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Assessment of gap-filling techniques applied to satellite phytoplankton composition products for the Atlantic Ocean

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Supplements

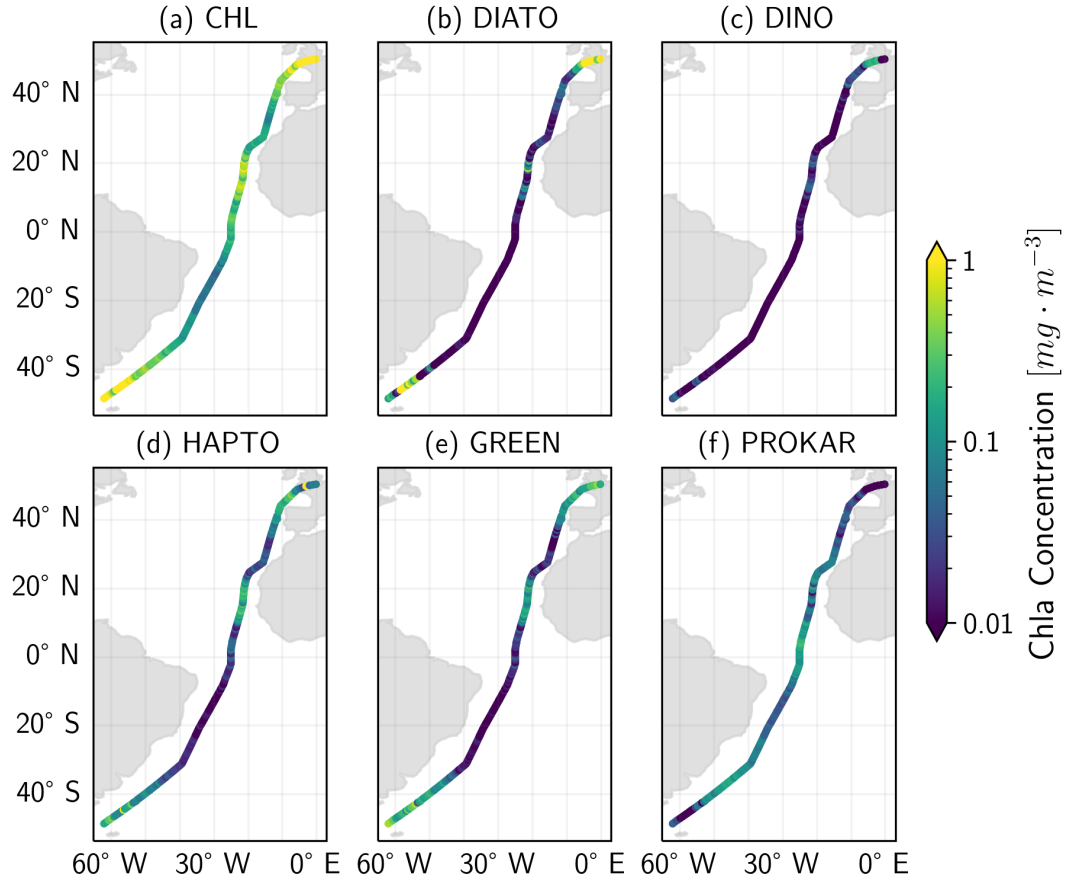

Figure S1: TChla and PFTs estimated from phytoplankton pigment derived from water samples using the HPLC technique. Dataset sourced from Bracher et al. (2020b) and processed with diagnostic pigment analysis following Xi et al. (2023a).

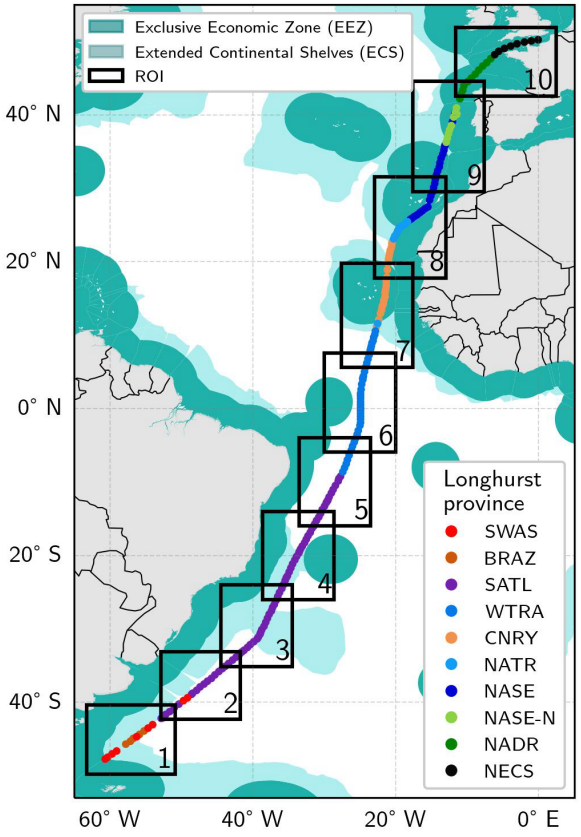

Figure S2: Regions of interest (ROI) analysed in this study, overlaid on the continental shelves region (Flanders Marine Institute, 2023, 2024) to emphasise coastal dynamics, and in situ measurements clustered by Bracher et al. (2020a) into Longhurst biogeographical provinces to highlight ecological zones. The in situ measurements clustered to Longhurst provinces are provided by Bracher et al. (2020b).

Table S1: DINEOF hyperparameters along with their distribution, selection range and optimal value.

Parameter	Description	Selection range	Distribution	Optimal value
α	Strength of Filter	[5e-3 – 5e-1]	Log-uniform	7.6e-2
P	Number of Iterations	[1 - 20]	Uniform	11
SST	Use SST in reconstruction	Boolean	Uniform	False
CV RMSLE on the validation dataset = 0.12				

Table S2: DINCAE hyperparameters along with their distribution, selection range and optimal value.

Parameter	Description	Selection range	Distribution	Optimal value
SST	Use SST in reconstruction	Boolean	Uniform	False
jitter_std	Standard Deviation of the noise	[0 – 0.1]	Uniform	0.035

epochs	Number of epochs to run the model	[600 – 1200]	Uniform	900
batch_size	Batch size	[16 – 64]	Uniform	29
enc_nfilter_internal	Number and size of layers	First layer = [32 – 64] Increase power = [1.5 – 2] Number of layers = [3 – 4]	Uniform Uniform Uniform	[60, 98, 159, 258]
ntime_win	Window of timeseries	[3, 5, 7]	Uniform	3
upsampling_method	Interpolation method in the decoder	[nearest, bilinear]	Uniform	Nearest
loss_weights_refine	Refinement control coefficient	$\alpha' + \alpha = 1$ α = [0 – 0.5] α' = [0.5 – 1]	Uniform	α = 0.32 α' = 0.68
Learning Rate	Learning rate of the optimiser	[1e-4 – 1e-3]	Log-uniform	1.49e-4
regularization_L2_beta	L2 regularisation weight	[1e-4 – 1e-2]	Log-uniform	9.2e-4
laplacian_penalty	Smoothness regularization	[False or True (1e-6 – 1e-2)]	Uniform (Log-uniform)	False
Fix Parameters				
skip-connection	Number of layers with skip-connection			All layers except the first
Optimizer	Method to adjust weights to minimise loss			Adam
Activation Function	Introducing non-linearities to the network			Leaky ReLU
CV RMSLE on the validation dataset = 0.12				