Expanded ensemble method for bubble nucleation

Jaakko Hällfors

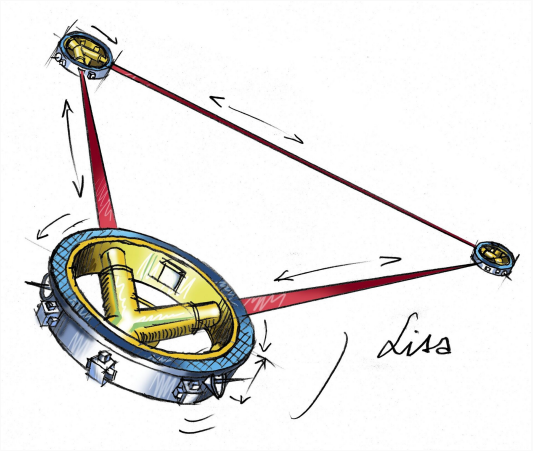
University of Helsinki

December 1, 2025

[arXiv:2502.14610]

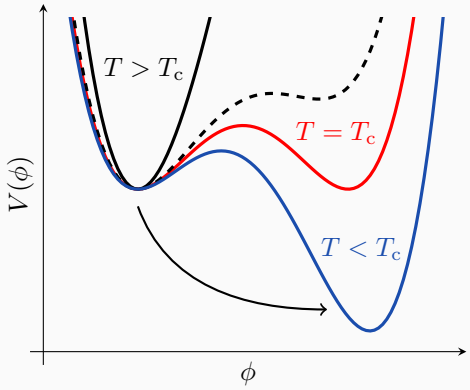
Cosmological phase transitions

- Many extensions of the standard model can have first order phase transitions
- These are expected to produce a model-dependent gravitational wave background
- Future GW observatories might be able to rule out models based on the detected background



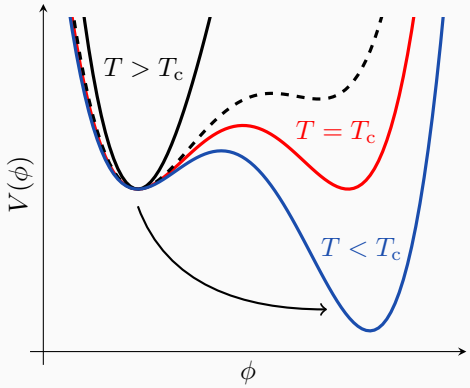
[European Space Agency]

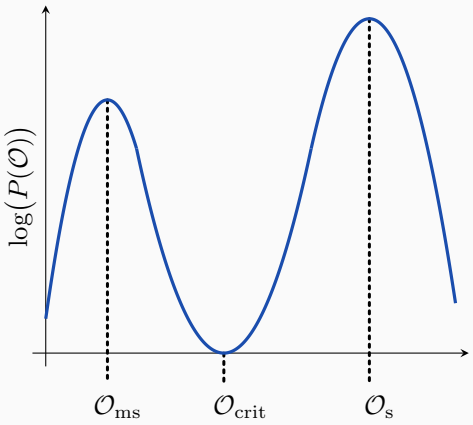
First-order phase transitions



- First-order phase transitions happen through bubble nucleation from the metastable to the stable phase
- The nucleation rate tells us how often bubbles of the stable phase appear

First-order phase transitions

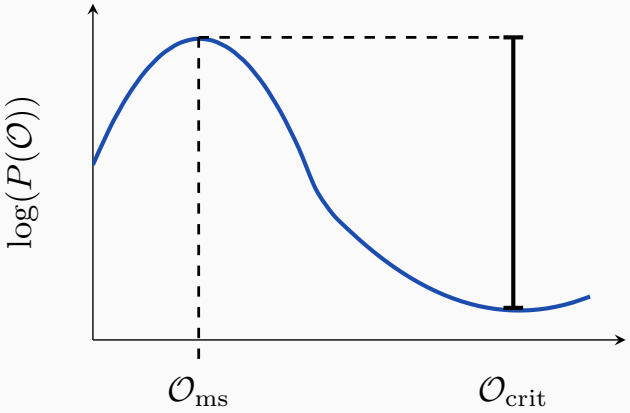




Computing the nucleation rate on the lattice

- The nucleation rate factorises into a statistical and dynamical parts
  [Moore and Rummukainen 2001]
- The statistical part is given by the probability of the critical bubble

$\Longrightarrow$ Just need to obtain $P(\mathcal{O}_{\mathrm{crit}})/P(\mathcal{O}_{\mathrm{ms}})$ using MCMC



Toy model

- Real two-dimensional scalar field

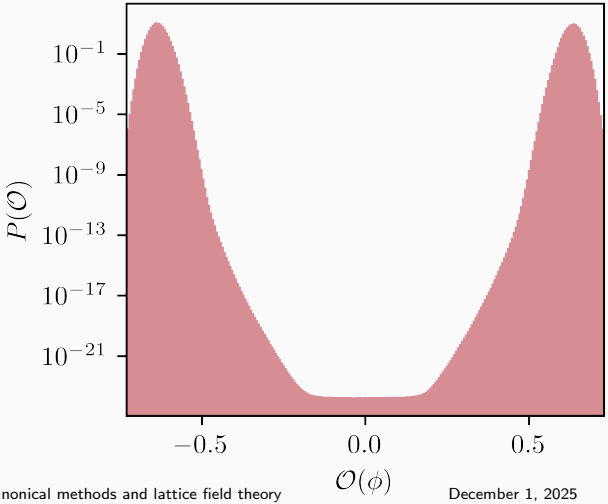
$$S(\phi) = (\partial_\mu \phi)^2 - m^2\phi^2 + \lambda\phi^4$$

- Degenerate minima at

$$\phi = \pm\sqrt{m^2/2\lambda}$$

- Define an order parameter as

$$\mathcal{O}(\phi) = \frac{1}{V}\sum_x \phi(x)$$



The usual way: Multicanonical MCMC

- Instead of trying to sample $P_{\mathrm{ca}}(\phi)$, choose a function $W(\mathcal{O})$ such that [Berg and Neuhaus 1991]

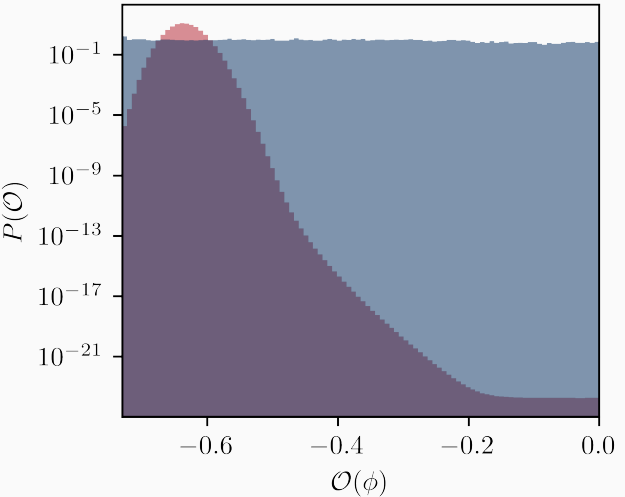
$$P_{\mathrm{muca}}(\phi) \propto \exp\left[-(S(\phi) + W(\mathcal{O}))\right]$$

and

$$P_{\mathrm{muca}}(\mathcal{O}) \approx \mathrm{Uniform}$$

$\Longrightarrow$ Suppression of the critical configurations is removed

- The weighting can be factored out afterwards

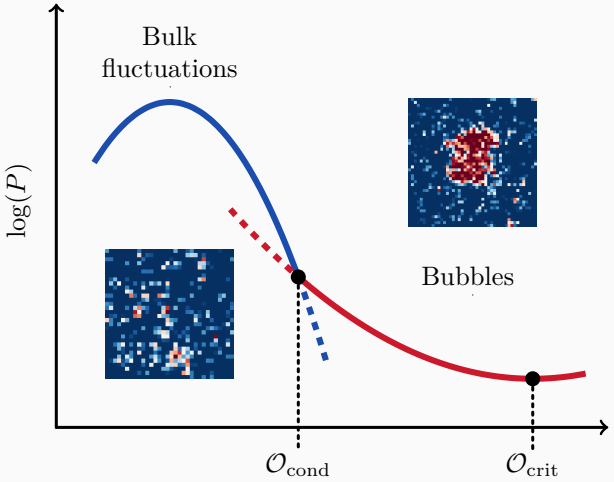


Condensation transition

- At some value $\mathcal{O} = \mathcal{O}_{\text{cond}}$ it becomes preferable to form a single localised bubble

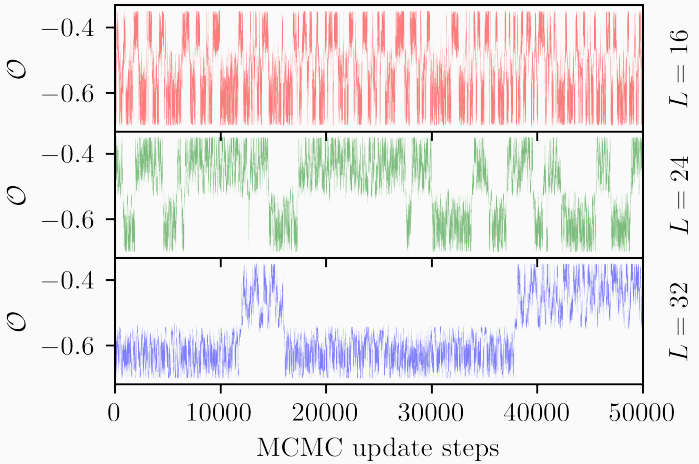
  [Binder 2003; Nußbaumer, Bittner, and Janke 2010]

- The transition occurs without a change in the order parameter
- Multicanonical weighting does not affect the transition



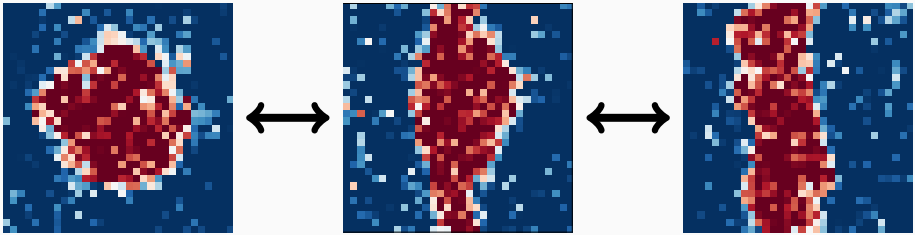
Problems

- Chain has trouble moving through the condensation transition
- Problem becomes (exponentially) worse as lattice volume is increased
- Large bubbles (small supercooling) become impractical to investigate



Something similar

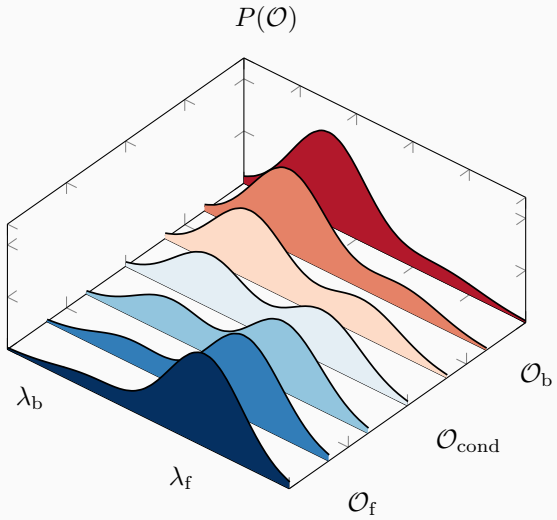
- For a periodic lattice, at some value $\mathcal{O}$ it becomes preferable to form a slab instead of a bubble
- As $\mathcal{O}(\phi_{\mathrm{b}}) = \mathcal{O}(\phi_{\mathrm{s}})$ MUCA does nothing
- Barrier arises from having to morph through deformed configurations that are unlikely for *any* value of $\mathcal{O}$



Structure of the condensation barrier

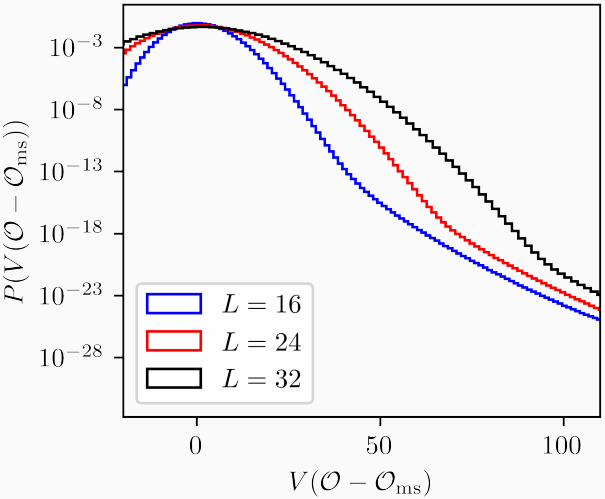
- The effect of the multicanonical weighting is to equalise the probability mass between canonical ensembles at different fixed $\mathcal{O}$

- Were it easy to define, λ would make a good order parameter near the transition



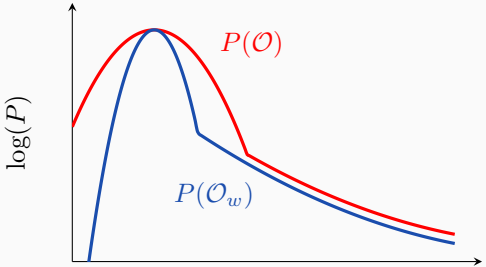
Increasing the volume

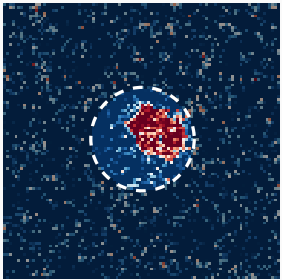
- As system volume is increased, the delocalised fluctuations of the metastable phase "mask" small bubbles
- The physical size of the bubble at the condensation transition increases, and so does the barrier
- Small variance in the metastable phase is preferable for the order parameter!



Weighted order parameters

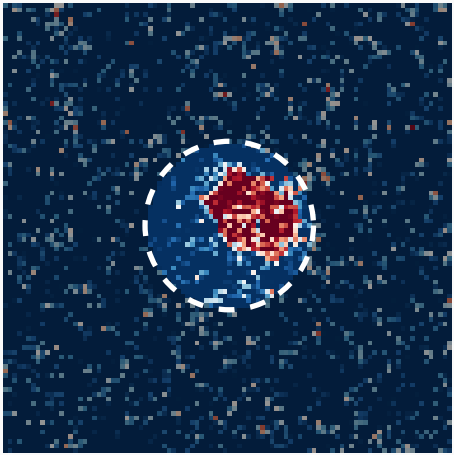
- What if we only measure $\mathcal{O}$ in some subvolume V_w and use that for multicanonical weighting?
- Near the peak $P(\mathcal{O}_w)$ looks like $P(\mathcal{O})$ in a smaller system with $V \approx V_w$
- Importantly, the condensation barrier in the new ensemble is also small





What have we achieved?

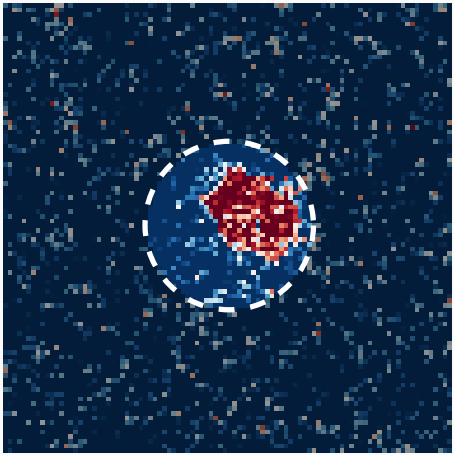
- We can now enhance the probability of small bubbles in arbitrarily large volumes
- We *can not* use it to create large bubbles, since they must fit inside the weighted area



What have we achieved?

- We can now enhance the probability of small bubbles in arbitrarily large volumes
- We *can not* use it to create large bubbles, since they must fit inside the weighted area

What's the use?

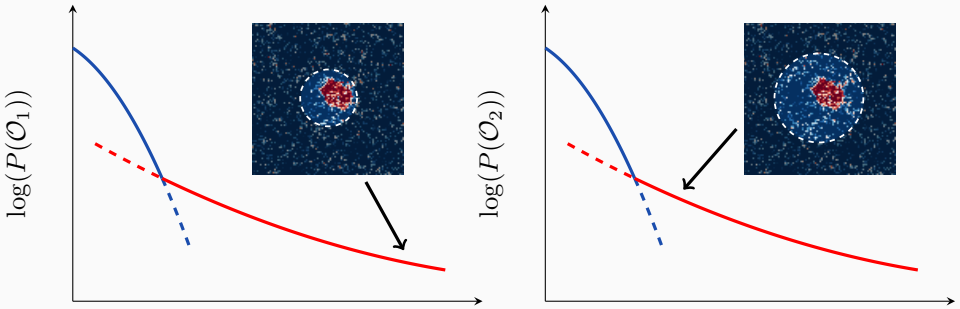


Size is relative

Consider two ensembles where one of the weighted volumes is slightly larger:

$\Longrightarrow$ The large bubbles of $\mathcal{O}_1$ are small bubbles of $\mathcal{O}_2$

$\Longrightarrow$ There is good phase space overlap between the two ensembles!



Method of expanded ensembles

- A more general form of simulated tempering
  [Lyubartsev et al. 1992]
- Multicanonical subensembles that use differently weighted order parameters
- Two types of MC updates:
  1. Change the field values
  2. Change the subensemble

$$P(\phi, i) = \frac{1}{\mathcal{Z}_i} \exp\big[-S(\phi) + W_i(\mathcal{O}_i(\phi))\big],$$

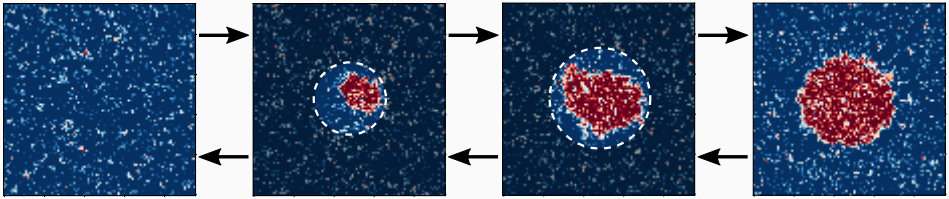
$$\mathcal{P}(i \to j) = \exp\big[W_j(\mathcal{O}_j(\phi)) - W_i(\mathcal{O}_i(\phi))\big]$$

Good phase space overlap is necessary for successful ensemble swaps!

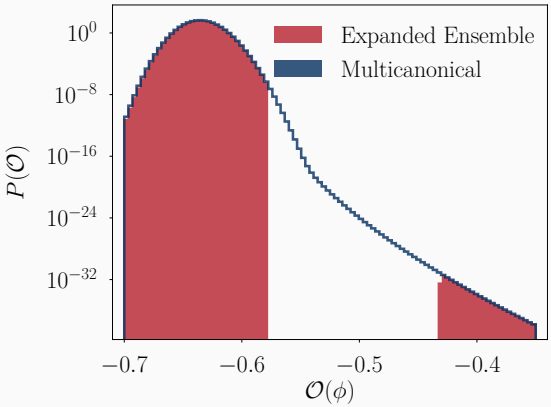
The construction

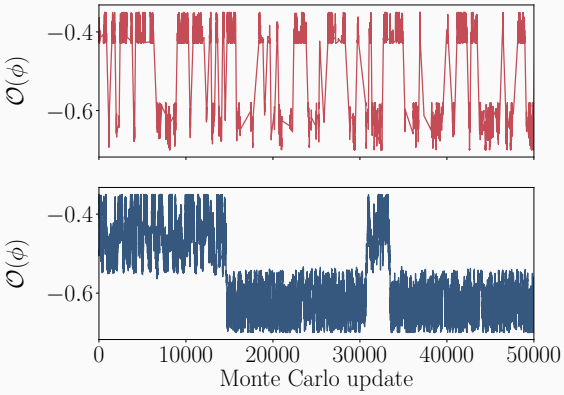
1. Start with a regular subensemble around the metastable peak
2. Add a subensemble that uses a small weighted area (condensation happens here!)
3. Add a chain of ensembles using larger and larger subvolumes
   restricted to their respective bubble branches

n. End on a second regular subensemble that sampled the bubble branch



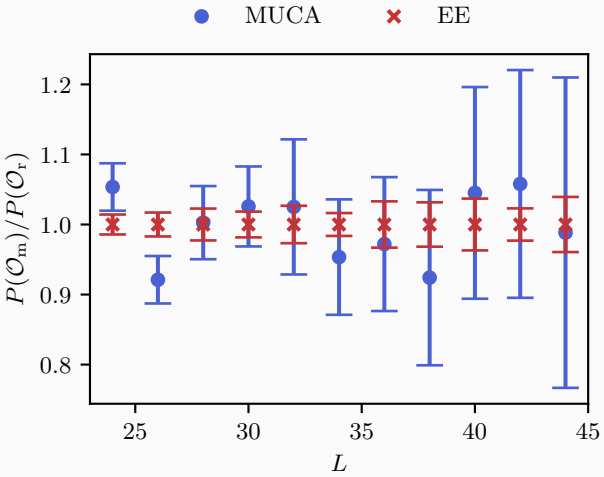
Comparison


Expanded Ensemble
Multicanonical
10^{0}
10^{-8}
10^{-16}
10^{-24}
10^{-32}
$P(\mathcal{O})$
-0.7
-0.6
-0.5
-0.4
$\mathcal{O}(\phi)$


-0.4
-0.6
$\mathcal{O}(\phi)$
-0.4
-0.6
$\mathcal{O}(\phi)$
0
10000
20000
30000
40000
50000
Monte Carlo update

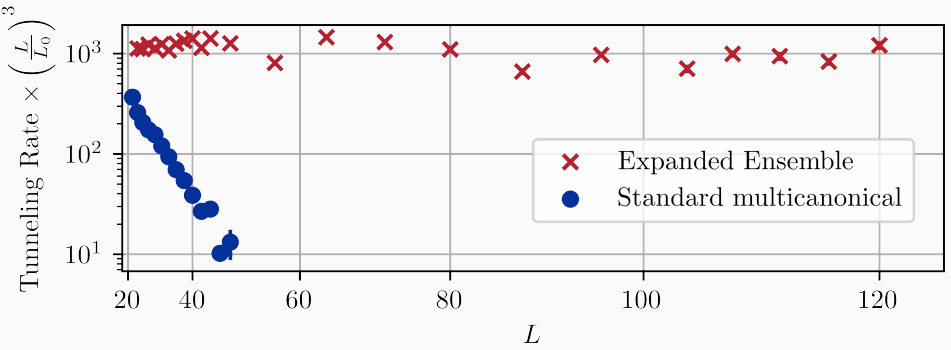
Bubble probability

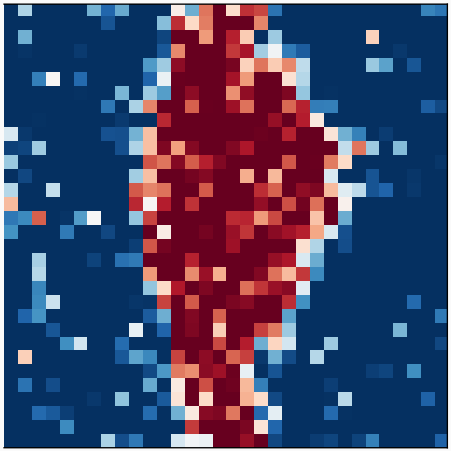
- Good agreement between the methods
- Much reduced errors using the expanded ensemble method



Tunneling rate

- Now slowing down appears to be no worse than power law
- Should generalise nicely to other order parameters



Future

- Check that the thin-wall limit is valid by simulating very large bubbles
- Try to apply the idea to similar problems
  1. Shape transitions?
  2. Something entirely different?