Visual Exploration of Rheological Test Results from Soft Materials

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ABSTRACT

Rheological testing of soft materials aims to characterize them through a complex combination of elastic and viscous properties. Its fundamental idea is to apply a force and register the resulting deformation of the material. These tests have applications in a wide range of domains from adjusting oil drilling muds for different rock strata to developing fast-drying paints and quality control in food processing. Yet, visual-interactive means for the explorative analysis of the resulting data are scarce if they exist at all. Hence, we present VAOS — an open-source visual analysis software for exploring the complex rheological properties of soft materials subjected to oscillatory tests. VAOS offers a specific focus on the visual analysis across multiple samples and test runs at once, which is currently not well supported by existing software. We showcase the utility of VAOS in a usage scenario and two expert interviews, effectively demonstrating the improved ability of scientists to swiftly obtain a rheological fingerprint of complex materials.

Index Terms: Human-centered computing—Visualization—Visualization systems and tools—Visualization toolkits

1 INTRODUCTION

Soft matter or materials (e.g., gels, pastes, or foams) have applications ranging from tribology of gears where they are used as lubricants, to packaging materials where they are used for cushioning and insulation. Soft materials are studied in a variety of ways, including microscopy and spectroscopy [7, ch.1.9]. But only with rheology — the focus of this paper — it is possible to understand their behavior during deformation or stress. Rheology is defined as “the study of how materials deform when forces are applied to them” [3]. Among different aspects, rheological studies often aim to measure the viscoelastic properties of a soft material — i.e., in which ways it behaves like a solid (its elastic properties) and in which ways it behaves like a liquid (its viscous properties) [16]. Viscoelastic properties of soft materials are critical, for example, to ensure appropriate swallowing of food products for patients or ketchup staying on top of the French fries throughout a meal.

The importance of understanding these properties and in particular of their dynamics — i.e., how they change at different temperatures or over time when processing the materials — can hardly be overstated. For example, the question at which pressure and temperature a liquid will turn into a gel mass or vice versa is of very practical relevance when pumping ingredients through the pipes of a food processing plant. But also for quality assurance of the end product, rheological tests are key — e.g., to ensure consistent oral haptics (i.e., chewing properties) of a food product, to obtain a toothpaste easy to squeeze from a tube, and to make a paint that is easy to spread on a wall but does not drip on the floor during its application. Hence, it is only logical to establish continuous rheological testing as integral part of the manufacturing line itself [15].

The crucial role of rheological testing has not only propelled the field into a scientific discipline in its own right [19, ch.3], but also accelerated the development of rheometers — i.e., the devices with which rheological studies are carried out. These devices impose a force on the soft material (the so-called stress) and measure the resulting deformation of the material (the so-called strain) [9]. Plotting the results of these tests, let alone their interactive exploration is still largely unsupported by current state-of-the-art software. It is not uncommon for material scientists working with these data to generate matrix representations by painstakingly pasting screenshots of individually generated plots into a table in PowerPoint — one table cell at a time. And when test results of multiple samples (e.g., the same material at different temperatures) need to be compared, these are usually printed out and placed side-by-side to determine similarities and differences.

To address this gap and to enable the domain scientists to explore their rheological test results in a visual-interactive manner, we present VAOS — an open-source visual analytics software for rheological data originating from oscillatory tests. VAOS was developed in close collaboration with food scientists, who are actively using the software in their research and teaching. What sets the software apart from other rheological analysis and diagramming tools is

- its interactivity that enables the visual exploration of the data through brushing & linking and details-on-demand;
- its flexibility in configuring the user interface according to the rheological analysis task at hand;
- its scalability to investigate and particularly to compare multiple samples with each other;
- its end-to-end support from importing the data to exporting the resulting graphs.

With VAOS, we make the following contributions towards enabling visual exploration of rheological test results:

- an open-source visual analytics software that is specifically geared for the data and tasks common in rheological studies;
- novel visualization techniques specifically tailored to enable the joint visual-interactive analysis of multiple samples;
- a use case from the food sciences illustrating the benefits of using VAOS and an evaluation through two expert interviews.

2 DOMAIN BACKGROUND AND RELATED WORK

A common way to study viscoelastic properties are oscillatory tests whereby either stress or deformations are applied. For these tests, the material under study is placed on a stationary base plate of the rheometer and covered by a top plate that can be rotated in both directions — see Figure 1. In response to the angular displacement (i.e., how much to the left and right it rotates) and its frequency (i.e., how often this rotation is exerted in a given time frame), the rheometer measures the sample’s deformation as:

- **Stress**: capturing the torque (rotational force) applied to the material

- **Deformation**: capturing the resulting deformation (i.e., from which angular displacement the deformation was measured).
Strain: capturing the angular displacement (deformation) observed on the material in response to the applied stress

Strain rate: capturing the speed of the deformation of the material – i.e., the rate at which the strain changes over time

In practice, though, these tests are often done the other way around: the material scientist specifies a desired strain and then the rheometer is tasked to find the amount of stress that results in this target strain – effectively switching independent and dependent variables of the test. The reason for favoring these so-called controlled strain experiments is that they permit to confine the material tests to realistic and plausible deformations.

For ease of testing, modern rheometers do not require the material scientist to enter different desired strains individually, but provide the possibility to do an amplitude sweep across a given range of strain amplitudes. Along such a sweep, the rheometer then takes measurements at specified points. Depending on the amplitude range being swept, a strain-controlled experiment is referred to either as SAOS (small amplitude oscillatory shear) or as LAOS (large amplitude oscillatory shear). SAOS experiments can be thought of as investigating a material’s response to small vibrations, as this is basically what small oscillations amount to. Whereas LAOS experiments look into processes that actually disrupt the structure of a material – e.g., kneading, stretching, or extruding. LAOS experiments are of high relevance to evaluate the quality of materials obtained from production processes. Depending on what happens to the material, rheology discerns between two cases which are also shown in Figure 2: On one hand, there is the “well-behaved”, so-called linear response whereby as the deformation occurs, a response proportional to the oscillatory stimulus is recorded. On the other hand, at larger deformations, a “disorganized”, so-called non-linear response to the rotational shear is recorded [8].

Due to the importance of following the material response also during the non-linear behavior, it is critical to make sense of their results. To that end, one can consider that by their nature these experiments deform the material sinusoidally due to the rotational oscillation [18]. This means that it must be possible to express stress and strain in the time domain as functions of sine and cosine, which can be derived from the raw data through Fourier transformation. In traditional SAOS rheology only the 1st harmonic of the Fourier transform is utilized. Unique for LAOS is the inclusion of higher harmonics – usually the 3rd and sometimes also the 5th harmonic. Higher odd harmonics beyond the 5th are usually written off as noise. Even harmonics are generally recognized as experimental errors like wall slip or inertia contribution [8].

The standard visualization of these data are Lissajous curves [5]. They show the relations between stress, strain, and strain rate as closed trajectories – either in 3D for the full data space, or in 2D projections for the viscous subspace (stress vs. strain) and the elastic subspace (stress vs. strain rate). Figure 3 gives an impression of these curves, and one can easily see how these plots of the Fourier transformed data from a LAOS experiment resemble the plot of the raw data from a SAOS experiment in Figure 2.

Lissajous curves are usually compared to the curves that would result from testing perfect elastic and perfect viscous materials: In the elastic perspective (stress vs. strain), the more the Lissajous curve looks like a full circle, the more viscous its properties; and the more it looks like a diagonal line, the more elastic properties it has.
VAOS is freely available at https://vis-au.github.io/vaos/ and its source code is open and reusable under a GPL3 license. A screenshot of VAOS was presented in Figure 5. In the following, we briefly outline the requirements for the software solution we built, as well as its implementation and feature set.

3 The VAOS Software

Our visualization software for rheological test results – VAOS – was designed and built in close collaboration with domain scientists. VAOS is freely available at https://vis-au.github.io/vaos/ and its source code is open and reusable under a GPL3 license. A screenshot of VAOS is shown in Figure 5. In the following, we briefly outline the requirements for the software solution we built, as well as its implementation and feature set.

3.1 Design Process and Requirements

To build a visualization software for the analysis of rheological test results, we held multiple workshops with domain experts from the Department of Food Science at Aarhus University, DK over the course of 6 months. These workshops were set up as informal meetings introducing us to the research field in general, the lab environment and equipment in particular, and – most importantly – the currently used analysis software. At the same time, the workshops also provided a context in which to showcase early software prototypes to facilitate their iterative design [11, p.33]. From these workshops, the following design requirements emerged:

[R1] Interactivity to be able to perform the visual data analysis within-sample and across-sample directly in the software, instead of having to rely on printouts.

[R2] Flexibility to configure the graphical interface so that it is in line with the data and analysis task at hand, instead of being confined to a potentially ill-fitting standard UI.

[R3] Scalability to cope with datasets spanning multiple rheological tests (within-sample or across-sample) instead of having to split these datasets manually into single test runs using Excel and only being able to analyze them individually.

[R4] Ease-of-use in having a self-contained software instead of packages to be run inside another environment for which – in the case of Matlab – even additional license fees arise, and in having export capabilities instead of relying on screenshots.

3.2 Design Decisions and Implementation

VAOS embodies a dashboard design [6, 17]. This provides a configurable multi-view setup that is enhanced with brushing & linking to allow for coordination across views, meeting requirement [R1]. The dashboard also permits to combine exactly those views needed for an interactive analysis task at hand [R2]. To not create additional effort for the user through this flexibility, a set of dashboard templates are already preconfigured in VAOS. The user can also add more such templates to reuse a view layout once found to be working well. This functionality is provided using the react.js framework.1 For processing, VAOS uses code adapted from the MITlaos package [4] with the Fourier transform being done through the @signalprocessing/transforms library.2 To visualize the results, VAOS relies on D3.js [1] for 2D plots and on Apache ECharts3 for 3D plots.

1https://reactjs.org
2https://github.com/yusufsaygili/signalprocessing
3https://echarts.apache.org
Figure 5: Screenshot of VAOS showing a view setup for investigating similarities between test runs. Three different samples are shown: M1, M2, and M3. Each of these samples was tested at strain amplitudes of 0.1%, 1%, 10%, 40%, and 100%. The results are shown in the elastic perspective (stress vs. strain) in all views. The Pipkin diagram at the top left shows the Lissajous curves for all samples. One can notice that the Lissajous curves for M2 and M3 at 100% strain amplitude are much “bulkier” (arrows #1 and #2) than the rather slim shapes of all other curves. They thus deviate more from the straight diagonal which indicates a perfect elastic material, meaning a lesser elastic contribution to the viscoelastic response. This can likewise be seen in the line chart showing the Centerpoint Distances where all Lissajous curves from the Pipkin diagram are “unrolled” as illustrated in Figure 6 and superimposed. As most of the Lissajous curves are rather homogeneous, most lines are overplotted by the last sample M3 shown in green. Only two lines stand out (arrow #3), which are the ones corresponding to M2 and M3 at 100% strain amplitude being placed further away from the perfect elastic curve shown in red than all other lines. The Similarity Map at the bottom left indicates the same by grouping the resulting curves into clusters of similar shape and thus of similar material properties. One can see that again M2 and M3 at 100% strain amplitude are placed far away from the majority of the test runs and even further away from the perfect elastic case shown in red (arrow #4). The Similarity Matrix details that observation: The rows and columns for M2 and M3 at 100% strain amplitude (arrows #5 and #6) are darker than the rest of the matrix cells, meaning that they are both somewhat different from the rest of the test runs. The only exception being the cells showing the pairwise similarity between them (arrow #7), which are lighter and thus indicate that the two deviating test runs are quite similar to each other, though. The diagonal in the matrix encodes the similarity to the perfect elastic case. From the darker cells on the diagonal (arrows #8 and #9), one can see that the two test runs in question are not as similar to the perfect elastic behavior as the remainder of the data.

Furthermore, VAOS supports comparative analyses among multiple test runs (within-sample or across-sample) in fulfillment of [R3] through visualizations showing similarities between rheological test results. These similarities are established through Dynamic Time Warping (DTW) [13] of the individual test runs’ resulting Lissajous curves – or, more precisely, between the 1D “pseudo timeseries” derived from the 2D Lissajous curves [14, 21]. In our case, we use and show only half of the “rolled out” curve as it is symmetric. This is also illustrated in Figure 6. We found DTW to be more robust in handling noisy data than using Euclidean distance. For the DTW computation, VAOS uses the dynamic-time-warping-2 library.4

Finally for its ease-of-use [R4], VAOS is made available as a ready-to-run standalone software based on the electron.js framework.5 MS Excel files can be imported using the library fast-xlsx-reader6. All charts can be exported as SVG or PNG images. All derived data – i.e., the results from the preprocessing – can be exported as a CSV file for further processing or plotting in other tools.

3.3 VAOS Overview and Features

Views can be freely added, removed, or rearranged on the dashboard. Where this makes sense, color scales are kept consistent across views (e.g., in the Centerpoint Distances chart and the Similarity Map). Brushing and linking allows to select test runs of interest in one view and others will then highlight them as well. Different view setups can be brought up from saved dashboard templates through the tabbed interface at the top of the screen. Global view parameters such as the perspective (elastic vs. viscous) to be used in all plots can be changed through the buttons at the bottom left of the screen.

Data import and export functionality is available via the side menu that can be brought up on demand, so as to not get in the way of the visual-interactive analysis. The side menu also gives access to more advanced parameter settings of the data preprocessing. This includes the points per quarter cycle (PPQC) setting (i.e., how fine-grained to subsample the data for the Fourier transform reconstruction) and the harmonics to include in the analysis based on a shown power spectrum. While for most rheological tests of soft materials only odd harmonics up to the third harmonic are considered, there are cases in which the inclusion of the fifth harmonic can be argued for based on its contribution to the overall response.

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5https://www.electronjs.org
6https://github.com/bigabdoul/fast-xlsx-reader
In addition, the common charts have been slightly upgraded where it seemed suitable. For example, in the Pipkin diagram shown in Figure 5, one can see additional line charts below the small multiples of the 2D Lissajous curves. These indicate, for example, the maximum stress (shown in brown) which was only visible and comparable in the layover plot, but not in the Pipkin diagram due to normalization. With the line chart, the user gets an indication of whether the stress is increasing, decreasing, or stable across the strain amplitude sweep. As quantitative measures of the Lissajous curves, derived metrics such as strain-stiffening ratio and strain-thickening ratio [20] are likewise added as lines to the Pipkin diagram.

For a more detailed overview of all functionalities available in VAOS, the interested reader is pointed to the materials available at https://vis-au.github.io/vaos/.

3.4 VAOS Scalability

In terms of visual scalability, VAOS is currently optimized for 5 samples stored in 5 separate Excel files, with 5 experimental settings (i.e., strain rates) stored as 5 individual sheets in each file. If necessary, VAOS can handle up to twice this number before becoming unwieldy to work with.

In terms of runtime scalability, VAOS can handle experimental data with up to 15,000 measurement points before the computation of the Fourier transform becomes noticeably long and hinders the analysis. This should not pose a critical limitation in practice though, as most rheological time series are much shorter. After all once the material is broken up, additional oscillations will not further change the material’s properties and yield different responses.

4 Evaluation of VAOS

To illustrate the usefulness of VAOS, we showcase its application to a set of rheological data derived from testing three different mozzarella samples, and we report on two expert interviews that we conducted.

4.1 Use Case Scenario

The testing of rheological properties of cheese is not only done for product quality assurance (e.g., ensuring the proper texture) but also for maintaining stable production processes despite natural ingredients whose properties can vary greatly. For example, cheese may be too sticky or too crumbly to be properly sliced [22]. Rheological tests can help in understanding process dynamics including crucial material properties during processing.

In this use case, we explore rheological test data extracted from mozzarella cheese sampled at different processing stages. Mozzarella is produced through kneading and stretching processes in combination with increased temperature in hot water or by steam injection. A better understanding of how its material properties change during these processes allows for a better process control and ultimately a more consistent quality. The three mozzarella samples tested in this use case were taken from different stages of the kneading process:

- M1 is a sample of the raw mozzarella curd derived from skimmed milk that has been condensed into a crumble. (see Figure 7 left)
- M2 is half-finished mozzarella sampled midway during the kneading process.
- M3 is the finished product. (see Figure 7 right)

Testing the rheological properties of these samples helps to optimally configure the kneading process. For example, in the raw mozzarella curd no protein network has yet formed, so that it can still be kneaded much more briskly at this stage than the close-to-finished cheese. By the end of the kneading process, the cheese is already much more compact and must be kneaded more gently and slowly to avoid over-kneading and thus breaking up the desired structure again.

Rheological tests of the material during processing will allow for process optimization at individual production steps.

Each of the three samples were tested with a 0.1%-100% strain amplitude sweep using an HR20 Discovery Hybrid Rheometer by TA Instruments.\(^7\) Five strain values were selected to be further processed and analyzed in the software: 0.1%, 1%, 10%, 40%, and 100%. The data are stored in three Excel files (one for each sample tested) with five sheets each (one for each strain amplitude).

After loading all three files into VAOS, we quickly check the contributions of the different harmonics to make sure we do not discard any relevant data as noise. Yet from the heatmap shown in Figure 8, one can clearly see that relevant contributions to the test results – indicated as red or orange cells – are only made by the 1st and 3rd order harmonic.

![Figure 6: Illustration of the transformation from a closed 2D Lissajous curve into a 1D “pseudo timeseries” showing the distances of the outline of the Lissajous curve from the curve’s center point.](image)

![Figure 7: Two of the three tested mozzarella samples: mozzarella curd (M1) on the left and the finished cheese (M3) on the right.](image)

![Figure 8: Heatmap of the normalized power of each harmonic order for sample M1 and the five different strain amplitudes tested.](image)

\(^7\)https://www.tainstruments.com/hr-20/
more on the elastic side of materials. For more viscous materials, one would instead start the visual analysis with the viscous perspective (i.e., plotting stress vs. strain rate). For M1, it can be seen that the required stress to reach a given target strain amplitude increases with the amplitude (brown line underneath the Lissajous curves indicating “max. stress”). At the same time, the Lissajous curves do not change much and their elliptic shapes remaining close to the diagonal indicates a viscoelastic response with a high elastic contribution. For M2 and M3 (the top two rows of the Pipkin diagram), this changes somewhat for high strain amplitudes of 100%, for which a clear deviation from that behavior can be seen from the somewhat more “bulky” curves. These two particular test runs – M2 and M3 at 100% – are also nicely singled out in the Similarity Map and differently colored in the Similarity Matrix. The implication from this observation is clear: At these high strain amplitudes, the already kneaded and compacted mozzarella would be broken up again, effectively destroying the product. As this behavior is not yet present in the results from the 40% test run, it is safe to assume that the threshold at which the mozzarella breaks up is somewhere between 40% and 100% strain amplitude.

These results illustrate that characterization of the non-linear response allows for samples to be separated from one another. This would not be possible with traditional linear rheology, which evaluates viscoelastic properties up until the end of the linear response – i.e., up to the point at which structural breakdown is introduced – thus only providing insight into parts of the response. By being able to cross this threshold into the nonlinear response, VAOS provides rheological analysis of the effects of food processing on structure formation. This enables entirely new possibilities for process design and process control in this domain.

4.2 Expert Interviews

We also conducted two expert interviews with domain scientists working with rheological data. The scientists work at two different universities in Denmark, with one being a senior material scientist [SMS] and the other being a junior food scientist [JFS] – both having experience in using rheology software. The interviews lasted about one hour each, starting with an introduction into VAOS and its capabilities, followed by a period in which the scientists could freely explore a demo dataset, pose questions, and make comments.

The perspectives of the two experts were complementary: JFS who spends a lot of time using rheological analysis software himself commented mainly on the detailed workflow from the raw data to the final analysis results. While SMS does not conduct rheological analyses himself in his day-to-day work, he is aware of the processes and software through his teaching and supervision of student projects. He commented more on the bigger picture of when, how, and for whom VAOS may be useful.

JFS was very positive about the software’s ability to create Pipkin diagrams out of the box. So far, she had to manually create the Pipkin diagrams by taking screenshots of each individual test run – i.e., combination of sample and strain amplitude – and manually piece them together into a matrix. Also, the ability to directly explore strain-stiffening and strain-thickening ratios was much appreciated, as with her current tooling this required a lot of manual effort.

SMS mentioned the usefulness of visualization in general and VAOS in particular for gaining a qualitative understanding of a material – e.g., how similar or different an unknown material is from a known one. He also commented about its accessibility as “you don’t have to be a mathematician to understand such visualizations”, making them perfect for reaching a wider audience. In particular the latter made him very eager to use VAOS in his future teaching.

From our observation of the interviews, we noticed that none of the two experts made much use of the linking & brushing features to explore the data in the multiple coordinated view setup. We believe this to be mainly for two reasons:

1. In both domains – food science and material science – visualization is used very much in a tradition that focuses on presentation rather than exploration. Current analytic workflows usually have visualizations as an end result that they produce to be included in a publication, instead of being the starting point and interactive control center from which to steer and manage the computational analysis in an informed way.

2. If visualizations are being shown and used in current software, they are displayed by themselves. The idea of having multiple visualizations side-by-side, being able to add or remove visualizations to that setup as needed for an analysis step, and the possibility of direct manipulation (i.e., brushing) in one diagram to see the effects in all others (i.e., linking) is too far out from the feature set of current software to even come to mind when using VAOS.

This points to the general challenge of introducing means of interactive data visualization in application domains where no tradition for such explorative, visually-driven, human-in-the-loop analysis exists. Enabling the domain scientists to see and leverage the full potential of this approach needs more than providing them with an easy-to-use software, as they will still use it in similar ways as they use the existing software. To leverage the full potential of VAOS, established analytic workflows need to be rethought and the role of visualization within them need to be redefined.

On top of that, JFS made the observation that LAOS rheology – i.e., the analysis of nonlinear material responses – is not the preferred rheological analysis method in food science, yet. Many of the connections between structural properties, their dynamics, and the registered rheological data are yet to be fully understood and LAOS rheology remains an evolving field. This also has implications for VAOS, as it will need to be constantly updated in order to stay in sync with the current state-of-the-art in LAOS rheology.

5 Conclusion

In this paper, we have presented VAOS – a software enabling the visual exploration of rheological test results – together with a first evaluation through a use case scenario and two expert interviews. In doing so, we advance the state-of-the-art in two important respects:

First and that being the main focus of this paper – we provide the domains of material science in general and food science in particular with a free software incorporating all the major analysis and diagramming features that are currently used for rheological test data as an interactive one-stop solution. From the expert feedback we got, we expect it to be readily picked up by rheology users and to be applied in research and teaching.

Second, this paper also serves to introduce the area of rheological analysis to the domain of visualization research as an application area that has so far not benefited from the advances visualization has made over the past 30 years. We hope it will pique the interest of other visualization researchers to look into this particular application domain as well. Interactive visual analysis holds the promise of not only advancing, but in fact accelerating the study of new, more sustainable biomaterials. With VAOS being available as open-source to build upon, we believe to have sufficiently lowered the hurdles to enter the field and to devise new visualization ideas.

Investigating new diagrams and visual-analytic features for VAOS will also be our next endeavor to further the impact of visualization on the field of rheology. In addition, following our observation from the expert interviews we also aim to integrate subtle means of user guidance [2] to make the domain experts more aware of interactive features and exploration possibilities within the software.

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