Rare event sampling with FRESHS

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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

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

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

→ 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

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

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Forward Flux Sampling (FFS)


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

- Transition rate
  \[ k_{AB} = \Gamma e^{-\beta \Delta G^*} \]

- Arrhenius equation

- kinetic pre-factor \( \Gamma \)

- \( \beta = 1/k_B T \)
Forward Flux Sampling

- Escape flux:
  \[
  \frac{\Phi_{A,0}}{\bar{h}_A} = \frac{\text{number of configurations at } \lambda_0}{\text{total simulation time}}
  \]

- Conditional probabilities:
  \[
  P(\lambda_n|\lambda_0) = \prod_{i=0}^{n-1} P(\lambda_{i+1}|\lambda_i)
  \]

- Transition rate:
  \[
  k_{AB} = \frac{\Phi_{A,n}}{\bar{h}_A} = \frac{\Phi_{A,0}}{\bar{h}_A} P(\lambda_n|\lambda_0)
  \]

- Advantage:
  \[
  P(\lambda_{i+1}|\lambda_i) \gg P(\lambda_n|\lambda_0)
  \]
  \[\Rightarrow\] 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)


- Focus on calculating the time-series of the probability of a rare event
- Phase space binning instead of hypersurfaces
- Reaction coordinate $\lambda$, 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 $\tau$.
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
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Input parameters
Workflow module
FRESHS Server
TCP/IP Socket Layer
Server machine
FRESHS Clients
Nodes 1...n
Simulation Software
Nodes 1...n
Configpoint DB
Ghost DB
Harnesses
The Flexible Rare Event Sampling Harness System

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

- Start a client:
  
  ```python
  python "$FRESHS"/client/main_client.py "$ESPRESSO" "$HARNESS"
  ```

- If things are working, start more clients 😊