Rare event sampling with

FRESHS

11.10.2012

Kai Kratzer[1]

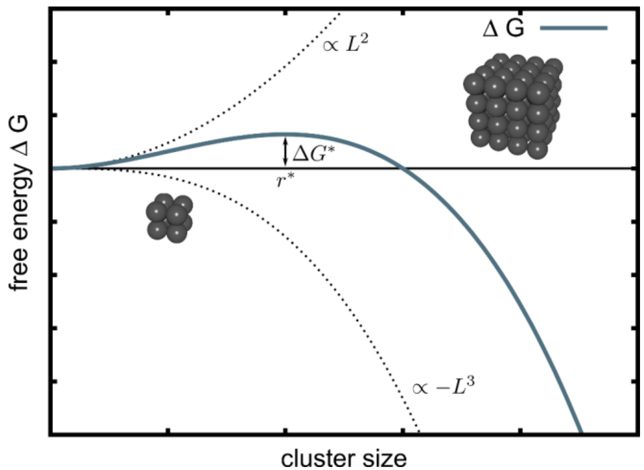
[1]Institute for Computational Physics, University of Stuttgart

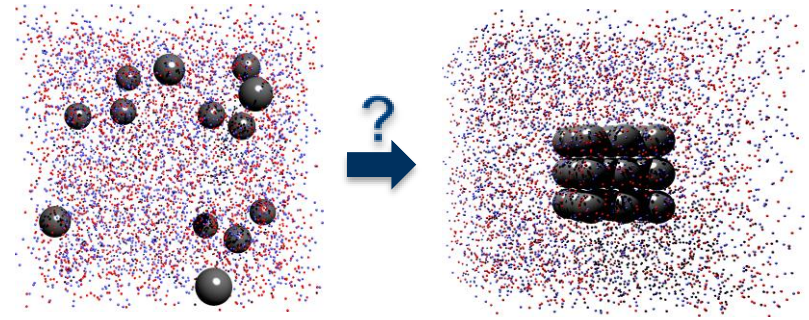
Outline

- Intro: Rare events & sampling methods overview
- Forward flux sampling (FFS)
- Stochastic process rare event sampling (S-PRES)
- Harness System (FRESHS)
- Conclusion

Rare Events: Examples

- Crystallization of charged macromolecules





Clusters smaller than a critical nucleus size are more likely dissolved than they continue to grow!

$$\Delta G = -\Delta G_V + \Delta G_S = -\mu\rho\frac{4}{3}\pi L^3 + 4\pi\sigma L^2$$

CNT: bulk term and surface term

→ **Long time scales**, **many particles:** Does not crystallize in available computation time

→ Computationally very expensive task, only few, if any, events are observed in a conventional simulation run

→ Rare event

- Macroscopic: Earthquakes, financial crashes, telecommunication failures
- Microscopic: Activated chemical reactions, protein folding, translocation of DNA through nanopores

Simulating rare events – methods overview

- Many rare event sampling methods have been developed recently [1], e.g.
  - Bennet-Chandler/reactive flux methods based on the transition state theory (TST)
  - Transition path sampling (TPS) and transition interface sampling (TIS)
  - Milestoning
  - The weighted ensemble method
  - The finite temperature string method (FTS)

equilibrium

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equilibrium and nonequilibrium

  - …
  - Forward flux sampling (FFS)
  - Stochastic process rare event sampling (S-PRES) [2]

[1] R. J. Allen, Ch. Valeriani, P. R. ten Wolde, J. Phys: Condens. Matter **21** 463102 (2009)
[2] J. T. Berryman and T. Schilling, J. Chem. Phys. **133**, 244,101 (2010)

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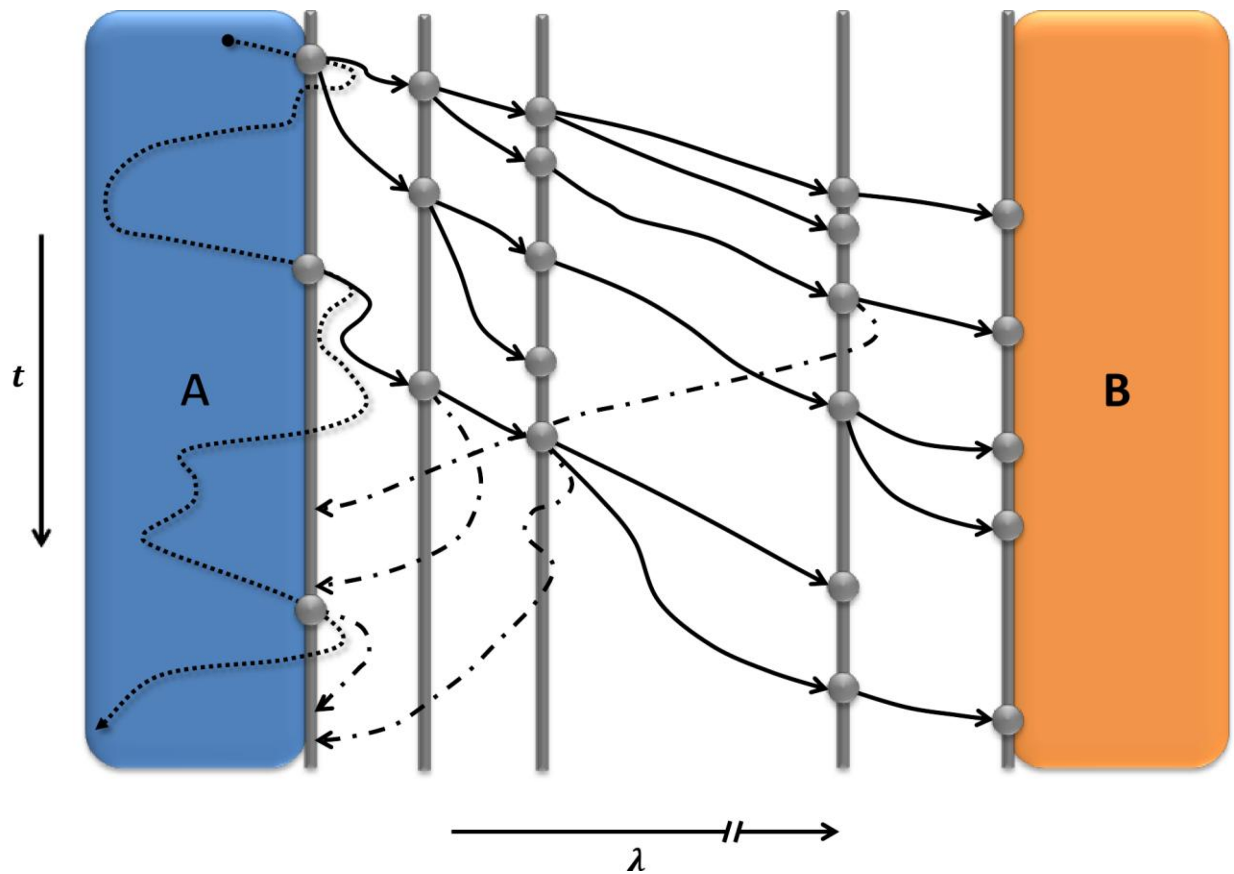
Forward Flux Sampling (FFS)

R. J. Allen, Ch. Valeriani, P. R. ten Wolde, J. Phys: Condens. Matter **21** 463102 (2009)

- Rare event: **Spontaneous**, **fluctuation-driven** transition



- Transition rate

$$k_{AB} = \Gamma e^{-\beta \Delta G^*}$$

- Arrhenius equation
- kinetic pre-factor Γ
- $\beta = 1/k_B T$

Forward Flux Sampling

- Escape flux: $$\frac{\overline{\Phi}_{A,0}}{\overline{h}_A} = \frac{\text{number of configurations at } \lambda_0}{\text{total simulation time}}$$
- Conditional probabilities: $$P(\lambda_n|\lambda_0) = \prod_{i=0}^{n-1} P(\lambda_{i+1}|\lambda_i)$$
- Transition rate: $$k_{AB} = \frac{\overline{\Phi}_{A,n}}{\overline{h}_A} = \frac{\overline{\Phi}_{A,0}}{\overline{h}_A} P(\lambda_n|\lambda_0)$$
- Advantage: $$P(\lambda_{i+1}|\lambda_i) \gg P(\lambda_n|\lambda_0)$$
  ➔ Much easier to sample than the whole process!
- FFS:
  Equilibrium and **nonequilibrium** systems with stochastic dynamics, **quasistatic**

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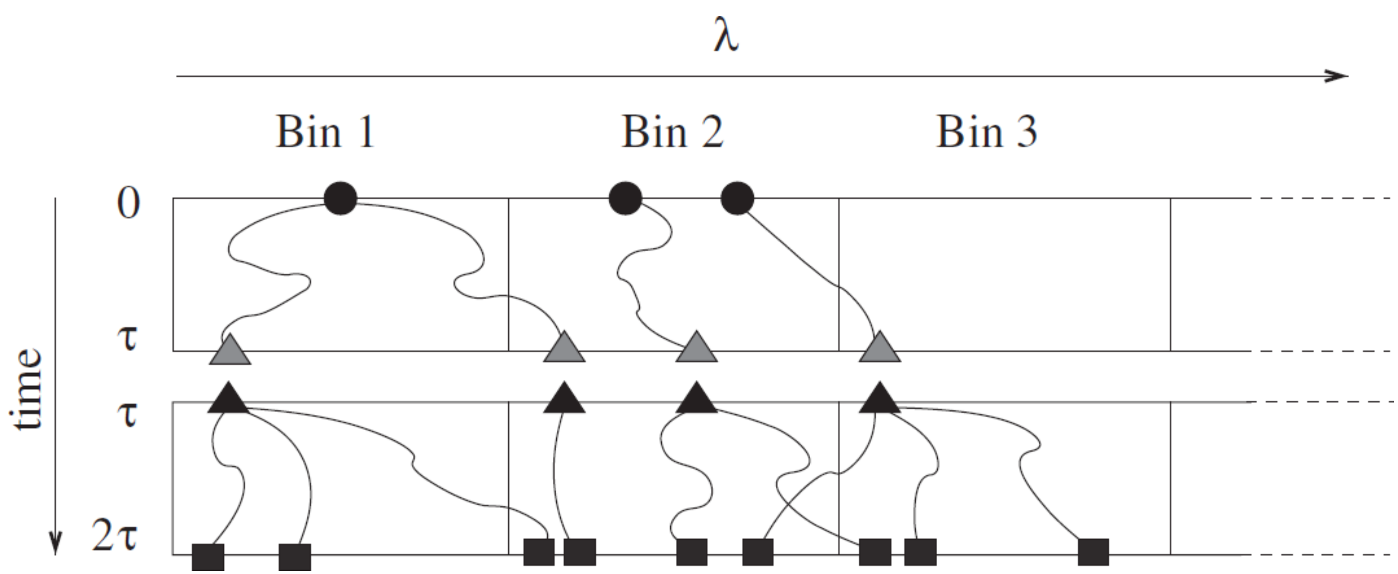
Stochastic Process Rare Event Sampling (S-PRES)

J. T. Berryman and Tanja Schilling, J. Chem. Phys. **133**, 244101 (2010)

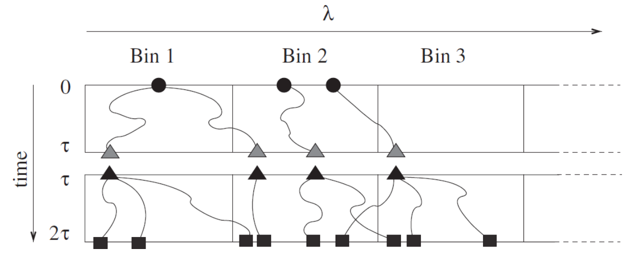
- Focus on calculating the **time-series** of the probability of a rare event
- Phase space binning instead of hypersurfaces
- Reaction coordinate λ, trajectory paths similar to FFS
- Now: Each trajectory fragment (shot) has a fixed duration for tracking the time evolution



Path generation: Symbols represent configurations, lines represent path segments of duration τ.

Stochastic Process Rare Event Sampling (S-PRES)

- Rosenbluth sampling is used to ensure dynamically adaptive sampling rates in the bins
- Fixed bins
  ➔ Time-dependent matrix of transition frequencies
  ➔ Extraction of observables and statistics



- S-PRES:
  Nonequilibrium and **nonstationary** systems with macroscopically **irreversible dynamics** and away from both stationary and metastable states
- Examples of events: quenching, aging, ignition, impact

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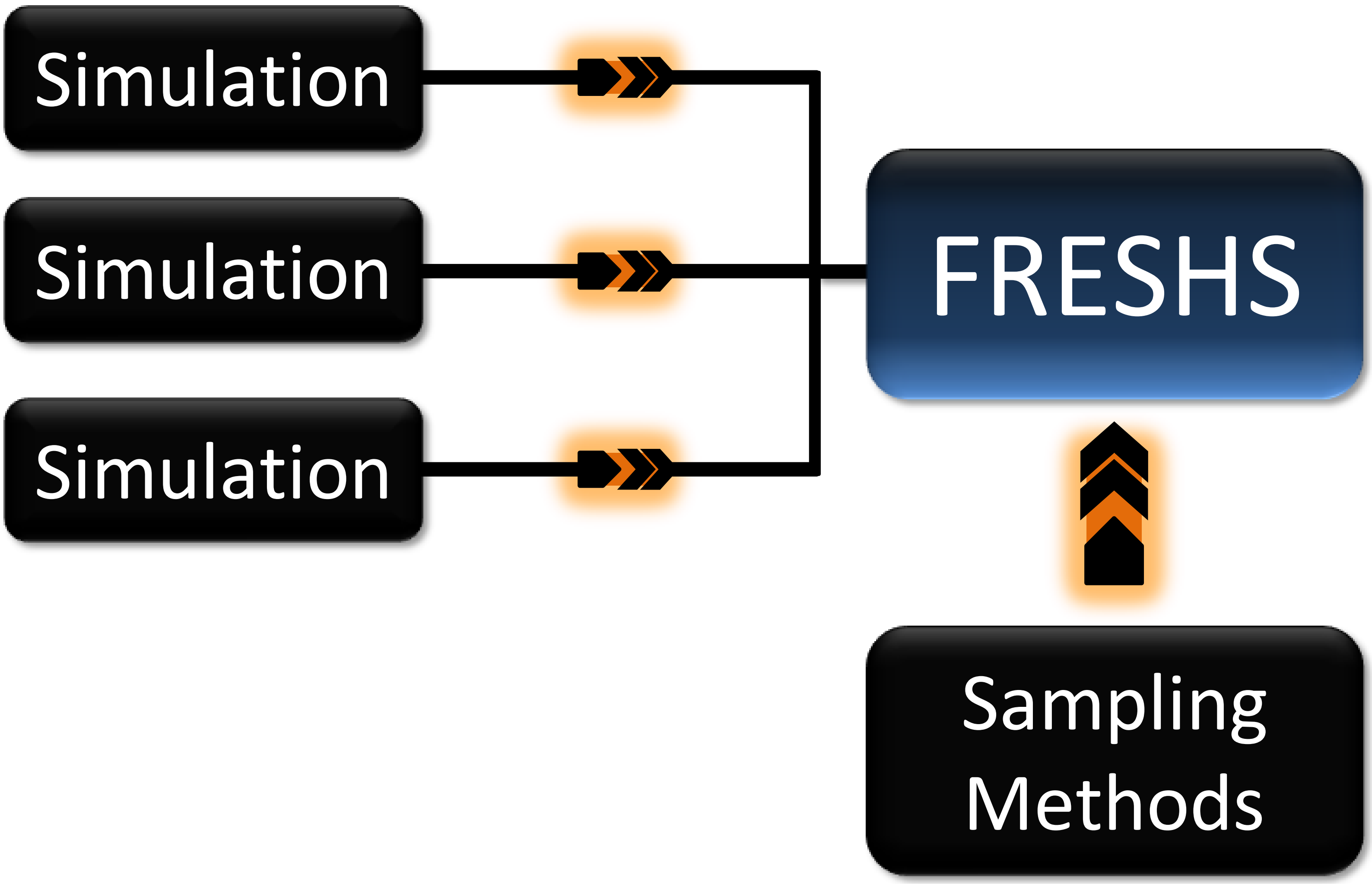
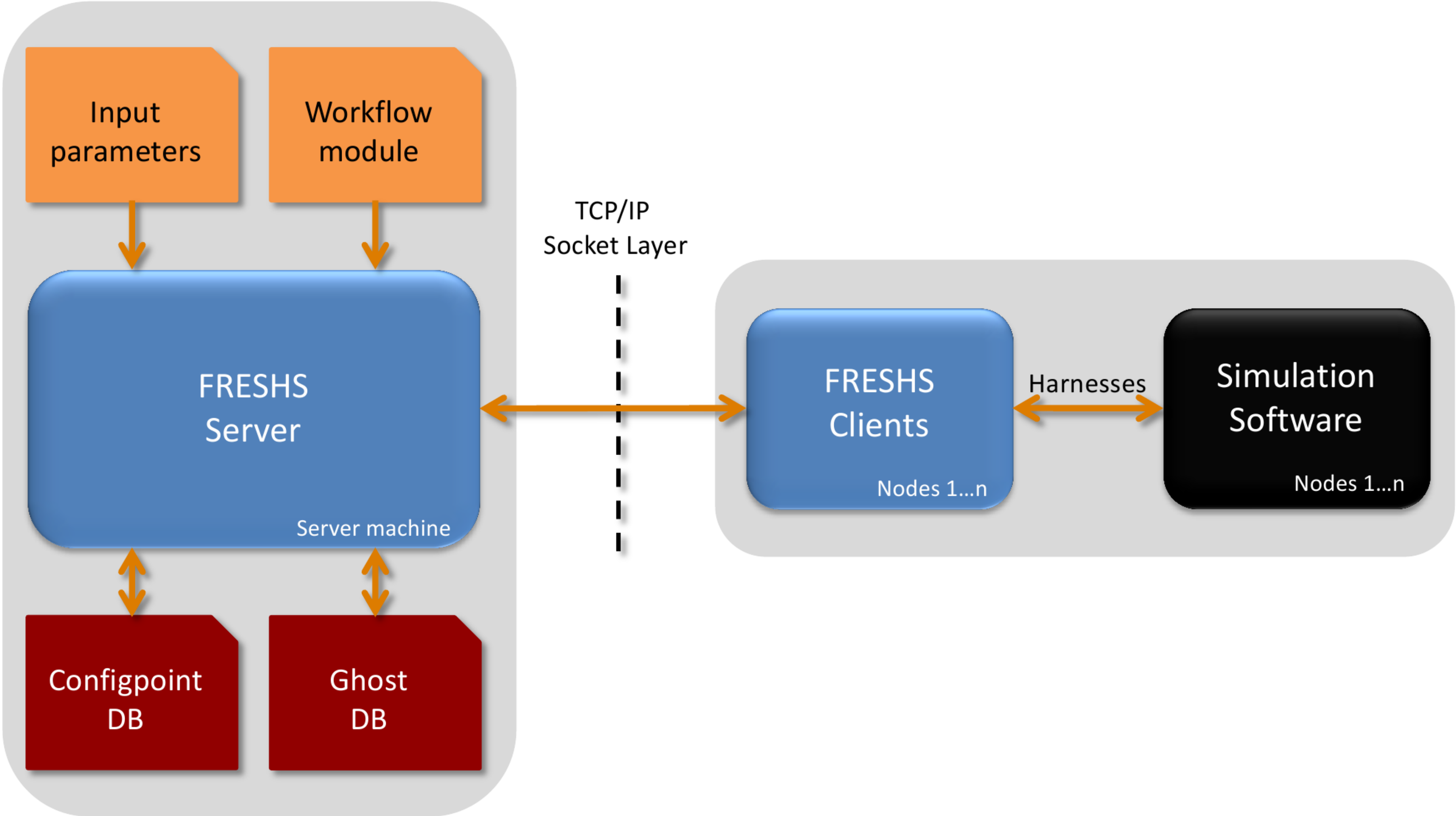
The Flexible Rare Event Sampling Harness System



The Flexible Rare Event Sampling Harness System



The Flexible Rare Event Sampling Harness System

FRESHS

- Asynchronous parallelization
  ➔ each path can be calculated by a different client

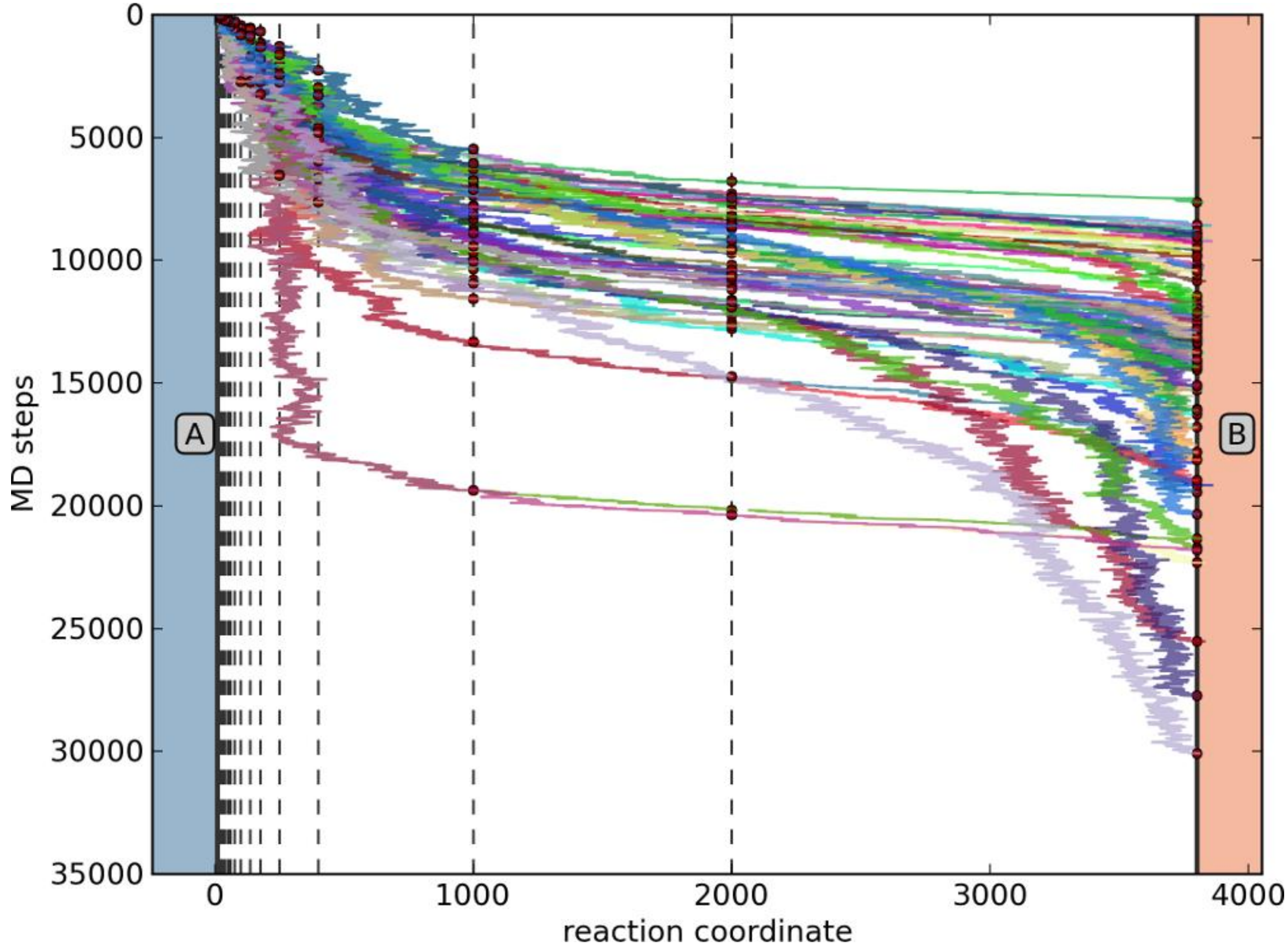
- Calculation of the physics can still be parallelized using OpenMP or MPI
  E.g. each client 1 node and 8 CPUs,100 clients connected
  ➔ 800 CPUs working for us

- Ghost runs to bridge the waiting time on interface change

Spin-off projects:

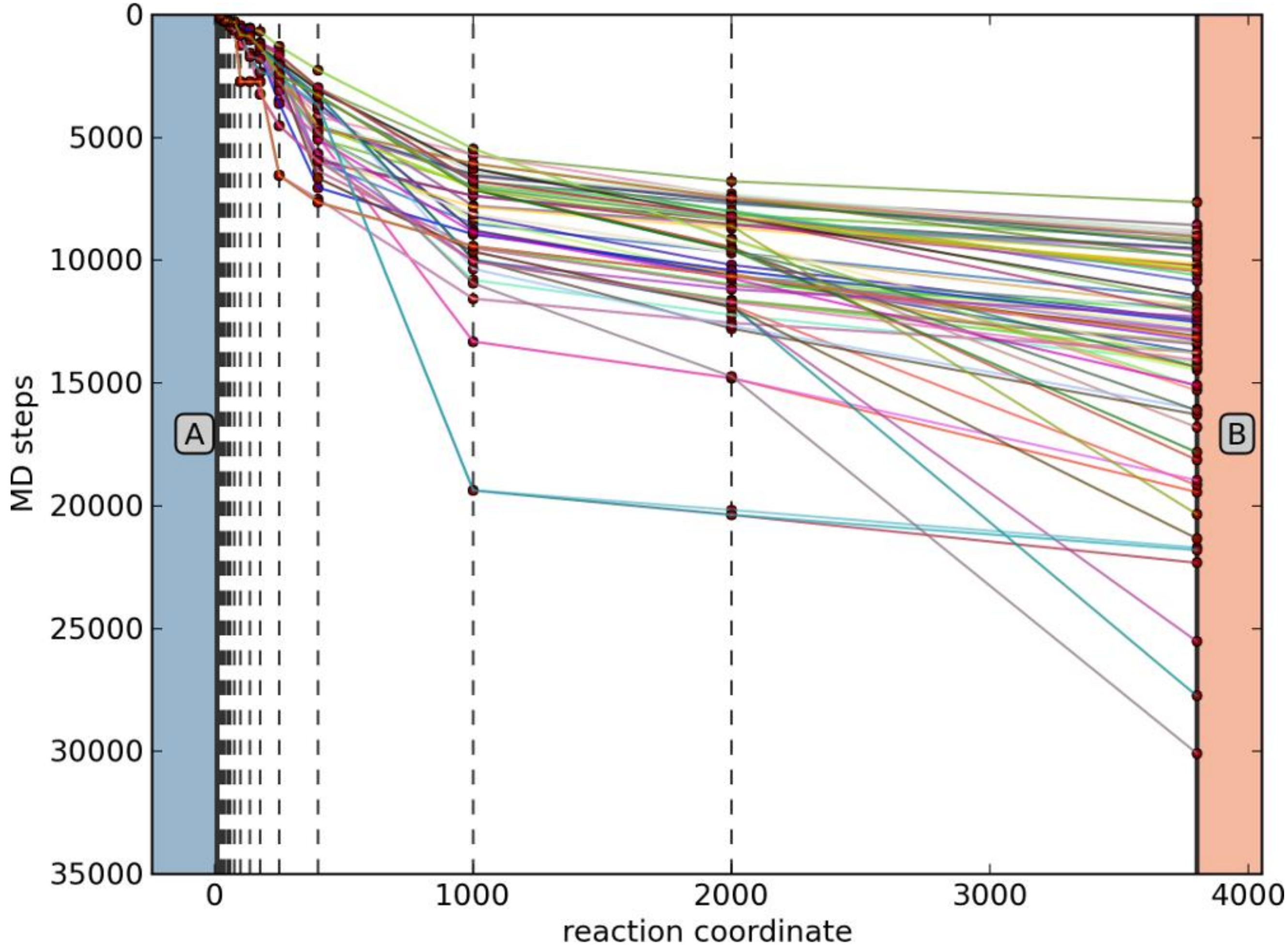
- A. Taudt: Gromacs & biological Systems, ICP / ITB
- J. Zeman: Kinetic Monte Carlo, Fe/Cu nucleation, ICP / IMWF
- S. Kesselheim: Translocation of DNA through nanopore, ICP

Results of a crystallization simulation - pathways



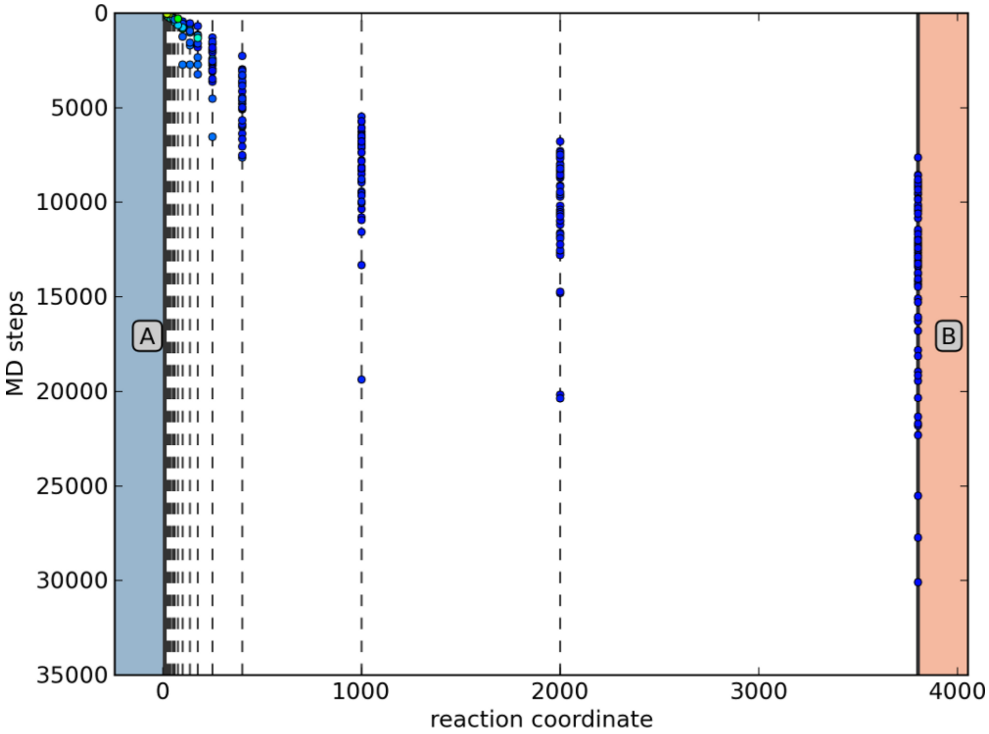
Successful pathways of the nucleation process: Fluctuations of the order parameter.

Results - backtracing

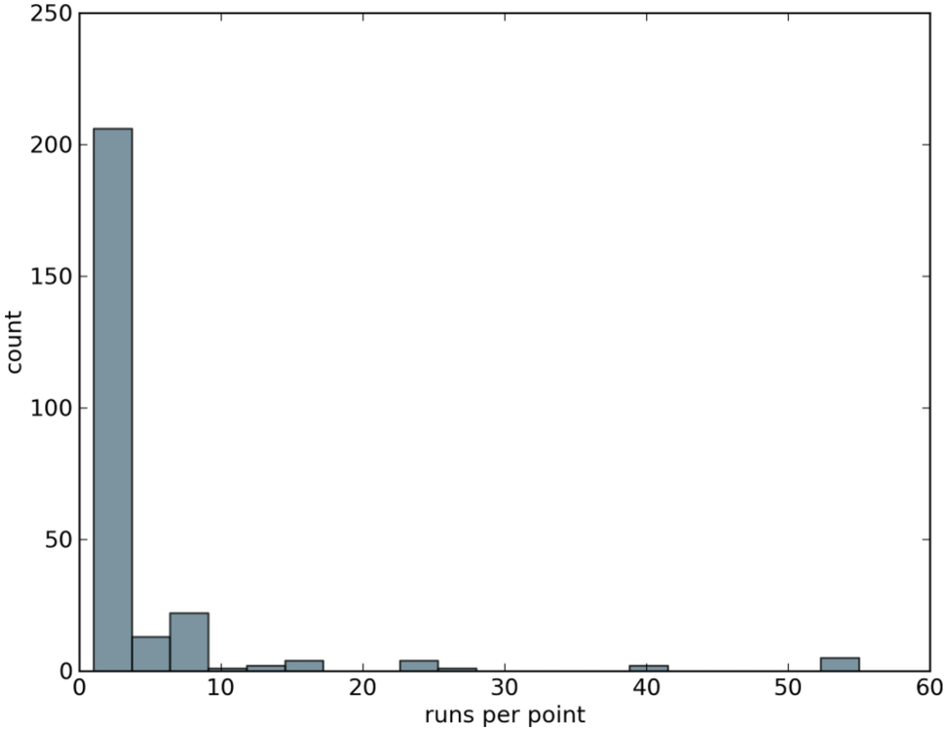


Backtrace of the successful runs. As many backtraces as points on border of state B.

Results - check of statistics



(a) BLUE = 1 run, RED = all runs.



(b) Histogram of the runs per point.

Conclusions

- Developed flexible framework for simulating rare events
  - ➔ Simulating quasistatic and dynamic systems in equilibrium and non-equilibrium
  - ➔ Farming on HPC hardware
  - ➔ Tested with ESPResSo, Gromacs, LAMMPS and various self-written simulation codes
  - ➔ Will be put open source soon

http://www.espressomd.org

SimTech Cluster of Excellence

FRESHS + ESPResSo

Now:

Hands-on Tutorial

Requirements for the hands-on session

- FRESHS & Tutorial: http://www.icp.uni-stuttgart.de/~kratzer/freshs_tut.tar.bz2
- ESPResSo: http://espressomd.org
- Python

Optional:

- Gnuplot
- A sqlite DB viewer, e.g. firefox sql browser plugin
- VMD

Getting started

- Unpack the tutorial package
- Open the lj_spres_tut.pdf
- Follow instructions in the pdf

E.g.

- Run the server:

  python "$FRESHS"/server/main_server.py "$CONF"

- Start a client:

  python "$FRESHS"/client/main_client.py "$ESPRESSO" "$HARNESS"

- If things are working, start more clients ☺