Modelling Dynamics of a Plume of Ionic Molecular Species Generated by Laser Ablation for Coupling to a Mass Spectrometer

R. J. Dwayne Miller

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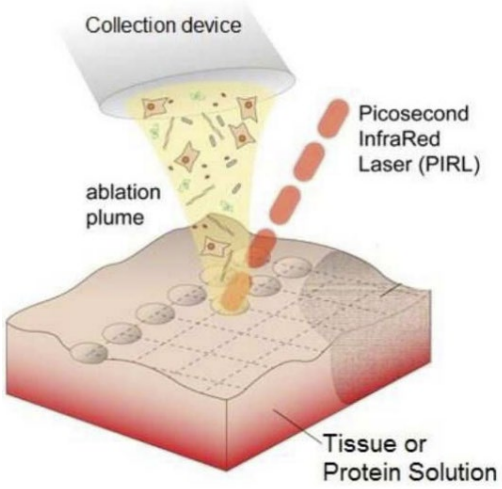
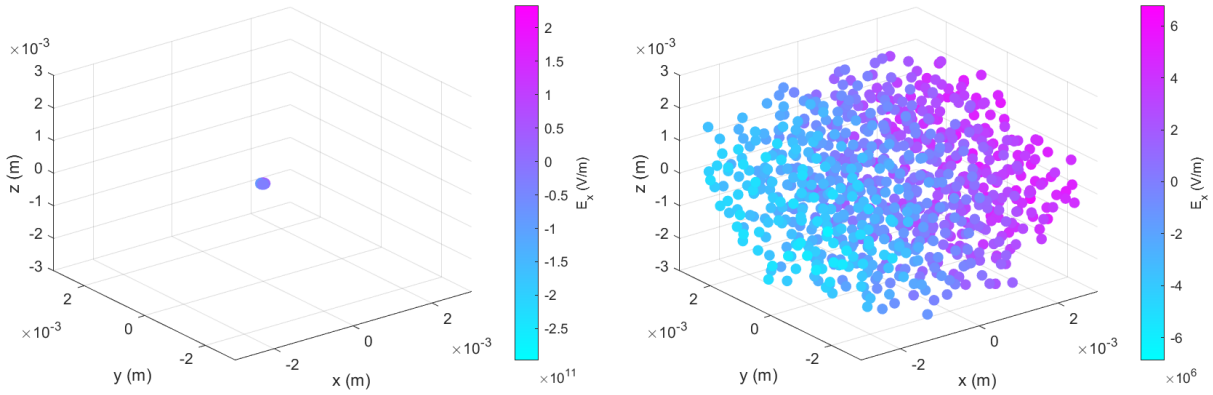
The Picosecond InfraRed Laser (PIRL) has been demonstrated to ablate intact molecules and proteins through the process of DIVE (Desorption by Impulsive Excitation). PIRL was specifically engineered to selectively excite the water in tissue, which acts as the propellant to drive intact molecules and proteins into the ablated plume [1, 2]. Coupled to a mass spectrometer, the PIRL-DIVE regime could unlock the door to the detection of the complete human proteoform and uncover the physics behind biomolecular and cellular functions.



Schematic of a PIRL tissue ablation and the produced protein plume collection [Miller].

However, low coupling efficiency into mass spectrometer (MS) systems presents a major barrier to this goal [3]. Space charge effects in the ionic cloud are a major factor contributing to this low coupling efficiency [3]. The limiting effect of space charge has been observed with electron diffraction experiments [4]. Modelling and understanding the ion dynamics in the accelerating ablation plume is necessary for optimising the coupling of ions into the inlet of the mass spectrometer.



Snapshots of the time evolution of the macroparticle spatial distribution and the electric field strengths of an ion cloud. (a) is the initial spatial distribution, (b) the ionic spatial distribution after 5 ns. [Madhoun]

The student will help build a simulation framework to study the space charge and molecular dynamics in an accelerating ionic cloud of various molecules. In particular, the student will study short range forces between "neutral" polar molecules such as water and other ionic molecules and compounds. The results of the simulation will guide the development and implementation of an experimental setup for laser ablation of drosophila embryos to optimize the collection of the ablated plume. This project is two-fold: first studying the ion dynamics in the acceleration regime for coupling into the inlet of the MS followed by optimizing the laser ablation for mass spectrometry of drosophila embryos for better understanding of the developmental stages of this species. The ongoing study will exploit the well-understood and fast development of Drosophila embryos to link protein distributions to biological functions [5].

The main tasks for this project are:

- Development and implementation of a new simulation code in C.
- Development and implementation of an experimental setup for laser ablation and optimisation of the ion collection of the ablated plume.
- Analysis of the detected mass spectra of biomolecules.

For inquiries, please contact Khaled Madhoun at khaled.madhoun@mail.utoronto.ca

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