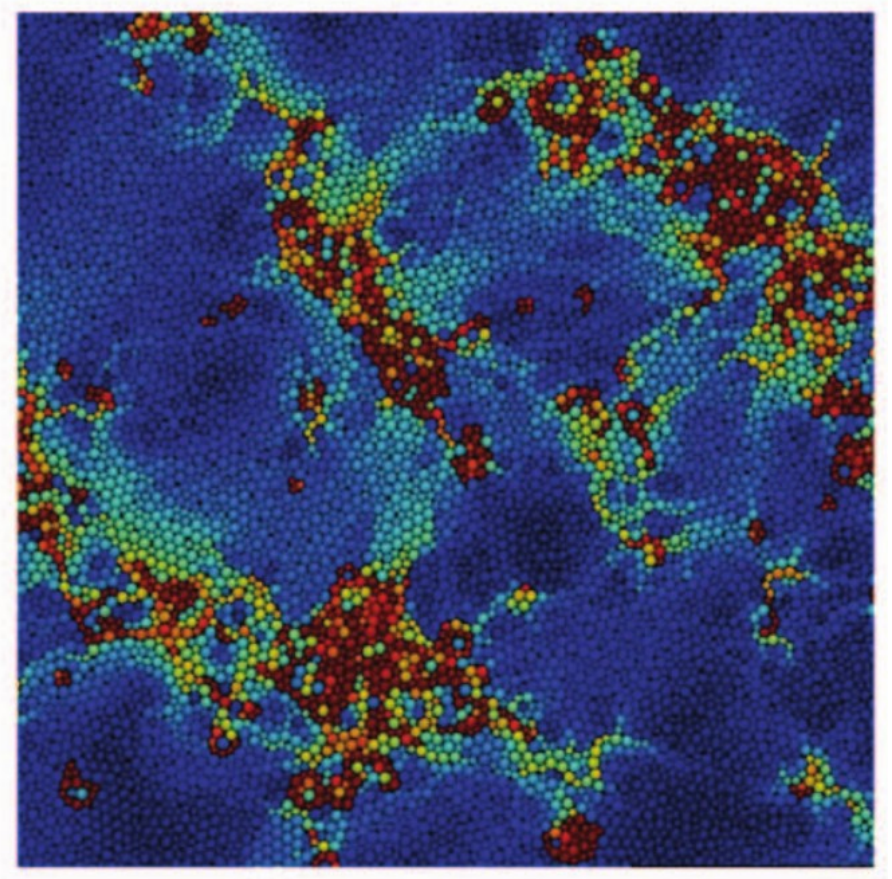

Applying Graph Networks-based Simulators to predict the dynamics of glassy systems

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Supercooled liquids

Slowed-down dynamics upon cooling down without any apparent **structural change**

Studied usually using as a binary system with a **Kob-Andersen** pair-potential

$$V_{ij} = V_{\alpha\beta} = 4\epsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{6} - \left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{12}\right]$$

$$\epsilon_{AA} = 1.0 \qquad \sigma_{AA} = 1.0$$
$$\epsilon_{AB} = 1.5 \qquad \sigma_{AB} = 0.8$$
$$\epsilon_{BB} = 0.5 \qquad \sigma_{BB} = 0.88$$

Machine Learning can help underpinning the structural markers of the glass transition

Physics-based approaches
(with Support Vector Machines or CNN)

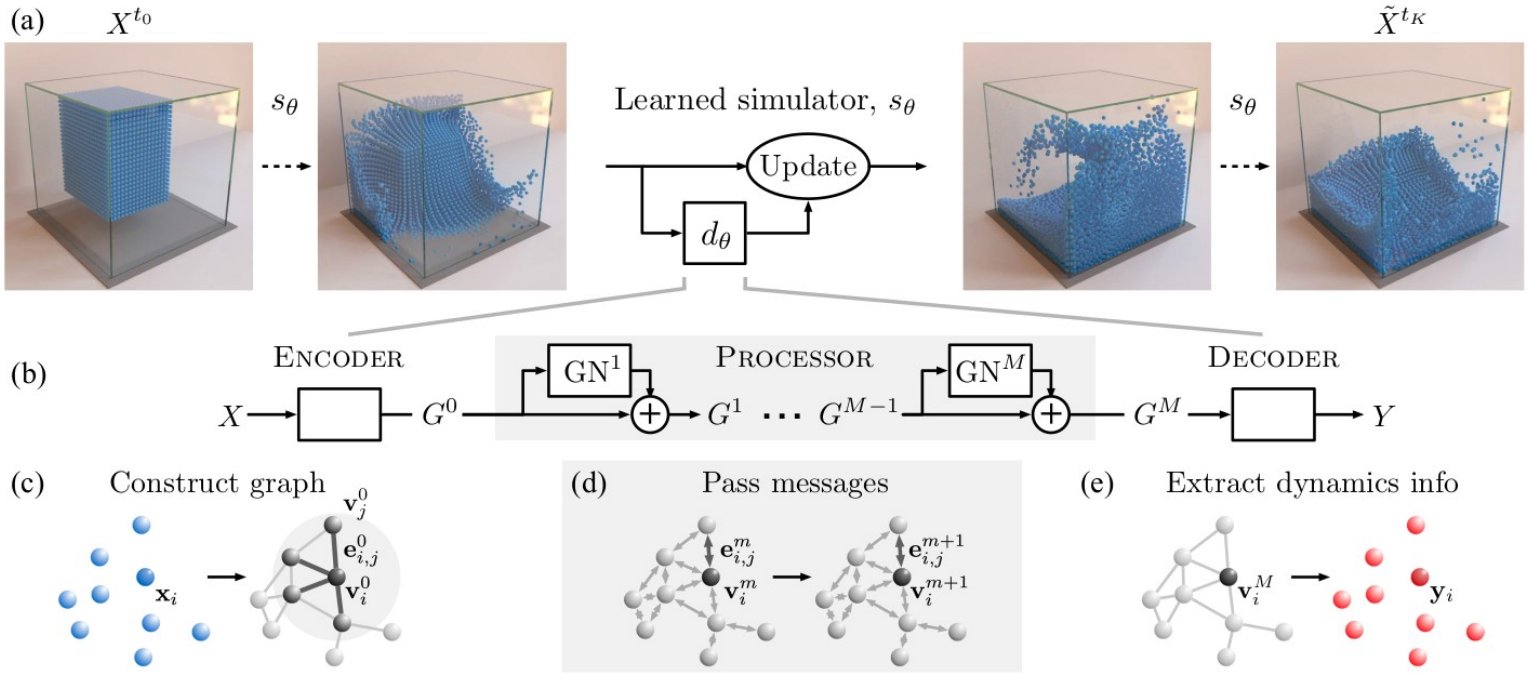
Handcrafted features depending on density and angular information

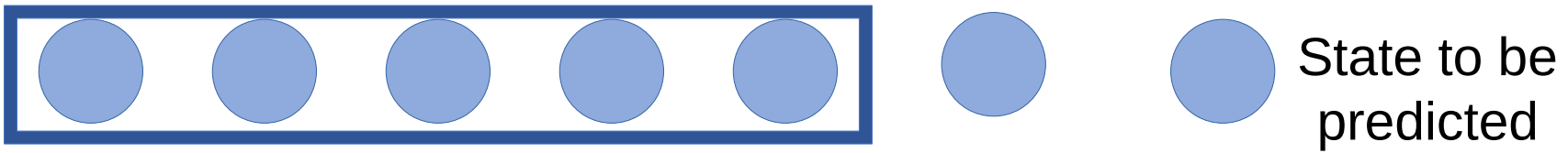
Graph Networks
(Interaction Networks)

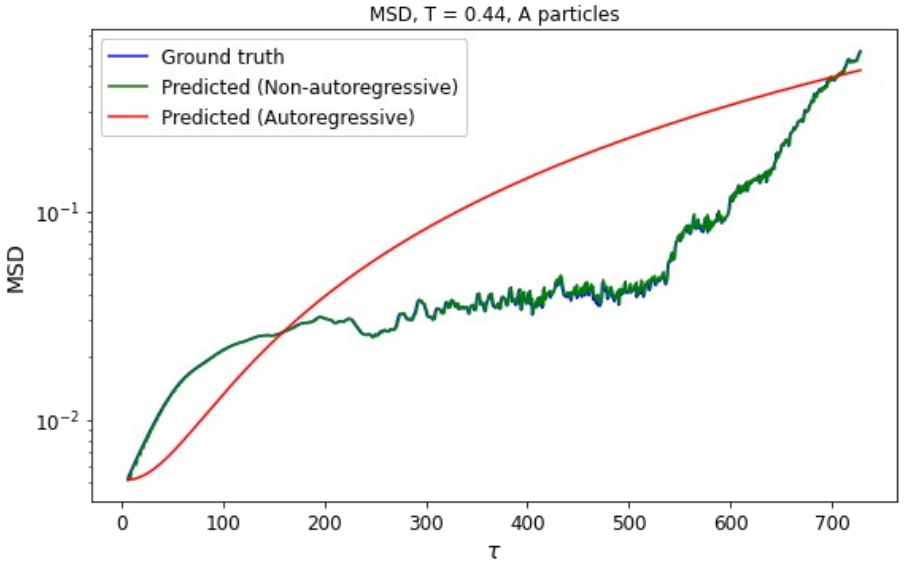
Takes particle positions as part of the input

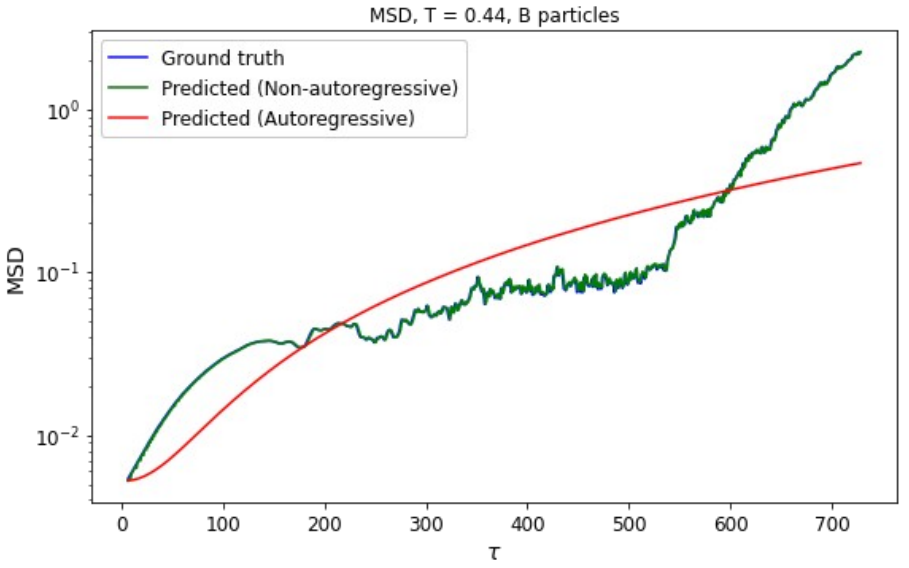
Can encode Object and Relational reasoning

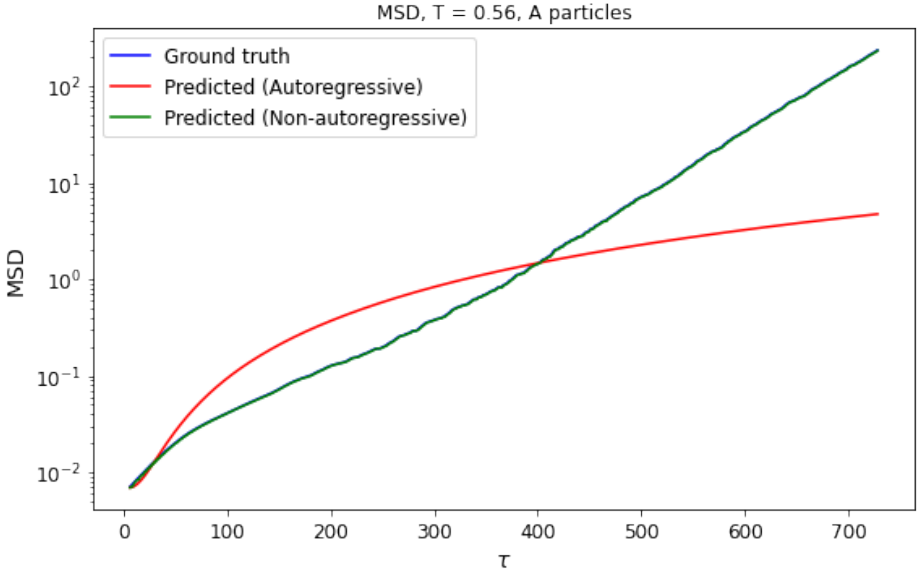
Graph Networks-based Simulators

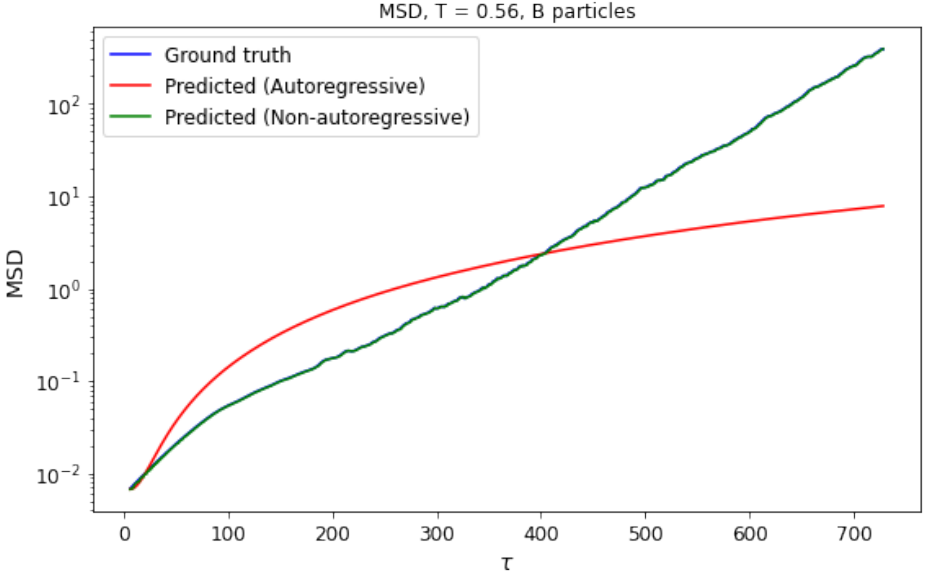





MSD, T = 0.44, A particles
Ground truth
Predicted (Non-autoregressive)
Predicted (Autoregressive)
MSD
τ


MSD, T = 0.44, B particles
Ground truth
Predicted (Non-autoregressive)
Predicted (Autoregressive)
MSD
τ


MSD, T = 0.56, A particles
Ground truth
Predicted (Autoregressive)
Predicted (Non-autoregressive)
MSD
τ


MSD, T = 0.56, B particles
Ground truth
Predicted (Autoregressive)
Predicted (Non-autoregressive)
MSD
τ

Areas of improvement

Towards a ‘physics-informed model’

Adapting hyperparameters (connectivity radius) to consider long-range interactions

Improving the noise given to the input

Changing the update mechanism (higher order)

Improving the expressivity

Improving our data: more simulations and longer trajectories

Bigger batch size

Complete hyperparameters study, making a deeper model

References

[1] Alvaro Sanchez-Gonzalez et al., **Learning to Simulate Complex Physics with Graph Networks**, 2020, https://arxiv.org/abs/2002.09405

[2] V. Bapts, T. Keck, A. Grabska-Barwińska, et al., **Unveiling the predictive power of static structure in glassy systems**, In *Nat. Phys.,* 16 (2020), https://doi.org/10.1038/s41567-020-0842-8

[3] Katharina Vollmayr-Lee, **Introduction to molecular dynamics simulations**, in *American Journal of Physics* (May 2020), https://doi.org/10.1119/10.0000654