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The Pixel Imaging Mass Spectrometer: towards reconstructing molecules

Pixel Imaging Mass Spectrometry is a new molecular imaging technique that relies on precision laser pulses to both align and strip molecules of their valence electrons thereby causing them to explode. The primary task of this experimental setup is the reconstruction of the disintegrated parent molecule through the systematic collection of the fragments of the explosion. The unique characteristics of the experimental setup provide an unprecedented resolution from other techniques. Experimentally obtained covariance maps reveal a partially hidden rich structure of the parent molecule and fragmentation dynamics. However, for larger molecules, the large number of fragment ions that are produced congest the the resulting time-of-flight spectrum and alternative strategies are required to resolve the structure of the parent molecule.

The underlying mathematical challenges of this problem that are unique to the pixel imaging mass spectrometer will be discussed, and a comparison of the forward model predictions with experimental data for the imaging of 3,5-dibromo-3',5'-difluoro-4'-cyanobiphenyl molecule will be presented. A brief survey of the established reconstruction methods for this type of problem will also be discussed.