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Introduction

This supporting information provides the computational performance of the VISIR-2 software (section S1), additional details about the identification of the vessel's performance (S2), two specific routes from both the ferry and the sailboat case studies (S3), all the bundles of 2022's optimal routes (S4), route duration metrics for direction-resolved sailboat routes (S5), and the computation of the angle of attack between vessel's heading and course (S6). Unless stated otherwise, all equation and table numbers should be understood to refer to those found in the main manuscript.

S1. Computational performance

The assessment consisted in profiling four (Grafi, Campi, Pesi, Tracce) among the VISIR-2 modules listed in Tab.4 of the main manuscript.
Corresponding computing time T_c was recorded for numerical problems of various sizes, indexed by either the number of coast points (N_c, for just Grafi) or the number of degrees of freedom (DOF, for all other modules). The DOF was obtained as the product of the number of graph edges E and the number of time steps N_T. A submodule granularity was ensured, with profiling at the level of the main phases of processing, and the outcome is documented in Fig.S1. Data were collected via methods from both the `time` and `cProfile` python modules. The profiling times shown here were obtained on an iMac computer with 3.8 GHz 8-Core Intel Core i7 processor and 32 GB 2667 MHz DDR4 memory. Instead, the performance coefficients provided in the main manuscript were derived from performance data relative to a HPC facility as described thereto.

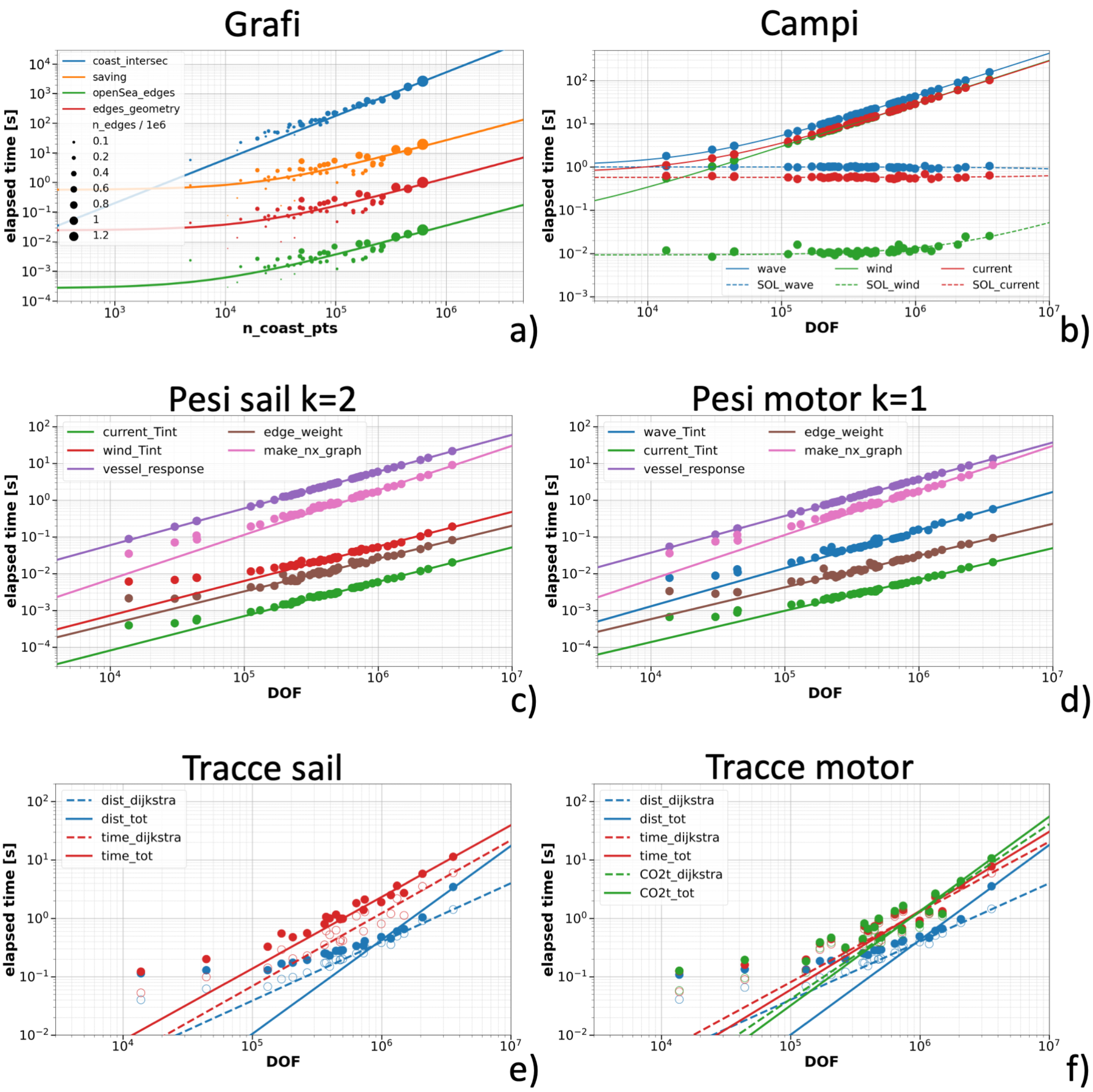

Fig. S1 Profiling of computing time for VISIR-2 main modules: a) Grafi; b) Campi; c) Pesi -sailboat version; d) Pesi - motorboat; e) Tracce- sailboat; f) Tracce - motorboat. The independent variable is the number of degrees of freedom (DOF) in the graph, but for a) where it is the number of shoreline points N_c. Markers refer to experimental data points and lines to least-square fits. In e-f) void markers refer to just the Dijkstra's component and full markers to the whole shortest path routine. The graph parameters were (ν,1/Δx)=(4,12/º). The *k* parameter in the titles of panels c) and d) refers to the number of iterations of Eq.A1.

submodule	description	fit fun	fit coeffs			
			a	std	b	std
coast_intersec	pruning coast-intersecting edges	y = ax ^ b	8.00E-06	3.00E-06	1.47E+00	3.41E-02
saving	node, edges, and coastline saving	y = a + bx	5.64E-01	3.37E-01	2.62E-05	2.06E-06
openSea_edges	find edges in open sea	y = a + bx	2.68E-04	3.83E-04	3.48E-08	2.34E-09
edges_geometry	edges center, orientation, and length saving	y = a + bx	2.39E-02	1.75E-02	1.38E-06	1.07E-07

Tab.S1 Fit coefficients of the T_c= *a* DOF*^{b} regressions for various components of the Grafi module. *Std* are the standard deviation errors on *a* and *b*. Based on data of Fig.S1.

submodule	description	fit fun	fit coeffs			
			a	std	b	std
wave	spatial interpolation of wave height and direction over edges	y = a + bx	1.06E+00	9.59E-02	4.32E-05	1.06E-07
SOL_wave	seaoverland application over waves fields		1.01E+00	7.04E-03	-9.63E-09	7.82E-09
wind	spatial interpolation of wind speed and direction over edges		4.94E-02	5.33E-02	2.96E-05	5.92E-08
SOL_wind	seaoverland application over wind fields		9.37E-03	3.64E-04	4.26E-09	4.04E-10
current	spatial interpolation of currents over edges		7.33E-01	3.05E-02	2.87E-05	3.38E-08
SOL_current	seaoverland application over currents fields		5.79E-01	6.65E-03	5.45E-09	7.38E-09

Tab.S2 As Tab.S1 but for the Campi module.

description	fit fun	fit coeffs							
		sail				motor			
		a	std	b	std	a	std	b	std
time interpolation of wave height and direction over timesteps	y = ax^b					9.33E-08	2.04E-08	1.04E+00	1.51E-02
time interpolation of currents over timesteps		1.29E-08	9.66E-10	9.45E-01	5.23E-03	5.43E-08	6.50E-09	8.52E-01	8.40E-03
time interpolation of wind speed and direction over timesteps		3.80E-08	9.70E-09	1.02E+00	1.77E-02				
STW evaluation		4.24E-06	3.66E-08	9.96E-01	5.99E-04	3.77E-06	8.28E-08	1.00E+00	1.52E-03
SOG and edge delay comupation		1.44E-07	3.75E-08	8.75E-01	1.83E-02	2.04E-07	3.58E-08	8.65E-01	1.23E-02
populating networkX graph		4.50E-08	1.53E-08	1.27E+00	2.32E-02	9.86E-08	2.45E-08	1.21E+00	1.70E-02

Tab.S3 As Tab.S1 but for the Pesi module. Data for the case *k*=1 in the iterative solution of the transcendental equation, Eq.A1.

submodule	description	fit fun	fit coeffs							
			sail				motor			
			a	std	b	std	a	std	b	std
wave_Tint	time interpolation of wave height and direction over timesteps	y = ax^b					5.67E-08	1.32E-08	1.07E+00	1.61E-02
current_Tint	time interpolation of currents over timesteps		1.49E-08	1.42E-09	9.35E-01	6.65E-03	1.40E-08	2.08E-09	9.41E-01	1.04E-02
wind_Tint	time interpolation of wind speed and direction over timesteps		1.26E-07	2.95E-08	9.41E-01	1.63E-02				
vessel_response	STW evaluation		5.93E-06	9.64E-08	1.00E+00	1.13E-03	5.11E-06	5.13E-08	9.98E-01	6.96E-04
edge_weight	SOG and edge delay comupation		1.15E-07	2.04E-08	8.93E-01	1.24E-02	1.92E-07	3.74E-08	8.69E-01	1.37E-02
make_nx_graph	populating networkX graph		1.02E-07	2.43E-08	1.21E+00	1.63E-02	9.25E-08	2.27E-08	1.22E+00	1.68E-02

Tab.S4 As Tab.S3, but for *k*=2.

submodule	description	fit fun	fit coeffs							
			sail				motor			
			a	std	b	std	a	std	b	std
dist_dijkstra	least distance route computation	y = ax^b	2.12E-07	8.01E-08	1.04E+00	2.59E-02	3.70E-07	1.05E-07	1.00E+00	1.96E-02
dist_tot	least distance route, track metrics and save ouput files		3.50E-08	3.40E-08	1.22E+00	6.59E-02	1.11E-07	8.77E-08	1.14E+00	5.39E-02
time_dijkstra	least time route computation		1.33E-06	5.47E-07	1.01E+00	2.82E-02	1.35E-06	4.92E-07	1.01E+00	2.52E-02
time_tot	least time route, track metrics and save ouput files		1.48E-06	7.98E-07	1.02E+00	3.70E-02	1.05E-06	5.15E-07	1.04E+00	3.37E-02
CO2t_dijkstra	least CO2 route computation						1.90E-07	9.54E-08	1.16E+00	3.43E-02
CO2t_tot	least CO2 route, track metrics and save ouput files						1.87E-07	1.10E-07	1.18E+00	4.04E-02

Tab.S5 As Tab.S1 but for the Tracce module.

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S2. Vessel performance

For both vessels considered in the manuscript, the ferry and the First-367 sailboat, a function with its seakeeping performance is identified starting from a look-up table (LUT). As explained in the main manuscript, the LUT stems from either a simulator (for the ferry) or a velocity prediction programme (VPP, for the sailboat). The function used to encode the seakeeping performance can be either a cubic spline or a neural network. The predictions (evaluations at new values of the independent variable) deriving from such functions are compared to the “observations” (data from the LUT) and relative scores are presented in this section.

S2.1 Ferry

The ferry is the 125-m long vessel which principal particulars are given in Tab.2 of the main manuscript. The scores (Pearson’s R^2 coefficient, root mean square error RMSE) from both the spline and neural network are given in the following two subsections. It is distinguished between the speed through water (STW) and the CO_2 emission rate.

S2.1.1 Spline

The Bspline method[1] is used, and the outcome is provided in the figure below.

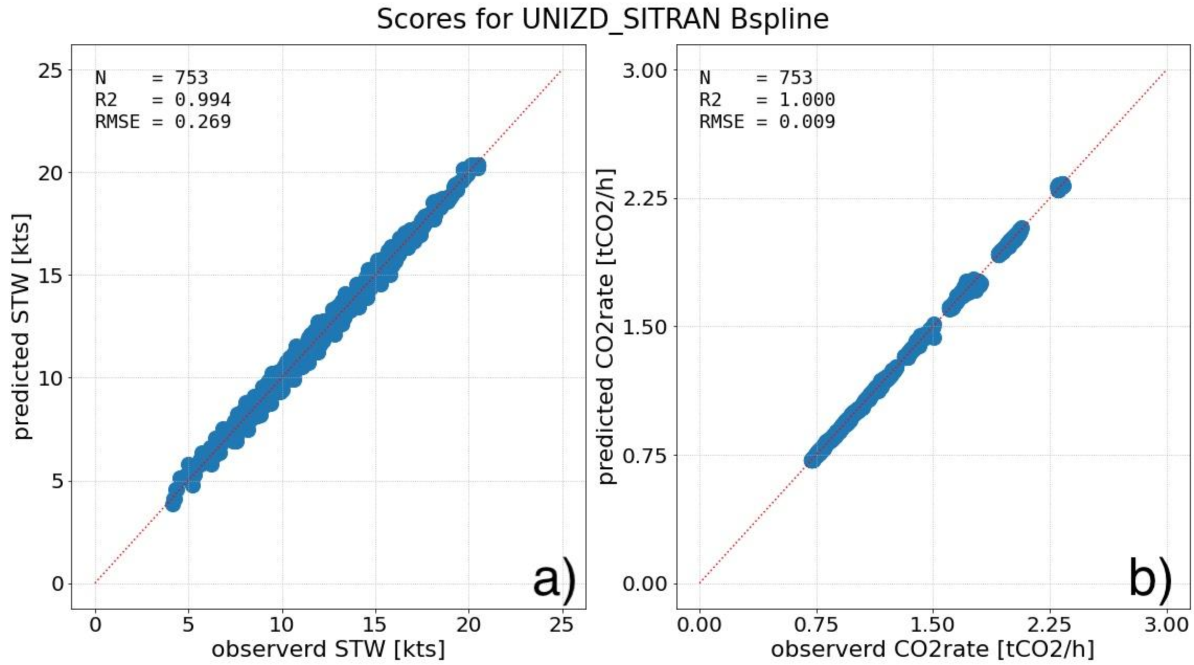

Fig.S2 Predicted vs, observed STW (a) and CO_2 emission rate (b) of the ferry, using the spline interpolation on the vessel’s LUT.

[1] https://docs.scipy.org/doc/scipy/reference/generated/scipy.interpolate.BSpline.html

S2.1.2 Neural Network

The parameters of the network are provided in Tab.S2 while its performance is assessed in Fig.S3 (for the STW variable) and Fig.S4 (for the CO_2 emission rate).

Regression variable	Hidden layers	alpha	Activation function	Max iterations
STW	112	1.E-04	relu	10,000
CO2rate	155, 25	1.E-05	relu	10,000

Tab.S2 parameters of the multi-layer perceptron of the ferry.

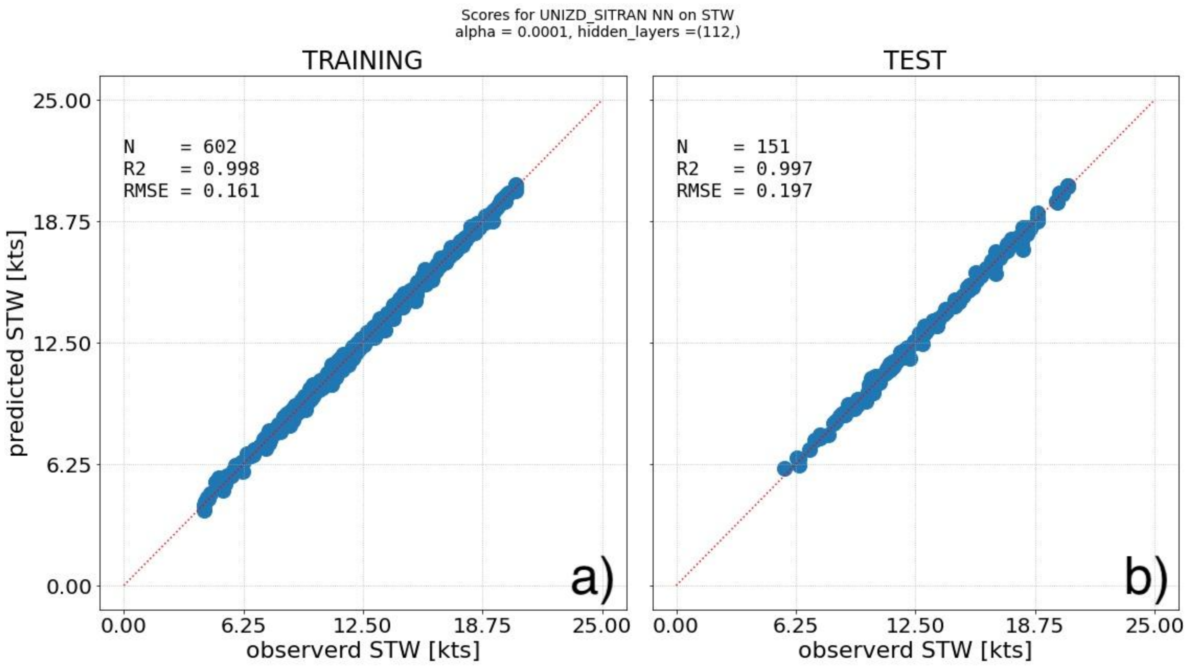

Fig.S3 Predicted vs. observed STW of the ferry for both the training (a) and the test dataset (b) of the neural network, with relative scores printed in the legends.

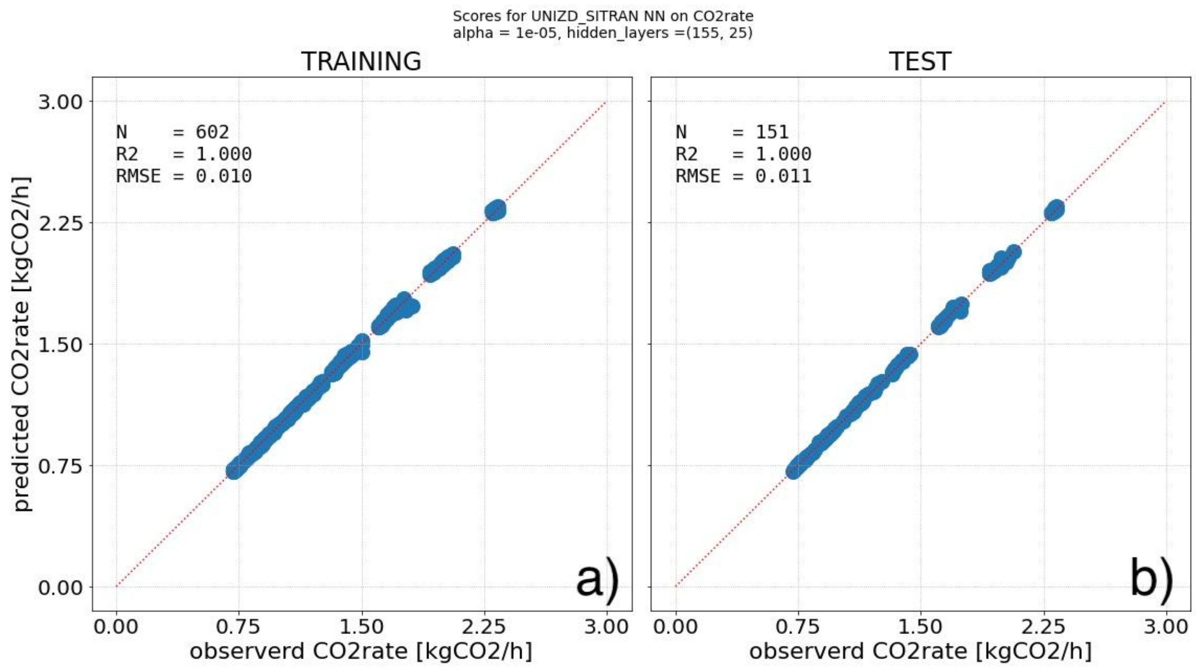

Fig.S4 Predicted vs. observed CO_2 emission rate of the ferry for both the training (a) and the test dataset (b) of the neural network, with relative scores printed in the legends.

S2.2 Sailboat

The sailboat is the about 11-m long Beneteau First-367 vessel which principal particulars are given in Tab.3 of the main manuscript. The scores (Pearson's R^2 coefficient, root mean square error RMSE) from both the spline and neural network are given in the following two subsections. It is distinguished between the speed through water (STW) and the leeway velocity.

S2.2.1 Spline

The Bspline method is used, and the outcome is provided in the figure below.

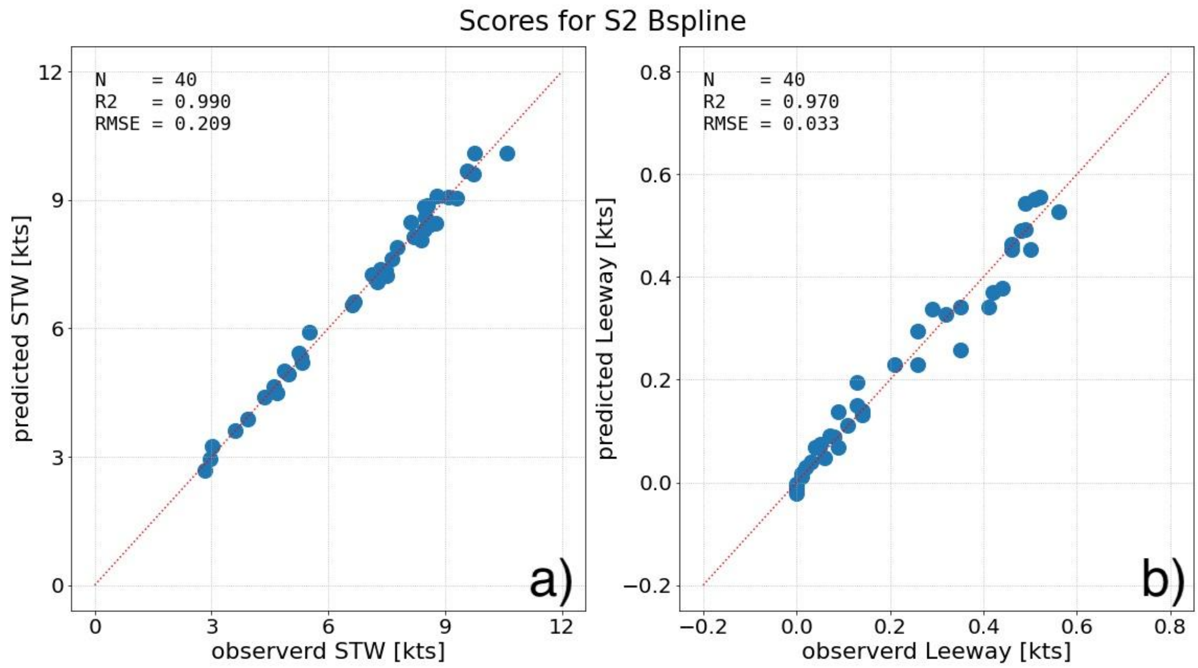

Fig.S5 Predicted vs, observed STW (a) and leeway velocity (b) of the First-367 sailboat, using the spline interpolation on the vessel's LUT.

S2.2.2 Neural Network

The parameters of the network are provided in Tab.S2 while its performance is assessed in Fig.S6 (for the STW variable) and Fig.S7 (for the leeway).

Regression variable	Hidden layers	alpha	Activation function	Max iterations
STW	25, 67	1.E-05	relu	10,000
Leeway	10, 49	1.E-04	relu	10,000

Tab.S3 parameters of the multi-layer perceptron of the sailboat.

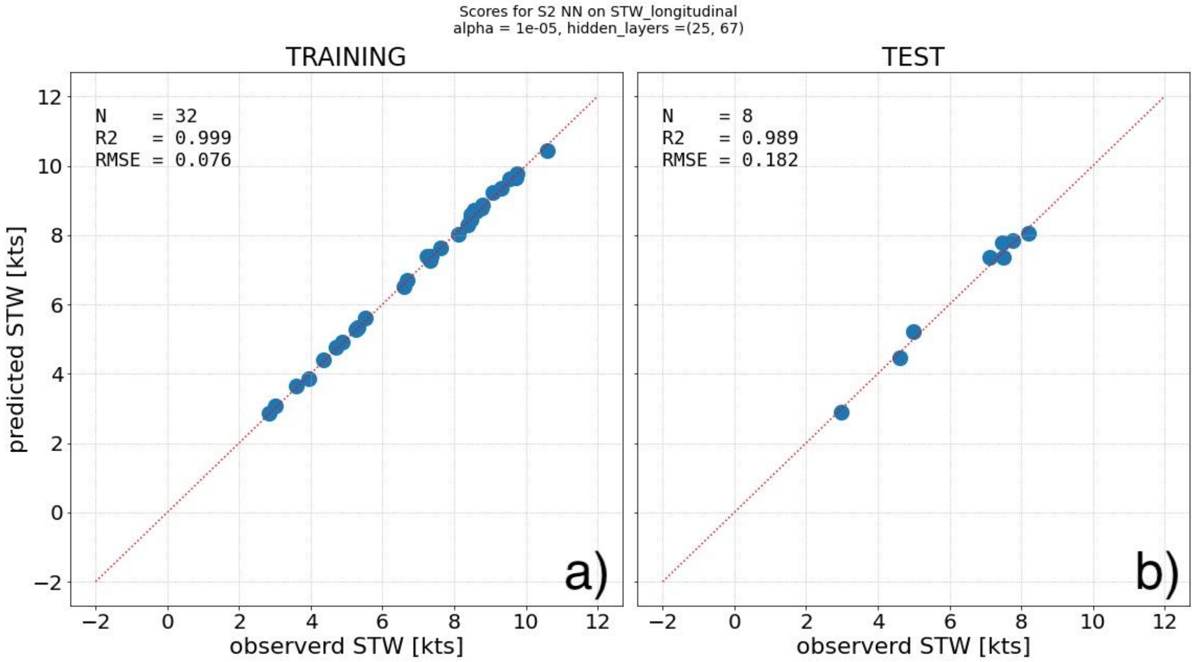

Fig.S6 Predicted vs. observed STW of the sailboat for both the training (a) and the test dataset (b) of the neural network, with relative scores printed in the legends.

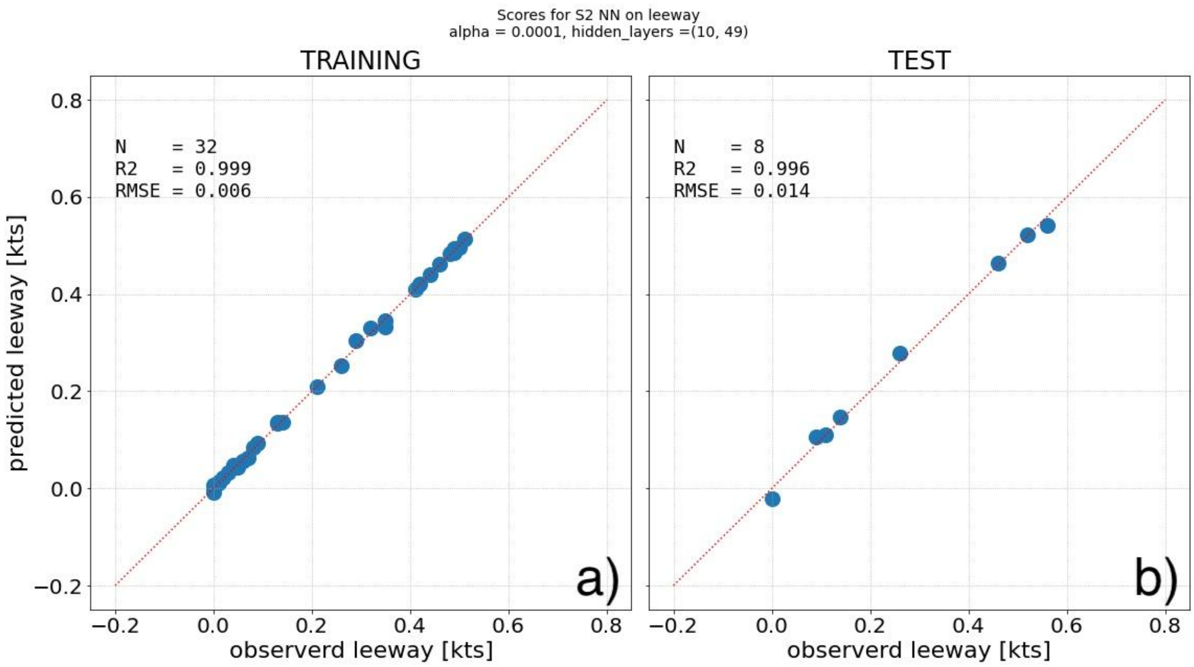

Fig.S7 Predicted vs. observed leeway velocity of the sailboat for both the training (a) and the test dataset (b) of the neural network, with relative scores printed in the legends.

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S3. Specific routes

In this section, specific and to some extent exceptional routes for both the ferry and the sailboat are presented.

S3.1 Ferry

Among the 2022's numerical experiments, there is just one least-CO2 route sailing East of Sardinia. For this special route it is therefore interesting to evaluate the marine conditions, the CO_2 savings, and the difference with the other optimal routes with the same departure time.

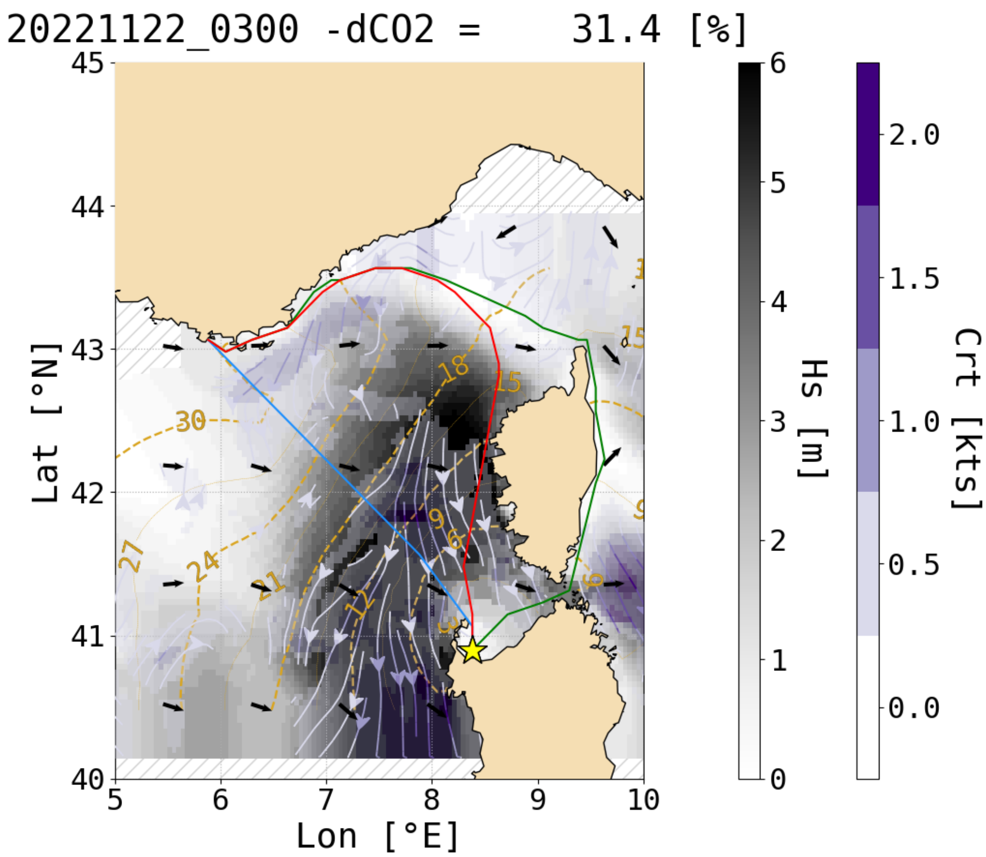

Fig.S8 Optimal Routes of the Ferry. For the specified departure date and time, the least-CO2 route is shown in green, the least-time route in red, and the least-distance route in blue. The significant wave height field is displayed in grey tones with black arrows, while the currents are depicted in purple tones with white streamlines. Environmental field values are not provided for the etched area. Additionally, isochrones of the CO2 -optimal route are shown at 3-hourly intervals. The engine load used was $\chi = 0.7$.

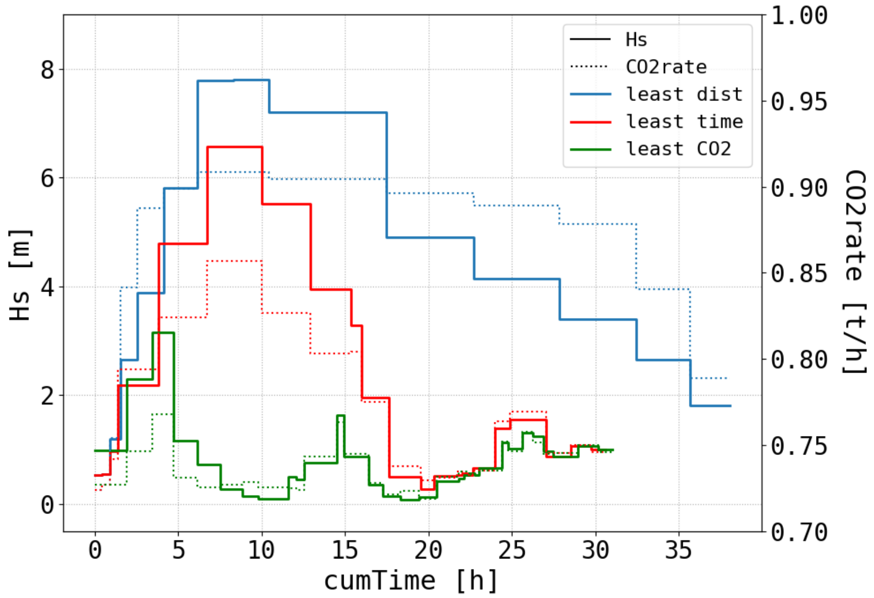

Fig.S9 Time-evolution or linechart of the three optimal routes shown in Fig.S11.

S3.2 Sailboat

Among the 2022's numerical experiments, there is just one least-time sailboat route with a duration longer than corresponding shortest-distance route. It is investigated more in depth here, highlighting its non-FIFO characteristics.

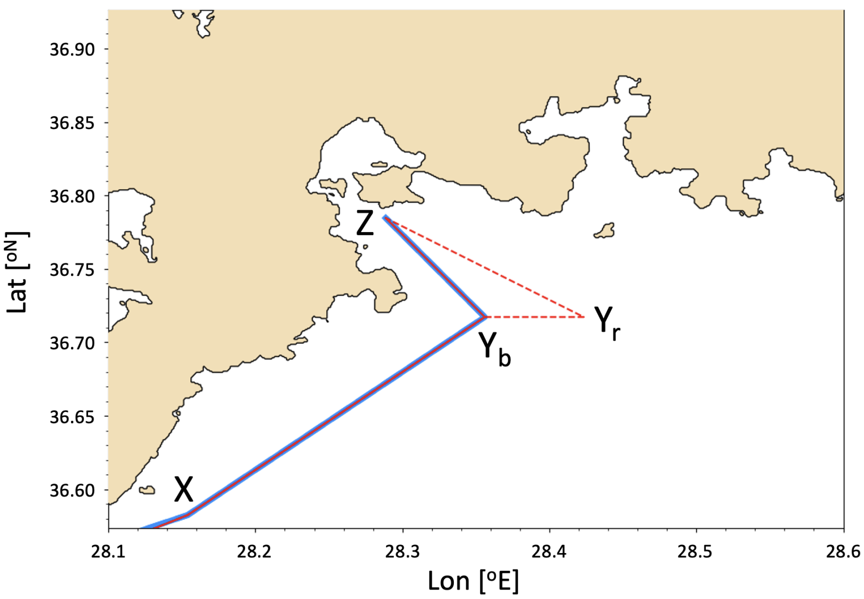

Fig.S10 Last three waypoints (x, Y, Z) of the geodetic (blue segments) and least-time (red segments) route for the eastbound route with departure on 2022-09-02 at 3:00 UTC. The least-time route sails either through Y_b or Y_r, depending on the actual $\Delta\tau$ value (s. Fig.S14).

From Fig.S11 it is seen that the (Y_bZ) leg was accessed (i.e. time of arrival at the Y_b node) via the least-time route a bit earlier than via the shortest-distance route. This is enough to find a not viable edge (because of the wind magnitude or direction). Consequently, the time-optimal route has to sail through the additional Y_r node, which eventually results in a longer total duration (31.31 hours) compared to the geodetic route (30.91 hours). However, as the time-step $\Delta\tau$ of the interpolated wind field (cf. Fig.4 in the manuscript) is reduced, more favourable wind conditions are experienced at Y_b. This allows completing the shortest-time route without sailing through Y_r and with a shorter duration than the geodetic.

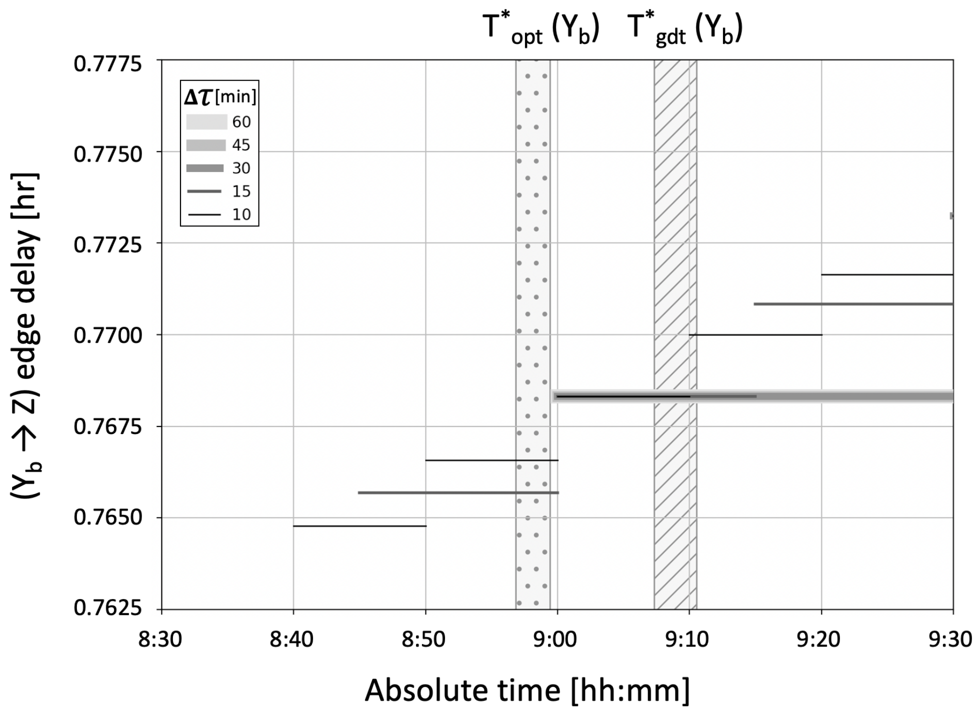

Fig.S11 Time for traversing the (Y_bZ) edge, depending on both the $\Delta\tau$ value and time of arrival at Y_b. depending on the actual $\Delta\tau$ value, the optimal and geodetic route access the Y_b node at the times within the etched stripes. If there is no horizontal segment with the style of a specific $\Delta\tau$ value, the (Y_bZ) edge is not available for sailing.

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S4. Bundles

Here the bundles comprising the solutions for all departure dates in 2022, both orientations, and several combinations of dynamic environmental fields are provided.

S4.1 Ferry

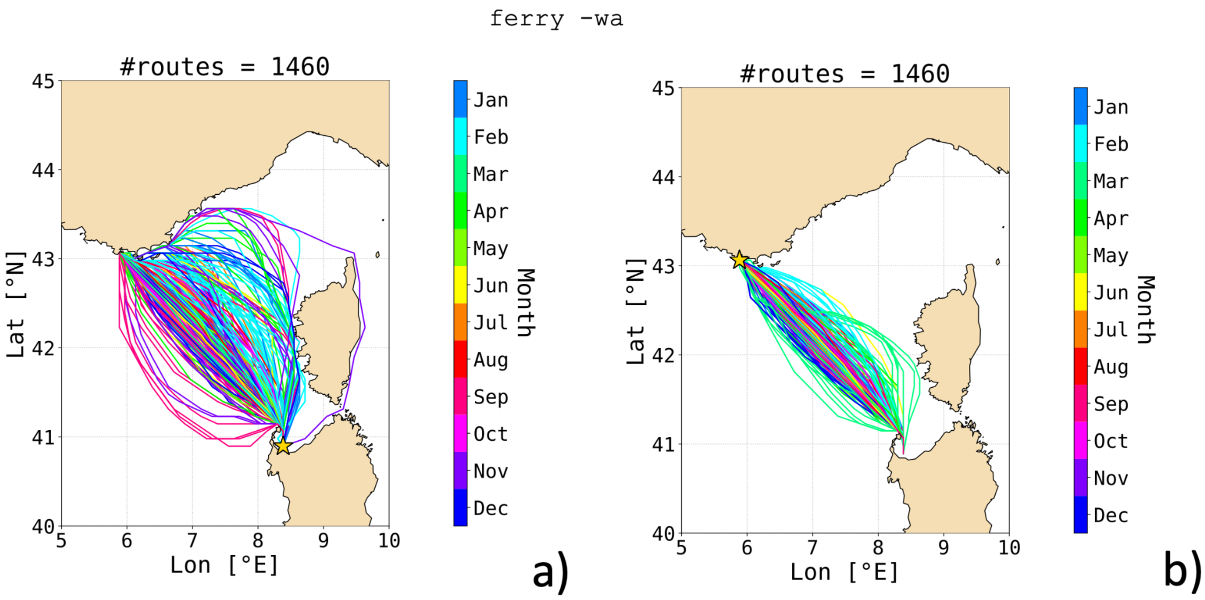

Fig.S12 Bundles for the ferry in case of a) northbound and b) southbound routes. Solutions for all the four engine load values χ = [70,80,90,100]% are shown. Just waves were accounted for.

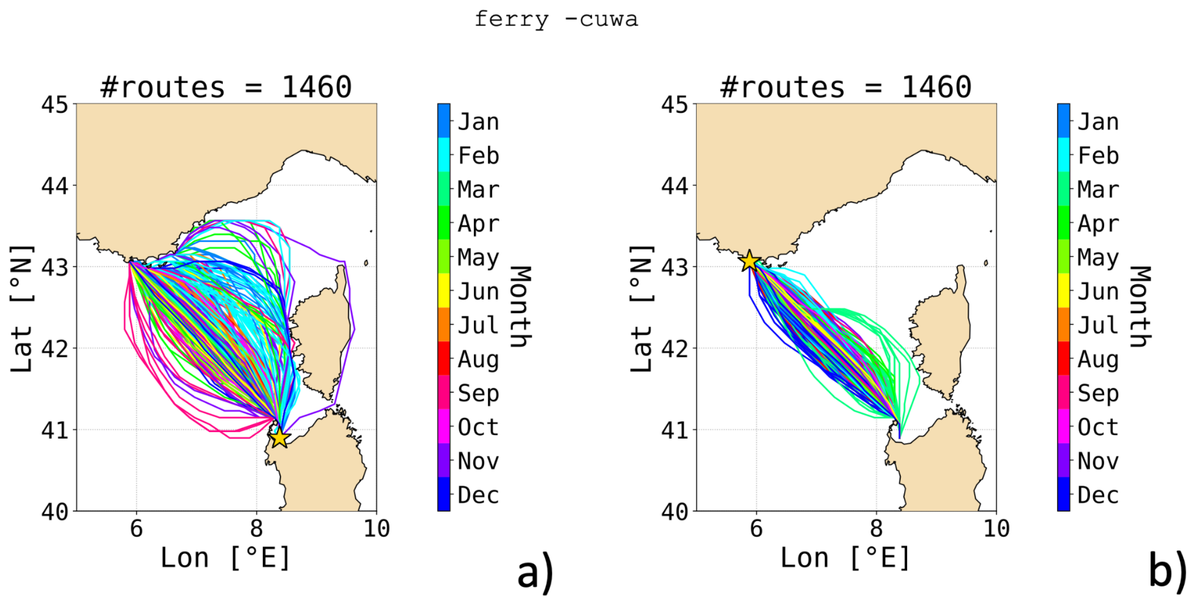

Fig.S13 As S12, but accounting for both waves and currents. Panel a) is identical to Fig.10b of the main manuscript.

S4.2 Sailboat

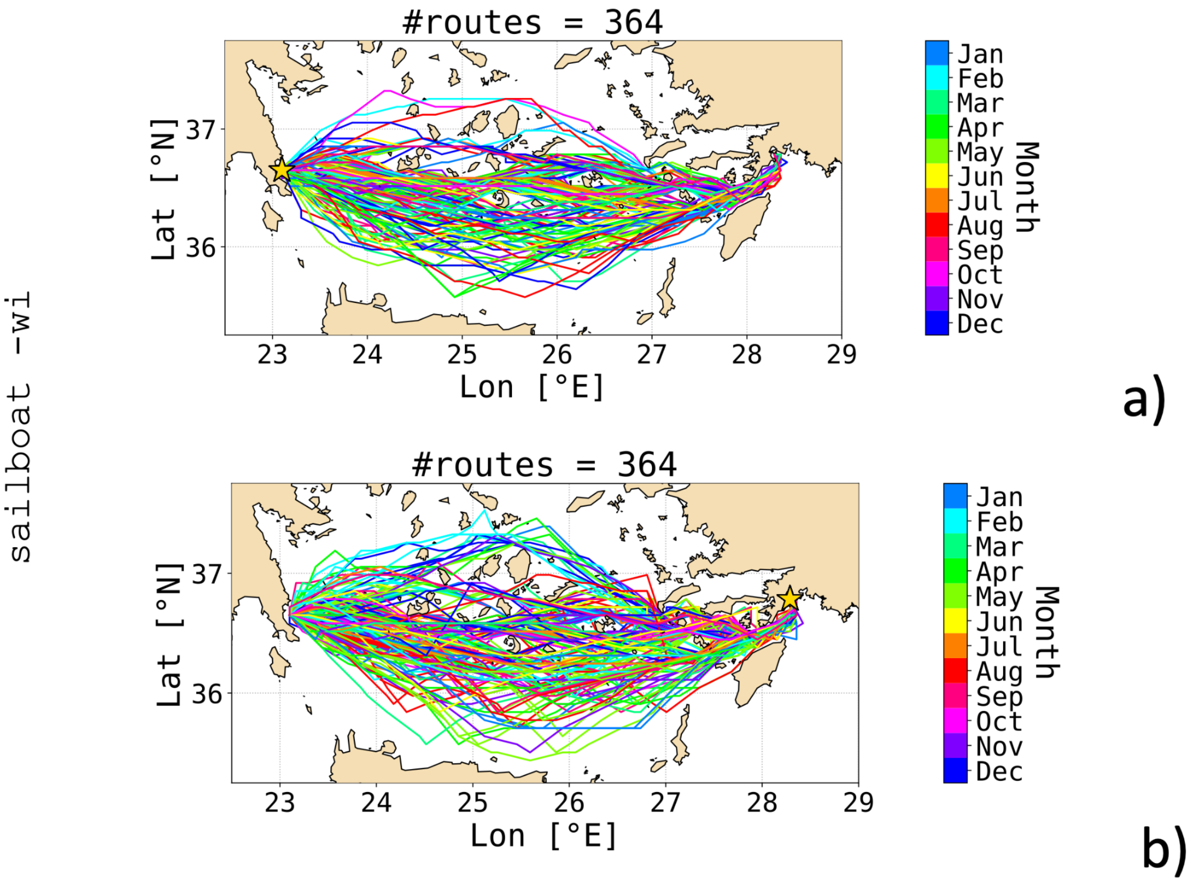

Fig.S14 Bundles for the First-367 sailboat in case of a) eastbound and b) westbound routes. Just wind was accounted for.

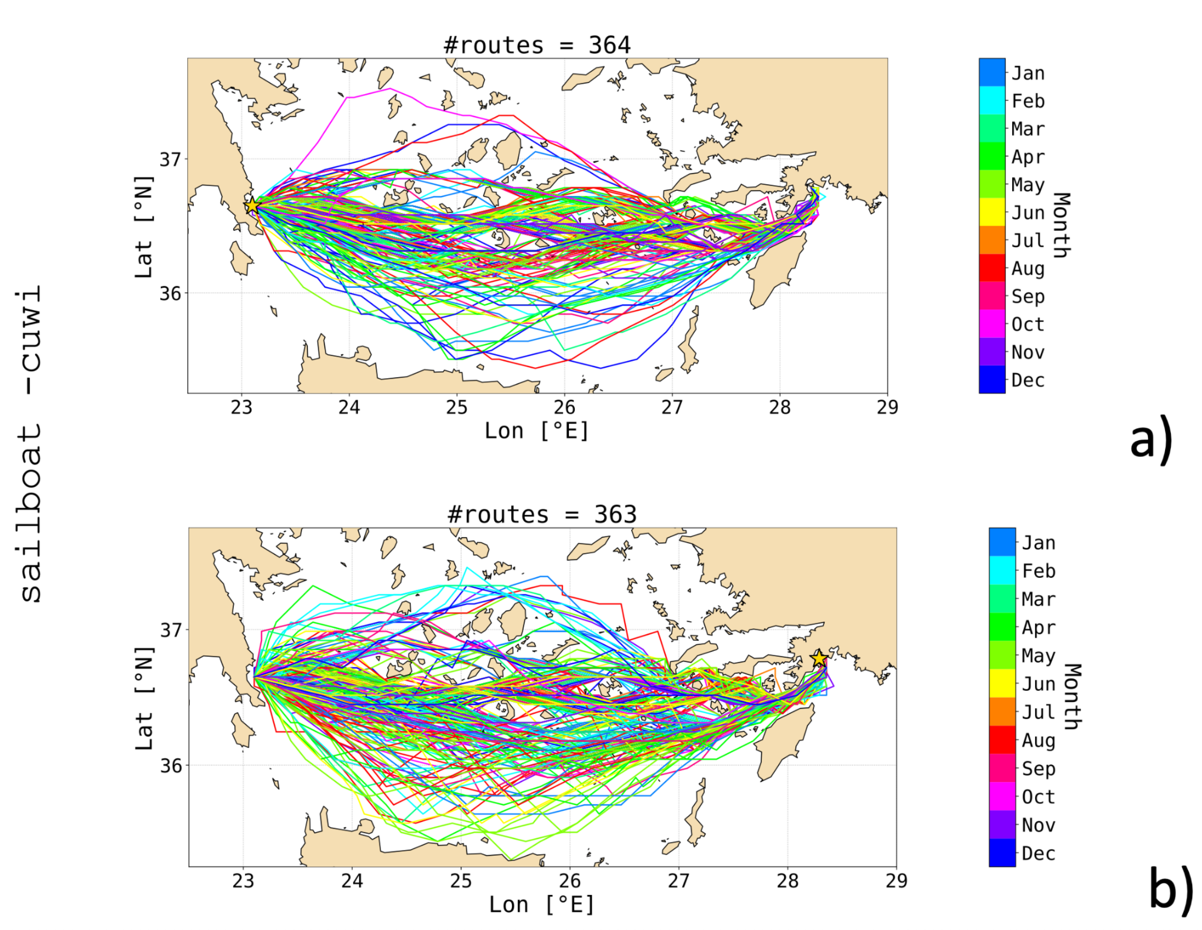

Fig.S15 As Fig.S14, but accounting for both wind and currents. Panel a) is identical to Fig.12b of the main manuscript.

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S5. Sailboat route metrics

Here the duration savings of the sailboat routes shown in Fig. 13 of the manuscript are broken out, depending on the sailing direction.

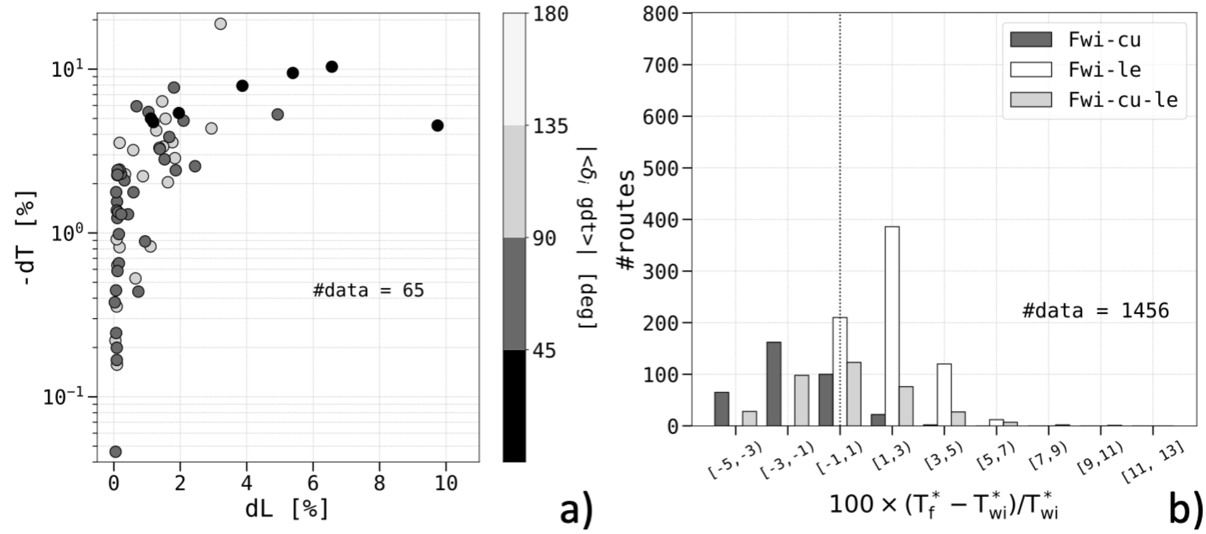

Fig. S16 For westbound routes (TRMRM-GRMON) only: a) Scatter plot of duration relative savings *-dT** vs. relative lengthening *dL* of optimal routes. The marker shape represents the average angle of attack of wind $|<\delta_i^{(gdt)}>|$ along the geodetic route as in legend. b) Histograms of relative route duration T^*_f with forcing combination *f* defined by the column colour, with respect to the duration T_{wi} of the wind-only optimal routes.

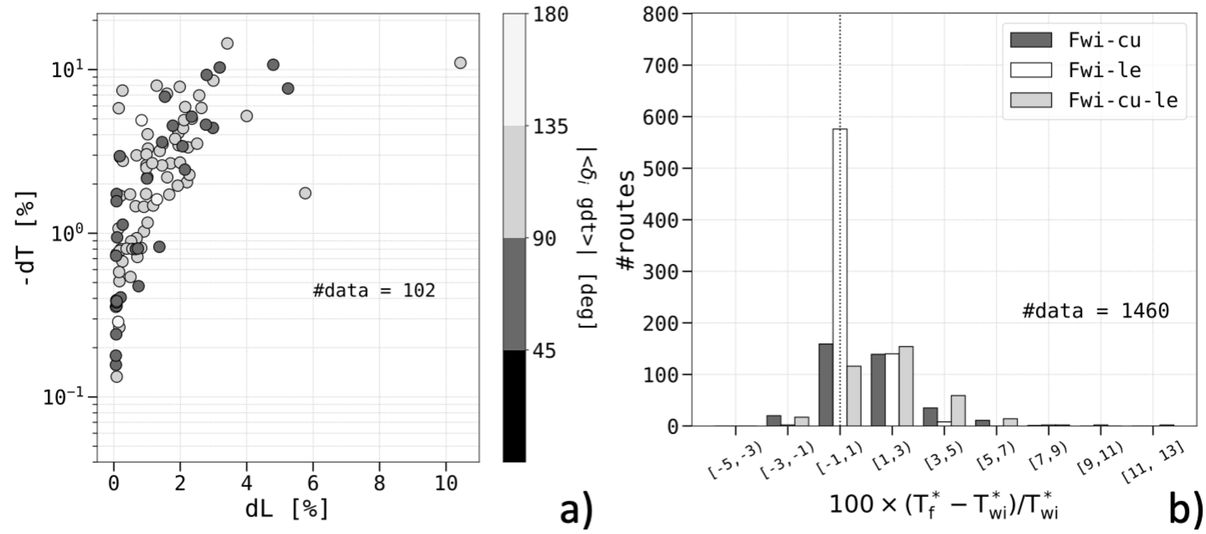

Fig. S17 as Fig.S16 but for eastbound routes (GRMON-TRMRM).

S6. Angle of attack

Here various plots regarding the computation of the angle attack δ between vessel's heading and course are provided.

S6.1 Ferry

The results in this section refer to the ferry described in the main manuscript.

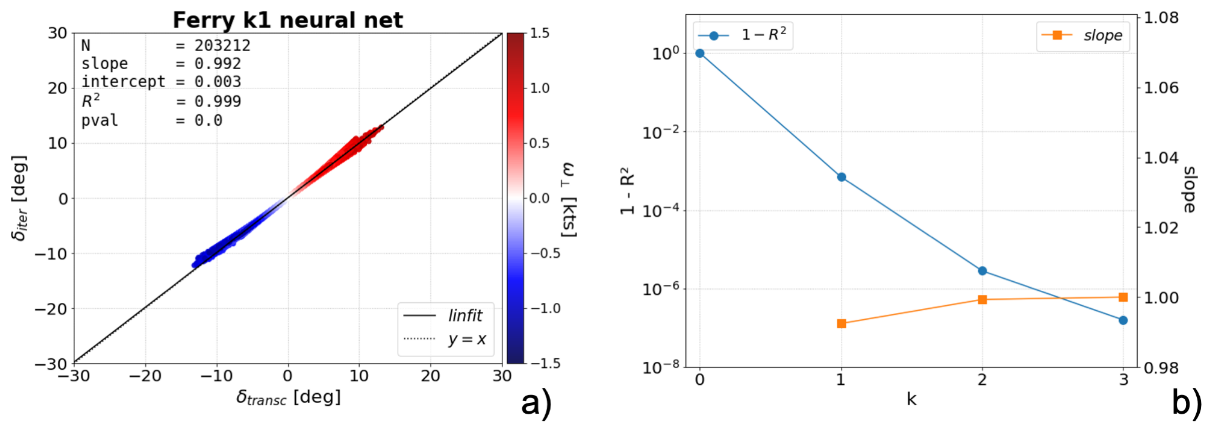

Fig. S18 Approximate vs. exact solution of Eq. 13 of the main manuscript, for the ferry. a) Iterative solution of Eq. A1 with *k* = 1 vs. exact solution, using the cross component of the effective flow $\omega_\perp$ as marker colour; b) unexplained variance (*R* is the Pearson's correlation coefficient) of the linear regression and fitted slope coefficient for various *k* values. The vessel's LUT was fitted via the neural network as explained in the main manuscript.

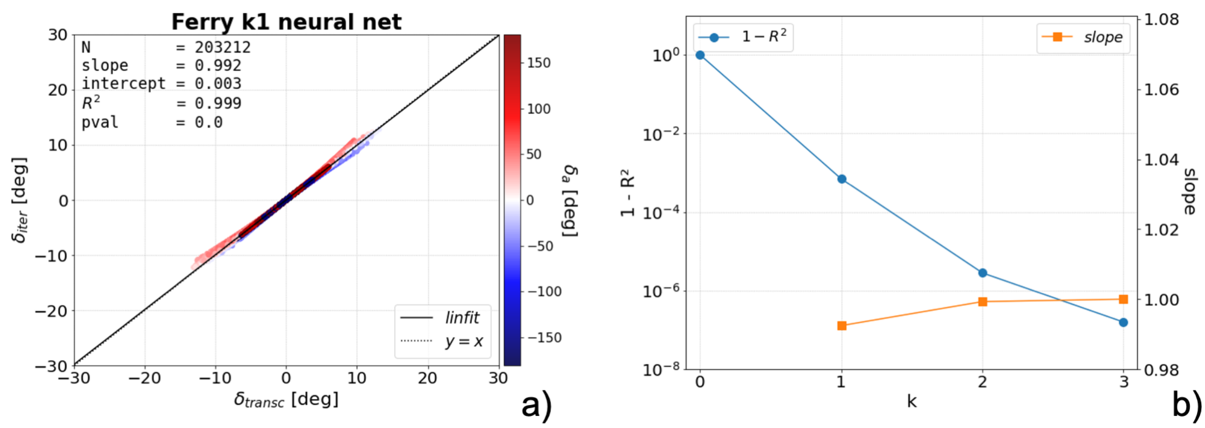

Fig. S19 As Fig.S18 but with wave angle of attack δ_a as marker colour.

S6.2 Sailboat

The results in this section refer to the sailboat described in the main manuscript (Sect. 4.2.1) and to some additional vessels (Sect. 4.2.2).

S6.2.1 First-367

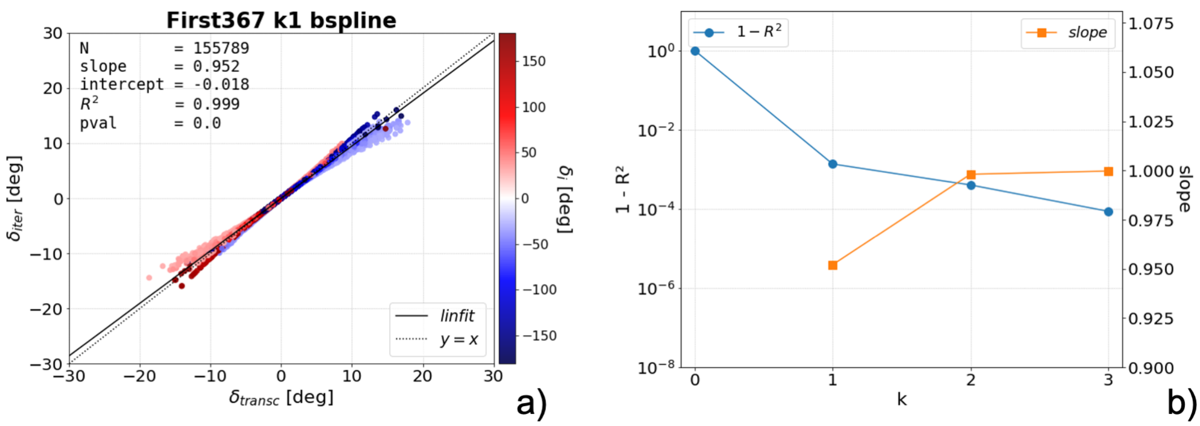

Fig. S20 Approximate vs. exact solution of Eq. 13 of the main manuscript, for the sailboat. a) Iterative solution of Eq. A1 with $k = 1$ vs. exact solution, using the cross component of the wind angle of attack δ_i as marker colour; b) unexplained variance (R is the Pearson's correlation coefficient) of the linear regression and fitted slope coefficient for various k values. The vessel's LUT was fitted via a cubic spline.

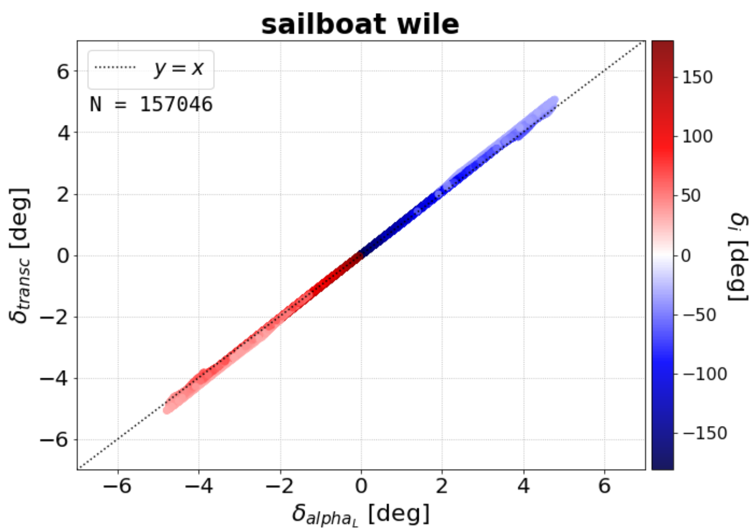

Fig. S21 Angle of attack δ from the exact solution of manuscript's Eq. 13 vs. the analytic solution in the absence of currents (Eq. 6). The marker colour refers to the wind angle of attack δ_i.

S6.2.2 Other sailboats

J24

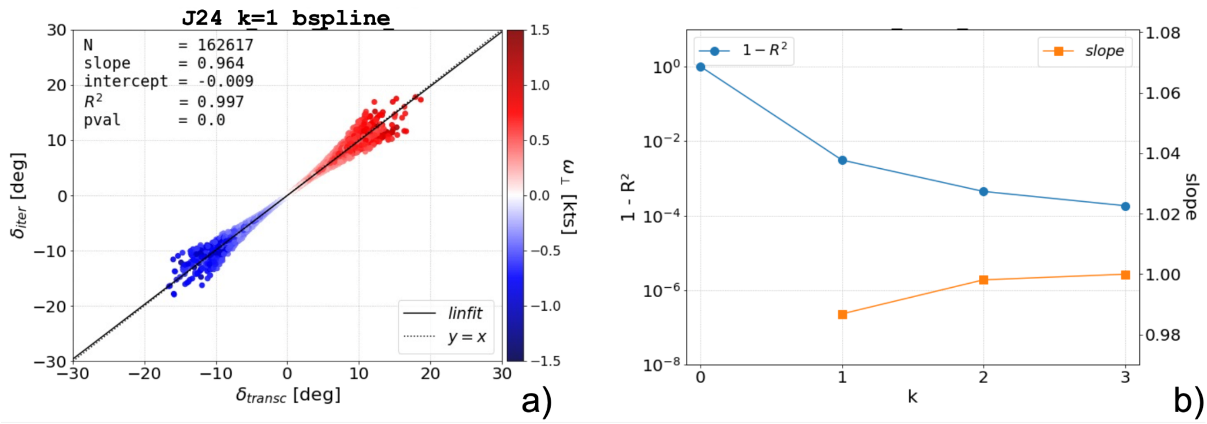

Fig. 22 Approximate vs. exact solution of Eq. 13 for a J24 sailboat. a) Iterative solution of Eq. A1 with k = 1 vs. exact solution, using the cross component of the effective flow $\omega_\perp$ as marker colour; b) unexplained variance (R is the Pearson's correlation coefficient) of the linear regression and fitted slope coefficient for various k values.

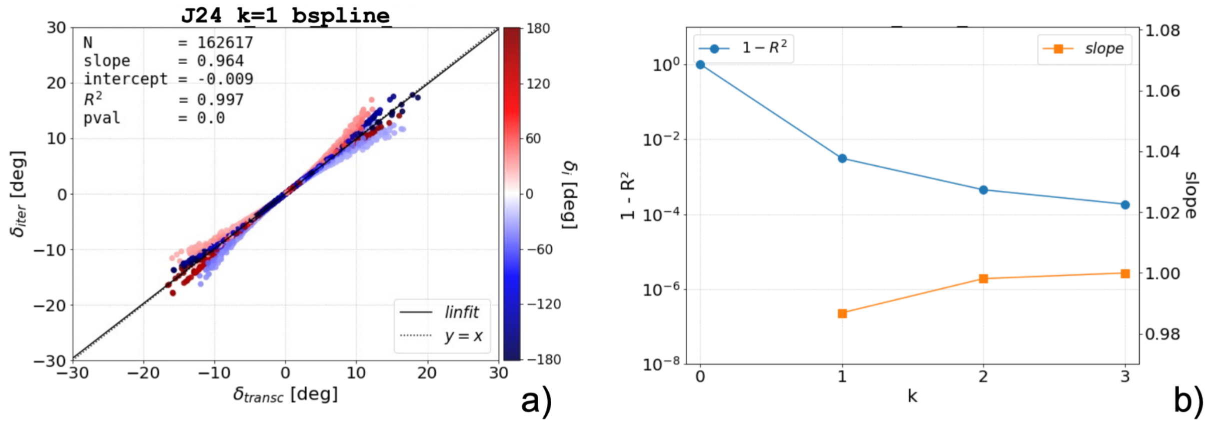

Fig. S23 As Fig.S22, but using the relative wind angle δ_i as marker colour.

Swan60FD

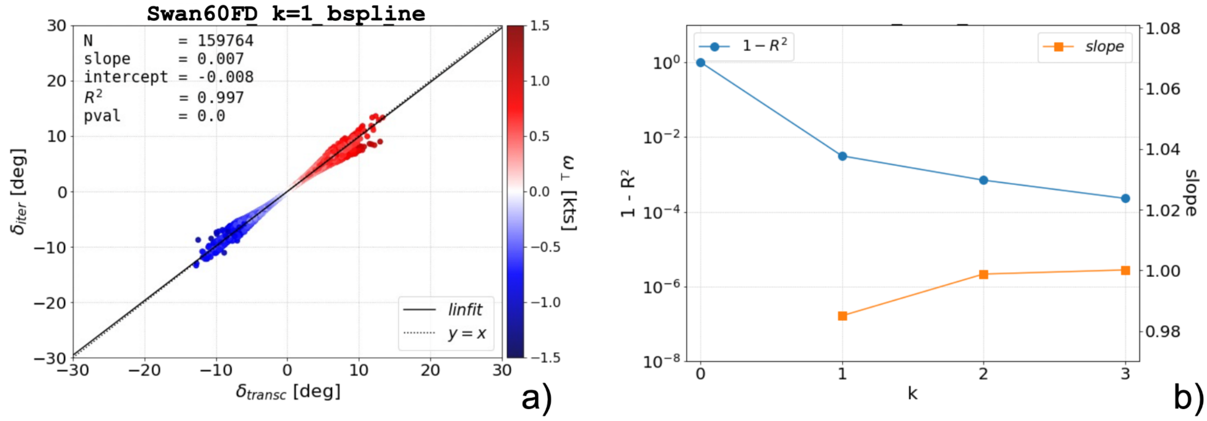

Fig. S24 Approximate vs. exact solution of Eq. 13 for a Swan-60FD sailboat. a) Iterative solution of Eq. A1 with *k* = 1 vs. exact solution, using the cross component of the effective flow $\omega_\perp$ as marker colour; b) unexplained variance (*R* is the Pearson's correlation coefficient) of the linear regression and fitted slope coefficient for various *k* values.

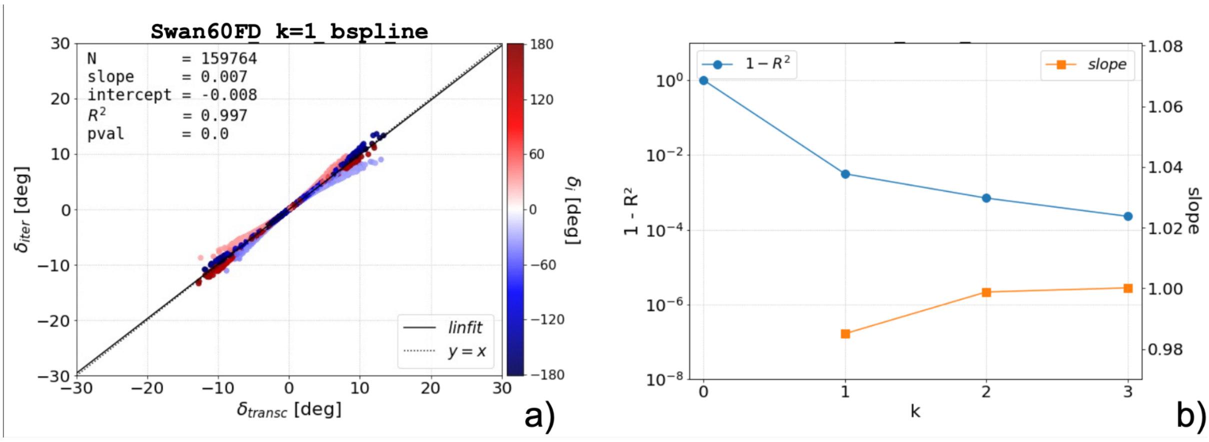

Fig. S25 As Fig.S24, but using the relative wind angle δ_i as marker colour.

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