Resolving Extended Space and Time Correlations in Molecular Dynamics Simulations of Strongly Magnetized Plasmas

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Research Results and Motivation

- Computed diffusion coefficients in a strongly magnetized one component plasma system using molecular dynamics (MD) simulations
- Significantly reduced particles required to obtain diffusion coefficients by using an elongated domain
- Examples of strongly magnetized plasmas include trapped antimatter, ultracold neutral plasmas, and magnetized dusty plasmas

Molecular Dynamics Simulations are Used to Compute Diffusion Coefficients

- Periodic boundaries are used to simulate an infinite plasma
- Using a randomly selected subset of the simulation particles, the velocity auto correlation function is calculated
- From the velocity auto correlation function, the self diffusion is calculated using the Green-Kubo relations for a magnetized plasma

$$D_{\parallel} = \frac{k_B T}{m}\int_0^{\infty} Z_{\parallel}(t)dt,$$

$$D_{\perp} = \frac{k_B T}{m}\int_0^{\infty} Z_{\perp}(t)dt,$$

$$D_{\wedge} = \frac{k_B T}{m}\int_0^{\infty} Z_{\wedge}(t)dt.$$

$$D = \lim_{t\to\infty}\langle|r(t)-r(0)|^2\rangle \qquad \langle|r(t)-r(0)|^2\rangle = 6t\int_0^t (1-\frac{s}{t})Z(s)$$

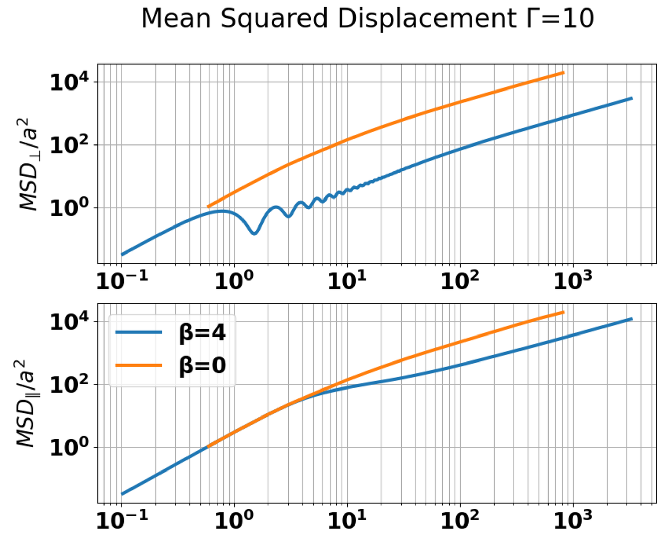
- The diffusion coefficient can be found by approximating $\lim_{t\to\infty}$ as the point which the mean squared displacement plot becomes linear on a log-log scale

Strong Magnetization Leads to Increased Temporal and Spatial Correlations Associated with Coulomb Collisions

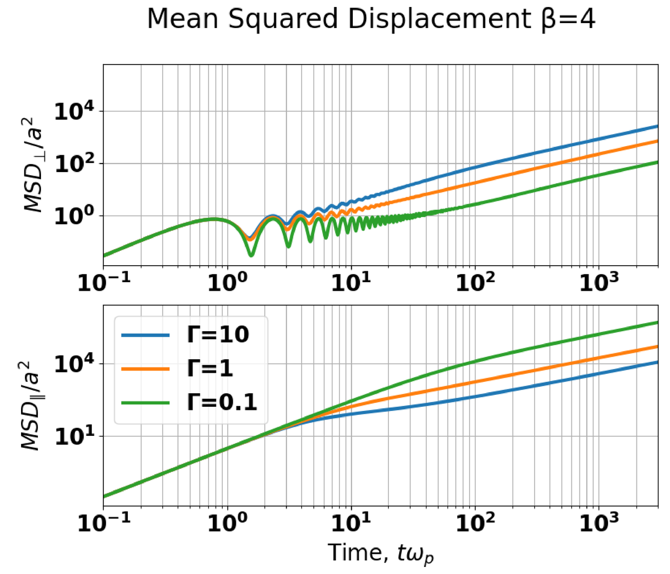
- Magnetized one component plasma is characterized by the magnetization strength (β) and coupling strength (Γ)

$$\Gamma = \frac{q^2/a}{4\pi\epsilon_0 k_B T} \qquad \beta = \frac{\omega_c}{\omega_p}$$

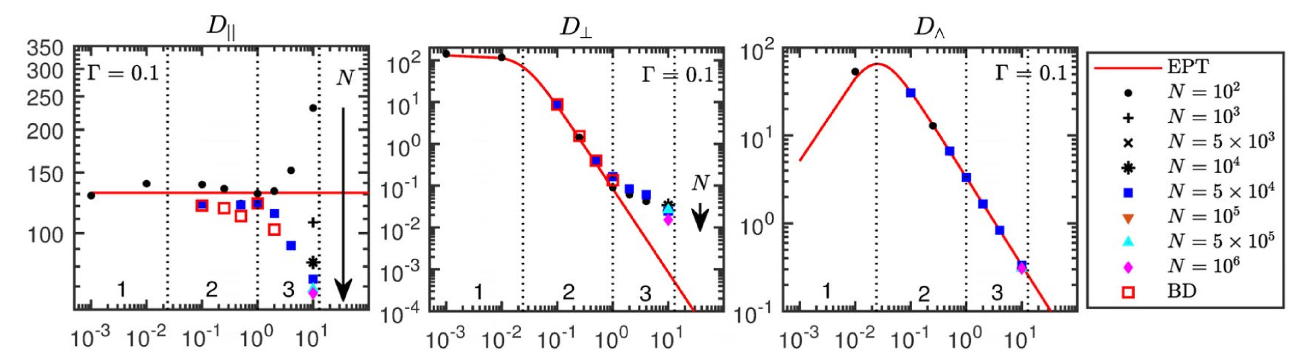
Mean Squared Displacement Γ=10



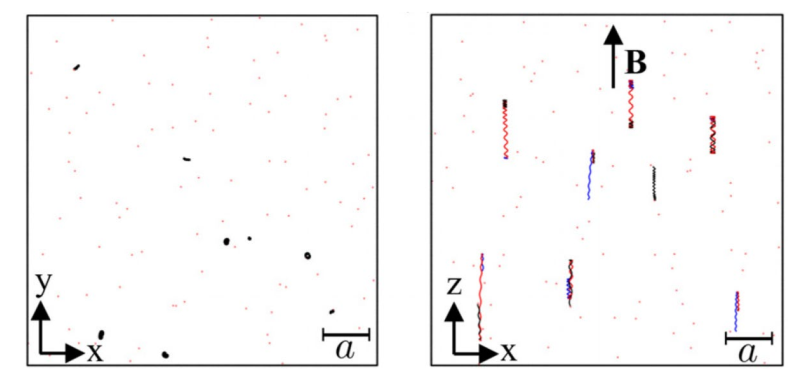
Mean Squared Displacement β=4



- Strong magnetization requires long simulation run time to reach the linear regime
- Weak coupling and strong magnetization decrease the timestep needed to resolve collisions
- Previous simulations required a large number of particles to resolve the long-range correlations because they used cubic domains [1]

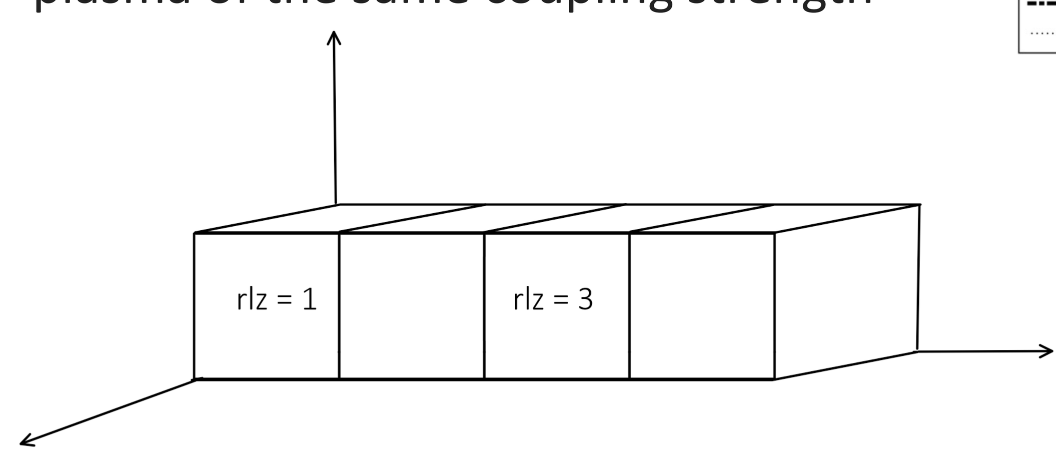


- Strong magnetization confines the motion to a small cylinder with a width characterized by the gyroradius and a length characterized by the collision mean free path [1]

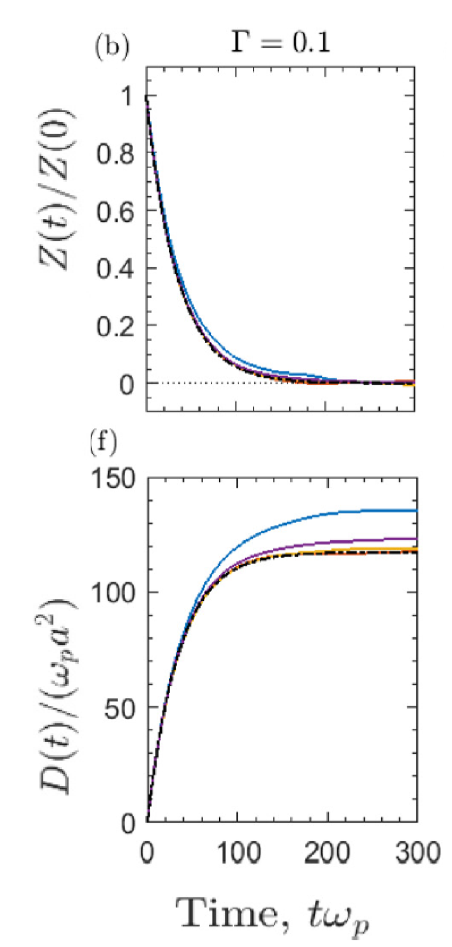


Elongated Boxes Can Capture the These Increased Correlations With Lesser Number of Particles

- The initial box size is set by the number of particles required for unmagnetized plasma of the same coupling strength



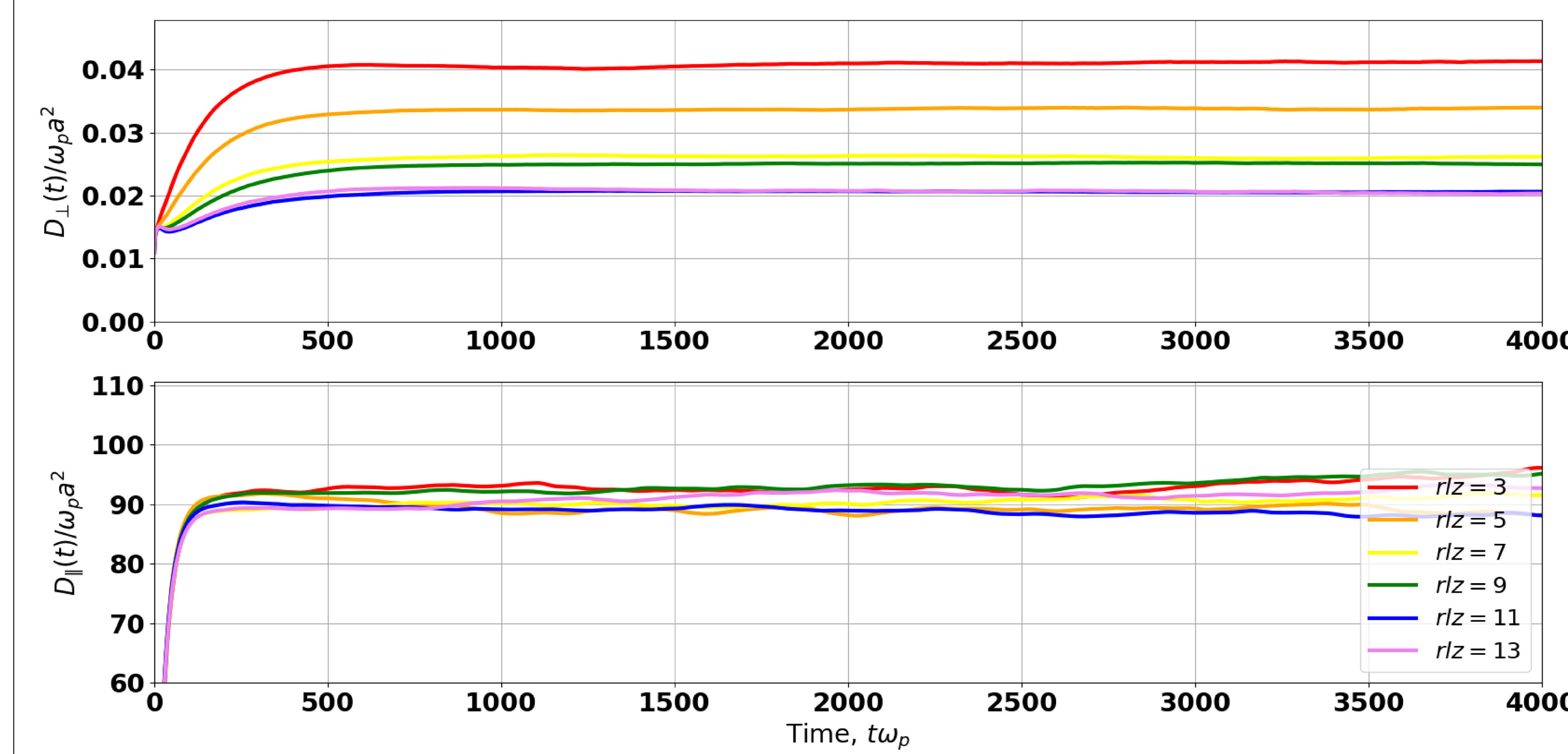
- Additional boxes are added along the magnetic field direction to capture the long-range correlations
- This significantly reduces the number of particles required as compared to using the cubic domain
- Computational cost is decreased with decreasing number of particles required



Velocity auto correlation function and self diffusion in unmagnetized one component plasma [1]

Convergence When Elongating the Domain in the Direction of the Magnetic Field

Self Diffusion [β=4, Γ=0.1, N=1000]



- Gyroaveraged plot of parallel and perpendicular self diffusion with respect to time in a one component plasma
- Convergence with increasing number of box lengths (rlz) where N is the number of particles in the initial cube, and the domain is stretched by adding additional cubes
- With elongated domain, Γ = 0.1, β=4 required 11,000 particles, corresponding to a significant reduction in the number of particles required

Diffusion Coefficients		
	$D\ \perp/\omega_p a^2$	$D\ \perp\parallel/\omega_p a^2$
Γ = 10	4.631×10^{-3}	1.998×10^{-2}
Γ = 1	1.171×10^{-2}	9.020×10^{-1}
Γ = 0.1	2.151×10^{-2}	9.049×10^{1}

Future Work

- Obtain diffusion coefficients using an elongated domain, continuing to explore the parameter space of β and Γ, particularly in strongly magnetized and weakly coupled regimes

References

[1] Vidal, Baalrud, Phys. Plasmas 28, 042103 (2021).

Acknowledgements

*This research was supported by US Department of Energy grant no. DE-SC0022202, and in part through computational resources and services provided by Advanced Research Computing (ARC), a division of Information and Technology Services (ITS) at the University of Michigan, Ann Arbor.