A PARALLIZED ALGORITHM FOR REAL-TIME CENTROID DETECTION FOR SINGLE-MOLECULE MAGNETIC TWEEZERS
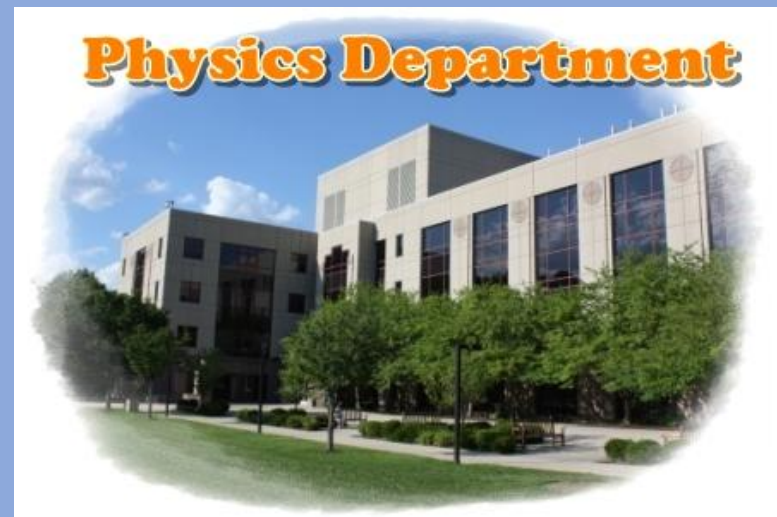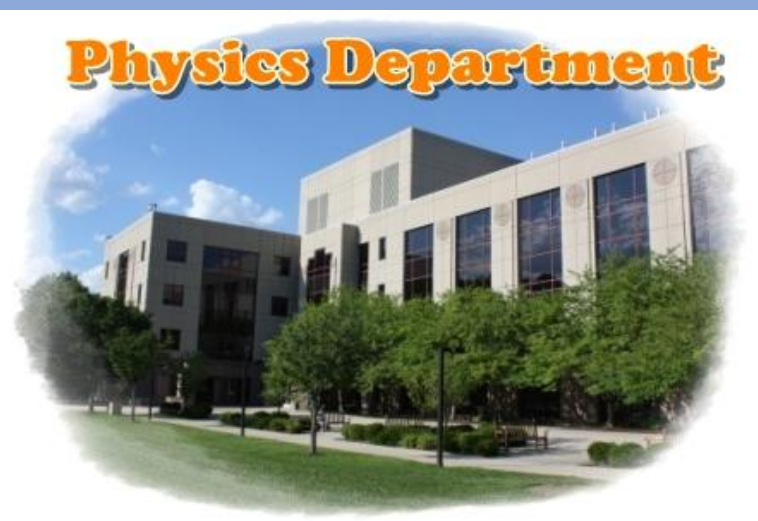
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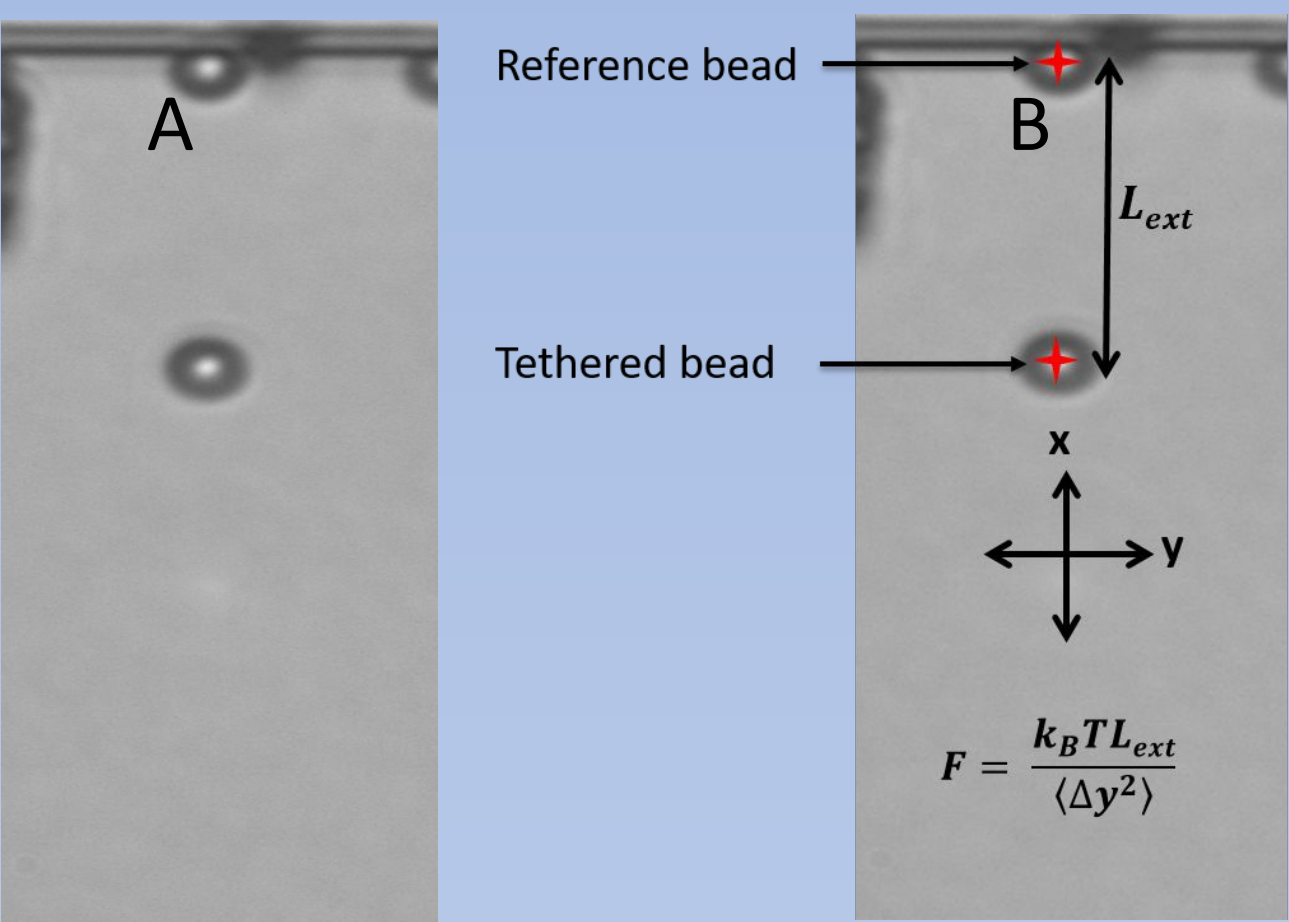[1]Abilene Christian University, [2]The Catholic University of America, [3]Colby College, [4]Vitreous State Laboratory (VSL)
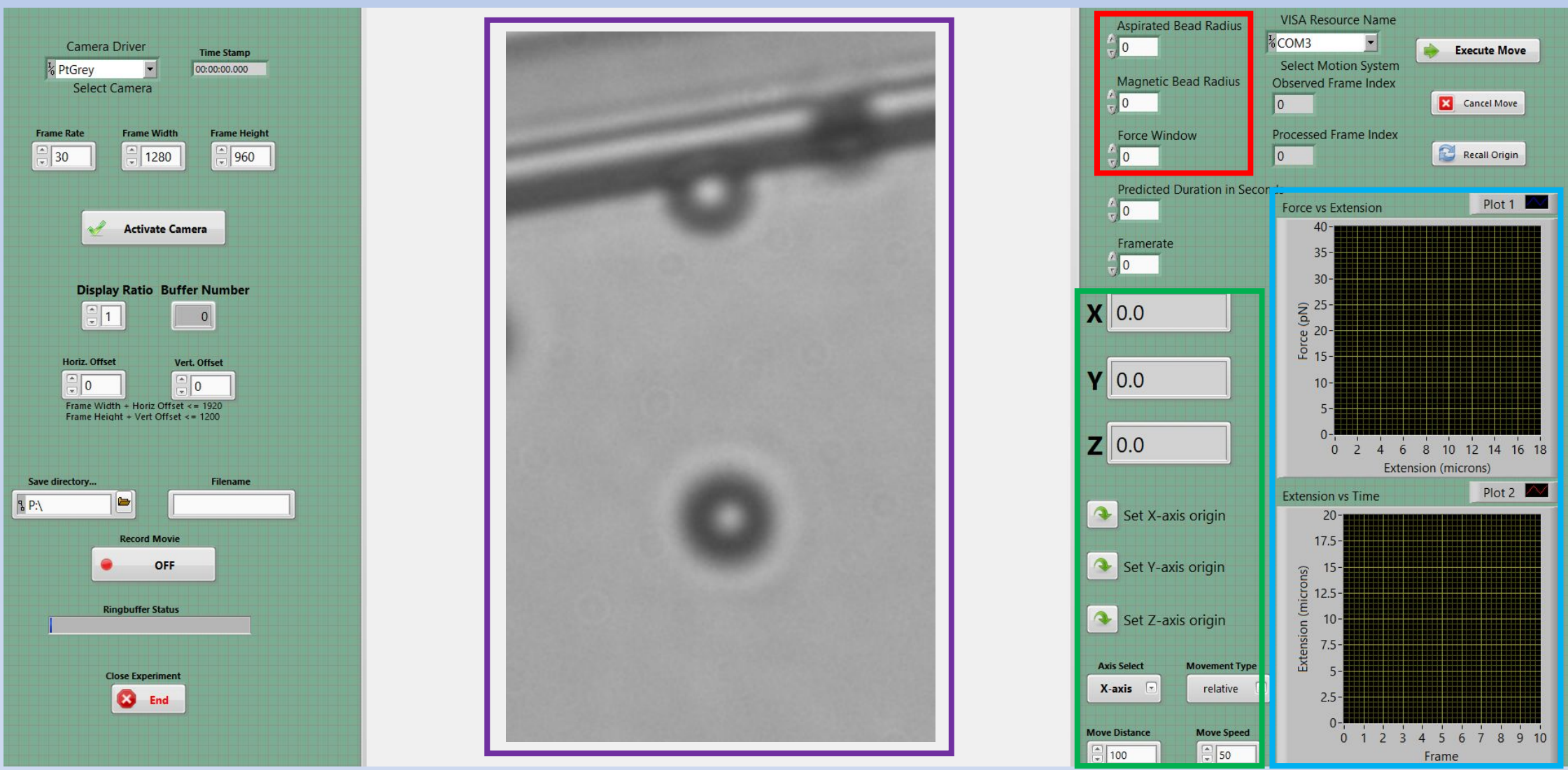
Abstract

Single-molecule magnetic tweezers have emerged as an important technique for measuring the elastic properties of single biomolecules. They utilize micron sized magnetic beads along with a permanent bar magnet and a high-speed camera. In some designs, each end of a single biomolecule, most commonly a single double stranded DNA molecule, bonds to a single magnetic bead. Most single-molecule magnetic tweezers currently in use rely on video-based tracking of the position of a single magnetic bead bonded to an end of the biomolecule. For dual-bead tethers, position coordinates of the bead are assigned in relation to the other bead tethered at the other end of the biomolecule, referred to as the reference bead. However, measurements can be inaccurate due to the inevitable mechanical drift of the reference bead. The single-molecule magnetic tweezers used in our lab is unique in that it tracks the positions of both magnetic beads simultaneously. This increases the accuracy of our measurements and resulting calculations because it directly takes the mechanical drift into account. Despite the increased accuracy of our system, our system suffers when it comes to efficiently processing our data. While some magnetic tweezers can process data in real time, our system takes upwards of 48 hours to analyze the data in its entirety. This is due to the serial nature of our data processing algorithm. The data must first be collected from the high-speed camera via a custom LabVIEW program, then delivered to a custom MATLAB algorithm, and finally plotted and displayed. Additionally, a fraction of all experiments does not yield usable data due to run-to-run variation in the setup. Therefore, we seek to accelerate our data processing flow in order to collect data, process the data, and display it simultaneously. Real-time data processing will allow us to further speed up our experiments by promptly terminating data collection of samples that produce unusable data. Our approach allows us to process data in real time by combining our LabView program with our MATLAB algorithm.

Principle of Experiment and Instrument Design

- (A) We use end functionalized λ-DNA with a contour length of 16.4 μm. The magnetic bead diameters are ~2.8 μm and the permanent magnet dimension are 3 mm $\times$ 2 mm $\times$ 1 mm. We manipulate the force by moving the magnet towards or away from the tethered bead.
- (B) Schematic of the Horizontal magnetic tweezers with its components.
- (C) Schematic of the sample cell. The overall dimensions of the sample cell are 60 mm $\times$ 40 mm $\times$ 1 mm; however, the enclosed region is 6 mm $\times$ 4 mm $\times$ 1 mm yielding a sample cell volume of ~24 μL. We perform our experiments at room temperature.

Image Analysis

- (A) A screen shot from a DNA-pulling experiment. The magnet is located near the bottom of the screen and is not visible in the field of view.
- (B) Using LabView and MATLAB algorithms, the centroids of the two beads are determined. The forces are calculated using the equipartition relation.
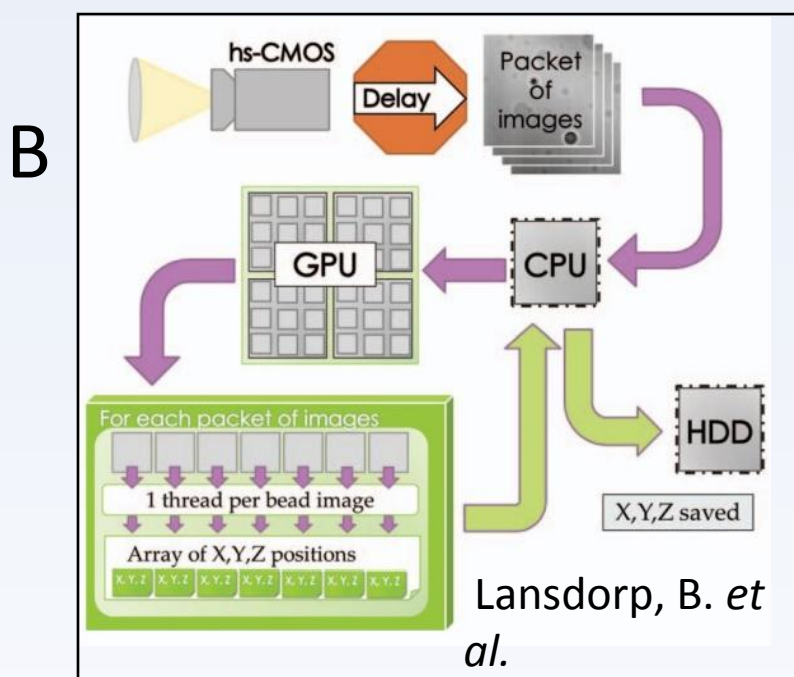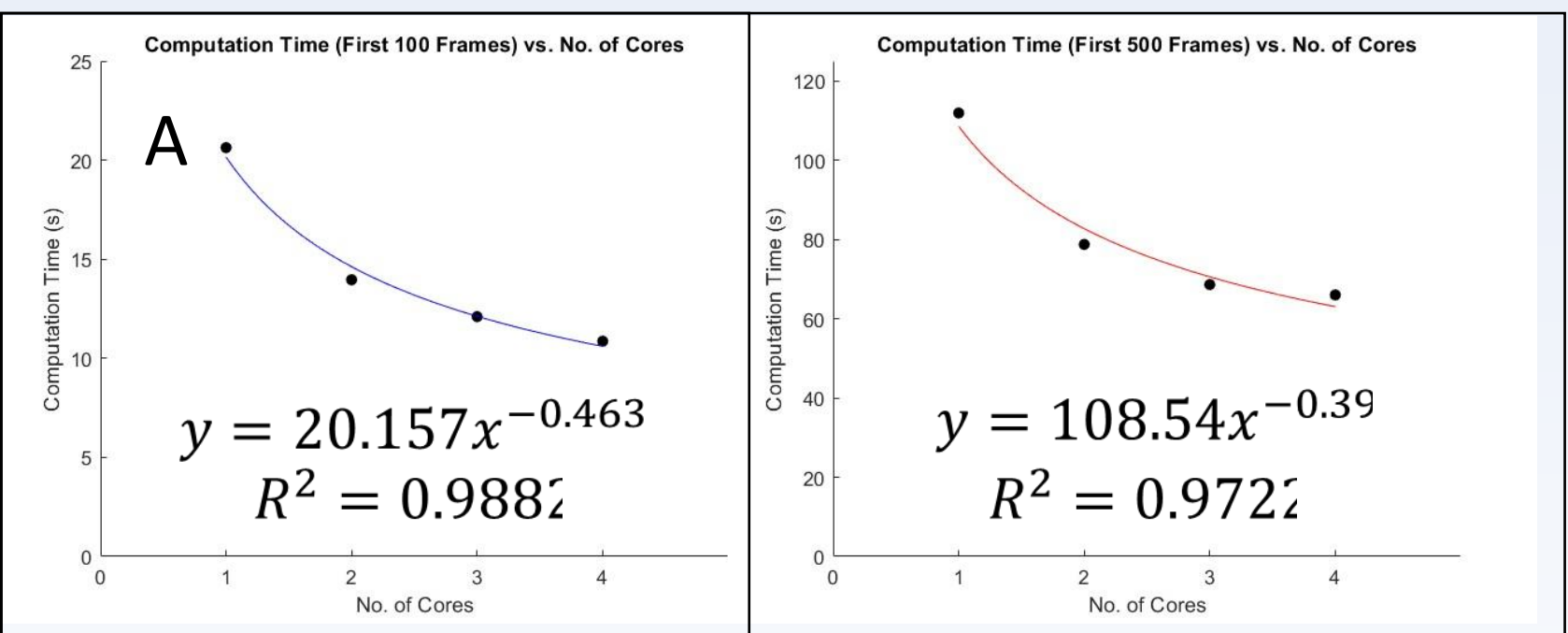
$$F = \frac{k_B T L_{ext}}{(\Delta y^2)}$$

LabVIEW Virtual Instrument Front Panel

- --- Here we enter information needed for the live calculations. Fixed magnetic Bead Radius and suspended Magnetic Bead Radius are used when calculating the distance between the beads and determining the coordinates of the bead centers. Force Window specifies the number of consecutive observation frames to use when determining the variance.
- --- Displays plots of calculated force and extension in real time.
- --- Allows us to control the speed and direction of motion of the sample stage.
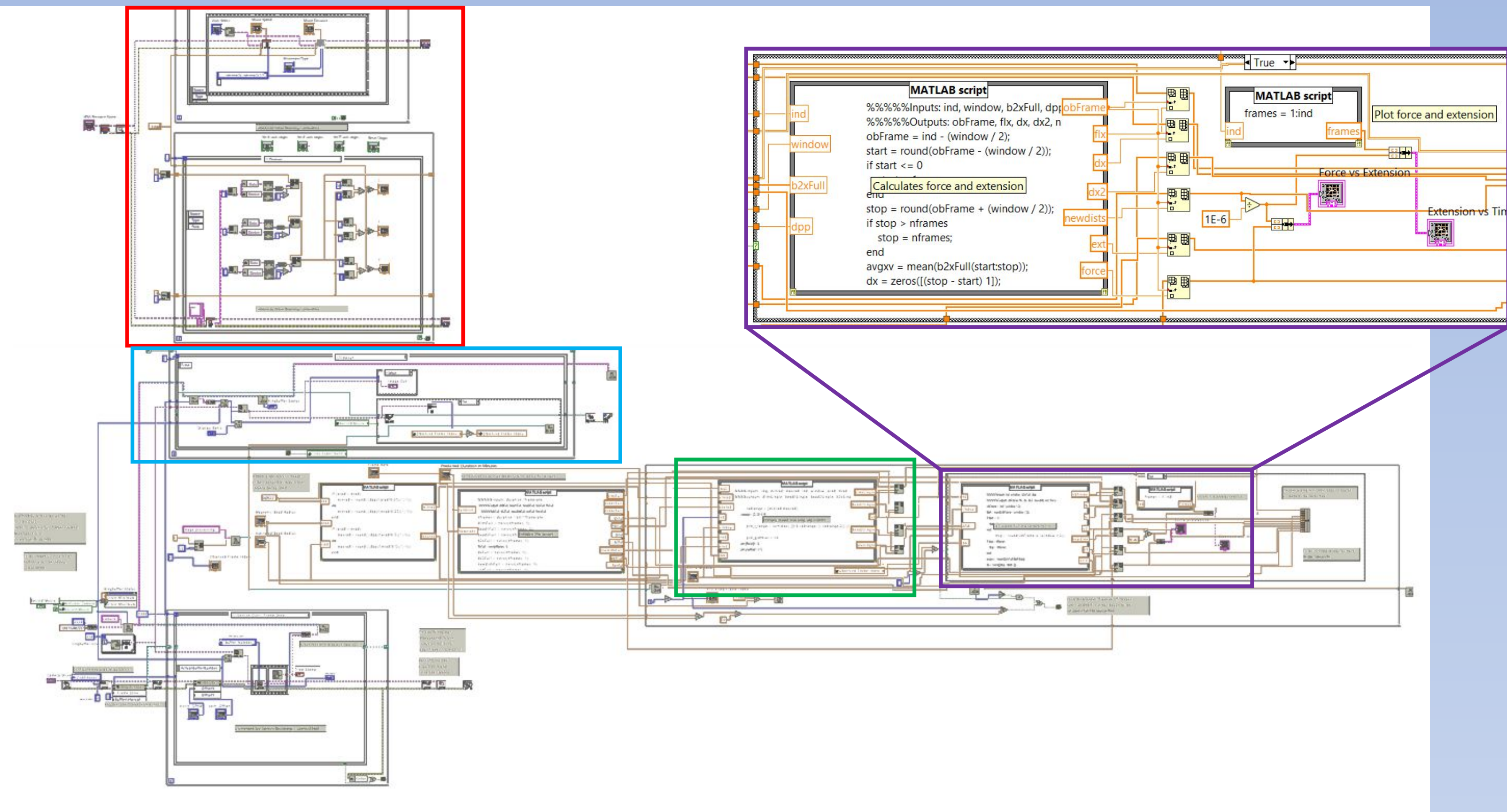- --- Live feed from high-speed camera.

Parallel Computing

- Our code can be parallelized to execute multiple computational tasks at once. We tested and recorded the effects of parallelization on our algorithm by distributing individual frames of the video to different cores of our computer's CPU (Central Processing Unit) for image processing. Our tests were performed on a computer equipped with an Intel® Core™ i7-10510U CPU processor, which contains 4 processing cores.
- We also parallelized our code using a GPU (Graphics Processing Unit). However, it decreases the computational speed of our image processing algorithm. This is because LabView and MATLAB, on their own, lack the ability to take full advantage of GPU parallel computing.

$$y = 20.157x^{-0.463}$$
$$R^2 = 0.9887$$

$$y = 108.54x^{-0.39}$$
$$R^2 = 0.9727$$

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- (A) shows how our parallelized algorithm's computation time decreases as the number of active CPU cores increases, as well as an exponential of best fit. We used a force window frame size of 500 for our measurements.
- (B) General schematic of data transfer in a GPU parallel computing bead tracking algorithm.

LabView Virtual Instrument Block Diagram

- --- Allows us to control the micromanipulators. The code accepts movement speed as input.
- --- Displays camera feed and places image/frame data into a queue.
- --- Bead tracking algorithm taken directly from our original MATLAB algorithm. Extracts image/frame data from the queue.
- --- Force and extension calculation algorithm. Here the code also plots the corresponding data in real time. This code only begins to execute after a specified number of frames have already been processed by the bead tracking algorithm. A "buffer" of frames is required in order to accurately calculate the variance, which is a necessary component of the force equipartition relation calculation.

Future Work

- We cannot advantageously implement GPU parallel computing into our current LabVIEW/MATLAB algorithm.
- We seek to rewrite our algorithm in the CUDA programming language, which specializes in GPU programming.

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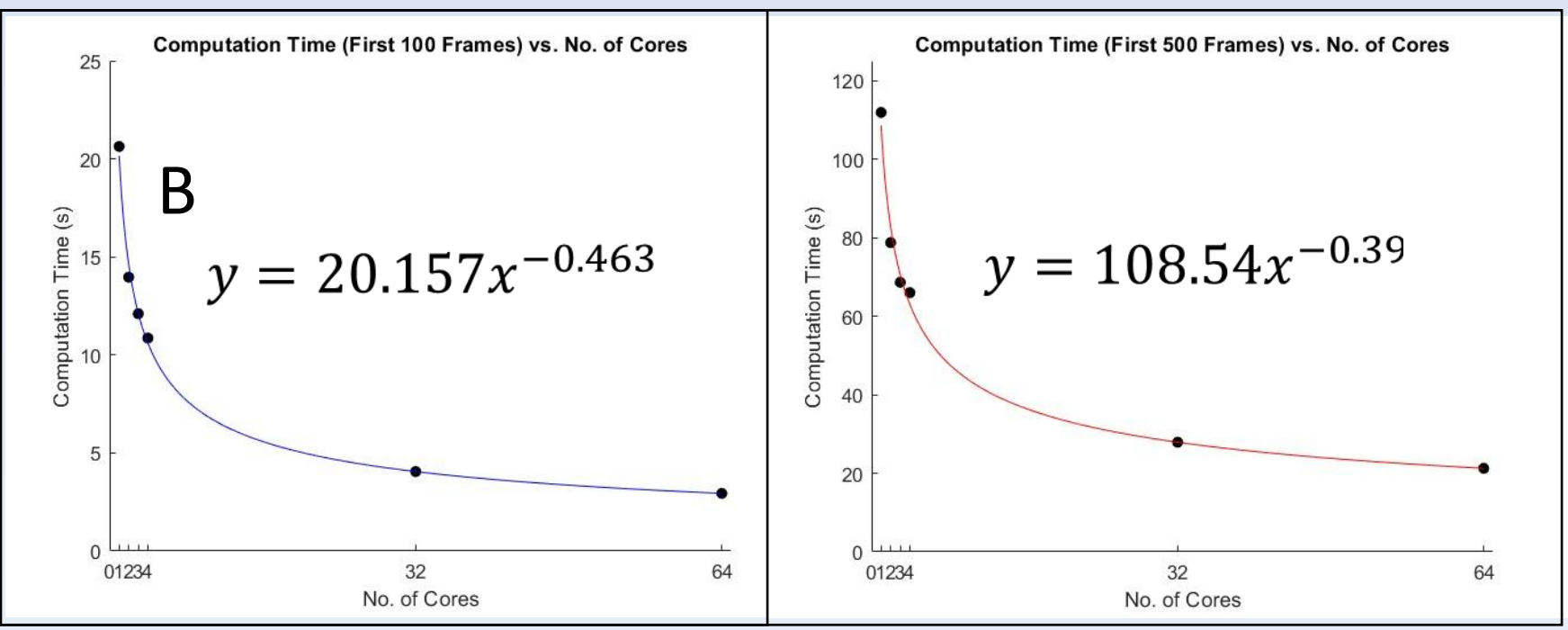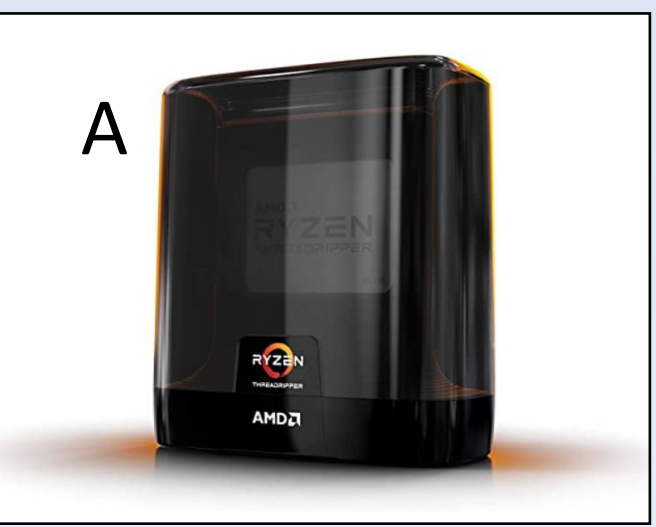
- (A) CPU processor we are considering investing in. It is an AMD Ryzen Threadripper PRO 3995WX. The price is ~$8,000.
- (B) Predicted improvement in processing speed for 32-core and 64-core processors based on observed processing times of our Intel® Core™ i7-10510U processor.
- (C) Motherboard we are considering investing in. It is compatible with AMD Threadripper processors and has 4 DDR4 RAM slots. It is an ASUS Pro WS WRX80E-SAGE SE WIFI AMD Threadripper Pro EATX. The price is ~$1,000.
- (D) RAM we are considering investing in. It is the Kingston FURY Beast RGB with 128 GB of memory and DDR4 memory technology. The price is ~$550.

References

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