

Discovering Optimal Observables for Inverse Design of Anisotropic Pair Potentials

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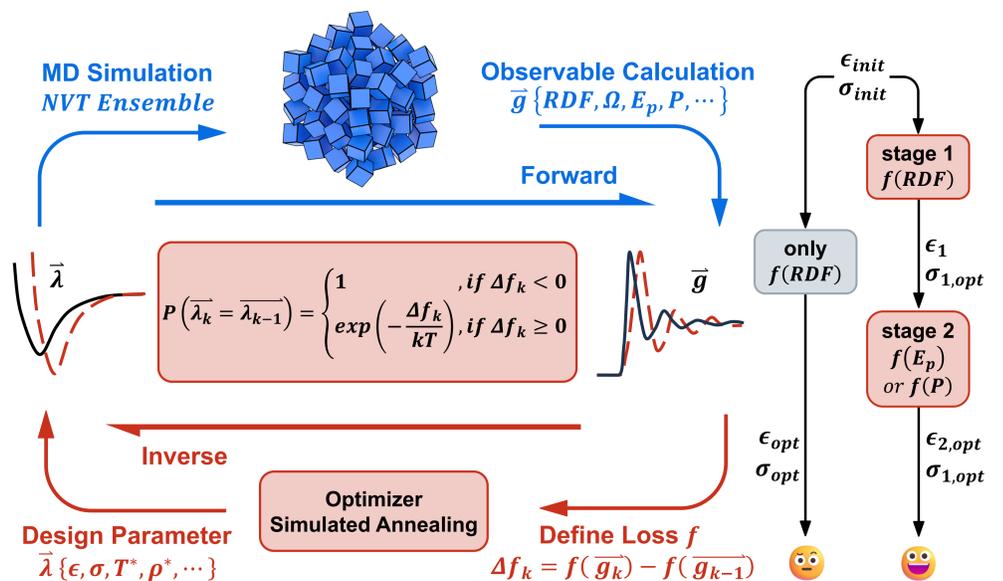
Motivation

- **Inverse design** can deduce interaction potentials from self-assembled structures [1], but the **choice of observables** remains the critical bottleneck for effective parameter recovery.
- **Goal:** leverage Molecular Dynamics (MD) simulations to identify generalizable observables, which can effectively recover the parameters of the **Anisotropic Lennard-Jones (ALJ)** potential [2].

Implementation Details

- **System:** 512 anisotropic 2D particles; MD via HOOMD-blue [3].
- **Inversion:** global optimization via Dual Annealing (SciPy) [4].
- **Observables:** radial distribution function (RDF), potential energy E_p , pressure P .
- **Validation Protocols** (for various particle geometry):
Single-parameter (σ): $T^* = 1.1$; $\epsilon = 1.0$ [energy]; $\rho^* \in \{0.4, 0.6\}$.
Multi-parameter (ϵ, σ): $T^* = 1.1$; $\rho^* = 0.4$.

Methodology



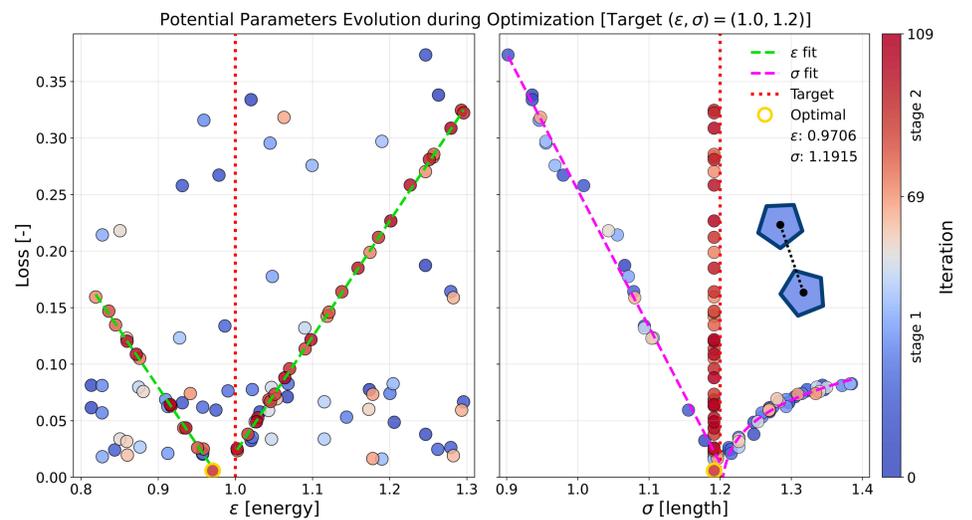
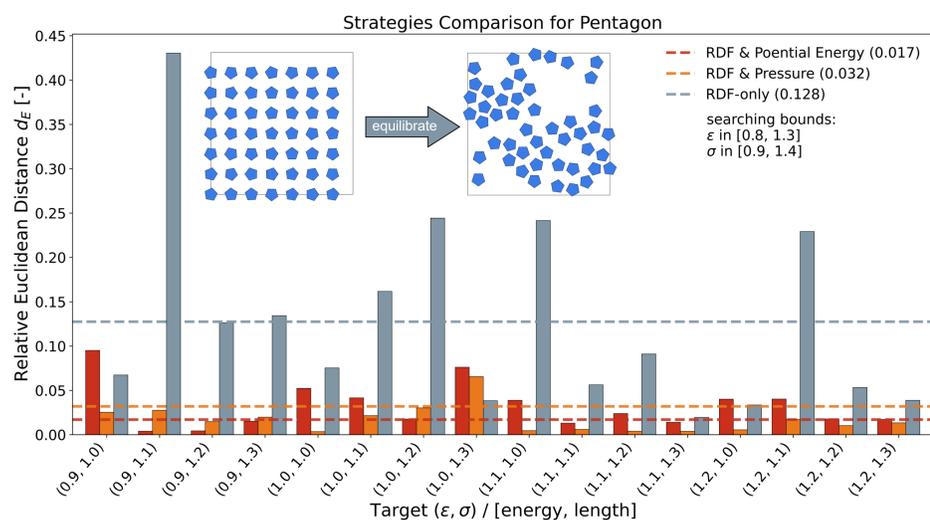
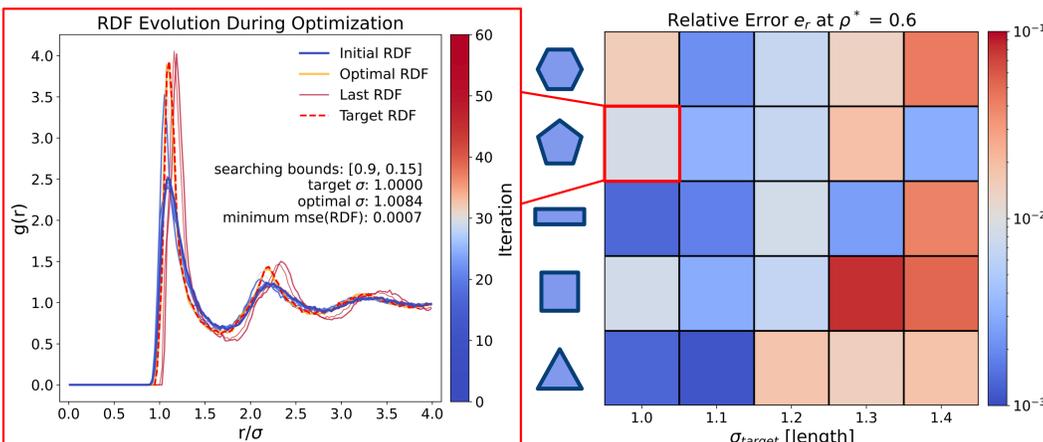
Results & Discussion

Effectiveness of RDF

- The relative error e_r between optimal and target σ is smaller than 2% in 21 out of 25 cases.
- Larger interaction distances σ lead to greater relative errors e_r .

Optimization Strategies Comparison

- Relative Euclidean distance $d_E = \|(\widehat{\delta}_\epsilon, \widehat{\delta}_\sigma)\|_2$ as the metric of fitness of an optimization strategy.
- Better to treat ϵ and σ separately with 2 observables, having one order magnitude smaller average d_E than with only RDF.



Conclusions

- RDF is an effective observable for determining distance-related parameters in the ALJ pair potential.
- Analyze the sensitivity of pair potential parameters to observables, and develop optimization strategies accordingly.

Outlook

- Capture the feedback from all observables simultaneously with other advanced multi-objective optimization algorithms.
- Focus on energy-related while experimentally accessible observables, e.g. enthalpy of vaporization or work of adhesion, etc.

Literature:

- [1] Sherman, Z. M., et al. J. Chem. Phys. 2020, 152 (14), 140902.
[2] Ramasubramani, V., et al. J. Chem. Phys. 2020, 153 (8), 084106.
[3] Anderson, J. A., et al. Comput. Mater. Sci. 2020, 173, 109363.
[4] Virtanen, P. et al., Nat. Methods 2020, 17 (3), 352-352.