Multi-Physics and Data-Driven Modeling for Electrospray Propulsion

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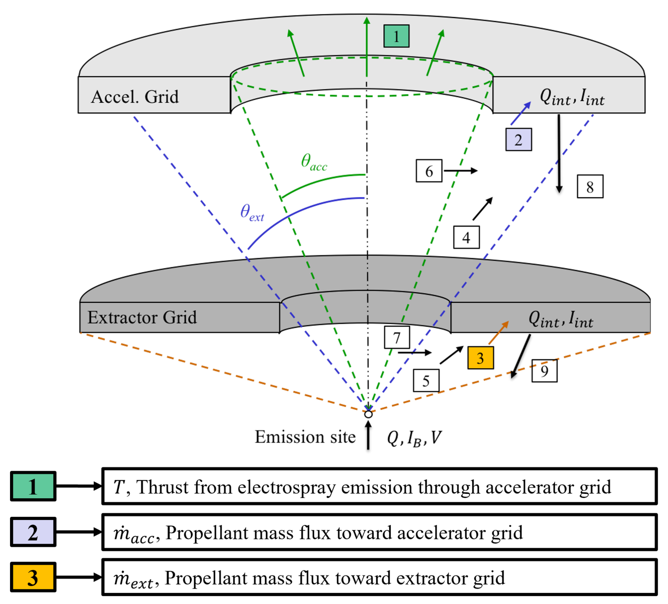
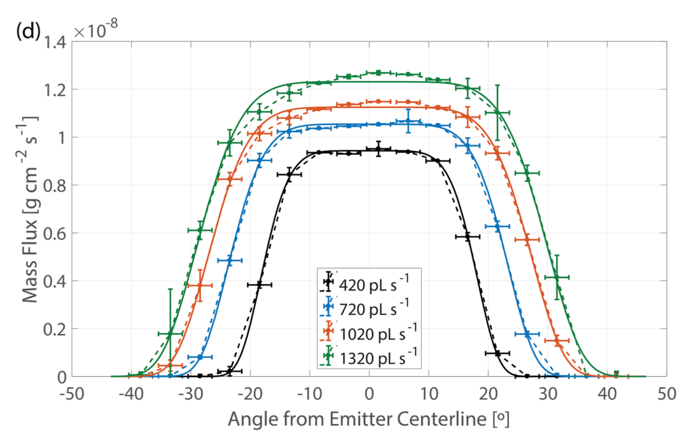
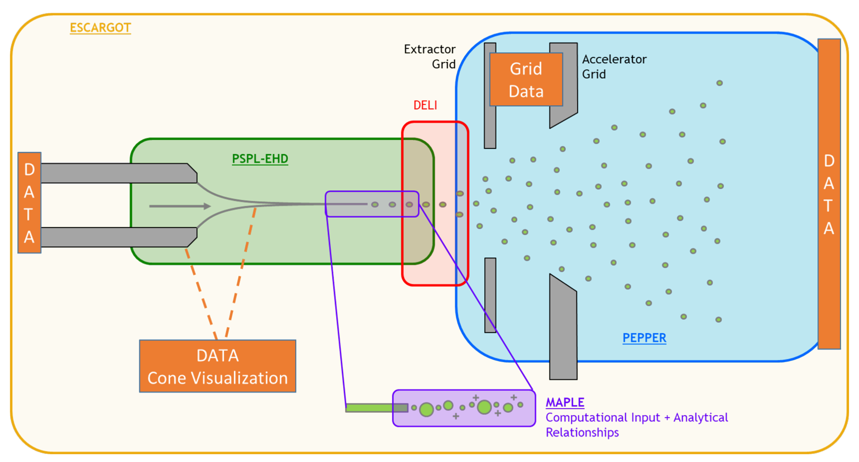
Motivation

Electrosprays have led to many scientific discoveries, from Nobel prize-winning **electrospray ionization** techniques, **quantum dot nanofabrication**, controlled **drug delivery**, to **spacecraft propulsion**. Electrosprays work by applying **strong electric fields** to highly-conductive **ionic liquids (ILs)** to generate a thin **liquid jet** and uniform stream of high-velocity **nanodroplets**.

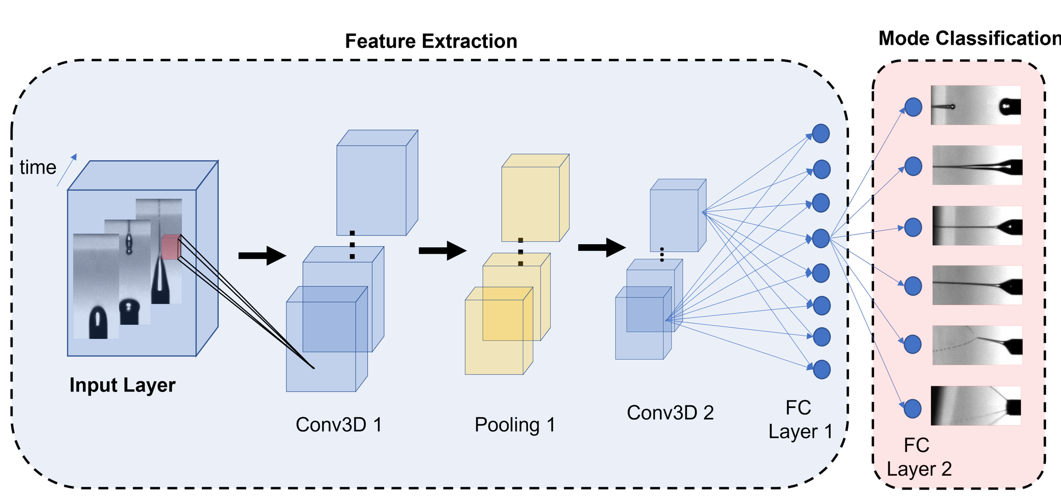




Understanding jet and droplet dynamics are critical to improving electrospray performance. To this end, the UCLA PESPL has coupled benchtop and *in vacuo* experimental testing with multi-scale computational modeling to investigate physics- and chemistry-based phenomena that are important to understanding electrospray operation. One intriguing but unexplained result from the data, is the **order 3 super-Gaussian shape** of the plume's mass flux profile.



Initial Design of 3D-Convolutional Neural Networks for Flow Reconstruction



Behavior and onset of temporal jet instabilities during electrospray operation are due to complex and often stochastic, electrohydrodynamics that is difficult to solve via computational fluid dynamics. To leverage high-speed microscopy of electrospray emission and plume expansion, convolutional neural networks (CNNs) can be used to reconstruct fluid flow data into a latent space representation for feature extraction. The proposed architecture is currently under investigation.

[1] D. Tran et al., **A Closer Look at Spatiotemporal Convolutions for Action Recognition**, 2018 IEEE/CVF Conference on Computer Vision and Pattern Recognition, 6450 (2018). [2] S. Wiewel et al., **Latent Space Physics: Towards Learning the Temporal Evolution of Fluid Flow**, Computer Graphics Forum 38 (2019).

Physics-based & Reduced-order Modeling

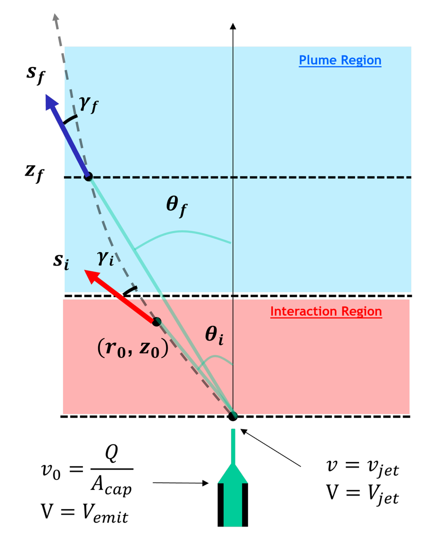
The governing equation for charged particle motion in a collision-less domain is

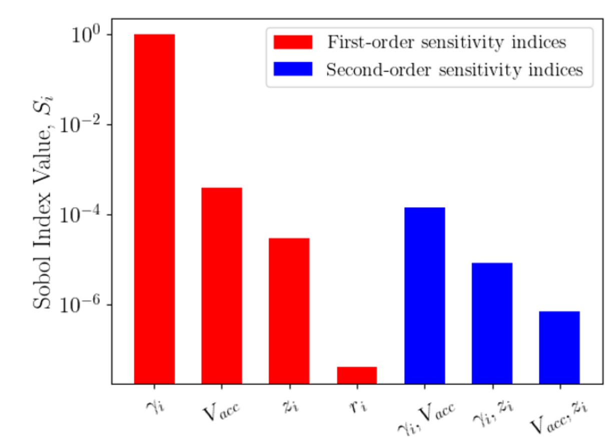
$$\frac{\mathrm{d}^2\vec{x}_i}{\mathrm{d}t^2} = -\left(\frac{q}{m}\right)_i \nabla\phi_{ext} = \left(\frac{q}{m}\right)_i \vec{E}_{ext}, \quad (1)$$

where $\vec{x}_i$ is the position of particle i, $\left(\frac{q}{m}\right)_i$ is the particle's specific charge, and ϕ_{ext} is the potential field from the electrodes. A model surrogate is used and defined by a **polynomial chaos expansion (PCE)**,

$$\mathbb{M}(\vec{X}) = \sum_{\alpha\in\mathbb{N}^d} y_\alpha \Psi_\alpha(\vec{X}), \quad (2)$$

where a basis set of orthogonal, Hermite polynomials, $\{\Psi_\alpha(\vec{X}), \alpha\in\mathbb{N}^d\}$, is bounded by the dimension d of the input parameter space $\vec{X}$. A **Sobol analysis** shows that angles of the emitted species entering the domain, γ_i, dominates the plume shape.



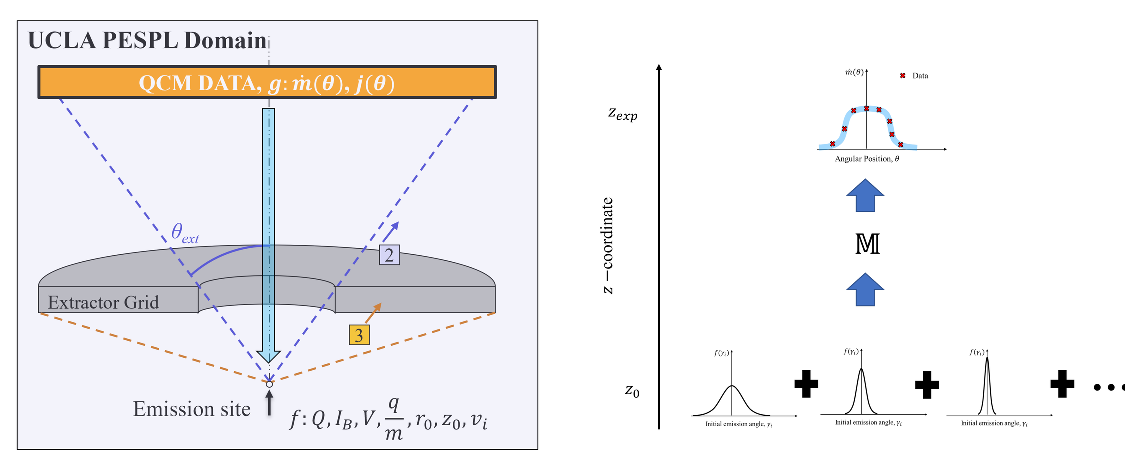


Inverse Problem Formulation

An inverse formulation can be used to help explain the super-Gaussian mass flux profiles. Formally, an inverse problem is defined by

$$g = \mathbb{M}(f) + \epsilon, \quad (3)$$

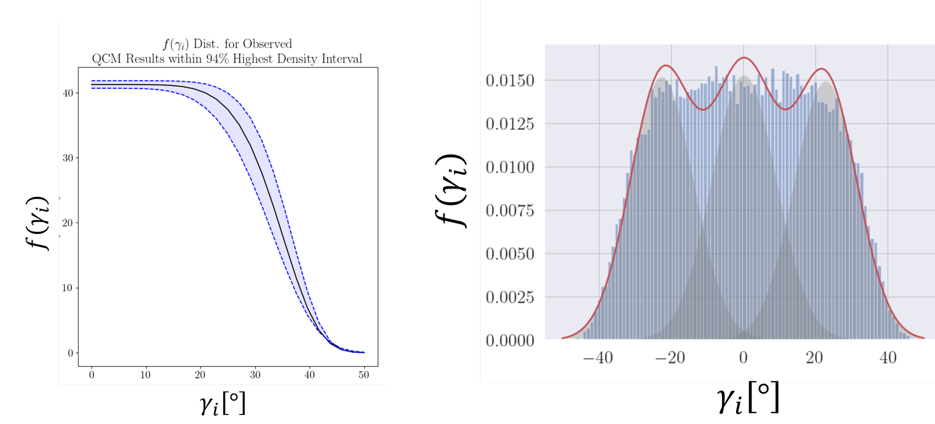
where some measured data, $g\in Y$, is the result of a forward problem where model parameters, $f\in X$, are mapped by an operator, $\mathbb{M}$, within observational noise, $\epsilon\in Y$.



A likelihood function using this formalism is used to solve the inverse problem,

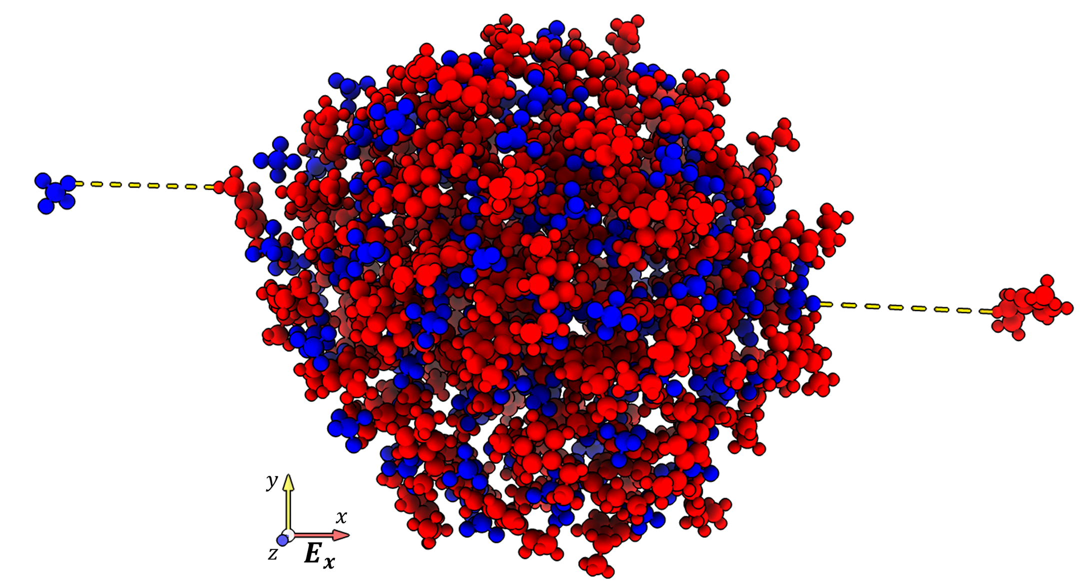
$$\mathrm{prob}(\dot{m}(\theta)_{UCLA}|\theta_i,\gamma_i,I) = \prod_i^N \sum_{j=1}^k \alpha_j \mathrm{prob}(\dot{m}(\theta)_i|\theta_i,\gamma_i,I) \quad (4)$$

where θ_i and γ_i are the uncertain parameters, we wish to quantify, $\dot{m}(\theta)_{UCLA,QCM}$ denotes the mass flux profile measurements provided by UCLA PESPL, and I represents any background knowledge available for this problem.



Molecular Simulation of Ionic Liquid Nanodroplets

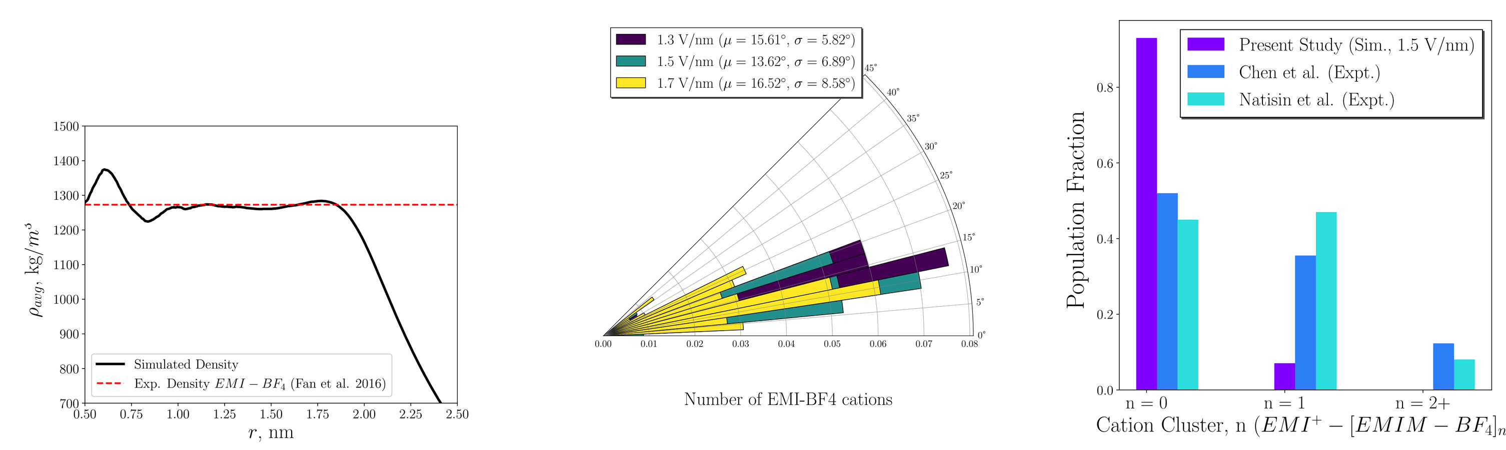
Classical molecular dynamics simulations of two imadazolium-based ionic liquids, EMI – BF_4 and EMIM – Tf_2N, were conducted to investigate effects of high-magnitude electric fields on **ion extraction** at nanodroplet-vacuum interfaces. **Initialization** of molecule positions was computed using optimal packing algorithms in Packmol; **equilibration** of quasi-spherical nanodroplets consisted of canonical (NVT) and microcanonical (NVE) ensemble calculations; **productions** runs were completed in the NVE ensemble for 24 unique droplet configurations.



125 EMI^+ cation (red) and BF_4^- anion (blue) pairs

Summary of Results

1. Electric field strengths past 1.5 V/nm resulted in droplet **breakup and fracturing**.
2. Simulations exhbitied preference to **monomer** emission compared to experiments.
3. Comparison between EMI – BF_4 and EMIM shows influence of **hydrogen bond strength** (and thereby cation-anion attractive forces) on emission timescales.



Future Work: Development of Transferable MD Force Fields

Improvement of future in-space propulsion technologies will depend on a **fundamental understanding of ionic liquid chemical break down mechanisms** in dynamic environments. Electrostatics are influenced by local dipole moments that cannot be accurately described by fixed-charge interatomic potentials; thus, **polarizable force fields** are being developed for various candidate propellants of interest to investigate structural, thermophysical, and dynamic properties.