

Multi-scale time integration schemes for three-dimensional hydrodynamic marine models

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A mathematician is a device
for turning coffee into theorems.

— Alfred Rényi.

Remerciements

Alleluia, c'est fini!

Si vous lisez ces lignes, c'est que j'ai obtenu mon diplôme de docteur. Je remercie tout d'abord toutes les personnes présentes pour fêter cela avec moi. Je pense notamment à mes amis Binchois, Carolos et Liégeois. Je n'oublie pas les amis chers que je me suis fait durant mes études à l'EPL. J'ai une pensée aussi pour ma famille de Belgique comme de France. Je tiens également à remercier les membres de mon jury pour leur lecture attentive de ce manuscrit ainsi que pour leurs conseils et suggestions lors de la défense privée qui fut plus excitante et excitée que prévu.

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La deuxième phase de la vie d'un bleu est la vie en régionale. C'est là que l'on apprend à connaître les autres membres, où l'on s'investit, s'épanouit et sort de son cocon. À la fin de l'année, on obtient son diplôme de bleu, preuve écrite et définitive qu'on est membre de la régionale. On n'est plus bleu mais loin d'être des anciens ou des Vi Sages, comme ils aiment se nommer. On comprend seulement que ce n'est que le début d'une chouette aventure. C'est un peu comme les quatre années qui suivent la confirmation. J'ai voyagé en Belgique et à l'étranger, jusqu'aux États-Unis. J'ai rencontré des gens extraordinaires lors de conférences. J'ai publié mon premier article, puis soumis mon deuxième. D'un point de vue personnel, j'ai eu l'opportunité de participer à de nombreuses reprises à la plus grande revue de la planète, voire de l'univers, pour ne pas dire du multivers. Je remercie cette revue pour tous les moments enrichissants et les rencontres incroyables qu'elle m'a permis de vivre.

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CHAPTER

Introduction

What we know is a drop,
what we don't know is an ocean.

— Isaac Newton.

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1.1 Ocean, the final frontier

(Ange) Pacific Ocean, the largest body of water on the planet, covers more than a third of the earth's surface. It is not for nothing that our planet is often referred to as the Blue planet. This expression alone underscores the vital importance of water on Earth. Oceans cover approximately 70 % of the planet's surface, playing a crucial role in climate and weather patterns.

Water bodies can be split into two groups: deep oceans and coastal ones. The first ones are vast and deep, with the deepest point, the Mariana Trench, reaching a depth of 11 km. The deep oceans are home to a wide variety of species, with the majority of marine life residing in the upper layers. They are also home to a variety of ecosystems, including hydrothermal vents, which are home to unique species. Coastal seas constitute a smaller fraction in terms of surface area and volume but hold significant biological importance, serving as habitats for numerous species and contributing significantly to primary production (Yool and Fasham, 2010).

The dynamics of coastal oceans differ greatly from those of deep oceans. Deep oceans exhibit much larger horizontal scales, leading to a greater influence of Earth's rotation and the curvature of the Earth. In contrast, coastal oceans and seas tend to have relatively shallow bathymetry. Surface winds and heat fluxes can have a pronounced effect on the water column due to this shallowness, with friction at the ocean bottom also playing a role, dissipating water movements. Additionally, coastal morphology can impose significant constraints on flow patterns.

These two worlds are not independent. The circulation in coastal seas is influenced by the currents neighboring oceans. These currents can transport heat, salt and nutrients, impacting the ecosystems in coastal areas. On the other hand, the coastal seas can also influence the oceans. Rivers, deltas and estuaries receive water from the continents and discharge it into the coastal seas. The water from these rivers can carry sediments, nutrients and pollutants, impacting the coastal environment. Moreover, heavy precipitation and evaporation also have an impact.

The coastal waters are crucial for humans, with an estimated 60 % of the global population living within 60 km of coastlines (Rao et al., 2008). Given urbanization and climate change trends, this percentage is expected to increase, highlighting the importance of coastal areas for food, natural resources and transportation. Human activities are increasingly impacting coastal environments, with industrialization, agriculture, overfishing, deforestation and population density exerting pressure on coastal zones (Crossland et al., 2005). These activities can lead to pollution, habitat destruction and the introduction of invasive species, among other issues.

Note that these are the first names of the author of this thesis on ocean models. As if everything had already been written...

One can understand that the hydrodynamics of these water bodies have significant effects on various species and ecosystems. In the studied areas, the motion of water is denoted as geophysical flows. Understanding these flows can help grasp the impact of human activities on coastal ecosystems. In this regard, in-situ measurements and remote sensing technologies such as radar and satellite imagery provide valuable information on water environments. Nonetheless, such data are often localized in time and space, costly to obtain and may be incomplete. For example, satellite imagery covers only the surface of the water. They are not able to provide information on the entire water column. To address this, numerical modeling serves as a valuable tool for simulating and predicting hydrodynamics in these environments. However, formulating appropriate equations and spatially and temporally discretizing them pose significant challenges. Furthermore, assembling the necessary inputs for these models can be complex. Despite these challenges, ongoing developments in numerical schemes aim to improve the precision and efficiency of these models, bringing them closer to reality.

1.2 Waves of numerical models

As outlined in the preceding section, numerical models have evolved into indispensable tools to understand the behavior of water flows. Over the past few decades, many models dedicated to studying hydrodynamic equations have been developed and extensively employed (Fringer et al., 2019). The advent of modern computers and the subsequent rise in computational power have paved the way for the development of increasingly complex models, enabling more detailed simulations. The origins of numerical modeling of geophysical flows can be traced back to the 1940s (Cushman-Roisin and Beckers, 2011). It was Hansen (1956) who pioneered the creation of a model capable of simulating regional storm surges and tide propagation within a two-dimensional framework. Subsequently, it took another decade before the development of the first general circulation model (Bryan and Cox, 1967; Bryan, 1969). Over the next fifty years, increasingly complex models continued to emerge.

To simplify the classification of these diverse models, in this thesis, they are sorted according to four key criteria. The first criterion relates to their application domain, followed by the methodology employed for discretizing the horizontal component of their 3D mesh. Similarly, the third criterion distinguishes them based on their approach to vertically extruding the horizontal mesh. Lastly, the spatial numerical method used serves as the fourth criterion.

1.2.1 Application domain

The first criterion, the application domain, is divided into two main categories: global ocean models and coastal models. The former encompass entire oceans basins, with spatial resolutions varying from a few kilometers to a dozen of kilometers. These models are used to study large-scale phenomena such as ocean currents, heat transport and the impact of oceans on climate. Models such as HYCOM (HYbrid Coordinate Ocean Model, [Bleck and Boudra \(1981\)](#)) are examples of this kind of model. For long climatic simulation, the conservation of tracers and water volume is very important. In contrast, coastal and regional models focus on specific areas, such as coastal seas, bays, or estuaries. These models are characterized by high resolution and are often used to study local phenomena over short periods of time. The resolution of these models can be as high as a few hundred meters. The bathymetry of these models is often more complex. The boundaries follow the coastlines making them more complex. These models are often forced by global models and serve to provide a more precise understanding of phenomena along the coasts, which are more influenced by human activities. Due to the areas of application and their small depth of these models, they can be more tidally and wind driven. Examples include COAWST (COupled Atmosphere, Wave and Sediment, [Warner et al. \(2005, 2008\)](#)), NEMO (Nucleus for European Modelling of the Ocean, [Irrmann et al. \(2022\)](#)), CROCO (Coastal and Regional Ocean COMMunity model, [Marchesiello et al. \(2021\)](#); [Hilt et al. \(2020\)](#)) and, last but not least, SLIM (Second-generation Louvain-le-Neuve Ice-ocean Model, ([Vallaey et al., 2018](#))), the model of interest throughout this thesis.

1.2.2 Horizontal spatial discretization

Regarding horizontal meshing, there are two main families: structured and unstructured meshes. The former divides the domain into a grid of elements of the same size like TRIM (Tidal, Residual, Intertidal Mudflat model, [Casulli \(1999\)](#); [Casulli and Zanolli \(2002, 2005\)](#)) or GETM (General Estuarine Transport Model, [Burchard and Bolding \(2002\)](#)). This generally allows for direct and efficient computational methods. However, they often struggle to reproduce the shape of the coastlines. Unstructured meshes have therefore emerged to address this limitation. The latter may involve mesh generation software such as GMSH ([Geuzaine and Remacle, 2008](#); [Lambrechts et al., 2008a](#)). Unstructured meshes, like UnTRIM (Unstructured Tidal, Residual, Intertidal Mudflat model, [Casulli and Roy \(2000\)](#)) or SCHISM (Semi-implicit Cross-scale Hydro-science Integrated System Model, [Zhang et al. \(2016\)](#)), are more flexible and can adapt to the shape of coastlines. However, they are generally more computationally expensive. The mesh of the Great Barrier Reef, shown in Figure [1.1](#), is an example of an unstructured mesh. It is denser along the coastlines

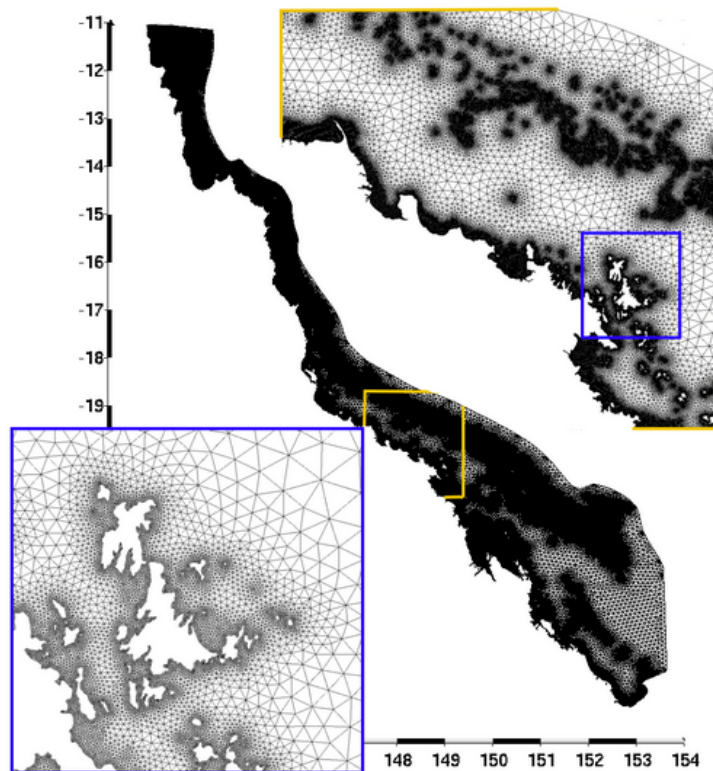


Fig. 1.1: Unstructured mesh of the Great Barrier Reef is denser along the coastlines and in shallow areas. It consists of 800,000 triangles, with resolutions varying from 200 meters to 5 kilometers.

and in shallow areas. It consists of 800,000 triangles, with resolutions varying from 200 meters to 5 kilometers.

1.2.3 Vertical spatial discretization

Regarding vertical spatial discretization, there are two main choices. The first option is to use a z-level model, which involves discretizing the vertical coordinates with fixed z values with only the top surface moving. MITgcm (MIT general circulation model, [Marshall et al. \(1997a\)](#)) or SUNTANS (Stanford Unstructured Nonhydrostatic Terrain following Adaptive Navier–Stokes Simulator, [Fringer et al. \(2006\)](#)) are examples of models that use this extrusion. This approach, while trying to follow the bathymetry, results in a stair-step effect in the domain's bottom. Such stair-step meshes make it easy to manage the

vertical cell size. Additionally, these models reduce errors in pressure gradients that may arise from steep bathymetry (Dawson and Aizinger, 2005). Aizinger and Dawson (2007) presented a three-dimensional barotropic model with this coordinate system and conducted a stability analysis. However, one issue with these models is that they can produce results overly dissipative due to the viscosity induced by vertical walls created by these staircases. To address this, another approach exists, known as sigma- or more generally, terrain-following vertical coordinates where all the horizontal surfaces move. As the name suggests, this discretization tends to follow the shape of the bathymetry by placing the same number of elements in each vertical layer. In addition to being more faithful to reality, it is also simpler to compute. One can cite the DELFT3D (Deltares Flexible mesh model, Deltares (2003)) or ROMS (Regional Ocean Modeling System, Shchepetkin A.F. (2005)) as examples of a model using this coordinate system. Figure 1.2 illustrates the difference between the two methods.

It is possible to combine both methods. This is called the hybrid model. It uses z-level coordinates in the lower layers and sigma coordinates in the upper layers. This model is particularly useful for simulating the different dynamics of the surface and the bottom of the ocean. At the surface, the changes of the sea surface elevation as well as the mixing of the water are well represented by the sigma coordinates. At the bottom where the motion of the flow is less dynamic, the z-level coordinates are used to better represent bathymetry gradients. At the interface between the two, the model can switch from one to the other.

A third method exists, known as isopycnal coordinates (Legg et al., 2006). This method involves discretizing the domain according to the density of the water. The vertical coordinate system is defined by the isopycnal surfaces, which are surfaces of constant density. HYCOM can be cited as an example. This method, by definition, eliminates vertical numerical diffusion of scalars and tracers. As there is no transport of scalars across isopycnal surfaces, no discrete vertical advection appears. However, it is more complex to implement and more computationally expensive. In the case of strong stratification, the isopycnal surfaces can be very steep in some regions, leading to a high number of elements in these regions. On the other hand, from the point of view of numerical methods, the isopycnal coordinates cannot be known beforehand. Surfaces of the same density have to be predicted, and then the mesh has to be updated. This can be computationally expensive.

1.2.4 Spatial numerical methods

Finally, the choice of spatial numerical method used to solve the equations is crucial. The three most prevalent methods are finite difference (FD), finite volume (FV) and finite element (FE) methods. Figure 1.3 illustrates the difference between the three methods.

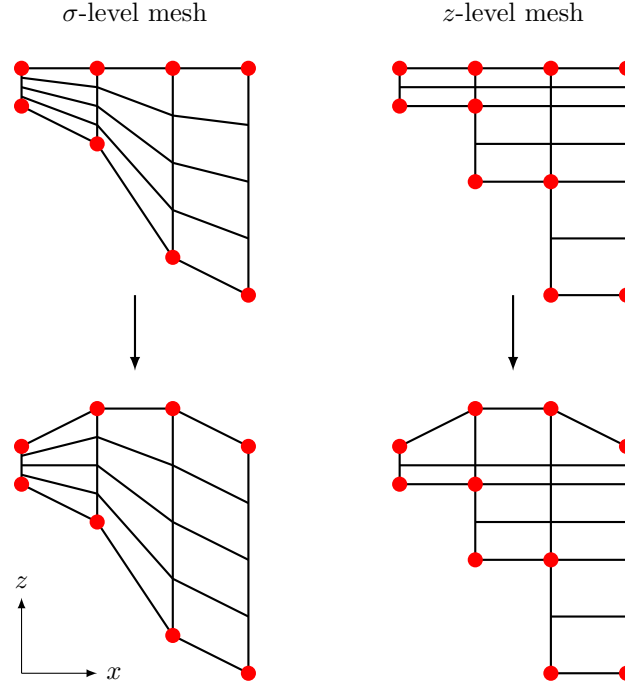


Fig. 1.2: Comparison between σ -level and z-level meshes. The σ -level mesh follows the bathymetry, while the z-level mesh has a constant vertical discretization. The σ -level mesh moves all the horizontal surfaces, while the z-level mesh only moves the top surface.

Finite difference is the simplest and most straightforward approach, involving discretizing the domain into a grid of points where the field values are assigned to nodes and their derivatives are approximated using differences. This method is typically employed in structured mesh models like COHERENS (COupled Hydrodynamical Ecological model for REgionNal Shelf seas, [Luyten et al. \(2003\)](#)).

On the other hand, the finite volume method relies on conserving mass within each cell, where each field maintains a constant value on the 3D or 2D elements. It is used by FVCOM (Finite Volume Coastal Ocean Model, [Chen et al. \(2003\)](#)), MPAS (Model for Prediction Across Scales–Atmosphere, [Skamarock et al. \(2012\)](#); [Ringler et al. \(2013\)](#)) or FESOM2 (Finite-volume Sea ice–Ocean Model, [Danilov et al. \(2016\)](#); [Wang et al. \(2008\)](#)) and its coastal branch FESOM-C ([Androsov et al., 2019](#)). It proves particularly well suited at simulating flows with discontinuities and can be used on both structured and unstructured meshes.

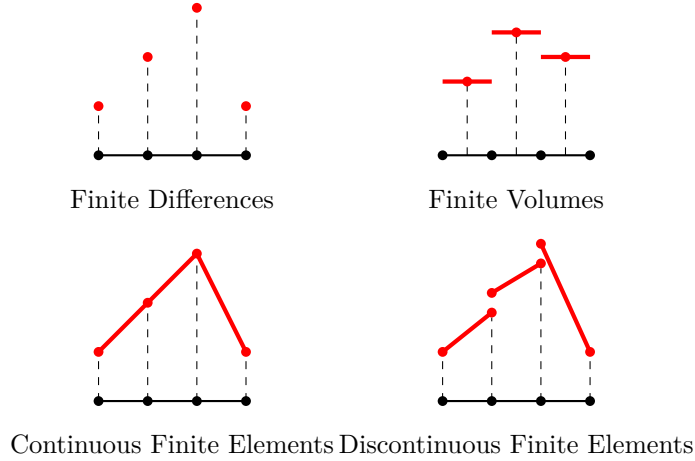


Fig. 1.3: Comparison between finite difference, finite volume and finite element methods. Finite difference discretizes the domain into a grid of points, finite volume put the field values on the elements and finite element method uses polynomials to approximate the field values.

Finite difference methods can be applied to various types of grids known as Arakawa grids ([Arakawa and Lamb, 1977](#)). These grids are distinct approaches to represent and compute orthogonal physical quantities, particularly velocity and mass-related quantities, on rectangular grids used in Earth system models for meteorology and oceanography. Figure 1.4 illustrates them. Named after the meteorologist Akio Arakawa, the Arakawa grids include the Arakawa A-grid, for instance, which evaluates all quantities at the same point within each grid cell, such as at the grid center or corners. It is the only unstaggered grid type. The Arakawa B-grid segregates the evaluation of the two sets of quantities, with velocities, for instance, evaluated at the grid center and scalar fields at grid corners. The Arakawa C-grid further distinguishes the evaluation of vector quantities compared to the Arakawa B-grid, such as evaluating velocity components at specific locations within the grid faces. The Arakawa C-grid is the most commonly used grid type in ocean models. There exist other Arakawa grids but these are the most used. Finite volume methods have also different ways to represent the fields but with more flexibility.

The finite element method is the most intricate yet versatile approach. It involves approximating the solution using polynomials. This method excels in handling complex geometries. When the basis functions are discontinuous between elements, this is a generalization of the finite volume method. ADCIRC (ADvanced CIRCulation model, [Luettich et al. \(1992\)](#)) or TELEMAC ([Janin et al., 1992](#); [Hervouet, 2007](#)) are an example of a model using this method.

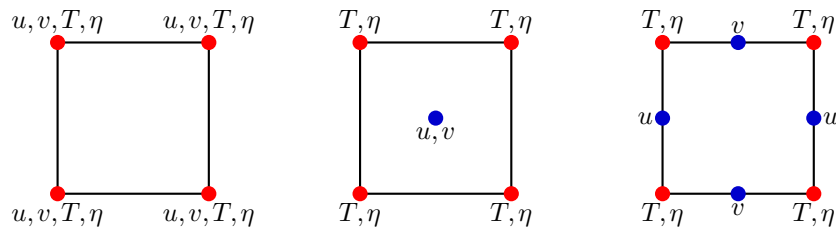


Fig. 1.4: Arakawa grids for finite difference. From left to right: A-grid, B-grid and C-grid. The A-grid evaluates all quantities at the same point in each cell, while the B-grid separates velocities at the grid center and scalar fields at grid corners. The C-grid further distinguishes vector quantities, evaluating velocity components at specific locations on grid faces.

1.2.5 Models for specific dynamics

It is worth noting that some models focus on specific aspects of dynamics. GOTM (General Ocean Turbulence Model, [Burchard et al. \(1999\)](#)), for instance, serves as the standard platform for turbulence parameterizations in coastal modeling, employing for instance the generic length scale (GLS) approach. Many parameterizations of turbulent eddy viscosity in coastal modeling use two-equation turbulence closure schemes ([Umlauf and Burchard, 2005](#)). These schemes typically involve a prognostic equation for turbulent kinetic energy and another equation for computing turbulent length scale. Examples include the Mellor–Yamada level 2.5 scheme ([Mellor and Yamada, 1982](#)), the $k - \epsilon$ model ([Jones and Launder, 1972](#); [Launder and Sharma, 1974](#)) and the $k - \omega$ model initially proposed by ([Saffman, 1970](#)).

Additionally, there are various biogeochemical models like COSINE (Carbon, Silicate and Nitrogen Ecosystem, [Chai et al. \(2002, 2003, 2007\)](#)), designed as a one-dimensional ecosystem model for the equatorial Pacific upwelling system. There are also several wave models. NHWAVE (Non-Hydrostatic Wave Model, [Ma et al. \(2012\)](#); [Shi et al. \(2016, 2019\)](#)), for instance, simulates non-hydrostatic waves using a 3D model. SWAN (Simulating Waves Nearshore, [Booij et al. \(1999\)](#)) and WaveWatch III ([Tolman, 2009](#)) employ a 2D phase-averaged wave model, while SWASH (Simulating Waves till SHore, [Zijlema et al. \(2011\)](#)) offers both two and three-dimensional wave models. Finally, there are models like MPAS and MPAS-atmosphere (Model for Prediction Across Scales, [Skamarock et al. \(2012\)](#); [Ringler et al. \(2013\)](#); [Klemp \(2011\)](#)) that couple ocean and atmosphere models.

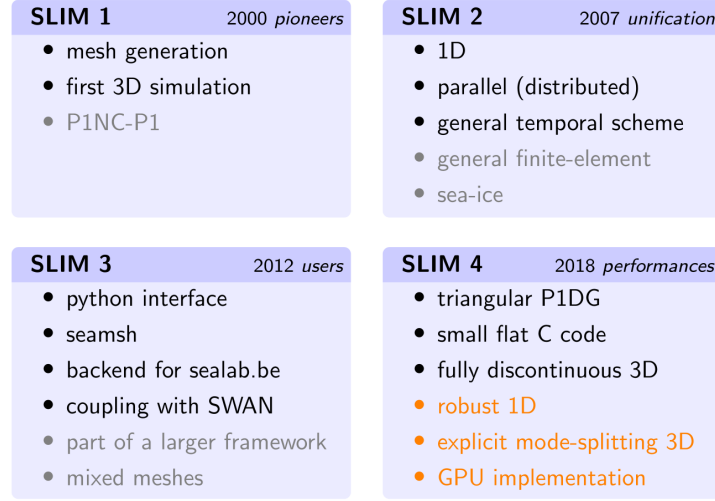


Fig. 1.5: The development of SLIM from 1999 to 2022 is depicted as follows: Modules developed and retained by the research team are represented in black. Modules that have been discontinued are shown in gray. Modules developed during this thesis or currently under development are highlighted in orange.

1.3 Once upon a time SLIM

This thesis was conducted within the framework of the multiscale coastal ocean model. SLIM employs the Discontinuous Galerkin (DG) finite element method to solve one-, two-, or three-dimensional hydrodynamic equations. It aims to simulate geophysical and environmental flows, particularly in domains with complex geometries. The evolution of SLIM can be divided into four main phases. The initial phase, often named the pioneer phase, was followed by an effort to consolidate all the different modules of SLIM created by different researcher. The third phase focused on implementing a user-friendly interface combining Python and C as well as a coupling with SWAN. The final phase aims to enhance performance by introducing new models, a streamlined C code and robust GPU utilization. This is illustrated in Figure 1.5.

SLIM, initiated in 1999, originally aimed at modeling coupled ice-ocean dynamics, with the goal of using the finite element method to take advantage of unstructured meshes in oceanography. Initially, a 2D model was developed, solving the shallow water equations. Various finite element pairs were evaluated. Hanert et al. (2003, 2004, 2005) presented three models. $P1 - P1$ places velocities and elevation at each node and interpolating fields via continuous linear functions. $P1 - P0$ uses constant elevation within each element. $P1^{\perp} - P0$, maintaining constant elevation within each element but calculating velocities

normal to the middle of each edge. [Le Roux et al. \(2005\)](#); [Bernard et al. \(2007\)](#) extended these efforts by proposing square elements or high-order interpolation polynomials, leading to the adoption of the Discontinuous Galerkin (DG) method, as shown by [Lambrechts et al. \(2008b\)](#). Apart from being well-suited for complex domains, DG is highly efficient for problems where advection dominates, ensuring local conservation, an important aspect of oceanic modeling. Moreover, it is easily parallelizable.

Subsequently, additional modules were added to address applications involving river flows with weak lateral variability, such as the Scheldt estuary and the Mahakam River. This model effectively captures the principal features and behaviors of unidirectional flow. Later, [Draoui et al. \(2020\)](#) developed and implemented a new robust and efficient 1D model for river flows.

Furthermore, coupling between the 2D model and SWAN was established to account for stress generated by waves ([Dobbelaere et al., 2022](#)). In this coupling, SLIM provides velocity and elevation information to SWAN, which predicts wave-induced stresses. Although relatively slow, this coupling is widely used in areas affected by extreme weather events.

For applications where the water column is not well mixed, particularly in cases of strong vertical shear or stratification, traditional 2D vertically averaged modeling is inadequate. Hence, the three-dimensional version of the model, SLIM3D, was devised to address such flows. It solves the Navier-Stokes equations under several assumptions, detailed in the following chapter. The spatial discretization of the three-dimensional baroclinic free-surface marine model is derived from a mesh of prisms extruded vertically from an unstructured two-dimensional mesh of triangles.

SLIM 3D has undergone development for a decade, passing through the hands of [White et al. \(2008\)](#), [Blaise et al. \(2010\)](#), [Comblen et al. \(2010\)](#) and [Kärnä et al. \(2013\)](#). However, upon commencement of this thesis, the operational code suffered from excessive numerical dissipation attributed to inaccuracies and approximations in the 2D-3D coupling and the temporal scheme used. The effect of this numerical diffusion can be seen in Figure 1.6. This thesis aims to address these issues.

1.4 What color is the grass on the other side of the fence?

Before exploring the specifics of this work and the developments made, it is essential to give a hint at the state of the art of the temporal splitting used in 3D models. One method is addressed here. Although using different temporal schemes, most of the other models use a coupling technique similar to it. They are therefore not shown.

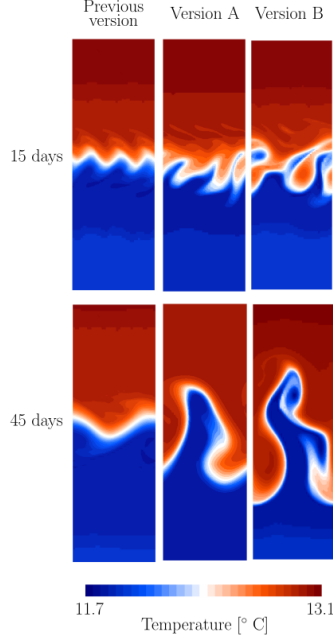


Fig. 1.6: The effect of numerical diffusion in the old version of SLIM3D on the temperature field in the baroclinic eddy test. The model is unable to capture large vortices or eddies. The version A is the improvement made by Valentin Vallaeys while the version B is the one made by Philippe Delandmeter during their thesis. Credit: Valentin Vallaeys

At the beginning of this thesis, one discontinuous Galerkin model serves as a direct challenger named Thetis. Similar to SLIM, it could resolve the 3D hydrodynamic equations on unstructured meshes from extruded triangles. But unlike SLIM, Thetis boasts second-order accuracy in both time and space as well as low numerical diffusion (Kärnä et al., 2018). This achievement was attributed to its use of a precise mode-splitting methodology and the choice of the second-order time integration scheme. Other 3D models employ similar approaches to Thetis regarding the coupling between 2D and 3D, such as MPAS (Model for Prediction Across Scales, Ringler et al. (2010); Thuburn et al. (2009)), ROMS, SUNTANS, FESOM2 or MOM. They usually use high order Adams-Bashforth or Adams-Moulton temporal scheme for the barotropic and baroclinic equations to have higher precision without increasing the computational cost.

The Thetis method and its derivations involve splitting the hydrodynamic equations into two separate ordinary differential equations. The first ODE

focuses on the slow terms, while the second addresses the fast dynamics. The slow terms are given to the fast terms through a source term. Then, the final value is obtained by assuring that the 2D component of the solution is equal to the value calculated by the fast iterations. Although this method seems efficient and accurate, it has some limitations. These models are not able to be conservative and consistent at the same time. The first one signifies that the total volume of water and the total tracer volume should stay the same in a closed domain. The second one means that the model should be able to solve coherently the volume equation and the tracer equation. To do so, the velocity field used in the tracer equation and the vertical velocity equation has to be divergence free and consistent with the new vertical coordinates given by the fast dynamics. Thetis guarantees strict local and global conservation of volume and tracers. However, the model is not strictly consistent without the use of slope limiters (Kärnä et al., 2018).

To be fully conservative and consistent as well as second order in time, an alternative approach is adopted in the thesis. The concept involves maintaining the solution as a single variable and splitting only the right-hand side of the ODE. By following this method, one unique ODE is solved where the slow and fast terms are interconnected through the right-hand-side (RHS).

1.5 Scope of this thesis

As previously discussed, the previous version of SLIM3D faced significant challenges mainly attributed to excessive numerical dissipation coming from its coupling and temporal scheme. Therefore, the primary objective of this thesis is to enhance SLIM3D to make it more accurate and robust. This involves introducing a new second-order split time-stepping scheme and proposing a novel coupling method to overcome the issues of the previous approach. Additionally, a spatial discretization analysis is conducted to ensure consistency and conservation of the model.

1.5.1 Explicit time stepping schemes

The primary focus of this thesis was to introduce a novel second-order split-explicit time stepping scheme, based on low storage Runge-Kutta methods. This scheme partitions the hydrodynamic equations into two components: slow dynamics and fast dynamics. Slow dynamics are computed using a time step Δt , while fast dynamics employ a time step ΔT . The slow dynamics use a second-order Runge-Kutta method with three steps, while the fast dynamics employ a two-step second-order approach. Coupling between slow and fast dynamics occurs through the slope of the right-hand side of the ODEs.

This new temporal scheme is combined with the DG method. Therefore, the spatial discretization has to be adapted to this new scheme. The first purpose

is to take into consideration the mass matrix appearing because of the Finite Element method. As the coordinate of the 3D mesh is obtained by extruding the 2D mesh in function of the elevation, their computation has to be made at relevant time. The second purpose concerns the tracer equation. The tracer equation is solved with the same time stepping scheme as the hydrodynamic equations but without iterations of the fast dynamics. In other words, the tracer equation is solved with the temporal method of the slow terms. In doing so, it is important to ensure the consistency and conservation of the tracer. To do this, a particular attention has to be paid to the velocity field used in the tracer equation. The velocity field has to be divergence free. Concretely, this means that the vertical velocity has to be computed with the same horizontal velocity as the tracer field. Moreover, this latter must be relevant with the new vertical coordinates given by the fast dynamics.

The accuracy of the scheme is evaluated through a series of test cases involving baroclinic flows, along with a laboratory application. These assessments indicate minimal numerical diffusion associated with the new scheme.

1.5.2 Implicit vertical schemes

While the split explicit scheme offers functionality in theoretical contexts, its applicability is limited when it comes to vertical dynamics. As discussed previously, the hydrodynamics can be divided into slow and fast dynamics, with slower terms potentially exhibiting two distinct longer characteristic timescales, resulting in a total of three timescales to consider.

In response to this temporal complexity, the next stage of this thesis introduces an innovative split second-order IMEX (IMplicit-EXplicit) temporal scheme. This scheme addresses the challenge by explicitly handling extremely short timescales with small time steps, while managing longer timescales both explicitly and semi-implicitly using larger time steps. The decision to solve a portion of the slower terms semi-implicitly is motivated by the fact that it does not significantly increase the overall computational cost, offering greater flexibility in time step selection without imposing a substantial burden on computational efficiency. This approach effectively manages the diverse temporal scales inherent in the equations, thereby optimizing computational resources.

The proposed IMEX scheme is applied to solve 3D hydrodynamic equations encompassing fast terms representing wave phenomena, slow terms describing horizontal aspects, and stiff terms for vertical dynamics. Results obtained from various test cases demonstrate the robustness and efficiency of the IMEX approach in simulating these complex systems.

Supporting publications

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., 2023. A split-explicit second order Runge-Kutta method for solving 3D hydrodynamic equations. *Ocean Modelling*, 186. <https://doi.org/10.1016/j.ocemod.2021.101695>

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., 2024. A multi-scale IMEX second order Runge-Kutta method for the 3D hydrodynamic equations. *Journal of Computational Physics* (under review)

De Le Court, M., **Ishimwe, A. P.**, Deleersnijder, E., Legat, V., Lambrechts, J., A GPU-based discontinuous Galerkin model for the three-dimensional hydrodynamic equations (in preparation)

Ishimwe, A. P., Moradi A., Manikantan A. T., Schuetz, J. A class of multirate multiderivative schemes (in preparation)

Conference talks

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., A new second order Runge-Kutta method for solving 3D hydrodynamic equations, American Geophysical Union, AGU23, New Orleans, USA, 2023

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., A Split-Explicit Runge-Kutta method for 3D hydrodynamic equations in SLIM, International workshop on Multi-scale Unstructured mesh numerical Modeling for coastal, shelf and global ocean dynamics, IMUM23, Venice, Italy, November 2023

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., A Split-Explicit second order Runge-Kutta method for solving 3D hydrodynamic equations, Computational Fluids Conference, CFC23, Cannes, France, April 2023

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., A Split-Explicit Runge-Kutta methods for 3D hydrodynamic equations for coastal applications, Advanced Computational Methods in ENgineering, ACOMEN22, Liege, Belgium, September 2022

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., A Split-Explicit Runge-Kutta methods for 3D hydrodynamic equations for coastal applications, European Geosciences Union Conference, EGU22, Vienna, Austria, May 2022

Ishimwe, A. P., Deleersnijder, E., Legat, V., Lambrechts, J., A Split-Explicit Runge-Kutta Methods for 3D Hydrodynamic Equations in Slim, Mathematical and Computational Issues in the Geosciences, SIAM21, Online, June 2021

CHAPTER 2

Ocean dynamics

Mathematics is no less vast than the sea.

— Victor Hugo.

This chapter aims to introduce and elucidate the scientific concepts highlighted in this thesis, which primarily focuses on two axes: the physics of oceanic flows and the numerical methods employed to simulate them.

Firstly, the fundamental hydrodynamic equations, their origins and the main assumptions necessary to derive them are presented. The most crucial assumption is the small aspect ratio of the studied domains, where the vertical scale is much smaller than the horizontal scale. An important aspect of this section is to demonstrate that two groups of phenomena can be distinguished: the slow ones and the fast ones. Consequently, the numerical schemes used to solve them must take this into account.

Secondly, the significance of selecting appropriate numerical methods is demonstrated. To do this, a model problem with two characteristic timescales, or in other words, two phenomena, is constructed. This model is designed to showcase the importance of using split-time methods, where a small timestep is used for fast terms and a larger timestep for slow terms. Through this model, an analysis of the influence of the ratio between characteristic velocities and an investigation of the ratio between the large and small timestep are conducted.

Finally, the hydrodynamic equations are simplified to create a toy model in the x-z plane. On this model, a first-order splitting is demonstrated to gain insight into the mechanism behind the split-time scheme. It is emphasized that no spatial discretization is performed to underscore the temporal integration. This means that derivatives are not discretized using methods such as finite element methods. Finally, a complete solved system is presented.

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2.1 A gyre of temporal and spatial scales

Hydrodynamics deals with the movement of fluids and the forces acting upon them. Various spatial scales are involved in this study, ranging from the predominantly unidirectional flow of rivers and streams to the three-dimensional dynamics within oceans. The focus often shifts towards coastal regions, which extend from the outer edge of the continental shelf to the shoreline and encompass the farthest saltwater influence in estuaries and rivers. These coastal domains occupy approximately 8 % of the Earth's surface. Generally, it is the coastal oceans that both influence and are influenced by human activities.

The governing equations are derived from the equations of continuum mechanics. As it is not feasible to represent everything explicitly, an averaging operator is applied to separate the resolved and unresolved processes, meaning the large-scale processes and the small-scale processes. This results in nonlinear equations where each process impacts the others. Parameterizations are used to address these interactions. For instance, turbulence is computed using a turbulent closure model. Furthermore, three main assumptions are applied: the f-plane approximation, the small aspect ratio and the Boussinesq assumptions.

Given that the Earth is not flat, it should be necessary to consider a change of coordinates when calculating the motion of oceans or other water bodies. However, according to the f-plane approximation (Ripa, 1996), if the horizontal scale of the domains under consideration is significantly smaller than the Earth's radius, it becomes acceptable to approximate the equations using the Cartesian coordinate system. Consequently, the governing equations are expressed in a coordinate system where the first two coordinates represent the horizontal dimensions, situated in the plane tangent to the Earth, while the third coordinate indicates the direction of the local vertical.

Moreover, in ocean modeling, the density of the domain closely approximates that of pure water, denoted as ρ_0 . Small variations in density occur due to observed differences in temperature and salinity (Gill, 1982; Jackett et al., 2006). The Boussinesq approximation assumes that these variations in inertia terms should be negligible. However, gravity, denoted g , is strong enough to cause significant differences in weight between regions with varying temperature or salinity levels. In other words, the density is considered constant except in the buoyancy term.

Finally, as stated before, the small aspect ratio assumption, δ , is based on the fact that the ocean's depth is significantly smaller than the horizontal dimensions, $L_v \ll L_h$. This assumption allows the removal of some terms of the Navier-Stokes equations when estimating the relative order of magnitude of their terms. For instance, the hydrostatic approximation is mainly due to the small aspect ratio.

For the three prognostic variables, $\mathbf{u} = (u, v)$, the horizontal velocities, and H , the total water depth, the governing equations are shown in Equations 2.1.

The first equation is obtained from the momentum equation, while the second equation represents the vertical integral of the continuity equation.

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla_h \cdot (\mathbf{u}\mathbf{u}) + \frac{\partial(w\mathbf{u})}{\partial z} = \nabla_h \cdot (\nu_h \nabla_h \mathbf{u}) + \frac{\partial}{\partial z} \left(\nu_v \frac{\partial \mathbf{u}}{\partial z} \right) \quad (2.1a)$$

$$\begin{aligned} & -f \mathbf{e}_z \times \mathbf{u} - g \nabla_h \eta - \frac{g}{\rho_0} \mathbf{q} - \frac{g}{\rho_0} \rho' |_{\eta} \nabla_h \eta \\ \frac{\partial H}{\partial t} &= -\nabla_h \cdot \int_{-b}^{\eta} \mathbf{u} dz \end{aligned} \quad (2.1b)$$

where w represents the vertical velocity. $\nabla_h = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y})$ stands for the horizontal gradient. The variable η corresponds to the free surface elevation while the parameter b stands for the bathymetry. H can be defined as $H = \eta + b$. ν_h and ν_v refer respectively to the horizontal and vertical viscosity. $\mathbf{U} = \int_{-b}^{\eta} \mathbf{u} dz$ is the transport. Additionally, the symbol f represents the Coriolis parameter. $\mathbf{q}$ represents the integral of the density deviation gradient. Finally, ρ' signifies the density deviation such that $\rho' = \rho - \rho_0$.

The vertical velocity is obtained from the continuity equation:

$$\frac{\partial w}{\partial z} = -\nabla_h \cdot \mathbf{u}. \quad (2.2)$$

The function of density deviation is based on a state equation that is influenced by water temperature or salinity. These fields are represented by the following advection-diffusion equations.

$$\rho' = \rho'(T, S), \quad (2.3)$$

$$\frac{\partial T}{\partial t} + \nabla_h \cdot (\mathbf{u}T) + \frac{\partial(wT)}{\partial z} = \nabla_h \cdot (\kappa_h \nabla_h T) + \frac{\partial}{\partial z} \left(\kappa_v \frac{\partial T}{\partial z} \right), \quad (2.4)$$

$$\frac{\partial S}{\partial t} + \nabla_h \cdot (\mathbf{u}S) + \frac{\partial(wS)}{\partial z} = \nabla_h \cdot (\kappa_h \nabla_h S) + \frac{\partial}{\partial z} \left(\kappa_v \frac{\partial S}{\partial z} \right), \quad (2.5)$$

where κ_h and κ_v stand for respectively the horizontal and the vertical eddy diffusivity.

Impermeability conditions are imposed on both the top moving, Γ_s , and bottom boundaries, Γ_b :

$$w - \frac{\partial H}{\partial t} - \mathbf{u} \cdot \nabla_h (H - b) = 0 \quad \mathbf{x} \in \Gamma_s \quad (2.6a)$$

$$w + \mathbf{u} \cdot \nabla_h b = 0 \quad \mathbf{x} \in \Gamma_b \quad (2.6b)$$

Bottom and surface stresses, $\boldsymbol{\tau}_b$ and $\boldsymbol{\tau}_s$ are also present and included in the model through the boundary conditions.

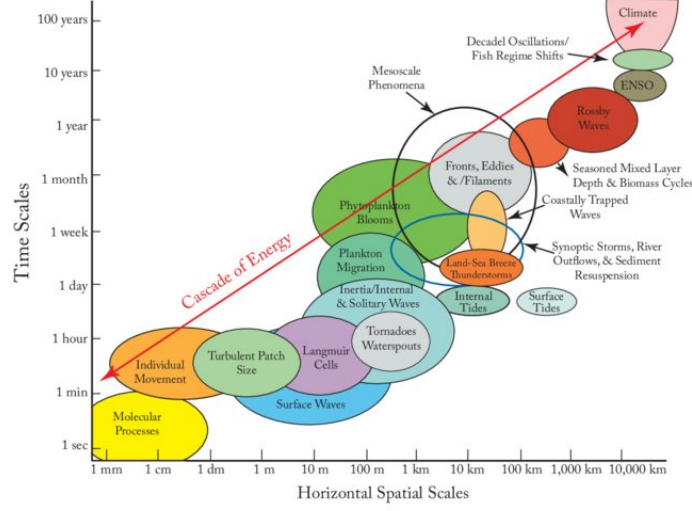


Fig. 2.1: Temporal and spatial scales of the ocean dynamics. Credit: [Nichols and Raghukumar \(2020\)](#).

$$\nu_v \frac{\partial \mathbf{u}}{\partial z} = \frac{\boldsymbol{\tau}_b}{\rho_0} \quad \mathbf{x} \in \Gamma_b \quad (2.7a)$$

$$\nu_v \frac{\partial \mathbf{u}}{\partial z} = \frac{\boldsymbol{\tau}_s}{\rho_0} \quad \mathbf{x} \in \Gamma_s \quad (2.7b)$$

2.1.1 Spatial and temporal scales of the ocean dynamics

Equations 2.1 are used to study the ocean's dynamics, which are characterized by a wide range of temporal and spatial scales illustrated in Figure 2.1. Spatially, two distinct category of scales can be distinguished: horizontal and vertical ones. Horizontal scales are significantly larger than vertical ones. Typically, horizontal scales range from 1 to 100 kilometers, while vertical scales range from a few meters to thousands of meters. Temporally, processes can be differentiated based on their time scales, corresponding to distinct dynamics with their own causes and consequences. In this section, some of these processes will be described. It is important to note that this list of processes is not exhaustive.

Between the fastest and the slowest, there can be a difference of several orders of magnitude. This is why the time-splitting method is used. The idea is to solve the equation by separating the stiff terms from the non-stiff terms. The stiff terms are solved with a small time step while the non-stiff terms are solved with a larger time step.

2.2 A dive into time splitting methods

The ocean's complex dynamics, as described in the previous section, are governed by the Navier-Stokes equations under the Boussinesq and the hydrostatic assumptions. These equations are notoriously difficult to solve analytically and, as a result, numerical methods are employed to approximate their solutions. The numerical methods used to solve these equations are based on the discretization of the spatial and temporal domains. The spatial domain is discretized into a grid while the temporal domain is discretized into time steps. The grid is composed of cells that can be either structured or unstructured. The grid and time steps are chosen to ensure that the numerical solution is accurate and stable. This section will focus on the temporal discretization. Given the following ODE:

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}, t) \quad (2.8)$$

where $\mathbf{y}$ is the state vector, t is the time and $\mathbf{F}$ is the right-hand side of the ODE.

As discussed in the previous section, the ocean's dynamics are characterized by a wide range of temporal scales. This makes the numerical solution of the hydrodynamics equations challenging as processes with a short time scale require a small time step. To address this issue, the temporal domain is split into different time scales and different numerical methods can be used to solve the ODEs associated with each time scale. This approach is known as temporal splitting.

The previous ODE is split into two parts: the fast part and the slow part. This gives

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}, t) + \mathbf{f}(\mathbf{y}, t) \quad (2.9)$$

where $\mathbf{F}$ is the fast part and $\mathbf{f}$ is the slow part.

One approach to solve this problem is to use the same time step and the same temporal method for both functions. This is possible if both processes have the same computational cost. One can use explicit time stepping schemes. These schemes are simple to implement and are computationally efficient. However, they are not always stable and the time step must be chosen carefully to ensure stability. Another way is to use implicit time stepping schemes. These schemes are more stable than explicit schemes, but they are more computationally expensive notably when the system is not linear. If the fast part has a computational cost much smaller than the slow part, one can use a different time step for each part. This approach is more efficient. The slow part can be solved with an explicit method while the fast part can be solved using explicit or implicit methods.

2.2.1 Time splitting

Let us recall the previous ODE. The purpose is to show the time splitting method and its impact on the numerical solution. To mimic the ocean dynamics, a simple two variable model is used. The objective is to construct a ODE with a fast and a slow part. Of course, these two parts must not be decoupled otherwise it should be enough to solve the fast part and the slow part separately and then combine the two solutions. A comparison with the 3D hydrodynamic equations can be done. The fast part can be associated with the external gravity waves while the slow part can be associated with the 3D motions. In the mathematical point of view, the fast part can be associated with the elevation equation and the gravity terms in the momentum equations.

The idea is to use a simple model to mimic this behavior. Sinusoidal function are used. The period is employed to define the characteristic time. This way, a sinusoidal function with small period is considered as the fast part while one with a large period is considered as the slow part. Here is the proposed ODE for variable $\mathbf{y} = (u, T)$:

$$\frac{\partial u}{\partial t} = 0.1 u \sin\left(\frac{t}{T}\right) + 0.2 \sin\left(\frac{t}{\alpha T}\right) - 0.04 u \quad (2.10)$$

$$\frac{\partial T}{\partial t} = 0.1 T \sin\left(\frac{t}{T_0}\right) \quad (2.11)$$

where u is the state variable, T is the period and t is the time. The first equation contains a fast and a slow part. The fast component corresponds to the first term, characterized by a short period of T , while the slow component is represented by the second term, featuring a longer period of αT with $\alpha > 1$. Additionally, there is a perturbation included. Conversely, the second equation exclusively encompasses a fast component with a fixed period of T_0 , corresponding to the initial period. This gives :

$$f_u(u, T, t) = 0.2 \sin\left(\frac{t}{\alpha T}\right) - 0.04 u \quad (2.12)$$

$$F_u(u, T, t) = 0.1 u \sin\left(\frac{t}{T}\right) \quad (2.13)$$

$$f_T(u, T, t) = 0 \quad (2.14)$$

$$F_T(u, T, t) = 0.1 T \sin\left(\frac{t}{T_0}\right) \quad (2.15)$$

with F_u and F_T the fast processes and f_u and f_T the slow ones.

To show the impact of the time splitting, a solution is computed by using an order 4 Runge-Kutta with a small time step. It is compared to a split-explicit Runge-Kutta of order 2. At this stage, the method for achieving this

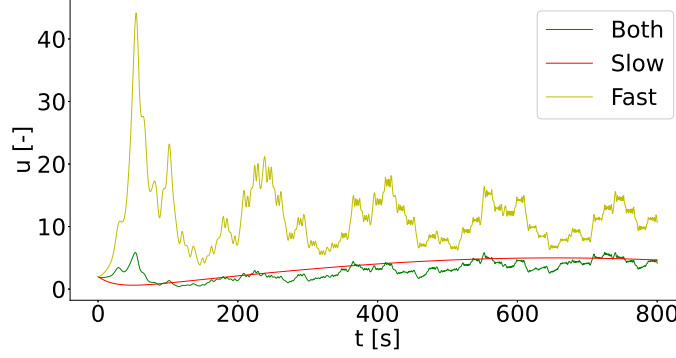


Fig. 2.2: Numerical solution of the fast and the slow part of the ODE for the variable u using an order 4 Runge-Kutta.

splitting is not explained. What is important for now is the analysis of the results obtained with a splitting approach.

α is set at 40. The initial condition is $u(0) = 2$ and $T(0) = 10$. The time domain is $[0, 800]s$. The time step for the slow and the fast part are respectively 100 and 5 s. This gives a ratio, M , of 20 between the time step of the slow and the fast part.

To see a representation of the fast and the slow part, they are solved separately. The results are shown in Figure 2.2 for the variable u . It is important to recall that these results are not the correct fast and slow solutions because the fast and the slow part are not decoupled. Regarding the solution, while the fast oscillations may be more apparent than the slow ones, it is the amplitude of the slow process that predominates.

The results of the split method for u and T are shown in Figure 2.3 and Figure 2.4 respectively. One can see that the results from the split-explicit Runge-Kutta of order 2 tend to match the results from the order 4 Runge-Kutta. This is a good indication that the time splitting method is working.

2.2.1.1 Impact on the computational time

If both the fast and slow processes involve equal computational costs, using explicit time splitting results in the computation being approximately twice as fast compared to using the full explicit method. Assuming a cost of 1 for the slow part and 1 for the fast part, explicit time splitting results in a cost of $1 + M$, while the full explicit method results in a cost of $2M$. This difference arises because, in the split explicit temporal method, the slow part is computed only

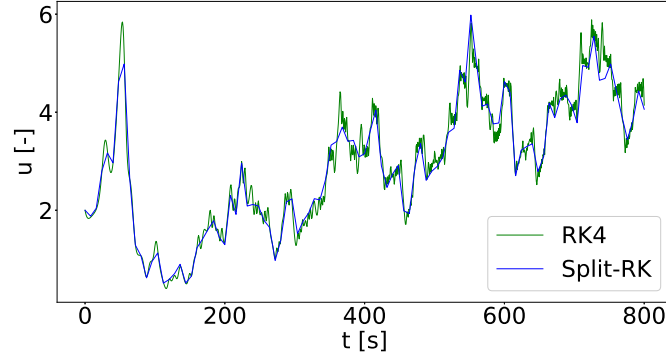


Fig. 2.3: Comparison of the numerical solution of the ODE for the variable u using an order 4 Runge-Kutta and a split-explicit Runge-Kutta of order 2.

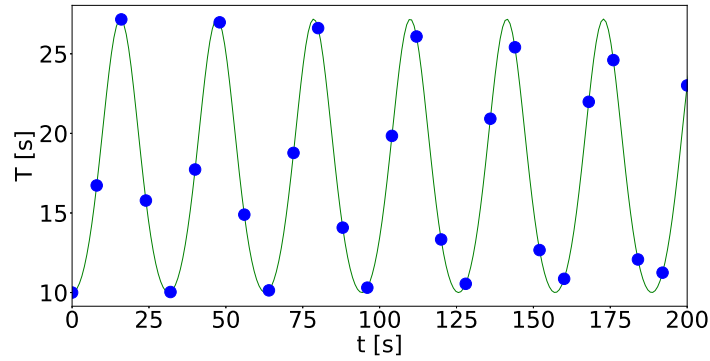


Fig. 2.4: Comparison of the numerical solution of the ODE for the variable T using an order 4 Runge-Kutta, in green, and a split-explicit Runge-Kutta of order 2, in blue.

once, while the fast part is computed M times. In contrast, for the full explicit method, both parts are computed M times.

Conversely, when the computational cost of the fast part is significantly lower than that of the slow part, explicit time splitting becomes much more efficient. For instance, if the slow terms require a cost of 1 and the fast terms a cost of 0.1, explicit time splitting costs $1 + 0.1M$, whereas the full explicit method costs $1.1M$. The advantages of using explicit time splitting become apparent. The larger the ratio M or the smaller the cost of the fast part, the more efficient explicit time splitting becomes.

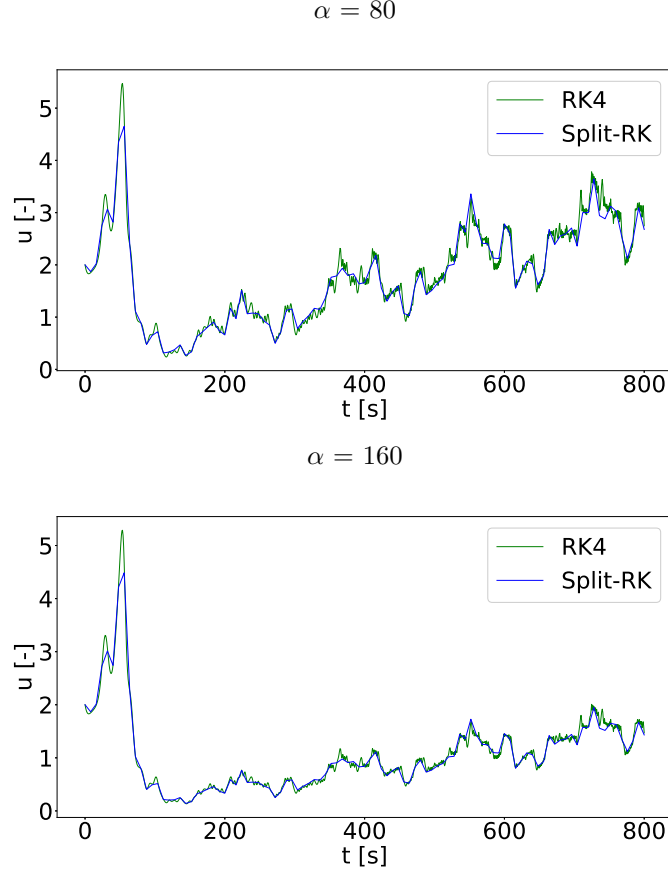


Fig. 2.5: Comparison of the split-method for different α corresponding to the ratio of the characteristic time of the slow part over the fast part.

2.2.1.2 Impact of the α parameter

An interesting thing to see is the influence of the α parameter. It represents the ratio of the period of the slow part over the period of the fast part. In other words, it is the ratio of the characteristic time of the slow part over the fast part. To see the impact of the α parameter, the ODE is solved for $\alpha = 80$ and $\alpha = 160$ instead of $\alpha = 40$ as before. The results are shown only for u in Figure 2.5. One can see that the split method is still working for the two values of α . The short and the long period are well resolved. However, the amplitude of the solution becomes smaller as α increases.

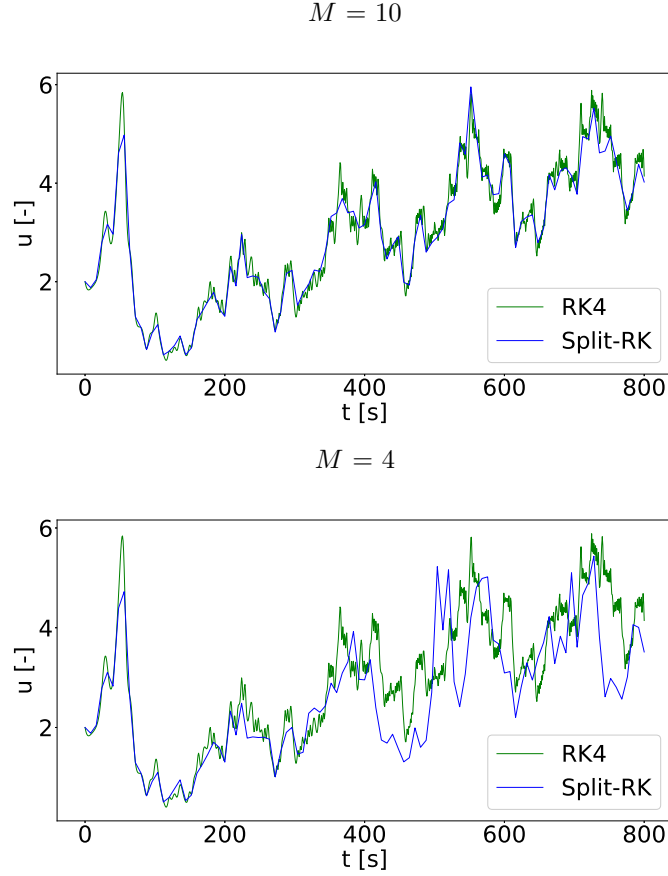


Fig. 2.6: Comparison of the split-method for different M parameter. M is the ratio of the time step of the slow part over the fast part.

2.2.1.3 Impact of the time step ratio

The impact of the integer time step ratio, M , is also interesting to see. For a fixed large time step, the time step of the fast processes varies. This shows the impact of the number of iterations of the fast part over the slow part. The bigger the ratio, the more iterations of the fast part are done. Increasing M does not change the results. This means that with a value of 10 for M , the fast part is already well resolved. The graph is not shown. On the other hand, decreasing M has a significant impact. The results are shown in Figure 2.6. As the value of M decreases, the split method is not working anymore. The short period is not well solved.

2.2.2 What about the 3D hydrodynamic equations?

The objective of this thesis is to split the 3D baroclinic ocean circulation equations into two parts: one corresponding to terms with a small characteristic time scale and the other to terms with a large characteristic time scale. The corresponding velocity scales have all been provided in the preceding sections. From these descriptions, it emerges that the fastest terms correspond to external gravity waves. Therefore, the approach is to solve these terms with a small time step and the others with a larger time step.

The splitting of the equations becomes

$$\begin{aligned}
 \mathbf{f}_u &= -\nabla_h \cdot (\mathbf{u}\mathbf{u}) - \frac{\partial(w\mathbf{u})}{\partial z} + \nabla_h \cdot (\nu_h \nabla_h \mathbf{u}) + \frac{\partial}{\partial z} \left(\nu_v \frac{\partial \mathbf{u}}{\partial z} \right) \\
 &\quad - f \mathbf{e}_z \times \mathbf{u} - \frac{g}{\rho_0} \mathbf{q} - \frac{g}{\rho_0} \rho' |_{\eta} \nabla_h \eta \\
 \mathbf{F}_u &= -g \nabla_h \eta \\
 f_H &= 0 \\
 F_H &= -\nabla_h \cdot \int_{-b}^{\eta} \mathbf{u} dz
 \end{aligned}$$

where $\mathbf{f}_u$ and f_H are the slow terms and $\mathbf{F}_u$ and F_H the fast ones.

A specific characteristic of 3D hydrodynamics equations is that these fast terms are essentially 2D terms. This implies that they are computed from variables with the same value along a vertical line. This observation makes the splitting strategy even more pertinent. Indeed, it implies that terms requiring frequent iterations are less expensive, while those needing a few computation are significantly more computationally demanding.

2.3 A toy model to sail between fast and slow phenomena

In the previous section, the time splitting method was applied to a simplified model. The results showed that the method was working. The next step is to apply this method to a simplified version of the 3D hydrodynamics equations. An $x-z$ model is used. The idea is to remove some terms while keeping the configuration of fast and slow terms. Only the external mode, the baroclinic pressure gradient and the advection are considered. The other terms are removed. The equations become

$$\frac{\partial u}{\partial t} + \frac{\partial(uu)}{\partial x} + \frac{\partial(wu)}{\partial z} = -\frac{g}{\rho_0} \int_z^\eta \frac{\partial \rho'}{\partial x} d\zeta - \frac{g}{\rho_0} \rho'|_\eta \frac{\partial \eta}{\partial x} \quad (2.16)$$

$$\frac{\partial H}{\partial t} = -\frac{\partial}{\partial x} \int_{-b}^\eta u dz \quad (2.17)$$

$$\frac{\partial T}{\partial t} + \frac{\partial(uT)}{\partial x} + \frac{\partial(wT)}{\partial z} = 0 \quad (2.18)$$

with

$$\frac{\partial w}{\partial z} = -\frac{\partial u}{\partial x}$$

$$\rho = 1000 - 0.2(T - 5)$$

As the objective is to show the time splitting method in a simplified model, a split-explicit Runge-Kutta of order 1 is used. This RK is also known as Euler explicit. As a reminder, here is its formulation for a scalar variable y and its derivative $\frac{\partial y}{\partial t} = f(y)$.

$$y_{n+1} = y_n + \Delta t f(y_n)$$

Algorithm 1 and Figure 2.7 show the time splitting method. The time step for the slow and the fast part are respectively ΔT and Δt . This gives a ratio, M , of $\frac{\Delta t}{\Delta T}$ between the time step of the slow and the fast part.

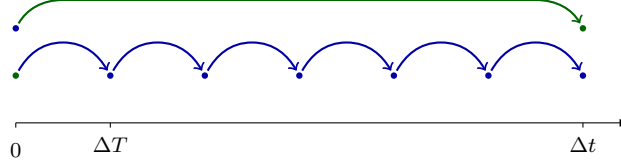


Fig. 2.7: Splitting method of order 1 for the x-z simplified hydrodynamics equations.. The slow part is computed once while the fast part is computed M times.

2.3.1 Split-explicit first order method

Algorithm 1: Splitting method of order 1 for the x-z simplified hydrodynamics equations.

Data: Model state variable u , z and M such that $\Delta t = M\Delta T$

$U, H \leftarrow \int_{-b}^{\eta} u dz, \int_{-b}^{\eta} 1 dz$

$k^{\text{slow}} \leftarrow f_u$

$K^{\text{fast}} \leftarrow 0$

for $j = 1, \dots, M$ **do**

$k_u^{\text{fast}}, k_H^{\text{fast}} \leftarrow F_u, F_H$

$H \leftarrow H + \Delta T k_H^{\text{fast}}$

$U \leftarrow U + \Delta T (k_u^{\text{fast}} + \int_{-b}^{\eta} k^{\text{slow}} dz)$

$K^{\text{fast}} \leftarrow K^{\text{fast}} + \frac{1}{H} k_u^{\text{fast}}$

end

$u \leftarrow u + \Delta t (k^{\text{slow}} + K^{\text{fast}})$

A complete description of the algorithm is given below. First, the slow part is computed.

$$k^{\text{slow}} = -u_n \frac{\partial u}{\partial x_n} - w_n \frac{\partial u}{\partial z_n} - \frac{g}{\rho_0} \int_z^{\eta} \frac{\partial \rho'}{\partial x_n} d\zeta - \frac{g}{\rho_0} \rho' \Big|_{\eta}^n \frac{\partial \eta}{\partial x_n}$$

The slope to move the slow from t^n to t^{n+1} is computed. Its vertical integral is used in the 2D loops.

Using the variable H and U , for each sub-iteration, the slopes of fast parts are computed. The first loop gives

$$k_u^{\text{fast}} = -gH \frac{\partial \eta}{\partial x_n}$$

$$k_H^{\text{fast}} = -\frac{\partial U}{\partial x_n}$$

The values of H and U are updated using both the slow and the fast parts.

$$\begin{aligned} H_{n,1} &= H_n + \Delta T k_H^{\text{fast}} \\ U_{n,1} &= U_n + \Delta T (k_u^{\text{fast}} + \int_{-b}^{\eta} k_u^{\text{slow}} dz) \\ K^{\text{fast}} &= K^{\text{fast}} + \frac{1}{H_n} k_u^{\text{fast}} \end{aligned}$$

This is repeated until the 2D variables reach $H^{n,M}$ and $U^{n,M}$ at t^{n+1} . The value of the final water height as well as the sum of all the slopes of the horizontal mean velocity are used to update the horizontal velocity.

$$\begin{aligned} H_{n+1} &= H_{n,M} \\ &= H_n + \sum_{j=1}^M -\Delta T \frac{\partial U}{\partial x_{n,j}} \\ u_{n+1} &= u_n + \Delta t k^{\text{slow}} + \Delta T K^{\text{fast}} \\ &= u_n + \Delta t \left(-u_n \frac{\partial u}{\partial x_n} - w_n \frac{\partial u}{\partial z_n} - \frac{g}{\rho_0} \int_z^{\eta} \frac{\partial \rho'}{\partial x_n} d\zeta - \frac{g}{\rho_0} \rho'_{|\eta}^n \frac{\partial \eta}{\partial x_n} \right) \\ &\quad + \sum_{j=1}^M -\Delta T g \frac{\partial \eta}{\partial x_{n,j}} \\ T_{n+1} &= T_n + \Delta t \left(-u_n \frac{\partial T}{\partial x_n} - w_n \frac{\partial T}{\partial z_n} \right) \end{aligned}$$

with

$$\begin{aligned} w_n &= \int_z^{\eta} -\frac{\partial u}{\partial x_n} d\zeta \\ \rho_n &= 1000 - 0.2(T_n - 5) \end{aligned}$$

2.3.2 Advantages of the splitting method

In the x-z model, the fast terms consist of 1D terms, computed from variables sharing the same value along a vertical line. Conversely, the slow terms are characterized as 2D terms, exhibiting varying values across the water height. In typical domains under study, the vertical dimension is discretized into a range of layers, usually between 20 and 40, though this number may be higher depending on the chosen vertical extrusion method. The number of horizontal elements depends on the domain's size.

Considering two 1D fields, H and U , with n horizontal degrees of freedom, the fast terms cost $2n$ iterations per 1D time step, which is relatively inexpensive compared to the slow terms. Each 2D variable requires between $20n$ and $40n$ iterations per 2D time step. Consequently, with three 2D variables— w , u and T —the total cost ranges from $60n$ to $120n$ iterations.

For a scenario with 30 degrees of freedom in the vertical, $n = 1000$ horizontal elements, and a time step ratio of $M = 100$, the slow terms require 90,000 iterations per 2D time step. Meanwhile, the fast terms need 2000 iterations per 1D time step. Thus, the split-explicit Runge-Kutta of order 1 totals 290,000 iterations per time step, significantly less than the full explicit Runge-Kutta of order 1, which costs 9,200,000 iterations per time step. Consequently, for this example, the time splitting method proves to be more or less 31 times faster than the full explicit method.

It is the difference between running your code and getting the results the next day after a good night's sleep and getting them the following month after 31 days of stress.

In conclusion, the computational efficiency of the explicit time splitting method becomes evident when considering the significant reduction in computational cost compared to the full method. By strategically allocating computational resources to fast and slow terms, the explicit time splitting method offers a practical solution for resolving hydrodynamic equations efficiently. This approach not only accelerates simulations but also maintains accuracy, making it a valuable tool for numerical modeling in hydrodynamics.

CHAPTER 3

A split-explicit second order Runge–Kutta method for solving 3D hydrodynamic equations

I'm a mathematician.
Mathematics has filled my life.

— Laurent Schwartz.

In the previous chapter, the different dynamics of the studied equations were presented, emphasizing the significance of a split-time method for their solution. A first-order split-time explicit method was illustrated on a simplified xy model of the equations.

The purpose of this chapter is to apply a second-order split-time scheme to the complete hydrodynamic equations. The primary objective is to reduce numerical diffusion, making second-order methods desirable. First-order temporal methods often lead to significant numerical diffusion, resulting in inaccurate or even false results. For instance, in terms of velocity, this implies a stronger viscosity than expected, causing vortices and similar mechanisms to disappear from the results.

Furthermore, the interest lies in the complete equations due to the necessity to respect certain essential physical properties, such as water conservation in

a closed domain. Therefore, careful consideration must be given to the choice of spatial discretization methods. In this thesis, the Discontinuous Galerkin Finite Element Method is used. It introduces mass matrices that reflect the volume of the mesh element. However, as the equations are solved in a domain with a free surface, these matrices change over time.

Initially, the temporal method is presented, explained through an ordinary differential equation. It is described via an algorithm and a scheme. Its convergence order is demonstrated on a linear model problem and the expression of its stability region is also calculated. A brief analysis is conducted.

Next, in the following section, the complete discrete model is showcased. The hydrodynamic equations are revisited and the finite element method is applied to each term. The fast discrete terms are distinguished from the slow terms. It is demonstrated how these terms interact, revealing the temporal and spatial coupling between them. The split-time scheme is applied to the discrete equations, showcasing how the physical properties of the continuous world are preserved in the discrete world. Four numerical test cases are conducted to demonstrate the efficiency of the split-time scheme in reducing numerical diffusion.

Before diving into the details of the split-time scheme, a presentation is made of the Thetis model, a well-known model in the field of marine hydrodynamics. The Thetis model uses a similar spatial discretization but with a different approach to the temporal coupling of the fast and slow dynamics. The presentation highlights the mechanism of the coupling.

Presentation of the Thetis model

The coupling, referred as the G-method in this thesis, between the 2D and 3D models stands as the pivotal element of the Thetis algorithm. Consequently, this section provides an overview of the coupling method. For illustration purposes, let us take the following ordinary differential equation:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}) + \mathbf{F}(\mathbf{y}), \quad t \in (0, T) \quad (3.1)$$

with the initial value $\mathbf{y}(0) = \mathbf{y}_0$. In this ODE, $\mathbf{f}(\mathbf{y})$ is the slope of slow dynamics while $\mathbf{F}(\mathbf{y})$ represents the fast one. The idea of the splitting method is to solve the slow terms with a time step Δt and the fast ones with a time step ΔT . The ratio between them is denoted M . Furthermore, the variable y can be split into two:

$$\mathbf{y} = \tilde{\mathbf{y}} + \bar{\mathbf{y}} \quad (3.2)$$

where $\tilde{\mathbf{y}}$ is the component of the slow dynamics and $\bar{\mathbf{y}}$ the fast ones.

In this example, $\mathbf{y}$ and $\tilde{\mathbf{y}}$ are vectors with numerous degrees of freedom (DOF). Each entries can have different value. $\bar{\mathbf{y}}$ is also a vector but possesses only one value for all its DOF. Consequently, in the previous sum, $\bar{\mathbf{y}}$ maintains identical values across all DOF. Additionally, the mean of all degrees for $\tilde{\mathbf{y}}$ amounts to zero. In simpler terms, the mean of all the entries of $\mathbf{y}$ is equal to $\bar{\mathbf{y}}$. This gives

$$\begin{aligned}\frac{1}{n} \sum_{i=1}^n \mathbf{y}_i &= \frac{1}{n} \sum_{i=1}^n (\bar{\mathbf{y}} + \tilde{\mathbf{y}}_i) \\ &= \bar{\mathbf{y}} + \frac{1}{n} \sum_{i=1}^n \tilde{\mathbf{y}}_i \\ &= \bar{\mathbf{y}}\end{aligned}$$

By considering that fast processes only need $\bar{\mathbf{y}}$, Equation 3.1 can be rewritten as follows:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}) + \mathbf{F}(\bar{\mathbf{y}}) \quad (3.3)$$

To explain the coupling, a splitting method composed of Euler explicit methods for the slow and fast terms is used. The idea of the G-method is to split the unique ODE into two ODEs. The first one is focused on the $\tilde{\mathbf{y}}$ while the second one solves $\bar{\mathbf{y}}$. The slow dynamics are, first, computed through $\tilde{\mathbf{y}}$ with this equation:

$$\frac{d\tilde{\mathbf{y}}}{dt} = \mathbf{f}(\mathbf{y}) \quad (3.4)$$

Using the Euler explicit method, the solution of this equation is:

$$\tilde{\mathbf{y}}^{n+1} = \tilde{\mathbf{y}}^n + \Delta t \mathbf{f}(\mathbf{y}^n) \quad (3.5)$$

The issue with these results is that the updated value of $\tilde{\mathbf{y}}$ may not be consistent. In other words, its average could be non-zero. To address this, the mean of $\tilde{\mathbf{y}}$ is subtracted from it. This gives:

$$\tilde{\mathbf{y}}^* = \tilde{\mathbf{y}}^n + \Delta t \mathbf{f}(\mathbf{y}^n) \quad (3.6)$$

$$\tilde{\mathbf{y}}^{n+1} = \tilde{\mathbf{y}}^* - \frac{1}{n} \sum_{i=1}^n \tilde{\mathbf{y}}_i^* \quad (3.7)$$

The approach is named the G-method because the mean subtracted from $\tilde{\mathbf{y}}$ represents the $\mathbf{G}$ term. $\mathbf{G}$ has the same value for all the DOF.

$$\mathbf{G} = \frac{1}{\Delta t} \frac{1}{n} \sum_{i=1}^n \tilde{\mathbf{y}}_i^* \quad (3.8)$$

Subsequently, the fast dynamics are estimated using $\bar{\mathbf{y}}$ with this $\mathbf{G}$ term. This constitutes the essence of the coupling method. Throughout the iterations of the fast phenomena, $\mathbf{G}$ remains the same. The fast dynamics are computed with the following equation:

$$\frac{d\bar{\mathbf{y}}}{dt} = F(\bar{\mathbf{y}}) + \mathbf{G} \quad (3.9)$$

Using M time step of order 1 with ΔT , the solution of this equation is:

$$\begin{aligned} \bar{\mathbf{y}}^1 &= \bar{\mathbf{y}}^n + \Delta T \mathbf{F}(\bar{\mathbf{y}}^n) + \Delta T \mathbf{G} \\ \bar{\mathbf{y}}^2 &= \bar{\mathbf{y}}^1 + \Delta T \mathbf{F}(\bar{\mathbf{y}}^1) + \Delta T \mathbf{G} \\ &\vdots \\ \bar{\mathbf{y}}^M &= \bar{\mathbf{y}}^{M-1} + \Delta T \mathbf{F}(\bar{\mathbf{y}}^{M-1}) + \Delta T \mathbf{G} \end{aligned}$$

Finally, the new value of $\mathbf{y}$ is computed by adding $\tilde{\mathbf{y}}$ and $\bar{\mathbf{y}}$.

$$\mathbf{y}^{n+1} = \tilde{\mathbf{y}}^{n+1} + \bar{\mathbf{y}}^M \quad (3.10)$$

As mentioned earlier, the Thetis model, although second order in space and time, fails to be conservative and consistent at the same time. To solve this problem, a new split-explicit Runge-Kutta scheme is developed in this thesis. This scheme is adapted to the discontinuous Galerkin finite element method. The new scheme is second order in time and is designed to conserve tracer and water volume as well as to be consistent.

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3.1 Introduction

Numerical simulation allows to understand processes taking place in the marine environment and, to some extent, predict their evolution. Formulating the relevant equations, selecting the values of the parameters and designing the initial and boundary conditions are challenges that have been addressed in various manners [Fringer et al. \(2019\)](#). Most estuarine, coastal and shelf sea models are based on the hydrostatic and Boussinesq approximations [Pearson et al. \(2017\)](#). However, for smaller-scale phenomena, the effects of non-hydrostatic equations are sometimes taken into account [Lermusiaux et al. \(2013\)](#).

Ocean models have to deal with large aspect ratio domains where the horizontal length scales can reach several thousands of kilometers while the depth is generally of the order of one kilometer or smaller. For this reason, various types of spatial and temporal discretizations have been developed which handle separately the horizontal and vertical directions. In the vertical direction, layered meshes, including terrain-following sigma-levels [Blumberg and Mellor \(1987\)](#); [Pan et al. \(2021\)](#), z-levels [Griffies et al. \(2005\)](#) and their generalization [Song and Haidvogel \(1994\)](#) are generally used. It is worth mentioning that, in some ocean models, isopycnal coordinates [Bleck and Smith \(1990\)](#) are used. In the horizontal direction, a large number of models (ROMS [Kumar et al. \(2012\)](#), POM [Weiss et al. \(2018\)](#), etc.) are based on structured grids, as the associated numerical methods are computationally efficient [Danilov et al. \(2008\)](#); [Blumberg and Mellor \(1987\)](#). This distinct advantage is partially offset by a lack of geometrical flexibility [Deleersnijder and Lermusiaux \(2008\)](#) to deal with complex topographical features and small-scale localised processes.

As a consequence, models based on horizontally-unstructured meshes are becoming increasingly popular, e.g., FVCOM [Chen et al. \(2003\)](#), SUNTANS [Fringer et al. \(2006\)](#), SCHISM [Zhang et al. \(2016\)](#), FESOM [Scholz et al. \(2013\)](#). These models use finite volume (e.g. FVCOM) or finite element (e.g. SCHISM) discretizations, or an approach lying in between them, namely the discontinuous Galerkin method e.g. SLIM [Dobbelaere et al. \(2022\)](#), [Vallaeys et al. \(2021\)](#). The latter, hereafter referred to as the DG method, is well suited for advection-dominated problem and leads to algorithms scaling very well on a large number of processors. They also facilitate the computation of explicit time methods and can easily be extended to higher order of accuracy in a natural way. On a given mesh, a DG method offers a higher precision than a classical finite element method with the same formal order of accuracy but requires significantly more discrete unknowns as well as the computation of additional terms at the boundaries between elements.

Since diffusion is very low in the deep ocean basins and water masses can remain unchanged for years, spurious mixing is a crucial issue in global circulation models [MacCready et al. \(2018\)](#). This mixing constitutes a problem even for coastal domains that are characterised by strong horizontal and vertical

density gradients [Geyer and MacCready \(2014\)](#); [MacCready and Geyer \(2010\)](#), small scale dynamics as internal waves and baroclinic eddies. As a result, an overly diffusive model cannot capture essential features like the intrusion of saline waters into embayments or the mixing in river plumes [Burchard and Rennau \(2008\)](#); [Hofmeister et al. \(2010\)](#); [Kärnä et al. \(2015\)](#); [Ralston et al. \(2017\)](#). The finite grid resolution and the numerical schemes, in particular the discretization of the advection, can introduce significant spurious numerical mixing [Burchard and Rennau \(2008\)](#); [Rennau and Burchard \(2009\)](#); [Hiester et al. \(2014\)](#).

To fully discretize the hydrodynamic equations, time integration methods are required. Splitting techniques are widely used e.g. [Wicker and Skamarock \(2002\)](#); [Knoth and Wensch \(2003\)](#); [Nilsen and Loseth \(1993\)](#); [Visbal and Gaitonde \(2002\)](#); [Robert and Kaper \(1986\)](#). The fast surface gravity waves propagating in a depth integrated 2D framework are coupled to the slower 3D dynamics. In a split-explicit scheme (SPEX), the 2D mode is solved explicitly with a small time step while the 3D one uses a larger time step [Gadd \(1978, 1980\)](#); [Killworth et al. \(1991\)](#); [Shchepetkin A.F. \(2005\)](#). Fast waves limit the time step. For long simulations, which are not uncommon in the marine domain, this can lead to a large number of time steps. This leans on computational and storage resources. In split-implicit schemes, the 2D and 3D modes generally use the same time-step but an implicit method is used for the 2D while the 3D is solved explicitly, e.g. [Dukowicz and Smith \(1994\)](#); [Marshall et al. \(1997b\)](#). Those schemes tend to be expensive for ocean models where the resolution of the nonlinear partial differential equations requires iterative methods.

The Second-generation Louvain-la-Neuve Ice-ocean Model (SLIM, www.slim-ocean.be) focuses on solving the hydrodynamic equations on an unstructured grid. As ocean and coastal domain can feature strong scalar field and velocity gradients, it is important to maintain a good quality of these fields. One drawback of many unstructured grid models is their excessive numerical diffusion that smooths out important physical features [Kärnä et al. \(2015\)](#); [Kärnä and Baptista \(2016\)](#); [Comblen et al. \(2010\)](#).

To address this issue, this work presents a new second order split-explicit Runge-Kutta (SPEX-RK) temporal scheme combined with the DG spatial discretization of SLIM. The objective is specifically to obtain a low numerical mixing, a second-order accurate, conservative and consistent tracer advection scheme. This requires a fully discontinuous treatment of the free surface motion in order to achieve conservation of water and tracer volumes both locally and globally. All horizontal terms are processed by an explicit method. Only the vertical terms are treated implicitly. This choice guarantees an easy and efficient parallelization of the model, as the evolution of each vertical column over a time step can be computed independently.

This article is organised as follows. It starts by introducing the split-explicit

Runge-Kutta time integrators in Section 3.2. In the next section, the hydrodynamic equations, their DG-FE discretisation, the integration of the temporal scheme in our marine model and the methods to ensure conservation and consistency are presented. In Section 3.4, various numerical results on different test cases are shown to validate our model. Finally, a conclusion is given at the end of this article in Section 3.5.

3.2 Split-Explicit Runge-Kutta methods

First of all, it is worth recalling the notion of stiffness of a problem. Let us consider an initial value problem associated with two different processes: a slow process and a fast one. Each process has its own characteristic timescale. When the magnitudes of the timescales are significantly different, the system is said to be stiff.

3.2.1 Temporal scheme

In practice, for an initial value problem with many processes, if the maximum value of the time step is mainly limited by a single term representing one process, the problem is said to be stiff. For illustration purposes, the following ordinary differential equation is taken into consideration:

$$\frac{dy}{dt} = f(y) + F(y), \quad t \in (0, T) \quad (3.11)$$

with the initial value $y(0) = y_0$.

The functions $f(y)$ and $F(y)$ correspond to the non-stiff (slow time-varying) and the stiff (fast time-varying) parts, respectively. Note that they could be the result of applying two different spatial discretizations for the two differential operators associated with slow and fast processes. To solve this type of equation, a splitting method can be used. For example, Runge-Kutta (RK) methods can be used with a big time step, Δt , for the temporal evolution of $f(y)$ and a small one, $\Delta T = \frac{\Delta t}{M}$ with M the closest suitable integer to the ratio between the characteristic timescales, for the temporal evolution of $F(y)$.

The main objective of this article is to obtain a second order temporal scheme. For this purpose, as pointed out in Knoth and Wensch (2013), one can use a Runge-Kutta of order 2 with 3 steps (RK3) for slow terms and a Runge-Kutta of order 2 with 2 steps (RK2) for the fast ones to ensure it. The combination of these two temporal scheme gives the SPEX-RK scheme. The RK3 is used to have a bigger stability region. For the random variables y_n and Y_n , respectively, the two chosen schemes are the following ones

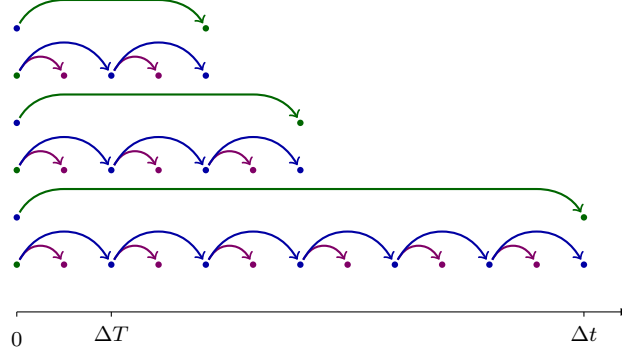


Fig. 3.1: Split-explicit scheme composed by RK3 and RK2. The green arrows represent the computation of each $f^{\text{slow}}(y)$ while the blue and the purple ones represent the computation of each $f^{\text{fast}}(y)$

$$\begin{aligned}
 y_{n+1} &= y_n + \Delta t k_3 & Y_{n+1} &= Y_n + \Delta T K_2 \\
 k_1 &= f(t_n, y_n) & K_1 &= F(t_n, Y_n) \\
 k_2 &= f(t_n + \Delta t/3, y_n + k_1 \Delta t/3) & K_2 &= F(t_n + \Delta T/2, Y_n + K_1 \Delta T/2) \\
 k_3 &= f(t_n + \Delta t/2, y_n + k_2 \Delta t/2)
 \end{aligned}$$

These RK are low-storage temporal schemes, meaning that for each evaluation of the solution, one just needs to keep few data in memory.

Let us describe the original SPEX-RK for Equation 3.11. Firstly, k_1^{slow} is computed using y_0 such that $k_1^{\text{slow}} = f(y_0)$. This allows the slow terms to reach $y_{n+\frac{1}{3}}$. A loop from 1 to $\frac{M}{3}$ moves the fast terms using RK2 to $Y_{n+\frac{1}{3}}$ by calculating k_1^{fast} and k_2^{fast} at each iteration. $Y_{n+\frac{1}{3}}$ and $y_{n+\frac{1}{3}}$ are added to obtain the total value of the variable. Afterwards, the same process is repeated with k_2^{slow} and k_3^{slow} . Finally, y_{n+1} is found by using k_3^{slow} . The whole process is summarised in the Figure 3.1 and the Algorithm 2. Although this temporal scheme uses two well-known RK, the resulting splitting is new.

Algorithm 2: SPEX-RK scheme for RK3 and RK2

Data: Model state variable y_n , $m = M/6$

```

 $y_0 \leftarrow y_n$ 
 $y \leftarrow y_n$ 
for  $i = 2m, 3m, 6m$  do
     $k^{\text{slow}} \leftarrow f^{\text{slow}}(y)$ 
     $y \leftarrow y_0$ 
    for  $j = 1, \dots, i$  do
         $k^{\text{fast}} \leftarrow f^{\text{fast}}(y)$ 
         $k^{\text{fast}} \leftarrow f^{\text{fast}}(y + \frac{1}{2}\Delta T(k^{\text{fast}} + k^{\text{slow}}))$ 
         $y \leftarrow y + \Delta T(k^{\text{fast}} + k^{\text{slow}})$ 
    end
end
 $y_{n+1} \leftarrow y$ 

```

3.2.2 Order of precision

While the [Knoth and Wensch \(2013\)](#) suggests that this scheme has a second order accuracy, it still needs to be verified through analysis. To achieve this, the Taylor series expansion of y_{n+1} must match the result of the temporal scheme up to order 2. The former can be expressed as:

$$\begin{aligned}
 y_{n+1} &= y_n + \Delta t y'_n + \frac{\Delta t^2}{2} y''_n + O(\Delta t^3) \\
 &= y_n + \Delta t (f_n + F_n) + \frac{\Delta t^2}{2} \left((f'_n + F'_n) (f_n + F_n) \right) + O(\Delta t^3) \quad (3.12)
 \end{aligned}$$

with $f_n = f(y_n)$ and $F_n = F(y_n)$.

A classic Runge-Kutta order analysis would compute each iteration of the residues, calculate the Taylor expansion for each of them and sum them up to obtain the final expression of y_{n+1} . For a SPEX-RK scheme, this is not practical to show the result of each 2D sub-steps, which involves too many terms to express. Instead, for clarity, only the evaluations of y at the 3D sub-steps are computed, which include $y_{n+\frac{1}{3}}$, $y_{n+\frac{1}{2}}$, and y_{n+1} . The result of a complete RK2 iteration is computed first. For a given k^{slow} and M , the first sub-iteration gives

$$\begin{aligned}
K_1 &= F_n \\
K_2 &= F\left(y_n + \frac{\Delta T}{2} (F_n + k^{\text{slow}})\right) \\
&= F_n + \frac{\Delta T}{2} (F_n + k^{\text{slow}}) F'_n + O(M\Delta T^2) \\
y_1 &= y_n + \Delta T (K_2 + k^{\text{slow}}) \\
&= y_n + \Delta T (F_n + k^{\text{slow}}) + \frac{\Delta T^2}{2} (F_n + k^{\text{slow}}) F'_n + O(M^3\Delta T^3)
\end{aligned}$$

The second sub-iteration yield

$$\begin{aligned}
K_1 &= F_n + O(M\Delta T) \\
K_2 &= F\left(y_1 + \frac{\Delta T}{2} (F_n + k^{\text{slow}})\right) \\
&= F_n + \frac{3\Delta T}{2} (F_n + k^{\text{slow}}) F'_n + O(M^2\Delta T^2) \\
y_2 &= y_1 + \Delta T (K_2 + k^{\text{slow}}) \\
&= y_n + 2\Delta T (F_n + k^{\text{slow}}) + \frac{4\Delta T^2}{2} (F_n + k^{\text{slow}}) F'_n + O(M^3\Delta T^3)
\end{aligned}$$

By recurrence, the last iteration produces the solution

$$y_M = y_n + M\Delta T (F_n + k^{\text{slow}}) + \frac{M^2\Delta T^2}{2} (F_n + k^{\text{slow}}) F'_n + O(M^3\Delta T^3)$$

This result is denoted $RK2(k^{\text{slow}}, M)$. To determine the order of accuracy of the global method, the RK3 method is unrolled.

$$\begin{aligned}
y_1 &= y_n \\
y_2 &= RK2(k_1^{\text{slow}}, \frac{M}{3}) \\
&= y_n + \frac{M}{3} \Delta T (F_n + f_n) + \left(\frac{M}{3}\right)^2 \frac{\Delta T^2}{2} (F_n + f_n) F'_n + O(M^3 \Delta T^3) \\
y_3 &= RK2\left(k_2^{\text{slow}}, \frac{M}{2}\right) \\
&= y_n + \frac{M}{2} \Delta T \left(F_n + f_n + \frac{M}{3} \Delta T (F_n + f_n) f'_n\right) \\
&\quad + \left(\frac{M}{2}\right)^2 \frac{\Delta T^2}{2} (F_n + f_n) F'_n + O(M^3 \Delta T^3) \\
&= y_n + \frac{M}{2} \Delta T (F_n + f_n) + \left(\frac{M}{2}\right)^2 \frac{\Delta T^2}{2} (F_n + f_n) \left(F'_n + \frac{4}{3} f'_n\right) + O(M^3 \Delta T^3) \\
y_{n+1} &= RK2\left(k_3^{\text{slow}}, M\right) \\
&= y_n + M \Delta T \left(F_n + f_n + \frac{M}{2} \Delta T (F_n + f_n) f'_n\right) \\
&\quad + M^2 \frac{\Delta T^2}{2} (F_n + f_n) F'_n + O(M^3 \Delta T^3) \\
&= y_n + M \Delta T (F_n + f_n) + M^2 \frac{\Delta T^2}{2} (F_n + f_n) \left(F'_n + f'_n\right) + O(M^3 \Delta T^3)
\end{aligned}$$

with $M \Delta T = \Delta t$

The final sub-step gives

$$y_{n+1} = y_n + \Delta t (f_n + F_n) + \frac{\Delta t^2}{2} \left((f'_n + F'_n) (f_n + F_n) \right) + O(\Delta t^3) \quad (3.13)$$

Comparing the two equations, it can be concluded that Equation 3.12 matches Equation 3.13. Therefore, the SPEX-RK scheme is a temporal scheme of order 3 locally and order 2 globally.

3.2.3 Stability Region

Typically, to determine the stability of a numerical method, it is standard practice to analyze the linear form of the underlying ordinary differential equation. In this particular case, the linear ordinary differential equation is given by Equation

$$\frac{dy}{dt} = \lambda y + \Lambda y \quad (3.14)$$

where λ and Λ represent the complex coefficients of the linear functions $f(y)$ and $F(y)$, respectively.

The amplification factor of the numerical solution at each time step is defined as the ratio between y_{n+1} and y_n . Using Algorithm 2, this factor can be expressed.

First, the complete RK2 iteration is calculated with a given k^{slow} and M . The initial sub-iteration produces the values for K_1 , K_2 , and y_1 .

$$\begin{aligned} K_1 &= \Lambda y_n \\ K_2 &= \Lambda \left(y_n + \frac{\Delta T}{2} (\Lambda y_n + k^{\text{slow}}) \right) \\ &= y_n \left(\Lambda + \Lambda^2 \frac{\Delta T}{2} \right) + k^{\text{slow}} \Lambda \frac{\Delta T}{2} \\ y_1 &= y_n \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right) + k^{\text{slow}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \end{aligned}$$

The subsequent sub-iteration produces y_2 , y_3 , and so on, until the last iteration is reached, which is y_M .

$$\begin{aligned} y_2 &= y_1 \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right) + k^{\text{slow}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \\ &= y_n \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right)^2 \\ &\quad + k^{\text{slow}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(1 + \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right) \right) \\ y_3 &= y_2 \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right) + k^{\text{slow}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \\ &= y_n \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right)^3 \\ &\quad + k^{\text{slow}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(1 + \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right) + \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right)^2 \right) \end{aligned}$$

By recurrence, the last iteration gives

$$\begin{aligned} y_M &= y_n \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right)^M + k^{\text{slow}} \Lambda \frac{\Delta T^2}{2} \sum_{i=0}^{M-1} \left(1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2} \right)^i \\ &= y_n A^M + k^{\text{slow}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^M}{1 - A} \right) \end{aligned}$$

with $A = 1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2}$ and $\Lambda \neq 0$, $\Delta T \neq 0$.

This result is denoted $RK2(k^{\text{slow}}, M)$ and it serves as the basis for deriving the amplification factor of the global method by unrolling the RK3.

$$\begin{aligned}
 y_1 &= y_n \\
 y_2 &= RK2\left(k_1^{\text{slow}}, \frac{M}{3}\right) \\
 &= y_n A^{\frac{M}{3}} + \lambda y_n \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^{\frac{M}{3}}}{1 - A} \right) \\
 &= y_n \left(A^{\frac{M}{3}} + \lambda \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^{\frac{M}{3}}}{1 - A} \right) \right) \\
 y_3 &= RK2\left(k_2^{\text{slow}}, \frac{M}{2}\right) \\
 &= y_n A^{\frac{M}{2}} \\
 &\quad + \lambda y_n \left(A^{\frac{M}{3}} + \lambda \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^{\frac{M}{3}}}{1 - A} \right) \right) \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^{\frac{M}{2}}}{1 - A} \right) \\
 &= y_n \left(A^{\frac{M}{2}} + \lambda A^{\frac{M}{3}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^{\frac{M}{2}}}{1 - A} \right) \right. \\
 &\quad \left. + \lambda^2 \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right)^2 \left(\frac{1 - A^{\frac{M}{3}}}{1 - A} \right) \left(\frac{1 - A^{\frac{M}{2}}}{1 - A} \right) \right) \\
 y_3 &= RK2\left(k_3^{\text{slow}}, M\right) \\
 &= y_n \left(A^M + \lambda A^{\frac{M}{2}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^M}{1 - A} \right) \right. \\
 &\quad \left. + \lambda^2 A^{\frac{M}{3}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right)^2 \left(\frac{1 - A^{\frac{M}{2}}}{1 - A} \right) \left(\frac{1 - A^M}{1 - A} \right) \right. \\
 &\quad \left. + \lambda^3 \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right)^3 \left(\frac{1 - A^{\frac{M}{3}}}{1 - A} \right) \left(\frac{1 - A^{\frac{M}{2}}}{1 - A} \right) \left(\frac{1 - A^M}{1 - A} \right) \right)
 \end{aligned}$$

Finally, the factor expression is

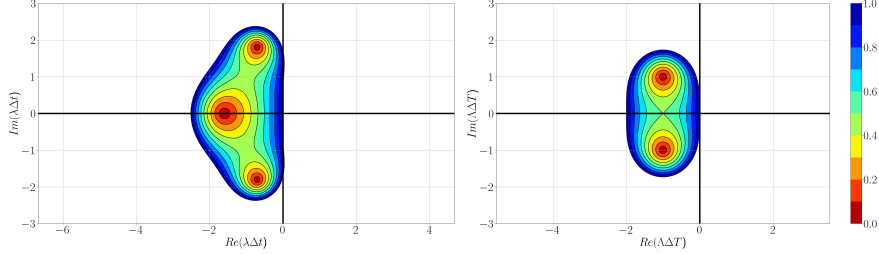


Fig. 3.2: Stability region with only one function with $M = 1$. The abscissa is the Real part while the ordinates is the Imaginary part of respectively $\lambda\Delta t$ and $\lambda\Delta T$. The bold lines are the origins.

$$\begin{aligned}
 \frac{y_{n+1}}{y_n} = & A^M + \lambda A^{\frac{M}{2}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \left(\frac{1 - A^M}{1 - A} \right) \\
 & + \lambda^2 A^{\frac{M}{3}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right)^2 \left(\frac{1 - A^{\frac{M}{2}}}{1 - A} \right) \left(\frac{1 - A^M}{1 - A} \right) \\
 & + \lambda^3 \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right)^3 \left(\frac{1 - A^{\frac{M}{3}}}{1 - A} \right) \left(\frac{1 - A^{\frac{M}{2}}}{1 - A} \right) \left(\frac{1 - A^M}{1 - A} \right) \quad (3.15)
 \end{aligned}$$

with $A = \left(\frac{\Lambda^2 dT^2}{2} + \Lambda dT + 1 \right)$ and $\Delta t = M\Delta T$.

The stability of the scheme depends on whether the norm of the amplification factor is less than or equal to 1. The stability region of the scheme is a function of three parameters: λ , Λ , and M , where the first two are complex and the last is a positive integer. The global stability region is too complicated to represent, as it is a 5D field. To facilitate the representation of the function, let us consider first the case where λ or Λ is null and $M = 1$. Figure 3.2 shows the corresponding stability regions, which match those of the classic RK3 and RK2 methods. Increasing the value of M affects both graphs: for RK3, the stability region is reduced but maintains the same shape, while for RK2, the region remains the same size but the area with a small amplification factor increases.

The focus is on the case where Λ is bigger than λ . For simplicity, a specific case is being considered that can be generalized. The magnitudes of $|\Lambda|$ and $|\lambda|$ are respectively 12 and 1, and M increases while ΔT decreases such that $M\Delta T$ remains constant. The factor M takes the value from the set [6, 12, 18, 24, 30]. The first entry in the set considers a factor smaller than the ratio between the eigenvalues of the fast and slow process. The second entry considers a factor

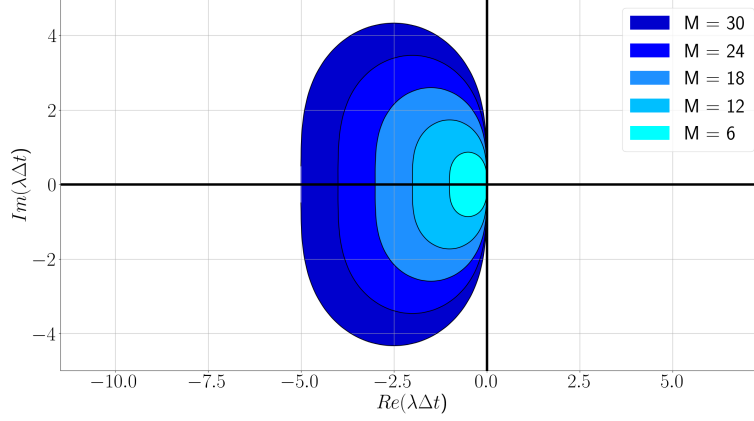


Fig. 3.3: Stability region with $\lambda = 1$ and $\Lambda = 12$ and $M = [6, 12, 18, 24, 30]$ while Δt stays the same. The abscissa is the Real part while the ordinates is the Imaginary part of $\lambda\Delta t$. The bold lines are the origins.

equal to the ratio, while the last values are greater than the latter. The stability regions are shown in Figure 3.3.

Each stability region has the shape of the classic RK2. When M is equal to the ratio, the region has the same size as the RK2. For a smaller M , the region is reduced, while for a larger M , the region is increased. This implies that when Δt is larger, M must be increased as well.

3.3 Model

The presented scheme is applied to the ocean. This study focuses on the three-dimensional hydrostatic equations with a focus on two ranges of timescales. The scale-separation stiffness can be described by the external Froude number. This dimensionless number characterises the ratio between the water velocity and the gravity wave speed.

3.3.1 Governing equations

The studied equations are derived from the Navier-Stokes equations under the hydrostatic hypothesis with the Boussinesq approximation. The first assumption means that the pressure force balances the weight of the water column. The Boussinesq approximation implies that density variations are neglected in all terms of the momentum equation, except the gravity term. Given the Carte-

sian horizontal and vertical coordinates $\mathbf{x} = [x, y, z]^T$, they take the following form

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla_h \cdot (\mathbf{u}\mathbf{u}) + \frac{\partial(w\mathbf{u})}{\partial z} = \nabla_h \cdot (\nu_h \nabla_h \mathbf{u}) + \frac{\partial}{\partial z} \left(\nu_v \frac{\partial \mathbf{u}}{\partial z} \right) \quad (3.16a)$$

$$- f \mathbf{e}_z \times \mathbf{u} - g \nabla_h \eta - \frac{g}{\rho_0} \mathbf{q} - \frac{g}{\rho_0} \rho' |_h \nabla_h \eta$$

$$\frac{\partial H}{\partial t} = - \nabla_h \cdot \int_{-b}^{\eta} \mathbf{u} dz \quad (3.16b)$$

$$\frac{\partial w}{\partial z} = - \nabla_h \cdot \mathbf{u} \quad (3.16c)$$

where ν_h , ν_v and ∇_h respectively represent the horizontal as well as the vertical viscosity and the horizontal gradient. $\mathbf{u} = (u, v)$ is the horizontal velocity vector while w is the vertical velocity. The horizontal total transport is represented by the variables $\mathbf{U} = \int_{-b}^{\eta} \mathbf{u} dz$ with η and b respectively the free surface elevation and the bathymetry. The height of the column is represented by H . f is the Coriolis parameter. $\mathbf{q}$ represents the integral of the density deviation gradient, $\mathbf{q} = \int_z^{\eta} \nabla_h \rho'$. The density deviation is obtained by a state equation depending on the water temperature or the salinity. The term with $\rho' |_h \nabla_h \eta$ serves as the surface condition for $\mathbf{q}$.

Water temperature and salinity are modeled by the advection-diffusion equation. This gives

$$\rho' = \rho'(T, S) \quad (3.17)$$

$$\frac{\partial T}{\partial t} + \nabla_h \cdot (\mathbf{u}T) + \frac{\partial(wT)}{\partial z} = \nabla_h \cdot (\kappa_h \nabla_h T) + \frac{\partial}{\partial z} \left(\kappa_v \frac{\partial T}{\partial z} \right) \quad (3.18)$$

$$\frac{\partial S}{\partial t} + \nabla_h \cdot (\mathbf{u}S) + \frac{\partial(wS)}{\partial z} = \nabla_h \cdot (\kappa_h \nabla_h S) + \frac{\partial}{\partial z} \left(\kappa_v \frac{\partial S}{\partial z} \right) \quad (3.19)$$

κ_h and κ_v stand for respectively the horizontal and the vertical diffusivity.

Furthermore, SLIM solves the equations in a three-dimensional domain Ω with a free moving surface. The lateral boundary Γ_l is fixed as well as the bottom boundary Γ_b . However, the surface boundary Γ_s varies in time with the vertical coordinates between $z = -b$ and $z = \eta$. The impermeability conditions are prescribed on the top and the bottom surfaces:

$$w + \mathbf{u} \cdot \nabla_h b = 0 \quad \mathbf{x} \in \Gamma_b \quad (3.20a)$$

$$w - \frac{\partial H}{\partial t} - \mathbf{u} \cdot \nabla_h (H - b) = 0 \quad \mathbf{x} \in \Gamma_s \quad (3.20b)$$

In addition, a slip condition is applied to account for bottom and surface stresses, $\boldsymbol{\tau}_b$ and $\boldsymbol{\tau}_s$,

$$\nu_v \frac{\partial \mathbf{u}}{\partial z} = \frac{\boldsymbol{\tau}_b}{\rho_0} \quad \mathbf{x} \in \Gamma_b \quad (3.21a)$$

$$\nu_v \frac{\partial \mathbf{u}}{\partial z} = \frac{\boldsymbol{\tau}_s}{\rho_0} \quad \mathbf{x} \in \Gamma_s \quad (3.21b)$$

3.3.2 Weak formulation

To obtain the weak formulation, the previous continuous equations have to be multiplied by a smooth 2D shape function $\phi_i(x,y)$ or 3D shape function $\phi_i(x,y,z) = \phi_{j,xy}(x,y) \phi_{k,z}(z)$ with j and k the indexes for respectively the horizontal and vertical discontinuous nodes. These equations are discretised with a discontinuous linear function space. They are then integrated by part to obtain volume terms and interface terms. The interface terms can be integrals on a horizontal triangle domain or a vertical squad domain.

In the weak form, the following notations are used for the volume and the interface integrals

$$\begin{aligned} \langle \bullet \rangle &= \int_{\Omega} \bullet dV \\ \langle \langle \bullet \rangle \rangle_{\partial \Gamma_h} &= \int_{\partial \Gamma_h} \bullet dS \\ \langle \langle \bullet \rangle \rangle_{\partial \Gamma_v} &= \int_{\partial \Gamma_v} \bullet dS \end{aligned}$$

Ω represents the domain while $\partial \Gamma$ represents the interfaces. In 3D, they can be vertical faces, Γ_v , or horizontal faces, Γ_h . In 2D, all the interfaces are edges.

The equation for $\mathbf{u}$ has 3D and 2D terms. The latter, corresponding to the fast processes, are split such that there are two types of functions spaces, 2D and 3D. In the interface integrals, a mean value is used for the terms with the horizontal velocities. It is computed such that

$$\{\mathbf{u} \cdot \mathbf{n}_h\} = \frac{\mathbf{u}_{right} \cdot \mathbf{n}_h + \mathbf{u}_{left} \cdot \mathbf{n}_h}{2} \quad (3.22a)$$

$$\{w\} = \frac{w_{right} + w_{left}}{2} \quad (3.22b)$$

where $\{\cdot\}$ represents the mean operator between values on both sides of the interfaces. The same reasoning is used for the terms with the vertical velocity.

What's more, in the vertical interfaces integrals, an upwind term is used, $\mathbf{u}^{up}$ in addition to the terms described before. Equation 3.16a becomes

$$\left\langle \phi_i \frac{\partial \mathbf{u}}{\partial t} \right\rangle = f_{3d}(\mathbf{u}) + \frac{1}{H} f_{2d}(H\mathbf{u}) \quad (3.23a)$$

with

$$\begin{aligned} f_{2d}(H\mathbf{u}) &= \left\langle g \frac{H^2}{2} \nabla_h \cdot \phi_i \right\rangle - \left\langle \left\langle g \frac{H^2}{2} \phi_i \cdot \mathbf{n} \right\rangle \right\rangle + \left\langle \phi_i g H \nabla_h b \right\rangle \\ &= \left\langle g \frac{H^2}{2} \nabla_h \cdot \phi_i \right\rangle - \left\langle \left\langle g \left(\frac{H_{left}^2 + H_{right}^2}{4} \right) \phi_i \cdot \mathbf{n} \right\rangle \right\rangle \\ &\quad + \left\langle \phi_i g H \nabla_h b \right\rangle \\ f_{3d}(\mathbf{u}) &= \left\langle \mathbf{u} \mathbf{u} \cdot \nabla_h \phi_i \right\rangle - \left\langle \left\langle \phi_i \mathbf{u}^{up} \{ \mathbf{u} \cdot \mathbf{n}_h \} \right\rangle \right\rangle_{\Gamma_h \cup \Gamma_v} + \left\langle w \mathbf{u} \frac{\partial \phi_i}{\partial z} \right\rangle \\ &\quad - \left\langle \left\langle \phi_i \{ w \} \mathbf{u}^{up} n_z \right\rangle \right\rangle_{\Gamma_h} - \left\langle \phi_i \mathbf{f} \times \mathbf{u} \right\rangle - \left\langle \phi_i \mathbf{q} \right\rangle + \text{Diffusion} \end{aligned}$$

The diffusive terms have not been developed for more clarity.

With $i = 1, \dots, n$, with n being the number of discontinuous nodes, the vertical velocity equation becomes

$$-\left\langle \frac{\partial \phi_i}{\partial z} w \right\rangle + \left\langle \left\langle \phi_i \{ w \} n_z \right\rangle \right\rangle_{\Gamma_h} = \left\langle \mathbf{u} \cdot \nabla_h \phi_i \right\rangle - \left\langle \left\langle \phi_i \{ \mathbf{u} \cdot \mathbf{n}_h \} \right\rangle \right\rangle_{\Gamma_h \cup \Gamma_v} \quad (3.24)$$

The weak formulation of the temperature, the salinity or a scalar field equation is derived analogously. For more clarity, the development are shown only for the temperature equation.

$$\begin{aligned} \left\langle \phi_i \frac{\partial T}{\partial t} \right\rangle &= \left\langle \mathbf{u} T \cdot \nabla_h \phi_i \right\rangle - \left\langle \left\langle \phi_i T^{up} \{ \mathbf{u} \cdot \mathbf{n}_h \} \right\rangle \right\rangle_{\Gamma_h \cup \Gamma_v} \\ &\quad + \left\langle w T \frac{\partial \phi_i}{\partial z} \right\rangle - \left\langle \left\langle \phi_i \{ w \} T^{up} n_z \right\rangle \right\rangle_{\Gamma_h} + \text{Diffusion} \end{aligned} \quad (3.25)$$

Unlike the previous horizontal velocities, H is a 2D variables. Therefore, the function space is 2D. In the interface integrals, stabilisation terms are added by means of the Lax-Friedrichs approximated solver. With $i = 1, \dots, n$, it gives

$$\left\langle \phi_i \frac{\partial H}{\partial t} \right\rangle = \left\langle \mathbf{U} \cdot \nabla_h \phi_i \right\rangle - \left\langle \left\langle \phi_i \mathbf{U}^* \cdot \mathbf{n}_h \right\rangle \right\rangle \quad (3.26a)$$

with

$$\mathbf{U}^* = \frac{(\mathbf{U}_{left} + \mathbf{U}_{right}) \cdot \mathbf{n}_h}{2} - c \frac{(H_{left} - h_{left}) - (H_{right} - h_{right})}{2}$$

$$c = \max \left(\sqrt{gH_{left}} + \left\| \frac{\mathbf{U}_{n,left}}{H_{left}} \right\|, \sqrt{gH_{right}} + \left\| \frac{\mathbf{U}_{n,right}}{H_{right}} \right\| \right)$$

3.3.3 3D and 2D link

In the weak form of the all previous equations, the integrals are made on the elements of the mesh. Three-dimensional volume terms are integrated on prisms, Ω , while the two-dimensional ones on triangles, Ω_{2D} . The 3D interfaces terms are either integrated on horizontal triangles, Γ_h , or vertical squads, Γ_h , while 2D ones on edges, Γ_{2D} . For ease of computation, all these integrals are done on parent elements denoted by $\hat{\Omega}$ or $\hat{\Gamma}$. The parent triangle is the unit triangle of area 0.5 while the parent vertical and horizontal edge are segments of length 2. These spatial transformations introduce new coefficients : A the area of the 2D horizontal extruded triangles, $h = h(x, y)$ the vertical height of each prisms and l the length of the edges of the mentioned triangles. By taking $h\mathbf{u}$ as the advection field instead of $\mathbf{u}$ for the vertical velocity in the weak form, it can be shown that the vertical integrals of the 3D terms become the terms with 2D velocity by using numerical integrals. The vertical sum of the 3D volume terms becomes

$$\begin{aligned} \sum_z \left\langle h\mathbf{u} \cdot \nabla_h \phi_i \right\rangle_{\Omega} &= \sum_z \left\langle 2A \left(\frac{h}{2} \mathbf{u} \right) \cdot \nabla_h \phi_i \right\rangle_{\hat{\Omega}} \\ &= \sum_z \sum_p \left(2A \left(\sum_q \left(\frac{h}{2} \mathbf{u} \right)_q \phi_{q,xy} \phi_{q,z} \right) \cdot \nabla_h \phi_i \right)_{\hat{\Omega},p} \\ &= \sum_p \left(2A \left(\sum_q (H\bar{\mathbf{u}})_q \phi_{q,xy} \right) \cdot \nabla_h \phi_{i,xy} \right)_{\hat{\Omega}_{2D},p} \\ &= \left\langle 2A (H\bar{\mathbf{u}}) \cdot \nabla \phi_{i,xy} \right\rangle_{\hat{\Omega}_{2D}} \\ &= \left\langle \mathbf{U} \cdot \nabla \phi_{i,xy} \right\rangle_{\Omega_{2D}} \end{aligned}$$

The vertical sum of the 3D vertical squad interface terms becomes

$$\begin{aligned}
\sum_z \left\langle \left\langle \{h \mathbf{u} \cdot \mathbf{n}_h\} \phi_i \right\rangle \right\rangle_{\Gamma_v} &= \sum_z \left\langle \left\langle \frac{l}{2} \left\{ \frac{h}{2} \mathbf{u} \cdot \mathbf{n}_h \right\} \phi_i \right\rangle \right\rangle_{\hat{\Gamma}_v} \\
&= \sum_z \sum_p \left(\frac{l}{2} \left\{ \sum_q ((H \bar{\mathbf{u}})_q \phi_{q,xy} \phi_{q,z}) \cdot \mathbf{n}_h \right\} \phi_i \right)_{\hat{\Gamma}_{2D,v}} \\
&= \sum_p \left(\frac{l}{2} \left\{ \sum_q ((H \bar{\mathbf{u}})_q \phi_{q,xy}) \cdot \mathbf{n}_h \right\} \phi_{i,xy} \right)_{\hat{\Gamma}_{2D,v}} \\
&= \left\langle \left\langle \frac{l}{2} \{H \bar{\mathbf{u}} \cdot \mathbf{n}_h\} \phi_{i,xy} \right\rangle \right\rangle_{\hat{\Gamma}_{2D,v}} \\
&= \left\langle \left\langle \{\mathbf{U} \cdot \mathbf{n}_h\} \phi_{i,xy} \right\rangle \right\rangle_{\Gamma_{2D,v}}
\end{aligned}$$

In the interface integrals, 3D stabilisation terms are added to match the Riemann solvers in the 2D equation.

3.3.4 Temporal integration and ALE formulation

For the temporal scheme, a split explicit second order Runge-Kutta method is used. It consists of a RK3 for the 3D part of the velocity equation and a RK2 for the 2D one. The two temporal schemes are those described in Section 3.2 with time steps Δt and ΔT respectively. The ratio, M , between the two time steps is the closest integer to the ratio of the highest propagation speed in the external mode to the highest speed of the external gravity waves. The variable y corresponds the horizontal velocity $\mathbf{u}$, the vertical coordinates represented by the vertical height of each prisms h , the temperature T and the salinity S while Y corresponds to horizontal total transport $\mathbf{U}$ and the water height H . All the other variables $\mathbf{w}$, $\mathbf{q}$, ρ' and η , can be obtained at any time from these primary variables. The finite element method introduces mass matrices. M^n is the global mass matrix at the time n . Therefore, to apply these two temporal schemes to our problem, one must take into account the change of the mass matrix through time in the algorithm. An arbitraty Lagrangian-Eulerian scheme is introduced to take into account the vertical displacement of the mesh. As the three-dimensional mesh follows the movement of the free surface, only the vertical coordinates move with time (e.g. [Clare et al. \(2022\)](#); [Pan et al. \(2019\)](#)).

A complete iteration of the three-dimensional hydrostatic equations is shown in Algorithm 3. First, $\mathbf{u}$ and h are used to obtain the 2D variables, $\mathbf{U}$ and H , at the beginning of the time step. Each external mode sub-iteration are done following the same process. For each sub-time step i , the horizontal terms

of the three-dimensional discretized velocity equations, $\mathbf{f}^{\text{hor}}$, is obtained. The friction terms are also computed in this term. This 3D residue is integrated over the water columns to obtained the 2D term $\mathbf{F}^{\text{hor}}$. The vertical terms without the friction terms can be omitted because their vertical integrals are zero. The two-dimensional variables are moved to the right sub-time using $\mathbf{F}^{\text{hor}}$. Throughout the iterations, the sum of all the residues of the 2D velocity equation multiplied by the small time step, $\mathbf{F}^{\text{fast}} = \sum_{j=1}^i \Delta T \mathbf{F}_{\mathbf{U}}$, is obtained. The new vertical height is known at the end of the internal sub-iteration. Therefore, the position of the mesh can be updated. Finally, the horizontal velocity is obtained by computing the vertical terms of three-dimensional velocity equations, $\mathbf{f}^{\text{ver}}$, taking into consideration the horizontal and the 2D terms.

$$M_{3d}\mathbf{u} - M_{3d}^0\mathbf{u}^0 = \frac{i\Delta t}{M}(\mathbf{f}^{\text{hor}} + \mathbf{f}^{\text{ver}}) + \frac{1}{2} \frac{h}{H} \mathbf{F}^{\text{fast}}$$

Algorithm 3: SPEX-RK iteration for the hydrodynamic equations,
 $m = M/6$

Data: Model state variable $\mathbf{u}, z$
 $\mathbf{U}, H \leftarrow \sum_z \frac{h}{2} \mathbf{u}, \sum_z \frac{h}{2}$
 $\mathbf{u}_0, h_0 \leftarrow \mathbf{u}, h$
 $\mathbf{U}_0, H_0 \leftarrow \mathbf{U}, H$
for $i=2m, 3m, 6m$ **do**
 $\mathbf{f}^{\text{hor}} \leftarrow f_{3d}^{\text{hor}}(\mathbf{u}, z)$
 $\mathbf{F}^{\text{hor}} \leftarrow \sum_z \mathbf{f}^{\text{hor}}$
 $\mathbf{U}, H \leftarrow \mathbf{U}_0, H_0$
 $\mathbf{F}^{\text{fast}} \leftarrow 0$
 for $j=1, \dots, i$ **do**
 $\mathbf{F}_{\mathbf{U}}, F_H \leftarrow F_{2d}(\mathbf{U}, H)$
 $\mathbf{F}_{\mathbf{U}}, F_H \leftarrow F_{2d}(\mathbf{U} + \frac{\Delta T}{2} M_{2d}^{-1}(\mathbf{F}_{\mathbf{U}} + \mathbf{F}^{\text{hor}}), H + \frac{\Delta T}{2} M_{2d}^{-1} F_H)$
 $\mathbf{U} \leftarrow \mathbf{U} + \Delta T M_{2d}^{-1}(\mathbf{F}_{\mathbf{U}} + \mathbf{F}^{\text{hor}})$
 $H \leftarrow H + \Delta T M_{2d}^{-1} F_H$
 $\mathbf{F}^{\text{fast}} \leftarrow \mathbf{F}^{\text{fast}} + \Delta T \mathbf{F}_{\mathbf{U}}$
 end
 Update the z coordinates based on H
 $\mathbf{u} \leftarrow M_{3d}^{-1} \left(M_{3d}^0 \mathbf{u}_0 + \frac{i\Delta t}{M} (\mathbf{f}^{\text{hor}} + \mathbf{f}^{\text{ver}}) + \frac{1}{2} \frac{h}{H} \mathbf{F}^{\text{fast}} \right)$
end

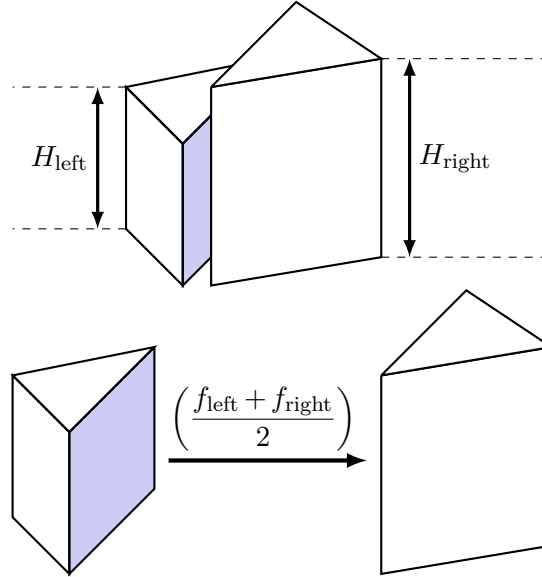


Fig. 3.4: Flux between two prisms in a discontinued mesh with 1 layer

3.3.5 Conservation and Consistency

In order to be coherent with the basic physics of hydrodynamic flows, the temporal scheme and the spatial discretisations must respect two main properties. The first one concerns tracer concentration through the domain and the second one the conservation of the amount of water and tracer. The general idea behind tracer consistency is that if the tracer concentration is uniform over the domain, then it should remain uniform at all time. The conservation states that the volume of water and tracer must remain constant in a domain isolated from its environment. To respect the tracer conservation and consistency, the temporal scheme as well as the discretisation of the method has to be chosen in a proper way. [White et al. \(2007\)](#) explains it for a different scheme.

3.3.5.1 Water conservation

All the discretised variables in the presented equations are discontinuous. The hydrodynamic velocities, the tracer concentration and especially the elevation have multiple values for the same points. The latter leads to a discontinued mesh. Two adjacent prisms have slightly discontinuous vertical coordinates. To ensure the water and tracer conservation, the focus is put on the fluxes [Berger and Howington \(2002\)](#). Unique fluxes are computed as the mean between the flux evaluated on the left and right prisms (see Figure 3.4).

The fluxes problems fixed, the water conservation still has to be demonstrated. The water height Equation 3.26a is analysed in a closed domain. The equation is summed up for each $i \in [0, m]$, m being the number of discontinuous nodes.

$$\sum_{i=1}^m \left\langle \phi_i \frac{\partial H}{\partial t} \right\rangle = \sum_{i=1}^m \left\langle \mathbf{U} \cdot \nabla_h \phi_i \right\rangle \quad (3.27)$$

$$+ \sum_{i=1}^m \left\langle \left\langle \phi_i \left(\frac{\mathbf{U}_{n,left} + \mathbf{U}_{n,right}}{2} - c \frac{H_{left} + H_{right}}{2} \right) \right\rangle \right\rangle \quad (3.28)$$

The sum and the integrals permute. By remembering that by definition the sum of ϕ_i and $\nabla \phi_i$ equals respectively to 1 and 0, the previous equation becomes

$$\left\langle \frac{\partial H}{\partial t} \right\rangle = \left\langle \left\langle \left(\frac{\mathbf{U}_{n,left} + \mathbf{U}_{n,right}}{2} - c \frac{H_{left} + H_{right}}{2} \right) \right\rangle \right\rangle \quad (3.29)$$

For each edge that is not at the boundary of the domain, the flux receives by the left element is the same as the flux gives by the right one. The normal vector of the two prisms are opposite. The sum of all the fluxes inside the domain is 0. At the boundaries, all the fluxes are zero because the domain is closed. The equation finally becomes

$$\left\langle \frac{\partial H}{\partial t} \right\rangle = 0 \quad (3.30)$$

This proves the water conservation.

3.3.5.2 Surface impermeability

In this section, the demonstration is done for one big time step using Δt but it stays valid for each sub-time step. To numerically ensure the conservation and the consistency of the tracer, the surface impermeability condition of continuity Equation 3.24 must be respected as stated in [Deleersnijder \(1993\)](#); [Campin et al. \(2004\)](#); [Deleersnijder and Campin \(1995\)](#). To achieve that, the following equation is used to compute the mesh velocity w_m . For each $i \in [0, m]$, m being the number of discontinuous nodes, it gives

$$\frac{\left\langle \phi_i \right\rangle^{n+1} - \left\langle \phi_i \right\rangle^n}{\Delta t} = - \left\langle w_m \frac{\partial \phi_i}{\partial z} \right\rangle^n + \left\langle \left\langle w_m^d \phi_i n_z \right\rangle \right\rangle_{\Gamma_h}^n \quad (3.31)$$

By summing only the vertical part of the ϕ_i , this equation can be simplified. The left-hand side (LHS) equals the integral of the difference of the water height between two 3D time step. In the right-hand side (RHS), only the fluxes through the horizontal interfaces remain.

Using the same reasoning as that for the water conservation, the sum of all the fluxes inside the domain is 0. The flux through the bottom boundaries is zero. Only the flux at the surface boundary remains. By removing n_z , the integral can be projected onto a flat 2D mesh. Equation 3.31 becomes

$$\left\langle \frac{\Delta H}{\Delta t} \phi_{j,xy} \right\rangle^n = \left\langle \left\langle w_m \phi_{j,xy} n_z \right\rangle \right\rangle_{\Gamma_s}^n \quad (3.32)$$

$$= \left\langle w_m \phi_{j,xy} \right\rangle_{\Gamma_s, 2D}^n \quad (3.33)$$

This shows that w_m at the surface matches the temporal evolution of the sea surface elevation between two 3D time steps. Thanks to the P_1^{DG} discretisation, this equality is satisfied for each node i at machine precision.

By analysing the equation of w , recalled below, the impermeability of the surface can now be demonstrated:

$$-\left\langle w \frac{\partial \phi_i}{\partial z} \right\rangle^n + \left\langle \left\langle \{w\} \phi_i n_z \right\rangle \right\rangle_{\Gamma_h}^n = \left\langle \mathbf{u} \cdot \nabla \phi_i \right\rangle^n - \left\langle \left\langle \{\mathbf{u} \cdot \mathbf{n}_h\} \phi_i \right\rangle \right\rangle_{\Gamma_h \cup \Gamma_v}^n$$

Applying the same reasoning as for the previous equations, the equation of the vertical velocity recalled above yields

$$\begin{aligned} \left\langle \left\langle w \phi_{j,xy} n_z \right\rangle \right\rangle_{\Gamma_s}^n + \left\langle \left\langle \{\mathbf{u} \cdot \mathbf{n}_h\} \phi_{j,xy} \right\rangle \right\rangle_{\Gamma_s}^n &= \left\langle H \mathbf{u} \cdot \nabla \phi_{j,xy} \right\rangle^n \\ &\quad - \left\langle \left\langle \{H \mathbf{u} \cdot \mathbf{n}_h\} \phi_{j,xy} \right\rangle \right\rangle_{\Gamma_v}^n \end{aligned} \quad (3.34)$$

The RHS of the previous equation is actually the RHS of the discretised water height equation (Equation 3.26a). As the equation of H is linear in the discrete field $\mathbf{U} = H \bar{\mathbf{u}}$,

$$\frac{\partial H}{\partial t} = -\nabla_h \cdot \mathbf{U},$$

by using the temporal mean of $\mathbf{U}$ over all the 2D small time steps in $\mathbf{u}$, $\mathbf{U}_{\text{mean}}$, this gives

$$\left\langle \left\langle w \phi_{j,xy} n_z \right\rangle \right\rangle_{\Gamma_s}^n + \left\langle \left\langle \mathbf{u} \cdot \mathbf{n}_h \phi_{j,xy} \right\rangle \right\rangle_{\Gamma_s}^n = \left\langle \left\langle \frac{\Delta H}{\Delta t} \phi_{j,xy} \right\rangle \right\rangle_{\Gamma_s}^n \quad (3.35)$$

$$= \left\langle \left\langle w_m \phi_{j,xy} n_z \right\rangle \right\rangle_{\Gamma_s}^n \quad (3.36)$$

By putting all the terms in the LHS and by introducing w_m , it becomes :

$$\left\langle \left\langle w \phi_{j,xy} n_z \right\rangle \right\rangle_{\Gamma_s}^n + \left\langle \left\langle \mathbf{u} \cdot \mathbf{n}_h \phi_{j,xy} \right\rangle \right\rangle_{\Gamma_s}^n - \left\langle \left\langle w_m \phi_{j,xy} n_z \right\rangle \right\rangle_{\Gamma_s}^n = 0 \quad (3.37)$$

This shows that the flux at the surface is zero for the weak formulation. In others words, the impermeability of the surface boundary represented by Equation 3.20b is satisfied by the weak formulation. In practice, to verify the top surface condition, two choices were made. Firstly, the temporally averaged 2D velocity, denoted $\mathbf{U}_{\text{mean}}$, is used in the tracer equation and in the computation of the vertical velocity on each 3D sub-time step. Secondly, in the advection term of the tracer equation, $h_v \mathbf{u}$ and h_v are used instead of $\mathbf{u}$ and the stability 3D terms are added to match the vertical velocity equation. In others words, the velocity field used is

$$h\mathbf{u} = h_{\text{mean}} \bar{\mathbf{u}}_{\text{mean}} + h_n \tilde{\mathbf{u}}_n$$

3.3.5.3 Conservation and Tracer consistency

The tracer equation is analysed to check the tracer conservation in a closed domain. For the sake of clarity, the diffusion terms are omitted but the same reasoning applied. The demonstration is done with one big time step like in the previous section. The tracer equation without the diffusion terms reads

$$\frac{\left\langle T \phi_i \right\rangle^{n+1} - \left\langle T \phi_i \right\rangle^n}{\Delta t} = \left\langle \mathbf{u} T \cdot \nabla \phi_i \right\rangle^n - \left\langle \left\langle T^{up} \{ \mathbf{u} \cdot \mathbf{n}_h \} \phi_i \right\rangle \right\rangle_{(\Gamma_h \cup \Gamma_v) - \Gamma_s}^n \quad (3.38)$$

$$\left\langle (w - w_m) T \frac{\partial \phi_i}{\partial z} \right\rangle^n - \left\langle \left\langle \{ w - w_m \} T^{up} \phi_i n_z \right\rangle \right\rangle_{\Gamma_h - \Gamma_s}^n$$

where the flux at the surface, Γ_s , is removed because it is null as demonstrated above. The fluxes at the vertical boundaries are null. The flux at the bottom is

also null. The Galerkin finite element being a conservative methods, the total tracer quantity is conserved in the domain.

To check the consistency, one should demonstrate that if the tracer concentration is uniform, it remains uniform. By putting the tracer concentration equal to 1 everywhere in the domain at time n and adding the surface flux (which is null), the Equation 3.38 becomes

$$\frac{\langle T\phi_i \rangle^{n+1} - \langle \phi_i \rangle^n}{\Delta t} = \langle \mathbf{u} \cdot \nabla \phi_i \rangle^n - \left\langle \left\langle \{\mathbf{u} \cdot \mathbf{n}_h\} \phi_i \right\rangle \right\rangle_{\Gamma_h \cup \Gamma_v}^n \\ \left\langle \left(w - w_m \right) \frac{\partial \phi_i}{\partial z} \right\rangle^n - \left\langle \left\langle \{w - w_m\} \phi_i n_z \right\rangle \right\rangle_{\Gamma_h}^n$$

The diffusion terms can be omitted because the gradient of an uniform fields is null. Using Equation 3.24, it becomes

$$\frac{\langle T\phi_i \rangle^{n+1} - \langle \phi_i \rangle^n}{\Delta t} = - \left\langle w_m \frac{\partial \phi_i}{\partial z} \right\rangle^n + \left\langle \left\langle \{w_m\} \phi_i n_z \right\rangle \right\rangle_{\Gamma_h}^n$$

By looking at the equation of w_m , the only solution for the concentration of the tracer at time $n + 1$ over the domain is 1.

3.4 Numerical tests and results

The 3D model is assessed by a set of numerical benchmarks. A first barotropic test checks the conservation and the consistency properties. Then, three test cases of increasing complexity demonstrate the precision of the proposed temporal scheme. A lock exchange test case evaluates the numerical mixing of the baroclinic solver in the z -direction. The correct size of the vortices produced by instabilities in a rotating baroclinic benchmark demonstrates the small amount of numerical dispersion introduced by the discrete model. Another more difficult instability test case confirms the presumed order of the global scheme.

3.4.1 Surface gravity waves

To check the conservation and the consistency of our model, the test proposed by Kärnä et al. (2013) is a very good candidate because this test is simple and smooth. It allows the properties to be checked easily. Moreover, the tracer is a passive scalar field.

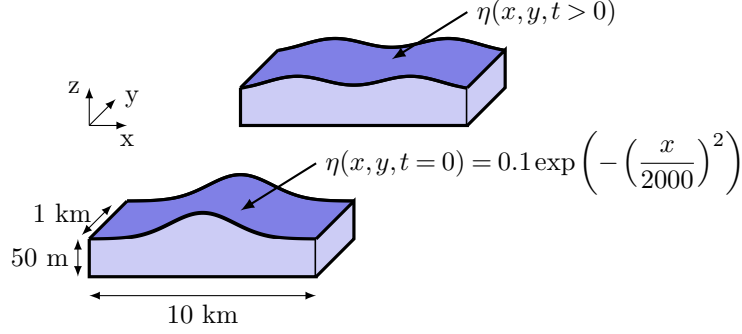


Fig. 3.5: Evolution of the surface gravity waves testcase

The propagation of surface gravity waves in a 10 km long and 1 km wide rectangular domain is considered. The depth is 50 m. All the vertical boundaries are impermeable. Bottom friction and vertical diffusion are omitted. The water density is constant throughout the simulation as illustrated. The free surface perturbation is initially set to the following function :

$$\eta(x, y, 0) = 0.1 \exp\left(-\left(\frac{x}{2000}\right)^2\right)$$

The horizontal and vertical resolution of the grid are 100 m and 2.5 m. The 3D time step is 10s while the 2D one is 0.33s. Simulation is performed with 800 3D time steps in order to reproduce the same result as [Kärnä et al. \(2013\)](#). For a field f and a reference field f^{ref} , the error on the domain Ω is computed with the L_2 norm as follows :

$$E = \|f - f^{ref}\|_{L_2} = \sqrt{\int_{\Omega} (f - f^{ref})^2 d\Omega}$$

In the first run, the tracer is set at an initial constant value $T_0 = 4$ PSU. Then, the simulation is launched with a non-constant tracer. It is set to 3 PSU at the surface and 4 PSU at the bottom with a linear transition. In both case, the tracer extrema deviation is of the order of 10^{-9} . This shows the consistency of the scheme. Regarding the conservation, the total water and tracer volume remains the same at the order of 10^{-13} .

A convergence analysis of the temporal scheme is performed using a constant tracer. The horizontal resolution is 140 m with 5 layers in the z-direction. The simulation is running for 1600 s with the following set of Δt : [16, 8, 4, 3.2, 2, 0.16] s and $M=18$. The solution obtained with the smallest time resolution is used as a reference. The theoretical second order convergence is observed in [Figure 3.6](#).

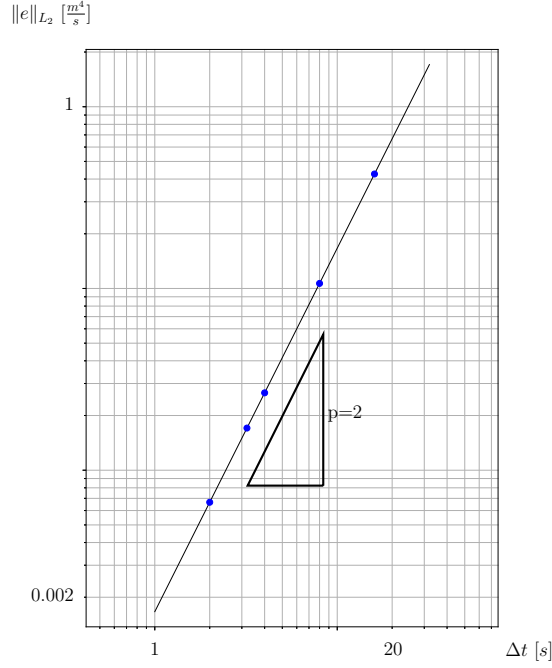


Fig. 3.6: Convergence analysis of the L_2 error on u in the surface gravity wave test case. The reference time step is 0.16 s. Tested time steps are 16, 8, 4 and 3.2 s.

3.4.2 Lock Exchange

The lock exchange test case is used to estimate the model spurious numerical vertical diffusion in a simple configuration where the solution is not too complex.

Initially, one half of the domain is filled with cold water ($T = 5^\circ\text{C}$) while the other half is filled with hot water ($T = 30^\circ$). The test case is a density driven flow. Warm water flows over the cold water. This is the setup of [Ilicak et al. \(2012\)](#) and [Petersen et al. \(2015\)](#). The domain is a 1 km wide and 64 km long box. The depth is 20 m. Closed boundaries conditions are imposed in the x-direction while the domain is periodic in the y-direction. The density is a function of the temperature only, so that Equation 3.17 becomes

$$\rho = 1000 - 0.2(T - 5)$$

resulting in a density difference of $\Delta\rho = -5.0 \text{ kg m}^{-3}$. The friction at the bottom of the domain is omitted. Tracer diffusion is set to 0. In the absence of bottom friction, assuming that all the potential energy is transformed into kinetic energy, Benjamin (1968) estimated the maximum speed of front propagation, using Bernoulli's equation for an ideal fluid, as

$$c = \frac{1}{2} \sqrt{gH \frac{\Delta\rho}{\rho_0}}$$

which is 0.495 ms^{-1} in this situation.

The mesh Reynolds numbers is defined by

$$Re_h = U \frac{\Delta x}{\nu_h}$$

where the characteristic velocity scale is $U = 0.5 \text{ ms}^{-1}$ and the grid horizontal and vertical resolution are 0.5 km and 1 m. The numerical instabilities due to internal pressure gradient are stabilized with a constant horizontal viscosity ν_h . Three runs are performed with $\nu_h = 1.0 \text{ m}^2\text{s}^{-1}$, $10.0 \text{ m}^2\text{s}^{-1}$, and $100.0 \text{ m}^2\text{s}^{-1}$, corresponding respectively to $Re_h = U \frac{\Delta x}{\nu_h}$, of 250, 25, 2.5 .

Figure 3.7 shows the initial deviation density field and the solution after 17h. Smaller mesh Reynolds number, i. e. higher horizontal viscosity, leads to a less noisy density front. The smooth interface between the dense and the light water produces less mixing. This speed gives a right front location at 62.3 km at 17h of simulation. For $\nu_h = 100 \text{ m}^2\text{s}^{-1}$, $10 \text{ m}^2\text{s}^{-1}$ and $1 \text{ m}^2\text{s}^{-1}$, the front is at 61 km, 60.75 km and 60.5 km respectively. When the interface became noisy, this means that a part of the potential energy is wasted in the noise. Therefore, the speed of front propagation is reduced. This explains the front locations. As show in Figure 3.7, those results are similar to those presented in Kärnä et al. (2018), Petersen et al. (2015) and Ilicak et al. (2012). Without the complications of topography, Coriolis force, bottom drag and surface forcing, and providing a sufficiently large horizontal viscosity is used, the model exhibits an admissible vertical mixing.

3.4.3 Baroclinic eddies

The baroclinic eddies test case of Ilicak et al. (2012) is used to check the model's ability to generate baroclinic eddies as well as its precision. Generating eddies of an appropriate size means that the temporal scheme of the model does not produce too much dissipation. Compared to the previous case, a fully 3D rotating flow is introduced.

This test represents an idealisation of the Antarctic Circumpolar Current. An unstable sinusoidal front separates cold water from hot water. Vortices develop at the front in function of the horizontal viscosity. The Coriolis parameter

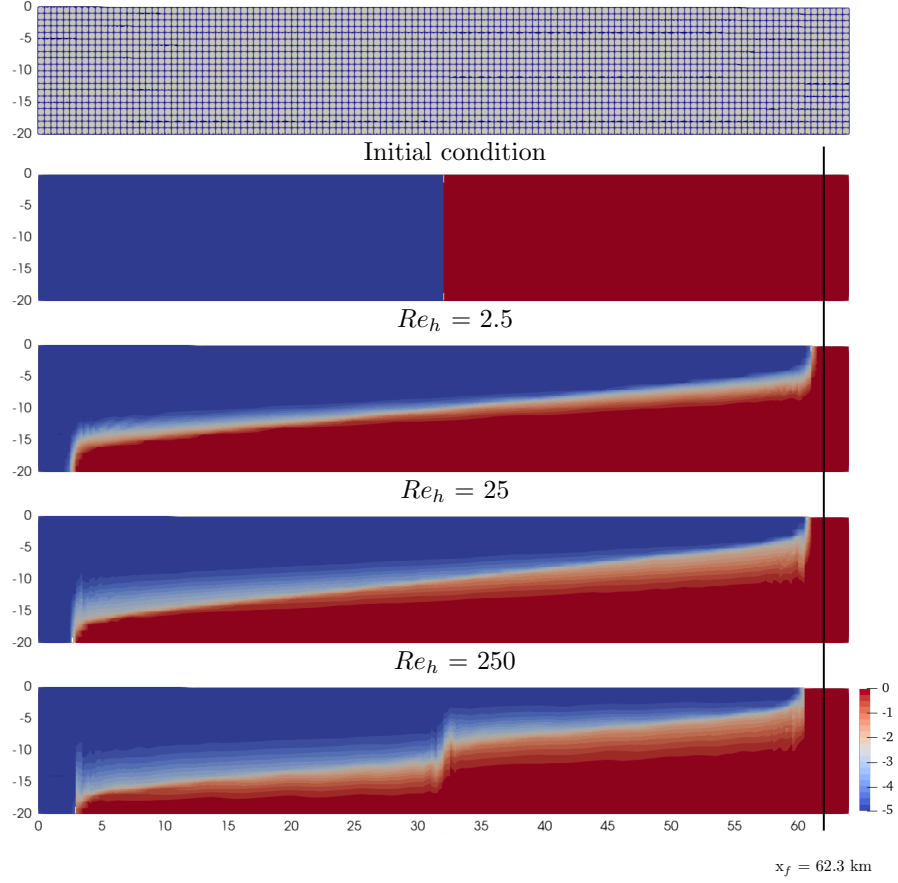


Fig. 3.7: Water deviation density, ρ' [kg/m^3], in the lock exchange test case for Z-X plane. At the top, we have the vertical mesh from the horizontal extruded mesh and the initial condition. We have successively the solution after 17h of simulation with respectively Re_h and ν_h : 2.5 - 100 m^2s^{-1} , 25 - 10 m^2s^{-1} , 250 - 1 m^2s^{-1} . The vertical line shows the theoretical position of the front

is taken as a constant $-1.2 \times 10^{-4} s^{-1}$. The domain is a three dimensional box, 500 km long delimited by impermeable boundaries in the meridional direction (y) and 160 km large with periodic boundaries in the zonal (x) direction. The depth is 1000 m. The quadratic bottom drag is defined :

$$\frac{\tau_b}{\rho_0} = C_d |\mathbf{u}_b| \mathbf{u}_b$$

where $\mathbf{u}_b$ is the horizontal velocity of the bottom element taken at the middle

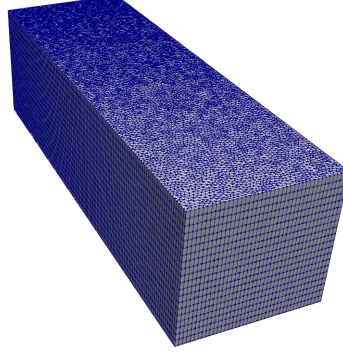


Fig. 3.8: Mesh of the computational domain of dimension 500 km x 150 km x 1 km. Number of 2D elements is 13686. Number of layers is 20.

point and C_d is 0.01. The density function is the same as in the previous test case. Salinity and vertical viscosity are again set at the same constant value.

The mesh is shown in Figure 3.8 to illustrate the domain. The simulation is performed in horizontal grid resolution of 4 km and the horizontal viscosity from $20 \text{ m}^2\text{s}^{-1}$ to $200 \text{ m}^2\text{s}^{-1}$. The characteristic speed being 0.1 ms^{-1} , this gives a mesh Reynolds numbers respectively from 20 to 2. The vertical resolution of the grid is 50 m.

The initial temperature field can be seen in Figure 3.9. Warmer surface temperature in the north is separated from colder surface temperature in the south by a sinusoidal transition band in the x-y plane. The temperature distribution in the north of the domain is a linear increasing function from the bottom :

$$T_0(z) = T_{bot} + (T_{top} - T_{bot}) \frac{z_{bot} - z}{z_{bot}} \quad (3.39)$$

where $T_{bot} = 10.1^\circ\text{C}$, $T_{top} = 13.1^\circ\text{C}$, and $z_{bot} = -975 \text{ m}$. The south part of the domain is uniformly cooler at $\Delta T = 1.2^\circ\text{C}$. The wide boundary is defined by

$$y_w(x) = y_0 - y_A \sin\left(2\pi k \frac{x}{L_x}\right) \quad (3.40)$$

where $y_0 = 250 \text{ km}$, $y_A = 40 \text{ km}$, $k = 3$ and $L_x = 160 \text{ km}$ so that there is three wavelengths of width L_x in a domain. This gives the following temperature distribution

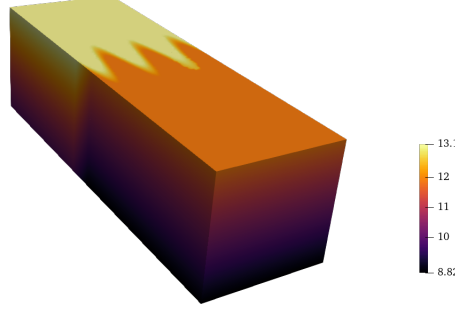


Fig. 3.9: Initial sea temperature field [$^{\circ}\text{C}$] in the eddy channel test case

$$T(x, y, z) = \begin{cases} T_0(z) & y_w(x) + \Delta y \leq y \\ T_0(z) - \Delta T \left(1 - \frac{y - y_w(x)}{\Delta y}\right) & y_w < y \leq y_w(x) + \Delta y \\ T_0(z) - \Delta T & y \leq y_w(x) \end{cases} \quad (3.41)$$

where $\Delta y = 40$ km and $\Delta T = 1.3^{\circ}\text{C}$. An additional perturbation is added to one of the wave crest to stimulate the instability

$$y'_w(x) = y_0 - \frac{y_A}{2} \sin\left(\pi \frac{x - x_2}{x_3 - x_2}\right) \quad (3.42)$$

$$T'(x, y) = \Delta T' \left(1 - \frac{y - y'_w(x)}{0.5\Delta y}\right) \quad (3.43)$$

that way the temperature is $T + T'$ within the range $x_2 \leq x \leq x_3$, $y'_w - \frac{\Delta y}{2} \leq y \leq y'_w + \frac{\Delta y}{2}$, where $x_2 = 110$ km, $x_3 = 130$ km and $\Delta T' = 0.3^{\circ}\text{C}$.

Figure 3.10 and Figure 3.11 show the evolution of the sea surface temperature for two different horizontal viscosities : $20 \text{ m}^2\text{s}^{-1}$ and $200 \text{ m}^2\text{s}^{-1}$. For the high viscosity numbers, the hot and the cold water tend to mix slowly. The velocity field has small values. This generates only a few eddies though these eddies are large and smooth. As time goes by, they dissipate quickly. At day 200, the eddies are less dense. For simulations with low viscosity numbers or bigger Re_h , the flow is much more chaotic and energetic. The eddies appear sooner than the previous ones but are globally smaller. Moreover, as time progresses, the mixing becomes more important. At day 200, for $\nu_h = 200 \text{ m}^2\text{s}^{-1}$ two areas can still be distinguished while, for $\nu_h = 20 \text{ m}^2\text{s}^{-1}$, the flow tends to be more homogeneous. These results show that our temporal scheme succeeds

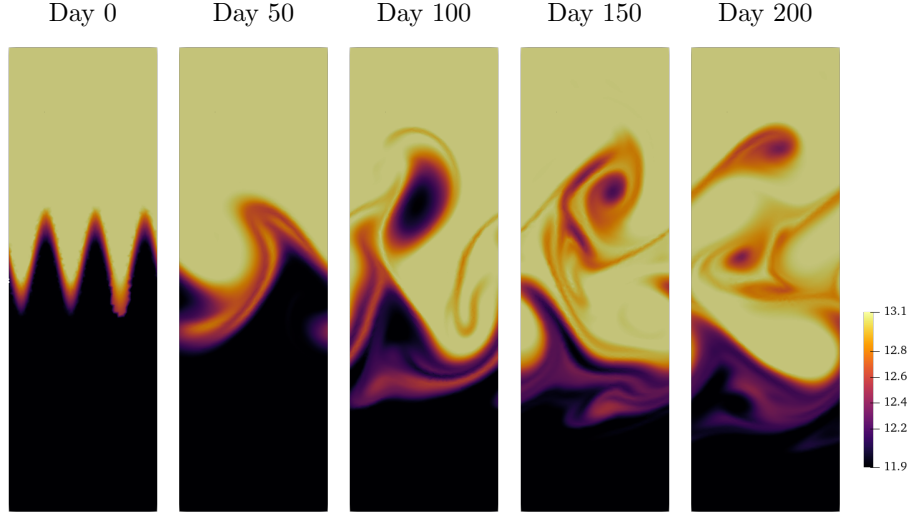


Fig. 3.10: Sea surface temperature field [°C] in the eddy channel test case for respectively $Re_h=2$ and $\nu_h=200 \text{ m}^2\text{s}^{-1}$

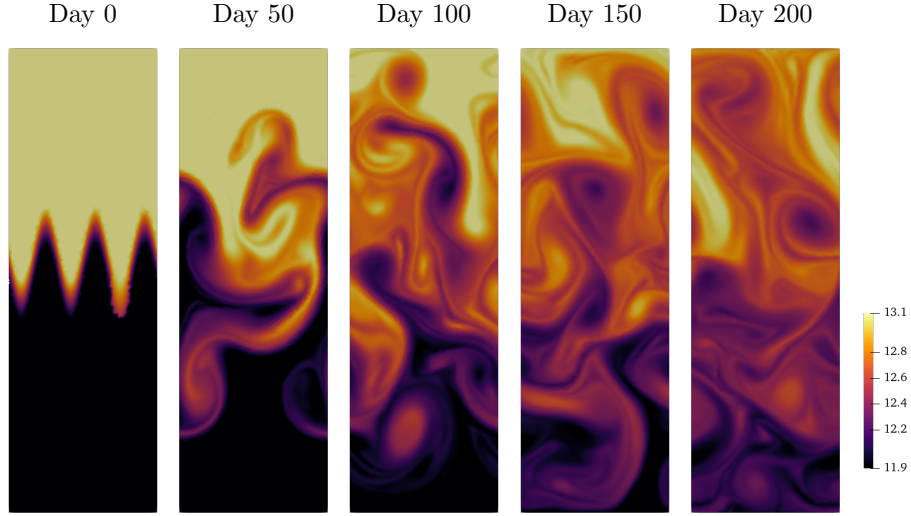


Fig. 3.11: Sea surface temperature field [°C] in the eddy channel test case for respectively $Re_h=20$ and $\nu_h=20 \text{ m}^2\text{s}^{-1}$

in capturing more mesoscale features as viscosity is decreased while rotation is taken into account.

A convergence analysis of the temporal scheme is performed with $\nu_h = 20$

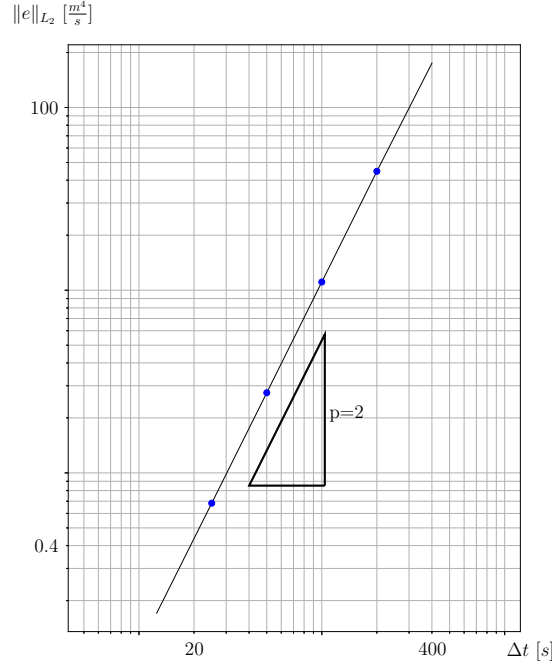


Fig. 3.12: Convergence analysis of the L_2 error on u in the eddies test case. The reference time step is 1.25 s. Tested time steps are 200, 100, 50 and 25 s.

m^2s^{-1} . The horizontal resolution is 20 km with 10 layers in the z -direction. The simulation is running for 2000 s with the following set of Δt : [200, 100, 50, 25, 1.25] s and $M=138$. The solution obtained with the smallest time resolution is used as a reference. In the model, the vertical terms are treated implicitly in the temporal scheme. All terms, including the vertical terms, are treated explicitly in this convergence analysis. The theoretical second order convergence is observed in Figure 3.12.

3.4.4 Eddies in a rotating stratified fluid

The last studied test case shows the ability of the model to handle the geostrophic adjustment of a freshwater cylinder and the development of unstable vortices. By having the right amount of unstable lobes, the order 2 of the temporal scheme can be confirmed. The setup is based on the experiments of [Griffiths and Linden \(1981\)](#) and [Saunders \(1973\)](#) which were numerically modelled by

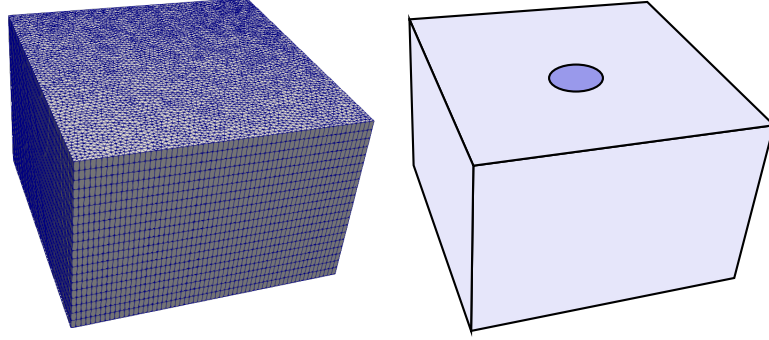


Fig. 3.13: [Left] Mesh of the computational domain of the vortices test case of dimension 30 km x 30 km x 20 m. Number of 2D elements is 5602. Number of layers is 20. [Right] Initial sea salinity field. The lower salinity is inside a 3 km radius and 10 m depth cylinder

James (1996) and Tartinville et al. (1998) neglecting all forms of mixing.

The represented area is supposed to be located at 52°N and hence the Coriolis parameter is $1.15 \times 10^{-4} \text{ s}^{-1}$. The domain is a box of salty water with a 30 km length for both the x-coordinates and the y-coordinates and a depth of 20 m. All the boundaries are closed. A cylinder of less salty water is put at the center of the top. As time goes by, the light cylindrical core sinks and spread out until it reaches a state of quasi-geostrophic equilibrium. The vortex can either remain stable and circular or either break up into a well-defined number of vortices depending on the initial parameters of the model.

Unlike the previous test case, the temperature field is set to a constant value while the salinity field represents a 10 m deep, 3 km radius cylinder of concentrated water in the upper part of the box. More precisely, inside the cylinder, the salinity is

$$S = 1.1 \left(\frac{d}{3} \right)^8 + 33.75 \quad (3.44)$$

with d the distance to the centre of the domain in km. Outside the cylinder, the ambient salinity is 34.85 PSU. The density is, in this case, only influenced by the water salinity which gives $\rho' = 0.78(S - 33.75)$. To use the same parameters as the previous articles focusing on this test case, ρ_0 is changed into 1025 kg m^{-3} . This gives an initial density difference of 0.858 kg m^{-3} between the most concentrated areas and the less ones. Horizontal and vertical viscosity and diffusivity are set to zero. Figure 3.13 displays the initial situation as well as the 3D mesh. the grid horizontal and vertical size are 0.5 km and 1 m.

The parameters determining the number of vortices can be reduced to a dimensionless number $\theta_0 = g' \frac{H_0}{f^2 R_0^2}$ which represents the ratio between the buoyancy force and the Coriolis force with $g' = g \frac{\Delta \rho}{\rho}$, the reduced gravity, H_0 , the initial depth of the cylinder and R_0 , the initial radius of the cylinder. The number of vortices called the zonal wavenumber of the instability also depends of these parameters. For this test case, [James \(1996\)](#) found out that the simulation should give a wavenumber 2 instability. [Tartinville et al. \(1998\)](#) have shown most of the models can give the expected spreading of the cylinder and the development of, respectively, anticyclonic circulation in the upper layer and cyclonic one in the lower layer of the domain. However, they have also demonstrated that models with no adequate advection schemes do not succeed in reproducing the 2 wavenumber instability after 144 hours of simulation. they suggested that models with only first-order horizontal advection scheme for momentum failed because the numerical viscosity should induce a too strong decrease of the kinetic energy. To be more precise, they said that the numerical modelling of low-diffusion marine systems where frontal instability processes are important requires the use of at least a second-order discretisation for the advection of momentum. Therefore, an order-four instability is created instead of an order-two one. This test case is not shown a lot because it is quite difficult to obtain the right number of vortices.

Figure 3.14 shows the evolution of the cylinder through time. The most important result is that the model and the numerical schemes presented in this article achieved to predict a wavenumber 2 instability. As expected after 144 hours, the cylinder breaks up and two vortices are appearing as time goes. Then, cyclonic vorticity appear in each lobe of the disturbance. As the lobes grow, closed cyclonic circulation is being established. These results match the experiments and the conclusions of [Griffiths and Linden \(1981\)](#). As the diffusivity is computed the same way than the viscosity, this demonstrates that the model does not produce an excessive amount of numerical viscosity and diffusivity.

3.5 Conclusion

This paper focuses on three-dimensional hydrostatic equations under the Boussinesq approximation with a specific emphasis on two different timescales. The hydrodynamic equations considered have a wave propagation speed that is greater than the advection speed, so it is important to choose an appropriate time scheme. A combined RK3 and RK2 scheme is used, and the equations are decomposed into fast and slow terms to allow for spatial discretization using discontinuous Galerkin methods on an unstructured grid. This approach offers several advantages, including easy parallelization for large scale or high resolution applications.

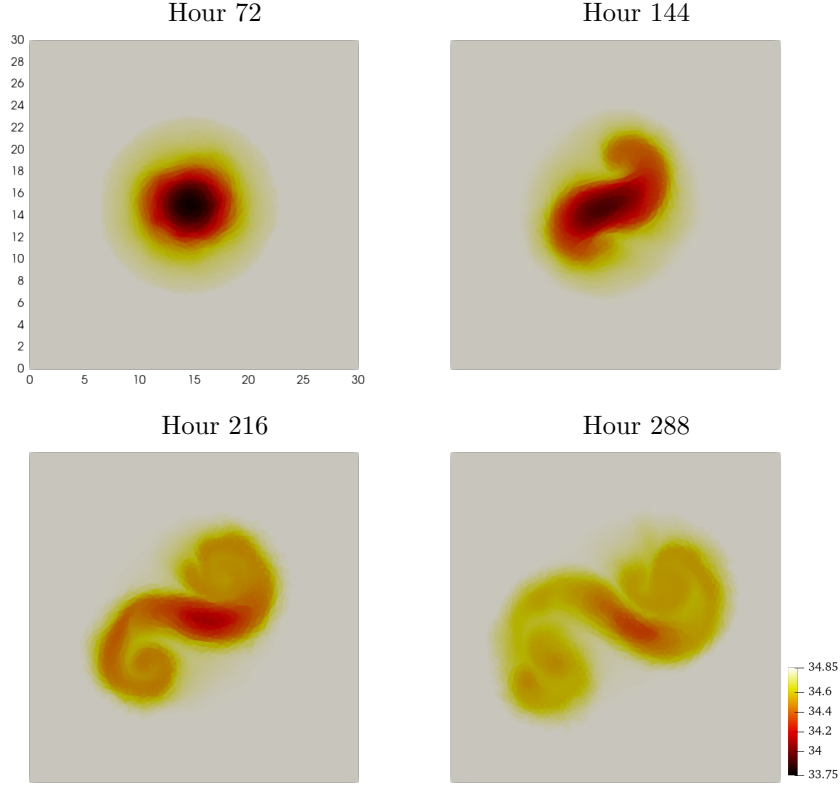


Fig. 3.14: Sea surface salinity field [psu] in the vortices test case during 288 hours

The goal of this approach is to limit numerical dissipation due to spatial and temporal discretization. The scheme is designed to be of order two temporally and spatially and completely discontinuous. This enables the vertical mesh to follow the displacement of the water surface, thereby maintaining the conservation of tracer and water fields throughout the simulations. The tracer is consistent due to the advection velocity field used, which is coherent with the vertical motion of the mesh. A mathematical demonstration has been performed to verify the order and stability of the scheme, demonstrating its effectiveness in accurately simulating hydrodynamic behavior.

To test the model, a gravitational wave benchmark, a lock-exchange, and an eddies producing test cases were used. The numerical results indicate that the proposed scheme achieves the expected numerical spatial accuracy and temporal second order. The scheme's complete discontinuity ensures that both the conservation of the tracer and its consistency are preserved, as well as the conservation of water. The model is able to capture the expected physical

behavior, including vortices, instabilities, and eddies, due to the reduction of numerical diffusion.

Furthermore, this new model can be expanded and generalized to any order as long as the splitting is well-done. The temporal splitting could mix any Runge-Kutta method, which can lead to obtaining higher orders of precision. An analysis of the optimal ratio between the two time steps, denoted as M , could be performed to help produce results more quickly with good precision. Overall, this new scheme offers many potential benefits for future use in ocean modeling, especially in large-scale simulations that require high accuracy and efficient computation. In the future, we plan to continue to explore these possibilities and improve the model's accuracy by implementing new equations and techniques, such as the wetting-drying model and the use of GPUs for acceleration.

CHAPTER 4

A multi-scale IMEX second order Runge-Kutta method for the 3D hydrodynamic equations

There aren't problems we ask to ourselves,
there are problems that arise.

— Henri Poincaré.

In the previous chapter, a purely explicit second-order split-time scheme was presented. This scheme aims to account for the various characteristic speeds of the phenomena described by the hydrodynamic equations. It also reduces numerical dissipation through its second-order temporal accuracy and the correct interactions between the internal and external mode.

However, although functional in theoretical cases, the presented scheme is unfortunately not applicable in practical scenarios. This limitation arises from the phenomena described by the vertical terms of the equations. Due to the small aspect ratio of the domains, vertical discretization typically results in small elements. Consequently, vertical phenomena impose very small time steps, with vertical diffusion being particularly problematic.

To address this, the aim of this section is to add an implicit component to the previously proposed temporal scheme. Specifically, vertical terms are

treated with the same time step as horizontal phenomena but with an implicit aspect to overcome the Courant-Friedrichs-Lewy (CFL) constraint.

In the first part of this chapter, the hydrodynamic equations are shown again, focusing on their impact on time steps. Terms are classified into three groups: fast 2D terms, slow 3D horizontal terms and stiff 3D vertical terms. The equations of the turbulence closure model are also discussed, detailing the influence of wind, friction and stratification. This section aims to establish a robust physical foundation for the equations to be solved.

In the subsequent part, an explanation of the various numerical choices leading to the second-order implicit-explicit split-time scheme is provided. Attention is given to ensuring the physical property of positivity of variables in turbulent closure equations. The new scheme, with its implicit component, is described, followed by a proof of its second-order accuracy and calculation of its stability region. Finally, an algorithm is presented, illustrating the application of the new temporal scheme to finite elements.

Ultimately, the model properties are addressed through two test cases. The first demonstrates the scheme's ability to reduce numerical diffusion, while network convergence confirms its order. The second test validates the accuracy of the numerical scheme.

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4.1 Introduction

Numerical simulation plays a pivotal role in unraveling complex physical phenomena. By solving differential equations, these simulations facilitate the understanding of processes occurring from the ocean to the atmosphere, encompassing terrestrial dynamics. Previous studies have tackled challenges involved in formulating appropriate equations, selecting relevant parameters, determining characteristic values and defining boundary conditions.

When employing numerical methods, the choice of temporal discretization requires thoughtful consideration. Not all equations share the same characteristics. For example, in the computation of discontinuous solution of hyperbolic conservation laws, TVD (total variation diminishing), TVB (total variation bounded), or ENO (essentially non-oscillatory) schemes are often used (Shu, 1988; Shu and Osher, 1988). These schemes are designed to preserve the discontinuities of the solution. For these equations, the choice of a temporal scheme is not as important as the one of the spatial discretization. However, the choice of a temporal scheme becomes more challenging when dealing with equations that exhibit multiple timescales. These equations are categorized as stiff, signifying that at least one of their processes possesses a notably high characteristic velocity in comparison to the studied physical phenomena. For instance, this is prevalent in equations related to atmospheric dynamics or oceanic behaviors. Managing these equations often involves temporal schemes with exceedingly small time steps for resolving all terms during computations, but this approach incurs significant computational costs.

However, for specific problems, the troublesome terms have remarkably lower computational costs. This could be due to the fast terms being calculated across significantly fewer degrees of freedom than the slower terms. For such problems, a split temporal method becomes advantageous, allowing the computationally cheaper, fast terms to be computed numerous times compared to the computations of the computationally expensive, slower terms. In specific cases, within the slower terms, equations may exhibit phenomena with two distinct velocities. For instance, problems with exceptionally small aspect ratios exhibit this characteristic, as seen in oceanic models, where the vertical dimensions are significantly smaller than the horizontal ones. In these cases, the fast terms representing wave velocity are resolved in a two-dimensional grid, while the other terms with smaller characteristic velocities are handled in 3D. In oceanic or atmospheric models, the fast phenomena represent wave propagation. Due to the substantial aspect ratio, vertical phenomena within the slower terms tend to exhibit smaller characteristic timescales than horizontal phenomena. For instance, vertical diffusion, often arising from a turbulent closure model such as $k - \epsilon$ as described in (Rodi, 1987; Canuto et al., 2001), imposes more stringent constraints on the time step than horizontal diffusion.

To efficiently solve these equations, this paper introduces a second-order

split implicit-explicit temporal scheme. The choice of second order is crucial in reducing the numerical dissipation of the overall scheme. For instance, in ocean applications, the numerical schemes used can introduce mixing rates of tracers and momentum than can be orders of magnitude larger than physical mixing (Burchard and Rennau, 2008; Rennau and Burchard, 2009; Hiester et al., 2014). This is particularly true for the discretization of the horizontal advection (Marchesiello et al., 2009; Griffies et al., 2000), but it can arise from the vertical advection and diffusion as well (Shchepetkin A.F., 2005) or various filters introduced to improve numerical stability (Zhang et al., 2016). This numerical dissipation can be reduced by using higher order schemes.

In a prior publication, a fully explicit second-order split scheme is introduced, drawing inspiration from Wicker and Skamarock (2002); Wensch et al. (2009); Knoth and Wensch (2003). This schemes find application in atmospheric models, specifically handling terms in an explicit manner. Since the equations are predominantly influenced by advection terms, implicit treatment is not deemed necessary. Subsequent works by Nilsen and Loseth (1993); Visbal and Gaitonde (2002); Robert and Kaper (1986) introduce diffusion terms in splitting and treat them implicitly. However, the primary goal is not to create a final second-order temporal scheme; rather, the focus lies in achieving a direct low-storage implicit solution tailored to handle viscous terms. Essentially, the aim is to substantially minimize the computational effort associated with simulating turbulent flows with the larger time step possible.

While theoretically usable, the scheme detailed in Ishimwe et al. (2023) presents challenges when transitioning to real-world scenarios due to the constraints imposed by vertical terms on the 3D time steps. Consequently, this paper introduces a semi-implicit facet to the stiff term, aiming to surmount the challenges encountered during realistic simulations and presents a comprehensive and practical scheme.

The temporal scheme is employed within the framework of 3D hydrodynamic equations and is implemented within the Second-generation Louvain-la-Neuve Ice-ocean Model (SLIM, www.slim-ocean.be). This software, developed in Louvain-la-Neuve through years as explained by (White et al., 2008; Blaise et al., 2010; Comblen et al., 2010), resolves them on unstructured grids. While structured grids are known for their great computational efficiency (Danilov et al., 2008; Danilov, 2013), unstructured meshes tend to be favored within coastal domains. This preference arises from their superior ability to accurately tackle intricate coastal topography and localized features (Deleersnijder and Lermusiaux, 2008; Pigott et al., 2013). The 3D mesh, composed of prisms, is obtained by extruding a 2D mesh of triangles. Typical approaches include terrain-following sigma-levels Blumberg and Mellor (1987); Pan et al. (2021), z-levels Griffies et al. (2005) and their generalization Song and Haidvogel (1994). Given the small aspect ratio of oceanic problems, the number of horizontal elements exceeds the number of vertical elements. For spatial discretization,

SLIM employs the Discontinuous Galerkin method. This method, as implied by its name, uses spatial discontinuous discretization, meaning each node possesses a value within each adjacent triangle. This geometrical flexibility gives many advantages. Practically, this enables efficient numerical resolution, as each triangle, or prism in 3D, can solve its linear system without being blocked by other elements. This combines really well with the split temporal scheme, as the fast terms are computed in a 2D grid, while the slow and stiff terms are computed in a 3D grid as explained by [Kärnä et al. \(2013\)](#). Even when deciding to resolve the vertical terms semi-implicitly, it does not diminish the method's effectiveness because the triangle-based systems become column-based systems for prisms. Furthermore, as mentioned earlier, the number of prisms per column is generally not excessive, ensuring these systems remain easily and efficiently solvable.

The structure of this article is as follows: it opens with an introduction to the hydrodynamic equations, highlighting their characteristic timescales. The subsequent section elaborates on the temporal scheme, detailing its construction, properties such as convergence order and the stability zone. Numerical results from diverse test cases are presented to effectively validate the model. Finally, the article concludes by summarizing the findings and implications of this study.

4.2 Governing physical equations

The temporal scheme outlined in this study is implemented in a coastal context, specifically targeting the three-dimensional hydrostatic equations derived from the Navier-Stokes equations. The study focuses on three distinct timescale ranges: one short and two long timescales. These latter are due to the small aspect ratio of the domain, which is a common characteristic of coastal areas. The short timescale is associated with external gravity waves, while the two longer timescales are related to the horizontal and vertical dynamics.

4.2.1 Hydrodynamic equations

Given the Cartesian horizontal and vertical coordinates $\mathbf{x} = [x, y, z]^T$, the studied equations take the following form

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \nabla_h \cdot (\mathbf{u}\mathbf{u}) + \frac{\partial(w\mathbf{u})}{\partial z} = \nabla_h \cdot (\nu_h \nabla_h \mathbf{u}) + \frac{\partial}{\partial z} \left(\nu_v \frac{\partial \mathbf{u}}{\partial z} \right) \\ - f \mathbf{e}_z \times \mathbf{u} - g \nabla_h \eta - \frac{g}{\rho_0} \mathbf{q} - \frac{g}{\rho_0} \rho' |_\eta \nabla_h \eta \end{aligned} \quad (4.1a)$$

$$\frac{\partial H}{\partial t} = - \nabla_h \cdot \int_{-b}^{\eta} \mathbf{u} dz \quad (4.1b)$$

$$\frac{\partial w}{\partial z} = - \nabla_h \cdot \mathbf{u} \quad (4.1c)$$

In the provided equation set, ν_h , ν_v and ∇_h respectively denote horizontal and vertical viscosity, which can be determined respectively by the Smagorinsky paramerisation (Smagorinsky, 1963; Blaise et al., 2007) and the $k - \epsilon$ turbulence closure model (Rodi, 1987; Kärnä, 2020) and the horizontal gradient. The horizontal velocity vector is denoted as $\mathbf{u} = (u, v)$, while w represents the vertical velocity. The variables $\mathbf{U} = \int_{-b}^{\eta} \mathbf{u} dz$ denote the total horizontal transport, where η and b stand for the free surface elevation and the bathymetry correspondingly. The column's height is symbolized by H and f denotes the Coriolis parameter. Additionally, $\mathbf{q}$ signifies the integral of the density deviation gradient, specifically defined as $\mathbf{q} = \int_z^{\eta} \nabla_h \rho' d\zeta$. The density deviation relies on a state equation that depends on the water temperature or salinity (Jackett et al., 2006). They are modeled by the following advection-diffusion equations

$$\rho' = \rho'(T, S) \quad (4.2)$$

$$\frac{\partial T}{\partial t} + \nabla_h \cdot (\mathbf{u}T) + \frac{\partial(wT)}{\partial z} = \nabla_h \cdot (\kappa_h \nabla_h T) + \frac{\partial}{\partial z} \left(\kappa_v \frac{\partial T}{\partial z} \right) \quad (4.3)$$

$$\frac{\partial S}{\partial t} + \nabla_h \cdot (\mathbf{u}S) + \frac{\partial(wS)}{\partial z} = \nabla_h \cdot (\kappa_h \nabla_h S) + \frac{\partial}{\partial z} \left(\kappa_v \frac{\partial S}{\partial z} \right) \quad (4.4)$$

κ_h and κ_v stand for respectively the horizontal and the vertical diffusivity.

The density deviation is defined as $\rho' = \rho - \rho_0$, where ρ_0 is the reference density.

Furthermore, SLIM tackles the equations within a three-dimensional domain Ω incorporating a free surface, managed using an Arbitrary Lagrangian-Eulerian (ALE) approach (Formaggia and Nobile, 2004). While the lateral boundary Γ_l and the bottom boundary Γ_b remain static, the surface boundary Γ_s dynamically moves over time, traversing the vertical coordinates between $z = -b$ and $z = \eta$. Impermeability conditions are imposed on both the top and bottom boundaries:

$$w + \mathbf{u} \cdot \nabla_h b = 0 \quad \mathbf{x} \in \Gamma_b \quad (4.5a)$$

$$w - \frac{\partial H}{\partial t} - \mathbf{u} \cdot \nabla_h (H - b) = 0 \quad \mathbf{x} \in \Gamma_s \quad (4.5b)$$

Also, a slip condition is implemented to accommodate bottom (Kärnä et al., 2013) and surface stresses, $\boldsymbol{\tau}_b$ and $\boldsymbol{\tau}_s$:

$$\nu_v \frac{\partial \mathbf{u}}{\partial z} = \frac{\boldsymbol{\tau}_b}{\rho_0} \quad \mathbf{x} \in \Gamma_b \quad (4.6a)$$

$$\nu_v \frac{\partial \mathbf{u}}{\partial z} = \frac{\boldsymbol{\tau}_s}{\rho_0} \quad \mathbf{x} \in \Gamma_s \quad (4.6b)$$

In the application of the temporal scheme to three-dimensional hydrodynamic equations, processes are grouped into three categories based on their timescales. Defining Δxy as the horizontal grid size and Δz as the vertical one enables to establish a value for the characteristic timescales. The following values are simplifications as the real characteristic timescales are more complex depending for example of the spatial discretization. However, they are sufficient to understand the main idea of the method.

- **External gravity waves**, corresponding to the fastest phenomena, involve elevation gradient and water height evolution treated in a 2D grid allowing to conserve computational resources while requiring a smaller time step. Their characteristic timescale is defined as

$$\Delta t \propto \frac{\Delta xy}{\|\bar{\mathbf{u}}\| + \sqrt{gH}}$$

- **Vertical processes** are represented by the 3D semi-implicit terms. Given the equations' application in shallow areas, using 3D meshes with thin vertical layers, these terms exhibit reduced temporal characteristics, justifying their semi-implicit handling. These terms encompass the vertical advection, the vertical diffusion and the friction parametered with a quadratic function, split into linear components (vertical diffusion) and nonlinear components (vertical advection and friction). The quadratic bottom drag is defined :

$$\frac{\boldsymbol{\tau}_b}{\rho_0} = C_d |\mathbf{u}_b| \mathbf{u}_b$$

where $\mathbf{u}_b$ is the horizontal velocity of the bottom element taken at the middle point and C_d is the drag coefficient. The characteristic timescale of these terms is

$$\Delta t \propto \max\left(\frac{\Delta z^2}{\nu_v}, \frac{\Delta z}{w}\right)$$

- **Horizontal processes** are treated explicitly. These terms include horizontal advection, horizontal diffusion, the wind effect and density-related terms. They also take into account the internal hydrostatic waves. They appear between two layers of water with different densities. They are not as fast as the external gravity waves. The characteristic timescale of these terms is defined as

$$\Delta t \propto \max\left(\frac{\Delta xy^2}{\nu_h}, \frac{\Delta xy}{\|\mathbf{u}\| + \sqrt{gH\rho'/\rho}}\right)$$

Finally, the missing term, the Coriolis force, with $\Delta t \propto \frac{1}{f}$, is treated semi-implicitly. This decision is due to the necessity for a centered temporal scheme to ensure that the Coriolis force vector, perpendicular to velocity, neither generates nor dissipates kinetic energy. The model dealing with semi-implicit terms is centered, hence justifying the inclusion of the Coriolis term among these semi-implicit terms. This does not significantly increase the computational cost as the Coriolis force is a linear source term.

4.2.2 Two equations turbulence closure model

The turbulence closure model known as the Generic Length Scale (GLS) by [Umlauf and Burchard \(2003\)](#) solves a pair of equations governing the turbulent kinetic energy (TKE), denoted k , and an auxiliary turbulent variable, represented by Ψ . These are advection-diffusion equations with source terms. Both k and Ψ are positive fields that obey:

$$\begin{aligned} \frac{\partial k}{\partial t} + \nabla_h \cdot (\mathbf{u}k) + \frac{\partial(wk)}{\partial z} &= \nabla_h \cdot (\nu_h \nabla_h k) + \frac{\partial}{\partial z} \left(\frac{\nu_v}{\sigma_k} \frac{\partial k}{\partial z} \right) + P - \epsilon + B \\ \frac{\partial \Psi}{\partial t} + \nabla_h \cdot (\mathbf{u}\Psi) + \frac{\partial(w\Psi)}{\partial z} &= \nabla_h \cdot (\nu_h \nabla_h \Psi) + \frac{\partial}{\partial z} \left(\frac{\nu_v}{\sigma_\Psi} \frac{\partial \Psi}{\partial z} \right) + \frac{\Psi}{k} (c_1 P - c_2 \epsilon + c_3 B) \end{aligned}$$

where σ_k and σ_Ψ are the Schmidt numbers for k and Ψ respectively. c_1, c_2, c_3 are constants determined by the model.

Contrary to the Zero-equation parametrizations such as Pacanowski and Philander ([Pacanowski and Philander, 1981](#)) or the K-profil Parametrization ([Large et al., 1994](#); [Roedel et al., 2018](#)) that parametrize the eddy viscosity as

a function of the mean flow state, these equations take into account prognostic turbulent variables. P is the production term of TKE while ϵ is the dissipation rate of TKE. B represents the buoyancy and is a production or destruction term depending on the stratification. P and B are defined as

$$P = \nu_v \left(\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right) \quad (4.7)$$

$$B = \kappa_v \frac{g}{\rho_0} \frac{\partial \rho}{\partial z} \quad (4.8)$$

The term P consistently holds a semi-positive value, indicating that horizontal velocity shear generates turbulence. P converts kinetic energy of the mean flow into turbulent kinetic energy. On the contrary, the sign of B can fluctuate: under stable stratification, where $\frac{\partial \rho}{\partial z} < 0$, or in simpler terms, denser water is positioned below lighter water, B adopts a negative value, converting turbulent kinetic energy into gravitational potential energy. Consequently, this stratification tends to inhibit turbulence. In the case of unstable stratification, B becomes positive, transforming potential energy into turbulence. [Burchard \(2002\)](#) emphasized that the numerical implementation of B and P should maintain energy conservation, ensuring that the increase in TKE caused by P aligns with the corresponding loss of kinetic energy of the mean flow. Additionally, the dissipation term, ϵ , is always positive and refers to the dissipation of TKE into heat mainly at the smallest scale of motion.

Concerning Ψ , the source terms are dependent of P , B and ϵ . But they are scaled by Ψ/k and the empirical constants c_1 , c_2 and c_3 . The meaning and the unity of the variable Ψ are not straightforward.

For instance, $p = -1$, $m = 1/2$ and $n = -1$ gives the $k - \omega$ model ([Wilcox, 1988, 2008](#)). In this model, Ψ represent the specific dissipation rate as it is proportional to ϵ/k . It is also known as the turbulence frequency ω as its units are in s^{-1} . The source terms are multiplied by ϵ/k^2 up to a coefficient.

When $p = 0$, $m = 1$ and $n = 1$, this is the $k - kl$ model from [Mellor and Yamada \(1982\)](#). In this case, Ψ is the product between the turbulent energy and the turbulent length scale. In this closure, the production and destruction terms are scaled by the turbulent length scale.

Finally, in the popular $k - \epsilon$ model, where $p = 3$, $m = 3/2$ and $n = -1$, Ψ is the TKE dissipation rate. This means that the source terms are multiplied by the ratio of the TKE dissipation rate and the TKE which is ω .

In numerous ocean models, the horizontal advection of k and Ψ is disregarded, assuming relatively long transport timescales. In addition, the vertical advection is disregarded, considering dimensional analysis on the continuity equation. The same applies to the horizontal diffusion.

The two equations become

$$\frac{\partial k}{\partial t} = \frac{\partial}{\partial z} \left(\frac{\nu_v}{\sigma_k} \frac{\partial k}{\partial z} \right) + P + B - \epsilon \quad (4.9)$$

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial z} \left(\frac{\nu_v}{\sigma_\Psi} \frac{\partial \Psi}{\partial z} \right) + \frac{\Psi}{k} (c_1 P + c_3 B - C_2 \epsilon) \quad (4.10)$$

The TKE dissipation rate, ϵ , is computed using the following equation:

$$\epsilon = c_0^{3+p/n} \frac{k^{3/2+m/n}}{\Psi^{1/n}} \quad (4.11)$$

where c_0 , m , n , p are constants. The values of these constants are also given by the model.

Finally, the vertical eddy viscosity and diffusivity, ν_v and κ_v , are computed using the following equation:

$$\nu_v = \frac{c_\nu}{c_0^{3+p/n}} k^{1/2-m/n} \Psi^{1/n} \quad (4.12)$$

$$\kappa_v = \frac{c_\kappa}{c_0^{3+p/n}} k^{1/2-m/n} \Psi^{1/n} \quad (4.13)$$

where c_ν and c_κ are non-dimensional stability functions that depend on the vertical gradient of the water velocity and density.

As there are no horizontal flux terms, there is no need for boundary conditions on the lateral boundaries. Regarding the boundaries at the surface and bottom of the domain, they are determined by the wall conditions. The boundaries flux for k are 0 while the Neumann conditions on Ψ are

$$\frac{\nu_v}{\sigma_\Psi} \frac{\partial \Psi}{\partial z} = -n \frac{\nu_v}{\sigma_\Psi} c_0^p k^m \kappa^n \left(\frac{\Delta z}{2} + z_{0,s} \right)^{n-1} \quad \mathbf{x} \in \Gamma_s \quad (4.14a)$$

$$\frac{\nu_v}{\sigma_\Psi} \frac{\partial \Psi}{\partial z} = n \frac{\nu_v}{\sigma_\Psi} c_0^p k^m \kappa^n \left(\frac{\Delta z}{2} + z_{0,b} \right)^{n-1} \quad \mathbf{x} \in \Gamma_b \quad (4.14b)$$

where $z_{0,s}$ and $z_{0,b}$ are the roughness length scales at the surface and bottom respectively. Δz is the vertical grid size. As the gradients cannot be computed right at the surface and bottom because Ψ can change rapidly. Therefore, the gradients are computed at the middle of the first and last vertical layers.

4.3 Temporal scheme

The aim of this section is to propose suitable time discretizations that efficiently resolve multiscale behaviour of a stiff problem. Several methodologies exist for

integrating systems of ordinary differential equations, which encompass multistep approaches dealing with the system in fully explicit, fully implicit, or split implicit–explicit manners. This study specifically explores the utilization of second-order split IMEX integrators. These temporal integrators partition the hydrodynamic equation’s right-hand side into three components: an explicit fast yet less computationally intensive part, an explicit non-stiff part and a semi-implicit stiff part with a smaller timescale than the previous one. To exemplify, let us consider the subsequent ordinary differential equation:

$$\frac{dy}{dt} = f^{xy}(y) + f^z(y) + F^{\text{fast}}(y), \quad t \in (0, T) \quad (4.15)$$

with the initial value $y(0) = y_0$. The notation $f^{xy}(y)$ represents the slow horizontal processes integrated explicitly, while $f^z(y)$ denotes the vertical terms treated semi-implicitly. $F^{\text{fast}}(y)$ symbolizes the 2D dynamics characterized by a short timescale.

The semi-implicit term needs to be further developed as it may contain non-linear operators. Resolving non-linear semi-implicit terms requires the use of non-linear solvers such as the ones based on the Newton-Raphson method. However, employing such solvers can significantly increase computational time. To address this issue, the semi-implicit terms are divided into linear and non-linear components. The non-linear portion is addressed as a product between an explicit coefficient and an implicit one, while the linear part is treated completely semi-implicitly. This approach allows for handling semi-implicit terms without a substantial increase in computational time. The previous equation becomes :

$$\frac{dy}{dt} = f^{xy}(y) + f^{z0}(y) + f^{z1}(y) y + F^{\text{fast}}(y), \quad t \in (0, T) \quad (4.16)$$

where $f^{z0}(y)$ and $f^{z1}(y) y$ are the linear and non-linear components of the semi-implicit term respectively.

The fundamental idea behind the method presented in this paper is to employ a split-time scheme composed of Runge-Kutta methods. These Runge-Kutta methods use two different time steps: Δt for the 3D evolving terms and $\Delta T = \frac{\Delta t}{M}$ for the fast terms, where M represents the largest integer close to the ratio of characteristic speeds. As the primary aim of this paper is to develop a second-order global scheme, the selection of these Runge-Kutta methods cannot be arbitrary.

4.3.1 Choice of the Runge-Kutta schemes

The choice of the temporal discretization methods involves several constraints. Depending on the equations, they can vary.

4.3.1.1 Hydrodynamic equations

For the hydrodynamic equations, the discontinuous Galerkin finite element method, when dealing with an advection problem, has eigenvalues along the imaginary axis. Due to diffusion terms, these eigenvalues are slightly shifted towards the left. In other words, they are not purely imaginary but remain very close to the axis. Therefore, when employing a temporal method of order one, an extremely small time step is required. Hence, the choice of a temporal scheme of order two is made. In aiming for a second-order scheme over the final time step, each term within the ordinary differential equation must be treated using, at minimum, a second-order method. In other words, it is imperative to identify an order two explicit Runge-Kutta method for the explicit terms along with a semi-implicit second-order Runge-Kutta for the linear semi-implicit stiff term. Moreover, a Runge-Kutta method capable of integrating a term comprising a product of functions, one handled explicitly and the other semi-implicitly, is necessary. One first easy direct choice is to use the same explicit RK for the fast term as the one used for the explicit slow terms.

By doing this choice, this gives the following split IMEX Runge-Kutta method for the 3D terms:

$$\begin{aligned} y_{n+i} = & y_n + \alpha_{00} \Delta t f^{xy}(y_n) \\ & + \beta_{00} \Delta t f^{z0}(y_{n+i}) \\ & + \gamma_{00} \Delta f^{z1}(y_n) y_{n+i} \end{aligned} \quad (4.17)$$

$$\begin{aligned} y_{n+1} = & y_n + \alpha_{10} \Delta t f^{xy}(y_n) + \alpha_{11} \Delta t f^{xy}(y_{n+i}) \\ & + \beta_{10} \Delta t f^{z0}(y_{n+i}) + \beta_{11} \Delta t f^{z0}(y_{n+1}) \\ & + \gamma_{10} \Delta f^{z1}(y_n) y_{n+i} + \gamma_{11} \Delta f^{z1}(y_n) y_{n+1} \\ & + \gamma_{12} \Delta f^{z1}(y_{n+i}) y_{n+i} + \gamma_{13} \Delta f^{z1}(y_{n+i}) y_{n+1} \end{aligned} \quad (4.18)$$

This constitutes the expression of the complete temporal scheme without constraints. Essentially, it forms a system with 12 unknowns: one coefficient representing the temporal position achieved at the end of the first sub-time step and eleven coefficients multiplying the slopes, or in other words, the derivatives in the form of α_{mn} , β_{mn} and γ_{mn} . The α_{mn} coefficients correspond to the explicit slow terms, while the β_{mn} coefficients are related to the semi-implicit stiff terms. Finally, the γ_{mn} coefficients are associated with the explicit-implicit cross terms. The indices m and n represent the stage number and the term number respectively. The first index m varies from 0 to 1, while the second index n varies from 0 to 1 for the first stage and from 0 to 3 for the second stage.

Additionally, in this model, we aim to enforce the final scheme to be low storage, implying the use of only a limited number of temporal values at each

stage of the method. This constraint is crucial as it significantly simplifies the method's implementation, particularly because the equations involve Arbitrary Lagrangian-Eulerian formulations. In essence, at each stage, a maximum of three temporal values are present: the value at the beginning of the temporal scheme, the value at the end of the current stage and the value used in the slope to move the variables. For the first stage, it does not change anything. However, for the second stage, this implies that the derivatives can not use simultaneously values at t_n and t_{n+i} . Consequently, this gives two choices. The first is to keep the value at t_n and the value at t_{n+1} in the right-hand side. This gives

$$\alpha_{11} = \beta_{10} = \gamma_{10} = \gamma_{12} = \gamma_{13} = 0$$

In this configuration, the second stage becomes

$$\begin{aligned} y_{n+1} = & y_n + \alpha_{10} \Delta t f^{xy}(y_n) \\ & + \beta_{11} \Delta t f^{z0}(y_{n+1}) \\ & + \gamma_{11} \Delta t f^{z1}(y_n) y_{n+1} \end{aligned}$$

One can see that this scheme is not second-order accurate by construction. Indeed, the value computed at the first stage is not used in the second stage. The right choice is to keep the value at t_{n+i} and at t_{n+1} in the right-hand side. This gives

$$\alpha_{10} = \gamma_{10} = \gamma_{11} = 0$$

The second time loop becomes

$$\begin{aligned} y_{n+1} = & y_n + \alpha_{11} \Delta t f^{xy}(y_{n+i}) \\ & + \beta_{10} \Delta t f^{z0}(y_{n+i}) + \beta_{11} \Delta t f^{z0}(y_{n+1}) \\ & + \gamma_{12} \Delta t f^{z1}(y_{n+i}) y_{n+i} \\ & + \gamma_{13} \Delta t f^{z1}(y_{n+i}) y_{n+1} \end{aligned}$$

Finally, the last constraint is to ensure that the scheme is second-order accurate. To achieve this, the Taylor series expansion of y_{n+1} must match the result of the temporal scheme up to order 2. The only way to do so is to take the following split IMEX Runge-Kutta method for the slow and stiff terms:

$$\begin{aligned}
 y_{n+\frac{1}{2}} &= y_n + \frac{1}{2}\Delta t f^{\text{xy}}(y_n) \\
 &\quad + \frac{1}{2}\Delta t f^{\text{z0}}(y_{n+\frac{1}{2}}) \\
 &\quad + \frac{1}{2}\Delta t f^{\text{z1}}(y_n) y_{n+\frac{1}{2}} \\
 y_{n+1} &= y_n + \Delta t f^{\text{xy}}(y_{n+\frac{1}{2}}) \\
 &\quad + \Delta t f^{\text{z0}}(y_{n+\frac{1}{2}}) \\
 &\quad + \Delta t f^{\text{z1}}(y_{n+\frac{1}{2}}) y_{n+\frac{1}{2}}
 \end{aligned} \tag{4.19}$$

The demonstration of the order of this scheme is done Section 4.3.3. Concerning the fast terms, they are computed with the same explicit Runge-Kutta method as the slow explicit terms. This gives

$$\begin{aligned}
 y_{n+\frac{1}{2}} &= y_n + \frac{1}{2}\Delta T F^{\text{fast}}(y_n) \\
 y_{n+1} &= y_n + \Delta T F^{\text{fast}}(y_{n+\frac{1}{2}})
 \end{aligned} \tag{4.20}$$

4.3.1.2 Two equations turbulence closure model

As for the turbulence closure equations, a second-order temporal scheme is also desirable to keep the global scheme of order 2. The aim is to use vertical viscosity and diffusivity value that are calculated at time $n + \frac{1}{2}$ in the diffusion terms of the hydrodynamic equations. To satisfy both constraints, the simplest choice is to employ the same temporal scheme as that described in the preceding section.

However, this is not sufficient. An additional requirement for these equations is that the scheme must be positive. This means that if a simulation starts with positive field values, they must remain positive throughout all the simulation regardless of the hydrodynamics.

Positive production terms pose no issues. The diffusion term in these equations also doesn't raise any concerns. The stability of the Runge-Kutta as well as the Finite-Volume methods guarantees the positivity of the variables under the diffusion. The only problematic terms is the destruction terms. The aim is to avoid situations where, within a time step, more is destroyed than what is produced and received by diffusion. This would result in a negative value for k or Ψ , which is not physically possible. Moreover, this can lead to negative viscosity or diffusivity coefficients. To avoid this, an appropriate approach involves using Patankar techniques (Patankar, 1980) on the destruction terms. As shown by Burchard et al. (2003), Patankar methods are employed to ensure the positivity of turbulent variables. Isgin and Ranocha (2023) demonstrated

the way to implement these techniques in a temporal scheme of order two. For the sake of brevity, the details of the demonstration of the order are not given here again.

The diffusion term and the positive production terms follow the temporal scheme presented before. The temporal scheme for destruction terms is the following:

$$\begin{aligned} y_{n+\frac{1}{2}} &= y_n + \frac{\Delta T}{2} D(y_n) \frac{y_{n+\frac{1}{2}}}{y_n} \\ y_{n+1} &= y_n + \Delta T D(y_{n+\frac{1}{2}}) \frac{y_{n+1} y_n}{\left(y_{n+\frac{1}{2}}\right)^2} \end{aligned} \quad (4.21)$$

where $D(y)$ is the negative destruction term.

4.3.2 Split IMEX Runge-Kutta method

In order to obtain the final scheme, one needs to combine the explicit and implicit Runge-Kutta methods for the 3D terms with the explicit Runge-Kutta method for the fast 2D terms. Coupling the fast terms with the slow explicit terms has already been done in [Ishimwe et al. \(2023\)](#). In the context of this model, coupling between stiff and fast terms proves to be notably intricate.

For the first sub iteration, the implicit aspect of this scheme anticipates computing the value of the variable $y_{n+\frac{1}{2}}$ for each iteration within the temporal loop of the fast scheme. However, this contradicts the core purpose of splitting. The aim is to compute the 3D terms a fixed number of times independent of the number of fast time steps. This requires taking inspiration from predictor-corrector methods to handle the connection between the implicit elements.

The description of the first sub-time step of the 3D component follows. Initially, before entering the temporal loop of the fast terms, the contribution of the slow and stiff terms must be calculated. During the evaluation of the slow explicit terms, a prediction of the implicit vertical terms is also computed. This prediction estimates the value of the implicit slope without considering the fast terms. Using this slope alongside the contribution from the explicit slow derivative advances the fast terms with a smaller time step. Following multiple Runge-Kutta iterations, the contributions of all fast slopes can be computed. By using these fast slopes along with the explicit slow slopes, the unknown variable's value can be calculated, this time incorporating the correct value for the implicit slope. Consequently, this yields the value of y at the midpoint of the time step.

Regarding the second sub-time step, upon close examination of the Runge-Kutta equations described in the preceding section, it is noticeable that the semi-implicit functions are no longer computed using the future value of y but rather utilizing the midpoint value. This implies that the second time step is

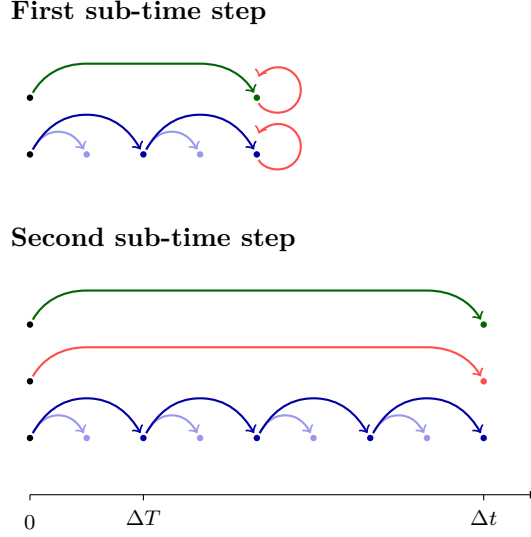


Fig. 4.1: Split IMEX scheme composed by two RK2 and one IRK2. The green and red arrows represent the computation of each explicit and semi-implicit stiff process while the blue ones represent the computation of each $f^{\text{fast}}(y)$

entirely explicit. Consequently, the coupling between the slow, the stiff and the fast terms becomes more straightforward and is directly inspired by [Ishimwe et al. \(2023\)](#). This implies that all 3D terms are computed before the temporal loops of the fast terms and then the entirety advances during the fast Runge-Kutta iterations.

The whole process is summarised in the Figure 4.1 and the Algorithm 4. While this temporal method uses two established RK methods, the resultant splitting mechanism is novel and unique.

4.3.3 Order of precision

The order of the scheme is obtained by comparing the Taylor series expansion of the scheme with the Taylor series expansion of the solution of the ODE. The order of the scheme is the highest order of the same terms between them. The expression of the Taylor series y_{n+1} is given by

Algorithm 4: split IMEX scheme of order 2

Data: Model state variable y_n , $m = M/2$

First sub-time step

```

fxy ← fxy(yn)
fz1 ← fz1(yn)
y* ← yn +  $\frac{\Delta t}{2}$ (fxy + fz0(y*) + fz1 y*)
fz0 ← fz0(y*)
y ← yn
Ffast ← 0
for j = 1, ..., M/2 do
    ffast ← ffast(y)
    ffast ← ffast(y +  $\frac{1}{2}\Delta T$ (ffast + fxy + fz0 + fz1 y*))
    y ← y +  $\Delta T$ (ffast + fxy + fz0 + fz1 y*)
    Ffast ← Ffast +  $\Delta T$ ffast
end
yn+ $\frac{1}{2}$  ← yn +  $\frac{\Delta t}{2}$ (fxy + fz0(yn+ $\frac{1}{2}$ ) + fz1 yn+ $\frac{1}{2}$ ) + Ffast

```

Second sub-time step

```

fxy ← fxy(yn+ $\frac{1}{2}$ )
fz0 ← fz0(yn+ $\frac{1}{2}$ )
fz1 ← fz1(yn+ $\frac{1}{2}$ )
Ffast ← 0
for j = 1, ..., M do
    ffast ← ffast(y)
    ffast ← ffast(y +  $\frac{1}{2}\Delta T$ (ffast + fxy + fz0 + fz1 yn+ $\frac{1}{2}$ ))
    y ← y +  $\Delta T$ (ffast + fxy + fz0 + fz1 yn+ $\frac{1}{2}$ )
    Ffast ← Ffast +  $\Delta T$ ffast
end
yn+1 ← yn +  $\Delta t$ (fxy + fz0 + fz1 yn+ $\frac{1}{2}$ ) + Ffast

```

$$\begin{aligned}
y_{n+1} &= y_n + \Delta t y_n' + \frac{\Delta t^2}{2} y_n'' + O(\Delta t^3) \\
&= y_n + \Delta t (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) \\
&\quad + \frac{\Delta t^2}{2} \left((f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n)' (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) \right) \\
&\quad + O(\Delta t^3)
\end{aligned} \tag{4.22}$$

with $f_n^{xy} = f^{xy}(y_n)$, $f_n^{z0} = f^{z0}(y_n)$, $f_n^{z1} = f^{z1}(y_n)$ and $F_n = F^{\text{fast}}(y_n)$.

A conventional Runge-Kutta order analysis involves calculating each iteration of the slopes and adding them to derive the final expression for y_{n+1} . However, in a split temporal scheme, showcasing the outcome of each 2D sub-step is not practical due to the multitude of terms involved. Therefore, for clarity, only the assessments of y at the 3D sub-steps, encompassing $y_{n+\frac{1}{2}}$ and y_{n+1} , are computed instead. However, rest assured that the comprehensive details of the small time-step 2D loops have been provided in the article [Ishimwe et al. \(2023\)](#). The result of a whole fast Runge-Kutta iteration has also been expressed. For a given k^{slow} and M , the result of the fast Runge-Kutta iteration is

$$y_M = y_n + M\Delta T \left(F_n + k^{\text{slow}} \right) + \frac{M^2\Delta T^2}{2} \left(F_n + k^{\text{slow}} \right) F'_n + O(M^3\Delta T^3)$$

$$y_n + \Delta t \left(F_n + k^{\text{slow}} \right) + \frac{\Delta t^2}{2} \left(F_n + k^{\text{slow}} \right) F'_n + O(\Delta t^3)$$

This result is denoted $RK2(k^{\text{slow}}, M)$. To determine the order of accuracy of the global method, the split IMEX RK2 method is unrolled. The two sub-steps are computed separately because the first sub-step is implicit, while the second sub-step is explicit. Moreover, the prediction of the implicit terms is analysed separately from the correction. In the first sub steps, the predicted 3D slope is denoted $k_1^{*,\text{slow}}$ and the corrected 3D slope is denoted k_1^{slow} . The former ones are computed without considering the fast terms while the latter ones are computed with the fast terms. The predicted slope is given by

$$\begin{aligned} k_1^{*,\text{slow}} &= f_n^{xy} + f_n^{*,z0} + f_n^{z1} y_n^* \\ &= f_n^{xy} + f_n^{z0} + f_n^{z1} y_n \\ &\quad + \frac{\Delta t}{2} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n) f_n^{i'} \\ &\quad + \frac{\Delta t}{2} f_n^{z1} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n) \\ &\quad + O(\Delta t^2) \end{aligned}$$

Following Algorithm 4, the value of $RK2(k_1^{*,\text{slow}}, \frac{M}{2})$ can be obtained. Consequently, the sum of the fast slopes can be computed. This sum is denoted F_1^{fast} and is given by

$$F_1^{\text{fast}} = \frac{\Delta t}{2} F_n + \frac{1}{2} \left(\frac{\Delta t}{2} \right)^2 F_n F'_n + O(\Delta t^3)$$

The value of $y_{n+\frac{1}{2}}$ can now be expressed as

$$\begin{aligned}
y_{n+\frac{1}{2}} = & y_n + \frac{\Delta t}{2} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) \\
& + \frac{\Delta t^2}{8} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) F_n' \\
& + \frac{\Delta t^2}{4} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) f_n^{i'} \\
& + \frac{\Delta t^2}{4} f_n^{z1} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) \\
& + O(\Delta t^3)
\end{aligned} \tag{4.23}$$

The second sub step computes explicitly the slow, the stiff and the fast terms. The slope denoted k_2^{slow} is

$$\begin{aligned}
k_2^{\text{slow}} = & f^{xy}(y_{n+\frac{1}{2}}) + f^{z0}(y_{n+\frac{1}{2}}) + f^{z1}(y_{n+\frac{1}{2}}) y_{n+\frac{1}{2}} \\
= & f_n^{xy} + f_n^{z0} + f_n^{z1} y_n \\
& + \frac{\Delta t}{2} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n)' \\
& + O(\Delta t^2)
\end{aligned}$$

The final value of y_{n+1} is given by $\text{RK2}(k_2^{\text{slow}}, M)$.

$$\begin{aligned}
y_{n+1} = & y_n + \Delta t (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) \\
& + \frac{\Delta t^2}{2} (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n) (f_n^{xy} + f_n^{z0} + f_n^{z1} y_n + F_n)' \\
& + O(\Delta t^3)
\end{aligned} \tag{4.24}$$

Comparing the Taylor series expansion of y_{n+1} (Equation 4.24) with the Taylor series expansion of the solution of the ODE (Equation 4.22), one can see that the order of the scheme is 2.

As stated before, the Patankar modified scheme is also of order 2. This is mentioned by [Isgin and Ranocha \(2023\)](#). The demonstration is done in [Kopecz and Meister \(2018\)](#).

4.3.4 Stability region

The stability region of a numerical scheme is the set of complex numbers z such that the numerical scheme applied to the linear ODE is stable.

4.3.4.1 Stability of the IMEX Runge-Kutta method

In the case of the split IMEX RK2 scheme, there are three different characteristic speeds. Therefore, this configuration should be taken into account. The linear ODE becomes

$$\frac{\partial y}{\partial t} = \lambda_{xy}y + \lambda_z y + \Lambda y$$

with respectively λ_{xy} , λ_z and Λ the complex coefficient of the linear function of the horizontal explicit terms, the vertical semi-implicit terms and the fast terms.

The amplification factor of the scheme is defined as the ratio between the value of y at the end of the time step and the value at the beginning of the time step. The result of the fast Runge-Kutta iterations, denoted $RK2(k^{\text{slow}}, M)$, is

$$y_M = y_n A^M + k^{\text{slow}} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^M}{1 - A}$$

with $A = 1 + \Lambda \Delta T + \Lambda^2 \frac{\Delta T^2}{2}$ and $\Lambda \neq 0$, $\Delta T \neq 0$.

Once again, the analysis of the complete temporal scheme is divided into two due to the specific configuration of this IMEX scheme. Indeed, the implicit aspect of the first sub-time step, coupled with its predictor-corrector nature, complicates the analysis. The value resulting from the prediction offers an insight into the scheme's treatment concerning the 3D terms and impacts the overall stability of the scheme.

The predicted value is

$$y^* = y_n \frac{1 + \frac{\Delta t}{2} \lambda_{xy}}{1 - \frac{\Delta t}{2} \lambda_z}$$

The corresponding slope is

$$\begin{aligned} k_1^{*,\text{slow}} &= \lambda_{xy} y_n + \lambda_z y^* \\ &= y_n \left(\lambda_{xy} + \lambda_z \frac{1 + \frac{\Delta t}{2} \lambda_{xy}}{1 - \frac{\Delta t}{2} \lambda_z} \right) \end{aligned}$$

The predicted value is then used to compute the fast Runge-Kutta iterations. The result of the fast iterations gives

$$\begin{aligned} y_{n+\frac{1}{2}}^* &= RK2(k_1^{*,\text{slow}}, \frac{M}{2}) \\ &= y_n A^{\frac{M}{2}} \\ &\quad + y_n \left(\lambda_{xy} + \lambda_z \frac{1 + \frac{\Delta t}{2} \lambda_{xy}}{1 - \frac{\Delta t}{2} \lambda_z} \right) \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^{\frac{M}{2}}}{1 - A} \end{aligned}$$

As Algorithm 4 shows, this value is only a prediction to obtain the fast slopes. They are combined with the slow explicit slope to obtain the final value using the correction of the implicit term. This gives the following expression

$$\begin{aligned} y_{n+\frac{1}{2}} &= y_n A^{\frac{M}{2}} + \lambda_{xy} y_n \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^{\frac{M}{2}}}{1 - A} + \frac{\Delta t}{2} \lambda_z y_{n+\frac{1}{2}} \\ &= y_n \left(\frac{1}{1 - \lambda_z \frac{\Delta t}{2}} \right) \left(\lambda_{xy} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^{\frac{M}{2}}}{1 - A} + A^{\frac{M}{2}} \right) \end{aligned}$$

Using this value, the slope of the second sub-time step, k_2^{slow} , can be computed.

$$\begin{aligned} k_2^{\text{slow}} &= \lambda_{xy} y_{n+\frac{1}{2}} + \lambda_z y_{n+\frac{1}{2}} \\ &= y_n (\lambda_{xy} + \lambda_z) \left(\frac{1}{1 - \lambda_z \frac{\Delta t}{2}} \right) \left(\lambda_{xy} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^{\frac{M}{2}}}{1 - A} + A^{\frac{M}{2}} \right) \end{aligned}$$

Consequently, the value of y_{n+1} can be expressed as

$$\begin{aligned} y_{n+1} &= RK2(k_2^{\text{slow}}, M) \\ &= y_n A^M \\ &\quad + y_n \left(\frac{\lambda_{xy} + \lambda_z}{1 - \lambda_z \frac{\Delta t}{2}} \right) \left(\lambda_{xy} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^{\frac{M}{2}}}{1 - A} + A^{\frac{M}{2}} \right) \\ &\quad \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^M}{1 - A} \end{aligned}$$

Finally, the amplification factor of the scheme is given by

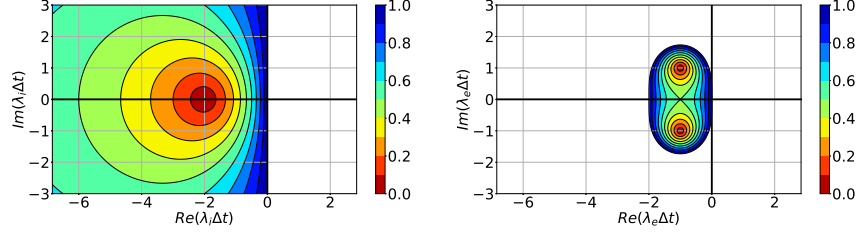


Fig. 4.2: Stability region with only one function with $M = 1$. The abscissa is the Real part while the ordinates is the Imaginary part of respectively $\lambda_z \Delta t$ and $\lambda_{xy} \Delta t$. The bold lines are the origins.

$$\frac{y_{n+1}}{y_n} = A^M + \left(\frac{\lambda_{xy} + \lambda_z}{1 - \lambda_z \frac{\Delta t}{2}} \right) \left(\lambda_{xy} \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^{\frac{M}{2}}}{1 - A} + A^{\frac{M}{2}} \right) \left(\Delta T + \Lambda \frac{\Delta T^2}{2} \right) \frac{1 - A^M}{1 - A}$$

The stability region of the scheme is a function of four parameters: λ_{xy} , λ_z , Λ and M , where the first three are complex and the last is a positive integer. Representing the global stability region proves to be highly intricate, given its 7D nature. To simplify the illustration of the function, let us examine the scenario where either λ_{xy} , λ_z or Λ equals zero and M equals 1. The fast term and the explicit slow term using the same temporal scheme, it is shown once. The stability regions depicted in Figure 4.2 align with those of the conventional RK2 methods and the Crank-Nicolson. Altering the value of M impacts both graphs: regarding the RK2 for the slow process, the stability region decreases while preserving its original shape; conversely, the semi-implicit process, the region stays unconditionally stable for all the negative values.

4.3.4.2 Stability of the Patankar Runge-Kutta method

In this section, an analysis of the second-order temporal scheme that incorporates the Patankar method is done for the destruction terms of the turbulence closure equations. This scheme is specifically designed to ensure the positivity of the solution of an equation containing a destruction term. To study its stability zone, the focus is on an ODE where the right-hand side comprises only a destruction term. As a reminder, $D(y)$ is negatively signed and may be a function of y . This results in the following ODE:

$$\frac{\partial y}{\partial t} = D(y)$$

The first step of the Patankar method moves the solution to $t = t + \frac{\Delta t}{2}$. This gives

$$\begin{aligned} y_{n+\frac{1}{2}} &= y_n + \frac{\Delta t}{2} D(y_n) \frac{y_{n+\frac{1}{2}}}{y_n} \\ \Leftrightarrow y_{n+\frac{1}{2}} &= \frac{y_n^2}{y_n - \frac{\Delta t}{2} D(y_n)} \end{aligned}$$

The final step of the Patankar gives

$$\begin{aligned} y_{n+1} &= y_n + \Delta t D(y_{n+\frac{1}{2}}) \frac{y_{n+1} y_n}{y_{n+\frac{1}{2}}} \\ \Leftrightarrow y_{n+1} &= \frac{y_n^5}{y_n^4 - \Delta t D(y_{n+\frac{1}{2}}) y_n \left(y_n - \frac{\Delta t}{2} D(y_n) \right)^2} \end{aligned}$$

This is the solution of the ODE for a generic destruction term. To study the stability of the scheme, the following case is considered

$$D(y) = \lambda_p y$$

with λ_p a complex number and the real part of λ_p negative.

The amplification factor of the scheme is given by

$$\begin{aligned} \frac{y_{n+1}}{y_n} &= \frac{y_n^4}{y_n^4 - \Delta t \lambda_p y_{n+\frac{1}{2}} \left(y_n - \frac{\Delta t}{2} \lambda_p y_n \right)^2} \\ &= \frac{1}{1 - \Delta t \lambda_p + \frac{\Delta t^2}{2} \lambda_p^2} \end{aligned}$$

The stability region is shown in Figure 4.3. The scheme is unconditionally stable for all the negative values of $Re(\lambda_p)$. This is consistent with the fact that the Patankar method is designed to ensure the positivity of the solution of an equation containing a destruction term. By definition, the latter is always negative. The figure also demonstrates that the stability region of the second-order Patankar scheme is the inverse of the stability region of a classical second-order Runge-Kutta scheme, with a sign change. This means that the region where the amplification factor is less than zero corresponds to the stability region of the Runge-Kutta scheme with a negative sign, whereas it is greater than zero.

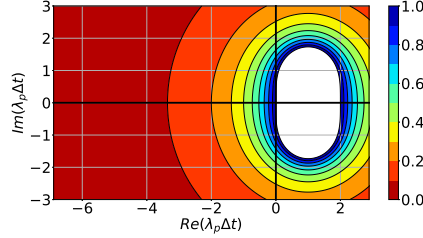


Fig. 4.3: Stability region of the Patankar method. The abscissa is the Real part while the ordinates is the Imaginary part of respectively $\lambda_p \Delta t$. The bold lines are the origins.

4.3.5 Application to the hydrodynamics equations

The split IMEX RK2 method is applied to the hydrodynamics equations presented in Section 4.2.1. Regarding spatial discretization, the first-order discontinuous Galerkin finite element method is employed. A comprehensive description of this method was previously detailed in [Ishimwe et al. \(2023\)](#). As the same methodology is used here, it is not reiterated in this paper.

The temporal method is implemented on these discretized equations. Nonetheless, the finite element method incorporates mass matrices. At time n , M^n represents the global mass matrix. Consequently, in order to employ the split IMEX temporal schemes for our specific problem, it is crucial to consider the evolution of the mass matrix throughout the algorithm.

To accommodate the vertical mesh displacement, an Arbitrary Lagrangian-Eulerian scheme is introduced. As the three-dimensional mesh tracks the free surface movement, solely the vertical coordinates experience temporal changes (e.g., ([Clare et al., 2022](#); [Pan et al., 2019](#))).

While not explicitly demonstrated in this article, it is emphasized that the proposed IMEX scheme still adheres to the properties outlined in the previous work. These include tracer consistency, conservation of water volume and conservation of tracer volume.

A complete iteration of the three-dimensional hydrostatic equations is shown in Algorithm 5.

4.4 Results

The 3D model is assessed by a set of numerical benchmarks. The correct size of the vortices produced by instabilities in a rotating baroclinic benchmark demonstrates the small amount of numerical dispersion introduced by the discrete model. The second-order accuracy of the scheme is demonstrated by

Algorithm 5: split IMEX iteration for the hydrodynamic equations,
 $m = M/2$

Data: Model state variable $\mathbf{u}, z$

$$\mathbf{U}, H \leftarrow \sum_z \frac{h}{2} \mathbf{u}, \sum_z \frac{h}{2}$$

$$\mathbf{u}_0, h_0 \leftarrow \mathbf{u}, h$$

$$\mathbf{U}_0, H_0 \leftarrow \mathbf{U}, H$$

First sub-time step

$$\mathbf{f}^{\text{xy}} \leftarrow f_{3d}^{\text{xy}}(\mathbf{u}, z)$$

$$\mathbf{f}^{\text{z1}} \leftarrow f_{3d}^{\text{z1}}(\mathbf{u}, z)$$

$$\mathbf{u}^* \leftarrow M_{3d}^{-1} \left(M_{3d}^0 \mathbf{u}_0 + \frac{\Delta t}{2} (\mathbf{f}^{\text{xy}} + f_{3d}^{\text{z0}}(\mathbf{u}^*, z) + \mathbf{f}^{\text{z1}} \mathbf{u}^*) \right)$$

$$\mathbf{f}^{\text{z0}} \leftarrow f_{3d}^{\text{z0}}(\mathbf{u}^*, z)$$

$$\mathbf{F}^{\text{xy}} \leftarrow \sum_z \mathbf{f}^{\text{xy}}$$

$$\mathbf{F}^{\text{z0}} \leftarrow \sum_z \mathbf{f}^{\text{z0}}$$

$$\mathbf{F}^{\text{z1}} \mathbf{U} \leftarrow \sum_z \mathbf{f}^{\text{z1}} \mathbf{u}^*$$

$$\mathbf{U}, H \leftarrow \mathbf{U}_0, H_0$$

$$\mathbf{F}^{\text{fast}} \leftarrow 0$$

for $j=1, \dots, m$ **do**

$$\mathbf{F}_{\mathbf{U}}, F_H \leftarrow F_{2d}(\mathbf{U}, H)$$

$$\mathbf{F}_{\mathbf{U}}, F_H \leftarrow F_{2d}(\mathbf{U} + \frac{\Delta T}{2} M_{2d}^{-1} (\mathbf{F}_{\mathbf{U}} + \mathbf{F}^{\text{xy}} + \mathbf{F}^{\text{z0}} + \mathbf{F}^{\text{z1}} \mathbf{U}), H + \frac{\Delta T}{2} M_{2d}^{-1} F_H)$$

$$\mathbf{U} \leftarrow \mathbf{U} + \Delta T M_{2d}^{-1} (\mathbf{F}_{\mathbf{U}} + \mathbf{F}^{\text{xy}} + \mathbf{F}^{\text{z0}} + \mathbf{F}^{\text{z1}} \mathbf{U})$$

$$H \leftarrow H + \Delta T M_{2d}^{-1} F_H$$

$$\mathbf{F}^{\text{fast}} \leftarrow \mathbf{F}^{\text{fast}} + \Delta T \mathbf{F}_{\mathbf{U}}$$

end

Update the z coordinates based on H

$$\mathbf{u}_{n+\frac{1}{2}} \leftarrow$$

$$M_{3d}^{-1} \left(M_{3d}^0 \mathbf{u}_0 + \frac{\Delta t}{2} (\mathbf{f}^{\text{xy}} + f_{3d}^{\text{z0}}(\mathbf{u}_{n+\frac{1}{2}}, z) + \mathbf{f}^{\text{z1}} \mathbf{u}_{n+\frac{1}{2}}) + \frac{1}{2} \frac{h}{H} \mathbf{F}^{\text{fast}} \right)$$

Second sub-time step

$$\mathbf{f}^{\text{xy}} \leftarrow f_{3d}^{\text{xy}}(\mathbf{u}_{n+\frac{1}{2}}, z)$$

$$\mathbf{f}^{\text{z0}} \leftarrow f_{3d}^{\text{z0}}(\mathbf{u}_{n+\frac{1}{2}}, z)$$

$$\mathbf{f}^{\text{z1}} \leftarrow f_{3d}^{\text{z1}}(\mathbf{u}_{n+\frac{1}{2}}, z)$$

$$\mathbf{F}^{\text{xy}} \leftarrow \sum_z \mathbf{f}^{\text{xy}}$$

$$\mathbf{F}^{\text{z0}} \leftarrow \sum_z \mathbf{f}^{\text{z0}}$$

$$\mathbf{F}^{\text{z1}} \mathbf{U} \leftarrow \sum_z \mathbf{f}^{\text{z1}} \mathbf{u}_{n+\frac{1}{2}}$$

$$\mathbf{U}, H \leftarrow \mathbf{U}_0, H_0$$

$$\mathbf{F}^{\text{fast}} \leftarrow 0$$

for $j=1, \dots, 2m$ **do**

$$\mathbf{F}_{\mathbf{U}}, F_H \leftarrow F_{2d}(\mathbf{U}, H)$$

$$\mathbf{F}_{\mathbf{U}}, F_H \leftarrow F_{2d}(\mathbf{U} + \frac{\Delta T}{2} M_{2d}^{-1} (\mathbf{F}_{\mathbf{U}} + \mathbf{F}^{\text{xy}} + \mathbf{F}^{\text{z0}} + \mathbf{F}^{\text{z1}} \mathbf{U}), H + \frac{\Delta T}{2} M_{2d}^{-1} F_H)$$

$$\mathbf{U} \leftarrow \mathbf{U} + \Delta T M_{2d}^{-1} (\mathbf{F}_{\mathbf{U}} + \mathbf{F}^{\text{xy}} + \mathbf{F}^{\text{z0}} + \mathbf{F}^{\text{z1}} \mathbf{U})$$

$$H \leftarrow H + \Delta T M_{2d}^{-1} F_H$$

$$\mathbf{F}^{\text{fast}} \leftarrow \mathbf{F}^{\text{fast}} + \Delta T \mathbf{F}_{\mathbf{U}}$$

end

Update the z coordinates based on H

$$\mathbf{u}_{n+1} \leftarrow M_{3d}^{-1} \left(M_{3d}^0 \mathbf{u}_0 + \Delta t (\mathbf{f}^{\text{xy}} + \mathbf{f}^{\text{z0}} + \mathbf{f}^{\text{z1}} \mathbf{u}_{n+\frac{1}{2}}) + \frac{1}{2} \frac{h}{H} \mathbf{F}^{\text{fast}} \right)$$

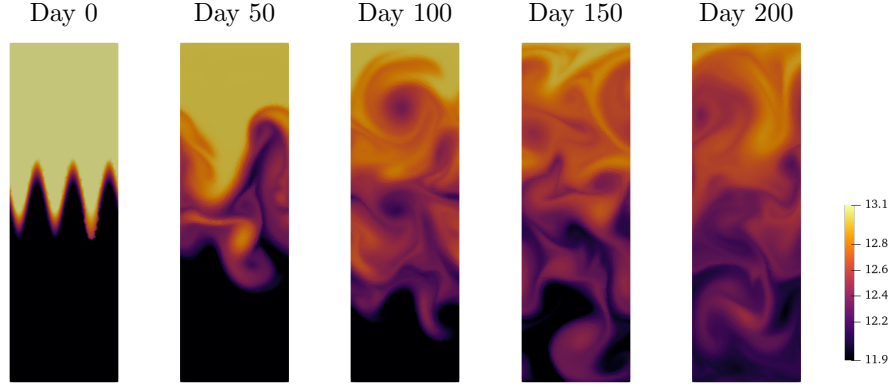


Fig. 4.4: Sea surface temperature field [°C] of the baroclinic eddies test case for 200 days with the split imex runge-kutta. The horizontal viscosity is $20 \text{ m}^2/\text{s}$.

the convergence of the error. Then, the ability of the model to reproduce the dynamics of the overflow mixing and entrainment is also demonstrated.

4.4.1 Baroclinic eddies

The baroclinic eddies test case, initially introduced in [Ilicak et al. \(2012\)](#), serves as a pivotal benchmark to assess the model capabilities of generating and accurately representing these eddies while minimizing numerical dissipation through the temporal scheme. It has been previously employed in a prior study. However, it is indispensable to include it in this research as it provides an effective means to test the second-order accuracy and performance of our model in this specific context.

This simulation, representing the Antarctic Circumpolar Current, replicates an unstable sinusoidal front dividing warm and cold water masses, resulting in the development of vortices under the influence of horizontal viscosity. Implemented within a three-dimensional box domain, spanning 500 km in length, 160 km in width and 1000 m in depth, the model incorporates impermeable boundaries along the meridional axis (y) and periodic boundaries along the zonal axis (x). Key parameters encompass a constant Coriolis parameter set at $-1.2 \times 10^{-4} \text{ s}^{-1}$, quadratic bottom drag coefficient of 0.01 and a density function formulated from temperature variations.

Its expression is given by

$$\rho(x, y, z) = 1000 - 0.2(T(x, y, z) - 5)$$

where T is the temperature in °C. The initial temperature distribution is given by [Ilicak et al. \(2012\)](#).

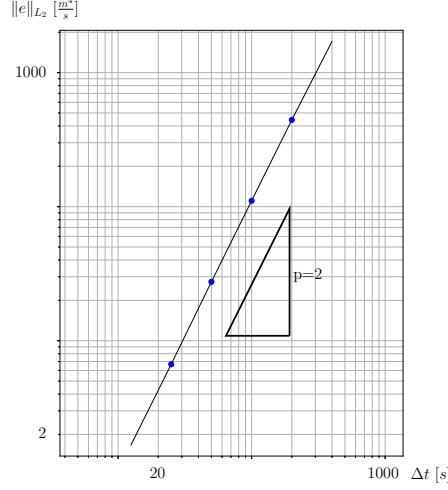


Fig. 4.5: Error convergence of the baroclinic eddies test case with the split imex runge-kutta.

This simulation employs a 4 km horizontal grid resolution coupled with a horizontal viscosity of $20 \text{ m}^2/\text{s}$. In Figure 4.4, the simulation showcases the initial temperature field, with warmer northern and colder southern surface temperatures separated by a sinusoidal transition band. The evolution of sea surface temperature over time further underscores the model's proficiency in capturing and reproducing mesoscale features, particularly evident when reducing viscosity while considering rotational influences.

Additionally, a convergence analysis of the temporal scheme is done in Figure 4.5. The error is computed with the L_2 norm as follows

$$E = \|f - f^{ref}\|_{L_2} = \sqrt{\int_{\Omega} (f - f^{ref})^2 d\Omega}$$

with f the variable of interest and f^{ref} the reference solution. The simulation is running for 2000 s with the following set of Δt : [200, 100, 50, 25, 1.25] s and $M=138$. The solution obtained with the smallest time resolution is used as a reference. The order of accuracy is obtained by computing the slope of the error versus the time step. The slope is 2.0 which confirms the second-order accuracy of the scheme.

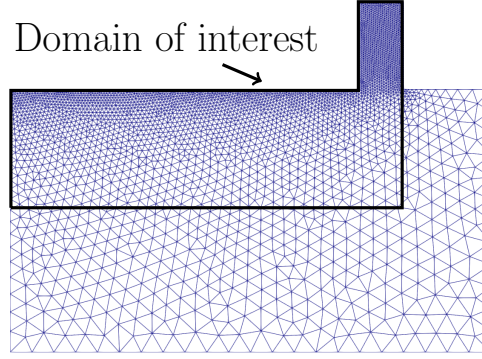


Fig. 4.6: Horizontal mesh of the DOME test case. The characteristic size at the entry is 5 km then becomes 50 km which produces 7234 triangles.

4.4.2 Dynamics of Overflow Mixing and Entrainment

The following test case is known as the Dynamics of Overflow Mixing and Entrainment, or DOME, test case (Ezer and Mellor (2004); Legg et al. (2006); Wang et al. (2008); Burchard and Rennau (2008)). This test aims to evaluate the method's performance in generating swirling patterns. The fluid flow is primarily influenced by gravity and the Coriolis effect. It serves as a simplified representation of the Denmark Strait overflow. In a stratified basin, dense water is introduced through a channel. Through a passive tracer, the movement of the water can be tracked.

The domain is a rectangular box measuring 1100 km in length and 600 km in width. The bathymetry is constant at 3600 m between $x = 0$ and $x = 300$ km. Then, it transitions to a slope, decreasing from 3600 m to 600 m between $x = 300$ km and $x = 600$ km. Finally, a 100×200 km channel is located at the northern part of the domain. Concerning boundary conditions, the eastern, southern and western boundaries are open with an elevation of 0 m. At the northern part of the channel, it is also open but additionally, along with a zero elevation, an incoming velocity with a maximum value of 0.75 ms^{-1} is applied, whose equation will be described later. The rest of the boundaries are closed. Figure 4.7 illustrates the domain.

The 3D grid is created from a horizontal grid illustrated in Figure 4.6 with a characteristic size of 5 km and contains 20 vertical layers, resulting in a horizontal mesh Reynolds number of 200.

Regarding temperature, initially, it varies between 10 and 20 degrees Celsius, with 10 degrees at the bottom of the basin and 20 degrees at the surface. The incoming water has a temperature mostly of 10 degrees. This equation is also described later. For the passive tracer, its concentration is 0 within the

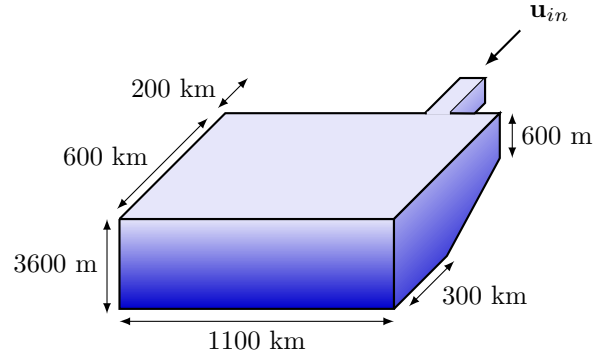


Fig. 4.7: Geometry of the DOME test case. The blue color represents the vertical gradient in density field. The arrow represents the incoming flow. The channel is 100 km wide and 200 km long with a depth of 600 m.

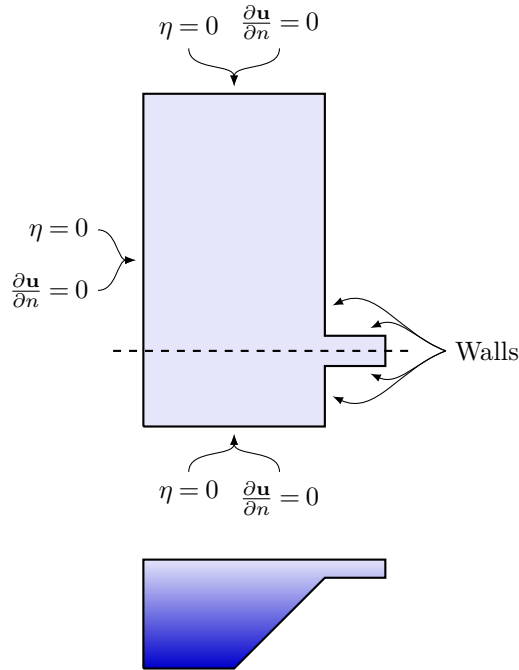


Fig. 4.8: Boundary conditions of the DOME test case

domain and 1 at the entrance of the channel, ensuring it represents an image of the velocity field. The Coriolis parameter is taken as a constant $1 \times 10^{-4} \text{ s}^{-1}$. The quadratic bottom drag coefficient is $2e^{-3}$. The horizontal viscosity and diffusivity are $18.75 \text{ m}^2\text{s}^{-1}$ and $10 \text{ m}^2\text{s}^{-1}$ respectively. The vertical viscosity and diffusivity are $0.1875 \text{ m}^2\text{s}^{-1}$ and $0 \text{ m}^2\text{s}^{-1}$ respectively.

The state equation of the density and the temperature field are given by

$$\begin{aligned}\rho(z) &= \rho_0 - 0.2(T(z) + 10) \\ T(z) &= \frac{z}{360} + 20\end{aligned}$$

with ρ_0 the reference density and z the vertical coordinate.

For x_w , the distance from the wall at $x = 800 \text{ km}$, the incoming velocity is given by

$$u_{in}(x_w, z) = -u_0 \exp\left(-\frac{x_w f}{u_0}\right) (1 - F(z^*))$$

with u_0 the maximum incoming velocity, f the Coriolis parameter. $F(z^*)$ is the following function

$$F(z^*) = \begin{cases} 1 & z^* \leq \frac{1}{5} \\ \frac{3z^*}{z^*+1} & -\frac{1}{6} < z^* \leq \frac{1}{5} \\ 0 & -\frac{1}{6} \leq z^* \end{cases}$$

with

$$z^* = \frac{z - h_0 \exp\left(-\frac{x_w f}{u_0}\right) - h_e}{h_0 \exp\left(-\frac{x_w f}{u_0}\right)}$$

where h_0 is the depth of the incoming flow set at 300 m and h_e the depth of the channel set at 600 m.

The incoming fluid temperature is given by

$$T_{in}(z) = \frac{10}{\Delta b_0} \min(-\Delta b_0 (1 - F(z), 0)) + 20$$

with Δb_0 the maximum buoyancy difference between the incoming fluid and the ambient fluid.

Finally, the maximum velocity, u_0 , is set by the following equation

$$u_0 = \sqrt{h_0 \Delta b_0}$$

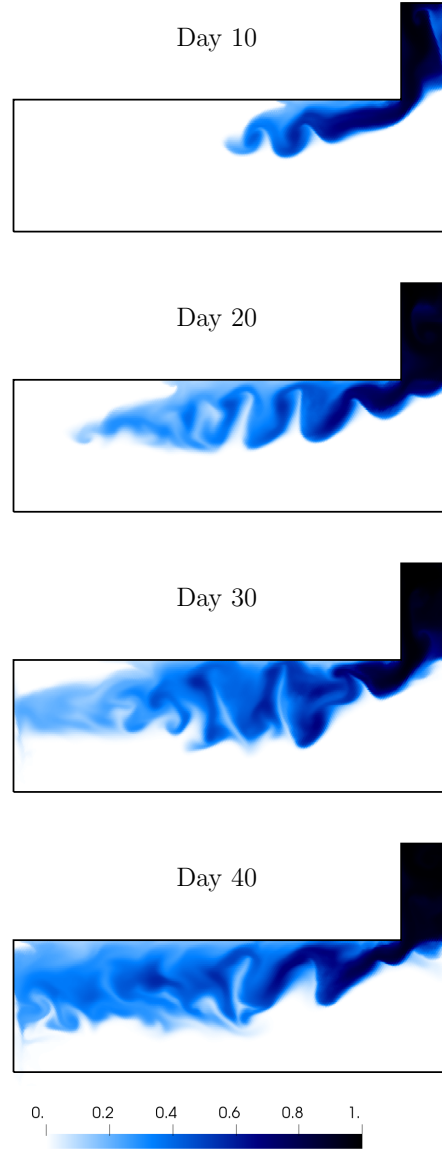


Fig. 4.9: Evolution of the passive tracer concentration in the bottom layer for the DOME test case. The maximum value of u_{in} is 0.75 m s^{-1} . The horizontal viscosity is $18.75 \text{ m}^2 \text{ s}^{-1}$. We have successive snapshots of the passive tracer concentration at 10, 20, 30, 40 days.

The simulation is run for 40 days with a time step of 60 s and a factor M of 30. The results can be seen in Figure 4.9. This is the evolution of the passive tracer in last layer. As the current flows into the basin, it derives westward, forming a coastal plume spanning about 150 km in width. This plume separates from the side boundary, continuing its westward journey along the bottom slope. Upon encountering the stratified ocean, this dense water mass becomes unstable, leading to the formation of swirling eddies and internal waves. The most robust eddies occur within the initial 300 km after the inlet ($x = 500\text{--}800$ km). Beyond this range, the plume becomes more mixed and less turbulent. The plume remains relatively shallow, with the majority of the passive tracer concentrated within 200 meters of the bottom. In terms of its extent, movement, and eddy patterns, the results are in good agreement with the results of Wang et al. (2008).

4.5 Conclusion

This study introduces an innovative split Implicit-Explicit temporal scheme of order 2 specifically designed to tackle the complex ODE equations characterized by three distinct timescales. The main goal of this approach is to limit numerical dissipation due to temporal discretization. This temporal scheme is tailored for equations with extremely stiff terms that are computationally inexpensive. Its semi-implicit aspect specifically targets equations with a high aspect ratio, where the vertical characteristic length is much smaller than the horizontal one. These equations tend to have a more restrictive vertical Courant-Friedrichs-Lewy constraint. For instance, this is applicable to atmospheric or oceanic problems.

This IMEX scheme has undergone extensive theoretical analysis to verify its second-order convergence and assess its stability across diverse scenarios, demonstrating its reliability and robustness in computational simulations.

The application of the IMEX scheme extends to solving intricate 3D hydrodynamic equations, subjecting it to test cases such as Baroclinic Eddies and DOME simulations. These tests serve as empirical evidence of the scheme's exceptional accuracy and computational efficiency in mimicking the complex fluid dynamics observed in oceanic phenomena.

The IMEX scheme, a noteworthy addition to oceanic modeling, stands as a groundbreaking tool capable of accurately capturing ocean behaviors across multiple timescales. Its adeptness in handling intricate dynamics while ensuring computational efficiency signifies a significant progress forward in the realm of oceanic simulations

CHAPTER 5

Conclusion

The secret of a good sermon is to have
a good beginning and a good ending,
then having the two as close together as possible.

— George Burns

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5.1 A small step for the hydrodynamic models, a giant leap for SLIM

To deepen our understanding of the intricate physical processes occurring in coastal waters and to predict their behavior accurately, the development of regional marine models is crucial. Coastal applications demand capturing the complex topographical features and relevant time and length scales associated with river-estuary-shelf sea systems. Unstructured grid methods offer promising solutions for addressing these multi-scale challenges due to their inherent flexibility. Numerical modeling serves as an indispensable tool for studying environmental flows in coastal regions. While forecasting remains a primary application, numerical models also facilitate testing assumptions about underlying processes, conducting sensitivity analyses regarding various parameters, and more.

My research primarily focused on developing temporal methods to tackle the complex multi-scale nature of coastal flows. Two-dimensional processes with small characteristic time live along with three-dimensional slow ones. Both have to be considered while solving the hydrodynamic equations. To limit the numerical dissipation, second order temporal methods are preferred. Moreover, the velocity field and the tracer equation must be consistent with the evolution of the domain. Given these characteristics of coastal flows and their equations, identifying suitable numerical methods presents a non-trivial challenge. This work addressed two key issues. Firstly, a splitting temporal scheme was devised and implemented to optimize computational efficiency by appropriately allocating resources for each process. Secondly, an implicit aspect was incorporated into the scheme to address the vertical restrictive terms, enhancing the model's ability to accurately simulate coastal dynamics.

5.1.1 A split-explicit scheme for the hydrodynamic equations

In Chapter 3, a novel split-explicit Runge-Kutta method for solving the 3D hydrodynamic equations is introduced. The theoretical aspects for this scheme are outlined in Chapter 2, using a simple ODE with fast and slow terms as an illustrative example. Unlike conventional splitting methods employed by others models, this approach aims to facilitate interaction between 2D fast processes and 3D dynamics through the slope of derivatives. This innovation enables the model to achieve second-order accuracy while accommodating the motion of the free surface, which results in dynamic changes to the 3D mesh over time. Given the use of the finite element method, these temporal variations in mesh geometry necessitate adjustments to the mass matrix, a challenge addressed in this thesis through the successful implementation of an Arbitrary

Lagrangian Eulerian scheme. This methodology ensures volume conservation of water throughout the simulation.

Furthermore, the model addresses the evolution of a scalar field, represented by the tracer equation. In this thesis, the tracer is advected by a divergence-free velocity, ensuring the scheme's consistency. Consequently, a uniform tracer remains uniform within a closed domain.

To assess the accuracy of the model, four test cases were conducted. The first evaluated the model's ability to simulate pure barotropic flow, while the second assessed its capability to compute the motion of a domain composed of two distinct densities. Subsequent benchmarks demonstrated the model's proficiency in generating vortices and eddies and handling internal waves between layers of different densities. Finally, laboratory experiments were replicated to assess the model's handling of geostrophic adjustment of a freshwater cylinder and the development of unstable vortices. Notably, the appearance of two lobes in these experiments indicates low numerical diffusion as well as a network convergence of order two.

5.1.2 An implicit component for the vertical terms

Chapter 4 introduced a significant advancement to the model with the introduction of an innovative split second-order IMEX temporal scheme. While vertical viscosity and diffusivity were previously regarded as unproblematic, it became evident that when computed from the turbulence closure model equations, they can impose significant constraints on the 3D time step. This constraint arises from the combination of the small vertical size of the extruded prism and the potential for high turbulent diffusion. Consequently, the hydrodynamic equations exhibit three characteristic timescales: one corresponding to fast 2D dynamics, the next representing horizontal slow 3D phenomena, and the final timescale for vertical stiff 3D dynamics.

The IMEX scheme effectively manages these temporal complexities by explicitly handling extremely short timescales with small time steps, while managing longer timescales semi-implicitly and explicitly using larger time steps. This hybrid approach strikes a balance between computational efficiency and accuracy, offering greater flexibility in time step selection without substantially increasing computational overhead. By efficiently managing the various temporal scales present in the equations, the IMEX scheme optimizes computational resources.

To validate the performance of the IMEX approach, two test cases were conducted. The first, focusing on eddies, assessed the scheme's convergence order and its ability to accurately simulate vortex and internal wave dynamics. The second test case evaluated the model's capability to generate swirling patterns of a dense fluid, demonstrating its effectiveness in handling complex flow phenomena.

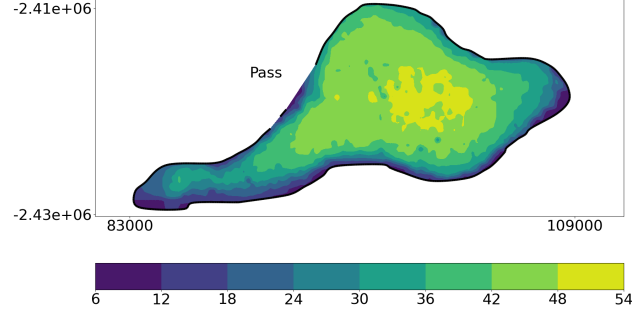


Fig. 5.1: Mururoa Atoll bathymetry [m]. Abscissa and ordinate are in meters.

5.1.3 Mururoa Atoll

The model was further validated through a real-world application: the flow within Mururoa Atoll in the South Pacific. This case study was conducted to assess the model's ability to accurately replicate the real flow patterns.

Mururoa Atoll is part of the Tuamotu Archipelago in French Polynesia. It features a semi-enclosed lagoon connected to the open ocean by a single pass approximately 5 km wide and 8 m deep. The lagoon has an average depth of 33 m, with a maximum depth of around 50 m. Figure 5.1 illustrates the atoll's bathymetry.

At the open boundary, only the semi-diurnal M2 component of the tide is imposed. The period is ≈ 12.4 hours, and the amplitude is 0.3 meters. At the surface, the wind stress is kept constant, $\tau = (-64 \times 10^{-3}, 0)$ N/m². At the bottom, the stress is calculated based on the bottom roughness length, which is set to 4×10^{-2} m in the lagoon and 8×10^{-2} m near the pass. The Coriolis parameter is defined as

$$f = 2\Omega \sin(\Phi)$$

where $\Omega = 7.292 \times 10^{-5} \text{ s}^{-1}$ and Φ is the latitude of the point. This gives a value of $f \approx 5.4e^{-5} \text{ s}^{-1}$ at the atoll. The eddy horizontal viscosity is obtained using the Smagorinsky model with a constant value of 0.01. The vertical viscosity is computed using the $k - \epsilon$ model.

Figure 5.2 illustrates the mesh used for the simulation. The mesh consists of triangles with a characteristic size of 100 m. The vertical mesh comprises 10 σ -levels. The model is run for 10 tidal cycles with a time step of 37 seconds.

The output is validated by comparing the model's results with [Tartinville et al. \(1997\)](#). The stream function, Φ , is used as a diagnostic tool to assess the model's performance. The stream function is defined as

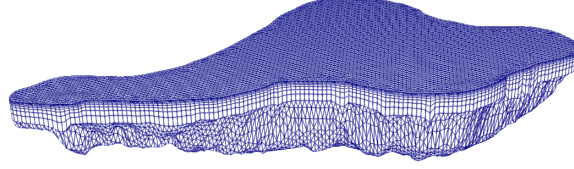


Fig. 5.2: Mururoa Atoll mesh composed of extruded horizontal triangles with a characteristic size of 100 m and 10 σ -levels.

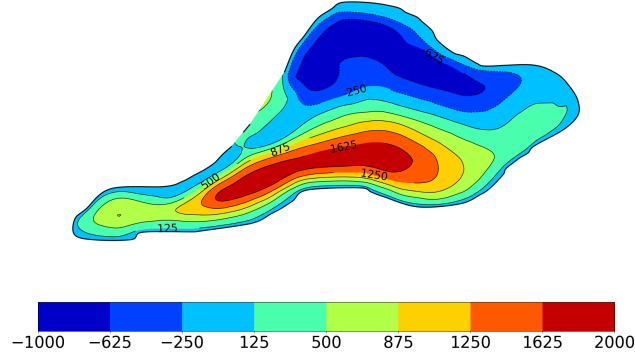


Fig. 5.3: Mururoa Atoll stream function $[\frac{m^3}{s}]$

$$\left(-\frac{\partial \Phi}{\partial y}, \frac{\partial \Phi}{\partial x} \right) = (U^*, V^*)$$

where U^* and V^* are the divergence-free transports obtained as the time average of $\mathbf{U}$ over the last tidal cycle. because of the impermeability of the ridge, the stream function should be constant at the boundaries. It is set at 0 in the results.

Figure 5.3 displays the stream function obtained from the model. The stream function is zero at the boundaries and shows a slow, counter-clockwise pattern in the northern part of the domain. In the southern part, a large clockwise gyre forms. Theses results are consistent with the stream function obtained by Tartinville et al. (1997), as shown in Figure 5.4 despite the fact they do not have the same extrema. The model seems to effectively capture the atoll's complex flow dynamics, including the rotating patterns and the interaction between the atoll and the surrounding ocean.

Finally, to study the dynamics of passive tracers, the residence time of the lagoon was computed. The residence time is defined as the time it takes for a

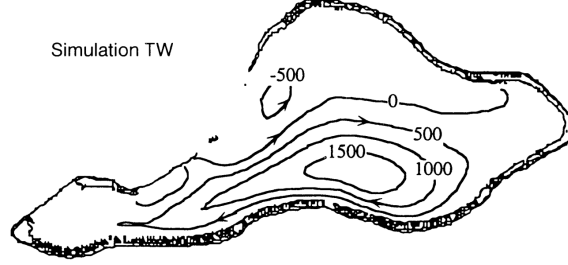


Fig. 5.4: Mururoa Atoll stream function [$\frac{m^3}{s}$] from Tartinville et al. (1997). The TW letters stand for tides and wind.

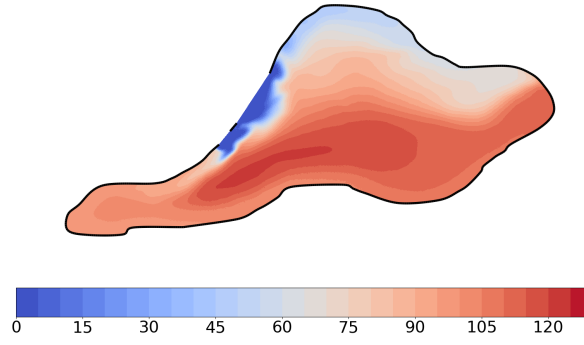


Fig. 5.5: Depth-averaged Mururoa Atoll residence time [days]

particle to leave the lagoon. This calculation is performed using the Eulerian approach, which involves running the simulation backwards in time until the residence time field stabilizes. Specifically, a passive tracer with a concentration of 1 is produced into the domain every second, while the concentration at the pass is set to 0. The velocities used for advection are the negatives of the divergence-free velocities obtained from the last tidal cycle of the hydrodynamic simulation. The horizontal and vertical diffusivities are based on the Okubo model and the $k - \epsilon$ turbulence model, respectively. The simulation continues until the concentration reaches a steady state.

Figure 5.5 shows the residence time distribution within the lagoon. The range extends from 0 to 120 days. Residence time is zero at the pass and increases with distance from the pass. The maximum residence time occurs in the middle of the southern part of the domain. This outcome aligns with the anticipated behavior of the lagoon.

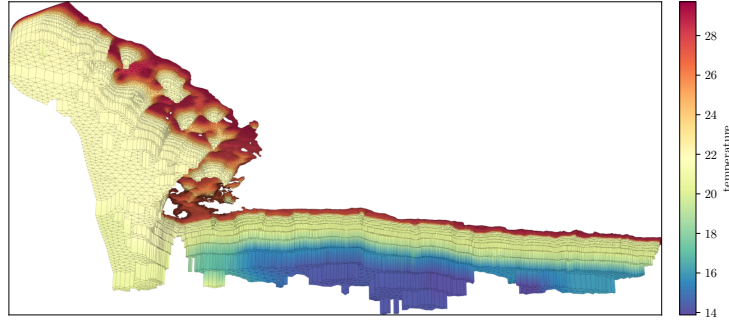


Fig. 5.6: Temperature field in the Tanganyika lake using a z -level mesh.

5.2 And now, for the encore

5.2.1 z -level 3D model

As previously discussed, SLIM3D uses a 3D mesh created from a 2D triangular mesh that undergoes vertical extrusion. Various methods exist for this extrusion process, with the σ -level mesh being the traditional choice used in all simulations presented in this thesis. This method is not strictly essential for the model. In scenarios with steep bathymetric gradients, it may be advantageous to employ a variable number of levels, which is where the z -level mesh becomes relevant.

However, adopting z -level meshes necessitates certain considerations. As the mesh must maintain consistent topology, this extrusion process results in discontinuous bathymetries. The boundaries at the vertical walls where the bathymetry is not constant are referred in this section to as "vertical bottoms" or "stairs." Figure 5.6 illustrates a typical z -level mesh configuration.

However, transitioning to z -level meshes requires certain adjustments, particularly regarding spatial discretization and the interaction between 2D and 3D terms. This section outlines potential steps for implementing a z -level model in the future.

5.2.1.1 The barotropic equations

Adapting the barotropic equations to a z -level mesh presents some straightforward adjustments. With the bathymetry now exhibiting discontinuities, the water height also becomes discontinuous. Consequently, at any given point, the difference between elevations is not necessarily equal to the difference in water height. Therefore, the barotropic equations need to be modified to accommodate this distinction. Instead of employing H as the variable representing water height, it's more appropriate to use η . This alteration necessitates rewriting all the 2D terms discussed in Chapter 3 in terms of η .

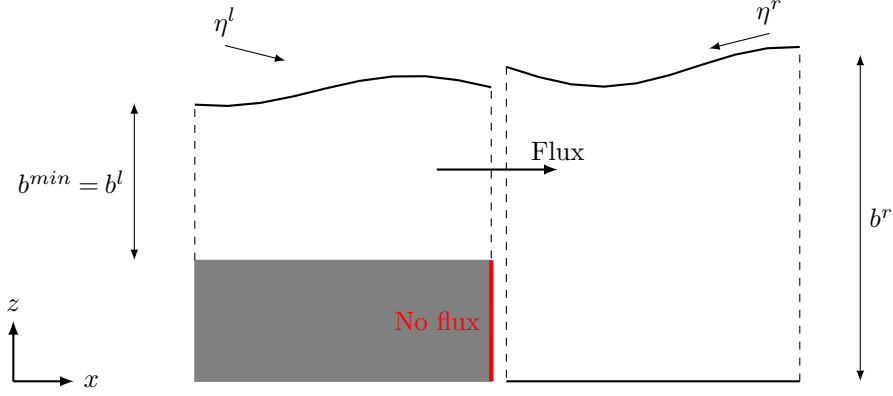


Fig. 5.7: Barotropic flux calculated in the 2D terms in a z -level mesh. The index l and r refer to the left and right elements.

- **Volume terms** remain unchanged. Each element continues to see its individual water height. The adjustment here is that H is now computed as $H = \eta + b$.
- **Flux terms** require adaptation. On the vertical bottoms, there is no flux by definition. Then, these 2D terms should only consider the flux occurring above the stairs. Figure 5.7 illustrates this concept. Consequently, the flux calculation should use $b_{\min}$, representing the minimum bathymetry between the two elements and include the corresponding elevation of the 2D elements. Concretely, in Equation 3.23a, the gravity term

$$-\left\langle\left\langle g - \left(\frac{H_{left}^2 + H_{right}^2}{4} \right) \phi_i \cdot \mathbf{n} \right\rangle\right\rangle \quad (5.1)$$

becomes

$$-\left\langle\left\langle g - \left(\frac{(b_{\min} + \eta^l)^2 + (b_{\min} + \eta^r)^2}{4} \right) \phi_i \cdot \mathbf{n} \right\rangle\right\rangle \quad (5.2)$$

5.2.1.2 The connection between the 2D and 3D models

Once the barotropic equations are adjusted, establishing the correct connection between the 2D and 3D models becomes imperative for maintaining model accuracy. These 2D terms, $\mathbf{F}_{2d} = \mathbf{F}_{flux} + \mathbf{F}_{vol}$, represent the force of $\sqrt{g\eta}$ along the water column. At the stairs, water pushes against the vertical walls. These forces should not be omitted, as they are essential for maintaining the model's accuracy. Then, the 2D terms are reintegrated into the 3D equations across the entire water height.

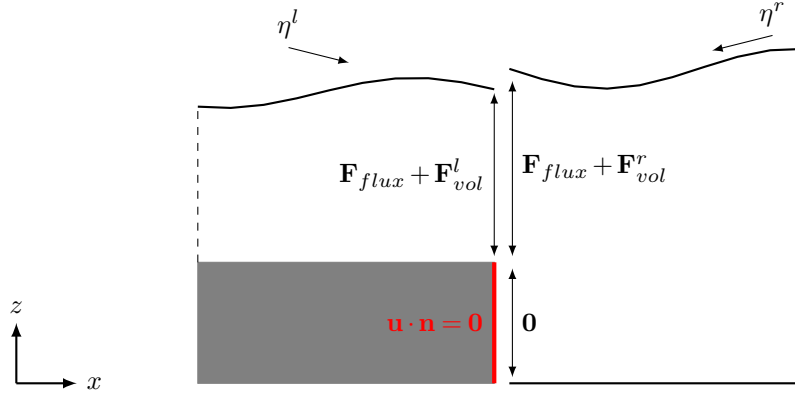


Fig. 5.8: 2D terms are put back into 3D terms above the stairs. Normal velocity is maintained at zero at the vertical bottoms by changing the matrices and the right-hand-side. The index l and r refer to the left and right elements.

This modification alone is insufficient. Physically, the normal velocity at the vertical bottoms must be zero. The adjustments made previously do not ensure this condition. Including gravity volume terms at the vertical bottoms would imply non-zero normal velocities. Therefore, it is necessary to enforce a zero normal velocity at these locations.

One straightforward approach to achieve this is by strongly imposing the normal velocity to be zero at the vertical bottoms. This involves modifying the entries of the mass matrix and the right-hand-side of the equations at these locations to enforce zero normal velocity. However, one must be cautious when implementing this approach. The sum of the 2D terms put in the 3D system should always gives back the terms of the 2D system. When nullifying the values of $\mathbf{F}_{2d}$ at the stairs, these latters should be reintegrated above the stairs. The simplest way to do so is to put all $\mathbf{F}_{2d}$ above the vertical bottoms. This is illustrated in Figure 5.8.

A penalty method using Lagrangian terms could also be efficient. The line and the column of the mass matrix and thr RHS are not modified. Instead, Lagrangian terms λ are added to the system to enforce the zero normal velocity. In this configuration, $\mathbf{F}_{2d}$ from the 2D terms are considered also on the stairs. Then, λ are subtracted on the vertical bottoms. To maintain the good vertical integral, λ are added above the stairs. This method is illustrated in Figure 5.9. The number of unknowns increase. Therefore, this approach breaks the structure of the mass matrix as it is no longer block diagonal. This could lead to a loss of efficiency in the solver. It would also introduce additional complexity during implementation.

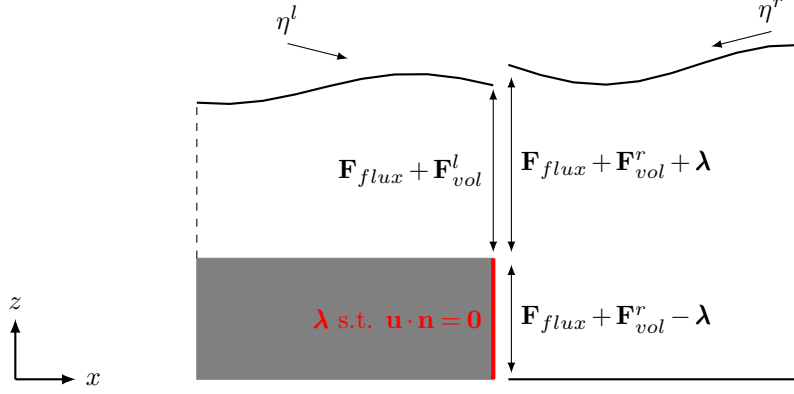


Fig. 5.9: 2D fluxes are put back into 3D terms along the water column. Normal velocity is maintained at zero at the vertical bottoms by adding Lagrangian terms. The index l and r refer to the left and right elements.

5.2.1.3 The velocities in the tracer equation

As described in Chapter 3, the tracer equation is advected by a 3D horizontal transport reconstructed from a combination of a 2D velocity, $h\bar{\mathbf{u}}_{\text{mean}}$, representing the motion of the 3D mesh, and the deviation of the 3D velocity, $h\tilde{\mathbf{u}}$. Here, h denotes the corresponding vertical height of a prism. This approach ensures that the 3D transport includes a 2D component that accounts for the mesh motion. Mathematically, this integration implies that the vertical sum of the 3D transport equals the 2D transport that has shifted with the elevation of the mesh. This is written as

$$\sum_z h\mathbf{u} = \sum_z (h\bar{\mathbf{u}}_{\text{mean}} + h\tilde{\mathbf{u}}) \quad (5.3)$$

$$= H\bar{\mathbf{u}}_{\text{mean}} \quad (5.4)$$

with $H\bar{\mathbf{u}}_{\text{mean}}$ the transport moving η from the beginning of the time step to the end of the time step. Subsequently, a vertical velocity is derived from this 3D transport, and the resulting divergence-free velocity is employed to advect the tracer.

This process must be adapted to the z -level mesh. The 2D velocity is still used to advect the tracer. However, there are two constraints to respect. The first one is that there is no flux at the vertical bottoms. An easy solution is to set the normal 2D velocity to zero at the vertical bottoms. Doing so, the integral of the 3D reconstructed velocities is not the 2D transport anymore.

To address this, all 2D velocity contributions should be positioned above the vertical bottoms. This adjustment ensures that the sum of the 3D transport

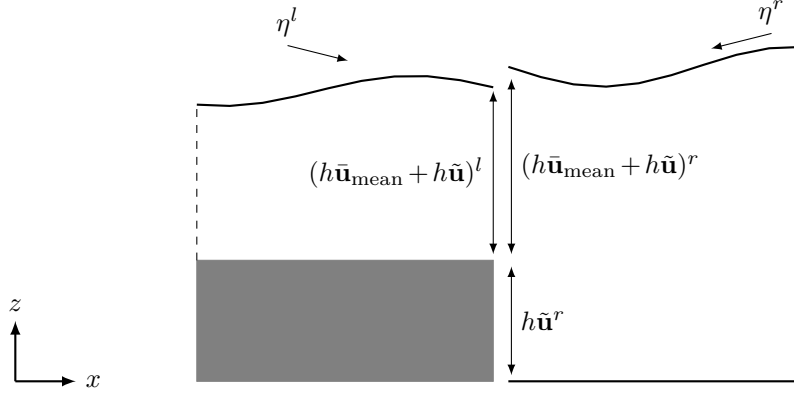


Fig. 5.10: 2D velocities is put back into 3D terms. The index l and r refer to the left and right elements.

aligns coherently with the mesh motion. Additionally, the computation of the deviation of the 3D velocity should adhere to this logic. This adaptation process is illustrated in Figure 5.10.

5.2.2 Non-hydrostatic effects

The model presented in this thesis is based on the hydrostatic assumption. However, in certain scenarios, non-hydrostatic effects may be significant. When considering processes over shorter scales relative to the depth, the non-hydrostatic pressure, which can be thought of as the pressure arising from fluid motion, can also become important. For instance, to be able to simulate waves where the horizontal wavelength is comparable to the vertical wavelength, the hydrostatic assumption is no longer valid. Swell waves on the beach, that are of the order of the depth or shorter, are strongly non-hydrostatic.

Mathematically, this implies that the vertical acceleration term in the momentum equation can no longer be neglected. In others words, the vertical velocity is no longer a function of the horizontal velocity. It becomes an prognostic variable. In figure 5.11, the lock-exchange problem is simulated with a hydrostatic model and a non-hydrostatic model. The non-hydrostatic model is able to capture complex vertical structures that the hydrostatic model cannot. ORCTM (Ocean Regional Circulation and Transport Model, [Huang et al. \(2023\)](#)) SUNTANS or ROMS ([Kanarska et al., 2007](#)) are examples of a model that has been developed to simulate non-hydrostatic effects.

To address this, the model would need to incorporate the vertical equation into the slow dynamics. Furthermore, the calculation of non-hydrostatic processes becomes computationally expensive because of the need to employ high

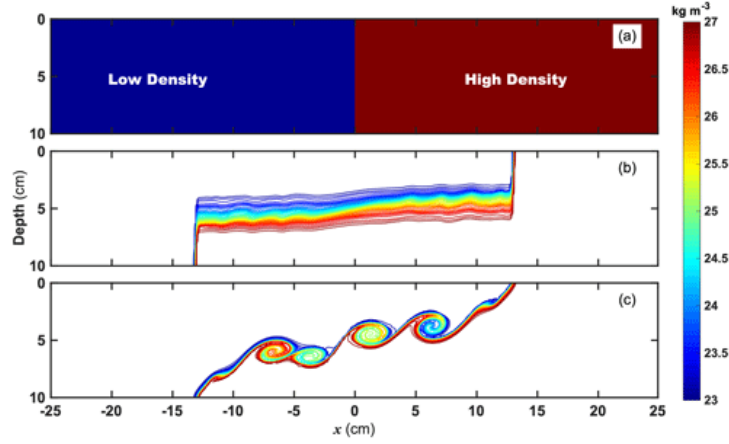


Fig. 5.11: Density deviation field in the lock-exchange test case for the initial condition (a) and for $t = 4.5$ seconds. The hydrostatic model is the middle image while the non-hydrostatic model is the bottom image. Credit: [Huang et al. \(2023\)](#)

grid resolution to resolve processes with short horizontal length scales. It is also expensive because solution of the non-hydrostatic pressure involves inversion of a large, linear system of equations, which can increase the computational cost of an ocean model by up to one order of magnitude ([Fringier et al., 2006](#)). This would require a significant overhaul of the model's structure.

Finally, to respect the consistency of tracer, a proper analysis of the tracer equation would be necessary. This enhancement would enable the model to simulate non-hydrostatic effects, such as internal waves, with greater accuracy.

5.2.3 Data assimilation

The performance of hydrodynamic models is frequently challenged by various sources of uncertainty, including model forcing, structure, and parameter estimation. Consequently, the model's predictions may differ from actual observations. This difference is noticeable in the model's ability to forecast three-dimensional fields like temperature and salinity, as well as two-dimensional variables like water elevation. To enhance the accuracy of state estimates, data assimilation techniques can be employed. By integrating observational data with model predictions, these methods enhance the model's accuracy not only at the current time but also throughout the entire simulation period, owing to improved initial conditions and boundary inputs.

The initial research on data assimilation dates back to ([Richardson, 1922](#)). Subsequently, numerous researchers have explored this field, leading to the emergence of diverse methods. Data assimilation has demonstrated its utility in

disciplines like oceanography (Bertino et al., 2003) and aerospace (Grewal and Andrews, 2010). Presently, two primary categories of assimilation techniques exist: variational analysis methods and sequential methods.

Variational methods use optimization techniques rooted in control theory to minimize a cost function, aiming to estimate unknown parameters. This cost function quantifies the difference between the model and the observed data, with its minimum representing the optimal parameter values. Notably, variational methods possess the capability to move backward in time, rendering them valuable for retroactive analysis of past model outcomes. In contrast, sequential methods adopt a probabilistic approach to generate diverse estimates of system states. The outcome of these methods is the mean of these states, which, when combined with their covariance, furnishes a comprehensive overview of the system's condition. Operating forward in time, sequential methods rely solely on past and present data. Within the variational analysis framework, two widely employed methods are the 3D Variational analysis (Courtier et al., 1998) and the 4D Variational analysis (Courtier et al., 1994; Klinker et al., 2000; Lorenc, 2003).

Due to its computational efficiency, as it does not require an adjoint model, attention shifts to one of the most prevalent sets of sequential methods in oceanography: the Kalman filters. Within the Kalman class of data assimilation techniques, the classic Kalman filter, also known as the Kalman-Bucy filter, serves as the foundational approach. This method was introduced by (Kalman, 1960), with the first practical application implemented by Schmidt (Schmidt, 1981). The fundamental principle involves calculating the mean and covariance of model values and updating them based on observational data. In recent years, two additional implementations have gained attention: the Extended Kalman Filter and the Ensemble Kalman Filter. The Extended Kalman Filter enhances the applicability of the filter to nonlinear models, while the Ensemble Kalman Filter employs ensembles to compute multiple potential model states. These ensembles facilitate the computation of the mean and covariance of the model state. The Ensemble Kalman Filter is currently the most widely used Kalman filter. Since its introduction by Evensen (1994), many researchers have embraced and improved upon this method. One notable enhancement is the incorporation of localization, with significant contributions from Hamill and Whitaker (Hamill et al., 2001) and Zhang and Oliver (Zhang and Olivier, 2010). They introduced two distinct approaches employing distance-dependent filters to mitigate background errors in large-scale models.

SLIM could greatly benefit from integrating this technique. Domain configurations, especially in coastal regions, can exhibit varying dynamics due to factors such as complex bathymetry or the presence of islands. These factors can vary significantly from one region to another and even within the same region. This is where the Ensemble Kalman Filter with localization becomes highly useful.

5.3 This is the end, Beautiful friend

As this thesis draws to a close, so does the journey of the past six years. The outcome is a numerical model capable of simulating complex 3D flows with a moving σ -level mesh. It can handle domains with areas of different density and can also be coupled with the turbulence closure model to estimate realistic vertical viscosity and diffusivity. At the time of writing, simulations on real domains are running successfully. These include applications in the U.S. Virgin Islands (Holstein et al., 2016; Holstein and Smith, 2016). An area in Kuwait has also been simulated using the new SLIM schema. The circulation offshore of Qatar regions also have been investigated. Mururoa atoll lagoon, a region of particular interest, has been successfully modeled. The model has been validated against previous results through a comparison of the velocity field and its the stream function (Tartinville et al., 1997; Tartinville and Rancher, 2000). The results are promising as the model has been able to obtained a residence time consistent with previous studies.

Additionally, thanks to the contributions of this thesis, ongoing enhancements to the 3D module of SLIM have been pursued by other researchers. Notably, significant improvements have been made to the speed the code through a rewrite to enable parallel execution on GPUs. Discontinuous Galerkin elements, due to their discontinuous nature, are particularly suited to this porting. New features have been added to the model, such as the ability to simulate the impact of heat flux on the water column. Precipitation and evaporation have also been added to the model. Furthermore, one significant avenue for enhancement has been under development: the incorporation of vertical discretization using z -level layers. This adaptation would empower the model to navigate realistic environments characterized by extensive bathymetric gradients.

Finally, perhaps the most fitting way to conclude this thesis is to express my gratitude to you, dear reader, dear beautiful friend. As my last words to you, I would like to thank you three times over.

Thank you.

Merci.

Ishimwe .

This word signifies "Thank you" in the author's native language, as well as being his last name. As I told you at the beginning, everything was already written.

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