Multifaceted Visual Analysis of Oceanographic Simulation Ensemble Data

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The analysis of multirun oceanographic simulation data imposes various challenges ranging from visualizing multifield spatio-temporal data over properly identifying and depicting vortices to visually representing uncertainties. We present an integrated interactive visual analysis tool that enables us to overcome these challenges by employing multiple coordinated views of different facets of the data at different levels of aggregation.

Oceanography scientists are interested in the unique properties of bodies of water such as the Red Sea and their influence on the ecosystem. It is therefore crucial to find potential relationships between these properties, such as recurring patterns or abnormalities. Vortices and water temperature are of particular interest, as they strongly influence the transport of salt and other particles in the ocean. Simulations of these properties produce large multifield spatio-temporal datasets with multiple simulation runs. A comprehensive analysis of such ensemble data is difficult to achieve by visualizing each volume individually due to the vast amount of data. To offer a faster way of analyzing such data, we propose interactive visual analysis methods for the different facets of the data and embed them into an integrated system. We apply our methods to the IEEE SciVis 2020 Contest data.[1]

The data consist of several simulation runs or members with slight perturbations in the initial conditions resulting in an ensemble, where each ensemble member might exhibit slightly different flow patterns and scalar quantities. One of our goals is the visualization of vortices and their impact on particle transport. We also analyze the correlation between vortices, salinity, and temperature, as well as their evolutions over time. Our methods incorporate the underlying uncertainty encoded in the given ensemble data.

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METHODS

The analysis tasks can be summarized as analyzing flow structures, multifield correlations, temporal evolution, and uncertainty within the ensemble. We propose respective task-driven methods operating on different data aggregation levels and analyze the interplay of different facets using coordinated views.

For the analysis of flow structures, vortex regions and their corelines are essential features. Density visualizations allow us to analyze the probability and frequency of their occurrence. To visualize the transport of particles, we demonstrate that geometric flow visualization can be employed effectively. For correlation analysis, parallel coordinates are known to be powerful. We apply them to analyze multifield correlations. Finally, we compare ensemble members and their temporal evolution by mapping them to a similarity space and visualizing them in a low-dimensional embedding of the similarity space.

Vortex Region Visualization

We extract and visualize vortex regions using Δ, λ_2, and Q criteria, as well as vorticity magnitude.[5] When aggregating over all simulation runs, we can compute a *probability field* for vortex regions, see Figure 1, or use an *uncertain vector field* representation.[8]

To visualize the resulting scalar fields as well as aggregated fields such as the ensemble mean, we employ a volume renderer, which is a GPU raycaster with configurable piecewise linear transfer functions and multifield functionality.[11]

Vortex Coreline Visualization

Analyzing the corelines of vortices helps us to understand their movement over time and rotational

THE 2020 IEEE SCIENTIFIC VISUALIZATION CONTEST

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Introduction

The SciVis Contest is an annual competition colocated with the IEEE VIS Conference as an associated event. Since 2004, the contest provides scientific datasets for visualization and data analysis by individuals and teams, stoking a competitive spirit in the visualization community. The competitive entries are judged and ranked by domain scientists and visualization experts.

The Contest Problem

The 2020 IEEE SciVis Contest was dedicated to creating novel approaches or state-of-the-art visualizations to assist domain scientists to better understand the complex transport mechanisms of eddies in the Red Sea under uncertainty. Eddies are clockwise or counterclockwise circular movements of water that play a major role in transporting energy and biogeochemical particles in the ocean. Advanced visualization techniques should enable for better detection capabilities and deeper knowledge of how regularly these eddies occur and how they behave.

The 50 different ensemble members of the dataset were generated with an ensemble data assimilation system based on the MIT ocean general circulation model (MITgcm) and the data research testbed (DART), together with remote sensing satellite observations. The Ensemble Adjustment Kalman filter (EAKF) was used for assimilation, it samples the ensemble members deterministically from the estimated posterior, assumed Gaussian–Kalman based, and conditioned on the available observations (satellite sea surface temperature, sea level anomalies, and *in situ* salinity and temperature data were assimilated). The dataset was simulated on the KAUST supercomputer Shaheen II with assistance of the KAUST Supercomputing Core Lab. It is freely available at https://kaust-vislab.github.io/SciVis2020/data.html.

Evaluation

We received seven quality submissions for the 2020 SciVis contest. A jury of nine domain scientists and visualization researchers (Thomas Theußl, Madhusudanan Srinivasan, Guoning Chen, Ibrahim Hoteit, Shehzad Afzal, Aneesh C. Subramanian, Bruce Cornuelle, Silvio Rizzi, and Theresa-Marie Rhyne) carefully reviewed all entries and selected the entry "Interactive Visual Analysis of Oceanographic Simulation Ensemble Data," by Hennes Rave, Johannes Fincke, Steffen Averkamp, Lehmensiek H. N. Tague, Beate Tangerding, Luca Wehrenberg, Tim Gerrits, Karim Huesmann, Simon Leistikow, and Lars Linsen as the overall winner. The winning team convinced the jury with a compelling presentation of their comprehensive tool that allows verification and exploration of domain science problems, including uncertainty, and illustration of some important domain science facts such as the outflow from the Red Sea into the Gulf of Aden.

This year's decision was extremely close and the jury decided to award an "Honorable Mention" to "The Use of 3D Optical Flow, Feature-Tracking and Token-Tracking Petri Nets to Analyze and Visualize Multiple Scales of Ocean Eddies," by Sedat Ozer, Karen Bemis, Weiping Hua, Arda Goktogan, Melike Aydogan, Kevin Guo, Dujuan Kang, Li Liu, and Deborah Silver.

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direction. To identify corelines, we find parallel vectors in the velocity and acceleration fields[9] and apply Sujudi–Haimes filtering.[10]

Coreline Density: By aggregating corelines from all runs into a single volume after convolution with a Gaussian kernel, we can visualize the density distribution of corelines for any time step. Additionally, aggregation over multiple time steps results in a frequency visualization of coreline occurrences, see Figure 2.

Merge-Tree: To track vortices over time, we match each coreline to the closest coreline of the same run at the subsequent time step, if their distance is lower than a user-adjustable threshold.

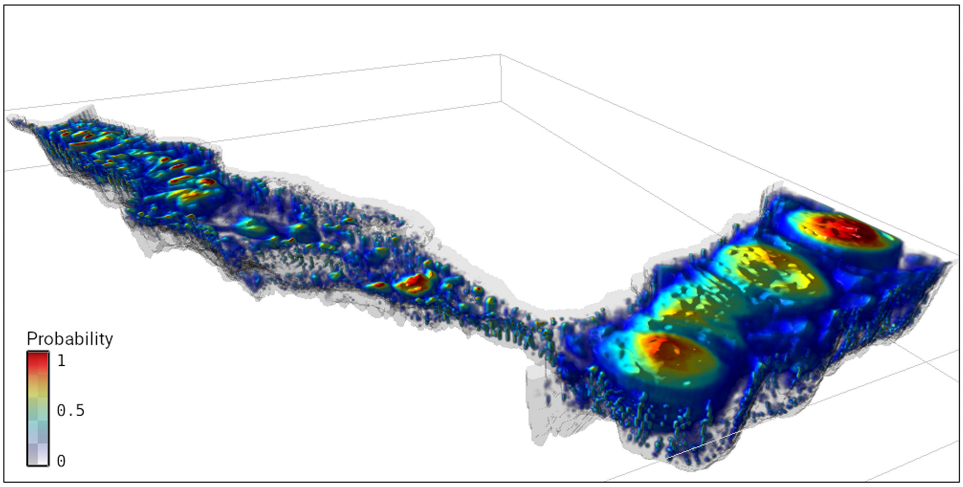

FIGURE 1. Probability of vortex regions computed over all runs (time step 0) using the λ_2 criterion, where the volume rendering is cropped at the top. Colors range from low-opacity blue to fully opaque red. Two of the large vortices in the Gulf of Aden are highly certain, while most vortices in the Red Sea are rather uncertain.

The distance of two corelines a and b is computed by

$$d(a,b) = \frac{1}{|a|}\sum_{a_i \in a} \min_{b_j \in b} ||a_i - b_j||_2$$

where a_i and b_j denote points on the corelines and $|a|$ the number of points on a. The matching result is encoded in a merge-tree visualization, which comprises two linked views, see Figure 3 (left): The top view shows nodes representing vortices over time from left to right. The bottom view depicts their respective spatial locations, shown from above. Connected paths indicate the movement of vortices over time as well as merging and splitting events. Cyclonic vortices are shown in blue, anticyclonic vortices in red. Vortices without a predecessor are depicted larger. The opacity encodes how often a vortex is found within a set of selected runs, i.e., vortices that appear in all selected runs are rendered fully opaque.

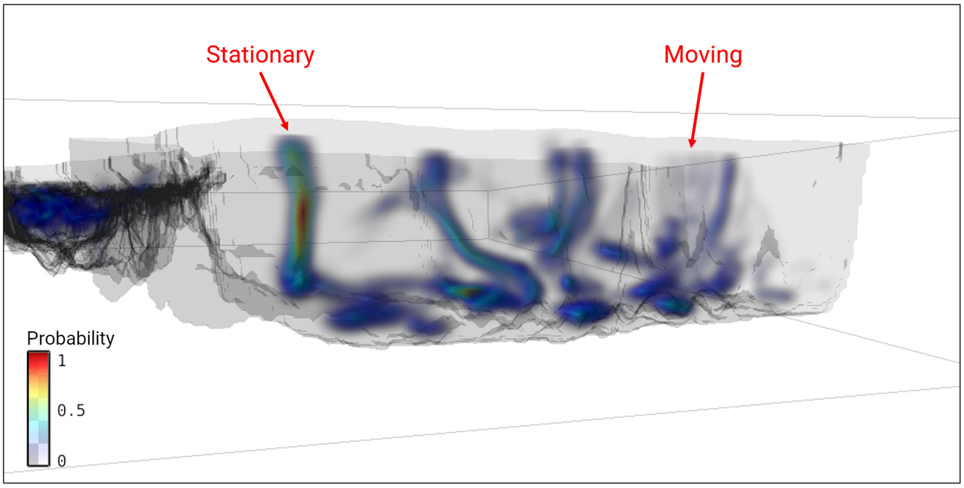

FIGURE 2. Coreline density visualization computed by aggregating all detected corelines of the ensemble mean over all time steps. Among the four large vortex regions in the Gulf of Aden, we observe that the two further in the West have a higher density than the two in the East, which indicates that the ones to the left move less over the simulated time interval.

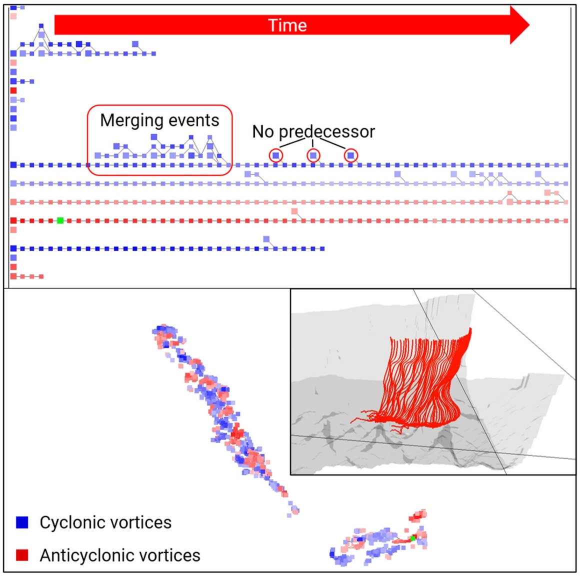

FIGURE 3. Merge-tree visualization of tracked vortices extracted from the ensemble mean. The hovered node is highlighted in green. *Inset:* Rendering of a tracked coreline, selected using the merge tree.

We can filter corelines by time, run, length, and rotational direction. By clicking on a vortex in either of the views, we can select/deselect it and, optionally, all of its successors. Selected vortices are displayed darker, see Figure 8. The corelines of all selected vortices can be rendered in a separate view and filtered by time to observe temporal evolution.

Approximate Parallel Vectors: As the parallel vectors operator only compares vectors of two volumes, we further implemented the approximate parallel vectors operator,[4] which extracts locations where the vectors of multiple vector fields are approximately parallel. We apply it to the velocities of all runs to find regions where the flow directions are aligned most.

Correlation Analysis

To analyze correlations between salinity, temperature, and vortex criteria, we use Parallel Coordinates.[7] Moreover, we use them to analyze temporal evolutions, where each axis represents one time step (in chronological order). We reduce visual clutter by showing line densities. Intervals along the axes can be selected via brushing. Brushing on multiple axes leads to the selection of the samples included in all brushed intervals.

The selected samples are rendered in a linked single-field volume rendering. Alternatively, the selections on multiple axes can be shown individually in a multivolume rendering, see Figure 4.

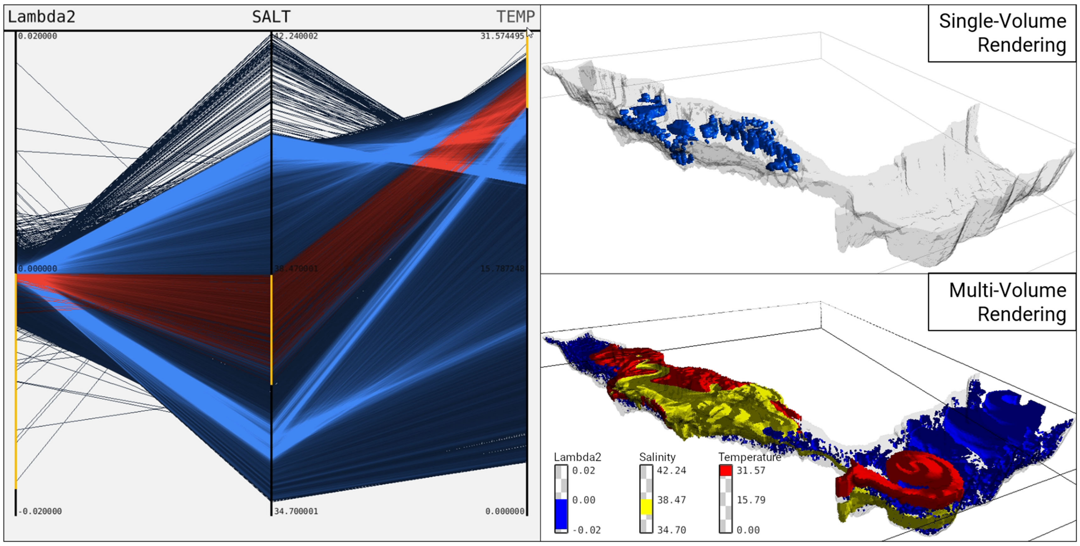

FIGURE 4. Interactive selection in parallel coordinates is supported by brushing on the axes, which can be linked to a multivolume renderer and a single-volume renderer to exhibit the spatial regions that correspond to the parallel coordinates selections. In the multivolume renderer, selections on the individual parallel coordinates axes are rendered using binary transfer functions with different colors (here, blue for λ_2, yellow for salinity, red for temperature). In the single-volume renderer, the intersection of the regions of the multivolume renderer is shown in blue. The visualizations use time step 0 of the ensemble mean.

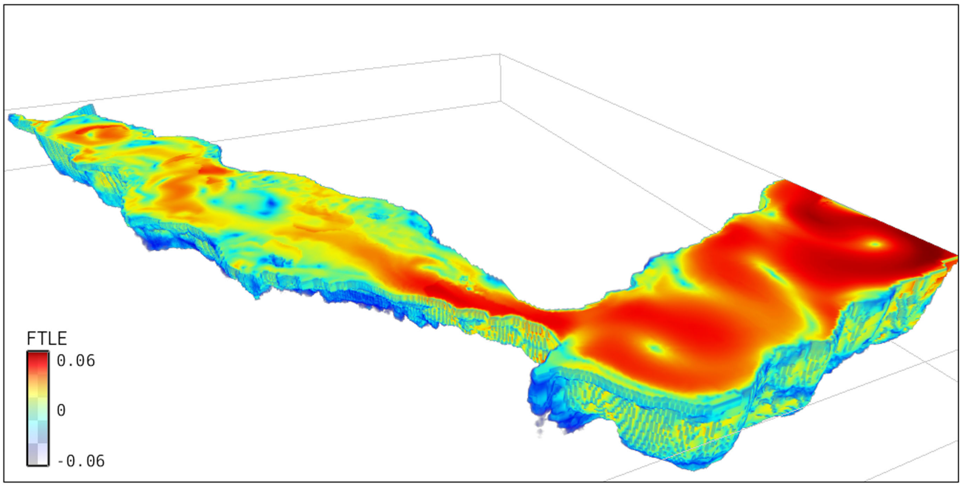

FIGURE 5. Particle separation over all time steps can be visualized by computing the FTLE field of the ensemble mean. High FTLE values (red) correspond to high particle separation. We observe the highest particle separation at surface levels near vortices and in the Bab-al-Mandab Strait.

Particle Transport

To analyze particle transport as well as the influence of vortices on it, we visualize particle separation and flow.

Particle Separation: We use forward finite-time Lyapunov exponent (FTLE)[6] fields to analyze particle separation in 3-D and over time for individual runs or the ensemble mean, see Figure 5.

Particle Flow: For single time steps, we use streamlines and color-code them by velocity magnitude, see Figure 6. For flow integration over multiple time steps, we implemented a pathline visualization, see Figure 10. These lines can be color-coded using any available measure such as salinity.

Comparing Ensemble Members

To capture the overall spatial similarities between individual runs of the given ensemble, we use similarity plots.[3] They show the temporal evolution of

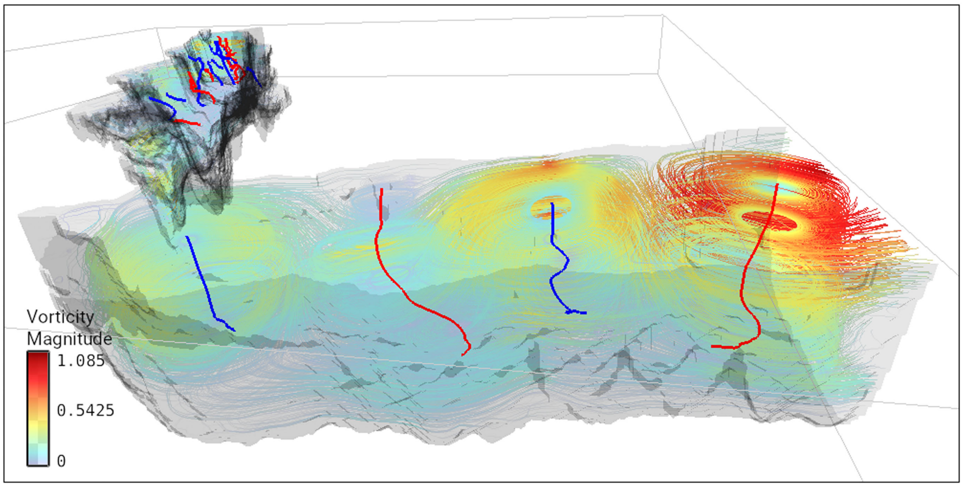

FIGURE 6. Steady flow behavior is analyzed by combining streamline and coreline visualizations, here for the ensemble mean at time step 0 for the Gulf of Aden. The streamlines' color encodes the velocity magnitude. The corelines have been filtered by length and color-coded according to their orientation (red: anticyclonic, blue: cyclonic). Corelines are surrounded by streamlines swirling around them, which allows for the detection of the vortices' region of influence.

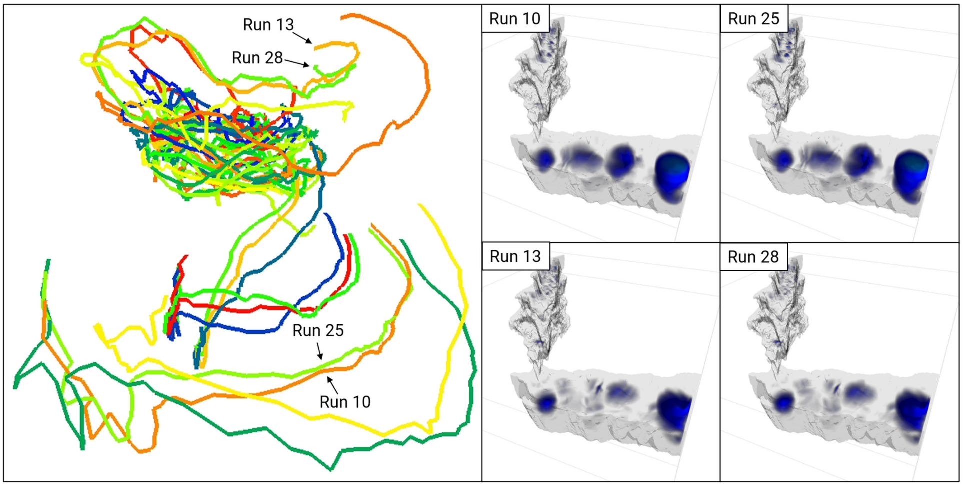

FIGURE 7. Similarity plots for the λ_2 fields represent each run by a (randomly colored) line to show how similar the spatio-temporal patterns of all simulation runs are. The 3-D similarity plot shows the first three principal components for interactive exploration. Identified groups are confirmed by volume renderings showing vortex regions ($\lambda_2 < 0$) in blue.

each simulation run by a curve in a low-dimensional embedding, where the closeness of curves in the embedding represents field similarity[2] of the respective simulation runs, see Figure 7. We can interactively switch between 1-D, 2-D, or 3-D embeddings.

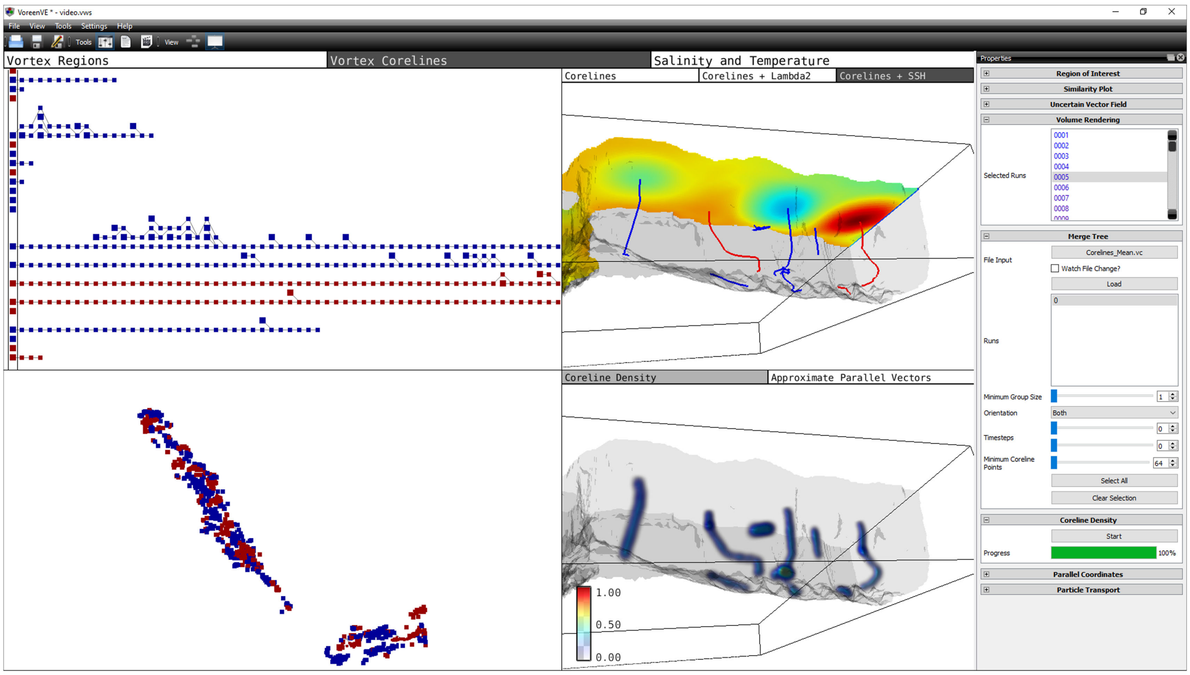

FIGURE 8. All visualization methods are embedded into an integrated interactive visual analysis tool with multiple coordinated views and respective interactive selection mechanisms. Overview visualizations show different facets of the entire ensemble in aggregated form and its evolution over time. Selections allow for a more detailed analysis of individual runs and time steps. The cameras of all spatial views are linked.

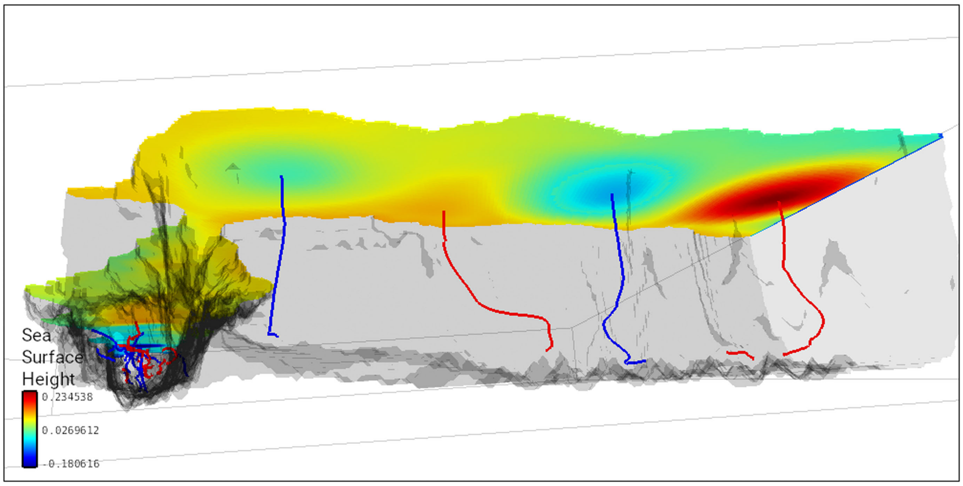

FIGURE 9. Visualization of the sea surface height in conjunction with major vortex corelines' (mean, time step 0, filtered by length) orientation reveals their correlation: Sea surface height is visualized using the jet color map where blue indicates decreased height and red indicates increased height. Vortex corelines are depicted in blue for vortices with cyclonic orientation and in red for vortices with anticyclonic orientation. We observe that cyclonic orientation and a decreased sea surface height correlate, as well as anticyclonic vortices and an increased sea surface height.

Analytical Workflow

The aforementioned visualizations are linked using multiple coordinated views, see Figure 8. In particular, the user is able to choose a region of interest, time step, or camera position, which then affects all selected views simultaneously.

The views include overview visualizations, such as similarity plots, parallel coordinates, or aggregated volume renderings, and detailed visualizations, such as streamlines or nonaggregated volume renderings. Typically, a user starts the analysis utilizing overview visualizations to detect interesting time steps and/or runs or to analyze correlations between different fields. Then, a detailed visualization can be used to examine possible findings more closely.

IMPLEMENTATION

Parts of the source code were published with release 5.2 of Voreen, an open-source rapid application development framework.[11] We converted the given ensemble from NetCDF to HDF5 format, which reduces the needed disk storage and accelerates loading of the dataset. In a second step, we mirrored the data at the *y*-axis to obtain a geographically correct representation of the Red Sea and adjacent waters. Subsequently, we precomputed mean, standard deviation, and vortex regions for multiple criteria of all runs at each time step for faster analysis.

RESULTS

Vortices: We begin the analysis by looking at probability fields for λ_2, Q, Δ, and vorticity magnitude criteria to get an overview of vortex regions. In further analyses, we only consider λ_2 criterion as it seems to extract vortex structures most reliably. We observe four large vortices in the Gulf of Aden, while many smaller vortices are located north of 18 $^\circ$N in the Red Sea, see Figure 1.

To capture the overall spatial similarity of vortex criteria between individual runs, we use similarity plots. By interacting with the 3-D embedding of λ_2 similarity plot, we are able to discern seven groups. We can confirm these observations by comparing representative runs of the groups, see Figure 7.

For the analysis of vortex corelines, the coreline density visualizations reveal locations where the probability of coreline occurrences is the highest, at a single time step or over time, see Figure 2. We observe that some vortices are more certain than others, i.e., they occur in all simulation runs. Also, some vortices are stationary, while others are moving, which can be confirmed using our tracking in combination with merge-tree interactions, see Figure 3. By superimposing corelines over the rendering of sea surface height, see Figure 9, we can identify a correlation with the rotational direction: The sea surface is higher near anticyclonic vortices and lower near cyclonic ones. The streamline visualization can be used to confirm the identified coreline positions, see Figure 6.

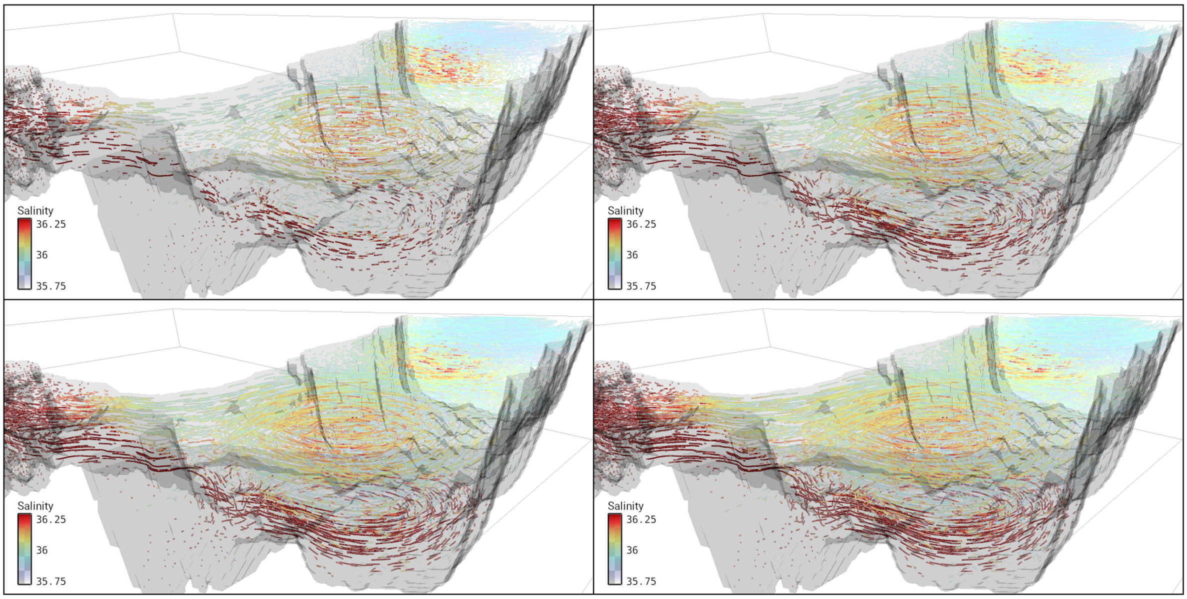

FIGURE 10. Unsteady flow visualization using 50,000 pathlines color-coded by the salinity values of the ensemble mean: The visualizations show pathlines when integrated up to time step 14 (top left), 29 (top right), 44 (bottom left), and 59 (bottom right), respectively. The series of visualizations show how low-salinity water flows from the Gulf of Aden into the Rea Sea at upper surface levels, while high-salinity water flows back from the Red Sea into the Gulf of Aden at lower surface levels and is taken up by the first major vortex structure.

Salinity and Temperature: Similar to λ_2 criterion, we can find groups of similar behavior in the similarity plots of salinity and temperature. Again, we can confirm these findings by comparing representative runs of the groups.

We utilize Parallel Coordinates to identify correlations between salinity and temperature: For a salinity above $39.1\ \mathrm{g\,m^{-3}}$, the temperature lies above 19 $^{\circ}$C. For a salinity below $35.25\ \mathrm{g\,m^{-3}}$, the temperature lies below 7.5 $^{\circ}$C. For a temperature below 18.1 $^{\circ}$C, the salinity lies below $37.2\ \mathrm{g\,m^{-3}}$. For vortex regions ($\lambda_2 < 0$), we cannot observe any clear local correlation between vortex regions and salinity or temperature, respectively. When visualizing the standard deviations of salinity and temperature over time, we observe a decrease, which implies that the runs become more similar with increasing simulation time.

Particle Transport: To visualize particle transport, we first calculate an FTLE field, see Figure 5. Particle separation is highest near vortices at the surface and in the Bab al-Mandab Strait. We additionally employ a pathline visualization, which shows that at the bottom of the Bab al-Mandab Strait, high-salinity water flows from the Red Sea into the Gulf of Aden, while low-salinity water flows in the opposite direction near the surface, see Figure 10. The high-salinity water is then transported by the large nearby vortex.

CONCLUSION

The authors would like to propose an integrated interactive tool for the analysis of oceanographic simulation ensemble data. It enables the visual analysis of vortices and their corelines in 3-D and over time using several vortex criteria as well as a merge tree for tracking and interactive filtering of vortices. We can analyze the impact of vortices on particle transport using FTLE fields, as well as streamline and pathline visualizations. Parallel Coordinate plots allow us to analyze the correlation between vortices, salinity, and temperature and their respective evolutions over time. We incorporated the multirun nature of the given ensemble using similarity plots and different kinds of uncertainty visualizations.

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