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Details-First, Show Context, Overview Last: Supporting Exploration of Viscous Fingers in Large-Scale Ensemble Simulations

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Abstract— Visualization research often seeks designs that first establish an overview of the data, in accordance to the information seeking mantra: "Overview first, zoom and filter, then details on demand". However, in computational fluid dynamics (CFD), as well as in other domains, there are many situations where such a spatial overview is not relevant or practical for users, for example when the experts already have a good mental overview of the data, or when an analysis of a large overall structure may not be related to the specific, information-driven tasks of users. Using scientific workflow theory and, as a vehicle, the problem of viscous finger evolution, we advocate an alternative model that allows domain experts to explore features of interest first, then explore the context around those features, and finally move to a potentially unfamiliar summarization overview. In a model instantiation, we show how a computational back-end can identify and track over time low-level, small features, then be used to filter the context of those features while controlling the complexity of the visualization, and finally to summarize and compare simulations. We demonstrate the effectiveness of this approach with an online web-based exploration of a total volume of data approaching half a billion seven-dimensional data points, and report supportive feedback provided by domain experts with respect to both the instantiation and the theoretical model.

Index Terms—theory, visualization design, details-first model, discourse paper, computational fluid dynamics

1 INTRODUCTION

A common goal in visualization is the design of techniques that provide both overview visualizations and support for feature exploration. Overviews can help the user find regions where further investigation in more detail might be productive [48]. Spatial features are, in turn, at the very core of most engineering and biomedical visualization endeavors, from vortices in flow simulations to bonding sites in protein structures.

While many such visualization designs follow the information seeking mantra: "Overview first, zoom and filter, then details on demand" [61], there are situations where providing an initial overview is not relevant or practical for users, while providing details is paramount. For instance, in a wide class of problems, including the problem illustrated in this paper, details do not have a precise definition, and their identification relies on internalized knowledge in the domain expert's head. As further argued by van Ham and Perer [66] in their alternative "Search, Show context, Expand on Demand" mantra for large graphs, there is also a significant class of scientific users who are not interested in global patterns in the data, but have specific questions about one or several specific data points. As a practical example, an astronomer who studies a class of quasars is typically not interested in an overview of the entire observable universe [36]. A step further, in computational fluid dynamics (CFD), domain scientists often work on the same problem for months, and have a good mental overview of the underlying data [15]. From an information theory perspective, Chen et al. [15] argue briefly that in such a case, having the direct ability to reach a detailed view (details-first) would reduce the cost of step-by-step zoom operations. Nevertheless, visualization textbooks only report the Overview-first mantra and the Search-first mantra [48].

Other arguments against first presenting global overviews to users are of a more practical nature. As illustrated in this paper, overviews may be derived from imprecisely-defined details and thus may not be

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Manuscript received 31 Mar. 2018; accepted 1 Aug. 2018. Date of publication 16 Aug. 2018; date of current version 21 Oct. 2018. For information on obtaining reprints of this article, please send e-mail to: reprints@ieee.org, and reference the Digital Object Identifier below. Digital Object Identifier no. 10.1109/TVCG.2018.2864849 readily available. In the case of large-scale multidimensional datasets, creating an overview may also not be feasible, in particular when a large dataset is being maintained at a centralized location, and transferring it to multiple client machines is not an option [41,45,66]. Last but not least, in some scientific problems, for instance in simulation ensemble visualization [52], the problem overview is not one spatial dataset, but a collection of datasets, whose summarization in an overview is not necessarily clear to the domain expert.

This discourse paper provides theoretical and practical evidence to support an alternative approach to the two established design mantras, Overview-first and Search-first. This alternative can be defined as "Details-first, Show context, Overview last", and supports situations where the main user workflow is oriented along spatial or spatiotemporal feature analysis, while the problem overview can only take the form of a summary. In this model, the analysis starts with the spatial feature(s) of interest, with the help of a computational back-end that can help identify and track those features over space and time. The detail features are then used to automatically filter the feature-context in space and time, while controlling the complexity of the visualization. Last, detail-derived calculations are used to summarize and compare collections of features and potentially datasets, presenting a summarization overview to the user.

We construct this alternative model with the help of scientific workflow theory [56] and of a practical example in the CFD domain, the exploration of viscous fingers in large-scale ensemble simulations [1]. Viscous fingers are areas of high concentration formed when a higher density fluid (e.g., oil) is poured into a lower density fluid (e.g., water); the fingering process is nondeterministic, and can lead to instability. To study this process, multiple stochastic simulations with nondeterministic properties must be executed, resulting in a simulation "ensemble." In turn, these simulation ensembles are nearly impossible to analyze computationally, due to the large number of parameters involved and the ill-defined nature of both the analysis process and the finger structures themselves.

Using this problem as a vehicle, the Details-first model allows domain scientists to explore a total volume of data approaching half a billion multi-dimensional data points through an interactive web-based application. The contributions of this work are:

- A Details-first, Show context, Overview-last model for the exploration of large-scale spatial data;
- A constructive instantiation of this model, using scientific workflow theory and the problem of viscous finger exploration; the

instantiation constructs methods for identifying and tracking finger structures over time, for filtering the spatiotemporal context of the computed features, and for supporting overview summarization;

- An evaluation of this model on a large-scale dataset, including feedback from CFD researchers on both the instantiation and the underlying theoretical model;
- A discussion of the merits, applicability and limitations of this approach, and of its fit with existing models.

2 BACKGROUND AND RELATED WORK

We begin our discussion with a brief review of relevant terminology and paradigms in visualization design. We then highlight representative work on detail identification for spatiotemporal CFD visualization; we follow with a summary of representative work that uses CFD details to visually filter data, and of work in ensemble visualization.

2.1 Relevant paradigms and terminology

Because the terms *overview*, *context*, and *detail* are overloaded in the literature, we describe briefly the two dominant design paradigms, give descriptions for each term below, and clarify their meaning and usage in the scope of this work.

Overview-First paradigm. Among the detail, context and overviewrelated guidelines for how to design visual interfaces, few are as widely cited as Shneiderman's 1996 Visual Information Seeking mantra: "Overview first, zoom and filter, then details on demand" [61]. The mantra provides an intuitive guideline to the interplay between the need for "a broad awareness of the entire information space" [48] and the need to see details, with a recommendation to designers that they should provide an initial overview to users. Multiple "uses of the term overview are found in the literature" [29].

Search-First paradigm. Shneiderman's overview-first guideline is most useful when handling datasets of moderate size [48]. In the case of large datasets, creating a useful overview for top-down analysis may simply not be feasible. For such situations, an alternative mantra is van Ham and Perer's 2009 approach to the exploration of large graphs: "Search, Show Context, Expand on Demand" [66]. This second approach to visual analysis is similar to the online map search process, where search results provide the starting point for exploring local neighborhoods. The mantra does not provide a formal definition for context.

Overview. The meaning of *overview* is diverse in the visualization literature. As Hornbaeck [29] notes, many authors [61, 63, 65] write about users gaining an overview of the information space, a process which Hornbaeck identifies as "overviewing". This process is akin to the design concept of "knowledge in the head" or "internalized knowledge" [50]. Yet Greene et al. [24] and Shneiderman [61] also note that "an overview is constructed from, and represents, a collection of objects of interest". Munzner's [48] discussion of overviews touches on both aspects: "broad awareness of the entire information space [...] and all items", but also "When the dataset is sufficiently large, some form of *reduce* action must be used in order to show everything at once." Last, while Shneiderman [61] discusses overviewing in his mantra paper as "seeing the entire collection", the mantra and subsequent examples refer to overview in the sense of a technical, user interface component ("knowledge in the world" [50]).

In this work, we adopt the Munzner dual definition. To distinguish between the two common uses, "spatial overview" denotes the spatial overview of one simulation (often internalized by domain experts), and "summarization overview" denotes a collection of objects of interest, constructed through reduction of the entire information space.

Detail. In general, detail denotes an individual feature, fact or item. In the Shneiderman mantra [61], detail is "implicitly defined in contrast to overview" [29]. Contrary to Shneiderman and Spence [63], Tufte does not contrast between overview and detail, and instead suggests that "to clarify, add detail". Munzner describes "a more detailed view that shows a smaller number of data items with more information about

each one" [48]. In scientific visualization and in this work, details are often spatial features, as described below.

Spatial Features as Details. In the context of information theory and CFD, Chen et al. [15] directly relate details to spatial features. Obermaier and Peikert [68] further note that the concept of feature in scientific visualization is derived from its definition in computer vision [12], where it describes a salient feature of an image, such as an edge or a ridge. For example, features in flow visualization include vortices, shock waves, isosurfaces, separation lines, and statistical features. Features and Soft-knowledge. Obermeier and Peikert [68] note that in the ideal case, features have a precise mathematical definition which does not depend on any "tuning" parameters. In contrast, other feature definitions involve a parameter and "require a visualization system where parameters can be controlled by the user." [68]. Similarly, Weber and Hauser [68] define features as data subsets of interest to the user, sometimes "due to prior knowledge". Last, Chen and Golan [16] introduce "soft information, knowledge, and priors" in the context of information theory in visualization, to capture known theories, intuition, belief, and meta-knowledge about a system.

In our work, details denote spatial features. Following Chen and Golan, *soft-knowledge features* denote those spatial features whose definition involves one or more parameters controlled by the user. The "soft" qualifier refers to the fact that this type of knowledge is difficult to capture and represent computationally.

Context. In general, context can denote either 1) a global setting, or 2) a local circumstance. In the visualization literature, the concept is similarly used. When describing the concept of focus+context, Card et al. [13] equate context with overview (a global view at reduced detail). Doleisch et al. [20] also describe context as "the rest of the [spatial] data", at a lower resolution, or in reduced style, for example using translucency. More generally, Furnas [22] explains that context, conceptually, is "any presentation of an information structure" that helps the user "to extract meaning, to understand something about [another focused/original] structure."

The van Ham and Perer [66] construction and usage of context is consistent with the locality aspect of the general vocabulary definition. In our work, context is defined similarly, along its locality aspect.

2.2 CFD Visualization

Feature Extraction. A common practice in the visual analysis of CFD spatiotemporal relationships is the detection, extraction, and exploration of features of interest over time [5,6,44]. Oftentimes, these approaches require the presence of clearly defined features in isomorphic structures, and are not directly relevant to our illustrative example: finger structures are soft-knowledge features. Favelier et al. [21] and Lukasczyk et al. [37] use an adaptation of Shepard's kernel method [59] to identify such features based on concentrations. Both these works rely on userdefined thresholds. In our recent work, neural networks have been trained to identify shock features based on descriptors such as the strain tensor and schlieren value at each timestep [45]. In a similar machine learning approach, Maries et al. [41] utilize K-means clustering to group and label points in areas of interest based on the velocity stress and strain tensor. Our finger identification method resembles Maries et al.'s [41] in that we define features based on groups of points with similar salt concentrations. However, we threshold the feature groups based on local-proximity and point concentration.

Feature Tracking. Most methods extract soft-knowledge features from each timestep separately and track how they progress over time [30, 57, 62]. These methods rely on the temporal and/or spatial coherence of attributes and location of the feature as it moves through time and space. Other methods [9, 25, 69, 70] use a contour-based, merge-tree ideology to enable tracking of regions of interest in combustion simulations. Our finger tracking solution builds upon the combined success of these spatiotemporal feature graphs.

Feature-based Filtering. CFD data is multivariate and dense, causing visual occlusion even at modest scales. In consequence, the body of work that uses details for filtering flow data is enormous. Here we report only on the works most relevant to our approach, where the features do not have a pre-defined formula for extraction. Multiple

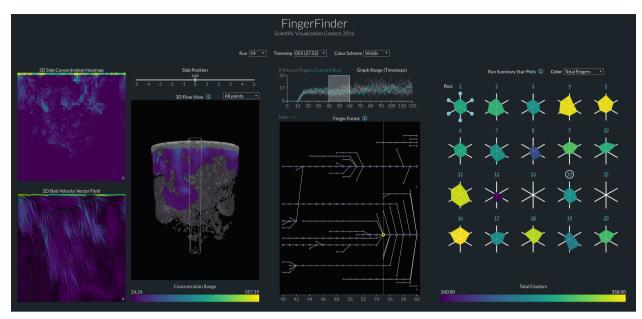


Fig. 1. The Details-first, Show Context, Overview Last model supports the interactive, web-based exploration of ensemble simulations. From left to right: detail and spatial-context panel comprising two 2D slices and a 3D flow view; a temporal-context panel comprising a time chart and a finger forest; overview panel showing a small multiple of Kiviat diagrams. Linked interaction and a computational back-bone allow users to identify fingers and track their evolution over time, and to analyze the data at multiple levels of detail.

coordinate views (MCV) have been deployed simultaneously to explore multivariate data and identify potential regions of interest [20]. These approaches harness linking-and-brushing techniques [27] to select and filter features between the multiple views. Furthermore, many of these approaches follow a focus+context style, where a general view or physical view is brushed to uncover specific features [27, 33, 52].

However, this approach is difficult in the case of temporal features users have to mentally integrate multiple samples across timesteps to understand the feature over time [46]. In our work, the data is automatically filtered based on the finger structures we extract.

Ensemble Visualization. Multiple simulations are often used to quantify and mitigate uncertainty in models that contain stochastic effects [53]. The resulting multiple simulation runs (collectively termed "a simulation ensemble") are often large, multivariate, multivalued and time-varying, and have been described as "awkward" [71] and difficult to visualize [32, 51]. Many ensemble visualizations aim to reduce complexity by presenting basic derived statistics such as the mean and standard deviation of observed properties [52, 53]. Alone, these techniques can capture ensemble variations between runs and provide strong indications of overall ensemble behavior. However, unlike our work, they may not capture more nuanced changes across time-steps or among ensemble members, and do not attempt to display user-defined spatial features.

Basic visual abstractions such as line charts, quartile charts, and histograms are commonly used in ensemble visualization to encode statistical parameters [28], as well as reduced spatial aggregate views [19,37] to display specific attributes at a specific time and location. To facilitate further exploration of ensemble members across space and time, these aggregate views are linked to range-based representations [26]. These representations may include colored overlays, multidimensional scaling projections [8], and various types of tracking graphs [9,37,69]. We use similar encodings for several of the features we compute.

3 MODEL INSTANTIATION

3.1 Constructive Example and Workflow Analysis

We illustrate the Details-first approach on a constructive example from the IEEE VIS 2016 Scientific Visualization Contest [1]. The visualization design (Fig. 1) was created in close collaboration with a CFD researcher with over seven years of experience in turbulent flow computational research, who is a co-author on this work.

Data and Tasks. The contest problem is centered on the spatiotemporal exploration of viscous fingers in large-scale ensemble simulations. One of the datasets provided is a simulation ensemble containing multiple stochastic simulation runs. Each simulation run in the ensemble captures the diffusion of an infinite salt source placed at the top of a cylinder filled with pure water. Over time, the higher-density salt diffuses into the water, forming structures known as viscous fingers. Each simulation is run using a Finite Pointset Method (FPM) approach with 250,000 points at the lowest resolution, and over 120 timesteps per simulation. In this ensemble, "the behavior of so-called viscous fingers is of primary interest. The six-dimensional nature and size of the data is the main challenge for visualization. Effective browsing, summarization, and data reduction strategies are needed to obtain meaningful insight into the data" [1]. The simulation ensemble cannot be analyzed purely computationally, due to the large number of parameters involved and the ill-defined nature of both the analysis process and the finger structures themselves.

Model Perspective. From a model perspective, the finger structures are defined based on soft-knowledge on the user side. Finger structures are typically visualized and identified via the use of concentration thresholds and contours. In this approach, a threshold is specified, and the structures are identified at the interface where concentrations are greater than or less than the threshold. This approach, which is not an exact formula for finger structure, is based on the knowledge that a) the features have higher concentration than surrounding areas, and that b) the features form blobs that are similar in shape to fingers. In other words, the finger structures are features that depend on the expert's soft-knowledge.

The second aspect weighing into the model perspective is that the details are here the finger structures and their evolution over time. The context is likely the physical volume around the spatial features, respectively the features' behavior over time across simulations. The overview, in turn, can be considered at two levels: 1) the spatial overview of all simulations, respectively 2) a summarization of the simulations. The spatial overview (a plain upright cylinder with 250K points) poses clutter and rendering time challenges, and its overall structure is also familiar to the domain experts. The summarization overview, in contrast, will likely be encoded by a visual abstraction unfamiliar to a CFD expert.

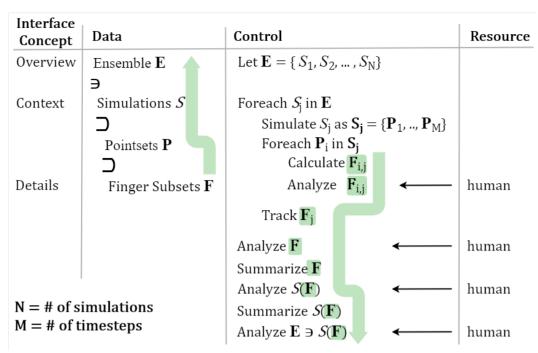


Fig. 2. Workflow decomposition of the finger calculation and exploration process along the main axes of scientific workflows: data, control, and (human) resource components. An additional column maps the data elements to the design components corresponding to overview, context and details. The Resource column only shows the steps where humans are involved; the remaining steps are computational. Note how the details **F** travel down the control flow, and up the data and the interface elements.

Scientific Workflow Analysis. Given these observations, let us consider the problem from a workflow perspective [39]. In particular, the finger calculation and exploration process can be decomposed along the main axes of scientific workflow theory [56]: data, control, and (human) resource components. In scientific workflow theory, *data* captures the information that is required during the execution of a workflow; *control-flow* describes the set of steps that make up the process and the way in which the thread of execution is routed between them; *resource* identifies the people and facilities that actually carry out the process. Figure 2 captures the data, control and resource elements for this problem, with an additional column mapping the data elements to the design components corresponding to overview, context and details.

This decomposition captures a number of traits of this workflow. First, the spatial features (i.e., details, highlighted in green in Fig. 2) are central to the entire process. Simulation summaries are a function of the finger characteristics, and the ensemble is a function of the simulation summaries, and thus also a function of the finger characteristics. In other words, the context is a function of details $(S(\mathbf{F}))$, and the overview is a function of details $(\mathbf{E} \sim (S(\mathbf{F})))$.

Second, a human is involved in all the analysis steps. Because finger structures are identified empirically, human input is necessary at that stage. Human input is necessary when selecting the set of measures used to characterize the finger structures. A human is further necessary when analyzing a simulation and extracting the measures that characterize the simulation in terms of its fingers, and when analyzing the entire ensemble.

In the following sections, we describe briefly the computational and human-input steps in this example, along with the visual encodings for each output, and then the resulting visualization design.

3.2 Finger Segmentation and Spatial Context Calculation

The description of the segmentation step captures the close interplay between human input and the feature identification process. In order to identify features within the data using the definition of a viscous finger (a contiguous area of "high" concentration), we run a custom clustering algorithm on the data. Along with determining the finger structures, this process simultaneously allows us to calculate the spatial context of the fingers.

Because the simulation data is mesh-free, and provided in the form of a seven-dimensional point cloud (point position, velocity and concentration), the first step was to construct an adjacency network that captures the local neighborhood of each point. Next, a simple clustering algorithm was run on this adjacency network, grouping together those points within the network which had a high concentration of above $\mu + \sigma/k$, where μ and σ are the mean and standard deviation of concentration for that timestep, respectively, and k = 7 was an empirical value determined through visual analysis. The clustering algorithm iteratively connects the nodes of the graph into clusters, based on the relative position of each point to its neighbors. For each point, the heuristic polls the cluster to which the neighboring points belong. If only one neighbor belongs to a cluster, the heuristic adds the point to that cluster. However, if the neighbors of the current point all belong to a different cluster, the heuristic combines those clusters and adds the current point to it.

Using the concentration heuristic alone can lead to all clusters near the saline top (which is a constant source of high saline concentration) being grouped together. To circumvent this artifact, the algorithm ignores points within 0.5 units of the top of the cylinder. In particular, the CFD expert noted that ignoring points immediately near the boundary condition is logical and acceptable because, by any definition of a finger, a constant source would satisfy the finger concentration condition. These empirical thresholds for the clustering can be calibrated, however the data will need to be reprocessed to perform the clustering again with the new thresholds.

The final clusters that result from this algorithm form the viscous fingers for that timestep. The algorithm assigns each cluster a unique cluster identifier. By keeping track of both cluster identifiers and point IDs, we can track the points whether or not they appear in one of the clusters as they move through time.

Finger Visualization. Finger structures and their spatial context are visually represented using 3D and 2D views (Fig. 3).

<u>3D View and Context.</u> Finger structures can be inspected in a 3D Flow View. Users can select the specific simulation and timestep to view.

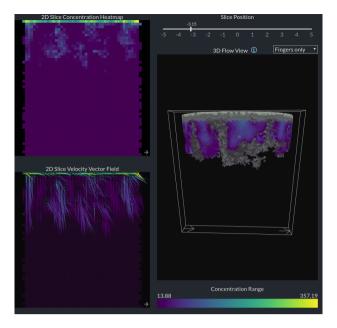


Fig. 3. Detail and spatial context. The 3D Flow View (right) provides the spatial context of finger structures. A vertical slab can be used to analyze finger structures in detail using 2D Views (left). This snapshot captures the formation of two large finger structures.

The cylindrical 3D view provides the context of the simulation domain, with the saline layer displayed at the top. Each point color is mapped to the concentration of that point. To provide further context, we display points considered by the finger clustering algorithm in gray (i.e., points of higher concentration).

Vertical Slab and 2D Views. To alleviate cluttering, a 3D vertical slab (cutting plane with depth) is used to carve out a subset of points for in-depth analysis. The slab points can be analyzed through linked views which show the concentration heatmap and velocity vector field of the data contained in the slab. We chose the slab representation, as opposed to a plane, because fingers are not restricted to 2D; the slab can be used to capture the finger depth along the cylinder cross diameter as well. The linked 2D views aggregate over the slab width the average value of the concentration and velocity, and help analyze in detail the finger concentration and velocity. Fingers may be viewed by moving the slab onto a specific viscous finger, which in turn allows the user to view the concentration heatmap and velocity vector field of the slab containing the finger. All viscous fingers are displayed by default. Specific viscous fingers can be also interactively highlighted in the 3D Flow view through the Finger Forest view described further below. Selecting a specific node of a tree highlights the finger in color (mapped to concentration).

Finger Properties and Analysis. To locate each cluster in the next timestep, several properties of each cluster are calculated and used, with input from the domain expert. From the finger segmentation output, this approach produced for each finger an attribute set which includes:

- · the number of points
- · the total concentration
- · the concentration-weighted average position of points
- · the concentration-weighted average velocity of points
- · the average magnitude of velocity
- · the concentration-weighted average magnitude of velocity
- · an axis-aligned bounding box around the feature

The first property is an average position of the points within the cluster, weighted by the concentration of the points. Second, the average velocity of the points in the cluster is calculated, also weighted by the concentration of the points. To find the cluster nearest to another in a different time step, the centers of concentration of the clusters are used, which are both corrected for the difference in time by adjusting the coordinates using the average velocity of the each cluster. The output of these algorithms are multiple clusters of points for each timestep, as well as the information linking these clusters to each other across multiple timesteps. The results of the data preprocessing are used for feature tracking, as well as in the simulation summarization.

From a model perspective, notice how extracting the details relies on soft knowledge on the user side; and how the domain expert input is essential to extracting the measures to characterize the features and their context.

3.3 Finger Tracking and Temporal Context Calculation

To track the fingers' evolution across a simulation, we run a two-stage algorithm on the finger clusters that were identified in the previous step. This process allows us to determine the temporal context of the finger evolution. This temporal context captures the appearance, dissipation, merging, and splitting of fingers.

The two-stage algorithm is based on the tracking graph algorithm proposed by Bremer et al. [9]. The algorithm first uses the size, position, concentration, and average velocity of the viscous fingers to label each cluster in each timestep with an ID, unique to each viscous finger over the course of the simulation: in other words, fingers within a single timestep can not share an ID, but fingers between timesteps can. In the second stage, these IDs are used to index the fingers into an adjacency list per timestep. A grouping procedure is then run on each pair of consecutive timesteps, constructing relationships between the fingers, over time. For each of the M-1 pairs of consecutive timesteps, the algorithm iterates over the two lists, comparing both finger properties and IDs. If the procedure finds a match between both properties and IDs, then the corresponding finger persisted between the timesteps and the two adjacency list entries for that ID are linked. Similarly, if the procedure finds a match between properties but not IDs, then the finger in the earlier timestep has merged into the finger in the later timestep, and the two adjacency list entries are connected. Finally, the procedure treats all unmatched nodes as either having split or dissipated, depending on whether the unmatched node is present in the later or prior timestep, respectively.

The trees output by the algorithm capture the evolution of each viscous finger throughout a simulation. We assign each tree the same ID as the viscous finger that is mapped by the tree root. By binding the finger structures to the trees, we can track the spatial features as they evolve. The linked IDs also allow us to select a node in the tree interactively and highlight that specific viscous finger in the 3D Flow view and 2D feature views.

Simulation Analysis. To analyze the finger evolution over time, we turn again to input from the domain expert. We will use two of the finger properties previously derived, as well as an additional parameter. These properties are: the number of points in each finger, the average concentration of the points in each finger, and now also the total number of fingers in the simulation.

Temporal Context Visualization and Filtering. The temporal context calculated in this step is shown in a temporal-encoding panel. The panel contains one horizontal, time-aligned tree for each finger in the simulation, as well as a Time Chart which can be used to control the temporal context shown.

<u>*Time Chart View.*</u> The Time Chart can be used to select the range of timesteps to be graphed in the Finger Forest. The number of fingers in each timestep is graphed for all simulations, with the graph for the current simulation highlighted in color.

Finger Forest View. The Finger Forest (Fig. 4) displays a set of horizontal, time-aligned trees that encode the evolution of fingers in a simulation, over the time interval selected in the Time Chart. Each node in a tree represents one viscous finger as that timestep, similar to the graphs of Bremer et al. [9]. The nodes are colored by the average concentration of the points in the finger, and the radius of each node is scaled by the number of points in the finger. The trees may merge or

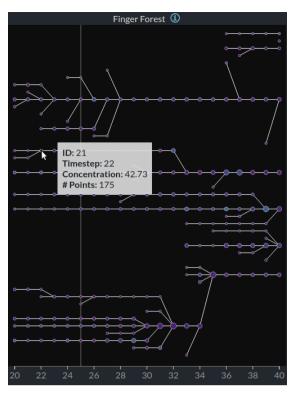


Fig. 4. Temporal context visualization. A Finger Forest shows one horizontal, time-aligned tree for each finger in the simulation. Each node in a tree represents one viscous finger as that timestep. Nodes are colored by the average concentration of the points in the finger, and the radius of each node is scaled by the number of points in the finger. The trees may merge or split according to the finger evolution over time. A vertical bar indicates the current timestep.

split according to the finger evolution over time. A vertical bar indicates the current timestep.

In order to minimize edge-crosses, we balance the trees using a heuristic similar to Widanagamaachchi et al.'s [69, 70]. The heuristic begins with the fingers in the last timestep and recursively enumerates and sorts the children of each finger based on the latest timestep in which that finger appears. For each enumerated finger, the heuristic then splits the nodes into two groups and positions them above and below the parent so that the oldest fingers are closest to the parent, and the most recent ones are furthest from the parent.

We note that both rendering a spatial overview and rendering a complete temporal overview would be impractical in this setting. A spatial overview of the entire information space would be affected by cluttering and rendering constraints. Similarly, a complete temporal overview would be affected by rendering constraints (computation time, minimal node size for visibility, minimizing edge crossings). From a model perspective, filtering by spatial and temporal context helps control visual complexity; these contexts are derived based on detail calculations.

3.4 Simulation Summarization and Ensemble Analysis

The last stage of the control-flow in our workflow decomposition (Fig 2) seeks to summarize the properties of the simulations that form the ensemble. These properties are derived from the finger properties, with input from the human expert. One of these properties characterizes the simulation as a whole; five additional properties are computed for each timestep, and averaged over the duration of the simulation:

- · the total number of unique fingers over the entire simulation
- · the number of fingers in each timestep
- · the average concentration of fingers in each timestep

- the average concentration of points in viscous fingers in each timestep
- the average finger speed (points' average magnitude of velocity) in each timestep
- the number of merges (not including fingers which disappear) in each timestep

Ensemble Analysis. The simulation properties are summarized in a small-multiple overview panel. The panel comprises one Kiviat diagram [34] per simulation. Kiviats are a graphical method of displaying multivariate data in the form of a two-dimensional chart, in which three or more quantitative variables are represented on axes starting from the same point. Unlike most radial plots, which tend to capture temporal sequences, the Kiviat relative position and angle of the axes is typically uninformative. Kiviat are equivalent to a parallel coordinates plot (PCP) in polar coordinates, and are seldom effective when more than two Kiviats are overlaid [42]. However, due to their closed polygon shape, which is a preattentive feature, Kiviats are particularly effective in small multiple form [40]. The axis ordering is not an issue, because each Kiviat uses the same axis ordering across the small multiple, resulting in similar polygon shapes for similar simulations.

Each Kiviat axis is mapped to one of the simulation properties. Hovering over each Kiviat axis shows how each property was computed. The Kiviats are further color-mapped to a simulation property selected by the domain expert, for example the total number of fingers in each simulation. In Fig. 1 right, note the similarity (diagram shape and color) between simulations 1, 3, 6, and 14. Simulation 12 stands out as an outlier. Simulations 13 and 15 are empty (no content at the 250K resolution). Through this small-multiple panel summarization, simulation properties can be compared between ensemble members. From a model perspective, these properties were also derived from detail calculations.

3.5 Design and Implementation

The model instantiation was developed through a parallel prototyping approach, which included 1) exploring encodings and potential properties, 2) evaluation with a computational flow dynamics (CFD) expert and revising properties, and 3) discarding a variety of measures as well as encodings (including parallel coordinate plots and scatterplots). The work benefited from repeated evaluation with and feedback from the CFD expert.

Figure 5 shows three iterations through the design process; the final design is shown in Fig. 1. Given that CFD experts were unlikely to be familiar with abstract representations of ensemble simulations, the original top-level design for the application adopted a multiple coordinated views approach. The approach has been shown to support visual scaffolding [38]—helping domain experts build from familiar visual representations towards unfamiliar representations. Within this approach, the design then tried to follow, left-to-right, an Overview-first, Filter, Details-on-Demand paradigm (Fig. 5 top and middle). Multiple cycles with the domain expert made it clear that, linked-views or not, their analysis always started with the finger structures, i.e., the details. The Details view was also the interface area where the domain expert spent most time. As in an Overview-first paradigm, subsequent analysis steps switched repeatedly between details, context, and overview.

Following a workflow decomposition along scientific workflow theory (Section 3.1), a Details-first design emerged (Fig. 5 bottom), which, unsurprisingly, turned out to be successful. A last attempt to emphasize the overview through an eye-catching color-scheme (Fig. 5 bottom, Kiviat panel) still failed to produce a single expert workflow that would lead with the overview, when evaluated with a small group of CFD researchers (Section 4). In the final design (Fig. 1), the color scheme for the overview is de-emphasized, completing the "Details-first, Show Context, Overview Last" model instantiation.

In this instantiation, the detail, context, and overview are tied together through brushing, linking and filtering. Specific viscous fingers can be highlighted in the 3D Flow View by selecting a node in the Forest Tree. If the selected viscous finger is from a different timestep than those currently displayed, the corresponding timestep is loaded into the

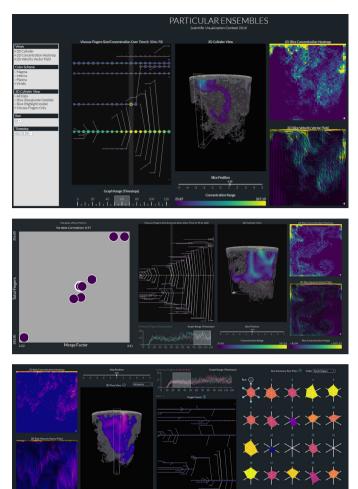


Fig. 5. Three snapshots through the design process. Top: Filter/Context-First, Details-Last iteration. Middle: Overview-First, Zoom and Filter/Context, Details-on-Demand iteration. Bottom: Details-first, Show Context, Emphasized Overview (through bold, eye-catching colors) iteration. The final design (de-emphasized overview) is shown in Figure 1.

3D Flow View, and the selected finger is highlighted. Selecting a finger from the Finger Forest also updates the 2D views by automatically moving the slab over the selected finger.

To implement this web-based instantiation, we used the d3.js and three.js Javascript libraries. The data provided by the contest website was downloaded as individual simulation packs, at its lower 250K resolution due to the size limitation of the web-based platform. We did not process and visualize every resolution of the data due to limitations in the amount of data a web-browser can import and render while still maintaining semi-realtime interaction rates. These limitations are a product of the environment we chose for development and, potentially, would not be a issue in a higher-performance setting. The analyses reported below were performed at interactive rates (2 fps under Google Chrome, Windows 10, 8GB, Intel i7-3537u @ 2.9 GHz).

4 EVALUATION

Visualization theories and models span a wide range, from mathematical abstractions and frameworks to guidelines and novel interpretations of different aspects of the development of visualizations in particular contexts [2, 3]. Validations of the resulting theories and models also cover a range of approaches. The "notable theoretical development" [18] of the Overview-first mantra was not accompanied by supporting evidence [61]. The Search-first mantra was introduced along a constructive example in the domain of large graphs of citations [66], with reported usage cases and no domain expert feedback. Last but not least, in the visualization design literature, a model or theory can be acceptably supported by as little as one to a few concrete examples coming from the experience of one to a few authors [35, 47, 54, 58].

In this work, in addition to the constructive example, we present as supporting evidence two scenarios performed by our CFD expert co-author, using the model instantiation. We further report instantiation feedback from senior CFD researchers, and theoretical model feedback from the CFD community. The evaluation is rounded by considering further evidence from reports in the visualization literature.

The scenarios below were completed online through web-based exploration of a total volume of data approaching half a billion sevendimensional data points. The two analyses were conducted by the domain expert using a 18 panel tiled display wall at 21.9 feet by 6.6 feet and 6144 by 2304 pixels; the application used the full height and 2/3 length of the tiled display. The visualization researchers took detailed notes. The usage of interface components (detail, context, overview) was noted based on both the expert's discourse and the physical motion cues as the expert walked from one interface area to another. The observed wall-display usage was consistent with the expert's observed interface usage on a regular display.

4.1 Domain Expert Scenarios

Exploring Finger Formation. In a first phase, we used the system repeatedly, over several weeks, to identify, define and refine the finger structures, and to derive the relevant characteristics used to generate the context and summarization overview. In this second phase, we investigate viscous finger formation throughout the first simulation run in the ensemble. After loading the run, the investigation begins with the Detail panel, where we notice the appearance of several fingers around timestep 25. Moving the 2D slab from side-to-side, we examine the salt concentration and velocity in detail. A large finger (Fig. 3) catches our interest: it appears larger and with higher concentration than others.

To get a better sense of the spatial and temporal context of this finger snapshot, we rotate the 3D Flow cylinder to center the finger in the slab, and also examine the temporal context panel. We notice a downward spike in the finger count between timesteps 20 and 40 in the Time Chart, so we center the *Finger Forest* over that range and advance the 3D Flow View to timestep 25.

We suspect that the decrease in fingers resulted from a few of the fingers merging together to form larger ones, so our analysis moves back from the 3D Viewer to the Finger Forest. As suspected, we notice that many of the nodes between timestep 20 and 40 have merged to form larger nodes. For example (Fig. 4), fingers 7 and 21 merge into a single larger node at timestep 22, shown close to the top of the view.

Another spike in the node count is around timestep 95, so we change the range of the Finger Forest to center around that timestep. We again notice that many of the smaller fingers begin to merge into one into one much larger finger by timestep 100. However, we also notice that many smaller fingers begin to form close to timestep 105, which appears to have the most new fingers. Sure enough, we observe in the 3D Flow View that while many of the fingers began to merge at the bottom of the cylinder, many new fingers began to form near the salt source.

Similar Simulation Analysis. In the second study we investigate two similar simulation runs. Again, we use the application URL to load the first run and visit the detail finger structures. Noticing low finger formation between timesteps 40 and 60, we center the context Finger Forest using the Time Chart. We observe that timestep 44 appears to have the highest finger formation in the selected range, so we next load that timestep into the 3D Flow View. We hypothesize that the decrease in finger count was caused by large fingers breaking apart to spawn smaller structures. Sure enough, the 3D Flow View displays larger fingers near the edges of the cylinder, with smaller fingers above and below. The Finger Forest further validates this inference, showing us that the majority of the structures in the range have both average high point counts and high concentrations.

Intuitively, we suspect that simulations with similar global properties might exhibit similar merge behavior, so we move to the diagrams in the overview panel. We begin to investigate the other simulations by hovering over the individual axes of the first Kiviat diagram. Starting at 12 o'clock and rotating clockwise, we observe the six computed summary statistics for average finger velocity, average finger density, total finger, fingers per timestep, merge factor, dissipation factor, average finger concentration, and average finger point concentration, respectively. The interface allows us to change the colormap of the diagrams based on one of the derived statistics. Changing the map to "Merge Factor", we observe the color and shape of runs 1, 3, 6 and 14 are similar (Fig. 1).

We decide to investigate simulation 14 in more detail, so we select its Kiviat diagram to load the data into the other views. To our surprise, we notice that the merge tree of run 14 differs from the previous run, over a similar range. Moving back to the 3D Flow View, we notice significantly more finger structures than in run 1, many of which are smaller in size and still forming at the top of the cylinder. These differences indicate that despite having similar global properties, the fingers of run 14 and run 1 do not follow the same structural formation and evolution.

4.2 Domain Expert Feedback

Instantiation Expert Feedback. We have collected feedback on this instantiation from two CFD researchers who worked directly with the online system, and two small groups of researchers (5 to 6 participants) who were given demonstrations of the work. One of the groups specialized in advanced computing at a national research laboratory, and included two CFD researchers; the second group consisted of three domain experts and two visualization researchers, as part of the SciVis Contest 2016. The feedback, reported below, was enthusiastic.

The first CFD researcher is a co-author on this work, and exclaimed repeatedly "I want this!" (for exploring supersonic and hypersonic flows and turbulent combustion), in particular with respect to the Details-first and temporal context exploration capabilities of the system. He noted that "Oftentimes in CFD we are details first because we are already familiar with the simulation and wish to investigate specific features in the data" and then: "When I say details first I mean that we look at specific regions or quantities. We are often interested in specific things happening at specific locations or specific times. A [summarization] overview without physical context lacks specificity and therefore is hard to extract meaning from, so we often perform [such] overviews at a later stage." "It is often very impractical to create an overview of the data as well. Seeing many, or all variables at many (or even some) times is extremely costly in real world datasets, e.g., 10.5TB." The expert noted that "This type of visualization can be used to investigate underlying physics of the temporal evolution of features of interest. It has applications to a wide range of CFD problems, notably vortex pairing and turbulent mixing."

The second CFD researcher is a senior investigator who studies computationally turbulence in the aerodynamics of aircrafts. His research involves running multiple dynamic simulations with soft-knowledge spatial features. He noted that standard CFD visualization systems (Paraview [4], VisIt [17]) are frequently employed in a typical CFD workflow to identify simple areas of interest ("Details-first"). Sometimes those features are then used offline to summarize multiple outcomes. However, that summarization is usually in the context of simulations that can be "easily summarized in terms of mean and standard deviation values while discarding lower-level features". In contrast, our instantiation "enabled analysis at multiple scales", allowed repeated refining of soft-knowledge features "within their original spatial setting" and the fluid reuse of those "spatially-derived characteristics to summarize multiple outcomes", well beyond state-of-the-art capabilities. The researcher was keen to have a similar system for his work.

Similar supportive feedback was collected from the larger groups. CFD experts were particularly excited about the smooth coupling of spatial feature characteristics to the temporal context ("extremely intuitive") and to the summarized overview. The spatial-feature based summarization was "more powerful than anything else [they] had seen." As in the reports above, group members spent most time operating in the finger detail space, where they were "immediately able to extract meaning to see the formation of fingers", and used the temporal context and overview mainly for navigation in the finger space. They expressed repeatedly interest in similar analysis tools for their research projects, which also study features based on soft-knowledge ("[the feature is] hard to define, but if you see it, you recognize it immediately"). Last, we quote feedback from the SciVis Contest contribution [10]: "extremely impressive due to the very well thought-out visualization design"; "clearly superior in visualization design", "very good and well-crafted", "in particular, the presentation of the ensemble[...], as well as the layout and linking of all views to facilitate interactive exploration, by far exceed all other submissions." This feedback attests to the value of our instantiation as a powerful tool for CFD analysis.

Theoretical Model Feedback. Our theoretical model sparked equal interest in the CFD community. After clarifying the visualization terminology, our CFD co-author engaged in numerous background readings and conversations with other domain experts. Particularly intrigued by the "overview" concept, he set out to find examples of overview usage in standard CFD visual workflows, as employed by a group of nine CFD researchers: two doctoral researchers who use routinely Paraview, an industry researcher and two doctoral researchers who use routinely VisIt, one doctoral researcher who uses routinely ANSYS [64], and a postdoctoral researcher and two senior researchers who are familiar with a variety of platforms. Through short discussions and observations, he sought to establish what software they use, what kind of plots they make, how do they use them, what is the first thing they do, and where, if at all, they use spatial or summarization overviews. He found out that no expert used spatial overviews in their everyday work. Summarization overviews were used, when necessary, last. He then compacted his findings in a common workflow description, best described as: 1) Details first (narrow down what is present); 2) Create filters, expressions, statistics within context; 3) Create a summarization overview of features (describe behavior of features as a whole over entire dataset); 4) Find something of interest then return to 1) Details and Repeat. In the group's assessment, much of this workflow stems from the fact that, very similar to the finger instantiation, a number of the physical phenomena they are investigating do not have concrete definitions. These CFD phenomena (e.g., turbulence or reattachment length) typically require a skilled user in order to be visually identified, separated, and investigated. As a result, it becomes difficult to draw conclusions from an overview first, when they "do not know exactly what is present in the data."

4.3 Supporting Evidence From the Literature

Chen et al. [15] were the first to note, in 2016, that in "many scenarios, we often observe that an experienced viewer may find [overview first and details on demand] frustrating, as the viewer knows exactly where the interesting part of a detailed representation is. For example, in flow simulation, scientists work on the same problem for months". Their anecdotal observation is reflected in a vast number of works in scientific visualization that support explicitly spatial feature exploration, and display the rest of the information primarily for context (e.g., [11, 20,27,31,33,52,60,72]). This collective evidence supports the "Details-first, Show Context" part of our argument.

Overviews (that are not used merely as context) are conspicuously rare in the scientific visualization literature. This observation is not surprising: summarization overviews tend to correlate with the relatively recent advent of ensembles of models and simulations. Nevertheless, the "Overview-last" part of our argument is also implicitly supported by a several examples of scientific visualization. While sometimes nominally providing an overview according to the Shneiderman mantra, these examples relegate their overview to the bottom or side of the visual analysis interface, and allocate it significantly reduced display space, compared to the "detailed view" [7, 19, 43, 49, 52, 67].

5 DISCUSSION

Model summary. This work is not a general critique of the "Overview first" mantra, but of its sometimes inappropriate application, without careful consideration of user and data workflows. At the same time, while instantiations of our alternative model are particularly common in flow visualization, they are in no way specific to the CFD domain:

"details-first" approaches also exist, anecdotally, in biology [14] and in journalism [55].

The alternative "Details-first, show context, overview last" model we advocate supports situations where the main user activities are oriented along (spatial) feature analysis. The model specifically applies to situations where the features are defined through soft-knowledge on the user side, and those features drive both the relevant context for the exploration process and the calculation of the summarization overview.

From a wider analytical perspective, the model applies to domain expert workflows that start with an in-depth exploration of one model or simulation, then seek to extrapolate or generalize the findings to a collection of models. In such workflows, including in forensic analysis, users may wish to start with the features of interest, in particular when those features are ill-defined and need repeated refinement. The relevance of user-driven refinement in our model is in agreement with Doleisch et al.'s observation: "for interactive analysis, in many cases, the *question of what actually is (or is not) considered to be a feature refers back to the user*: depending on what parts of the data the user (at an instance of time) is most interested in, features are specified accordingly." [20]. Our model enhances this observation and frames it in a "details-first" paradigm.

When those features have an inherent spatial structure (3D or Cartesian coordinates), the model further emphasizes, formally, the importance of providing the spatial and temporal context of those features. This model aspect is also in agreement with observations in the literature: "[Feature localization] is usually *provided in the context of simulation data*, that has some spatial context." [20], and with feedback from our CFD co-author ("CFD/ensemble features are not meaningful outside of their context."). Our model instantiation shows how a computational back-end can help identify and track features over space and time, and use those details to automatically filter the spatial and the temporal context. The "Show context" step of the model has the triple benefit of 1) helping anchor the features in space and time; 2) reducing visual clutter by controlling complexity of the visualization; and 3) improving rendering times for large scale datasets, in particular in online, platform-agnostic, web-based environments.

Last, this model extends the use of spatial details into the calculation of summarization overviews. In our model instantiation, extracted spatial features and calculations over those features are used to summarize and compare simulation ensembles.

Relationship to other models and theories. Similar to the van Ham and Perer approach [66], the Details-first model signals a set of limitations of the Shneiderman mantra [61]. In contrast to the van Ham and Perer mantra, the present model emphasizes the importance of Details (not Search for a particular item) for a class of problems, and the relevance of user input in specifying and refining those details. In a further departure from the van Ham and Perer approach, where overviews are circumvented as being both impractical and not relevant under specific circumstances, our model handles situations where summarization overviews are necessary. In particular, our model extends and provides a frame for the use of details into the calculation of such overviews.

The Details-first model further relates to Chen et al.'s Information Theory framework [15]. Our model encompasses their anecdotal observation that, in particular in flow visualization, the Shneiderman mantra can be suboptimal when the user is already intimately familiar with the overview. Beyond agreeing with their observation, this work highlights: 1) the tight connection that exists between the user "knowledge in the head" [50] and the very definition of spatial features; and 2) how those details can propagate into the construction of filtering operations, and then into the construction of summarization overviews.

The model's "overview last" aspect may also be related to the principle of visual scaffolding [38], captured by the domain experts' typical resistance to unfamiliar visual encodings.

Limitations and falsifiability. The different mantras have complementary strengths and limitations. Our model may not be necessary when the analysis can be conveniently broken into two separate processes, for example feature detection and simple statistical summarization. Our full model also does clearly not apply: to situations where overviews are irrelevant (use Search instead, or default to Detailsfirst, no overview); when user prior knowledge is not relevant, when global changes are likely, or when each search starts from scratch (use Overview-first instead); or when the features are well-defined and computable, or not at the very core of the user activity (a variety of other approaches apply, including pure computation).

Our observational evaluation draws on a left-to-right, multi-view instantiation, designed and evaluated with small groups of experts, several from the same labs. Such multi-view instantiations take advantage of the complementarity of multiple representations, and also have the potential to facilitate multiple user workflows [38, 40]. In practice, we have not observed domain expert analysis workflows that did not lead with the details view. A formal user study to analyze the likelihood of different mantras would be interesting, although beyond the scope of this discourse paper. Any such study should take particular care in the participant selection, given the central soft-knowledge aspects of our model, and the limited availability of domain experts.

Although multi-views have the potential to relieve workflow-related design constraints, we note that the model principle still applies, in the designer-assigned color scheme, size and location of overviews and context views in the overall design. However, extensions of this paradigm to single-view, reduced screen space settings, may be particularly limiting, considering the complementary benefits of summarization overviews. A step further, the process of overview summarization itself may miss an unexpected global change.

Finally, this model is likely not the only other possible alternative to the two established mantras. There may be further circumstances under which this model will be falsified, in accordance to Karl Popper's assessment that a theory in the empirical sciences can never be proven, although it can be falsified [23].

6 CONCLUSION

In conclusion, this work introduces and documents an alternative "Details-first, show context, overview last" approach to visualization design. The approach supports situations where the user activities are oriented along (spatial) feature analysis. This work further highlights the tight connection that can exist between user input and the definition of spatial features, and then how those details can propagate into the construction of filtering operations, and then into the construction of overviews. A model instantiation demonstrates the effectiveness of this approach with an online web-based exploration of a total volume of data approaching half a billion seven-dimensional data points. The approach is supported by endorsements from CFD domain experts. The applicability of this model extends beyond flow visualization to domain expert workflows that start with an in-depth exploration of one model or simulation, then seek to extrapolate or generalize the findings to a collection of models. Conversely, this model is not appropriate in situations involving novice users or when features are well-defined and computable. Overall, adoption of a particular design mantra should take into account the benefits, limitations, and possible co-existence of each approach, with careful consideration of data, user knowledge and interests, and user workflows.

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