Plan Overview

A Data Management Plan created using DMP Tool

Title: Unraveling the Spatiotemporal Dynamics of Inertio-Elastic Turbulence using Measurements and Data-Infused Simulations

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Project abstract:

When polymers are added to a solvent, even in very dilute solutions, they markedly change the behavior of the fluid in intriguing ways, such as reducing the drag force of flow past objects. Polymer-induced drag reduction in marine transport applications can result in 20-25% decrease in frictional energy losses and can thus have a major impact on society in the form of reduced fuel consumption and carbon dioxide emissions. However, the changes induced in the time-varying three-dimensional fluid dynamics are often counter-intuitive and poorly understood. In some configurations, the polymeric solution can introduce new flow instability mechanisms that would not be possible in typical fluids; yet in other regimes, the same forces can also have the seemingly opposite effect of mitigating the energetic eddying motions of turbulence. Direct imaging of the evolution of turbulent flow structures is needed, and it requires a technique with very high resolution and sensitivity. The research plan to achieve this goal is tightly coupled with an education and outreach plan that includes both curriculum development and supplemental lectures and interactive

lab demonstrations for Engineering Innovation through summer programs for high-school and college-level STEM students at both universities. The research involves detailed experiments using a unique imaging system to probe how a polymeric jet injected into a surrounding Newtonian fluid becomes unstable. These visualizations will enable a detailed characterization of the mixing between the polymeric jet and the surrounding fluid and the amplification rate of jet instability. The results from the experiments will be complemented by first-of-their-kind measurement-infused simulations of the same configuration. By directly integrating the measurements into the simulations, computations will probe the exact same flow and provide all the additional details that cannot be measured directly in the laboratory. The coupled results from both the experiments and simulations will provide an unprecedented view of the mechanisms through which polymer solutions alter turbulent flow instabilities. Ultimately, such insights will explain how molecular parameters such as chain extensibility and flow elasticity control polymer drag reduction and help guide selection of novel biopolymer sourced additives that can serve as cheap and environmentally friendly substitutes for traditional drag reduction agents such as synthetic polymers derived from hydrocarbon resources. This award reflects NSF's statutory mission and has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.

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Unraveling the Spatiotemporal Dynamics of Inertio-Elastic Turbulence using Measurements and Data-Infused Simulations

Products of Research

What types of data (experimental, computational, or text-based), metadata, samples, physical collections, models, software, curriculum materials, and other materials will be collected and/or generated in the course of the project? The DMP should describe the expected types of data to be retained, managed, and shared, and the plans for doing so. What descriptions of the metadata are needed to make the actual data products useful and reproducible for the general researcher? For collaborative proposals, the DMP should describe the roles and responsibilities of all parties with respect to the management of data (including contingency plans for the departure of key personnel from the project) both during and after the grant cycle.

At MIT, high-speed (4000 fps), high-resolution (500 pixels by 1000 pixels) Schlieren and particle image velocimetry (PIV) videos, each with a size of approximately 10GB, will be recorded for this project using a Phantom Miro m320s camera and stored in the format of Phantom high speed cameras (.cine). The raw unprocesssed video data can then be viewed, edited, and exported using the phantom camera control (PCC) software which is available online for free (https://www.phantomhighspeed.com/resourcesandsupport/phantomresources/pccsoftware). The digital video can be exported as vertical stacks of TIFF images and will be processed using the license-free image processing software ImageJ (https://imagej.nih.gov/ij/).

For Schlieren imaging analysis at MIT, in-house developed MATLAB codes will be used and the output (for example spatial maps of the scale of segregation saved as text files (.txt). For our PIV analysis, the exported stack of TIFF images will be used as an input for the free PIVLab MATLAB Package. The output of the PIV analysis, i.e., two-dimensional velocity profiles is exported as txt files. This text file (.txt) will then be used by in-house MATLAB codes for Dynamic Mode Decomposition.

At MIT, the data produced in the shear rheology, capillary breakup extensional rheology (CaBER), and capillary viscometry experiments will be stored as text (.txt) and Microsoft Excel Worksheet (.xlsx) files.

At JHU, high-fidelity, spatially- and temporally- resolved simulations will be performed during the proposed activity. During these simulations, statistical quantities will be computed and three-dimensional velocity, pressure and conformation fields will also be stored over regular time intervals. A single snapshot from a $512 \times 256 \times 256$ grid is therefore 2.5GB, and a time-resolved evolution of a single simulation will require 1TB. Overall it is anticipated that 10TB of RAID storage are needed for redundant storage from a few flow conditions.

The data will initially be hosted on the local RAID system for fast access and processing, and will subsequently be moved to archival storage.

Data Formats and Standards

In what format and/or media will the data or products be stored (e.g., hardcopy notebook and/or instrument outputs, ASCII, html, jpeg or other formats)? Where data are stored in unusual or not generally accessible formats, how may the data be

converted to more accessible formats or otherwise made available to interested parties? When existing standards are absent or deemed inadequate, this should be documented along with any proposed solutions or remedies. In general, solutions and remedies to providing data in an accessible format should be offered with minimal added cost.

Question not answered.

Dissemination, Access and Sharing of Data

What specific dissemination approaches will be used to make data available and accessible to others, including any pertinent metadata needed to interpret the data? In this case, "available and accessible" refers to data that can be found and obtained without a personal request to the PI, for example by download from a public repository. What plans, if any, are in place for providing access to data, including websites maintained by the research group and contributions to public databases/repositories? For software or code developed as part of the project, include a description of how users can access the code (e.g., licensing, open source) and specific details of the hosting, distribution and dissemination plans. If maintenance of a website or database is the direct responsibility of the research group, what is the period of time the website or database is expected to be maintained? What are the practices or policies regarding the release of POST-AWARD MANAGEMENT data – for example, are they available before or after formal publication? What is the approximate duration of time that the data will be kept private? "Data sharing" refers to the release of data in response to a specific request from an interested party. What are the policies for data sharing, including, where applicable, provisions for protection of privacy, confidentiality, intellectual property, national security, or other rights or requirements? Research centers and major partnerships with industry or other user communities should also address how data are to be shared and managed with partners, center members, and other major stakeholders; publication delay policies (if applicable) should be clearly stated.

The data generated from the proposed research will be open to the research community, and will be disseminated at conferences, workshops and through the research webpages of the PI-McKinley (http://nnf.mit.edu/) and PI-Zaki (https://engineering.jhu.edu/zaki/).

Metadata documentation regarding the format of the data, its storage and access will also be made available to the community. On the MIT side, DSpace@MIT (https://dspace.mit.edu/) and on the JHU side Sharepoint (https://livejohnshopkins-my.sharepoint.com/) will be the primary places to share the documentation and processed data sets. In addition, algorithms developed during the course of the proposed activity will be available to the public under an open-source license.

The metadata for each individual Schlieren or PIV video will include imaging information and details on the fluid composition, flow parameters, and the specific geometry of each individual experiment. Imaging information includes frame rate, exposure time, magnification, numerical aperture, depth of focus and field of view (based on pixels) of the camera for each individual video. The fluid composition detail includes the type of polymer solute (e.g. polyethylene oxide (PEO)), composition of the solvent (e.g. water or sucrose/water) as well as the concentration and molecular weight of the solute. The metadata will be available as a separate technical report through DSpace@MIT as well is in header information of each data file.

The metadata for each simulation includes the flow and computational parameters, including the Reynolds and Weissenberg numbers, the polymer concentration and maximum extensibility, geometric values, domain sizes and resolution. For measurement-infused simulations, a link to the metadata for the experimental measurements will be included. The metadata will be available as a technical report through JHU-Sharepoint.

Re-Use, Re-Distribution and Production of Derivatives

What are your policies regarding the use of data provided via general access or sharing? For data to be deemed "re-usable," it must be accompanied by any metadata needed to reproduce the data, e.g., the means by which it was generated, detailed analytical and procedural information required to reproduce experimental results, and other pertinent metadata. Practices for appropriate protection of privacy, confidentiality, security, intellectual property, and other rights should be communicated. The rights and obligations of those who access, use, and share your data with others should also be clearly articulated. For example, if you plan to provide data and images on your website, will the website contain disclaimers or condition regarding the use of the data in other publications or products?

Question not answered.

Archiving of Data

When and how will data be archived and how will access be preserved over time? For example, will hardcopy logs, instrument outputs, and physical samples be stored in a location where there are safeguards against fire or water damage? Is there a plan to transfer digitized information to new storage media or devices as technological standards or practices change? Will there be an easily accessible index that documents where all archived data are stored and how they can be accessed? If the data will be archived by a third party, please refer to their preservation plans (if available). Where no data or sample repository exists for collected data or samples, metadata should be prepared and made publicly available over the Internet and the PI should employ alternative strategies for complying with the general philosophy of sharing research products and data as described above

The experimental data produced at MIT, will be stored on an internal desktop hard drive which is password protected and is automatically backed up to the cloud hourly and daily by MIT's CrashPlan PROe (https://ist.mit.edu/backup). The experimental samples will be preserved inside a temperature controlled refrigerator at constant temperature . Reserve samples of the polymer batches will be stored as dry powders for the duration of the proposed research. Gel Permeation Chromatography profiles of the molecular weight distribution for each specific polymer batch will also be stored and used to calculate the relevant microstructural measures.

The numerical simulations data produced at JHU will initially be hosted on the local RAID system for fast access and processing, and will subsequently be moved to archival storage.

The full set of experimental samples and experimental and numerical data will be preserved long after the completion of the work at both MIT and JHU. In particular the essential data that are required to

reproduce all the results from the project will be available freely to the public via DSpace@MIT (see below) and Institute for Data Intensive Engineering and Science (IDIES) at JHU.