Towards Automated Sample Delivery at MFX

K. Karpos[1], R. C. Alvarez[1], S. Zaare[1], A. Pableo[1], J. Gilletti[1], R. Nazari[1], R. G. Sierra[2], M. Hunter[2], R. Kirian[1]

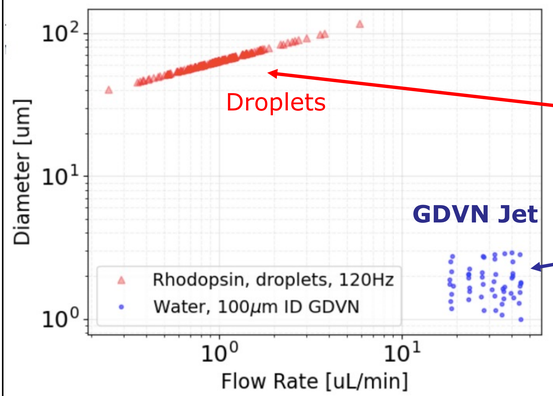
1. Arizona State University, 2. SLAC National Accelerator Lab

Introduction

Gas Dynamic Virtual Nozzles (GDVN) have been one of the primary sample delivery methods for serial femtosecond crystallography (SFX) and solution scattering experiments at XFEL beamlines. Due to high costs and difficult sample development methods, a reliable triggered droplet system is being pursued through a SLAC/ASU collaboration.

As part of the push towards triggered droplets, an automated analysis pipeline is being developed to provide active jet/droplet feedback.

Motivation



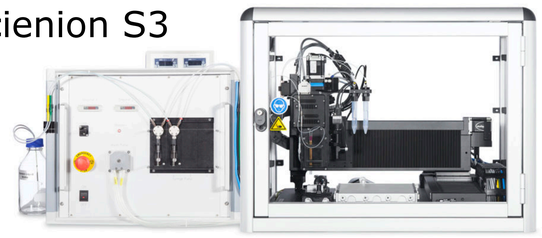
With a triggered droplet system, we expect:

- ~500-fold improvement in efficiency
- 30-fold reduction in sample consumption
- 20-fold reduction in measurement time

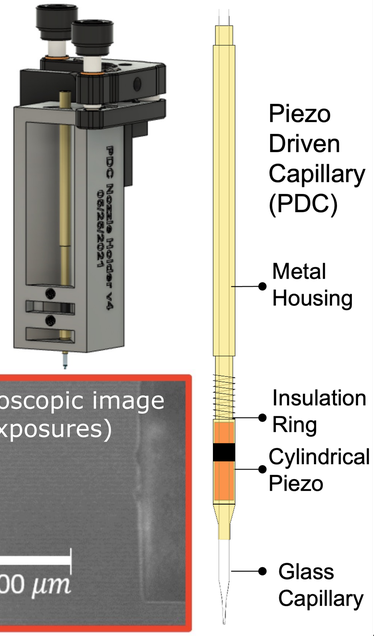
GDVNs often have a 90% data rejection rate due to jet scatter problems. Droplets have shown to be stable and repeatable, potentially decreasing the data rejection rate significantly.

The PDC

Scienion S3



Right: Custom 3D printed mounting system. Future models may include Peltier cooling or a localized humid environment



Hardware Interfaces

Goal:

- Full Python control of hardware in the Kirian Lab

Completed:

- Harvard Apparatus Syringe Pump
- Sensirion Liquid Flow Sensors
- Bronkhorst Mass Flow Sensors
- IDS Cameras
- Shimadzu FastCam Cameras

Open-Source Python Code:

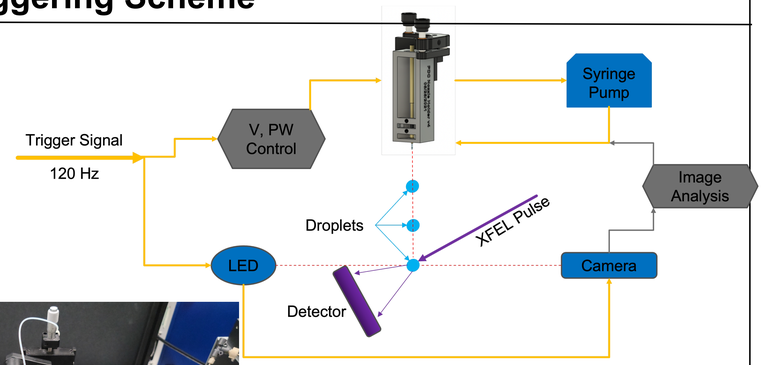
gitlab.com/kirianlab/hardware_interfaces

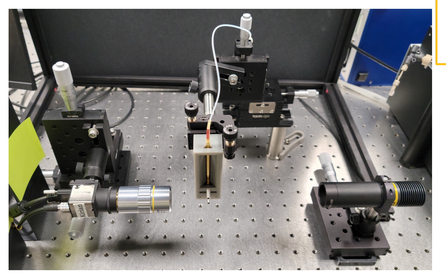
Triggering Scheme

Goal:

- Trigger the PDC without the full S3 for the upcoming X459 in-house beamtime at MFX
- Write Python control software for ease of use during a beamtime

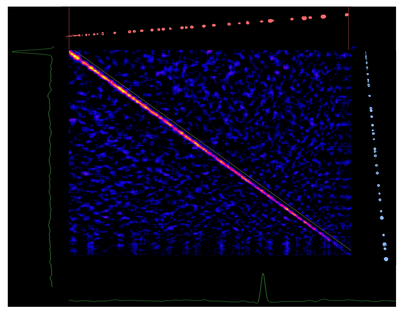
Given a trigger signal from the beamline, a triggering scheme can be developed to control a stroboscopic imaging system alongside many components in the hardware interfaces repository.

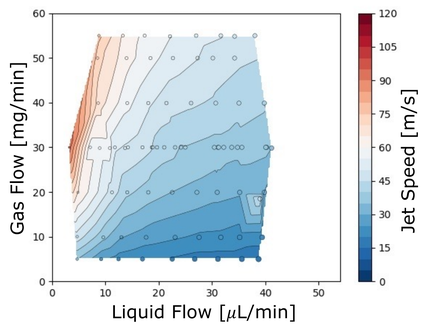




- Can achieve repetition rates between 60 and 10000 Hz
- See Daniel Rosenberg's poster for more information

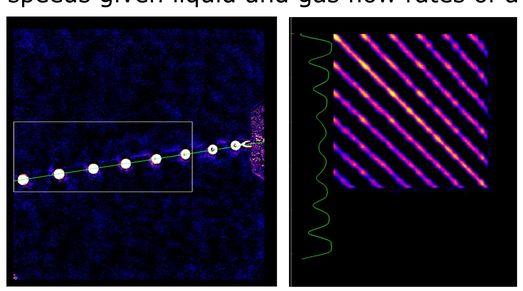
Automated Live Analysis





Top (left): Pearson Cross Correlation Matrix (PCC), used to determine correlated droplets in sequential frames. Pink pixels ⇒ high correlation. Deviation from white line gives jet speed.

Top (right): Automatically generated phase diagram, shows jet speeds given liquid and gas flow rates of a GDVN in vacuum.



Left: Automated jet analysis software applied to periodic droplets. PCC shows highly correlated droplets at regular intervals.

Conclusions

The development of an automated live analysis system has shown promise in rapid GDVN characterization, providing a useable parameter space for a given sample and GDVN design.

This analysis software will be used in combination with a triggered droplet system to characterize droplet volumes and speeds.

Acknowledgments

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