

# Molecular Dynamics Simulations

# Jérôme Daligault Applied Math. and Plasma Theory, T-5



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# **Objectives**



Explore the potentially fruitful analogies between Quark-Gluon Plasmas and Warm Dense Matter to provide physical insights and theoretical guidance on the effects of strong coupling on b-jet stopping power phenomenology

**Coulomb coupling strength** 

 $\Gamma = \frac{E_{pot}}{E_{kin}} = \frac{q^2 / a}{k_B T}$ 





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#### **Methods: molecular dynamics**





# Methods: molecular dynamics of dE/dx Los Alamos

Classical Molecular Dynamics

$$\begin{cases} m \frac{d^2 \mathbf{r}_i}{dt^2} = -\nabla_{\mathbf{r}_i} \left[ \sum_{i \neq j} \frac{q^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] - \nabla_{\mathbf{r}_i} \left[ \sum_i \frac{Qq}{|\mathbf{R} - \mathbf{r}_i|} \right] \\ M \frac{d^2 \mathbf{R}}{dt^2} = -\nabla_{\mathbf{R}} \left[ \sum_i \frac{Qq}{|\mathbf{R} - \mathbf{r}_i|} \right] & (1 \le i \le N) \\ + \text{ PBC} \end{cases}$$

- We developed an MD code to perform dE/dx
- We determined viscosity coefficient and location of viscosity minimum
- We are performing extensive parameter study of dE/dx

M/m , Q/q ,  $\Gamma$ 





# Effect of strong coupling on dE/dx



We are developing a theory  $-\frac{dE(V)}{dx} = \frac{mM}{4(m+M)V^2} \int d\vec{v} \frac{F_{MB}(v)}{v} \int_{|v-V|}^{v+V} dv_r v_r^4 \sigma_{tr}(v_r) \left(\frac{M-m}{M+m} + \frac{V^2 - v^2}{v_r^2}\right)$ 

binary collisions including strong coupling effects dynamical dielectric effects neglected

renormalized binary scattering cross section



# Strong coupling vs non-linear effects

### Weak coupling theory breaks down for $\Gamma > 0.1$ but strong coupling effects arise together with non-linear effects



## Summary



 Performed simulations to understand how strong coupling effects affect transport properties and stopping power of plasmas
1<sup>st</sup> milestone met, 2<sup>nd</sup> well underway

- We will now work with DR team members (I. Vitev) to figure out what these findings tell us about QGP's

- Work done in collaboration with 2017 summer student David Bernstein, Univ. of Iowa. David has started a PhD on this topic

- Publications: Phys. Rev. E 96, 043202 (2017) 95, 013206 (2017)
- Manuscript on dE/dx in preparation

- Talks: 2017 APS-DPP (contr.) 2017 White Dwarfs Physics Wkp (invited) Charged Particle Transport Wkp (invited)



