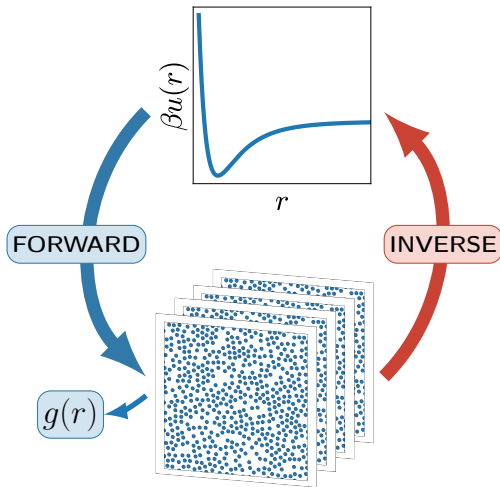**D. Paolino**, O. Coquand, L. Berthier

A simulation-free Boltzmann inversion method

Forward (Usual Statistical Mechanics)
From Hamiltonian to macroscopic behavior.
Validated via direct numerical simulations.
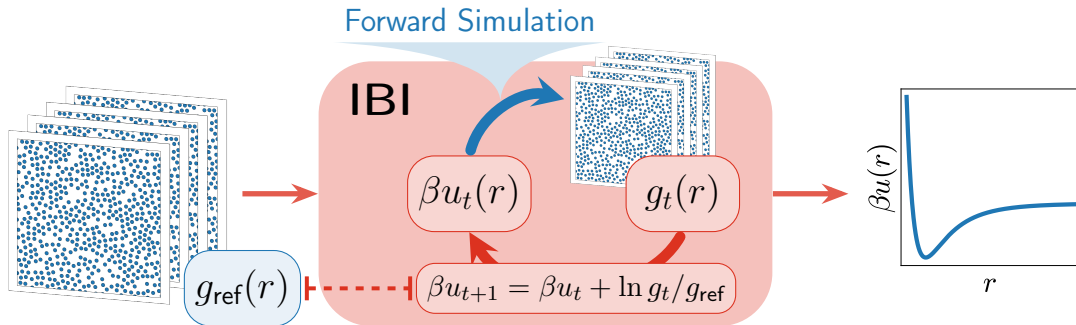
Inverse Approach
From configurations to potential.

- No exact solutions for $N > 2$.
- Numerical methods require multiple simulations.

Iterative Boltzmann Inversion (IBI)

Observable: $g(r) = \frac{1}{\rho N} \sum_{i<j} \langle \delta(r - r_{ij}) \rangle \iff \beta u(r).$

Bottleneck: Each iteration demands a full forward simulation.

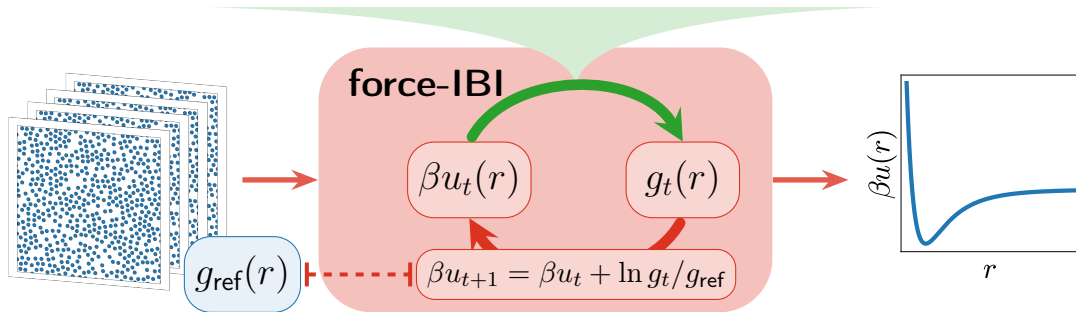- Expensive CPU time
- Expensive SSD space

W. Schommers, A pair potential for liquid rubidium from the pair correlation function, Physics Letters A 43, 157 (1973).
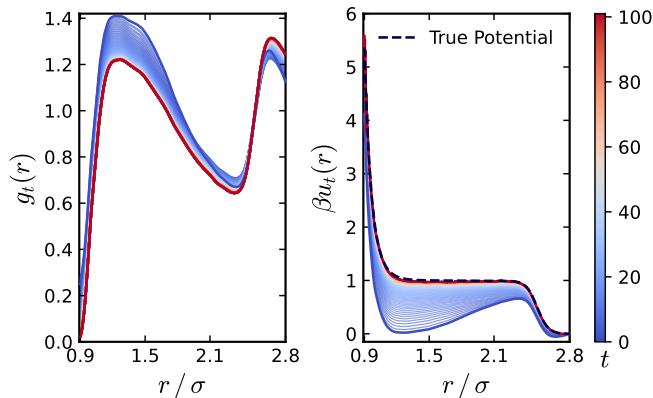
New simulation-free method: force-IBI

Idea: Integrate by parts $g(r) = \frac{1}{\rho N} \sum_{i<j} \langle \delta(r - r_{ij}) \rangle$ with $\frac{\partial}{\partial r_{ij}} e^{-\beta U}$ and $\int \mathrm{d}r_{ij} \delta(r - r_{ij})$:

$$g(r) = \frac{1}{\rho N} \sum_{i<j} \left\langle \frac{\mathbf{r}_{ij}}{\Omega_d r_{ij}^d} \cdot \beta(\mathbf{f}_i - \mathbf{f}_j)\theta(r_{ij} - r) \right\rangle$$

force-IBI

$\beta u_t(r)$ $g_t(r)$

$g_{\mathsf{ref}}(r)$ $\beta u_{t+1} = \beta u_t + \ln g_t / g_{\mathsf{ref}}$

$\beta u(r)$ r

Improvements: Inversion can be performed by averaging on the input configurations.

Tests: Recover potential shapes from simulated configurations.

Results:

- Accurate reconstruction of all test profiles.
- Convergence in < 30 seconds on standard hardware.
- Ready to be applied to any set of configurations.

Slides and article (in preparation) at: https://paolinodavide.github.io