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Langevin Meeting

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Convergence in Divergence Identity

Run FFT Poisson solve on $[-1, 1]^3$ to compute $\boldsymbol{D}(\tilde{v})$ and identities, then rescale ($\tilde{v} = v/v_{max}$).

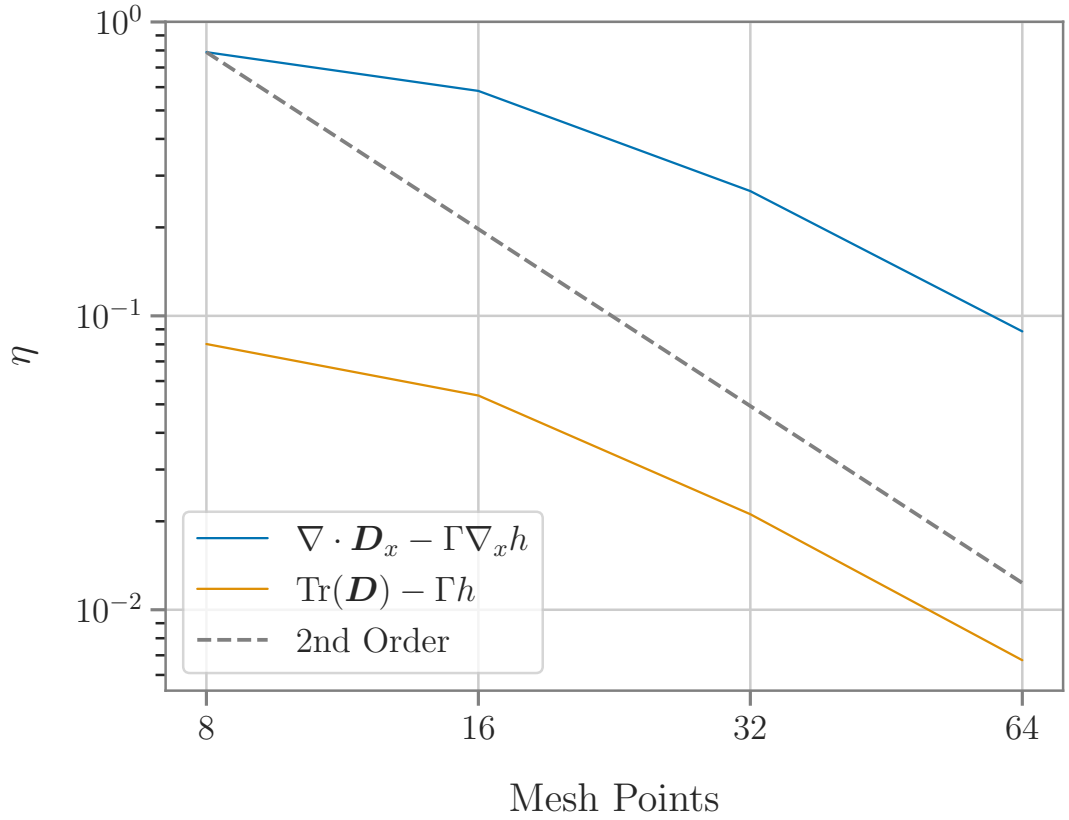

Figure 1: Add missing scaling after computing divergence on [-1,1] (Relative Error: $\eta = \frac{|x_{\text{appr}} - x|}{|x|}$).

Testcase Scaled to DIH Magnitude at Iteration 100

We actually see convergence for Langevin input (HOCKNEY and VICO results are very similar).
Potential causes why coeff.'s are nevertheless too small:

- DIH violates some assumption we make in the derivation of the FP coefficients
- ...

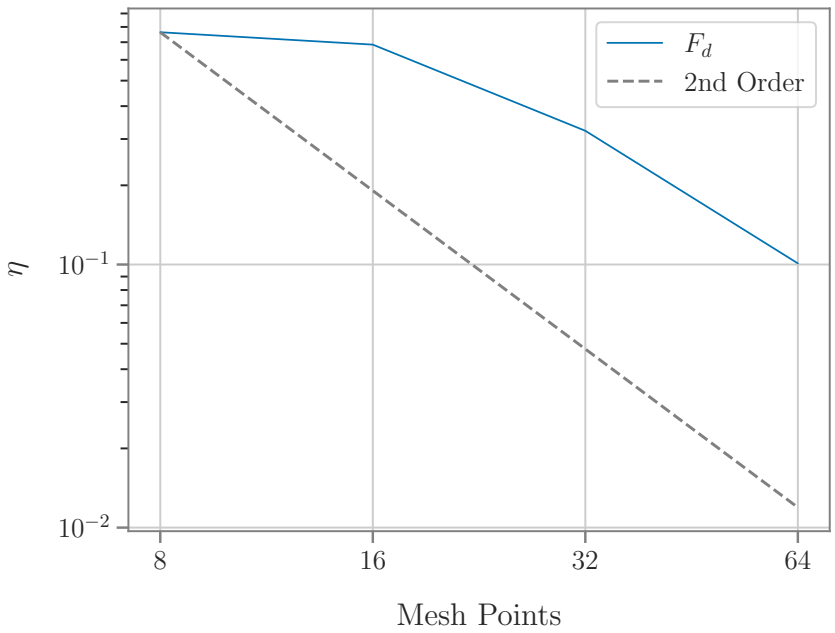

Figure 2: Relative Error Friction Coefficient F_d.

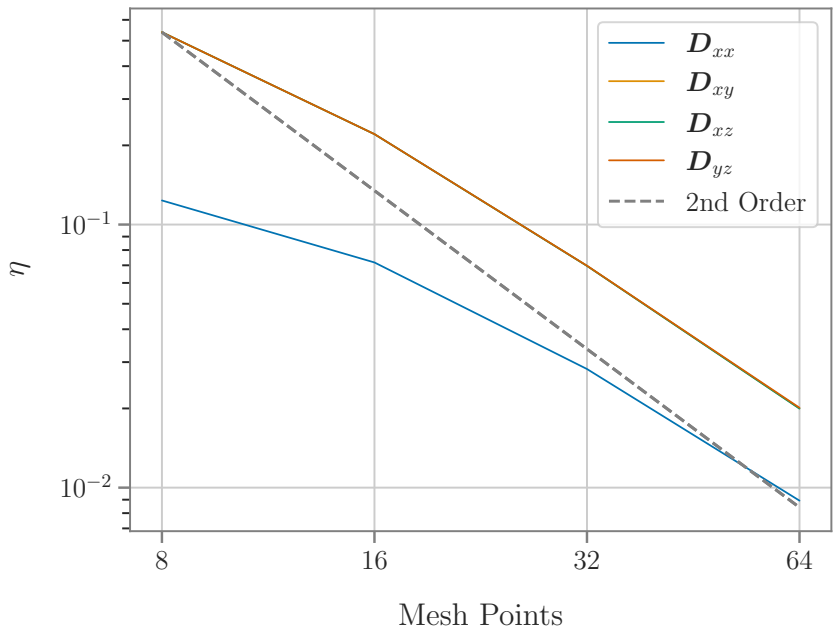

Figure 3: Relative Error Diffusion Matrix $\boldsymbol{D}$.

Charge Density B.C.

- Until now we used periodic b.c.'s for $\rho(\boldsymbol{r})$ since we compared our implementation to Ulmer's
- Open b.c.'s crash as the domain must start at $(0.0)^3$
- All test-cases conform to this, but ours is centered around $(0.0)^3$

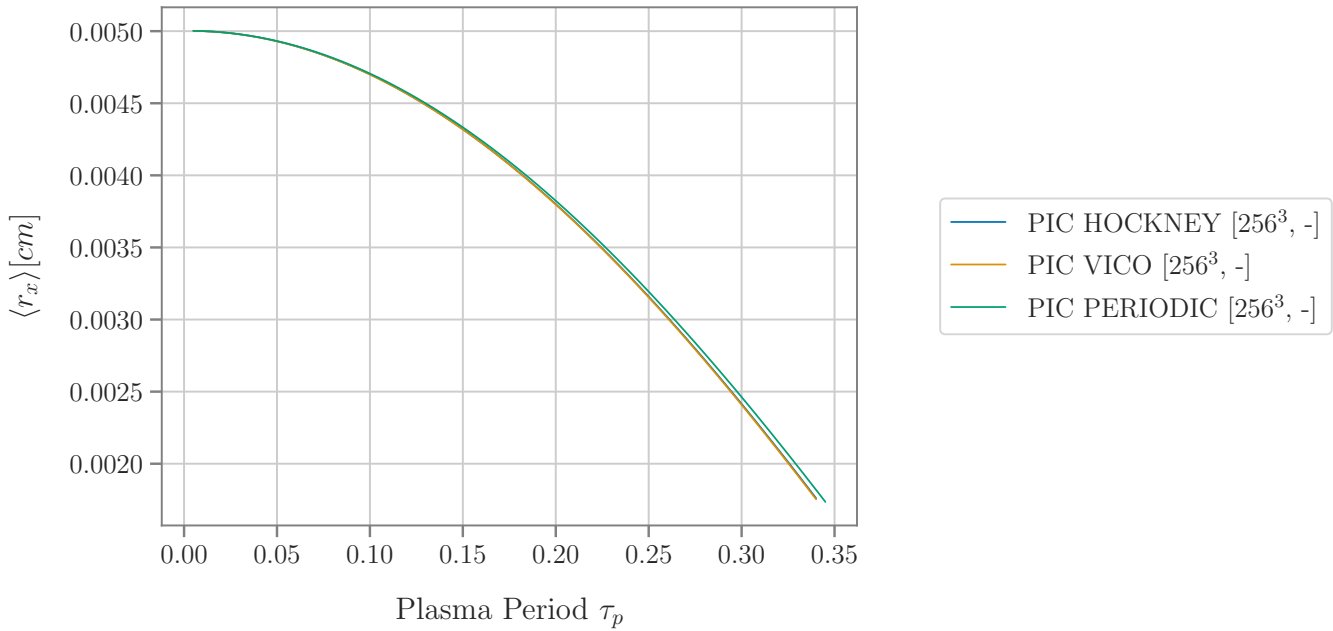

Figure 4: DIH with shifted mesh domain starting at $(0.0)^3$. Sphere moves to origin, causing the simulation to crash.

TODOs

- Continue writing
- [Test performance of E-Field solve for using open b.c. solvers]