}$. With $\Delta x_{i,j\pm 1/2}$ and $\Delta y_{i\pm 1/2,j}$ denoting the length 706 and width at the lateral edges, the vertical interfaces of the finite volume 707 have the areas $A_{i\pm 1/2,j,k} = \Delta y_{i\pm 1/2,j,k}$ and $A_{i,j\pm 1/2,k} = \Delta x_{i,j\pm 1/2} h_{i,j\pm 1/2,k}$. 708 With these notations, the volume-integral of the layer height equation (29) 709 reads as 710

$$\Delta x_{i,j} \Delta y_{i,j} \partial_t h_{i,j,k} + \left(\Delta y_{i+1/2,j} h_{i+1/2,j,k} u_{i+1/2,j,k} - \Delta y_{i-1/2,j} h_{i-1/2,j,k} u_{i-1/2,j,k} \right) + \left(\Delta x_{i,j+1/2} h_{i,j+1/2,k} v_{i,j+1/2,k} - \Delta x_{i,j-1/2} h_{i,j-1/2,k} v_{i,j-1/2,k} \right) + \Delta x_{i,j} \Delta y_{i,j} \left(w_{i,j,k+1/2}^{s} - w_{i,j,k-1/2}^{s} \right) = 0,$$
(38)

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with $u_{i\pm 1/2,j,k}$, $v_{i,j\pm 1/2,k}$, and $w_{i,j,k\pm 1/2}^{s}$, denoting area-averaged velocities at the 712 respective interfaces. Tracer mass conservation requires the finite-volume ⁷¹⁴ discretisation of e.g. the salinity equation of the following form:

$$\begin{aligned} \Delta x_{i,j} \Delta y_{i,j} \partial_t h_{i,j,k} S_{i,j,k} \\ &+ \left(\Delta y_{i+1/2,j} h_{i+1/2,j,k} u_{i+1/2,j,k} \widetilde{S}_{i+1/2,j,k} \right) \\ &- \Delta y_{i-1/2,j} h_{i-1/2,j,k} u_{i-1/2,j,k} \widetilde{S}_{i-1/2,j,k} \right) \\ &+ \left(\Delta x_{i,j+1/2} h_{i,j+1/2,k} v_{i,j+1/2,k} \widetilde{S}_{i,j+1/2,k} \right) \\ &- \Delta x_{i,j-1/2} h_{i,j-1/2,k} v_{i,j-1/2,k} \widetilde{S}_{i,j-1/2,k} \right) \\ &+ \Delta x_{i,j} \Delta y_{i,j} \left(w_{i,j,k+1/2}^{S} \widetilde{S}_{i,j,k+1/2} - w_{i,j,k-1/2}^{S} \widetilde{S}_{i,j,k-1/2} \right) = \\ &- \Delta y_{i+1/2,j} \left(h_{i+1/2,j,k} J_{\tilde{x},i+1/2,j,k}^{S} \right) + \Delta y_{i-1/2,j} \left(h_{i-1/2,j,k} J_{\tilde{x},i-1/2,j,k}^{S} \right) \\ &- \Delta x_{i,j+1/2} \left(h_{i,j+1/2,k} J_{\tilde{y},i,j+1/2,k}^{S} \right) + \Delta x_{i,j-1/2} \left(h_{i,j-1/2,k} J_{\tilde{y},i,j-1/2,k}^{S} \right) \\ &- \Delta x_{i,j} \Delta y_{i,j} \left(J_{z,i,j,k+1/2}^{S} - J_{z,i,j,k-1/2}^{S} \right), \end{aligned}$$

$$(39)$$

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with the interfacial salinity values $\widetilde{S}_{i\pm 1/2,j,k}$, $\widetilde{S}_{i,j\pm 1/2,k}$ and $\widetilde{S}_{i,j,k\pm 1/2}$ and the volume averaged salinity $S_{i,j,k}$. For constant tracers and zero turbulent tracer fluxes the tracer equation must recover (38).

The natural spatial discretisation which results from the volume-inte-719 gration carried out in (38) and (39) suggests to locate the discrete velocity 720 points $u_{i\pm 1/2,j,k}$, $v_{i,j\pm 1/2,k}$, and $w_{i,j,k\pm 1/2}^{s}$ at the centres of the 6 interfaces of the 721 finite volume. The natural location for the volume-averaged salinity $S_{i,j,k}$ 722 (and consequently also of the potential temperature $\theta_{i,j,k}$ and the buoyancy 723 $b_{i,j,k}$ would then be the centre of the finite volume, see Fig. 2. This would 724 be in accordance with the classical Arakawa C-grid (Arakawa and Lamb 725 (1977)), where velocity points and *pressure points* (salinity, potential tem-726 perature, buoyancy, and thus also pressure) are staggered in space. Such a 727 grid layout guarantees that (38) and (39) can be discretised at second order 728 in space without any interpolations of velocity components. For the volume-729 integrated u- and v-velocity equations (not shown here; note that for the 730 w-velocity no dynamic equation has to be integrated) separate (staggered) 731

finite volumes have to be constructed for which transport velocities have to 732 be interpolated to the respective interfaces (which has to be done for any 733 staggered or non-staggered grid layout). Turbulent quantities (such as verti-734 cal eddy viscosity/diffusivity and turbulent kinetic energy) are best located 735 at the w-points, such that also for the turbulence equations specific finite 736 volumes centred around the w-points need to be constructed. There is one 737 disadvantage of the fully staggered grid layout: The respectively other hori-738 zontal velocity component for the calculation of the Coriolis terms needs to be 739 interpolated from four adjacent velocity points in order to be second-order in 740 space. A grid layout which avoids this by collocating u- and v-components at 741 the corners of the finite volume is given by the B-grid (which still is staggered 742 with respect to vertical velocity and pressure points). Therefore large scale 743 ocean models for which an accurate spatial discretisation is essential typi-744 cally use the B-grid, whereas coastal ocean models have traditionally been 745 written as C-grid models (see also Sec. 8.1). An excellent overview over the 746 discretisation of the linearised shallow water equations and its accuracies in 747 A- (all discrete points collocated), B- (only horizontal velocity points collo-748 cated), C- (all staggered), and D-grids (as C-grid, but with u- and v-velocity 749 locations exchanged) is given by Beckers and Deleersnijder (1993). 750

⁷⁵¹ 5. Choices for mode splitting and wetting & drying

An essential feature of coastal ocean models is the consideration of a temporally and spatially variable free surface, see (2) in section 2.2. Due to the presence of a free surface, fast surface gravity waves are part of the numerical solution, and drying and flooding in shallow areas of the domain is possible. Both issues require special numerical techniques that will be outlined in the following two subsections.

758 5.1. Mode splitting

Within the EVD-treatment (see Section 4.2.3) the layer-integrated continuity equation (29) serves as a diagnostic equation for the grid-related vertical velocities $w_{k+1/2}^{s}$, and the layer heights h_k are determined in terms of the total water depth D and the free surface elevation η . In this case a prognostic equation for the free surface elevation must be derived from the vertical sum of the layer-integrated continuity equation (29) and consideration of the kinematic boundary conditions (14a) and (14b):



Figure 2: Control volume for cell-centered variables (top), C-grid staggering showing the location of the dependent variables in the horizontal (bottom, left) and in the vertical (bottom, right).

$$\partial_t(\eta + H) = \partial_t D = \partial_t \left(\sum_{k=1}^{k_{\max}} h_k\right) = -\partial_x \left(\sum_{k=1}^{k_{\max}} h_k u_k\right) - \partial_y \left(\sum_{k=1}^{k_{\max}} h_k v_k\right) - (E - P)$$
(40)

The direct numerical integration of the set (40) and (29)–(33) is possible. However, within an explicit temporal discretisation the time step is strongly constrained by the celerity of the fastest surface gravity waves. Alternatively, an implicit discretisation offers larger time steps (Casulli and Cheng, 1992), but also requires the inversion of a penta-diagonal system for the free surface elevation.

Since surface gravity waves are solely represented by the barotropic mode, the computational costs can be significantly reduced by splitting the governing equations into the barotropic and remaining baroclinic mode. Usually the slightly depth-dependent barotropic mode is approximated by the depthintegrated equations (also called external mode), given by (40) and the vertical sum of the layer-integrated momentum equations (30) and (31):

$$\partial_t D + \partial_x \left(D\bar{u} \right) + \partial_y \left(D\bar{v} \right) = -(E - P),$$
(41a)

$$\begin{array}{ll} & \overset{780}{781} \\ & \overset{781}{782} \\ & \partial_t \left(D\bar{u} \right) + \partial_x \left(D\bar{u}\bar{u} \right) + \partial_y \left(D\bar{v}\bar{u} \right) \\ & = f D\bar{v} - g D\partial_x \eta - D\frac{1}{\rho_0} \partial_x p_a + \tau^{\rm s}_{\rm x}(\bar{u},\bar{v}) - \tau^{\rm b}_{\rm x}(D,\bar{u},\bar{v}) + D\widetilde{F}^{\rm h}_{\rm x}(D,\bar{u},\bar{v}) + S_{\rm x}, \\ & (41b) \\ & & (41b) \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\$$

 $D \equiv \sum_{k=1}^{k_{\max}} h_k, \tag{42}$

⁷⁹² the barotropic transports,

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$$[D\bar{u}, D\bar{v}] \equiv \sum_{k=1}^{k_{\text{max}}} [h_k u_k, h_k v_k], \qquad (43)$$

⁷⁹⁴ and the barotropic-baroclinic interaction terms:

$$S_{[x,y]} = \partial_{x} \left(D\bar{u}[\bar{u},\bar{v}] \right) - \sum_{k=1}^{k_{\max}} \partial_{x} \left(h_{k}u_{k}[u_{k},v_{k}] \right) - \sum_{k=1}^{k_{\max}} \partial_{y} \left(h_{k}u_{k}[u_{k},v_{k}] \right) - D\widetilde{F}_{[x,y]}^{h}(D,\bar{u},\bar{v}] - \sum_{k=1}^{k_{\max}} \partial_{y} \left(h_{k}u_{k}[u_{k},v_{k}] \right) + D\widetilde{F}_{[x,y]}^{h}(D,\bar{u},\bar{v}) + \sum_{k=1}^{k_{\max}} h_{k}\widetilde{F}_{[x,y]}^{h}(h_{k},u_{k},v_{k}) + D\widetilde{F}_{[x,y]}^{h}(D,\bar{u},\bar{v}) + \tau_{[x,y]}^{s}(u_{k_{\max}},v_{k_{\max}}) + \tau_{[x,y]}^{b}(D,\bar{u},\bar{v}) - \tau_{[x,y]}^{b}(h_{1},u_{1},v_{1}) + \sum_{k=1}^{k_{\max}} h_{k}F_{[x,y],k}^{IP}.$$
(44)

The remaining 3D equations (30)-(33), as well as the turbulence closure 802 equations (section 3.2) and other tracer equations such as biogeochemical 803 model equations represent the internal (baroclinic) mode. With (42), (43)804 and (44) the splitting into external and internal mode equations is exact. 805 But, as mentioned above, it does not exactly separate the slightly depth-806 dependent fast barotropic dynamics from the slow baroclinic ones. Therefore, 807 the time-stepping of the internal mode might still be constrained by some 808 fast dynamics. 809

A careful stability analysis of the linearised (flat-bottom) version of the external mode (41a)–(41c),

$$\partial_t \eta = -H \left(\partial_x \bar{u} + \partial_y \bar{v} \right); \quad \partial_t \bar{u} = -g \partial_x \eta + f \bar{v}; \quad \partial_t \bar{v} = -g \partial_y \eta - f \bar{u}, \quad (45)$$

has been carried out by Beckers and Deleersnijder (1993). For an explicit 813 discretisation on an equidistant C-grid, the stability criterion would be $\Delta t \leq$ 814 $\Delta x/(2gH)^{1/2}$, which means for $\Delta x = 1000$ m and a depth of H = 200 m a 815 maximum timestep of $\Delta t \approx 5$ s. Compared to that, the stability criterion 816 for discretising the internal mode is typically given by the advection terms. 817 For an explicit one-stage two-level discretisation (Durran, 2013) of the linear 818 advection equation the stability criterion is $\Delta t \leq \Delta x/u_{\text{max}}$, which would for 819 a typical maximum velocity of $u_{\rm max} = 1 \,{\rm m \, s^{-1}}$ give a maximum timestep of 820 $\Delta t = 200$ s, which is a factor of about 40 larger. Non-linear systems retaining 821 all terms tend to have comparable timestep criteria. 822

If the surface elevation and the barotropic transports are not integrated 823 prognostically as part of the internal mode, but provided by the external 824 mode, an explicit temporal discretisation of the internal mode is not con-825 strained by the celerity of the fastest surface gravity waves anymore, but 826 only by the much slower internal motions. In this case the internal mode can 827 be integrated explicitly with a timestep which, for coastal oceans, is $\mathcal{O}(10^1)$ 828 times larger than that constrained by the celerity of shallow water surface 829 gravity waves. Since this increased timestep is usually already almost re-830 quired to resolve the dynamical processes in e.g. tidally dominated coastal 831 oceans, the overhead of an implicit treatment of the 3D internal mode equa-832 tions would be by far not balanced by the possible slight further increase of 833 the timestep. Therefore, the prognostic integration of the internal mode is 834 usually performed explicitly. 835

The prognostic integration of the external mode can be either carried out implicitly with the same timestep as used for the explicit integration of the internal mode, or explicitly within a series of smaller timesteps constrained by the celerity shallow water surface gravity waves. Both methods have their own merits and complications. Such a different numerical treatment of the two modes is called mode splitting and has first been introduced by Madala and Piacsek (1977).

⁸⁴³ 5.1.1. Semi-implicit external mode computation

Let (41a)–(41c) being solved simultaneously, with the transports $D\bar{u}$ and 844 $D\bar{v}$ in (41a) being temporally weighted such that they are between the levels 845 of the old and the new surface elevation, and equivalently, with η in (41b) and 846 (41c) being temporally between the old and new transports. then, a semi-847 implicit time stepping scheme for the external mode results. With the weight-848 ing parameter $0 \le \gamma \le 1$, this can be expressed as $X^{n+\gamma} = (1-\gamma)X^n + \gamma X^{n+1}$ 849 for any quantity X which is treated semi-implicitly (with superscripts de-850 noting the number of time step). For $\gamma = 0$, the scheme would be fully 851 explicit, for $\gamma = 1$ the scheme would be fully implicit and for $\gamma = 0.5$, the 852 Crank-Nicolson scheme is obtained. The schemes are more stable (and more 853 implicit) the more the bias is towards the new time step, i.e., the larger γ is. 854 This procedure gives a linear system of equations with a matrix of dimension 855 $N \times N$ with N denoting the number of free-surface grid boxes. Depending 856 on the treatment of the Coriolis terms (explicit or semi-implicit), and when 857 calculating non-linear terms explicitly, each row of the matrix has 5 or 9 858 non-zero entries, such that the matrix is very sparse. One of the challenges 859

for solving these large systems of equations is to find accurate (typically iterative) solvers which are efficient also on massively parallel high-performance computers. An early example for a semi-implicit coastal ocean model including semi-implicit treatment of the Coriolis term has been presented by Backhaus (1985). This semi-implicit scheme is unconditionally stable for $\gamma \geq 0.5$.

To avoid the requirement of solving large linear systems of equations 866 due to the semi-implicit treatment of the external mode, a directional-split 867 method had been introduced by Peaceman and Rachford (1955), in which 868 in an alternating manner the external mode is solved along one and then 869 along the other coordinate direction. This method is called Alternating Di-870 rections Implicit (ADI). Many models in coastal engineering had adopted 871 this approach (see, e.g., Pietrzak et al., 2002). While ADI is easier to handle 872 computationally than a semi-implicit treatment without directional splitting, 873 additional errors due to the splitting have to be considered. 874

The advantage of the semi-implicit treatment is the relatively easy cou-875 pling between the external and the internal mode, since both are computed 876 with the same time step. A disadvantage of implicit schemes is the demand-877 ing computation of large and sparse linear system on parallel computers. 878 While the Crank-Nicolson scheme is energy-conserving (but still sensitive to 879 instabilities arising from the discretisation of other terms), a larger degree 880 of implicitness $(\gamma \rightarrow 1)$ stabilises the scheme, a procedure which however 881 for larger time steps might become too dissipative (Walters et al. (2009)). 882 In tidal or tsunami simulations this sets a practical limitation to the overall 883 model time step. 884

⁸⁸⁵ 5.1.2. Explicit external mode computation

In order to provide a reasonable free surface elevation and barotropic transports for updating the internal mode from stage ⁿ to stage ⁿ⁺¹, the external mode is integrated explicitly within a subcycle of M_{max} timesteps from stage ^{n,0} to stage ^{n,M_{max}}. The timestep of the external mode Δt_{2D} is constrained by the celerity of shallow water surface gravity waves, whereas the internal mode is integrated with a larger internal timestep $\Delta t_{3D} = M \Delta t_{2D}$ with $M \leq M_{\text{max}}$.

It is easy and accurate to discretise the external mode with an explicit-intime solver. In the following a time-staggered two-level scheme is outlined. Staggering in time between the surface elevations and the barotropic transports would still guarantee second-order in time accuracy. This would be achieved by subsequently calculating the surface elevation and the barotropic transports with using the newly updated transports and elevations on the right hand sides, see section 7.3. In the following the focus will be on volume and tracer mass conservation. Therefore, the discretisation of the momentum equations will be not presented in detail. A time-staggered discretisation of the free-surface equation (41a) is given by:

$$\frac{\eta^{n,m+1} - \eta^{n,m}}{\Delta t_{2D}} + \partial_x (D\bar{u})^{n,m+1/2} + \partial_y (D\bar{v})^{n,m+1/2} = -(E-P)^{n,m+1/2}$$

$$= -(E-P)^{n,m+1/2}$$
(46)

Following Shchepetkin and McWilliams (2005) a filtered surface elevation is provided to the internal mode,

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$$\langle \eta \rangle^{n+1} \equiv \sum_{m=0}^{M_{\text{max}}} a_m \eta^{n,m},$$
 (47)

with normalised filter weights $\sum_{m=0}^{M_{\text{max}}} a_m = 1$. If the initial surface elevation of each external mode cycle is reset to $\eta^{n,0} \equiv \langle \eta \rangle^n$, the compatible surface elevation equation resolved by the internal mode can be derived from (46) as

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$$\frac{\langle \eta \rangle^{n+1} - \langle \eta \rangle^n}{\triangle t_{3\mathrm{D}}} + \partial_x \left\langle \left\langle D\bar{u} \right\rangle \right\rangle^{n+1/2} + \partial_y \left\langle \left\langle D\bar{v} \right\rangle \right\rangle^{n+1/2} = -\left\langle \left\langle E - P \right\rangle \right\rangle^{n+1/2} \quad (48)$$

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919 920 with

$$\langle\langle\psi\rangle\rangle^{n+1/2} \equiv \sum_{m=0}^{M_{\text{max}}-1} b_m \psi^{n,m+1/2} \tag{49}$$

and $b_m \equiv \frac{1}{M} \sum_{m'=m+1}^{M_{\text{max}}} a_{m'}$. The general filter applied in (47) offers different types of filtering. Deleersnijder (1993) proposed to provide the instantaneous surface elevation $\langle \eta \rangle^{n+1} = \eta^{n,M}$ and averaged barotropic transports $\langle \langle [D\bar{u}, D\bar{v}] \rangle \rangle^{n+1/2} = \sum_{m=0}^{M-1} [D\bar{u}, D\bar{v}]^{n,m+1/2}$ to the internal mode. This treatment corresponds to $M_{\text{max}} = M$, $a_m = \delta_{mM}$, $b_m = 1$ and involves no reset of the external quantities, i.e. $\eta^{n+1,0} = \eta^{n,M}$ and $[D\bar{u}, D\bar{v}]^{n+1,0-1/2} =$ $[D\bar{u}, D\bar{v}]^{n,M-1/2}$. In order to stabilise the retained fast dynamics within the ⁹²⁸ internal mode and to prevent aliasing errors Griffies (2007) suggested to pro-⁹²⁹ vide an averaged surface elevation $\langle \eta \rangle^{n+1} = \frac{1}{2M+1} \sum_{m=0}^{2M} \eta^{n,m}$ to the internal ⁹³⁰ mode, obtained by $M_{\text{max}} = 2M$, $a_m = \frac{1}{2M+1}$ and $b_m = \frac{2M-m}{M(2M+1)}$. Non-uniform ⁹³¹ filter weights, centered around $m = M < M_{\text{max}}$, were presented by Shchep-⁹³² etkin and McWilliams (2005) to offer more frequency-selective filtering. ⁹³³ Volume conservation requires that the layer-integrated continuity equa-

Volume conservation requires that the layer-integrated continuity equation (29) in the internal mode,

$$\frac{h_k^{n+1} - h_k^n}{\Delta t_{3D}} + \partial_x \left(h_k u_k \right)^{n+1/2} + \partial_y \left(h_k v_k \right)^{n+1/2} + \left(w_{k+1/2}^{s,n+1/2} - w_{k-1/2}^{s,n+1/2} \right) = 0,$$
(50)

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⁹³⁷ recovers (48) when vertically summed. Thus

$$\sum_{k=1}^{k_{\max}} h_k^{n+1} \equiv \langle \eta \rangle^{n+1} + \langle H \rangle^{n+1} = \langle D \rangle^{n+1}, \qquad (51a)$$

$$\sum_{k=1}^{k_{\max}} \left[h_k u_k, h_k v_k \right]^{n+1/2} \equiv \left\langle \left\langle \left[D\bar{u}, D\bar{v} \right] \right\rangle \right\rangle^{n+1/2} \tag{51b}$$

$$w_{\cdot}^{\mathrm{s},n+1/2} = \langle \langle F_{\cdot} - P \rangle \rangle^{n+1/2}$$

(51c)940 941 $w_{k_{\max}+1/2} \equiv \langle \langle E - P \rangle \rangle$ Compatibility condition (51b) can be obtained by shifting the velocity pro-942 files obtained from the baroclinic momentum equations (30) and (31). It 943 should be noted again, that for tracer mass conservation the discrete tracer 944 equations must recover (50) for constant tracers. Therefore, the shifting 945 of velocity profiles must be done before the grid-related vertical velocity is 946 diagnosed from (50) and the tracer equations are integrated. At the end of 947 each internal timestep, the interaction-terms (44) can be updated in terms of 948 each internal timestep, the interaction-terms (44) can be updated in terms of $\langle \langle [D\bar{u}, D\bar{v}] \rangle \rangle^{n+1/2}$, $[h_k u_k, h_k v_k]^{n+1/2}$ and $F_{[x,y],k}^{\text{IP},n+1}$. Since these interaction-terms are held constant over the next external subcycle, integrating the barotropic transports from $(D\bar{u})^{n+1,0-1/2}$ to $(D\bar{u})^{n+1,M_{\text{max}}-1/2}$, a time lag is introduced. 949 950 951

952 5.2. Drying and flooding

In many coastal areas intertidal flats are an important topographic feature. During high water those areas are inundated and during ebb tide they may fall dry, approaching zero water depth $D \rightarrow 0$, but never becoming negative. To understand how this is reflected in the mathematical formulations for coastal ocean dynamics, it is instructive to reformulate the depth-integrated continuity equation (41a) into an advection equation for the water depth:

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$$\partial_t D + \bar{u}\partial_x D + \bar{v}\partial_y D = -\left(\partial_x \bar{u} + \partial_y \bar{v}\right) D - (E - P).$$
(52)

The conservative form (41a) shows that total water volume is conserved. The 960 advective form (52) demonstrates positivity of the water depth, because its 961 total derivative depends on a sink term which vanishes for decaying water 962 depth. The divergence stays bounded, because for frictionally dominated 963 regimes the depth-integrated momentum equations (41b) and (41c), and the 964 quadratic bed friction (77) guarantee bounded depth-mean velocities. The 965 evaporation E which reduces the water depth must be numerically treated 966 such that it vanishes for vanishing water depth. 967

Various ways have been proposed in coastal ocean models to guarantee the two major properties (i) volume conservation (for incompressible flow) according to (41a) and (ii) positivity according to (52), also numerically.

It should be straight-forward to directly discretise one of the equations. Usually (41a) is used as a basis. In contrast, for a vertically integrated model, Stelling and Duinmeijer (2003) successfully applied a first-order upstream scheme to discretise the advection equation (52), and later Zijlema et al. (2011) postulated that positivity could also be achieved using a Total Variation Diminishing (TVD) scheme with the MUSCL limiter (van Leer (1979)).

Given that the spatial discretisation is for a C-grid (section 4.3), and in 978 order to conserve volume locally and globally, the transports $\bar{u}D$ and $\bar{v}D$ need 979 to be identical to the sum of the layer-integrated transports used in (29). 980 This consistency of local and global volume conservation is also essential 981 for the conservation of momentum and tracers. Therefore, a numerical re-982 calculation of $\bar{u}D$ and $\bar{v}D$ in (41a) would require a correction to the layer-983 integrated transports calculated prognostically in (30) and (31). This is 984 the general principle of conservative drying and flooding: to manipulate the 985 layer-integrated momentum equations in a physically sound and reasonable 986 way, and to use the same transports in (41a). 987

There are various approaches to this, all of them leaving a thin film of water in dry cells, where the dynamics is manipulated in some way to avoid zero or negative water depth. In early coastal ocean models (Flather and Heaps, 1975; Backhaus, 1976, 1985; Jungclaus and Backhaus, 1994), a number of rules were defined on how to reduce fluxes out of a grid cell when

the application of these fluxes would lead to negative water depth (or the 993 undercut of a prescribed minimum water depth). Also the wetting and drying 994 schemes of Oey (2005) and Warner et al. (2013) are based on this principle. 995 The method works reliably, but to guarantee positive water depth, it has to 996 be taken into account that reduction or shut-off of fluxes around one grid cell 997 would change the net fluxes into the neighboring cells, such that an iterative 998 procedure might become necessary. This problem has been partially solved 999 by Warner et al. (2013), by shutting off all transports around a cell when the 1000 water depth at the old time step is below the critical depth, see also Defne and 1001 Ganju (2015) who simulated a large lagoonal back-barrier estuary at the US 1002 east coast including extensive intertidal flats. Moreover, the direct correction 1003 of fluxes might in some models lead to spatially and temporally oscillating 1004 patterns of dry and wet cells. Furthermore, shutting on and off transports 1005 instantaneously could lead to complications in turbulence closure models, 1006 since the bed stress which largely determines the eddy viscosity profiles (via 1007 the turbulent kinetic energy and the macro length scale of turbulence, see 1008 section 3.2.1) would be suddenly switched on or shut off regularly. 1009

In some models (e.g., Casulli and Cattani, 1994) the water depth at the transport points of a C-grid is chosen as the minimum depth between the adjacent pressure points, with the consequence that velocities feel the shallow water and bed friction strongly reduces the volume transport. This however might lead to significantly delayed drying and flooding processes (Burchard and Bolding, 2002).

In order to avoid explicit switching on or off of transports in drying cells, Burchard et al. (2004) (see also Burchard and Bolding, 2002) proposed the following measures when calculating the layer-integrated momentum equations:

• A critical water depth $D_{\rm crit},$ and a minimum water depth, $D_{\rm min}$ are 1020 defined with $D_{\rm crit} > D_{\rm min}$ (see fig. 3). Typical values would be $D_{\rm crit} =$ 1021 $0.2 \,\mathrm{m}$ and $D_{\min} = 0.05 \,\mathrm{m}$. To simplify the dynamics in very shallow 1022 water with $D < D_{crit}$, many terms in the layer-integrated momentum 1023 equations are reduced by a factor linearly decreasing between 1 (for 1024 $D = D_{\text{crit}}$ and 0 (for $D = D_{\min}$), which basically reduces the local 1025 dynamics to an external pressure gradient - friction balance. Such a 1026 balance supports reduction of local transports, since the friction coeffi-1027 cient calculated from the law of the wall in the lowest grid box increases 1028 towards infinity for the water depth converging towards zero, see equa-1029


Figure 3: Sketch explaining the geometry of bathymetry and surface elevation approximations as it is defined in GETM. This figure has been modified from Burchard et al. (2004).

1030 tion (76).

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• Additionally, when the surface elevation in one grid box is below the 1031 bottom coordinate plus the minimum depth in any adjacent cell (which 1032 often happens at steep bathymetry in shallow water and relatively 1033 coarse horizontal resolution, see fig. 3, where $\eta_{i+1,j} < -H_{i,j} + D_{\min}$), a 1034 virtual surface elevation is defined from which the external pressure gra-1035 dient $(\partial_x \eta, \partial_y \eta)$ is calculated. In that case, $\tilde{\eta}_{i+1,j} = \max\{\eta_{i+1,j}, -H_{i,j} +$ 1036 D_{\min} , and the surface elevation gradient is calculated as $(\tilde{\eta}_{i+1,j} - D_{\min})$ 1037 $\eta_{i,j})/\Delta x$. In the extreme case shown in fig. 3 water volume would ac-1038 tually flow against the elevation gradient, because $\eta_{i,j} < -H_{i,j} + D_{\min}$. 1039

• Despite the above measures, direct reduction or shut-off of transports surrounding a grid cell may still be necessary at singular locations. To stabilise the drying and flooding algorithm, increasing the minimum and critical water depth is often a preferred option.

Using these algorithms Gräwe et al. (2016) could carry out a stable and multiannual simulation of the entire Wadden Sea of the South-Eastern North Sea
at a horizontal resolution of 200 m.

¹⁰⁴⁷ 6. Treatment of open boundary conditions and model nesting

Coastal ocean models focus on limited areas of interest and thus data are 1048 needed to force the models at open boundaries, see Section 2.5. The data can 1049 typically come from an external source (e.g. climatology, coarser resolution 1050 run on a wider domain) following a one-way (coarse \rightarrow fine) approach. In 1051 comparison, in a two-way approach, the external data (a numerical model) 1052 feel the local coastal solution through a feedback term. Local and external 1053 models generally differ on several key points among them grid resolution (in 1054 space and time) and physics. Across the interface, inflow and outflow can 1055 occur. In the case of inflow conditions, the quality of the local solution is 1056 strongly dependent on the quality of external data while in the case of out-1057 flow, the main issue is to prevent wave reflection at the interface. A two-way 1058 approach helps in maintaining some consistency between local and external 1059 solutions, at least when the physics of the two models are close. In both one-1060 way and two-way approaches, the design of the boundary conditions must be 1061 carefully done. Due to the complexity of the physics, the scale heterogene-1062 ity in space and time, ideal boundary conditions are not achievable and a 1063 reasonable choice relies on a compromise between accuracy and robustness. 1064 Section (6.1) briefly introduces the general framework. Section (6.2) treats 1065 the problem of model forcing in a one-way approach (open boundary con-1066 ditions). Section (6.3) introduces two-way approaches. Some considerations 1067 on discrete approximations are given in Section (6.4). 1068

1069 6.1. General framework

¹⁰⁷⁰ We consider a domain $\Omega_{\rm loc}$ embedded in a domain $\Omega_{\rm ext}$ as shown in Figure ¹⁰⁷¹ 4. The local and external solutions, $\phi_{\rm loc}$ and $\phi_{\rm ext}$, are integrated according ¹⁰⁷² to

$$\partial_t \phi_{\rm loc} + L_{\rm loc}(\phi_{\rm loc}) = f_{\rm loc} \text{ in } \Omega_{\rm loc}, \quad \partial_t \phi_{\rm ext} + L_{\rm ext}(\phi_{\rm ext}) = f_{\rm ext} \text{ in } \Omega_{\rm ext}.$$

¹⁰⁷³ L_{loc} and L_{ext} are spatial differential operators, f_{loc} and f_{ext} model forcings. ¹⁰⁷⁴ ϕ is the vector of prognostic state variables. The models interact through a ¹⁰⁷⁵ transition area Γ that, depending on the boundary conditions, may be re-¹⁰⁷⁶ stricted to a single interface γ .

¹⁰⁷⁷ Let $\Delta x_{\rm loc}$ and $\Delta x_{\rm ext}$ (resp. $\Delta t_{\rm loc}$ and $\Delta t_{\rm ext}$)) be the grid (resp. time) steps on ¹⁰⁷⁸ $\Omega_{\rm loc}$ and $\Omega_{\rm ext}$. Today, the availability of global/regional operational or reanal-¹⁰⁷⁹ ysis products allows to consider the case where typical values of time/grid



Figure 4: The local domain $\Omega_{\rm loc}$ embedded in the exterior domain $\Omega_{\rm ext}$. $\Omega_{\rm loc}$ has an artificial interface γ and possibly a transition area Γ on which boundary conditions are prescribed.

1080 steps obey:

$$\frac{\Delta x_{\text{ext}}}{\Delta x_{\text{loc}}} \approx \frac{\Delta t_{\text{ext}}}{\Delta t_{\text{loc}}} \approx 2 - 10.$$

¹⁰⁸¹ The model interactions across the interface γ and/or within the transition ¹⁰⁸² area Γ are described in the next Sections.

1083 6.2. Open boundary conditions (OBC) and one-way interaction

We start with a description of the two main classes of OBC methods: 1084 relaxation methods which aim to relax the local solution towards the ex-1085 ternal solution within the transition area Γ and radiation methods which 1086 propagate out the information to prevent waves reflection. Simple radiation 1087 methods are appropriate only for a wave equation, the extension to general 1088 hyperbolic systems using a characteristic variables approach is explained in 1089 (6.2.2). Advanced open boundary conditions like Perfectly Matched Layer 1090 (PML) and Absorbing Boundary Conditions (ABC) (see Nataf, 2013) will 1091 not be discussed here since their derivations require very simplified problems 1092 and they have still to be validated in realistic applications. In (6.2.4), we dis-1093 cuss the specificities of local mesh refinement when the local computational 1094 grid is nested within a coarser resolution grid and also mention the impact 1095

¹⁰⁹⁶ of variabilities at interfaces. For a review of open boundary conditions, the ¹⁰⁹⁷ reader is referred to Palma and Matano (2000); Blayo and Debreu (2005).

1098 6.2.1. Relaxation and radiation methods:

Relaxation methods. Basic Dirichlet (a.k.a. clamped) boundary conditions do not perform well (except for certain basic equations): this abrupt forcing generates inconsistencies and discontinuities near the interface γ . The flow relaxation scheme (FRS) (Davies, 1976) relaxes the interior solution towards external data in the transition area Γ near the boundary and can be written under the following relaxation (or nudging) form (Martinsen and Engedahl, 1987) (considering ϕ as a scalar variable and omitting the model forcing):

$$\partial_t \phi_{\rm loc} + L_{\rm loc}(\phi_{\rm loc}) = -\frac{1}{\tau} (\phi_{\rm loc} - \phi_{\rm ext}) \quad \text{in } \Omega_{\rm loc},$$
 (53)

The right hand side of (53) is the relaxation term. τ is a relaxation time scale. $\lambda = \frac{1}{\tau}$ is a positive function, which decreases away from the lateral boundary γ and vanishes outside of Γ . At the discrete level, the right hand side of (53) can be solved implicitly to remove associated stability constraints. It is difficult to prescribe the size of the transition area Γ and the variation of λ within Γ , since they depend on the space and time scales of the phenomena (Kållberg, 1977). Typical profiles of λ are based on quadratically or exponentially decreasing functions of the distance to the boundary γ .

Due to the smallness of the coastal model domain, it may also happen 1114 that the large scales of the solution are better reproduced in the external 1115 domain Ω_{ext} . It is particularly the case when the external model makes use 1116 of data assimilation techniques (reanalysis product or operational forecast). 1117 In this situation, there is a potential benefit to relax the large scales of the 1118 local solution to the ones computed by the external model while the small 1119 scales features are still governed by the coastal model evolution. To this aim, 1120 spectral nudging methods (Waldron et al., 1996) can be viewed as a FRS 1121 scheme which acts on the whole local domain on specified (large) scales. It 1122 can be written under the following form: 1123

$$\partial_t \phi_{\rm loc} + L_{\rm loc}(\phi_{\rm loc}) + \Lambda(\phi_{\rm loc} - \phi_{\rm ext}) = 0 \quad \text{in } \Omega_{\rm loc}, \tag{54}$$

where the operator Λ is now a low pass filter acting on the whole Ω_{loc} domain. The expression of Λ may be based on Fourier transform of $(\phi_{\text{loc}}, \phi_{\text{ext}})$ (with relaxation coefficients fixed in the Fourier space), on Gaussian correlation kernels and more simply on iterative Laplacian smoothing. When applied to
coastal modelling, the nudging term is usually reduced near the coast where
the external model may have a coarser representation of the coastline.

Finally, most of the time, the FRS scheme is associated to a sponge layer that damps the small scales near the boundary using increased viscosity/diffusivity ν :

$$\partial_t \phi_{\rm loc} + L_{\rm loc}(\phi_{\rm loc}) = -\frac{1}{\tau} (\phi_{\rm loc} - \phi_{\rm ext}) + \nu_{\Gamma} \,\Delta \phi_{\rm loc} \quad \text{in } \Omega_{\rm loc}. \tag{55}$$

Radiation methods. In the case of outflow conditions, the FRS scheme will only behave well (and in particular will prevent waves reflection) when the external data is already an accurate representation of the solution. In other cases, radiation methods can be used to propagate out the disturbances. The basic radiation methods solve the Sommerfeld radiation condition (56) at the interface,

$$\partial_t \phi_{\rm loc} + c \,\partial_n \phi_{\rm loc} = 0 \qquad \text{on } \gamma, \tag{56}$$

and corresponds to the transport of ϕ through γ at the phase speed projected 1139 to the boundary, c (∂_n denotes a derivative perpendicular to and towards the 1140 outside of teh boundary). Obviously this boundary condition is only ex-1141 act for a wave propagation problem and when c is known. In practice, c1142 $\left(=-\partial_t \phi_{\rm loc} \left(\partial_n \phi_{\rm loc}\right)^{-1}\right)$ is estimated at the discrete level using internal values 1143 (Orlanski, 1976), leading to different implementations, including, in two di-1144 mensions, variants taking into account tangential derivatives (Raymond and 1145 Kuo, 1984). Besides the evaluation of the phase speed c, the relevancy of this 1146 type of boundary condition for non-monochromatic and/or dispersive waves 1147 is questionable. 1148

The radiation condition is valid only for outflow conditions (e.g. c > 0 at an eastern boundary). In other cases, relaxation methods as described in the previous paragraph are more appropriate. Radiation and relaxation methods can be combined to give:

$$\partial_t \phi_{\rm loc} + c \,\partial_n \phi_{\rm loc} = -\frac{\phi_{\rm loc} - \phi_{\rm ext}}{\tau_{\gamma}} \qquad \text{on } \gamma.$$
 (57)

where τ_{γ} , the relaxation time scale, has different values $\tau_{\rm in}$, $\tau_{\rm out}$ according to inflow ($\tau_{\gamma} = \tau_{\rm in}$) or outflow ($\tau_{\gamma} = \tau_{\rm out}$) conditions (Marchesiello et al., 2001). During inflow conditions c is set to zero and $\tau_{\rm in}$ is small leading to a strong relaxation towards external solution. $\tau_{\rm out}$ is large but not infinity in order to ¹¹⁵⁷ prevent the internal solution to drift for external data. Note that even if (57) ¹¹⁵⁸ is written at the interface γ , it is most of the time associated to a relaxation ¹¹⁵⁹ term active on the whole transition area Γ . For consistency, the boundary ¹¹⁶⁰ value of the relaxation time scale τ defined in (53) should be greater than ¹¹⁶¹ τ_{out} .

1162 6.2.2. Characteristic methods

As mentioned previously, radiation methods are only valid when the tem-1163 poral evolution of the state variable is governed by a wave equation. They 1164 can be extended to more general cases by looking at the hyperbolic parts 1165 of the equations. By definition hyperbolic systems can be decomposed into 1166 a series of wave propagation problems whose solutions are the characteristic 1167 variables. The problem is then well posed if the incoming characteristics vari-1168 able are specified and the outgoing characteristic extrapolated from internal 1169 values (Blayo and Debreu, 2005). 1170

¹¹⁷¹ Considering a one-dimensional version of the linearised barotropic equation ¹¹⁷² (45)

$$\partial_t \eta = -H \partial_x \bar{u}, \quad \partial_t \bar{u} = -g \partial_x \eta,$$

¹¹⁷³ the two characteristics are given by

$$w_{\pm} = \bar{u} \pm \sqrt{\frac{g}{H}} \eta$$

and propagate with speeds $c_{\pm} = \pm \sqrt{gH}$ (i.e. $\partial_t w_{\pm} + c_{\pm} \partial_x w_{\pm} = 0$). At 1174 open boundaries, the incoming characteristics are prescribed $(w_{\rm loc} = w_{\rm ext})$ 1175 and the outgoing characteristic are computed from internal values. The com-1176 putation of outgoing characteristic variables at the boundary can be based 1177 on simple extrapolation techniques or on the application of upwind biased 1178 schemes. It is well known that the specification of the incoming characteris-1179 tics of the barotropic equations is equivalent to the Flather boundary condi-1180 tion (Flather, 1976) (which can also be obtained by a Sommerfeld radiation 1181 condition for \bar{u} , with $c = \sqrt{gH}$, and a 1D version of the continuity equa-1182 tion). At an eastern boundary where $w_{-} = \bar{u} - \sqrt{\frac{g}{H}} \eta$ must be prescribed, 1183 the Flather boundary condition reads 1184

$$\bar{u} = \bar{u}_{\text{ext}} + \sqrt{\frac{g}{H}} \left(\eta - \eta_{\text{ext}}\right)$$
(58)

and where η is given by another boundary condition (e.g. $\partial_x \eta = 0$). The use of the full characteristic method gives instead:

$$\bar{u} = \frac{1}{2} \left(w_{+,\text{int}} + w_{-,\text{ext}} \right) = \frac{1}{2} \left(\bar{u}_{\text{ext}} + \bar{u}_{\text{int}} \right) + \frac{1}{2} \sqrt{\frac{g}{H}} \left(\eta_{\text{int}} - \eta_{\text{ext}} \right)$$
(59)

1187 and

$$\eta = \frac{1}{2} \sqrt{\frac{H}{g}} \left(w_{+,\text{int}} - w_{-,\text{ext}} \right) = \frac{1}{2} \left(\eta_{\text{ext}} + \eta_{\text{int}} \right) + \frac{1}{2} \sqrt{\frac{H}{g}} \left(\bar{u}_{\text{int}} - \bar{u}_{\text{ext}} \right), \quad (60)$$

where $w_{+,\text{int}} = \bar{u}_{\text{int}} + \sqrt{\frac{g}{H}} \eta_{\text{int}}$ is computed from internal values. The Flather type boundary condition (58), or some of its variants, is used in most of the coastal ocean models where it is assumed that surface gravity waves are indeed dominant for the specification of the boundary conditions. If \bar{u}_{ext} is not known but only η_{ext} (e.g. tidal conditions), a reduced model (e.g. geostrophic balance) may be used to deduce \bar{u}_{ext} .

1194 6.2.3. 3D models

The 3D primitive equation models support the propagation of internal 1195 gravity waves whose characteristics can be obtained through a vertical nor-1196 mal mode decomposition. Setting 3D boundary conditions on the original 1197 state variables without taking into account these propagations renders the 1198 problem ill-posed (Oliger and Sundström, 1978). A remedy can be to add 1199 a small vertical viscosity in the hydrostatic balance equations (7) (Témam 1200 and Tribbia, 2003). Characteristics-based methods can formally be extended 1201 to 3D-based on a vertical mode decomposition (Jensen, 1998; Blayo and De-1202 breu, 2005) resulting into a series of shallow water models. However the 1203 number of assumptions used in their derivations (in particular the linearisa-1204 tion around an horizontally constant background density field and a constant 1205 background state velocity field, typically the barotropic solution) make them 1206 difficult to apply in practice. In addition, the staggering of the grid variables 1207 on an Arakawa C-grid add some difficulties to the discrete implementation 1208 of a combination of variables at different grid locations, thus introducing a 1209 number of additional assumptions. That is why, in 3D primitive equation 1210 models, the preceding relaxation/radiation boundary conditions are usually 1211 applied on each of the prognostic variables $(\eta, \bar{u}, \bar{v}, u, v, T, S)$, with a Flather-1212 like boundary condition for the barotropic part. 1213

1214 6.2.4. Local mesh refinement (one-way nesting)

One-way nested models can use any of the preceding boundary condi-1215 tions with parameters adjusted according to the space and time refinement 1216 factors which are here assumed to be relatively small. One-way nesting may 1217 be performed online (Penven et al., 2006) or offline (Mason et al., 2010). The 1218 key element for a choice between these two approaches is the spatio-temporal 1219 variability of the boundary conditions. When this variability is high, online 1220 nesting, with high frequency / high resolution exchanges between local and 1221 external domains, is more efficient. Indeed storage and performance issues 1222 limit the frequency/resolution of the outputs made during the coarse reso-1223 lution run. However in an offline approach, the obvious advantage is that 1224 the area covered by the local (high resolution) domain does not have to be 1225 known in advance, i.e. before running the external (coarse resolution) model. 1226

1227 6.3. Two-way interaction

We consider now a two-way interaction between the external and local models. The external model feels the local model by a feedback of the local solution. We differentiate between traditional two-way nesting algorithms where the local domain corresponds to a local grid refinement of the external domain and more general two-way coupling algorithms.

We will not detail here the interpolation/update operators between the two models. The reader is referred to Debreu and Blayo (2008) for their design, in particular in terms of scale selectivity and conservation.

1236 6.3.1. Two-way nesting

¹²³⁷ Two-way nesting algorithms have been reviewed in Debreu and Blayo ¹²³⁸ (2008). In this paragraph, we describe strongly coupled models which even-¹²³⁹ tually can be viewed as a single model with an abrupt change of resolution ¹²⁴⁰ at the high/coarse resolution grids interface γ .

Grid interactions. In two-way nesting applications, the feedback from the 1241 high to the coarse resolution grid prevents the two solutions to drift. In the 1242 limit of equal local and external grid resolutions $(L_{\text{ext}} = L_{\text{loc}})$ the original 1243 solution (without nesting) should be recovered. This implies a strong cri-1244 terion on the forcing of the local model: the boundary conditions have to 1245 act on the difference between external and local solutions. We will call this 1246 a consistency condition. Typically, the sponge layer in (55) should now be 1247 written 1248

$$\partial_t \phi_{\rm loc} + \ldots = \nu_\Gamma \Delta (\phi_{\rm loc} - \phi_{\rm ext}) \quad \text{in } \Omega_{\rm loc},$$
 (61)

¹²⁴⁹ and if radiation conditions are used, (57) should be replaced by:

$$\partial_t (\phi_{\rm loc} - \phi_{\rm ext}) + c \,\partial_n (\phi_{\rm loc} - \phi_{\rm ext}) = -\frac{\phi_{\rm loc} - \phi_{\rm ext}}{\tau}.$$
 (62)

In a sense, in these equations, the temporal and spatial scales of the external solutions are not assumed to be much more larger than those of the local domain so that the simplification occurring in (55) and (57) cannot be made. Condition (62) was used in Perkins et al. (1997).

Elliptic systems and/or time splitting. The discrete versions of L_{ext} and L_{loc} 1254 may involve the solution of an elliptic system. This occurs for example when 1255 an implicit treatment of the surface gravity waves is applied, see Section 1256 (5.1.1), or if a nonhydrostatic kernel is involved (leading to the solution 1257 of a Poisson system), see Section 8.2. In that case, special care must be 1258 taken in order to get to correct solution (i.e. continuity of the solution and 1259 its derivatives). For being properly treated, the implicit solver has to be 1260 transformed into a multi-resolution solver which includes the grid interactions 1261 (e.g., paragraph 2.2.1 of Debreu and Blayo (2008) and Haley and Lermusiaux 1262 (2010); Cailleau et al. (2008)). 1263

Similarly, when an explicit mode splitting scheme is employed (see Section 5.1), the models should be coupled at the barotropic time step instead of at the baroclinic time step (Debreu et al., 2012). This also allows to satisfy the consistency condition previously mentioned.

Vertical refinement. Most of the current two-way nested models apply only 1268 horizontal mesh refinements. Local vertical refinements (e.g. increase of res-1269 olution in surface and/or bottom boundary layers) are difficult to manage 1270 for several reasons. Vertical parameterizations (see Section 3.2.1) involve im-1271 plicit solvers due to stability constraints and, so, as for horizontal implicit 1272 solvers (paragraph above) are more difficult to tackle on multiresolution grids. 1273 Coupling between barotropic and baroclinic modes (see Section 5.1) can also 1274 become cumbersome if only part of the water column is computed on the 1275 fine grid. Instead of a local vertical mesh refinement, a local change of verti-1276 cal coordinate systems is achievable. In coastal applications, the capacity to 1277 change locally the vertical coordinate systems (4.2) can become crucial for 1278 some applications. Indeed, mesh refinement along coastal areas with very 1279 small water depths may require some local adaptation of the parameters of 1280

the vertical coordinate systems (parameters of the terrain-following coordinates, number of layers, ...). In that case, vertical remapping has to be applied between coarse and fine grids.

Time refinement. In traditional applications, horizontal mesh refinement is 1284 most of the time coupled with time refinement in order to satisfy stability 1285 conditions. If the main stability constraint is given by external gravity waves 1286 propagation (cf 5.1), at a velocity of \sqrt{gH} , we may expect that, when refining 1287 the grid near the coast and so with smaller depths, the time step does not have 1288 to be reduced. This is certainly the case for some applications, but generally 1289 having the possibility to refine the time steps may become important when 1290 the actual time step is constrained by other phenomena (e.g. drying and 1291 flooding, advection ...). 1292

1293 6.3.2. Two-way coupling

Less strong local/external coupling may also be of interest, particularly 1294 when the space and time refinement factors are large and/or if the models 1295 $L_{\rm ext}$ and $L_{\rm loc}$ have different physics. In that case, two-way relaxation methods 1296 may also be of interest. The spectral nudging method introduced in Section 1297 6.2.1 can be extended to two-way interactions. The smooth semi-prognostic 1298 method (Sheng et al., 2005) is an example of such a technique. More gen-1299 erally, grids interactions can be (weakly) incorporated in any assimilation 1300 scheme coupling at the same time the assimilation of observations and the 1301 grid interactions. 1302

1303 6.4. Discrete point of view

In addition to the preceding continuous formulations, a number of ques-tions arise when taking into account the model discretisations.

1306 6.4.1. Implementation of boundary conditions

We already mentioned the discretisation of the Sommerfeld radiation con-1307 dition, including the sensitivity to the computation of the normal wave speed 1308 in 2D. The discrete implementation of boundary conditions has to deal with 1309 the time stepping algorithm and the grid staggering. As an example, Mason 1310 et al. (2010) proposed a stable implementation of a 2D characteristic method 1311 for the barotropic equations on a staggered C-grid. This paper introduces a 1312 stable treatment of the outgoing characteristics (computation of \bar{u}_{int} and η_{int} 1313 in (59)). 1314

1315 6.4.2. Link with internal numerical schemes

More generally, the problem of open boundary conditions and model 1316 nesting is also fundamentally tied to the discrete internal schemes (e.g. im-1317 plicit/explicit treatment, time integration scheme, discrete conservation prop-1318 erties, diffusive terms). All these aspects interact with an efficient implemen-1319 tation of the boundary conditions. The trivial example is the use of a first-1320 order upwind biased scheme for a simple advection equation: the original 1321 equation $\partial_t \phi + c \partial_x \phi = 0$ is hyperbolic and thus requires only one boundary 1322 condition at inflow, otherwise over-specification occurs. However, the modi-1323 fied equation (i.e. including spatial truncation errors) is of parabolic nature 1324 $\partial_t \phi + c \partial_x \phi = \mu \partial_{xx} \phi + \mathcal{O}(\Delta x)^2, \mu = c \frac{\Delta x}{2}$ and allows for the specification of boundary conditions both at inflow and outflow boundaries. Indeed, in prac-1325 1326 tice the numerical scheme will naturally take into account only external data 1327 at inflow. Similarly if a dispersive scheme is used to discretise the spatial 1328 derivative (e.g. second-order centered), radiation methods will not perform 1329 well even in the monochromatic wave case. This makes the derivation of a 1330 very general OBC difficult and may also explain why some boundary condi-1331 tions work for some models and not for others. 1332

A promising approach concerning the derivation of boundary conditions is the summation-by-parts approach (Svärd and Nordström, 2014) that can make the link between internal schemes and boundary conditions (possibly weekly imposed) according to a discrete energy estimate.

Sanity control. At the discrete level, some basic sanity controls can be made. 1337 This is particularly important for one- and/or two-way nesting. The consis-1338 tency condition has been mentioned previously: assuming that the same 1339 numerical/physical choices are made for the local and external solution, a 1340 simulation with spatial and temporal refinement equal to one should lead 1341 to the same solution with or without nesting. This has several implications 1342 on the formulation of the boundary conditions, the choice of the number of 1343 ghost cells and the treatment of barotropic/baroclinic coupling. 1344

The second sanity control is to verify the constancy preservation (see Section 7.1): in absence of sinks and sources, if a tracer is globally initialised to a constant value, the tracer should remain constant on both grid and with the same value. This has again several implications on the way interpolation/update schemes are constructed and the consistency of barotropic and baroclinic exchanges.

¹³⁵¹ 7. Numerical treatment of single terms and processes

This section discusses discrete algorithms that are commonly used for 1352 the solution of the governing equations formulated in Sec. 3 and 4. Origi-1353 nally, coastal ocean models were discretised using numerical methods loosely 1354 inherited from large scale ocean models, namely second-order in space and 1355 Leapfrog-in-time schemes (Blumberg and Mellor, 1987). However, over the 1356 years, the numerics of those models have evolved toward the use of more 1357 advanced discretisation techniques, more similar to techniques used in other 1358 fields of computational fluid dynamics, in order to accommodate to the spe-1359 cific constraints of coastal applications. Indeed, as discussed in Sec. 2, coastal 1360 ocean dynamics is characterised by strong vertical and horizontal gradients, 1361 long waves, rapid variations on short time and spatial scales as well as large 1362 dissipation and velocities near the bottom which all require specific numer-1363 ical treatments. The diversity of methods in use in coastal models is large 1364 so that the discussion can only focus on techniques which are more widely 1365 used or are expected to become more widely used. Since the numerical re-1366 quirements for each process can be rather different, this section considers 1367 separately sub-systems of the full system of primitive equations. However, 1368 it should not overshadow the fact that a numerical kernel must be designed 1369 as a whole, not just as an advection or a wave propagation equation since 1370 interferences between numerical methods used for different processes exist. 1371

There often exists some confusion to properly characterise the class of dis-1372 cretisation techniques used in state-of-the-art oceanic coastal models. Since 1373 there are significant differences in truncation error between finite-difference 1374 and finite-volume advection-diffusion schemes (e.g. Leonard, 1995), clarifica-1375 tions are needed. As far as the tracer conservation is concerned, it is obvious 1376 that they must be interpreted in a finite-volume sense, meaning that for a 1377 given tracer q the discrete quantity $q_{i,j,k}$ is the average over a control vol-1378 ume $\mathcal{V}_{i,i,k}$ (Fig. 2). For the momentum equations, the generally adopted 1379 formulation is inherited from Lilly (1965) who introduced a discretisation 1380 approach which has the property to conserve energy in a discrete sense as 1381 long as second-order centered schemes are used. Momentum advection terms 1382 in Lilly (1965) can be viewed as a finite-volume discretisations provided that 1383 proper horizontal metric terms are added. However, not every term in the 1384 momentum equation can be cast in a flux divergence form (e.g. Coriolis term, 1385 curvilinear metric terms). For those terms momentum components should 1386 1387 be interpreted in a finite-different sense. Note that the fact that tracer values are cell-averaged implies that the pressure deduced from the hydrostatic relation is a point-wise value located on cell interfaces in the vertical. Generally
speaking, discretisation techniques in most existing structured-grid oceanic
coastal models can be classified as finite volume discretisations. The arrangement on the computational grid is shown in Fig. 2. We now give more details
on the specifics of different terms.

1394 7.1. Tracer and momentum advection

1399

¹³⁹⁵ We consider here the advection equation written in a conservative way ¹³⁹⁶ for a layer-averaged quantity q_k (q can either represent a tracer or horizontal ¹³⁹⁷ momentum components when a flux-form of nonlinear terms is used) along ¹³⁹⁸ with the continuity equation (29)

$$\partial_t (h_k q_k) + \partial_x (h_k u_k q_k) + \partial_y (h_k v_k q_k) + \delta_k (w^s q) = 0,$$

$$\partial_t h_k + \partial_x (h_k u_k) + \partial_y (h_k v_k) + \delta_k (w^s) = 0,$$
(63)

using the notations introduced in Sec. 4 and the definition of a vertical differ-1400 ence located at the centre of the cell $k, \delta_k(a) = a_{k+1/2} - a_{k-1/2}$ for any quantity 1401 a. We retain the continuity equation here to emphasise that the advection 1402 equation must be conservative while satisfying a constancy preservation prop-1403 erty (i.e. if q is initialised with a constant, it remains so). An overview of the 1404 time and space discretisations of (63) used in large and mesoscales oceanic 1405 models can be found in Lemarié et al. (2015). Broadly speaking, it is well 1406 known that classical even-ordered linear advection schemes tend to produce 1407 unphysical oscillations which can be controlled by an explicit scale-selective 1408 dissipation whose coefficients A_M and A_c must be tuned to ensure no build-1409 up of grid scale noise. On the contrary, odd-ordered linear advection schemes 1410 are inherently dissipative near the grid-scale (e.g. App. B in Soufflet et al., 1411 2016), but are not oscillation free with the exception of the first-order upwind 1412 scheme which can not, however, be considered seriously due to its unaccept-1413 able artificial diffusion. The linear compact implicit schemes (Lele, 1992) 1414 are a very attractive alternative but they require a matrix inversion which 1415 makes them tractable for vertical advection only. Note that an important 1416 constraint on the vertical advection is that the oceanic interior vertical mixing 1417 is exceptionally weak so that upwind schemes in models with quasi-Eulerian 1418 vertical coordinate or dissipative remapping schemes in models with an ALE 1419 1420 coordinate (see section 4.2) must be avoided.

1421 7.1.1. Design of numerical models

In practice, several strategies coexist in the coastal community. A first 1422 choice is to consider simple second-order centered schemes supplemented by 1423 an explicit diffusion and a non-dissipative time-stepping algorithm in order 1424 to ensure energy consistency of the whole code at a discrete level (Marsaleix 1425 et al., 2008). A second choice is to rely exclusively on standard high-order 1426 upwind schemes in the horizontal direction and low-dispersive centered ad-1427 vection schemes in the vertical (e.g. fourth-order compact schemes), without 1428 any explicit dissipation, combined with a high-order predictor-corrector time-1429 stepping algorithm using a method of lines (e.g. Shchepetkin and McWilliams, 1430 2005). In this case, it is accepted that strong gradients will generate over-1431 shoots and undershoots and that there is an uncontrolled sink of kinetic en-1432 ergy and tracer variance in the model caused by dissipative truncation errors. 1433 This last point is, however, generally not worrisome as long as a first-order 1434 upwind scheme is avoided. As an alternative to the method of lines, where 1435 space and time discretisations are considered separately, a coupled space-time 1436 approach¹ could be used for advective terms (e.g. Hundsdorfer and Trompert, 1437 1994; Daru and Tenaud, 2004). This type of approach can be viewed as a 1438 conservative semi-Lagrangian approach where the characteristics are tracked 1439 in space-time. The resulting schemes are one-step schemes with interfacial 1440 fluxes depending on the local Courant number $\alpha^x = u_k \Delta t / \Delta x$. They have 1441 the property to be free of computational mode, exact for a Courant number 1442 $\alpha^x = 1$, and to be easily extended to arbitrary high-order of accuracy (e.g. 1443 Daru and Tenaud, 2004). Examples of such schemes are the first-order up-1444 wind scheme, the Lax-Wendroff scheme or the QUICKEST scheme which are 1445 respectively first, second and third order accurate in space and time. What-1446 ever the strategy used (uncoupled or coupled space and time), it is generally 1447 preferable to prevent spurious numerical oscillations by using non-oscillatory 1448 schemes which are more computationally demanding but provide a way to 1449 ensure nonlinear stability. Since non-oscillatory schemes are expected to be 1450 increasingly used to simulate coastal flows, we provide additional comments 1451 on this point to highlight the associated delicacies. 1452

¹The coupled space and time approach is also known in the literature as flux-form semi-Lagrangian approach, as well as transient interpolation method, or direct space-time discretisation.

1453 7.1.2. Nonlinear stability and flux correcting/limiting methods

Numerical methods with an order of accuracy larger than one are prone to 1454 numerical oscillations. A nonlinear stability criteria often considered is that 1455 the numerical solution must not oscillate without bounds. Using the notion 1456 of total variation (TV) as a measure of the overall amount of oscillations, nu-1457 merical schemes have been constructed to ensure that the total variation is ei-1458 ther bounded (TVB) or diminishing (TVD) (Harten, 1983; Shu, 1987). Since 1459 TVD schemes necessarily degenerate to first order accuracy near smooth ex-1460 trema, they are prone to clipping errors manifested by the appearance of a 1461 flat plateau in the solution due to an excess of diffusion. To avoid this type of 1462 error, a less stringent constraint is the monotonicity-preservation (MP) which 1463 relaxes the TVD constraint near extrema (e.g. Suresh and Huynh, 1997; Daru 1464 and Tenaud, 2004). Flux correcting/limiting is generally used to impose the 1465 TVD, TVB or MP stability conditions (e.g. Durran, 2010). Historically, 1466 the flux limiting/correcting methods were derived in a coupled space and 1467 time framework using the second-order Lax-Wendroff scheme. They can be 1468 easily extended to higher-order accuracy using one-step coupled time-space 1469 approach of arbitrary high order (e.g. Daru and Tenaud, 2004). However 1470 if a method of lines is used the time and space dimensions are decoupled 1471 therefore the constraints on total variation must be imposed both in time 1472 and space. For this purpose, a family of Runge-Kutta (RK) schemes satis-1473 fying the TVD property has been derived by Shu (1988) and Gottlieb and 1474 Shu (1998). These RK schemes are TVD over a range of time-steps which 1475 is generally smaller than the stability range given by the more traditional 1476 CFL-type condition. Note that a consequence of the TVD, TVB and MP 1477 stability constraints is a better control of numerical oscillations hence those 1478 constraints could be used not only for momentum advection as a way to limit 1479 spurious mixing by reducing the grid Reynolds number (Ilicak et al., 2012), 1480 but also for the advection of tracers and layer thickness subject to mono-1481 tonicity or positivity constraints. There is an abundant literature on the 1482 comparison of different flux limiting/correcting strategies, see Mohammadi-1483 Aragh et al. (2015) for a recent study in the oceanic modelling context. Note 1484 that in multi-dimensions, the TVD, TVB or MP properties are generally ap-1485 plied independently in each spatial directions. It can be shown that in this 1486 case the resulting scheme does not strictly satisfy those properties anymore. 1487 Nonetheless this approach generally provides acceptable results. 1488

1489 7.1.3. Multidimensional aspects and stability constraints

The extension of one-dimensional advection schemes to multi-dimensions in the context of a method of lines is straight-forward since the necessary transverse terms are discretised in a transparent way. If a quasi-Eulerian vertical coordinate is used, the stability constraint in three dimensions reads

$$\alpha^x + \alpha^y + \beta \alpha^z \le \alpha^\star \tag{64}$$

where α^{\star} is the CFL stability constraint associated to the numerical schemes 1495 used for the time and space discretisations, and β a coefficient arising from 1496 the fact that different advection schemes with different stability criteria may 1497 be used in the horizontal and vertical directions. Typical values of α^* and β 1498 can be found in Lemarié et al. (2015). As far as the coupled space and time 1499 approach is concerned, a simple application of the one-dimensional fluxes in 1500 each spatial direction would result in a scheme that can be at most first-1501 order accurate, whatever the order of accuracy of the 1D fluxes, and the 1502 scheme would be unconditionally unstable. To overcome this issue a direc-1503 tional splitting can be used to introduce the necessary transverse terms in 1504 the discretisation. A simple method to introduce transverse terms while pre-1505 serving constancy is the splitting of Bott (2010). With this type of approach 1506 the stability constraint is given by 1507

$$\max\left\{\alpha^x, \alpha^y, \alpha^z\right\} \le 1$$

¹⁵⁰⁸ which is less stringent than (64).

For coastal applications, Shchepetkin (2015) has emphasised the severe 1509 stability constraint potentially imposed by vertical advection. Several ways 1510 can be used to mitigate this issue (i) use a semi-implicit advection scheme 1511 (ii) use a local time-step for vertical advective terms based on the maximum 1512 vertical Courant number in each water column *(iii)* use a quasi-Lagrangian 1513 vertical coordinate which is subject to a gentle Lipschitz stability condition 1514 rather than the usually severe CFL condition (e.g. White et al., 2009). This 1515 last remark applies to models using rezoning/remapping strategies because 1516 models using a transport algorithm instead of remapping (e.g. Hofmeister 1517 et al., 2010) will still be subject to a CFL type stability constraint. 1518

1519 7.2. Internal pressure gradient errors

Since in coastal ocean models the use of bottom-following coordinates is mandatory (see Sec. 2.1), the coordinate surfaces may intersect with isopycnal or geopotential surfaces at a relatively large angle when the bathymetry is steep. This makes it significantly harder to accurately compute the internal horizontal pressure gradient since the pressure is not known along constant horizontal surfaces. Using the notations introduced in Sec. 4, for a generalised vertical coordinate s, the x-component of the internal horizontal pressure gradient (HPG) is expressed using the chain rule

$$\frac{1}{\rho_0} \left(\partial_x p \right)_z = \frac{1}{\rho_0} \left[\left(\partial_x p \right)_s - \partial_z p \left(\partial_x z \right)_s \right], \tag{65}$$

where p is the hydrostatic pressure deduced from the hydrostatic relation (7). 1529 The subscript s is denoting differentiation with respect to constant s. In an 1530 arbitrary general coordinate the two terms in rhs are nontrivial, of opposite 1531 sign and may be large compared to the order of magnitude of their difference, 1532 except for two special cases: For isopycnal coordinates, the first term van-1533 ishes. The second term in the rhs is sometimes referred to as compensating 1534 hydrostatic term which vanishes for geopotential coordinates (s = z). At a 1535 discrete level, unbalanced truncation errors in the computation of the two 1536 large terms in the rhs will interfere with each other and give rise to a possibly 1537 large pressure-gradient error leading to hydrostatic inconsistency manifested 1538 by unphysical spontaneous motions, even in the absence of lateral density 1539 gradients (i.e., $\rho = \rho(z)$). A very large body of literature is dedicated to this 1540 subject (e.g. Blumberg and Mellor, 1987; Mellor et al., 1994; McCalpin, 1994; 1541 Burchard and Petersen, 1997: Lin, 1997; Shchepetkin and McWilliams, 2003; 1542 Adcroft et al., 2008; Marsaleix et al., 2011; Berntsen, 2011) where different 1543 strategies have been followed to reformulate (65) in a way more convenient 1544 for the discretisation. Those strategies are generally motivated either by 1545 achieving a high-order accuracy to cancel the two terms in (65) in the case 1546 of a flat stratification (e.g. McCalpin, 1994; Shchepetkin and McWilliams, 1547 2003) or by ensuring an energetic consistency (e.g. Marsaleix et al., 2008). 1548 In this latter case, the aim is to make sure in a discrete sense that the change 1549 of kinetic energy due to the work of pressure forces is balanced by the change 1550 of potential energy due to buoyancy forces. This balance occurs only with a 1551 linear equation of state and involves the discrete advection for density (e.g. 1552 Shchepetkin and McWilliams, 2003, App. A). 1553

¹⁵⁵⁴ Mainly three strategies have been followed in practical applications to ¹⁵⁵⁵ reformulate and discretise (65). (i) A first strategy is to directly use the ¹⁵⁵⁶ hydrostatic assumption (6) to express p in terms of density integrals

$$^{1557} \qquad \frac{1}{\rho_0} \left(\partial_x p\right)_z = \frac{g}{\rho_0} \left[\left(\partial_x I_\rho(z)\right)_s + \rho \left(\partial_x z\right)_s \right], \qquad I_\rho(z) = \int_z^\eta \rho(x, y, \xi) d\xi, \quad (66)$$

assuming a zero atmospheric pressure gradient at the surface. When dis-1558 cretising this form of pressure gradient, averaging of $I_{\rho}(z)$ in the vertical and 1559 ρ in the horizontal are needed since the only term computed at its natural 1560 position is $(\partial_r z)_{\epsilon}$. According to Shchepetkin and McWilliams (2003) this 1561 explains why this approach is often prone to large hydrostatic inconsisten-1562 cies. However, high-order schemes have been proposed in McCalpin (1994) 1563 to compute the horizontal derivatives and horizontal averaging of ρ combined 1564 with a spectral representation in the vertical. Note that high-order methods 1565 in the vertical should be used with care in case of strongly stratified flows 1566 because density is generally not smooth on the grid scale, especially with 1567 coarse vertical resolution. *(ii)* a second and intuitive approach consists in 1568 computing the pressure (i.e. $I_{\rho}(z)$) and then to vertically interpolate the 1569 result at an horizontal surface of reference before differentiating (e.g. Lin, 1570 1997; White et al., 2009). This is the preferred option in atmospheric mod-1571 els. In Lin (1997) a flux-form finite-volume approach based on this concept 1572 is adopted. *(iii)* the preferred approach for most oceanic models is to use 1573 a *density-Jacobian* discretisation. As done in (8) and (9), by combining the 1574 Leibniz rule and the hydrostatic relation we easily obtain that 1575

$$\frac{1}{\rho_0} \left(\partial_x p\right)_z = g \frac{\rho(\eta)}{\rho_0} \partial_x \eta - \int_z^\eta \underbrace{\left[\left(\partial_x b\right)_s - \partial_{z'} b\left(\partial_x z'\right)_s\right]}_{\mathcal{J}_{x,z'}(b,z')} dz' \tag{67}$$

where the buoyancy b is defined in Sec. 3. Compared to the straight-forward approach (66) differentiation comes first and integration then. The density-Jacobian formulation clearly shows that if $s = \rho$ only one term is nonzero and the pressure gradient term can be computed accurately provided that proper care is taken to the equation of state (Adcroft et al., 2008). The Jacobian in (67) must be computed at cell corners, if we refer to Fig. 5 a standard second-order discretisation reads

$$(\mathcal{J}_{x,z})_{i+1/2,k+1/2} = \frac{1}{2\Delta x} \{ (1+r_x)b_{i+1,k+1} + (1-r_x)b_{i+1,k} - (1-r_x)b_{i,k+1} - (1+r_x)b_{i,k} \}$$

$$(68)$$

1583

with $r_x = -\frac{z_{i+1,k+1/2} - z_{i,k+1/2}}{z_{i+1/2,k+1} - z_{i+1/2,k}}$ the grid slope. This discretisation of the Jacobian has been widely used in coastal models for years. It can be shown that the standard second-order Jacobian discretisation corresponds to a discrete



Figure 5: Elementary computational stencil of the standard second-order density Jacobian $\mathcal{J}_{x,s}$. The distances involved in the computation of the grid slope r_x are reported.

form of Green's theorem. Indeed, (68) can be written as the sum of four line 1587 integrals discretised using a simple trapezoidal rule. In an attempt to fur-1588 ther reduce the pressure gradient errors, Shchepetkin and McWilliams (2003) 1589 have introduced a high-order (cubic) discretisation for those line integrals. 1590 In their work, care has been taken to the robustness of the scheme even in 1591 case of non-smooth density fields. The resultant scheme turned out to be a 1592 significant step forward compared to existing approaches. Note that besides 1593 the imbalance in the truncation errors in (65) there is an other source of pres-1594 sure gradient error stemming from the use of a nonlinear equation of state 1595 including compressibility of seawater (Dukowicz, 2001). Ways to remove this 1596 source of error by rearranging the terms in the equation of state are presented 1597 in Shchepetkin and McWilliams (2003), Adcroft et al. (2008) or Marsaleix 1598 et al. (2011). This latter source of error is sometimes overlooked, however it 1599 must be stressed that the careless inclusion of compressibility terms into the 1600 equation of state would have significant dynamic consequences. 1601

The value of the parameter r_x in (68) is a good qualitative indicator of discretisation errors. For $r_x = 0$ the grid is flat and the pressure gradient term reduces to a single term while for $|r_x| = 1$ there is a 45 degrees slope between the grid and the horizontal direction, and (68) reduces to a simple differentiation of two terms in the diagonal. More generally, for $|r_x| \leq 1$ we expect the

discretisation to be fairly accurate since it is based on vertical interpolations, 1607 this is the so-called "hydrostatic consistency" situation (Fig. 5). Values of 1608 $|r_x|$ greater than 1 generally lead to a degradation of the accuracy due to 1609 the need of vertical extrapolation to compute the pressure gradient term. 1610 This corresponds to a situation of "hydrostatic inconsistency", see Haney 1611 (1991). A strong requirement to avoid the emergence of spurious motions 1612 is thus to keep the value of r_x at a reasonable level. To do so several ways 1613 are commonly used concurrently, (i) bathymetry smoothing (e.g. Martinho 1614 and Batteen, 2006) is systematically used in terrain-following coordinates to 1615 limit the maximum slopes (ii) the function responsible for the vertical place-1616 ment of grid points is designed in such a way to minimise the departure of 1617 the vertical coordinate isosurfaces from the horizontal direction (e.g. Schär 1618 et al., 2002; Shchepetkin and McWilliams, 2009; Berntsen, 2011; Lemarié 1619 et al., 2012b) (iii) a quasi-Lagrangian vertical coordinate whose layer distri-1620 bution in the rezoning step can be chosen to reduce grid slopes or to follow 1621 isopycnals (e.g. Burchard and Petersen, 1997; White et al., 2009; Hofmeis-1622 ter et al., 2010). Note that trying to confine the maximum grid slopes at 1623 the bottom to quickly obtain nearly flat coordinate isosurfaces when going 1624 toward the surface must be done with care in the sense that large pressure 1625 gradient errors at depth will affect the circulation in the upper layers anyway 1626 through baroclinic-barotropic coupling. Besides the approaches discussed so 1627 far, we could imagine alternative strategies. For example, the coordinate 1628 system could be determined using only the low-frequency variations in the 1629 bathymetry and high frequencies could be handled using an immersed bound-1630 ary method (e.g. Lundquist et al., 2010). Other alternatives could be the use 1631 of well-balanced discretisations (Botta et al., 2004) or to express horizon-1632 tal momentum using the covariant velocity components instead of the usual 1633 contravariant components (Weller and Shahrokhi, 2014). Eventually, as em-1634 phasised by Mellor et al. (1994), the interaction between pressure gradient 1635 and other terms in the equations should be further clarified, especially the 1636 interaction with active tracers advection. More specifically, the interplay 1637 between numerically-induced mixing of active tracers and HPG errors is ex-1638 pected to play a crucial role in the time-evolution of circulation errors (e.g. 1639 Lemarié et al., 2012b, Sec. 6.2). However, the importance of HPG errors in 1640 simulations of coastal currents is difficult to evaluate in practical applications. 1641 The competing effects of the model dynamics, its sensitivity to the horizon-1642 tal/vertical grid resolution and discrete numerical algorithms, are tricky to 1643 untangle. 1644

1645 7.3. Inertia-gravity waves

Most of the work on the discretisation of inertia-gravity waves was mainly 1646 concerned with finding the most appropriate variable arrangement among 1647 the Arakawa grids A to E by looking at discrete dispersion relations (e.g. 1648 Mesinger and Arakawa, 1976). Here we restrict ourselves to the C-grid ar-1649 rangement which is the preferred option in coastal models since the Rossby 1650 radius of deformation is generally properly resolved, with the exception of 1651 fjord-type systems such as the Baltic Sea, where very high resolution < 1 km1652 is required (Holtermann et al., 2014). Typical space-time discretisation tech-1653 niques can be found in Beckers and Deleersnijder (1993) or Lemarié et al. 1654 (2015) and are summarised below. 1655

1656 7.3.1. Inertial oscillations

¹⁶⁵⁷ In the absence of other terms but Coriolis terms in (30) and (31) we ¹⁶⁵⁸ obtain the equations of free motion on a rotating plane

1659

$$\partial_t(h_k u_k) = f h_k v_k; \quad \partial_t(h_k v_k) = -f h_k u_k. \tag{69}$$

A characteristic of the Coriolis acceleration is that it is directed perpendic-1660 ular to the velocity direction. Hence, it does not play any role in the kinetic 1661 energy budget, which forms an important constraint for the discretisation 1662 (e.g. Arakawa and Lamb, 1977). In (69), the quantity $fh_k v_k$ must be given 1663 at u-points and $fh_k u_k$ at v-points. If (69) is semi-discretised in space, this 1664 constraint is trivially satisfied locally on an Arakawa B-grid, since u and 1665 v are collocated, but can only be satisfied globally on an Arakawa C-grid. 1666 Considering that the Coriolis frequency f is cell centered, the following dis-1667 cretisation of the rhs in (69)1668

1669

$$(fh_k v_k)_{i+1/2,j} = \overline{f_{i,j}h_{i,j,k}}\overline{v}_k^{y^x}, \qquad (fh_k u_k)_{i,j+1/2} = \overline{f_{i,j}h_{i,j,k}}\overline{u}_k^{x^y}, \qquad (70)$$

where \bar{m} is an averaging operator in the direction m (m = x, y), ensures that 1670 all the terms associated to the Coriolis force cancel when a kinetic energy 1671 equation is derived from (30) and (31) (Sec. III.C in Arakawa and Lamb, 1672 1977). In (70), the horizontal variations of the curvature metric terms have 1673 been ignored for clarity. An alternative energetically-consistent discretisation 1674 providing a different logic for the cancellation of the terms when the kinetic 1675 energy budget is formed at the discrete level has been introduced in Espelid 1676 et al. (2000) and reads 1677

$$(fh_k v_k)_{i+1/2,j} = f_{i+1/2,j} \overline{(h_k v_k)}_{i+1/2,j}^w; (fh_k u_k)_{i,j+1/2} = f_{i,j+1/2} \overline{(h_k u_k)}_{i,j+1/2}^w,$$
(71)

¹⁶⁷⁹ where $\overline{\cdot}^w$ is a weighted average defined as

$$(h_k v_k)_{i+1/2,j}^w = \frac{w_{i+1/2,j,k}}{4} \sum_{n=0}^{n=1} \sum_{m=0}^{m=1} \frac{(hv)_{i+n,j-m+1/2,k}}{w_{i+n,j-m+1/2,k}}; \ w_{i+1/2,j,k} = \sqrt{\frac{gh_{i+1/2,j,k}}{|f_{i+1/2,j}|}}$$

for each layer k, same rationale applies to $\overline{(h_k u_k)}_{i,j+1/2}^w$. Compared to (70), this formulation requires the Coriolis parameter to be defined at u and v points and allows more freedom in the way to define the thickness layer h_k at cell interfaces.

When the time dimension is discretised, the energy conservation prop-1685 erty is less straight-forward to ensure. First, a simple forward Euler step 1686 to integrate (69) would be unconditionally unstable. The use of a (semi)-1687 implicit scheme would remove stability constraints. This approach is essen-1688 tially adopted in models which treat the gravity waves in a semi-implicit way 1689 (e.g. Walters et al., 2009). In general, for coastal applications, the baroclinic 1690 time-step is much smaller than the inertial period meaning that the Coriolis 1691 term is not expected to impose any limitation on the time-step. For this 1692 reason explicit schemes are generally preferred. To circumvent the stabil-1693 ity issues of the Euler forward step, a Forward-Backward in Time (FBT) 1694 approach is often used (Bleck and Smith, 1990) 1695

1696

and is stable for
$$f \Delta t \leq 2$$
. In (72), s is either 0 if n is even or 1 otherwise.
The major drawbacks of this approach are that it requires to switch at each
time-step the order of integration of the u and v components and it is not
energetically-consistent even if the spatial discretisation is. Other popular
explicit schemes to integrate (69) include the third-order Adams-Bashforth
scheme (stable for $f \Delta t \leq 0.72$) and the leapfrog scheme (stable for $f \Delta t \leq 1$)
which both globally ensure that there is no false generation of kinetic energy
since u and v are considered at the same moment in time.

1705 7.3.2. Internal gravity waves

Elements about the temporal discretization of external gravity waves are introduced in Sec. 5.1 so that we focus here on internal gravity waves. The numerical integration of those waves is generally studied on the followingone-dimensional subsystem

$$\partial_t p_q + \rho_0 c_q^2 \partial_x u_q = 0$$

$$\rho_0 \partial_t u_q + \partial_x p_q = 0.$$
(73)

1710

for a given vertical mode q (q = 0 corresponds to the barotropic mode) with 1711 c_q the gravity wave speed associated with $q^{\rm th}$ vertical mode. The details to 1712 derive (73) from the full three-dimensional equations can be found, e.g., in 1713 Lemarié et al. (2015). In (73), the term $\partial_x u_q$ in the first equation can be 1714 traced back to the horizontal divergence in the continuity equation and the 1715 term $\partial_x p_q$ in the second equation to the horizontal pressure gradient term in 1716 the primitive equations. The stability constraint imposed by internal gravity 1717 waves reads 1718

$$\Delta t \sqrt{c_1^2 \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)} \le \alpha_{\text{igw}}^{\star}$$

where α_{igw}^{\star} is the CFL stability criterion depending on space and time discretization used for internal waves and c_1 the speed of the fastest internal wave. Typical values for α_{igw}^{\star} can be found in Lemarié et al. (2015) and Tab. 1. Following Hallberg (1997) and Shchepetkin and McWilliams (2008), a general family of two-level schemes for the time integration of (73) in a forward manner is

1726

1719

$$p_{q}^{\star} = p_{q}^{n} - c_{q}^{2} \Delta t \, \partial_{x} (\rho_{0} u_{q}^{n}) \rho_{0} u_{q}^{\star} = \rho_{0} u_{q}^{n} - \Delta t \, \partial_{x} \left(\vartheta p_{q}^{\star} + (1 - \vartheta) p_{q}^{n} \right) p_{q}^{n+1} = p_{q}^{n} - c_{q}^{2} \Delta t \, \partial_{x} \left(\varsigma \rho_{0} u_{q}^{\star} + (1 - \varsigma) \rho_{0} u_{q}^{n} \right) \rho_{0} u_{q}^{n+1} = \rho_{0} u_{q}^{n} - \Delta t \, \partial_{x} \left((1 - \varphi) \left[(1 - \varepsilon) p_{q}^{n+1} + \varepsilon p_{q}^{\star} \right] + \varphi p^{n} \right)$$

$$(74)$$

where the parameters ϑ , ς , ε and φ can be chosen to improve both accu-1727 racy and stability. As reported in Tab. 1, the general discretization (74) 1728 encompasses several well-known schemes presented in the literature. Among 1729 the various alternatives, by far the simpler strategy is the so-called forward-1730 backward approach (e.g. Mesinger and Arakawa, 1976). Other alternatives 1731 include the time staggering of tracers and momentum (e.g. Backhaus, 1985) 1732 or the use of a larger stencil in time (Brown and Campana, 1978; Shchepetkin 1733 and McWilliams, 2005). Of interest for the coastal modeling community, 1734 Rueda et al. (2007) showed that the original implementation of the Casulli 1735

	Forward- Backward	Casulli and Cattani (1994)	Rueda et al. (2007)	Shchepetkin and McWilliams (2008)
ϑ	-	-	1/6	13/24
5	0	0	1/2	1/4
φ	0	1/2	1/2	1/4
ε	0	0	0	5/18
α_{igw}^{\star}	1	unstable	1	$\sqrt{3}$
Order of accuracy	2^{nd}	1^{st}	3^{rd}	3^{rd}

Table 1: Parameter values $(\vartheta, \varsigma, \varepsilon, \varphi)$ in the general two-level forward-time integration scheme (74) corresponding to different alternatives existing in the literature. The associated stability constraint α_{igw}^{\star} and order of accuracy are also given. For simplicity the parameters reported for the Shchepetkin and McWilliams (2008) scheme have been slightly modified compared to the original paper without compromising its properties.

and Cattani (1994) time-integration scheme with a semi-implicit treatment 1736 of the external gravity waves is baroclinically unstable for the integration 1737 of internal gravity waves unless a backward Euler scheme is used for the 1738 external mode. As far as the spatial discretisation is concerned, the over-1739 whelming majority of oceanic models consider simple second-order schemes 1740 to compute $\partial_x u_q$ (i.e. the continuity equation) and $\partial_x p_q$ (i.e. the horizontal 1741 pressure gradient). However studies by Blayo (2000) and Demange et al. 1742 (2014) emphasised that higher-order approximations of both the pressure 1743 gradient term and the horizontal divergence in the continuity equation allow 1744 a significantly better representation of internal waves propagation, compared 1745 to standard algorithmic choices. 1746

1747 7.4. Orientation of diffusion tensor and numerically-induced mixing

In (8), (9), (15), and (17), the horizontal turbulent fluxes are oriented in 1748 a direction (\tilde{x}, \tilde{y}) to be defined. In the case of a stratified flow, if the verti-1749 cal coordinate $s \neq \rho$ it is well known that maintaining the diffusion tensor 1750 along the coordinate lines can be responsible for non-physical mixing of water 1751 masses and associated spurious baroclinic currents (e.g. Barnier et al., 1998). 1752 It is thus relatively common for non-isopycnic models to implement a rota-1753 tion of the diffusion tensor in a direction non-aligned with the computational 1754 grid (e.g. Stelling and Van Kester, 1994; Griffies et al., 1998). However, the 1755

implementation of such a rotation tensor turned out to be very delicate no-1756 tably to avoid unphysical undershooting and overshooting and to maintain 1757 reasonable accuracy in case of large slopes, similarly to the HPG calculations 1758 (Beckers et al., 1998, 2000; Lemarié et al., 2012a). Since for a generalized 1759 coordinate it is expected that the slope between the isopycnal direction and 1760 the direction of the computational grid is larger than for a classical z coor-1761 dinate, a good compromise is generally to rotate the explicit diffusion in the 1762 geopotential direction rather than the physically correct isopycnal direction. 1763 This allows to avoid delicacies associated with the computation of isopycnal 1764 slopes in unstratified regions and at the intersection with the surface and the 1765 bottom. 1766

A non negligible amount of non-physical mixing of water masses can also 1767 be due to the advection operator. Indeed, as mentioned earlier, oceanic 1768 coastal models generally rely either on high-order linear upwind schemes or 1769 on flux correcting/limiting approaches to discretise horizontal advection. The 1770 associated truncation errors are dissipative. Much effort have been recently 1771 directed toward the quantification and/or modification of physical orienta-1772 tion of this mixing of numerical nature (e.g. Burchard and Rennau, 2008; 1773 Marchesiello et al., 2009; Ilicak et al., 2012; Klingbeil et al., 2014). For ex-1774 ample, Marchesiello et al. (2009) showed that the dissipative truncation error 1775 associated to a third-order upwind scheme in a terrain-following coordinate 1776 model was greatly exceeding the small level of physically acceptable mixing 1777 observed in the oceanic interior. The physical results proved to be greatly 1778 improved by splitting the third-order upwind scheme between a centered and 1779 a diffusive part and when the diffusive part is rotated in the isopycnal direc-1780 tion (Marchesiello et al., 2009; Lemarié et al., 2012b). This approach, which 1781 is viable only for linear advection schemes, required a thorough analysis of 1782 the biharmonic isopycnal mixing operator to obtain a stable and sufficiently 1783 accurate discretisation for large slopes (Lemarié et al., 2012a). However, this 1784 methodology has some limitations: the rotated operator is derived under the 1785 small slope approximation which may no longer be valid in coastal applica-1786 tions (Lemarié et al., 2012b, Sec. 2.4.2) and it is unclear how the diffusion 1787 operator behaves in case of fast temporal variations of isopycnals. An alter-1788 native approach to have more control on the orientation of mixing for coastal 1789 applications is the use of quasi-Lagrangian approach (e.g. Hofmeister et al., 1790 2010; Leclair and Madec, 2011). Besides the orientation of the diffusion ten-1791 sor, Ilicak et al. (2012) emphasised that spurious diapycnal mixing can be 1792 aggravated if the grid Reynolds number is too large (i.e. if the velocity field 1793

is not smooth on the grid scale). Useful diagnostics to help characterising the
amount and/or orientation of spurious mixing can be found in Ilicak et al.
(2012) and Klingbeil et al. (2014). Note that even if much of the attention
is on the advection operator, a non-negligible amount of numerical mixing
could also be associated to other terms in the equations (Soufflet et al., 2016).

1799 7.5. Bottom friction

Due to the relatively thick bottom boundary layers in the coastal ocean, see (1), an accurate discretisation of bottom friction is required. The nolike slip bottom boundary condition for u and v (12) is typically not directly discretised, because a vertical resolution on scales of millimetres would be required to obtain sufficient accuracy. Instead, it is assumed that the velocity profiles in the lowest grid box of an ocean model follow the law of the wall:

$$[u(z'), v(z')] = \frac{[u_*^{\rm b}, v_*^{\rm b}]}{\kappa} \ln\left(\frac{z' + z_0^{\rm b}}{z_0^{\rm b}}\right),\tag{75}$$

with the bottom roughness length, $z_0^{\rm b}$, the bottom friction velocity vector, $(u_*^{\rm b}, v_*^{\rm b})$ and the distance from the wall, z' = z + H. With (75), the discrete bottom boundary condition has the form of a quadratic friction law

$$\frac{\tau_{[\mathbf{x},\mathbf{y}]}^{\mathbf{b}}(h,u,v)}{\rho_{0}} = \left(\frac{\kappa}{\ln\left(\frac{h/2+z_{0}^{\mathbf{b}}}{z_{0}^{\mathbf{b}}}\right)}\right)^{2} \cdot [u,v] \left(u^{2}+v^{2}\right)^{1/2}$$
(76)

1806

 $= c_d \cdot [u,v] (u^2 + v^2)^{1/2}.$

1811 In (76),

1812

$$\tau_{[\mathbf{x},\mathbf{y}]}^{\mathbf{b}} = \rho_0 \left[u_*^{\mathbf{b}}, v_*^{\mathbf{b}} \right] \left(\left(u_*^{\mathbf{b}} \right)^2 + \left(v_*^{\mathbf{b}} \right)^2 \right)^{1/2} \tag{77}$$

is the bed stress vector, c_d is the non-dimensional bottom drag coefficient, 1813 h is the thickness of the lowest grid box, and (u, v) is the velocity vector in 1814 the lowest grid box. Note that for the limit of $h \to 0$ we obtain $c_d \to \infty$ and 1815 thus retain the original no-slip condition (12). The numerically calculated 1816 bed stress vector calculated in (76) is then used in the bottom boundary 1817 condition (13). In situations when the near-bottom velocity profile deviates 1818 strongly from the law of the wall, e.g. when stratification due to high sedi-1819 ment concentrations or a wave-enhanced bottom boundary layer (or both) are 1820

present, the vertical resolution needs to be sufficiently high. One other possibility would be to parameterise such unresolved processes (Burchard et al. (2008); Warner et al. (2008)). Specific care needs to be taken for the bottom (and surface) boundary conditions when turbulence closure models are used. As shown by Burchard and Petersen (1999) and Burchard et al. (2005b), flux
boundary conditions for turbulent quantities provide much higher accuracy in reproducing the law of the wall than Dirichlet boundary conditions.

1828 7.6. Numerical treatment of turbulence closure equations

The discretisation of turbulence closure budget equations requires spe-1829 cific care, since turbulence quantities are often non-negative scalars such as 1830 the turbulent kinetic energy (TKE) k or its dissipation rate ε . Furthermore, 1831 these quantities often cover several orders of magnitude across fairly short 1832 time and spatial scales such as in oscillating tidal flow. The problem of a 1833 straight forward, explicit-in-time discretisation of the TKE equation is best 1834 demonstrated for the idealised case of freely decaying homogeneous turbu-1835 lence. In this case the TKE budget equation (24) simplifies to the following 1836 form: 1837

$$\partial_t k = -\varepsilon. \tag{78}$$

An explicit discretisation of (78) would be

$$\frac{k^{n+1}-k^n}{\Delta t} = -\varepsilon^n \quad \Rightarrow \quad k^{n+1} = k^n - \Delta t \varepsilon^n, \tag{79}$$

where *n* denotes a variable on the old time level and n + 1 denotes a variable on the new time level. With (79) the time-step criterion for positivity of k^{n+1} is $\Delta t < \varepsilon^n/k^n$, which for example in tidal flow might require very small time steps during slack tide, when production is small and dissipation is high. A solution to this problem has been proposed by Patankar (1980):

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$$\frac{k^{n+1}-k^n}{\Delta t} = -\varepsilon^n \frac{k^{n+1}}{k^n} = -c_{\varepsilon} \frac{k^{n+1} (k^n)^{1/2}}{l^n}$$

$$\Rightarrow k^{n+1} = \frac{k^n}{1+\Delta t \frac{\varepsilon^n}{k^n}} = \frac{k^n}{1+\Delta t c_{\varepsilon} \frac{(k^n)^{1/2}}{l^n}},$$
(80)

which gives unconditionally positive results for k^{n+1} . Note that the second equalities in equations (80) are derived by using the cascading relation (26). This so-called Patankar trick is used in almost all discretisations of turbulence closure budget equations, including those for other parameters such as the dissipation rate ε and the turbulence frequency ω , see Deleersnijder et al. (1997) and Burchard et al. (2005b) for details. The Patankar trick may also be applied to sink terms in biogeochemical models to guarantee positivity, but to obtain conservation of state variables, source terms must be treated accordingly (Burchard et al. (2005a)).

Another issue of the numerical treatment of turbulence closure models is 1856 the energy-consistency between mean flow and turbulence. Physically, the 1857 kinetic energy extracted from the mean flow due to vertical stress divergence 1858 is a source of turbulent kinetic energy transferred as shear production P. The 1859 same applies to the exchange of energy between mean potential energy and 1860 turbulence kinetic energy which is transferred as buoyancy production B. 1861 Burchard (2002b) shows how a consistent energy exchange can be obtained 1862 also on the numerical level. 1863

1864 8. Existing coastal ocean community models

Previous sections have discussed the various choices that have to be made 1865 when designing a numerical model with a focus on coastal applications. The 1866 present section gives an overview of the specifics of some existing hydro-1867 static and non-hydrostatic structured-grid models to illustrate the diversity 1868 of methods in use in coastal models and their evolution over the years. We 1869 have strived here to present a fair description of past and ongoing develop-1870 ments, however the reader must be warned that omissions and inaccuracies 1871 in the model description are inherent to this type of exercise. 1872

1873 8.1. Hydrostatic structured-grid models

In this subsection examples of structured-grid oceanic models used in 1874 practice to tackle research or engineering applications related to coastal en-1875 vironments are given, see Tab. 2 for a list of the most popular models histor-1876 ically used in this context. In this list we can find models originally designed 1877 for shallow seas applications (e.g. BOM, COHERENS, GETM, HAMSOM, 1878 Mars3D, MOHID), as well as mesoscale oceanic models, like NCOM, POL-1879 COMS, POM or ROMS, adapted to handle nearshore and coastal scales (e.g. 1880 Oey, 2005; Uchiyama et al., 2010; Warner et al., 2013). More recently, global 1881 climate models (e.g. NEMO, Hycom) are also sometimes used to study shelf 1882 processes provided some adjustments in their numerical formulation (e.g. 1883

Leclair and Madec, 2011; Lahaye et al., 2011). Finally, models specifically 1884 designed for commercial/engineering applications (e.g. Delft3D, ECOM-si, 1885 MIKE 3, TRIM3D) can also be used for real case studies (e.g. Cheng et al., 1886 1993). As summarised in Tab. 3, the choice of discrete algorithms in oceanic 1887 models bear the imprints of their original target application and development 1888 time. In the 90's the situation was very clear: climate models were generally 1889 discretised on a B-grid using a geopotential coordinate under the rigid-lid 1890 assumption and leapfrog (LF) time-stepping (Griffies, 2004) while mesoscale 1891 models, largely inspired by POM, made use of a C-grid, a terrain-following 1892 coordinate and an explicit free surface. At that time coastal and engineering 1893 models were predominantly C-grid models based on a semi-implicit free sur-1894 face and baroclinic foward in time methods influenced by Backhaus (1985) 1895 and Casulli and Cheng (1992). Nowadays, the distinction between the differ-1896 ent class of models is less clear because newly developed models are generally 1897 designed to handle a larger range of spatio-temporal scales permitted by the 1898 advances in computational power and the maturity of nesting strategies (see 1899 Sec. 6). In early 2000's, the emergence of models like ROMS, GETM or 1900 Hycom came with a thorough rethinking of several model components like 1901 time-stepping algorithms (Shchepetkin and McWilliams, 2005), vertical coor-1902 dinate (Bleck, 2002; Burchard and Beckers, 2004), turbulent closure schemes 1903 (Umlauf and Burchard, 2003), or open boundary conditions (Marchesiello 1904 et al., 2001) which increased further the diversity of models. Tab. 3 reflects 1905 the variety of models and modelling techniques that are presently used. How-1906 ever some general trends can be distinguished : 1907

- Models originally developed with coastal applications in mind are characterized by 2-level (one-step) time-stepping with a coupled space and time treatment of advective terms. This choice combines simplicity and ease to implement monotonicity-preserving advection.
- The majority of models based on a coupled space and time approach 1912 favour the superbee slope limiter to impose the TVD property. This 1913 choice corresponds to the upper boundary of the TVD region and leads 1914 to the least numerical diffusion among the existing slope limiters (e.g. 1915 Cushman-Roisin and Beckers, 2011). However, this limiter tends to 1916 erroneously amplify the gradients. According to Durran (2010), the 1917 monotonized centered limiter is expected to provide superior results in 1918 terms of accuracy. Other flux-limiter methods currently used for prac-1919 tical applications is the ultimate quickest scheme (or equivalently the 1920

so-called P2-PDM scheme). Note that the WENO or FCT approaches 1921 are still relatively marginally used. 1922 • As motivated in Sec. 3.2.1, the overwhelming majority of coastal mod-1923 els rely on TKE-based vertical closure models. A dynamic equation for 1924 TKE is solved either in combination with a diagnostic mixing length 1925 or with a second dynamic equation for a length related quantity. 1926 • The recently developed models are almost exclusively based on an ex-1927 plicit external mode computation which allows more accuracy in the 1928 computation of fast barotropic waves and is expected to provide en-1929 hanced scalability and performance on parallel computers. 1930 The vertical coordinate system is one of the aspect that focuses the 1931 most attention nowadays. The general trend is to allow more flexibility 1932

in the definition of the coordinate within the Arbitrary Lagrangian-Eulerian framework.

1935 8.2. Non-hydrostatic models

 $1942 \\ 1943$

Within the last decade several existing coastal ocean models were extended to abandon the hydrostatic pressure assumption (POM: Kanarska and Maderich (2003), BOM: Heggelund et al. (2004), ROMS: Kanarska et al. (2007), Symphonie: Auclair et al. (2011), GETM: Klingbeil and Burchard (2013)). Scaling analysis shows that the nonhydrostatic pressure contribution, formally defined by

$$\partial_z p_{\rm nh} = -\left(\partial_t w + \partial_x \left(uw\right) + \partial_y \left(vw\right) + \partial_z \left(ww\right) - f_{\rm h}u - F_{\rm z}\right),\tag{81}$$

cannot be neglected when approaching sufficiently high spatial resolutions
that promote processes with significant vertical accelerations (Marshall et al.,
1996
1997; Klingbeil and Burchard, 2013). Practical examples on coastal ocean
scales are flows above irregular topography, high-frequency internal gravity
waves or gravity plumes. In order to simulate these processes in a physically
correct way, the vertical momentum balance must not be degenerated to (7)
anymore.

For solving the full set of incompressible Navier-Stokes equations algorithms were implemented on top of the hydrostatic model kernels that do not require a complete rewrite of the existing kernels. These were usually based on either the classical projection method (Chorin, 1968; Témam, 1969)

Model	Acronym	website						
BOM	Bergen Ocean Model	http://www.mi.uib.no/BOM/						
COHERENS	COupled Hydrodynamical Ecological	http://odnature.naturalsciences.						
	model for REgioNal Shelf seas	be/coherens/						
Delft-3D	Deltares flow	http://oss.deltares.nl/web/delft3d						
ECOM-si	Estuarine, Coastal and Ocean Model	http://woodshole.er.usgs.gov/						
	(semi-implicit)	operations/modeling/ecomsi.html						
GETM	General Estuarine Transport Model	http://www.getm.eu/						
HAMSOM	Hamburg Shelf Ocean Model	https://wiki.zmaw.de/ifm/TO/						
	-	Hamsom/modelhistory						
ROMS	Regional Oceanic Modeling System	·						
$\hookrightarrow \operatorname{Rutgers}$		https://www.myroms.org/						
$\hookrightarrow UCLA$		http://research.atmos.ucla.edu/						
		cesr/ROMS_page.html						
$\hookrightarrow \mathrm{AGRIF}$		http://www.romsagrif.org/						
Mars3D	Model for Applications at Regional Scale	http://wwz.ifremer.fr/mars3d/						
MIKE 3	Danish Hydraulic Institute	https://www.mikepoweredbydhi.com/						
MOHID	MOdelo HIDrodinâmico	http://www.mohid.com/						
NCOM	Navy Coastal Ocean Model	http://www.dtic.mil/dtic/tr/						
		fulltext/u2/a508063.pdf						
POLCOMS	Proudman Oceanographic Laboratory	http://cobs.noc.ac.uk/modl/						
	Coastal Ocean Modelling System	polcoms/						
POM	Princeton Ocean Model	http://www.ccpo.odu.edu/POMWEB/						
Symphonie	Sirocco Ocean Model	http://sirocco.omp.obs-mip.fr/						
		ocean_models/S-model						
TRIM-3D	Tidal Residual, Intertidal Mudflat							
Hycom	HYbrid Coordinate Ocean Model	https://hycom.org/						
NEMO	Nucleus for the European Modeling of the	http://www.nemo-ocean.eu/						
	Ocean							

Table 2: Summary of most significant oceanic models historically used for applications to three-dimensional coastal studies. The ROMS code has three variants referred to as ROMS-Rutgers, ROMS-UCLA, and ROMS-Agrif (see Shchepetkin and McWilliams, 2009, for more details). Hycom and NEMO are examples for large scale models which are also applied to the coastal ocean.

Turb. closure	MY2.5	k - ε	$k^{-\varepsilon}$	MY2.5	GOTM	$k - \varepsilon$	GLS	KPP	КРР	GLS	$k^{-\varepsilon}$	GOTM	MY2.5	MY2.5	MY2.5	TKE	GLS	КРР	GLS
Vertical discret.	×	s	z & s	s	adapt.	α	s	s	s	s	s	s	hyb z/s	δ	s	s	1	hyb z/s/ ρ	z & s
Tracer advec.	TVD Superbee	TVD Superbee	UP3 w/ Forester fltr	C2	TVD	upstream	MPDATA	UP3	WEN05Z	QK3	Ultimate QK3	TVD Superbee	FCT(UP3)	PPM w/ limiters	MPDATA	SUP3	TVD Van-Leer	FCT(C2)	FCT(C2)
Mom. advec.	TVD Superbee	TVD Superbee	UP3	C2	TVD	upstream	UP3	UP3	UP3	QK3	Ultimate QK3	upstream	SUP3	PPM w/ limiters	C2	C4	SL	Enstrophy- conserving	SUP3
External Time- stepping	LF-TR	1	ADI	θ -scheme	FB	θ -scheme	LF-AM3	Gen FB	Gen FB	ADI	ADI	ADI	θ -scheme	FB	LF	LF	θ -scheme	LF	LF
Internal Time- stepping	LF-AM3	2-level	ADI	2-level	2-level	2-level	LF-TR	LF-AM3	LF-AM3	2-level	2-level	2-level	LF	2-level	LF	LF	2-level	LF	LF
Mode splitting	SPE	SPI/SPE	IdS	IdS	SPE	IdS	SPE	SPE	SPE	IdS	IdS	IdS	IdS	SPE	SPE	SPE	IdS	SPE	SPE
Horz grid	C	C	C	υ	C	U	υ	C	υ	C	C	C	C	В	C	C	C	C	C
Introd. ref.	Svendsen et al. (1996)	Luyten et al. (1999)	Gerritsen et al. (2004)	Blumberg (1992)	Burchard and Bolding (2002)	Backhaus (1985)	Haidvogel et al. (2000)	Shchepetkin and McWilliams (2005)	Penven et al. (2006)	Lazure and Salomon (1991)	Pietrzak et al. (2002)	Martins et al. (2001)	Martin (2000)	Holt and James (2001)	Blumberg and Mellor (1978)	Johns et al. (1992) Marsaleix et al. (1998)	Cheng et al. (1993)	Bleck (2002)	Madec et al. (1991)
	BOM	COHERENS	Delft-3D	ECOM-si	GETM	HAMSOM	ROMS (Rutgers)	ROMS (UCLA)	ROMS (Agrif)	Mars3D	MIKE 3	MOHID	NCOM	POLCOMS	POM	Symphonie	TRIM-3D	Hycom	NEMO

those listed here). Acronyms represent the following: FB=Forward-Backward, Gen = generalised, ADI = Alternating Di-rection Implicit, SPE=SPlit-Explicit, SPI=SPlit-Implicit, (S)UP3= (Split) third-order UPwind, QK3=third-order quickest, LF=Leapfrog, PPM=Piecewise Parabolic Method, TVD=Total Variation Diminishing, C2=second-order centered, C4=fourth-Table 3: Properties of some structured-grid coastal ocean models (note that the models might have many more choices than order centered, TR=trapezoidal, AM3=third-order Adams-Moulton interpolation, MPDATA=Multidimensional Positive Definite Advection Transport Algorithm.

or the pressure correction method (van Kan, 1986). Both methods require 1955 the solution of a Poisson equation for either the nonhydrostatic pressure 1956 (Kanarska and Maderich, 2003; Heggelund et al., 2004) or its correction (Ka-1957 narska et al., 2007: Auclair et al., 2011), which should be derived by inserting 1958 the discrete momentum equations into the discrete incompressibility condi-1959 tion to force a divergence-free final velocity field. The specific characteristics 1960 of coastal ocean models demand for some adaptations and care, e.g. for the 1961 consistent coupling of the free surface to the corrected nonhydrostatic veloc-1962 ities or the numerical treatment of the additional diagonals in the coefficient 1963 matrix that is neither symmetric nor positive-definite in general. Strategies 1964 to avoid the additional diagonals, only caused by the cross-terms of the ver-1965 tical coordinate transformation, were presented by Heggelund et al. (2004) 1966 and Berntsen and Furnes (2005). Following Berntsen and Furnes (2005), 1967 Keilegavlen and Berntsen (2009) demonstrated that simulations with the 1968 nonhydrostatic pressure defined directly in σ -coordinates showed no signifi-1969 cant deviations to results obtained with the pressure defined in z-coordinates. 1970 An alternative algorithm for weakly nonhydrostatic regimes (e.g. internal lee 1971 waves) that avoids the Poisson equation was presented by Klingbeil and Bur-1972 chard (2013). They treat the nonhydrostatic pressure as the hydrostatic one, 1973 i.e. diagnose the time-lagged right-hand side of (81), integrate it vertically 1974 and insert it into the horizontal momentum equations. 1975

¹⁹⁷⁶ 9. Future perspectives

The present review of the numerics of structured-grid coastal ocean models gives an overview of the numerical methods available for todays coastal ocean models. There is no single model which combines all those methods. Thus, by just recombining existing methods, todays model platforms may be further improved.

But what are the future challenges in coastal ocean modelling? There are various trends which will drive further developments. One driver is certainly the ever ongoing growth of computational resources allowing for higher spatial resolution, better process representations, integration into regional Earth system models of growing complexity, application of more elaborate data assimilation schemes, and use of large ensemble simulations with high numbers of individual model simulations for better representation of model statistics.

1989 Non-hydrostatic and Boussinesq assumption

The possible higher spatial resolution will in many coastal ocean scenarios 1990 allow for resolving non-hydrostatic processes. In cases where the horizontal 1991 resolution becomes substantially smaller than the water depth, hydrostatic 1992 models would loose their predictability when for example relatively short 1993 internal waves still propagate at their hydrostatic phase speed. Therefore, 1994 one challenge to the developers of coastal ocean models is to allow for efficient 1995 non-hydrostatic pressure calculation in situations where needed. As discussed 1996 in section 8.2, there are only a few of such examples among the structured-1997 grid models. The challenge would therefore be that models automatically 1998 analyse whether in some regions the non-hydrostatic pressure contribution is 1990 relevant, and if so, the non-hydrostatic dynamics should be applied. On other 2000 (e.g., shallower) parts of the model domain it might be ignored. It should 2001 however be kept in mind that diagnosed non-hydrostatic pressure might also 2002 be a numerical artefact (Vitousek and Fringer, 2011). 2003

Another possibility to consistently add non-hydrostatic effects, while avoid-2004 ing the costly direct solution of a 3D Poisson equation for the pressure, is to 2005 relax both the hydrostatic and Boussinesq assumptions (Auclair et al., 2016). 2006 Since relaxing the Boussinesq assumption reintroduces the acoustic waves, an 2007 acoustic mode must be considered on top of the internal and external modes. 2008 This three-mode approach has the advantage to be completely explicit (i.e. 2009 local in space) and thus to have very good properties in terms of scalabil-2010 ity. However, it raises new challenges to derive consistent open boundary 2011 conditions to couple models based on different modeling assumptions. 2012

2013 Physics-dynamics coupling

The development of numerical models generally dissociates the dynamical 2014 kernel, which handles the resolved scales, from the "physics", that account 2015 for under-resolved processes. However, both components are strongly cou-2016 pled since there is constantly a transfer of information back and forth from 2017 the dynamics to the physics so that the dynamical core must not violate 2018 physical principles. Energy-consistency is certainly one important example 2019 of such coupling. As discussed in section 7.1, most advection schemes are 2020 not variance conserving, which means for the momentum budget violation of 2021 kinetic energy conservation. The rate of numerical dissipation can be diag-2022 nosed (e.g. Klingbeil et al., 2014) and it can be shown that more complex 2023 advection schemes limit the numerical dissipation (Mohammadi-Aragh et al., 2024 2015). Another source of energy-conservation violation is due to the exchange 2025

between mean kinetic energy and potential energy. This exchange is repre-2026 sented by the pressure-gradient term in the momentum equations and the 2027 advection terms of the potential temperature and salinity equations. Since 2028 those terms are discretised completely independently, energy-consistency is 2029 not given. Another issue is the energy consistency between loss of mean 2030 kinetic energy due to vertical stress divergence and production of turbu-2031 lent kinetic energy (see section 7.6 and Burchard, 2002b). Generally better 2032 energy-consistency may also be achieved by more suitable choices for verti-2033 cal coordinates. As discussed in section 4.2, generalised vertical coordinates 2034 give a high degree of freedom to construct an optimised vertical grid lay-2035 out. This flexibility needs to be better exploited in the future to improve the 2036 performance of coastal ocean models. 2037

It should be briefly mentioned that also the physics of coastal ocean models (as well as for large scale ocean models) is generally not energy-consistent, since e.g. the energy lost by horizontal stress divergence is not reintroduced into any other energy compartment of the model. This is an important issue which could however not be further discussed in this numerical review (see e.g., the discussion by Eden et al., 2014).

2044 Multi-resolution strategies

One other aspect of ongoing discussions in the coastal ocean developers 2045 community is the optimal layout for horizontal grids. In both, structured-2046 grid and unstructured-grid models, substantial progress has been made in 2047 the past. While unstructured-grid models have the better ability to solve 2048 multi-scale problems, the numerical cost per nominal grid point is up to one 2049 order of magnitude larger than for structured-grid models. It does there-2050 fore depend on the kind of problem to decide which type of model is better 2051 suited. For complex domains such as lagoon systems or estuarine networks, 2052 unstructured-grid models are the better choice while for classical coastal or 2053 shelf sea scenarios structured-grid models are more efficient. Structured-grid 2054 models have gained flexibility due to more flexible grids (such as curvilinear 2055 grids, see section 4.3 or two-way nesting, see section 6.3). Flexible multi-level 2056 nesting strategies reducing the number of masked grid points (land points) in 2057 the model domain might in the future help to better tackle multi-scale prob-2058 lems using structured grids. And there are efforts to increase the efficiency 2059 of unstructured-grid models. Both types of models - structured-grid models 2060 with flexible nesting and unstructured-grid models - might in the future sup-2061 port horizontal mesh-adaptivity to resolve moving or intermittent dynamic 2062

features (as for example done in larger scale models to follow hurricanes). It
depends on the success of such developments which type of model is gaining
more ground in the future of coastal ocean modelling.

2066 Coupling with other earth system compartments

Finally, stand-alone hydrodynamic coastal ocean models will always have 2067 a limited area of application. All such models are developed to also func-2068 tion as hydrodynamic core of coupled model systems. Most common is the 2069 coupling to biogeochemical models, where the hydrodynamic model provides 2070 advective and turbulent transports as well as the light regime and many 2071 other potential functional links between hydrodynamics and biogeochemistry. 2072 Without accurate physical and numerical representation of the hydrodynam-2073 ics (e.g., in terms of the mixed-layer depth), biogeochemical models will have 2074 no predictability. Links between hydrodynamics and biogeochemistry may 2075 be complex. One tool to flexibly provide such a link is FABM (Framework 2076 of Biogeochemical Models, Bruggeman and Bolding (2014)). 2077

Coupling to several other Earth system compartments is common, such as 2078 to statistical surface wave models, sea ice models, atmospheric models, ben-2079 thic models, and hydrological models. Several comprehensive system models 2080 exist, such as COAWST (Warner et al., 2008), interactively coupling hydro-2081 dynamics (from ROMS) with surfaces waves, atmosphere, biogeochemistry, 2082 sediment transport and benthos to study complex coastal ocean scenarios 2083 in hindcast and sensitivity mode, or NEMO-Nordic (Gröger et al., 2015), 2084 coupling hydrodynamics (from NEMO) with atmosphere, sea ice, biogeo-2085 chemistry, and hydrology for the purpose of regional climate downscaling 2086 and sensitivity scenarios. It is obvious that all coupling interfaces to other 2087 compartments require hydrodynamic process adaptations on the side of the 2088 hydrodynamic module, and that those need to be numerically discretised 2089 with care. It is expected that in the future, such complex coupled model 2090 systems will be much more widely used, such that quite some pressure to 2091 further develop hydrodynamic model will be generated. 2092

Despite the substantial growth of computational resources, regional climate system models with run-times of typically more than a century and which maybe executed as large ensemble runs with many individual simulations will require high accuracy at relatively low resolution. Therefore the development of efficient and accurate numerical schemes at low resolution will be an important task also for the future.
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