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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 $N_\tau$. 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 $(\nu, 1/\Delta x) = (4, 12^\circ)$. The $k$ parameter in the titles of panels c) and d) refers to the number of iterations of Eq.A1.

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

Tab. S1 Fit coefficients of the $T_c = a \cdot \text{DOF}^b$ regressions for various components of the Grafi module. Std are the standard deviation errors on $a$ and $b$. Based on data of Fig.S1.
Tab.S2 As Tab.S1 but for the Campi module.

<table>
<thead>
<tr>
<th>submodule</th>
<th>description</th>
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<th>fit coeffs</th>
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<tr>
<td>wave</td>
<td>spatial interpolation of wave height and direction over edges</td>
<td>$y = a + bx$</td>
<td>1.06E+00</td>
</tr>
<tr>
<td>SOL_waves</td>
<td>seafloor land application over waves fields</td>
<td>1.01E+00</td>
<td>7.04E-03</td>
</tr>
<tr>
<td>wind</td>
<td>spatial interpolation of wind speed and direction over edges</td>
<td>4.94E+00</td>
<td>5.33E-02</td>
</tr>
<tr>
<td>SOL_wind</td>
<td>seafloor land application over wind fields</td>
<td>9.37E-03</td>
<td>3.64E-04</td>
</tr>
<tr>
<td>current</td>
<td>spatial interpolation of currents over edges</td>
<td>7.33E-01</td>
<td>3.05E-02</td>
</tr>
<tr>
<td>SOL_current</td>
<td>seafloor land application over currents fields</td>
<td>5.79E-01</td>
<td>6.65E-03</td>
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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.

<table>
<thead>
<tr>
<th>submodule</th>
<th>description</th>
<th>fit fun</th>
<th>fit coeffs</th>
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</thead>
<tbody>
<tr>
<td>sail</td>
<td>time interpolation of wave height and direction over timesteps</td>
<td>$y = ax^b$</td>
<td>9.33E-08</td>
</tr>
<tr>
<td>motor</td>
<td>time interpolation of currents over timesteps</td>
<td>1.29E-08</td>
<td>9.66E-10</td>
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<tr>
<td>time_interp_w_t</td>
<td>time interpolation of wind speed and direction over timesteps</td>
<td>3.80E-08</td>
<td>9.70E-09</td>
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<tr>
<td>STW_evaluation</td>
<td>4.24E+06</td>
<td>3.66E+08</td>
<td>9.96E+01</td>
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<tr>
<td>SOG and edge delay computation</td>
<td>1.44E+07</td>
<td>3.75E+08</td>
<td>8.75E+01</td>
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<tr>
<td>populating network graph</td>
<td>4.50E+08</td>
<td>1.33E+09</td>
<td>1.27E+02</td>
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</table>

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

<table>
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<th>description</th>
<th>fit fun</th>
<th>fit_coeffs</th>
</tr>
</thead>
<tbody>
<tr>
<td>wave_Tint</td>
<td>time interpolation of wave height and direction over timesteps</td>
<td>$y = ax^b$</td>
<td>5.67E-08</td>
</tr>
<tr>
<td>current_Tint</td>
<td>time interpolation of currents over timesteps</td>
<td>1.49E-08</td>
<td>1.42E-09</td>
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<tr>
<td>wind_Tint</td>
<td>time interpolation of wind speed and direction over timesteps</td>
<td>1.26E+07</td>
<td>2.95E+08</td>
</tr>
<tr>
<td>vessel_response</td>
<td>5.93E+06</td>
<td>9.64E+08</td>
<td>1.00E+00</td>
</tr>
<tr>
<td>edge_weight</td>
<td>SOG and edge delay computation</td>
<td>1.15E-07</td>
<td>2.04E-08</td>
</tr>
<tr>
<td>make_w_graph</td>
<td>populating network graph</td>
<td>1.02E-07</td>
<td>2.43E-08</td>
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</tbody>
</table>

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.

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\(^1\) [https://docs.scipy.org/doc/scipy/reference/generated/scipy.interpolate.BSpline.html](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 CO₂ emission rate).

<table>
<thead>
<tr>
<th>Regression variable</th>
<th>Hidden layers</th>
<th>alpha</th>
<th>Activation function</th>
<th>Max iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>STW</td>
<td>112</td>
<td>1.E-04</td>
<td>relu</td>
<td>10,000</td>
</tr>
<tr>
<td>CO₂rate</td>
<td>155, 25</td>
<td>1.E-05</td>
<td>relu</td>
<td>10,000</td>
</tr>
</tbody>
</table>

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 CO₂ 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 R² 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).

<table>
<thead>
<tr>
<th>Regression variable</th>
<th>Hidden layers</th>
<th>alpha</th>
<th>Activation function</th>
<th>Max iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>STW</td>
<td>25, 67</td>
<td>1.E-05</td>
<td>relu</td>
<td>10,000</td>
</tr>
<tr>
<td>Leeway</td>
<td>10, 49</td>
<td>1.E-04</td>
<td>relu</td>
<td>10,000</td>
</tr>
</tbody>
</table>

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 CO₂ 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 $\chi = 0.7$. 
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.

From Fig.S11 it is seen that the (Yₜ,Z) leg was accessed (i.e. time of arrival at the Yₜ 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, 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 Δτ of the interpolated wind field (cf. Fig.4 in the manuscript) is reduced, more favourable wind conditions are experienced at Yb. This allows completing the shortest-time route without sailing through Y, and with a shorter duration than the geodetic.

Fig.S11 Time for traversing the (YbZ) edge, depending on both the Δτ value and time of arrival at Yb, depending on the actual Δτ value, the optimal and geodetic route access the Yb node at the times within the etched stripes. If there is no horizontal segment with the style of a specific Δτ value, the (YbZ) 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 $\chi = [70,80,90,100]$% 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 \( |< \delta^{(opt)}_i >| \) 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 $\delta$ 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 $\omega_x$ 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 $\delta_{w}$ 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 $\delta_i$ 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 $\delta$ 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 $\delta_i$. 

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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 \( \omega \) 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 \( \delta \) 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 $\delta_i$ as marker colour.

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