GULF18, a high-resolution NEMO-based tidal ocean model of the Arabian/Persian Gulf

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Abstract. The sensitivity of a shelf sea model of the Gulf area to changes in the bathymetry, lateral and vertical resolution, vertical coordinates and external forcing is explored. Two new Gulf models with a resolution of 1.8 km named GULF18-3.6 and GULF18-4.0 differing only in the vertical coordinate system and the NEMO codebase employed (NEMO-3.6 and NEMO-4.0.4, respectively) are introduced. We compare them against the existing 4 km PGM4 model, which is based on

5 NEMO-3.4 and is developed and used by the Met Office. PGM4 and GULF18-3.6 use a similar type of quasi-terrain-following vertical levels while GULF18-4.0 employs the multi-envelope method to discretise the model domain in the vertical direction. Our assessment compares non-assimilative hindcast simulations of the three Gulf models for the period 2014-2017 against available observations of tides, hydrography and surface currents. Numerical results indicate that both high resolution models have higher skill than PGM4 in representing the sea surface temperature and the water column stratification on the shelf.

10 In addition, in the proximity of the shelf-break and the deep part of the domain GULF18-4.0 generally presents the highest accuracy, demonstrating the benefit of optimising the vertical grid for the leading physical processes. For the tides and the surface currents the three models give comparable results. However, our tidal harmonic analysis suggests that future work may be needed in order to get real benefit from using a more realistic bottom topography as in the case of the GULF18 models.

1 Introduction

15 The Arabian/Persian Gulf (hereafter, "Gulf") is a shallow, semi-enclosed sea located between the Arabian Peninsula and the south west of Iran and connected to the open Indian ocean via the Strait of Hormuz, the Gulf of Oman and the Arabian Sea. It is an elongated shelf sea representing the main supply of water for industrial and domestic usage for all its surrounding countries. The Gulf region can be impacted by various natural and anthropogenic factors that can importantly affect the quality of its waters and influence the equilibrium of its marine ecosystem (Richlen et al., 2010; Al Shehhi et al., 2014; Zhao and

20 Ghedira, 2014; Gherboudj and Ghedira, 2014). For example, the Gulf area represents one of the major oil-rich regions of the World, where the risk for oil spills and illicit discharges with potential adverse ecological impacts is extremely high (Essa et al., 2005; Zhao et al., 2014, 2015). Therefore, it is of fundamental importance to understand and accurately predict the short-term

dynamics and state of the waters of this basin as well as its climatic and anthropogenic-induced variability.

25   The Gulf dynamics arise from complex interactions between topography, atmospheric fluxes of heat (Al Senafi et al., 2019), freshwater and momentum, river discharges and tides (see for example the exhaustive review given by Hyder et al. (2013)). A general wind- and buoyancy-driven cyclonic inverse estuarine circulation transports low salinity water originating from the Arabian sea and primarily entering the basin from the northern part of the Strait of Hormuz towards the northwestern and southeastern areas of the Gulf (Reynolds, 1993; Johns et al., 1999; Al Senafi and Anis, 2020b). Here, the combination of large

30   evaporation and shallow depths leads to the formation of highly saline waters which leave the Gulf through the deep part of the Strait of Hormuz forming dense bottom waters cascading at the shelf-break (e.g., Shapiro et al. (2017)). Tidal currents are strong and important in controlling the stratification and fronts formation of the basin (particularly close to the Strait of Hormuz, e.g. Matsuyama et al. (1998); Pous et al. (2013); Li et al. (2020)). Whilst early modelling studies found the tidal residual flow to be weak and to not contribute significantly to the main circulation of the Gulf (e.g. Pous et al. (2013)), more

35   recent numerical efforts (e.g. Mashayekh Poul et al. (2016)) showed strong tide-induced residual currents of the order ≈ 15 $cm\ s^{-1}$ in the Strait of Hormuz, more than 5 times greater than previous studies.

Few 3D numerical models of the Gulf hydrodynamics exist in literature. For example, Pous et al. (2015) used a 9 km resolution regional implementation of the MARS3D model (Lazure and Dumas, 2008) with 30 terrain-following σ-levels to describe

40   the intraseasonal to interannual variability in the Gulf circulation and exchange through the Strait of Hormuz. Similarly, Al Azhar et al. (2016) implemented the Regional Ocean Modeling System (ROMS, Shchepetkin and McWilliams (2005)) in the Gulf region with a resolution of 5 km and 25 terrain-following s-levels to study the sensitivity of the model to different vertical turbulence mixing and light penetration schemes. Hyder et al. (2013) presented and evaluated the forecasting skills of PGM4, a regional tidal implementation of the Nucleus for European Models of the Ocean (NEMO) (Madec and NEMO-team, 2016)

45   numerical code with a horizontal resolution of 4 km and 31 s-levels. Shapiro et al. (2017) used the NEMO ocean model with a resolution of $\approx 1.8\ km$ and 52 hybrid s-z levels (Shapiro et al., 2013) to characterise the seasonal variability of the dense outflow from the Gulf into the Gulf of Oman. Likewise, Vasou et al. (2020) used NEMO with a resolution of $\approx 2.6\ km$ and 50 z-levels with partial steps to study the variability of the water mass exchange between the Gulf and the Indian Ocean. Recently, Lorenz et al. (2020) applied the General Estuarine Transport Model (GETM; Klingbeil and Burchard (2013)) with a resolution

50   of $\approx 1.8\ km$ and 40 adaptive vertical layers (Hofmeister et al., 2010) to investigate the properties of the exchange flow of the Gulf.

In this paper we describe and assess GULF18, a new 1.8 km resolution tidal ocean model of the Gulf area, against observations and PGM4, the model developed and used by the Met Office (Hyder et al., 2013). The aim of this study is to explore the

55   impact of using a more realistic bottom topography and coastline, increasing the lateral and vertical resolution, optimising the vertical discretisation scheme for the leading physical processes and updating the external forcing on the accuracy of a Gulf

model .

Some of these developments were motivated by the lessons learned from the operational ocean forecasting system that the
Met Office runs for the north-west European shelf (NWS). For example, Graham et al. (2018a, b) and Tonani et al. (2019)
showed that resolving the internal Rossby radius both on the shelf and in the deep ocean improves the accuracy of the sim-
ulated mesoscale dynamics, better resolving important circulation patterns of the NWS such as the European slope currents
or the across shelf transport. Similarly, Siddorn and Furner (2013) and O'Dea et al. (2017) demonstrated the importance of
increasing the vertical resolution, especially in the case of haline ocean fronts in shallow, tidally-mixed areas or for the fluxes at
the sea surface. More recently, Bruciaferri et al. (2020) and Wise et al. (2021) proved that using a multi-envelope s-coordinate
system (Bruciaferri et al., 2018) allows significant improvements in the accuracy of an ocean model including shelf and deep
ocean areas when compared to traditional models employing geopotential or terrain-following levels.

At the time when the model development was carried out, the latest available stable version of the NEMO code was v4.0.4
(Madec and NEMO-team, 2019). This new version of the code differs significantly from v3.4 (Madec and NEMO-team, 2012),
the release used by PGM4. For this reason, two GULF18 models differing only in the NEMO code version and the vertical
discretisation scheme are developed and compared to PGM4 in this study, allowing a better understanding and assessment of
the impact of each model development included in this new configuration.

Freely accessible observations of the water column physical properties for oceanographic research purposes are scarce in
the Gulf (Hyder et al., 2013) and extensive efforts have been spent in this study to gather all the possible available observations
to validate the skill of our models. To the best of our knowledge, freely accessible and reasonably recent (collected during the
last decade) datasets cover the 2014-2017 span. While such a period is not long enough to evaluate the skill of our models on
climatic time scales, it is suitable to assess their ability in predicting the short term variability of the Gulf dynamics.

The paper is organised as follows. Section 2 details the main features of the new GULF18 model, highlighting the key
differences with the existing PGM4 model in the model domain geometry (Sec. 2.1), vertical discretization schemes (Sec. 2.2),
model core and physics (Sec. 2.3) and external forcing and initialisation (Sec. 2.4). After, Sec. 3 describes the methodology to
assess models' skill while Sec. 4 presents and discusses our main results for tides (Sec. 4.1), sea surface temperature (Sec. 4.2),
water column stratification (Sec. 4.3) and sea surface currents (Sec. 4.4). Finally, Sec. 5 summarises our main conclusions and
future development's plans.

2 GULF18 ocean model

In this study, two different GULF18 models are developed and compared to the existing PGM4. Both GULF18 configurations
share the same bathymetry and horizontal grid but they differ in the vertical discretisation scheme and the version of the NEMO

MODEL PARAMETERS		PGM4	GULF18-3.6	GULF18-4.0
DOMAIN, HORIZONTAL GRID AND BATHYMETRY (SEC. 2.1)				
Bathymetry		GEBCO 2008 + ad-hoc modific.	GEBCO 2014	
Horizontal grid	*Number of points*	244×172	584×432	
	Resolution [km]	≈ 4.3	≈ 1.8	
Land-Sea mask & coastline		from bathymetry + ad-hoc modific.	from bathymetry	
VERTICAL DISCRETISATION (SEC. 2.2)				
Discretisation scheme		vanishing quasi-sigma Song and Haidvogel (1994)	vanishing quasi-sigma Siddorn and Furner (2013)	multi-envelope Bruciaferri et al. (2018)
Number of levels		31	52	
Surface level thickness[m]		$\approx 0.3 - 6$	1	
DYNAMICAL CORE AND PHYSICS (SEC. 2.3)				
NEMO code		v3.4-stable	v3.6-stable	v4.0.4
Reference density	$[kg\ m^{-3}]$	1027	1020	1026
Lateral SGP	*Harmonic diffusivity* $[m^2 s^{-1}]$	3D-constant 50	Smagorinsky-like $1-30$	3D-constant 2
	Bi-harmonic viscosity $[m^4 s^{-1}]$	3D-constant -1.0×10^{10}	3D-constant -4.5×10^8	Mesh size and depth dependent $[-3.84 \times 10^8, -4.54 \times 10^8]$
Penetrative solar radiation		POLCOMS fixed length scale formulation	NEMO RGB formulation	
EXTERNAL FORCING (SEC. 2.4)				
Surface boundary conditions		Flux formulation	Large and Yeager (2009) BULK formulae	
Tidal forcing		TPXOv7.2	FES2014	
Rivers		1	5	

Table 1. Summary of the differences between the currently operational PGM4 configuration and GULF18-3.6 and GULF18-4.0 ocean models.

90 code employed. The first model, named GULF18-3.6, uses NEMO v3.6 (Madec and NEMO-team, 2016) and vanishing quasi-sigma (VQS) vertical levels (Dukhovskoy et al., 2009) similarly to PGM4. The second configuration, named GULF18-4.0, is based on NEMO v4.0.4 (Madec and NEMO-team, 2019) and employs the multi-envelope (ME) method (Bruciaferri et al., 2018) to discretise the domain in the vertical direction. Table 1 summarises the main differences between both GULF18 configurations (hereafter GULF18-*) and PGM4. In the next sections, the key components and parametrizations of GULF18-* along with their main differences with PGM4 are outlined and discussed.

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2.1 Domain, horizontal grid and bathymetry

GULF18-* and PGM4 configurations cover the same area extending from $47° \ 36' \ E$ to $57° \ 38' \ E$ and from $23° \ 03' \ N$ to $30° \ 30'$ N in the zonal and meridional directions, respectively. In addition, they also share the same single open boundary with the adjacent Indian Ocean located in the Gulf of Oman (see Fig. 1a and b).

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Both GULF18 configurations and PGM4 implement a regular geographical horizontal grid with grid lines aligned with parallels and meridians. However, PGM4 uses 244×172 grid points in the zonal and meridional directions, respectively, corresponding to a nominal lateral resolution of $\approx 4 \ km$, while GULF18-3.6 and GULF18-4.0 discretise the horizontal domain with 584×432 grid points, achieving a nominal resolution of $\approx 1.8 \ km$. Considering that in the Gulf the first baroclinic Rossby
105   radius is of order a few km (Hyder et al., 2013), PGM4 can be classified as an eddy-permitting model while GULF18-* configurations are eddy-resolving except in limited areas near the coast where the Rossby radius is very small.
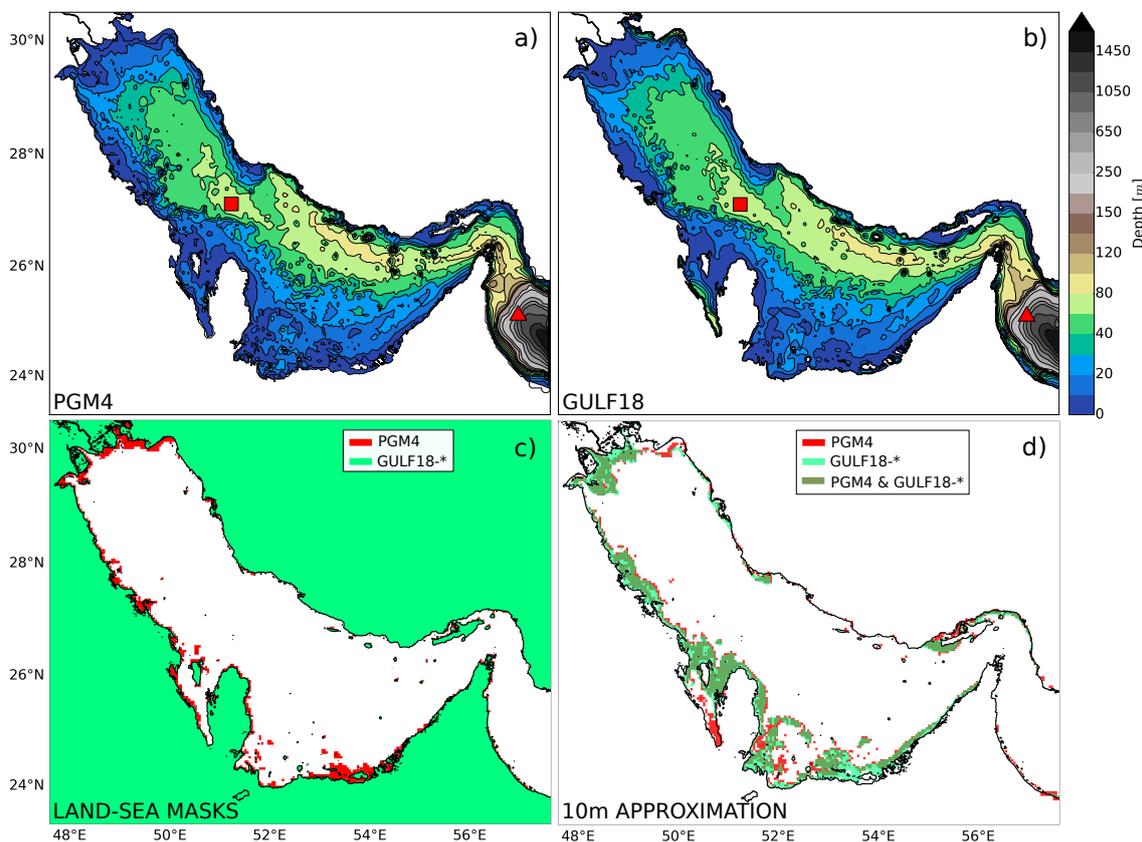
In both GULF18 configurations the bottom topography $H(x,y)$ (with x and y representing the zonal and meridional directions, respectively) is computed from the 30 arc-second resolution General Bathymetric Chart of the Oceans (GEBCO) 2014
110   dataset (see Fig. 1b). In the deep part of the domain (depth $> 300 \ m$) GULF18-* bathymetry is merged with the bottom topography of the Met Office GO6 global ocean configuration at $1/12°$ resolution ((Storkey et al., 2018)). Conversely, the PGM4 model bathymetry is based on the GEBCO 2008 dataset with some additional smoothing to alleviate horizontal pressure gradient errors with terrain-following vertical coordinates (especially in the proximity of the shelf-break, see Fig. 1a) and ad-hoc modifications to widen the channels around Bahrain and the Gulf of Salwa in order to minimise salinity drift due to evaporation
115   (Hyder et al., 2013).

In order to deal with the large tidal excursion characterising the Gulf area, GULF18-* and PGM4 models apply the same strategy of setting the minimum depth of their bottom topography to $10 \ m$ - i.e. the model bathymetry is modified deepening to $10 \ m$ at every grid point where the original depth is shallower than this threshold. Such a crude modelling choice represents
120   the only available solution when tidal ranges are large but the numerical model employed has no wetting-and-drying capability. Figure 1c presents the land-sea mask of GULF18-* (in green) and PGM4 (in red) ocean models while Fig. 1d illustrates the areas where the minimum depth parameterization is applied only in PGM4 (in red), only in GULF18-* (in light green) or in both ocean configurations (in dark green). Both figures clearly show that in the case of PGM4 the land-sea mask and coastline significantly diverge from the original model bathymetry, including important ad-hoc modifications, especially in the northern
125   and southern regions of the domain and in the proximity of Bahrain. In these areas, PGM4 model sets to land all those ocean grid points where the depth is $< 3 \ m$. On the other hand, GULF18-* land-sea mask and model coastline perfectly agree with the original model bathymetry: this modelling choice was preferred since starting from v4.0 the NEMO code is equipped with a wetting-and-drying algorithm (O'Dea et al., 2020) which could be employed in the future to have a more realistic represen-

Figure 1. Upper row: bottom topography of PGM4 (a) and GULF18-* (b) models; Bottom row: Land-sea mask (c) and grid cells where the 10 m approximation has been applied (d) only in PGM4 (red), only in GULF18-* (light green) or in both configurations (dark green). The red square and triangle in panel a and b represent the location where the profiles of models' levels vertical distribution shown in Fig. 4 are extracted.

tation of the water level evolution.

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2.2 Vertical discretisation

In the vertical direction, GULF18-3.6 and PGM4 models implement a vanishing quasi-sigma (VQS) vertical discretization scheme where computational surfaces follow an envelope bathymetry surface rather than the actual model bottom topography (Dukhovskoy et al., 2009; O'Dea et al., 2012). Such an envelope is computed smoothing the model bathymetry with the Mart-

135 inho and Batteen (2006) algorithm to ensure that the maximum value of the slope parameter $r = |H_a - H_b|/(H_a + H_b)$, with H_a and H_b the depths of adjacent grid points (Mellor et al., 1998), is less than a given threshold r_{max}. This solution allows one to have computational surfaces that are less tilted than in pure terrain-following models, hence reducing the errors in computing horizontal pressure gradients (e.g. Shapiro et al. (2013); Bruciaferri et al. (2018)). However, since computational surfaces
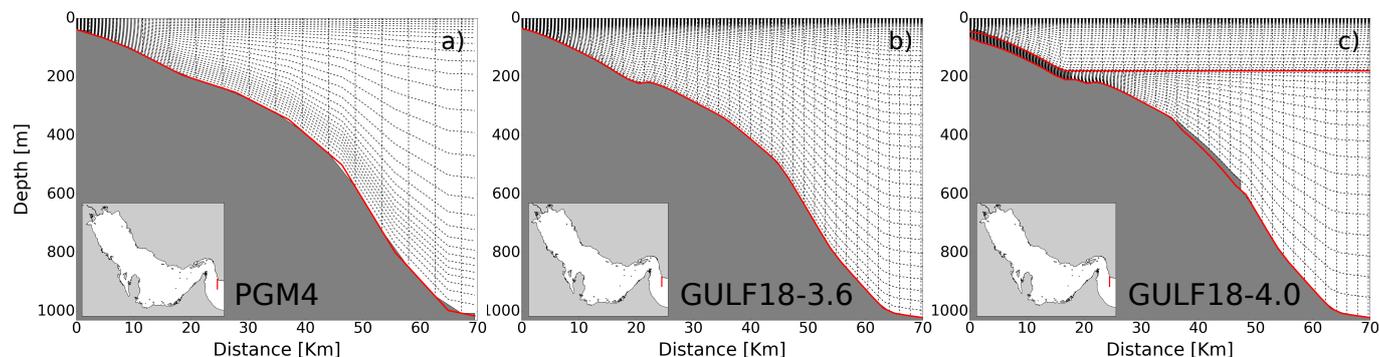
Figure 2. Example of cross-sections showing the model bathymetry and the numerical mesh of PGM4 (a), GULF18-3.6 (b) and GULF18-4.0 (c) configurations. In the case of PGM4 (a) and GULF18-3.6 (b), the red lines represent the envelope bathymetry; in the case of GULF18-4.0 (c), they identify the generalised upper and deeper envelopes $H_e^1(x,y)$ and $H_e^2(x,y)$.

are no longer strictly terrain-following, model cells are masked out in those grid points where the envelope is deeper than
140   the model bathymetry. As a result, when a too severe r_{max} threshold is used, the model bathymetry can include 'saw-tooth'
structures similar to z-level steps that can potentially affect the accuracy of the bottom boundary layer dynamics represented
by the model, including cross-shelf cascading and tides (Bruciaferri et al., 2020; Wise et al., 2021).

Both GULF18-3.6 and PGM4 models use a gentle maximum slope parameter threshold $r_{max} = 0.3$ to generate their enve-
145   lope bathymetry (see panels a and b of Fig. 2). In the case of GULF18-3.6, this r_{max} value was chosen after sensitivity tests
for horizontal pressure gradient errors (HPGE) and tidal dynamics accuracy. The HPGE test is a classical (e.g., Haidvogel
and Beckmann (1999)) idealised numerical experiment where the model is initialised with no horizontal density gradients and
neither external forcing nor explicit diffusion is applied. In this type of problem, the analytical solution for ocean currents is
$0\ m\ s^{-1}$. However, when model levels are not aligned with geopotential surfaces finite difference mathematics may introduce
150   errors in the computation of the pressure gradient force generating undesired numerical spurious currents (e.g., Mellor et al.
(1998); Berntsen (2002)). GULF18-3.6 sensitivity tests showed that whilst decreasing the r_{max} did not significantly reduce
HPGE (after 30 days models using r_{max} equal to 0.3 or 0.1 developed similar basin averaged spurious currents of $\approx 4\ cm\ s^{-1}$),
using a more severe r_{max} had a negative impact on the accuracy of the tidal dynamics represented by the model (e.g., the Mean
Absolute Error of the simulated M2 tidal component increased by $\approx 1\ cm$ when the r_{max} was reduced from 0.3 to 0.1).

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GULF18-4.0 model discretises the vertical domain via a multi-envelope (ME) s-coordinate system (Bruciaferri et al., 2018).
This is a generalised vertical coordinate system where model levels are curved and adjusted to arbitrarily defined surfaces (aka
envelopes) rather than following geopotential levels, the actual bottom topography or a single envelope bathymetry, as is the
case for the GULF18-3.6 and PGM4 models. In such a way, computational levels can be optimised for the leading dynamics
160   in different sub-domains of the model (see Bruciaferri et al. (2018, 2020) for the details).
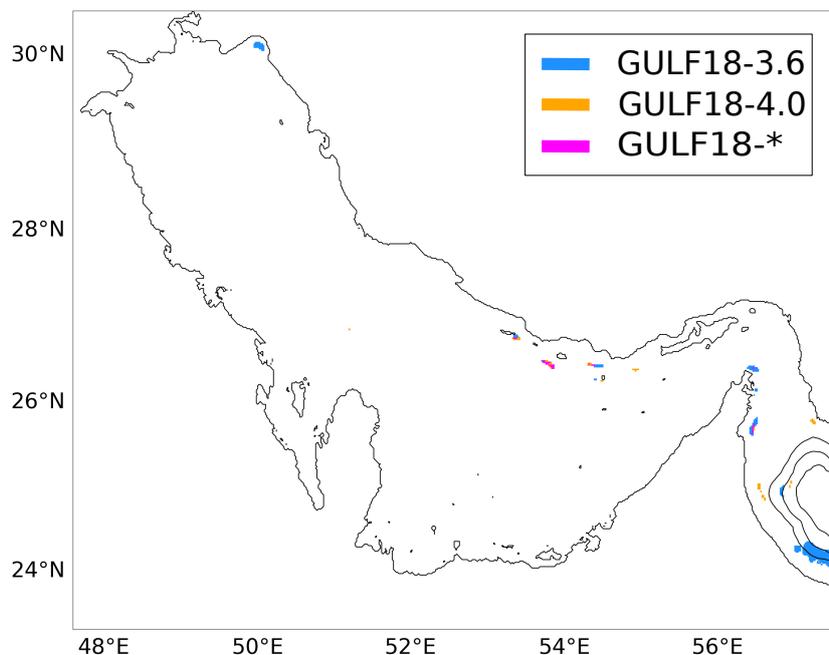
Figure 3. Grid points where spurious currents diagnosed via a HPGE test were $> 5\ cm\ s^{-1}$ only in GULF18-3.6 (blue), only in GULF18-4.0 (orange) or in both high resolution configurations (magenta).

In the case of a shelf sea model such as GULF18, the physical processes that a vertical grid should be able to accurately represent and prioritise are the strong tides and vertical mixing on the shelf, the cross-shelf transport and dense water cascading at the shelf-break and the turbulent exchanges with the atmosphere at the surface (Simpson and Sharples, 2012). Keeping this in mind, the ME vertical grid of GULF18-4.0 is configured using 2 envelopes (see Fig. 2c):

– the upper envelope $H_e^1(x,y)$ follows the actual topography $H(x,y)$ from a minimum depth of $10\ m$ to a maximum depth of $180\ m$ and is smoothed via the Martinho and Batteen (2006) algorithm to have $r_{max} = 0.3$;

– the deeper envelope is computed as $H_e^2(x,y) = max\{H_e^1(x,y) + h,\ H(x,y)\}$, where $h = 30\ m$ represents a user-defined offset parameter, and the Martinho and Batteen (2006) smoothing algorithm is applied to ensure that $r_{max} = 0.1$

Wise et al. (2021) showed that in a NWS model using a ME system with envelopes optimised to have HPGE $< 5\ cm\ s^{-1}$ gives significantly increased accuracy compared to VQS levels. Learning from this experience, both GULF18-4.0 envelopes were additionally smoothed at grid points where HPGE (assessed with a HPGE test) were larger than $6\ cm\ s^{-1}$ in the case of $H_e^1(x,y)$ and $3\ cm\ s^{-1}$ for $H_e^2(x,y)$, with target r_{max} parameters equal to 0.09 and 0.04, respectively. In the case of the upper envelope, a less restrictive threshold is applied than Wise et al. (2021) since GULF18-3.6 sensitivity tests showed that the accuracy of the simulated tidal dynamics is highly sensitive to how the model represents the bottom topography.
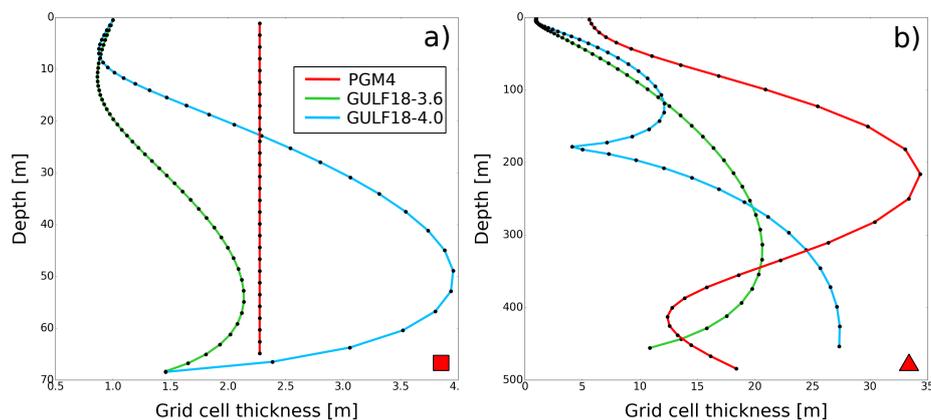
Figure 4. Model cell thickness as a function of depth for PGM4 (in red), GULF18-3.6 (in green) and GULF18-4.0 (in blue) models in two representative locations of the shelf (a) and the deep basin (b), respectively. The location of the two profiles is identified by the red square (panel a) and triangle (panel b) in Fig. 1.

Figure 3 shows the model cells where the maximum (in the vertical and time) spurious velocities were $> 5 \, cm \, s^{-1}$ only in GULF18-3.6 (in blue), only in GULF18-4.0 (in orange) and in both GULF18-* configurations (in magenta) after a 30 days-long HPGE test. Numerical results show that the multi-envelope configuration chosen for GULF18-4.0 allows the use of a 3D

180 varying r_{max} parameter which reduces the large HPGE affecting GULF18-3.6 in the proximity of the continental slope while minimising the number of undesired artificial saw-tooth structures on the shelf and shelf-break.

Both GULF18-* configurations use 52 computational surfaces to discretise the vertical domain while PGM4 employs 31 model levels. Figure 4 presents the vertical resolution of PGM4 (in red), GULF18-3.6 (in green) and GULF18-4.0 (in blue)

185 models at two representative locations of the shelf (a) and the deep basin (b), respectively. The vertical distribution of PGM4 computational surfaces is stretched according to the Song and Haidvogel (1994) function while GULF18-3.6 uses the Siddorn and Furner (2013) stretching formulation. In the case of GULF18-4.0, 35 ME s-levels are allocated to the upper sub-zone (i.e., between the free surface and the upper envelope) stretched according to Siddorn and Furner (2013) while 17 levels are used in the deeper part of the domain distributed to ensure that the vertical coordinate transformation and its Jacobian are continuous

190 (see Bruciaferri et al. (2018) for the details). Because of the Siddorn and Furner (2013) stretching formulation, the surface vertical level of GULF18-* configurations has a constant thickness of $1 \, m$ while in PGM4 it ranges from $0.3 \, m$ on-shelf to $6 \, m$ off-shelf (Fig. 4). In addition, PGM4 presents uniformly distributed vertical levels in areas shallower than $150 \, m$, while GULF18-* models switch off model levels' stretching only in areas shallower than $50 \, m$ (Fig. 4a).

195 As shown in Fig. 2c and Fig. 4b, GULF18-4.0 is configured to have increased resolution in the proximity of the maximum depth of the upper envelope, which corresponds to the depth where the shelf-break occurs ($\approx 200 \, m$). Such increased reso-

lution near the envelopes is a feature of the ME system which help to mitigate potential inaccuracies when simulating dense water cascading down a steep topography in those areas where model levels are not strictly terrain-following (see Fig 2c and experiment two of Bruciaferri et al. (2018)).

200 2.3 Dynamical core and model physics

GULF18-4.0 is based on NEMO v4.0.4 (Madec and NEMO-team, 2019), GULF18-3.6 on NEMO v3.6-stable (Madec and NEMO-team, 2016) while PGM4 uses NEMO v3.4-stable (Madec and NEMO-team, 2012). NEMO v4.0.4 presents numerous differences from v3.4-stable, while v3.6-stable can be considered an intermediate release between the two - see http://forge.ipsl.jussieu.fr/nemo/wiki/Changelog for a comprehensive list of the main features of each NEMO release.

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GULF18-* configurations build upon, and thus share, many of the core features of PGM4 model. For example, in order to accurately resolve the important tidal dynamics PGM4 and GULF18-* configurations implement a similar non-linear free surface via the NEMO variable volume layer (Levier et al., 2007) and time-splitting algorithms, using baroclinic and barotropic time-steps of $60\ s$ and $2\ s$, respectively. In addition, the three models also use the same pressure Jacobian scheme to compute

210 hydrostatic pressure gradients and the Energy and ENstrophy (EEN, Arakawa and Lamb (1981)) conserving scheme to advect momentum. Similarly, the 2nd order Flux Corrected Transport (FCT) scheme, referred to as Total Variance Dissipation (TVD) scheme in the case of NEMO v3.4 (PGM4) or v3.6 (GULF18-3.6), is applied by all models to advect active tracers along with a non-linear equation of state based on EOS-80 formulation UNESCO (1983). The three models agree also on the turbulent bottom boundary layer formulation, implementing an implicit logarithmic bottom friction with a roughness length z_0 of 3×10^{-3}

215 m and a minimum drag coefficient C_D of 2.5×10^{-3}. Finally, PGM4 and GULF18-* models implement the General Length Scale (GLS) turbulent closure scheme with similar settings to compute the vertical eddy viscosity and diffusivity coefficients.

GULF18-* and PMG4 configurations present also some important differences in the physics they implement (see Table 1). One major difference concerns the formulation of the lateral eddy fluxes. PGM4 is an eddy permitting model that needs to

220 parameterize some of the mesoscale and the full sub-mesoscale eddy turbulence. Therefore it uses a Laplacian operator with a 3D constant diffusivity of $50\ m^2\ s^{-1}$ for tracers and a bi-harmonic operator with a constant viscosity of $-1 \times 10^{10}\ m^4\ s^{-1}$ for momentum. On the other hand, GULF18-* configurations are eddy-resolving almost everywhere and therefore need to parameterise only the sub-mesoscale eddy fluxes. Both GULF18-* configurations use a horizontally aligned Laplacian operator for tracers and an along-levels oriented bi-harmonic operator for momentum. In the case of GULF18-3.6, it was chosen to test a

225 Smagorinsky-like diffusivity ranging between $1\ m^2\ s^{-1}$ and $30\ m^2\ s^{-1}$ while for GULF18-4.0 it was preferred a 3D constant diffusivity of $2\ m^2\ s^{-1}$ (the correspondent eddy velocity and length scales are $U_{scl} = 0.01\ m\ s^{-1}$ and $L_{scl} = 200\ m$, respectively). In the case of momentum, GULF18-3.6 applies a constant mixing coefficient of $-4 \times 10^8\ m^4\ s^{-1}$ while GULF18-4.0 uses a mesh size and depth dependent viscosity ranging between $3.84 \times 10^8\ m^4\ s^{-1}$ and $4.54 \times 10^8\ m^4\ s^{-1}$ (the correspondent velocity scale is $0.85\ m\ s^{-1}$).

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In the case of PGM4, the NEMO code was modified to include a POLCOLMS-style scheme for the penetration of the incoming solar short-wave radiation and the model was set to use a fixed 1-D attenuation length scale of 6.49 m (Hyder et al., 2013). In contrast, GULF18-* configurations employ the standard NEMO RGB light penetration scheme.

2.4 External forcing and initialisation

235 Ocean simulations discussed in this manuscript are free-running (i.e., with no data assimilation) numerical experiments spanning five years, from 2013 to 2017. Each model is initialised from rest with temperature and salinity fields computed by PGM4 on 16 January 2013 (in the case of GULF18-* configurations a pre-processing 3D regridding procedure was applied). The first year of the simulations is considered as spin-up time and hence is not included in the analysis.

240 At the surface, GULF18-* and PGM4 are forced with atmospheric fields from the Numerical Weather Prediction (NWP) configuration of the global Met Office Unified Model (Walters et al., 2019). NWP hindcast data are available at a horizontal resolution of $\approx 25\ km$ before 2014-07-17, $\approx 17\ km$ from 2014-07-17 to 2017-07-13 and $\approx 10\ km$ after 2017-07-13 and include three-hourly data for heat and freshwater fluxes, while the momentum flux is provided with a hourly resolution. A major difference between GULF18-* and PGM4 configurations is the way they compute the boundary conditions at the surface.

245 While PGM4 uses directly prescribed NWP fluxes (i.e., the NEMO flux formulation), GULF18-* models apply the Common Ocean-ice Reference Experiment (CORE) bulk formulae (Large and Yeager, 2009) to NWP atmospheric fields to compute momentum, heat and freshwater fluxes at the air-sea interface.

At the single open boundary in the Gulf of Oman, GULF18-* and PGM4 apply a Flather (1976) radiation boundary condi-
250 tion to propagate tidal energy in the domain. In the case of GULF18-*, tidal elevation and velocity are derived from eight tidal constituents extracted from FES2014 gridded tidal analysis (Lyard et al., 2021) while PGM4 uses the TPXOv7.2 dataset (Egbert and Erofeeva, 2002). In this study, GULF18-* and PGM4 configurations are one-way nested within the Met Office Indian Ocean FOAM $1/12°$ model (Storkey et al., 2010). GULF18-* and PGM4 models use the flow relaxation scheme (Martinsen and Engedahl, 1987) to relax temperature and salinity fields to the values specified by the Indian Ocean FOAM $1/12°$ model
255 over a ten point relaxation zone and the Flather boundary condition to add Sea Surface Height (SSH) and barotropic currents from the Indian Ocean FOAM system to the tidal constituents.

GULF18-* and PGM4 use climatological river run-off forcing. However, in PGM4 only the Shatt al-Arab (Tigris and Euphrates) river inflow at the Gulf's head is considered, while in GULF18-* domain also the Zohreh, Helleh, Mond and Minab
260 rivers are included.

3 Models' evaluation approach

In this study we assess and compare the skills of PGM4, GULF18-3.6 and GULF18-4.0 models in reproducing the observed Gulf ocean dynamics during the period 2014-2017. Such a time-frame was chosen considering the number of available observations for the validation.

265   In addition to the hydrodynamics simulations, we conduct also Lagrangian experiments to assess the accuracy of the surface dynamics reproduced by our three Gulf models. Numerical experiments consisted of forcing a Lagrangian particle transport model with surface current velocities computed by PGM4 and GULF18-* models to numerically reproduce the trajectories of satellite-detected drifter tracks.

        The next three Sections describe the observational datasets used for the verification (Sec. 3.1), the set-up of the additional
270 Lagrangian simulations (Sec. 3.2) and the metrics used in the assessment (Sec. 3.3).

3.1 Observational datasets
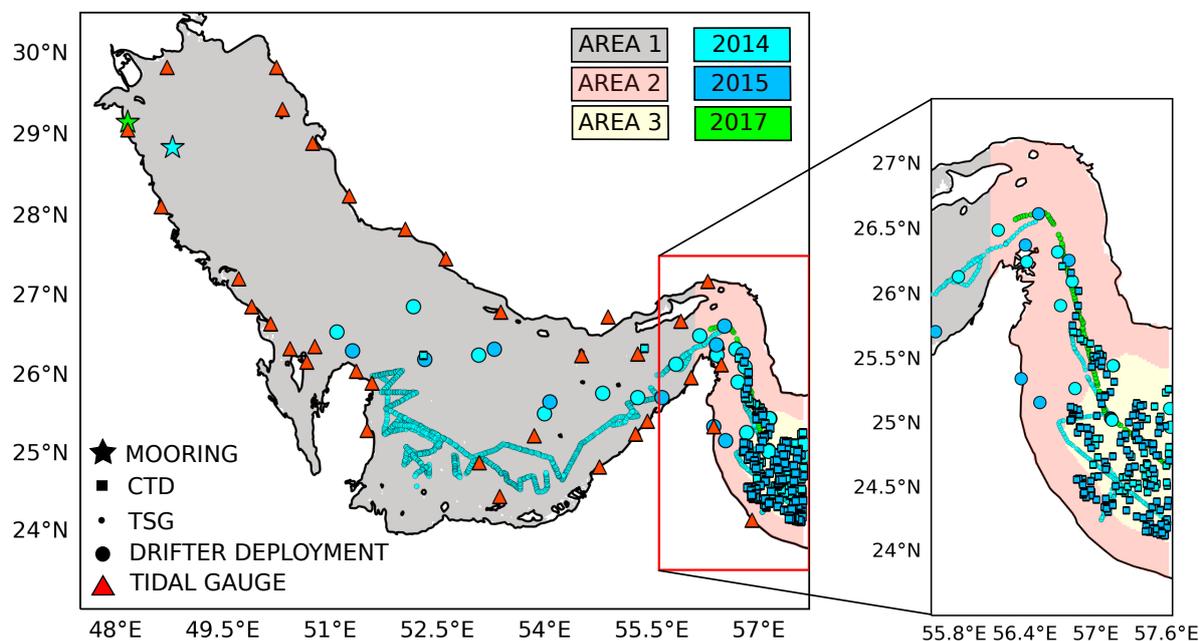
Figure 5. Map describing the three areas applied to analyse models' results together with the location and the temporal availability of the observations used in this study.

Observations used to validate the numerical results include:

- Tidal constituents' amplitude and phase data computed by Pous et al. (2013) and Mashayekh Poul et al. (2016) conducting harmonic analysis on 34 tide-gauges recorded water-level time-series (see red triangles in Fig. 5 for location of the tide-gauges' included in the analysis).

- The Met Office Operational Sea surface Temperature and sea Ice Analysis (OSTIA) dataset (Donlon et al., 2012). This is a high resolution analysis of the global ocean sea surface temperature (SST) produced by combining satellite and in-situ SST observations with an accuracy (RMSE) of 0.57°C and zero bias (Donlon et al., 2012).

- The global ocean, near real-time (NRT), in situ quality controlled observational dataset (Wehde et al., 2021) from the Copernicus Marine Environment Monitoring Service (CMEMS). This dataset includes profiles of temperature (T) and salinity (S) from Conductivity-Temperature-Depth (CTD) measurements, T and S observations from ThermoSalinoGraphers (TSG) and satellite-tracked iSphere drifters trajectories. The locations of CTD and TSG measurements (squares and small circles, respectively) and where drifters were deployed (big circles) are shown in Fig. 5.

- Two hydrographic observational datasets. The first dataset includes 3 months measurements from mid-January to mid-April 2014 at a mooring station located approximately 44 km off the coast of Kuwait and 120 km south of the Gulf's northern tip (see cyan star in Fig. 5 for location). The nominal water depth at mooring station was 23 m. The mooring was equipped with four high resolution temperature sensors (RBR, SOLO T) sampling at 2 Hz and two CTDs (RBR, XR-420) sampling every 18 seconds. Unfortunately, only the six instruments described above were recovered from the lower half of the mooring station and used for analysis. The second dataset includes 12 day measurements in July 2017 at mooring station located approximately 4 km off the coast of Kuwait (see green star in Fig. 5 for location). The nominal water depth at mooring station was 23 m. The mooring was equipped with nine high resolution temperature sensors (RBR, SOLO T) sampling up to 16 Hz and two CTDs (RBR, XR-420) sampling every 4 seconds. These two datasets are the only observations that provide time series of the water column vertical thermal structure in the northern Gulf, and several studies have analysed these data (e.g., Li et al. (2020); Al Senafi and Anis (2020b, a)).

Not all the observations are covering the entire period of the numerical experiments, see Table 2 and Fig. 5. The model validation has been tailored on the uneven distribution of the different type of observations.

MEASURED VARIABLE	INSTRUMENT	AVAILABLE OBSERVATIONS				UNITS
		2014	2015	2016	2017	
Water column T	CTD profiler	61	136	—	—	num. of downcasts
	Moored CTD	80			14	days of the timeseries
Water column S	CTD profiler	55	136	—	—	num. of downcasts
Near-surface T/S	TSG sampler	1978	—	—	111	num. of measurements
Lagrangian trajectories	iSphere drifters	17	11	—	—	num. of trajectories

Table 2. Number and type of T/S and Lagrangian observations available for this study. The location of the measurements is shown in Fig. 5.

Geoscientific
Model Development
Discussions

3.2 Lagrangian simulations of iSphere drifters

iSphere drifters are half submerged spherical drifting buoys transported by surface ocean currents, wave-induced drift and the direct leeway of the wind (e.g., De Dominicis et al. (2016)). However, since the aim of our Lagrangian simulations was to validate ocean currents, in order to facilitate the results' interpretation it was preferred to not include the Stokes' drift in our Lagrangian simulations, similarly to Barron et al. (2007); Carniel et al. (2009); Amemou et al. (2020).

We use OpenDrift Lagrangian framework (Dagestad et al., 2018; Dagestad and Röhrs, 2019) with a 4th order Runge-Kutta scheme and a timestep of $3600 \; s$ to integrate the following initial value problem for the drifter position $\boldsymbol{x}(t) = (x(t), y(t))$:

$$\begin{cases} \dfrac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{u}(\boldsymbol{x}(t), t) + \boldsymbol{u}_w(\boldsymbol{x}(t), t) + \boldsymbol{u}'(\boldsymbol{x}(t), t) \; , & \text{(1a)} \\ \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \; , & \text{(1b)} \end{cases}$$

where $\boldsymbol{x}_0$ is the initial drifter position at time t_0, $\boldsymbol{u}(\boldsymbol{x}(t), t)$ represents the surface Eulerian currents computed by the three Gulf models, $\boldsymbol{u}'(\boldsymbol{x}(t), t) = \alpha \, R$ with $R \in [-1, 1]$ and $\alpha = 0.04 \; m \; s^{-1}$ is used to simulate sub-grid turbulent diffusion and $\boldsymbol{u}_w(\boldsymbol{x}(t), t)$ is the wind drag velocity parameterised as $\boldsymbol{u}_w(\boldsymbol{x}(t), t) = \gamma \, \boldsymbol{U}_{10}(\boldsymbol{x}(t), t)$, with $\boldsymbol{U}_{10}(\boldsymbol{x}(t), t)$ the wind velocity at 10 m (from NWP fields) and $\gamma = 0.01$ in agreement with De Dominicis et al. (2016).

In order to maximise the usability of the observational dataset and to reduce the separation distance between observed and simulated track to an acceptable level (e.g., Dagestad and Röhrs (2019)), available satellite-tracked drifters trajectories were chunked into segments of 48 h duration. Then, similarly to Bruciaferri et al. (2021), for each segment 100 numerical drifters were released at the same initial location and time and the drift 48 h ahead was computed.

3.3 Evaluation metrics

In the case of tidal components and T/S measurements, the accuracy of PGM4 and GULF18-* models is quantified using the following metrics:

– Mean Bias Error:

$$MBE = N^{-1} \sum_{i=1}^{N} x_{i,m} - x_{i,o} \tag{2}$$

– Root Mean Square Error:

$$RMSE = \left[N^{-1} \sum_{i=1}^{N} (x_{i,m} - x_{i,o})^2 \right]^{1/2} \tag{3}$$

– Correlation coefficient:

$$r = \frac{\sum_{i=1}^{N} (x_{i,m} - \overline{x}_m)(x_{i,o} - \overline{x}_o)}{\left[\sum_{i=1}^{N} (x_{i,m} - \overline{x}_m)^2 (x_{i,o} - \overline{x}_o)^2 \right]^{1/2}} \tag{4}$$

where N is the total number of available observations, $x_{i,m}$ and $x_{i,o}$ are the values of the ith realisation of model and observational datasets, respectively, with mean values $\overline{x}_m = N^{-1} \sum_{i=1}^{N} x_{i,m}$ and $\overline{x}_o = N^{-1} \sum_{i=1}^{N} x_{i,o}$.

325

For T/S observations, metrics are computed bilinearly interpolating hourly model outputs on the geographical location of each T/S measurement. Then, in the case of hydrographic datasets, both observed and modelled profiles are also linearly interpolated on 26 reference depths with increased vertical resolution (from $2.5\ m$ to $25\ m$) in the first $200\ m$ of the water column. Harmonic analysis for computing models' tidal constituent amplitudes and phases is carried out using hourly Sea Surface
330 Height (SSH) model fields for the year 2014. Then, the comparison with observations is conducted considering the closest grid point to the location of each tide-gauge.

The accuracy of the Lagrangian simulations is quantified using the Liu and Weisberg (2011) skill score (ss). This metric evaluates the separation between modelled and observed drifter trajectories normalized by their total length:

$$335 \quad s = \frac{\sum_{i=0}^{N} d_i(\boldsymbol{x}_s(t_i), \boldsymbol{x}_o(t_i))}{\sum_{i=0}^{N} l_{oi}(\boldsymbol{x}_o(t_0), \boldsymbol{x}_o(t_i))} , \tag{5}$$

where N is the total number of observed drifter positions in a given trajectory, t_i is the time at which the ith drifter position has been recorded, t_0 is the time at which the drifter has been deployed, d_i are distances between simulated $\boldsymbol{x}_s(t_i)$ and observed $\boldsymbol{x}_o(t_i)$ drifter positions at time t_i and l_{oi} is the length of the observed trajectory at time t_i. The skill score ss is then defined as

$$ss = \begin{cases} 1 - s & , \text{if } s \leq 1 , \\ 0 & , \text{if } s > 1 , \end{cases}$$

340 so that $ss = 1$ indicates a perfect simulation while $ss = 0$ identifies a simulation with no skill. For each drifter simulation, 100 particles were released at the same initial location and time and the skill score of each numerical track was computed following Bruciaferri et al. (2021).

Whilst increasing the resolution of an ocean model typically allows one to better resolve finer-scale features, metrics based
345 on direct point matchup between interpolated model data and observations could not improve with higher granularity. This is due to the double penalty effect (e.g., Crocker et al. (2020)): features correctly predicted but misplaced with respect to the observations are penalised twice, for not occurring at the observed location and at the same time for occurring at the location where they were not observed. In this study, we found at least comparative performance of the high resolution GULF18 models with PGM4 using traditional verification techniques for the majority of the metrics included in the analysis. However, in
350 the case of the surface currents assessment it was preferred to include in the analysis only those trajectories that presented a skill score $ss \geq 0.35$ for all the three Gulf models to avoid a potential double penalty bias, resulting in a total of 183 iSphere trajectories (145 in 2014 and 38 in 2015).

Models' evaluation metrics are computed considering the entire basin or dividing the domain in three zones as shown in

355 Fig. 5: the shelf area (longitude $< 56.1°E$, grey zone), the deep basin (depth $> 300\ m$, yellow area) and the shelf-break zone (longitude $> 56.1°E$ and depth $< 300\ m$, pink area).

4 Results and discussion

4.1 Tidal harmonics

The Gulf presents a complex tidal regime, characterised by tidal standing waves varying from being primarily semi-diurnal

360 to diurnal and a large tidal range, with M2 peak amplitudes $> 1\ m$ throughout the whole domain (e.g. Proctor et al. (1994); Hyder et al. (2013)). The Gulf topography includes a shallow zone near the closed end which combines with an asymmetric cross-sectional depth profile (see Fig. 1). This particular conformation of the basin leads the generation of resonant interactions between semi-diurnal and diurnal waves resulting in tidal amplification at the northern end of the basin and a Kelvin-Taylor type system of amphidromic points shifted towards the coast to which the reflected Kelvin wave is bound (Roos and Schutte-

365 laars, 2011). Consequently, semi-diurnal constituents present two amphidromic points in the northwestern and southern ends of the Gulf while diurnal constituents have a single amphidromic point in the central western part of the basin (Pous et al., 2013).
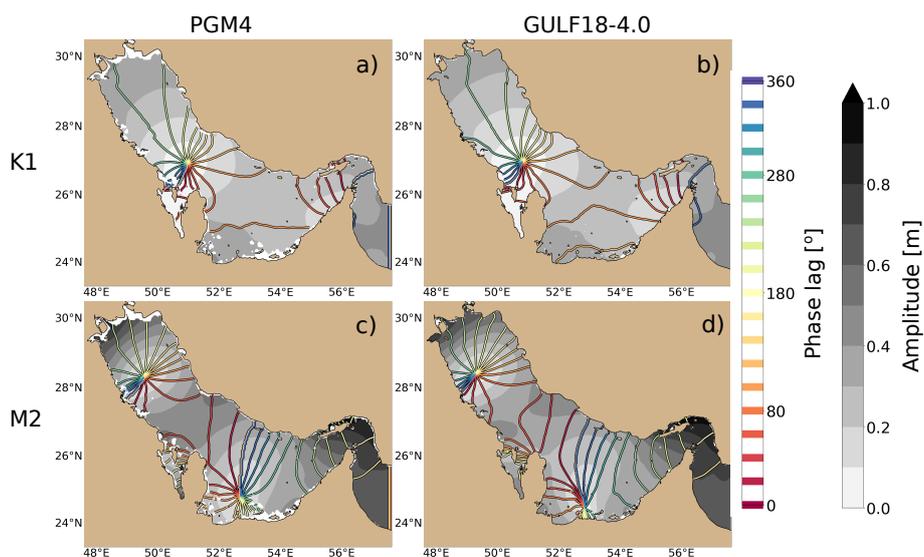

Figure 6. K1 (top panels) and M2 (bottom panels) co-tidal plots for PGM4 (a,c), and GULF18-4.0 (b,d). Shading shows amplitude (m) while contours present the phase lag (°). GULF18-3.6 maps are not shown for clarity, being very similar to GULF18-4.0 results.

Figure 6 presents co-tidal charts of the principal diurnal (K1, top row) and semi-diurnal (M2, bottom row) components of

370 PGM4 (a,c) and GULF18-4.0 (b,d) models (for clarity, here and in Fig. 7a,b only GULF18-4.0 results are shown, being the

differences between the two GULF18 configurations almost negligible). In general, the three models reproduce the typical pattern of the amphidromic points of the Gulf as in Pous et al. (2013). The main differences between PGM4 and GULF18-* models are where the coastline and the bathymetry differ the most, i.e. near the coasts of Qatar, Bahrain and south UAE.
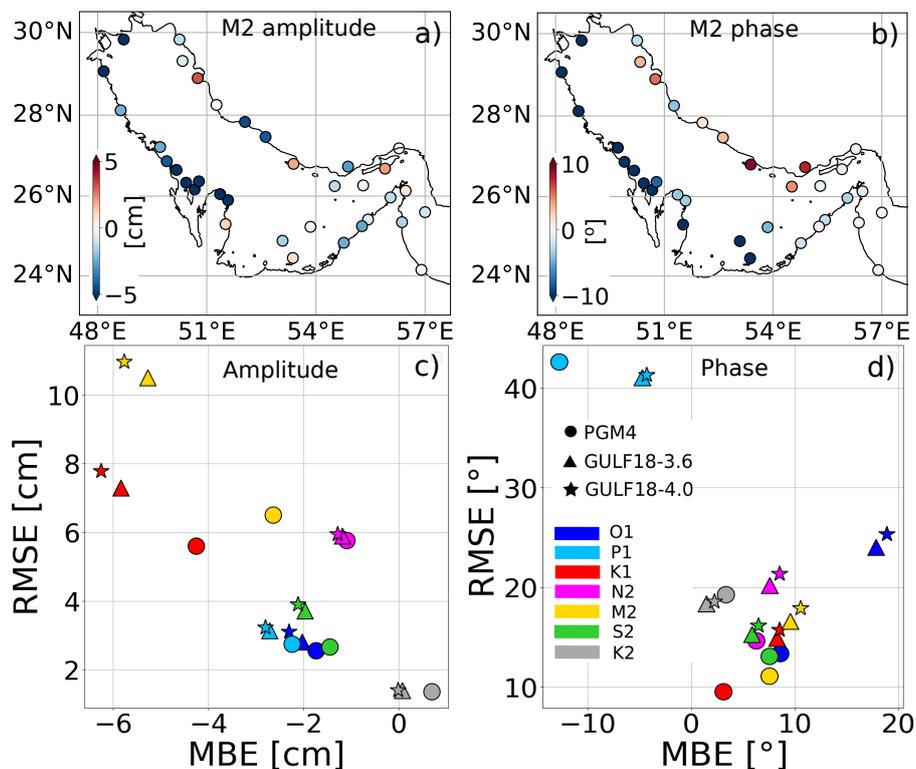
Figure 7. Upper row: difference in the absolute errors $|x_m - x_o|$ of PGM4 and GULF18-4.0 models for M2 amplitude (a) and phase (b) for each tide-gauge included in the assessment; Bottom row: Root Mean Square Error (RMSE) against Mean Bias Error (MBE) of amplitude (c) and phase (d) of the seven tidal components included in the assessment from harmonic analyses of model sea surface height and tide gauges.

375   The upper row of Fig. 7 presents the difference in the absolute errors of PGM4 and GULF18-4.0 models for M2 amplitude (a) and phase (b) for each tide-gauge included in the assessment. Similarly to Fig. 6, PGM4 has smaller errors than GULF18-* along the northwestern and western coast, especially in the proximity of Kuwait, Bahrain and Qatar. In those areas PGM4 bathymetry and land-sea mask were importantly modified (see Fig. 1) in order to improve the accuracy of the tidal dynamics represented by the model (Hyder et al., 2013). On the other hand, along the Iranian coast GULF18-* configurations seems

380   to have slightly improved accuracy. This is probably due to the better representation of the coastline in the higher resolution models which can affect the propagation of coastally-trapped Kelvin waves, especially in the case of near-resonantly forced Kelvin waves in channel-like basins (Griffiths, 2013).

The bottom row of Fig. 7 presents the RMSE against MBE of amplitude (c) and phase (d) computed by the models with
respect to tide-gauges measurements for the seven tidal components included in the assessment. In general, the solutions of the
three models for the phase lag are similar while for the amplitude, PGM4 seems to have a slightly better accuracy in the case
of M2 and K1 components - e.g., in the case of M2 PGM4 presents MBE$= -2.6\ cm$ and RMSE$= 6.5\ cm$, GULF18-3.6 has
MBE$= -5.3\ cm$ and RMSE$= 10.5\ cm$ while GULF18-4.0 shows MBE$= -5.8\ cm$ and RMSE$= 11.0\ cm$.

Shallow water waves propagate with a wave celerity proportional to $(gH)^{1/2}$, where H is the water depth and g the gravi-
tational acceleration. Therefore, when applying the 'minimum depth approximation' as it is the case in our three models, the
simulated tidal wave speed would be higher than the observed one. Hence, it is likely that the decreased accuracy of M2 and
K1 amplitudes and phases in the north-western part of GULF18-* domain could be partly explained considering that in those
areas GULF18-* models apply more often the minimum depth approximation in comparison to PGM4, as it is shown in Fig.
1d - see in particular the coastal areas near the closed end of the domain, which is where tidal waves are reflected and most of
the resonant interactions occur.

The small differences between GULF18-3.6 and GULF18-4.0 models (Fig. 7c and d) can be probably explained considering
the additional smoothing of the upper envelope of GULF18-4.0 to reduce HPGE (see Sec. 2.2 for the details) and the different
value of the reference density used by the two models (see Tab. 1), similarly to O'Dea et al. (2017).

4.2 Sea surface temperature

SST strongly influences fluxes of heat, moisture and momentum across the ocean-atmosphere interface and the importance of
more accurate SST simulations is widely recognised, both for long (e.g., Minobe et al. (2008)) and shorter (e.g., Mahmood
et al. (2021)) timescales. In this section, we assess the skill of PGM4 and GULF18-* models in predicting the SST of the Gulf
in the period 2014-2017.

Figure 8 presents monthly time-series of basin averaged MBE, RMSE and correlation coefficient r of the three Gulf
models with respect to OSTIA SST observed signal while Tab. 3 reports annual averages and standard deviations of mod-
els' MBE and RMSE. SST from model outputs was retrieved considering the temperature of the first model level. Nu-
merical results demonstrate that the three models reproduce a seasonal and interannual variability in good agreement with
OSTIA observations, with GULF18-* configurations having consistently improved accuracy in comparison to PGM4, both
in terms of MBE and RMSE. Mean metrics indicate that generally PGM4 is affected by a persistent warm bias (MBE$=
0.31 \pm 0.31°$C, RMSE$= 0.66 \pm 0.29°$C) while GULF18-3.6 presents a close to zero bias but larger RMSE and variability
(MBE$= 0.04 \pm 0.38°$C, RMSE$= 0.51 \pm 0.26°$C) than GULF18-4.0, which has a slightly cold bias and the smallest RMSE and
variability (MBE$= -0.11 \pm 0.26°$C, RMSE$= 0.46 \pm 0.26°$C).
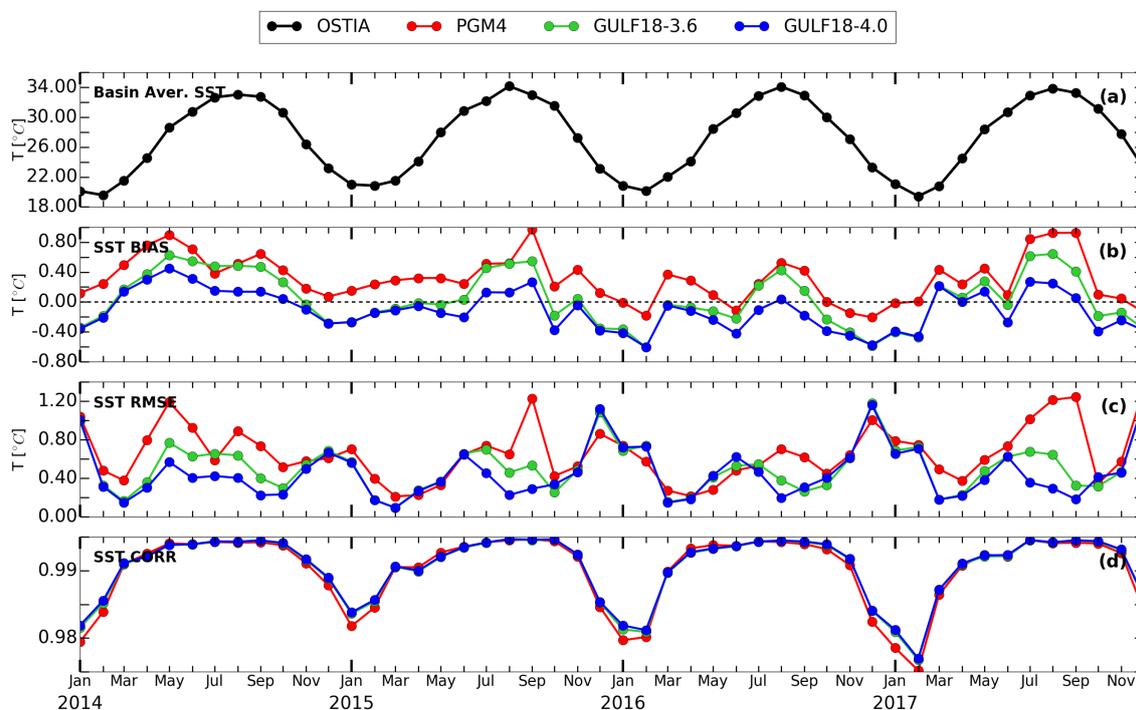
Figure 8. Monthly time-series of basin averaged OSTIA SST (a) and MBE (b), RMSE (c) and correlation coefficient r (d) of PGM4 (in red), GULF18-3.6 (in green) and GULF18-4.0 (in blue) models.

Figure 9 explores the spatial distribution and the seasonal variability of models' errors. In general, GULF18-* configurations significantly reduce PGM4 inaccuracies throughout the domain and for all the seasons, with GULF18-4.0 presenting the
420 largest improvements. In winter (DJF), GULF18-* models are able to mitigate the PGM4 warm bias in the central-eastern part of the domain and Strait of Hormuz and to reduce the marked cold bias of PGM4 along the western coast of the basin. In spring (MAM), both high resolution models present an overall small positive bias in contrast to the widely spread across the domain SST overestimation of PGM4. This seems to be the case also in autumn (SON), although GULF18-4.0 seems to be affected by a slightly cold anomaly (especially in the central western part of the domain) that it is not present in GULF18-3.6.
425 In summer (JJA), both GULF18-* configurations perform well, with GULF18-4.0 presenting the largest reduction of PGM4 errors, especially for the warm bias in the southern part of the domain and the cold anomaly in the proximity of the shallow closed end of the basin. In addition, both GULF18-* seem to introduce an SST underestimation in northern-central part of the domain which appears to be more intense in the case of GULF18-4.0.

430 SST biases often affect ocean models, particularly in summer when inaccuracies in the atmospheric forcings and/or in the upper mixed layer physics may be larger (e.g., Ezer and Mellor (2000), Hordoir et al. (2019) and Bruciaferri et al. (2020)) and SST data assimilation is typically used to constrain such model deficiencies (e.g, O'Dea et al. (2012); Hyder et al. (2013)).

19

MODEL	2014		2015		2016		2017	
	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE
PGM4	0.45 ± 0.25	0.73 ± 0.24	0.36 ± 0.22	0.58 ± 0.28	0.11 ± 0.24	0.54 ± 0.22	0.33 ± 0.37	0.79 ± 0.33
GULF18-3.6	0.21 ± 0.33	0.54 ± 0.23	0.04 ± 0.29	0.47 ± 0.26	-0.15 ± 0.30	0.50 ± 0.27	0.05 ± 0.37	0.54 ± 0.26
GULF18-4.0	0.06 ± 0.24	0.43 ± 0.23	-0.20 ± 0.19	0.42 ± 0.26	-0.29 ± 0.20	0.50 ± 0.28	-0.10 ± 0.27	0.47 ± 0.28

Table 3. Annual means and standard deviations of MBE and RMSE of SST fields reproduced by PGM4, GULF18-3.6 and GULF18-4.0 models in comparison to OSTIA SST observations. Annual metrics for the correlation coefficient r are not presented since the three models show very similar high values (> 0.99) during the whole simulated period.

In the case of our models, the improved accuracy of GULF18-* configurations in comparison to PGM4 could be due to differences in the horizontal resolution and sub-grid physics, the formulation of the surface boundary conditions, the light penetration schemes, the rivers forcing and the thickness of the first model level (as shown by Siddorn and Furner (2013)). One of the aims of this study was to assess the impact of the vertical coordinate system on the accuracy of a Gulf model. Therefore, a sensitivity test was conducted running GULF18-3.6 with a vertical coordinate system similar to the one of PGM4 (i.e., with an upper model level having a 2D varying thickness) to assess whether using a constant level thickness throughout the domain is important in terms of SST accuracy. Numerical results showed a basin averaged signal very similar to the original GULF18-3.6 simulation, suggesting a minor impact of the vertical coordinate system on the accuracy of the simulated SST.

GULF18-4.0 presents slightly improved accuracy in comparison to GULF18-3.6. This is consistent with the fact that the two models differ only in the NEMO code revision, the vertical coordinate system below the sub-surface and some numerical/physical choices. Since the two GULF18 configurations present similar vertical resolution in the upper part of the water column, it is likely that the differences between the two models can be attributed to their different formulation of the diffusivity and viscosity (see Sec. 2.3 for the details).

4.3 Water column stratification

In this Section, the accuracy of PGM4 and GULF18-* models in reproducing the thermal and haline stratification of the Gulf during the period 2014-2017 is assessed against CTD measured T/S profiles, TSG sub-surface T/S observations and T time-series from two on-shelf moorings of the Kuwait coast.

Table 4 presents the average MBE and RMSE of the three Gulf models against CMEMS CTD measured T/S profiles for the three analysis areas defined in Sec. 3.3 and for the total domain. Overall, basin averaged metrics indicate that GULF18-4.0 has higher T accuracy when compared to PGM4 and GULF18-3.6, with larger improvements in 2014 than 2015, especially with respect to PGM4. To the contrary, in the case of S there does not seem to be a clear pattern - in 2014 GULF18-4.0 presents the highest accuracy while in 2015 it results to be the less precise, with differences in the basin averaged metrics of the models
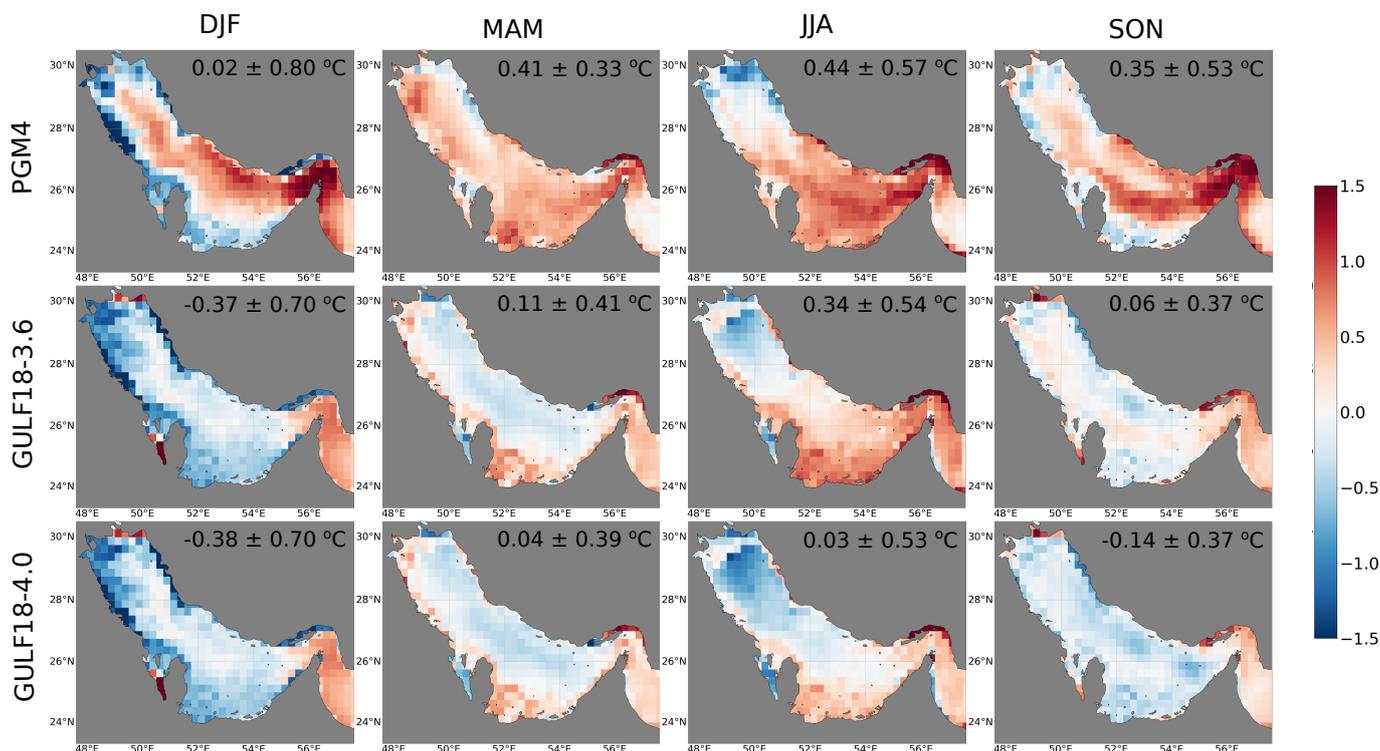
Figure 9. Seasonal SST anomalies (model minus observations) for PGM4 (top row), GULF18-3.6 (middle row) and GULF18-4.0 (bottom row) models. All panels show 4-year mean anomalies for the period 2014-2017, with spatially averaged mean errors and standard deviations reported in each panel.

$< 0.03 \; PSU$.

Figure 10 presents T and S models' errors as a function of depth for the three areas considered in the analysis. In general, the three models seem to broadly overestimate T and S in the upper 200 m of the water column, suggesting that the GLS turbulent closure scheme might need some tuning to improve the vertical mixing in the surface mixed layer.

On the shelf (Area 1), a limited number of available observations (two T profiles in 2014) seems to indicate that both GULF18-* configurations may have improved accuracy in comparison to PGM4. Panel 10a presents the on-shelf vertical distribution of T MBE and RMSE of the three models in 2014. Both GULF18-* configurations have improved accuracy in the proximity of the upper (0-10 m) and bottom (40-50 m) boundary layers with respect to PGM4, with GULF18-4.0 presenting slightly higher skill near the surface. This is probably due to the fact that in the upper and bottom mixed layers the two GULF18-* models have increased vertical resolution in comparison to PGM4 (see Fig. 4). Similarly, the better performance of GULF18-3.6 at medium depths ($\approx 20 - 40 \; m$) could be explained by its higher vertical resolution in this depth range with

a) TEMPERATURE $[^\circ C]$

MODEL	2014								2015							
	AREA 1 (2)		AREA 2 (12)		AREA 3 (47)		TOTAL (61)		AREA 1 (0)		AREA 2 (15)		AREA 3 (121)		TOTAL (136)	
	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE
PGM4	1.48	2.81	0.64	0.80	0.50	1.14	0.56	1.12	-	-	1.30	1.60	0.60	1.06	0.68	1.12
GULF18-3.6	0.70	1.80	0.39	0.60	0.67	1.28	0.62	1.16	-	-	0.90	1.34	0.79	1.20	0.80	1.22
GULF18-4.0	0.59	2.10	0.22	0.53	0.51	1.13	0.46	1.05	-	-	0.72	1.25	0.66	1.11	0.66	1.12

b) SALINITY $[PSU]$

MODEL	2014								2015							
	AREA 1 (0)		AREA 2 (11)		AREA 3 (44)		TOTAL (55)		AREA 1 (0)		AREA 2 (15)		AREA 3 (121)		TOTAL (136)	
	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE	MBE	RMSE
PGM4	-	-	0.10	0.16	0.10	0.23	0.10	0.21	-	-	0.20	0.47	0.09	0.22	0.10	0.25
GULF18-3.6	-	-	0.03	0.10	0.10	0.23	0.09	0.20	-	-	0.08	0.42	0.09	0.22	0.09	0.24
GULF18-4.0	-	-	-0.02	0.09	0.08	0.21	0.06	0.18	-	-	0.05	0.43	0.10	0.25	0.09	0.27

Table 4. Mean MBE and RMSE of PGM4, GULF18-3.6 and GULF18-4.0 models when compared against CMEMS CTD T (a) and S (b) profiles for the three areas defined in Sec. 3.3 as well as for the whole domain in 2014 and 2015 (values between parenthesis indicate the number of observations included in the average).

respect to the other two models.

Panels 10b, 10d and 10f, 10h show the vertical distribution of T and S models' errors, respectively, in the Strait of Hormuz and near the shelf-break (Area 2). Generally, in this area GULF18-4.0 presents the smallest MBE and RMSE in the upper $\approx 100\ m$ for both T and S in 2014 and for T in 2015 while PGM4 has typically larger errors than GULF18-4.0 in the upper $\approx$ 120 m of the water column for T in both years and for S in 2014. GULF18-3.6 has lower accuracy than GULF18-4.0 for T in the period 2014-2015 and for S in 2014, while there seems to be not a clear general pattern in comparison to PGM4. The higher skill of GULF18-4.0 in comparison to PGM4 can be probably explained by the lower vertical resolution of the latter model in the upper 300 m of the water column in Area 2 and 3, as depicted in Fig. 4. In the case of the two GULF18-* configurations, while the higher vertical resolution of GULF18-4.0 at depths between 100 m and 200 m (see Fig. 4b) is likely to play a role, the lower accuracy of GULF18-3.6 can be probably partially attributed also to its larger inaccuracies in computing HPGs in the proximity of the shelf-break (see Fig. 3), in agreement with the findings of Wise et al. (2021) for a model of the European NWS.

In the deeper part of the domain (Area 3), GULF18-4.0 and PGM4 present, in general, a similar higher accuracy than GULF18-3.6 for T, while for S there is not a clear pattern (see Tab. 4). Figures 10c, 10e and 10g, 10i report the vertical distribution of models' MBE and RMSE in Area 3. In the upper $\approx 100\ m$ of the water column PGM4 seems to have a similar (or slightly better in 2015) skill than GULF18-4.0 for T, while GULF18-3.6 shows the lowest accuracy. For S, in the upper $\approx 200\ m$ of the water column GULF18-* models show consistently better accuracy than PGM4, with GULF18-3.6 showing
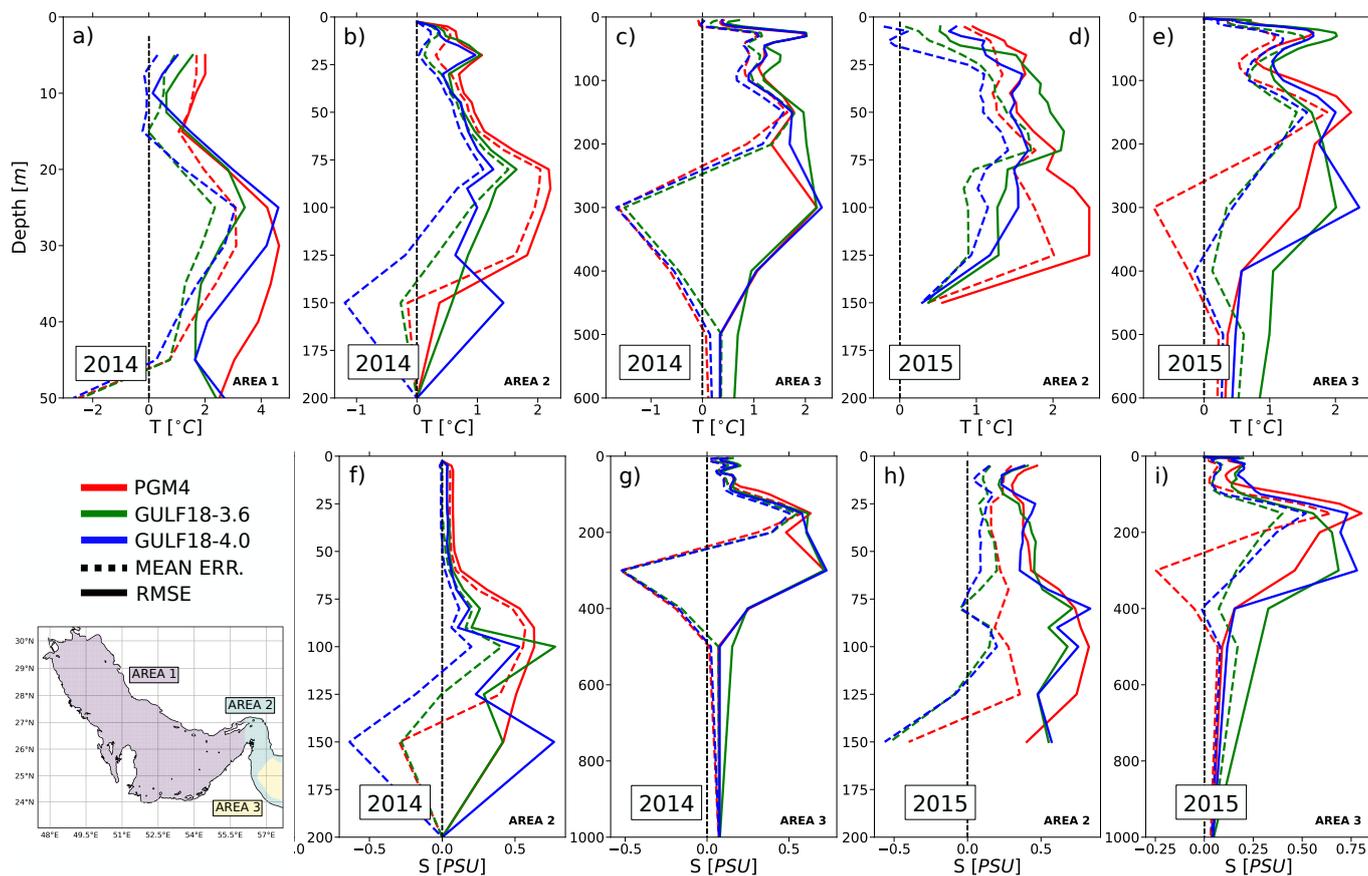
Figure 10. Vertical profiles of temperature (T, top row) and salinity (S, bottom row) MBE (dotted line) and RMSE (solid line) averaged over the three analysis areas defined in Sec. 3.3 for PGM4 (red), GULF18-3.6 (green) and GULF18-4.0 (blue) in 2014 and 2015. During the 2014-2015 period there were no available S observations for Area 1. Also, in 2015 there were no available T observations for Area 1.

the best improvements, especially in 2015. Below $\approx 200~m$, where the dynamics is typically more stagnant, PGM4 shows consistently better accuracy than the new GULF18-* configurations.

490   In Area 3, the dynamics of the three models is strongly influenced by the exchanges with the adjacent Indian Ocean. As explained in Sec. 2.4, all the three models apply a T/S relaxation zone of 10 grid points at the single lateral open boundary. However, given the coarser resolution of the 4 km model, this will result in a wider buffer zone in the case of PGM4, creating T/S fields that are smoother and more heavily nudged to the data assimilating forcing at the open boundary. To the contrast, in the case of GULF18-* models the dynamics of Area 3 is less influenced by the open boundary and can evolve more freely.

495   Therefore, whilst the good skill of the PGM4 here is partly due to the fact that a large portion of the deep area is strongly relaxed to the data assimilating solution forcing the open boundary, the higher skill of GULF18-4.0 for T and both GULF18-* for S in the upper part of the water column can be considered a model improvement over PGM4.
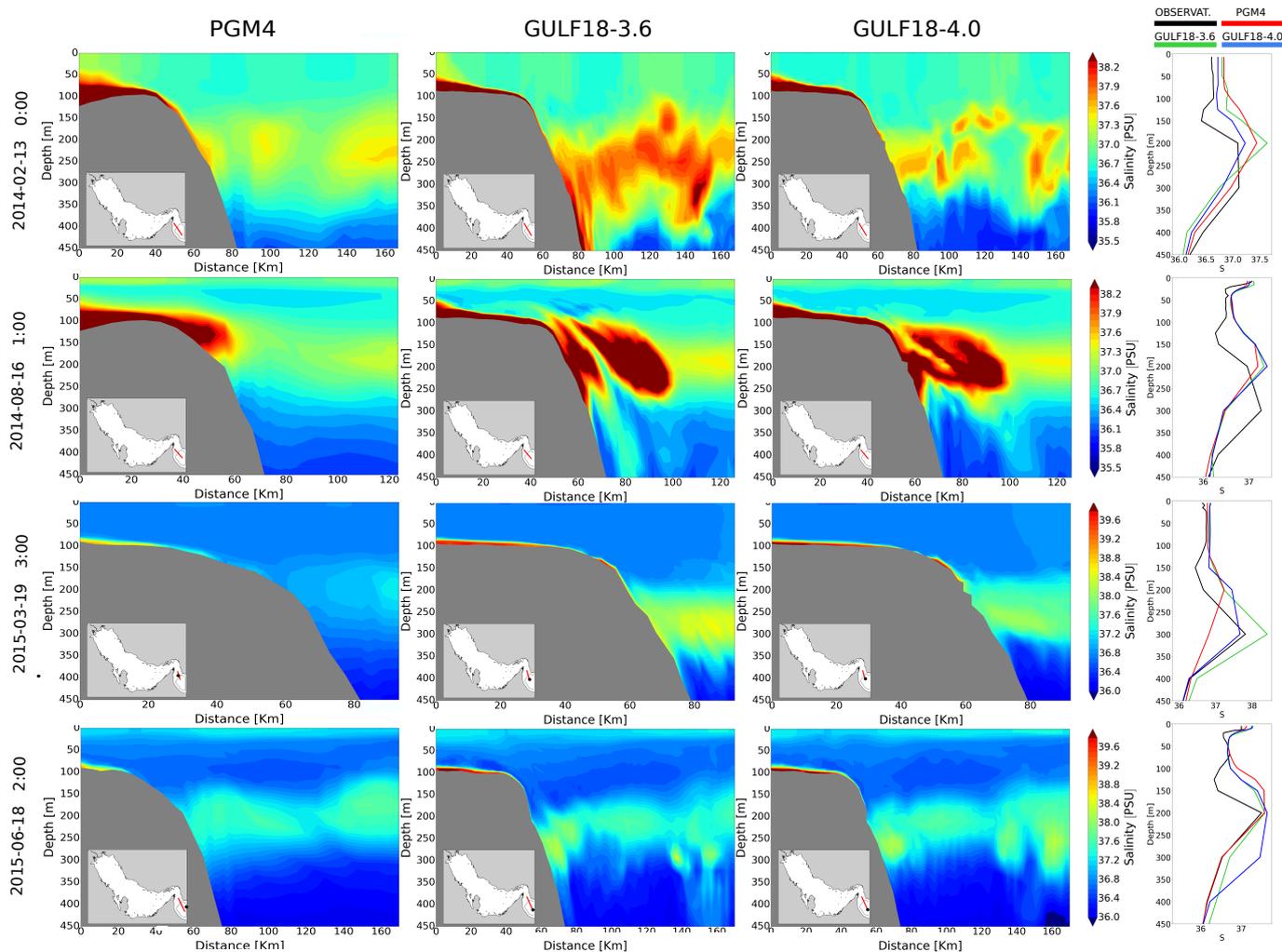
Figure 11. Examples of PGM4, GULF18-3.6 and GULF18-4.0 cross-sections representing salinity-driven cascading events occurred in 2014-2015. The location of the cross-sections is shown in the insets. The leftmost column of each row shows observed and modelled S profiles located at the off-shore end of each cross-section.

In order to better understand the reasons behind the general improvements of GULF18-* configurations at the shelf-break (Area 2) and the upper part of the water column in Area 3, in Fig. 11 we investigate how the three models represented four salinity-driven cascading events observed in 2014-2015. Measured and modelled salinity profiles at the off-shore end of each cross-section are shown in the leftmost column of each row. In the case of GULF18-* models, gravity currents seems to be affected by less numerical diffusion, enabling a stronger and more coherent cascading signal than in PGM4, where the solution appears to be generally smoother, more spread and less accurate in comparison to observations. The vertical grid of GULF18-4.0 has higher resolution in the proximity of the upper envelope (see Sec. 2.2). This enhanced vertical resolution seems to be able to mitigate potential errors in the deeper part of the domain where model levels are not strictly terrain following, resulting

24

a) TEMPERATURE [$°C$]				
MODEL	**2014**		**2017**	
	MBE	RMSE	MBE	RMSE
PGM4	0.68	0.91	0.61	0.70
GULF18-3.6	0.44	0.78	0.35	0.41
GULF18-4.0	0.19	0.68	0.32	0.39
b) SALINITY [PSU]				
MODEL	**2014**		**2015**	
	MBE	RMSE	MBE	RMSE
PGM4	0.59	1.07	-0.02	0.07
GULF18-3.6	0.86	1.45	-0.07	0.10
GULF18-4.0	0.71	1.33	-0.07	0.09

Table 5. Average MBE and RMSE of PGM4, GULF18-3.6 and GULF18-4.0 models when compared against CMEMS TSG T (top row) and S (bottom row) sub-surface hourly measurements collected in 2014 (from 23 to 25 March and from 21 May to 1 June) and 2017 (from 1 to 2 March). The location of the observations is shown in Fig. 5.

in GULF18-* models having similar accuracy when simulating bottom intensified gravity currents.

Table 5 reports the average MBE and RMSE of the three models with respect to TSG sub-surface (between 0 and 5 m)
510 hourly observations of T and S. In 2014, TSG measurements are located in the shallow southern part of the shelf (area 1) while in 2017 they are along a transect crossing Area 2 (see Fig. 5). For T, the assessment against TSG, SST and CTD observations seems to agree - GULF18-* configurations consistently present higher accuracy than PGM4, with GULF18-4.0 showing the larger improvements. For S, the general outcome is that PGM4 seems to present a better skill, especially in 2014.

515 We conclude the analysis of this Section by assessing how the models represented the evolution of the thermal stratification of the water column against two mooring temperature time-series collected in 2014 (Fig. 13) and 2017 (Fig. 14) off the coast of Kuwait (see Fig. 5 for the location). Unfortunately, in 2014 instruments attached to the upper part of the mooring failed to record and only bottom observations are available. In general, GULF18-3.6 shows an average MBE with magnitude of $\approx 0.2 - 0.4°C$, corresponding to a slightly cold bias with respect to observations, especially in the first ≈ 20 days of the
520 time-series (Fig. 13c and e). Conversely, in comparison to observations PGM4 presents a consistent warm bias for the first two months of the assessed period, with larger errors than GULF18-3.6 (the average difference of the absolute value of GULF18-3.6 and PGM4 MBEs is $\approx -0.3/-0.6°C$). On the other hand, GULF18-4.0 presents a very similar solution to GULF18-3.6, with differences between the magnitude of their MBEs of $\approx \pm 0.3°C$.

525 In July 2017, all the three models present a cold bias in comparison to observations. In the case of GULF18-3.6, cold anomalies of $\approx 1°C$ mainly interest the upper part ($\approx 10 - 15$ m) of the water column (Fig. 13c and e). The same occurs for
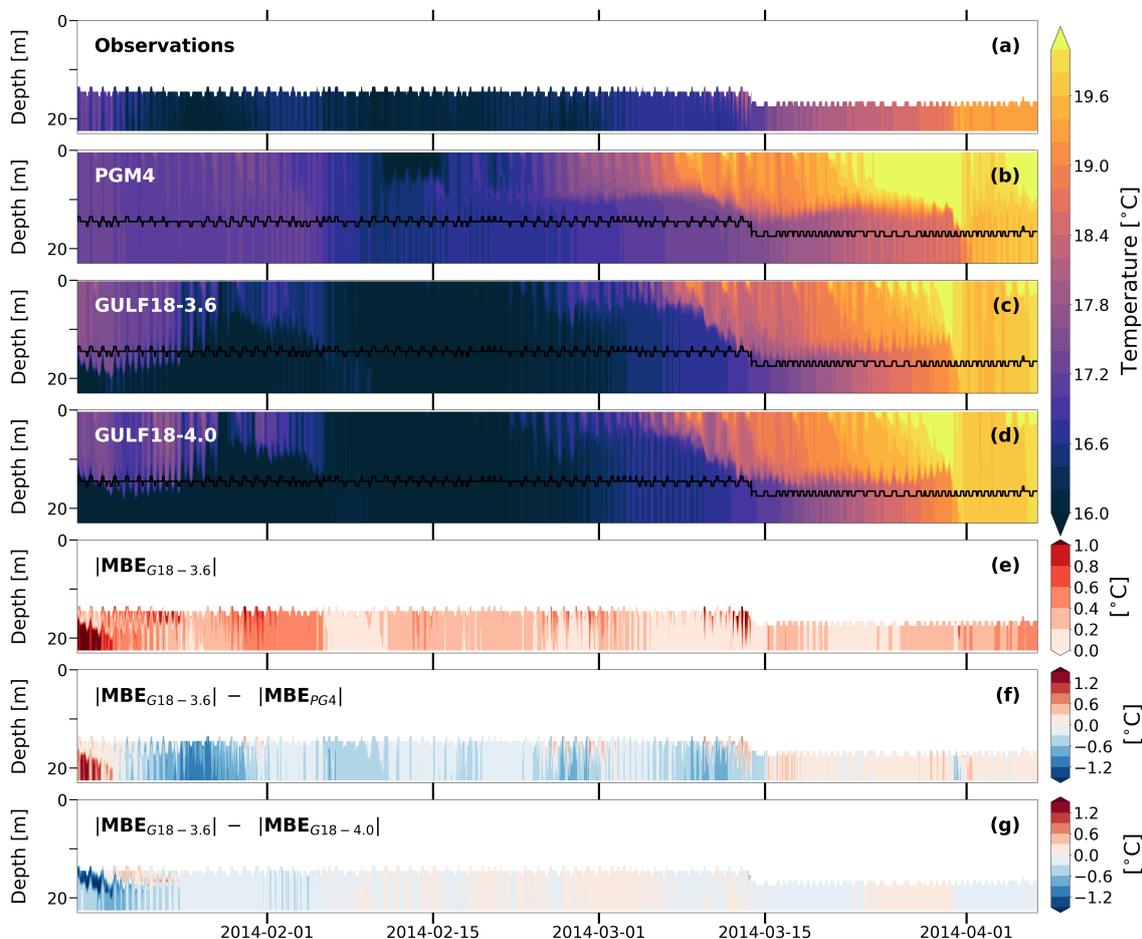
Figure 12. Hourly time-series of: a) mooring temperature profiles observed from 16 January to 6 April 2014 off the coast of Kuwait in the location identified by the cyan star in Fig. 5; temperature profiles computed by PGM4 (b), GULF18-3.6 (c) and GULF18-4.0 (d) and interpolated in the location of the mooring; absolute value of GULF18-3.6 MBE (e); differences between the magnitude of GULF18-3.6 MBE and the absolute value of PGM4 (f) and GULF18-4.0 (g) MBEs, respectively. Instruments attached to the upper part of the mooring failed to record and only bottom observations are available for this period.

GULF18-4.0, although with slightly colder values of $\approx 1.2°C$ on average (Fig. 13d and g). Conversely, PGM4 is affected by very strong and consistent cold biases larger than $2°C$, especially at depth (Fig. 13b and f). The analysis presented in Fig. 9 for the seasonal variability of SST errors seems to agree well with the results shown here: PGM4 presents a cold bias in summer (JJA) in the northern-west corner of the domain off Kuwait coasts that is not present in GULF18-* configurations.

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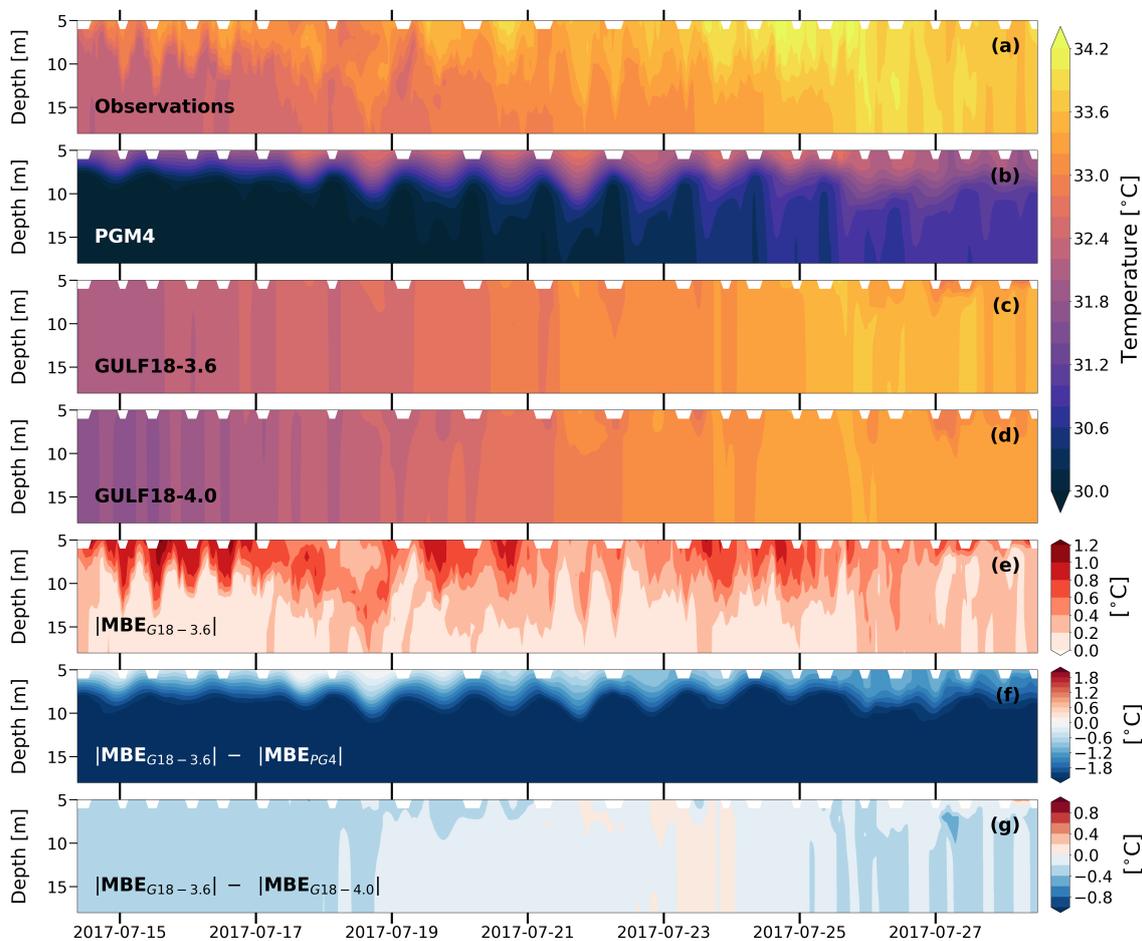
Figure 13. The same as in Fig. 12 but for the period from 14 to 28 July 2017.

4.4 Sea surface currents

One of the main purposes of an ocean forecasting system is to provide accurateise data on the sea surface circulation to support, for example, search and rescue or oil spill and plastic dispersal monitoring and control operations (e.g. Proctor et al. (1994); Breivik et al. (2013)). Therefore, in this Section we evaluate the skill of PGM4 and GULF18-* models in drift prediction against a total of 183 48 h long observed drifters trajectories.

Table 6 presents the mean skill score ss and standard deviation of our Lagrangian simulations for the three areas defined in Sec. 3 as well as for the whole domain during the period 2014-2015. In general, numerical trajectories simulated using surface currents from PGM4 and GULF18-* show similar basin averaged $ss > 0.65$ and standard deviations < 0.15, demonstrating a consistently good agreement with satellite-tracked drifters for all the three models.

MODEL	2014				2015			
	AREA 1 (60)	AREA 2 (59)	AREA 3 (26)	ENTIRE DOMAIN	AREA 1 (32)	AREA 2 (6)	AREA 3 (0)	ENTIRE DOMAIN
PGM4	0.69 ± 0.16	0.66 ± 0.12	0.50 ± 0.09	0.65 ± 0.15	0.70 ± 0.10	0.56 ± 0.11	–	0.68 ± 0.11
GULF18-3.6	0.71 ± 0.12	0.64 ± 0.15	0.57 ± 0.13	0.66 ± 0.14	0.67 ± 0.12	0.64 ± 0.10	–	0.67 ± 0.12
GULF18-4.0	0.69 ± 0.14	0.64 ± 0.14	0.56 ± 0.09	0.65 ± 0.14	0.67 ± 0.14	0.64 ± 0.10	–	0.66 ± 0.13

Table 6. Average Skill Score ss and standard deviation of numerical Lagrangian simulations for the year 2014 and 2015. Metrics are computed for each of the three areas defined in Sec. 3 and shown in Fig. 5 and the whole domain. Values between parenthesis indicate the number of tracks included in the averages.

Metrics averaged over the three analysis areas can help us to identify regions where models present some differences. On the shelf (Area 1), the majority of the tracks considered in the analysis are located in the southern side of the central Gulf. Here, a well known cyclonic circulation pattern driven by the inflow of surface water through the Strait of Hormuz generates a
545 southward coastal flow along the entire southern coast of the Gulf (Reynolds, 1993). Figure 14 shows that, in this area, most of our satellite-tracked drifters consistently drifted in a southerly direction, demonstrating such a cyclonic flow. In addition, in this area Lagrangian simulations using currents from PGM4 or GULF18-* present similar averaged ss (differences are ≤ 0.03) and variability, suggesting that the three models are representing a comparable southward coastal circulation in the central part of the Gulf which transports the numerical drifting buoys in good agreement with the real ones.

550

In the proximity of the Strait of Hormuz and the shelf-break (Area 2), Lagrangian simulations seems to be quite similar in 2014 (differences in the average ss are ≤ 0.02), while in 2015 GULF18-* surface currents seem to have higher accuracy ($+8\%$) than the ones simulated by PGM4. Figure 15a presents examples of numerical and observed trajectories in Area 2. The visual inspection of the actual simulated tracks seem to indicate that in general PGM4 surface currents are slightly weaker than
555 the real ones. Because of the Song and Haidvogel (1994) stretching function, in Area 2 and 3 PGM4 presents a surface layer thickness $> 5\ m$, while GULF18-* models, using a Siddorn and Furner (2013) stretching formulation, present a uniform $1\ m$ grid cell thickness at the surface (see Fig. 4). Hence, it is possible that part of the inaccuracies of PGM4 surface currents may be explained considering the too coarse resolution of the upper model layer, that may cause underestimation of the upper ocean shear and generates too weak grid cell averaged surface currents. Likewise, the larger lateral diffusivity of PGM4 may play
560 also a role in simulating smoother current fields. However, it is also possible that in the case of 2015 metrics under-sampling (6 tracks against 59 in 2014) may be affecting the results.

In the deep portion of the domain (Area 3), GULF18-* models presents higher accuracy ($+6/7\%$) than PGM4 in 2014 while for 2015 there are no available observations. The visual inspection of entire satellite-detected trajectories (see Fig. 15b for
565 some examples) indicates the presence of a clockwise gyre in the western part of the Gulf of Oman, in agreement with existing literature (e.g. Reynolds (1993)) and the three models generally simulate consistent trajectories following such an anti-cyclonic circulation (Fig. 15b). Probably, also in this area the reduced accuracy of PGM4 currents could be explained by a too coarse
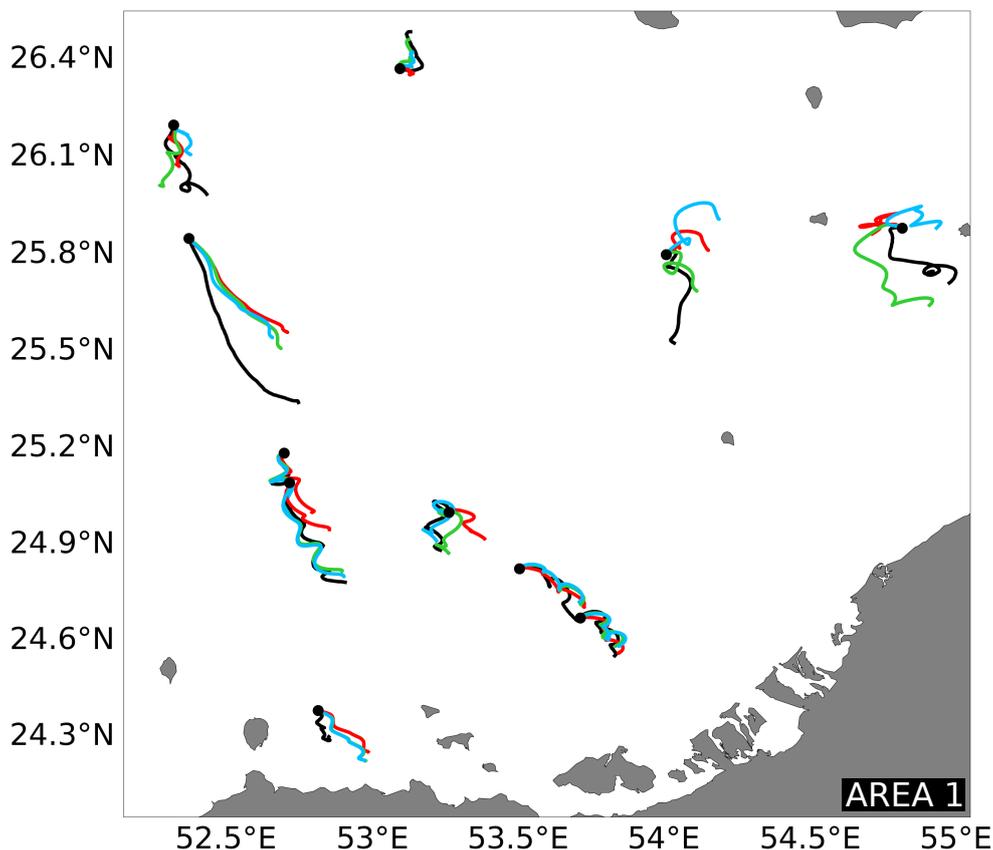
Figure 14. Examples of iSphere simulations located on the shelf (Area 1) during the 2014-2015 period. Observed drifter tracks are shown in black while numerical trajectories computed forcing the Lagrangian model with ocean surface currents from PGM4, GULF18-3.6 and GULF18-4.0 are shown in red, green and blue, respectively.

vertical resolution at the surface and a too large lateral diffusivity.

5 Conclusions and future work

This study explores the sensitivity of a shelf sea model of the Gulf area to changes in the bathymetry, lateral and vertical resolution, vertical coordinates and external forcing. To this end, two high resolution (1.8 km, 52 vertical levels) Gulf models named GULF18-3.6 and GULF18-4.0 differing only in the vertical discretization scheme and the NEMO codebase (NEMO-v3.6 against NEMO-v4.0.4, respectively) have been developed and compared against the existing Met Office PGM4 model (4 km, 31 vertical levels, NEMO-v3.4). Both PGM4 and GULF18-3.6 use similar flavours of quasi-terrain-following vertical levels while GULF18-4.0 employs generalised multi-envelope (ME) vertical coordinates. The assessment compares non-assimilative hindcast integrations of the three Gulf models spanning the period 2014-2017 against available observations of the tidal dy-
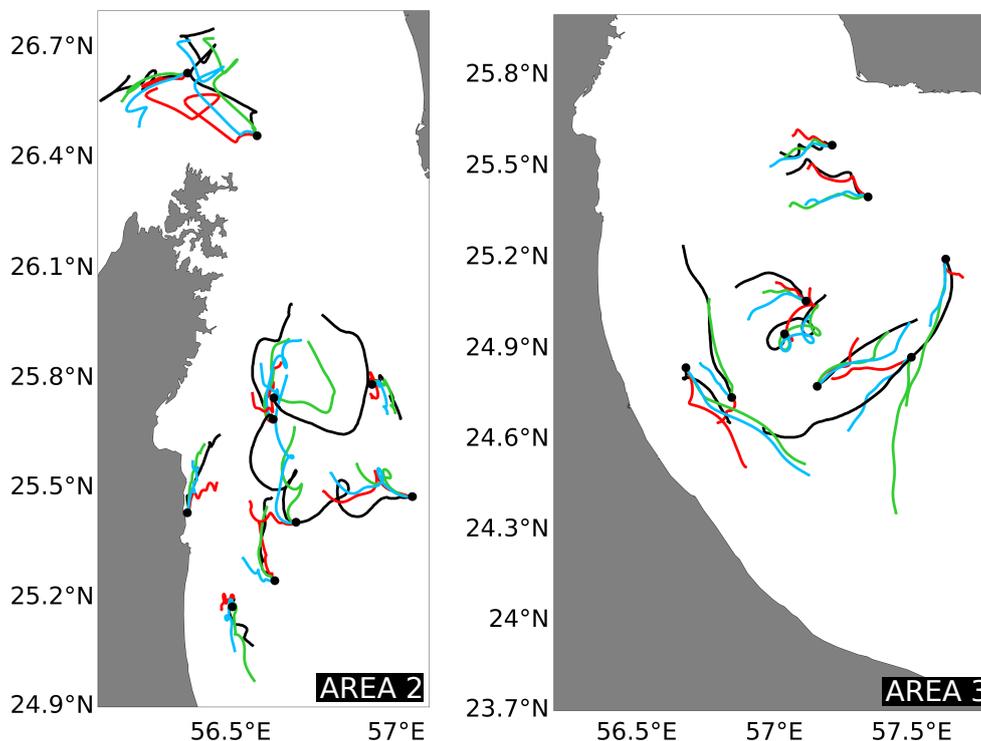
Figure 15. The same as Fig. 14 but for the Strait of Hormuz and shelf-break (Area 2, a) and the deep part of the domain (Area 3, b)

namics, sea surface temperature, water column stratification and ocean currents at the surface.

580   Numerical results indicate that, overall, PGM4 and both GULF18 models give a comparable representation of the majority of the tidal constituents, despite their considerable differences in the domain geometry and tidal forcing. The three models use the same strategy of limiting the minimum depth of the model domain to deal with the large tidal excursion of the Gulf basin. Such a crude parameterization seems to be particularly penalizing in the case of the new high resolution models suggesting that, in order to get real benefit from using a more accurate and detailed bathymetry, the physical processes explicitly resolved

585   by the model must be improved as well, in agreement with previous studies (e.g. Graham et al. (2018a); O'Dea et al. (2020)). Therefore, one future development will be the implementation of a wetting and drying algorithm to obtain a more realistic representation of the water level evolution.

GULF18-3.6 and GULF18-4.0 present similar skill for the tidal dynamics. This seems to indicate that using a ME vertical coordinate system optimised to reduce errors in the computation of the pressure force does not have significant detrimental

590   impact on the accuracy of the simulated tides, in agreement with the findings of Wise et al. (2021).

Both GULF18 configurations present significantly reduced sea surface temperature (SST) biases in comparison to PGM4, improving the RMSE by $\approx 20\%$ in the case of GULF18-3.6 and $\approx 29\%$ for GULF18-4.0. While the increased resolution is

likely to partially play a role in this, improvements are probably mainly due to processes that directly affect the local SST such
595   as the surface fluxes formulation, river forcing and the light penetration scheme.

Although the two GULF18 models differ in the vertical coordinate system, they present similar resolution near the surface.
Therefore, it is likely that the overall slightly better SST accuracy of GULF18-4.0 over GULF18-3.6 is due to the different
sub-grid physics settings and the version of the NEMO code employed.

GULF18-4.0 seems to introduce a slightly cold bias in summer and autumn. Umlauf and Burchard (2005) showed the im-
600   portance of carefully tuning the GLS vertical mixing scheme when dealing with stably stratified marine environment, as is the
case for the shallow parts of the Gulf. Therefore, future work could involve sensitivity numerical tests to improve the vertical
mixing at the surface.

Available observations of the water column thermal stratification indicate that both GULF18 configurations may have higher
605   accuracy than PGM4 on the shelf, especially in the proximity of the upper (0-10 m) and bottom (40-50 m) boundary layers.

Similarly, in the proximity of the shelf-break both GULF18 models represent a more accurate vertical stratification than
PGM4, with an average reduction of the RMSE of $\approx 22\%$ for temperature and $\approx 25\%$ for salinity. This is probably due to
their more realistic bathymetry and enhanced vertical resolution in the upper 300 m of the water column, which allows the two
GULF18 models to represent, for example, a more realistic saline dense water cascading at the shelf-break.

610   In the deep part of the domain, both high resolution configurations present a similar accuracy to PGM4 for temperature
while for salinity there seems to be not a clear pattern. The good accuracy of PGM4 is probably due to the fact that, in this
area, a larger portion of the model domain is strongly relaxed to the data assimilating solution forcing the open boundary. To
the contrary, the improvements of GULF18 models are probably due to their higher horizontal and vertical resolution and their
updated formulations of the atmospheric, river and light penetration forcings.

615   Our assessment seems also to suggest that, in general, GULF18-4.0 might have higher accuracy than GULF18-3.6 in repre-
senting the water column stratification, especially in the upper ≈ 120 m near the shelf-break. This is probably due to the larger
inaccuracies of GULF18-3.6 in computing the pressure gradient force in areas where the bottom topography is particularly
steep, in agreement with the findings of Wise et al. (2021) for a model of the north-west European shelf.

620   Numerical trajectories simulated forcing a Lagrangian model with surface currents from PGM4 and GULF18 models present
similar accuracy, with basin averaged $ss > 0.65$ and standard deviations < 0.15, demonstrating a good agreement with satellite-
tracked drifters. This is the case especially on the shelf and near the shelf-break (differences in the ss are less than 3%), areas
where tidal currents are stronger. Hence, these results seem to support the conclusions of our tidal harmonic analysis, indicating
that PGM4 and both GULF18 models might simulate tides with comparable accuracy.

625   In the deeper area of the domain PGM4 shows lower accuracy than the two high resolution models (-6%). In this area,
barotropic tides are less important and the surface transport is mainly controlled by the wind-driven circulation. It is likely that
the poorer skill of the PGM4 model might be due to its too coarse lateral and vertical resolution which ultimately generate too

Geoscientific
Model Development
Discussions

weak and smoother grid cell averaged surface current fields.

630   In conclusion, our results indicate that both GULF18 models are broadly more accurate than the PGM4 model, proving the benefit of increasing the horizontal and vertical resolution and using a more realistic and detailed bathymetry. In addition, we found GULF18-4.0 to be generally more accurate than GULF18-3.6, demonstrating the advantage of optimising the vertical grid for the prevailing physical processes at stake, in agreement with previous numerical studies (e.g. Bruciaferri et al. (2020); Wise et al. (2021)).

635

In a future study, data assimilation could be applied to the GULF18-4.0 model to assess and understand the additional predictive skill that might be obtained on short-term forecasting time-scales. Similarly, GULF18-4.0 could be also used for longer hindcast integrations to assess its skill on climatic time-scales and for future climatic projections of the Gulf marine environment.

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