Future Prediction in Brownian Dynamics Simulations Using Deep Neural Networks

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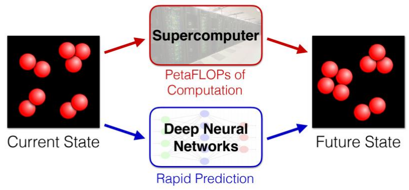
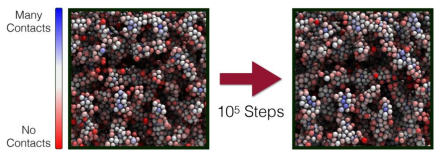
Motivation

- Scientists utilize molecular dynamics (MD) and Brownian dynamics (BD) to study dynamic or non-equilibrium properties of materials.[1]
- The principle challenge of MD/BD simulations is the prohibitive computational cost to simulate phenomena that occur at long time scales.
- The goal is to predict the future states of simulations using deep neural networks and bypass explicit computation of every time step:



Data & Features

- 14,400 simulation trajectories — list of particle positions (x,y,z) at a given time step — generated using the LAMMPS Molecular Dynamics Simulator.[2]
- Simulation undergoes slow arrested phase separation with different system parameters (volume fraction and interparticle attraction strength).[3]

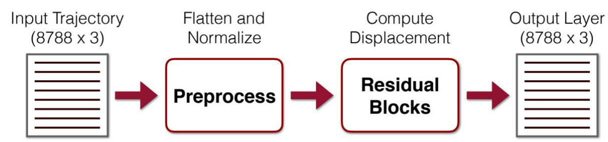


Images rendered from simulation snapshots undergoing slow phase separation, separated by 10^5 time steps. Particle colors indicate number of contacts

- Each input and output snapshot contains (x, y, z) positions of 8,788 particles: i.e. 26,364 floating point numbers.
- Particle motion is mildly stochastic and largely deterministic; particles with few contacts are free to diffuse while particles with many contacts move less.

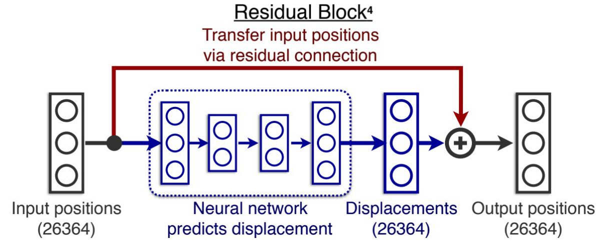
Model

Model Architecture



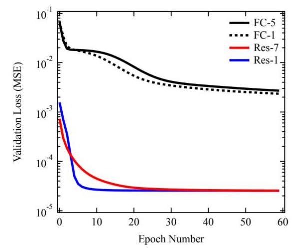
- Mean-squared error (MSE) for loss function.
- Use Adam optimizer with L2 regularization.
- Scan over architectures and hyperparameters.

Residual Block[4]



Results

- Our model accurately predicts particle positions with small MSE.
- Residual networks result in significantly smaller loss compared to simple plain networks with only fully connected layers.



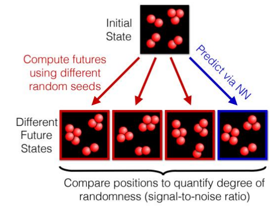
	Mean-Squared Error		
	Training	Validation	Test
FC-1	2.41E-03	2.35E-03	2.34E-03
FC-5	2.81E-03	2.71E-03	2.74E-03
Res-1	2.61E-05	2.55E-05	2.48E-05
Res-3	2.60E-05	2.55E-05	2.48E-05
Res-5	2.60E-05	2.56E-05	2.49E-05
Res-7	2.60E-05	2.55E-05	2.48E-05

Plain (fully connected) Nets: FC-(# of Layers)
Residual Nets: Res-(# of Residual Blocks)

Discussion and Conclusions

Bayes Error Quantification

- Different random seeds in simulations result in different realizations of future states.
- Mean-squared difference of particle positions are compared across simulated and predicted outcomes.



	Mean-Squared Error	
	Mean	SD
Simulations	1.90E-05	8.90E-06
Res-7	2.48E-05	1.11E-05

- Residual networks are able to predict future positions with randomness comparable to actual simulations

- L2 regularization (λ = 0.0001) suppresses overfitting.
- Learning rate α = 0.00005, achieves slow training but small loss.
- Batch size 512 achieves a balance of speed and performance.
- Residual block size with 3 fully-connected hidden layers each with O(1000) neurons provide accurate displacement predictions.

Conclusions and Future Work

- Successfully developed a deep neural network for predicting future states in Brownian Dynamics simulations.
- Utilizing a residual network structure to focus on displacement significantly improves performance.
- Future work should visualize and interpret what and how each residual block is computing displacements.
- Future work should extend current architecture for variable number of particles.

Acknowledgements and References

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[1] Chen, Jim C., and Albert S. Kim. "Brownian dynamics, molecular dynamics, and Monte Carlo modeling of colloidal systems." Advances in colloid and interface science 112.1-3 (2004): 159-173.

[2] Erban, Radek. "From molecular dynamics to Brownian dynamics." Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 470.2167 (2014): 20140036.

[3] Zia, Roseanna N., et al. "A micro-mechanical study of coarsening and rheology of colloidal gels: Cage building, cage hopping, and Smoluchowski's ratchet." Journal of Rheology 58.5 (2014): 1121-1157.

[4] He, Kaiming, et al. "Deep residual learning for image recognition." Proceedings of the IEEE conference on computer vision and pattern recognition. 2016.