Thermodynamic Field Estimator: $\{\mathbf{x}_i, \mathbf{v}_i\} \rightarrow \{\rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x})\}$

Basic Assumption: At any moment, there exist continuous, slowly-varying thermodynamic fields $\{\rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x})\}$, and atoms conform to certain single-particle distribution

$$dP = f\left(\mathbf{x}, \mathbf{v} | \rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x})\right) d\mathbf{x} d\mathbf{v}.$$

Inverse Problem: Given a set of particle data, $\{\mathbf{x}_i, \mathbf{v}_i\}, i = 1..N$; how can one determine the "actual" set of continuous fields?

Usual Approach: Divide the cell into bins and average over each bin.

Shortcomings: Neglect **intrinsic spatial coherency** of particle data, given by the belief that the "actual" fields are **continuous** and **slowly-varying**.

Maximum Likelihood Inference:

Given particle data, the "most probable" fields are which that maximizes the total probability,

$$P = \prod_{i=1}^{N} f\left(\mathbf{x}_i, \mathbf{v}_i | \rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x})\right).$$

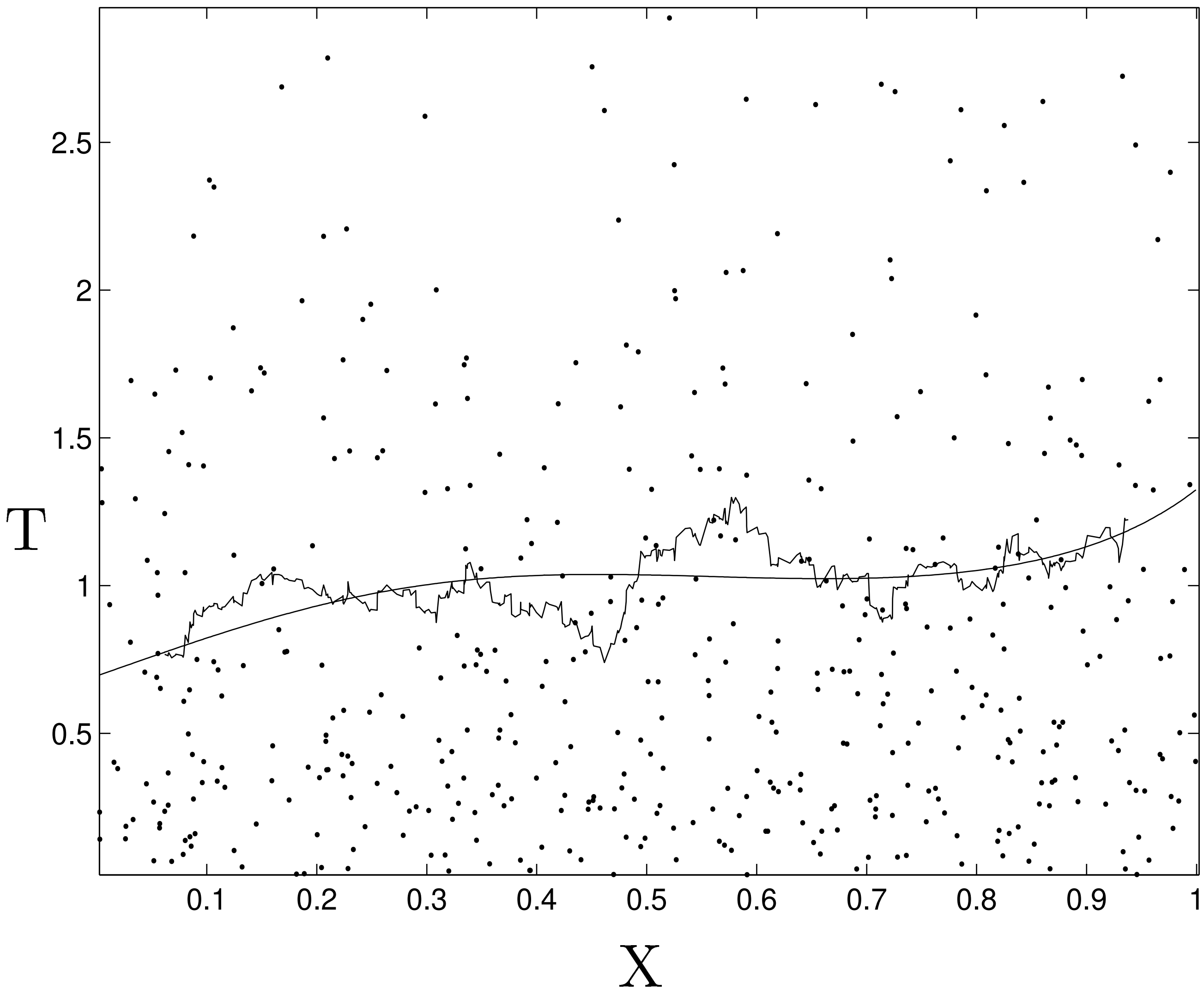
- Basis expansion of target fields in **low-order** Chebyshev polynomials (equivalent to assigning "priors" to fields with small spatial gradients).
- Conjugate gradient optimization of basis coefficients; two-step relaxation procedure.

– Continuous and slowly varying;   obtaining analytical forms

– "Maximal" utilization of given information

– Value at any point depends on all data (holographic)

– More expensive



Example **1**: Snapshot during a thermal conduction MD simulation. Dots are individual atom kinetic energies; zigzag line is from $w = 0.12$ sliding-bin average; smooth curve is by 4th-order TFE.