Two-Photon Double Ionization of H_2

X. Guan and K. Bartschat (Drake U.), L. Koesterke (TACC), B.I. Schneider (NSF)

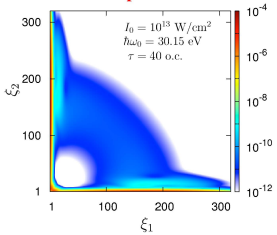
Goal: Resolve large discrepancies in previous calculations of this fundamental process.

Steps taken: 1) Optimized existing FEDVR code for Stampede
2) Sampled parameter space (photon energy, pulse duration) with about
100 runs (3000 cores and 10-20 hours of wallclock time each)

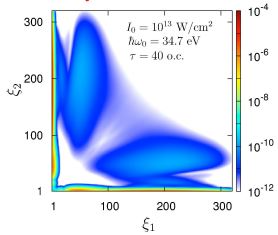
Findings: Discrepancies are due to surprisingly strong dependence of theoretical predictions on laser parameters and (previously unresolved) effect of autoionizing states.

Broad Impact: These calculations support/explain very expensive FEL experiments.

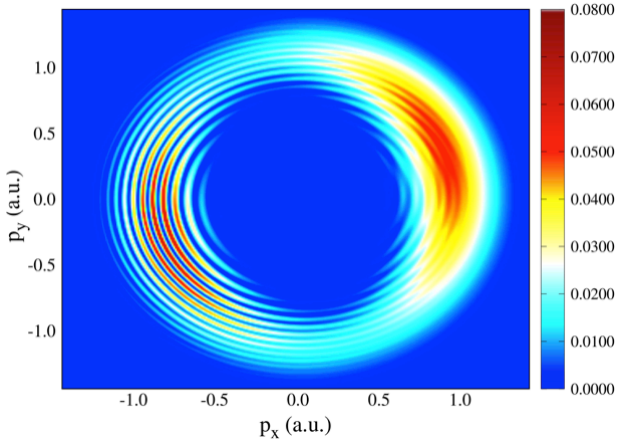
Sample Results for Electron Probability Distribution



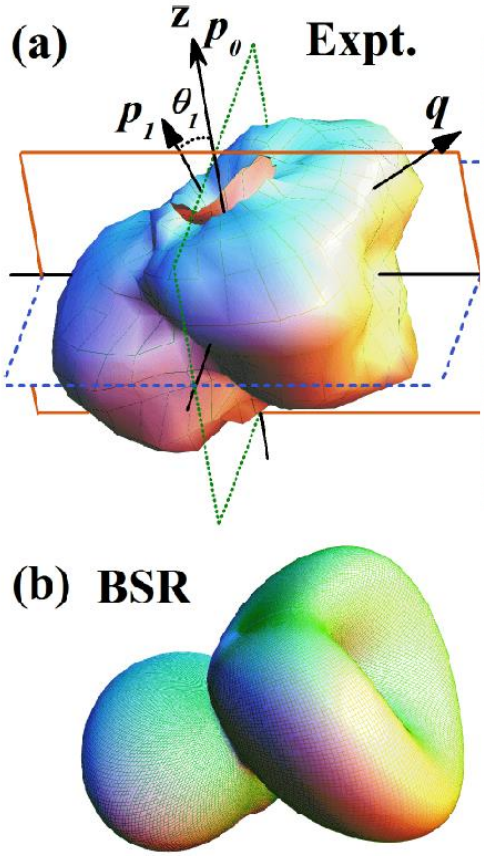
Effect of **autoionizing states** on non-sequential double ionization



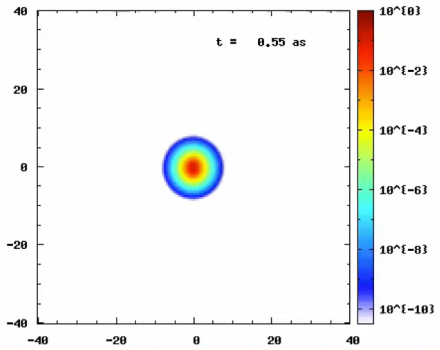
Competition between **direct** and **sequential** double ionization



Photoelectron Momentum Distribution for Ar Ionization in Strong Electromagnetic Field



Ionization of Ar(3d) by electron Impact: Experiment(a) and Theory(b)



H^+_2 Ionization in strong, ultrafast electromagnetic field