

# A micro-macro acceleration method for the Monte Carlo simulation of SDEs

K. Debrabant, G. Samaey and P. Zieliński

University of Southern Denmark and University of Leuven

#### Goals:

- 1. accelerate weak simulation of SDEs with fast micro-dynamics and slow evolution of observables
- 2. investigate the assumptions underlying the method and the quality of the resulting approximations

## Coarse Projective Integration

Framework to extrapolate the long time dynamic behavior of multiscale systems using appropriately initialized microscopic simulation on short time-scales

#### Lifting

Create ensemble of initial micro-states consistent with current macro-state

#### ■ Simulation

Run the micro solver with initial data for short macroscopic time

#### **■** Restriction

Compute a number of macro-states (averaging) to approximate the time derivative of macro-states

Idea: maximally exploit the information that is present in a (prior) microscopic state available from the previous instance of Coarse Projective Integration

Matching – Alternative for Lifting

#### Methodology

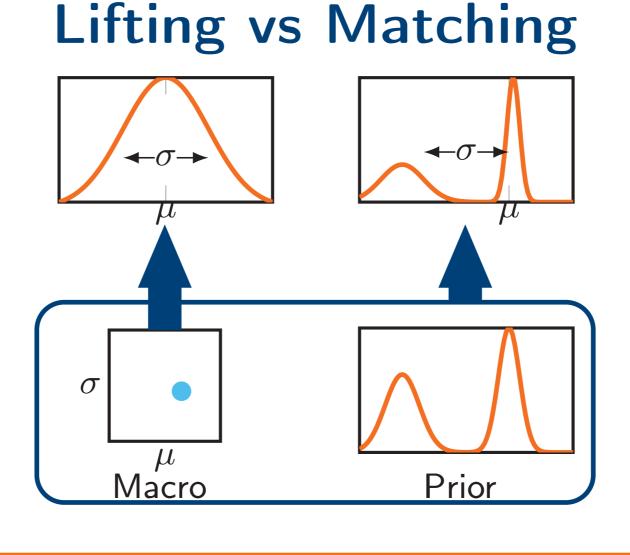
Search for minimal perturbation of prior state consistent with current macro-state

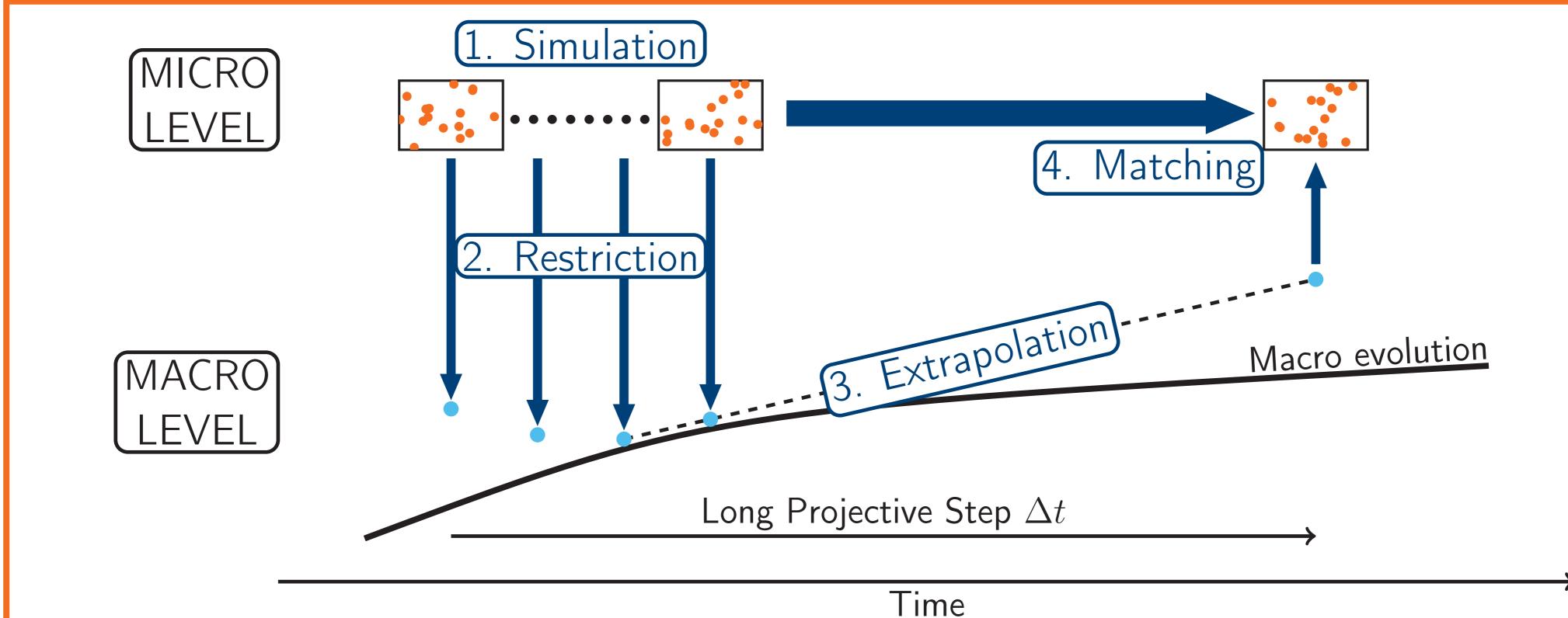
#### Advantage

Avoids numerical modeling error associated with Lifting

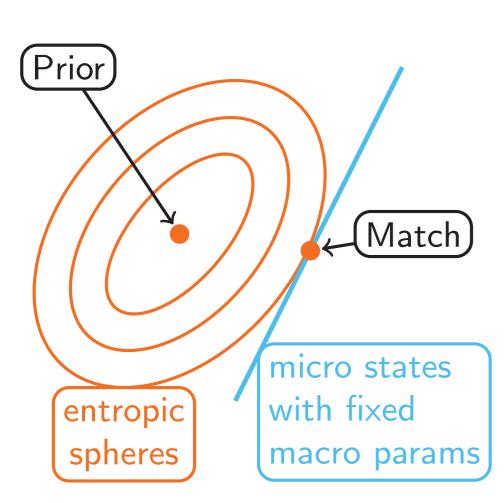
#### Analysis

Prove weak convergence to full microscopic dynamics





## Matching via Entropy Optimization



 $L^p$  norm:

$$\mathcal{I}(\phi|\pi) = \frac{1}{p} \int |\phi - \pi|^p$$

Logarithmic entropy:

$$\mathcal{I}(\phi|\pi) = \int \phi \log \frac{\phi}{\pi}$$

Hellinger distance:

$$\mathcal{I}(\phi|\pi) = \int (\sqrt{\phi} - \sqrt{\pi})^2$$

## Convergence for $L^2$ norm

Crucial components for analysis:

#### ■ hierarchy of macro-states

- $\rightarrow$  parametrized by the number of variables L
- ightarrow uniquely determines the micro-states as  $L
  ightarrow\infty$

#### consistency of matching

ightarrow bounds the matching error as  $\mathcal{O}(\Delta t/L)$ 

Global Weak Error  $\sim \mathcal{O}(1/L + L \cdot \Delta t)$ 

### **Proof and example with FENE dumbbells:**

K.Debrabant, G.Samaey, P.Zielinski, (2015) arXiv:1511.06171

