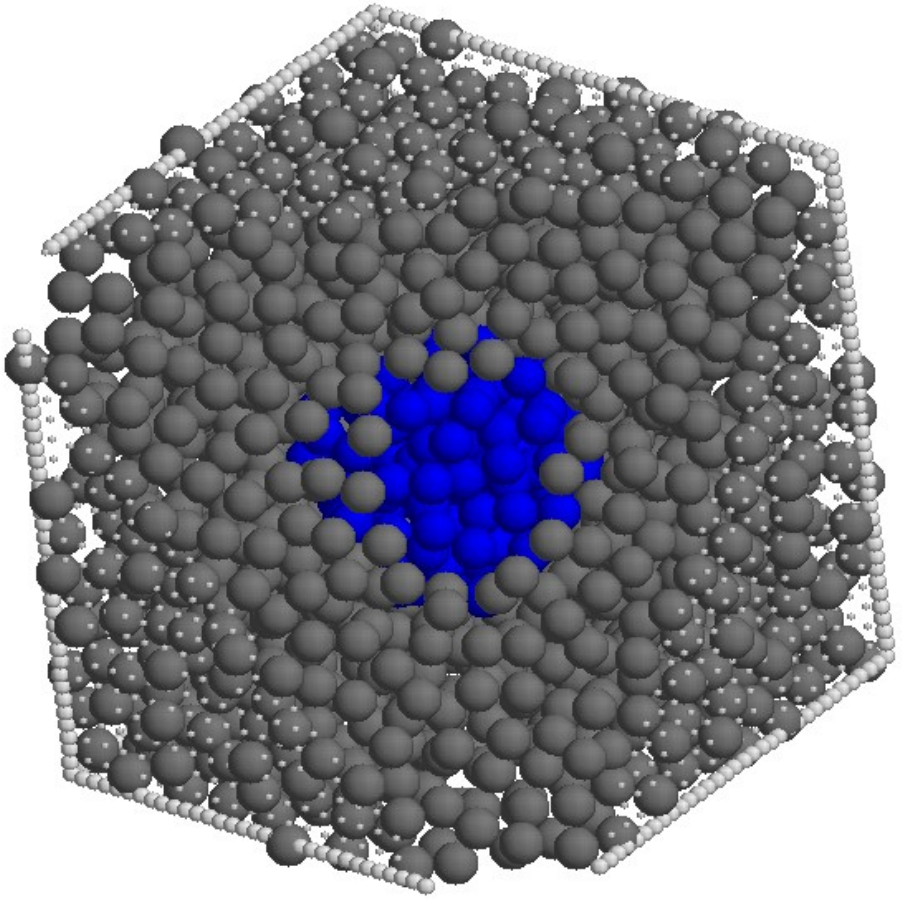
Numerical Simulations in Supercooled Liquids and Cavities



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Background

- Supercooled liquids are liquids below melting temperature (They “should” be Solid/Cristal)
- If we keep on lowering T, we get a glass.
- Glass: very viscous material, very large relaxation time, out of equilibrium.

- If there a Thermodynamical or just a Dynamical transition? (frustation)

Numerical Simulations

- Usually with simple particles (i.e. Lennard-Jones).
- Monte Carlo or Molecular dynamics simulations.
- The slow dynamics takes place also in simulations: It is hard to equilibrate the system.

- Usually Periodic Boundary Conditions (PBC). We, however perform Amorphous Boundary Conditions (ABC).

Why ABCs?

- The super Arhenius growth on relaxation upon cooling suggest there is a growing correlation length.
- There has been a great effort to find different types of order with no success.
- We look for Order Agnostic correlation lengths. i.e. We try to get evidence for order, without knowing what kind of order is.

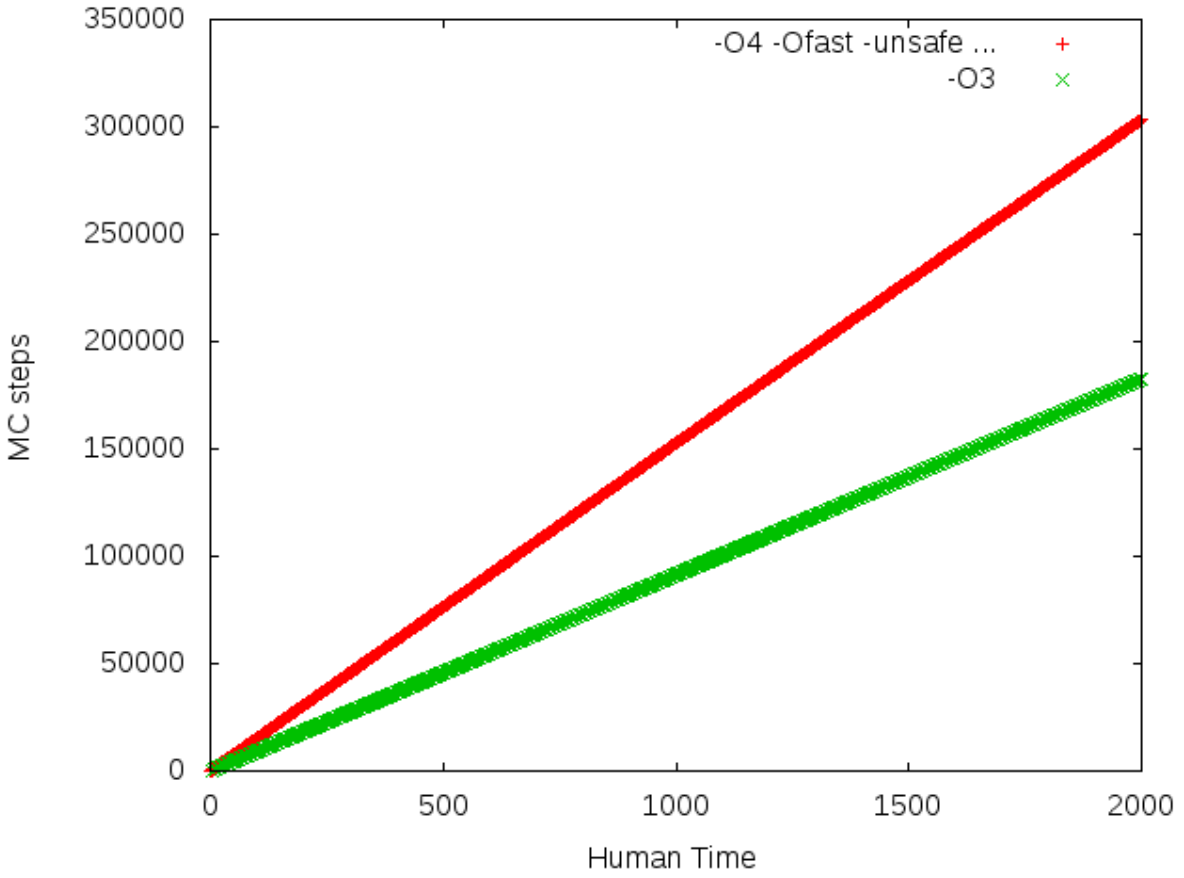
Speed Up strategies (ABCs and PBCs)

- Use Cells (divide the problem into boxes), so, when calculating observables, we don't visit every neighbor.
- Use Swap dynamics when available. Different kinds of particles, not always possible.
- Parallel Tempering.

New Trick!!!!

-O4 -Ofast -mavx -funsafe-math-optimizations

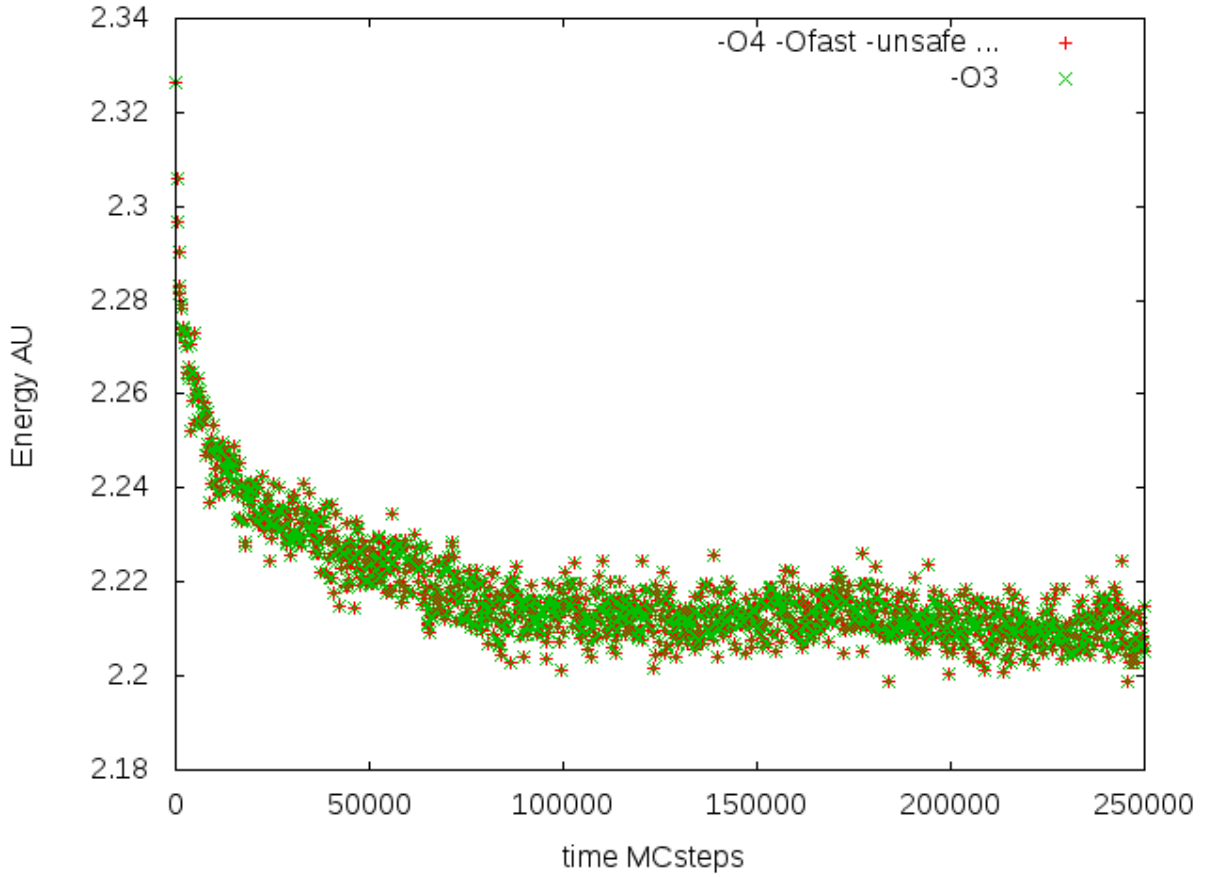
- It's FASTER!



New Trick!!!!

-O4 -Ofast -mavx -funsafe-math-optimizations

- Same Results



Boxes

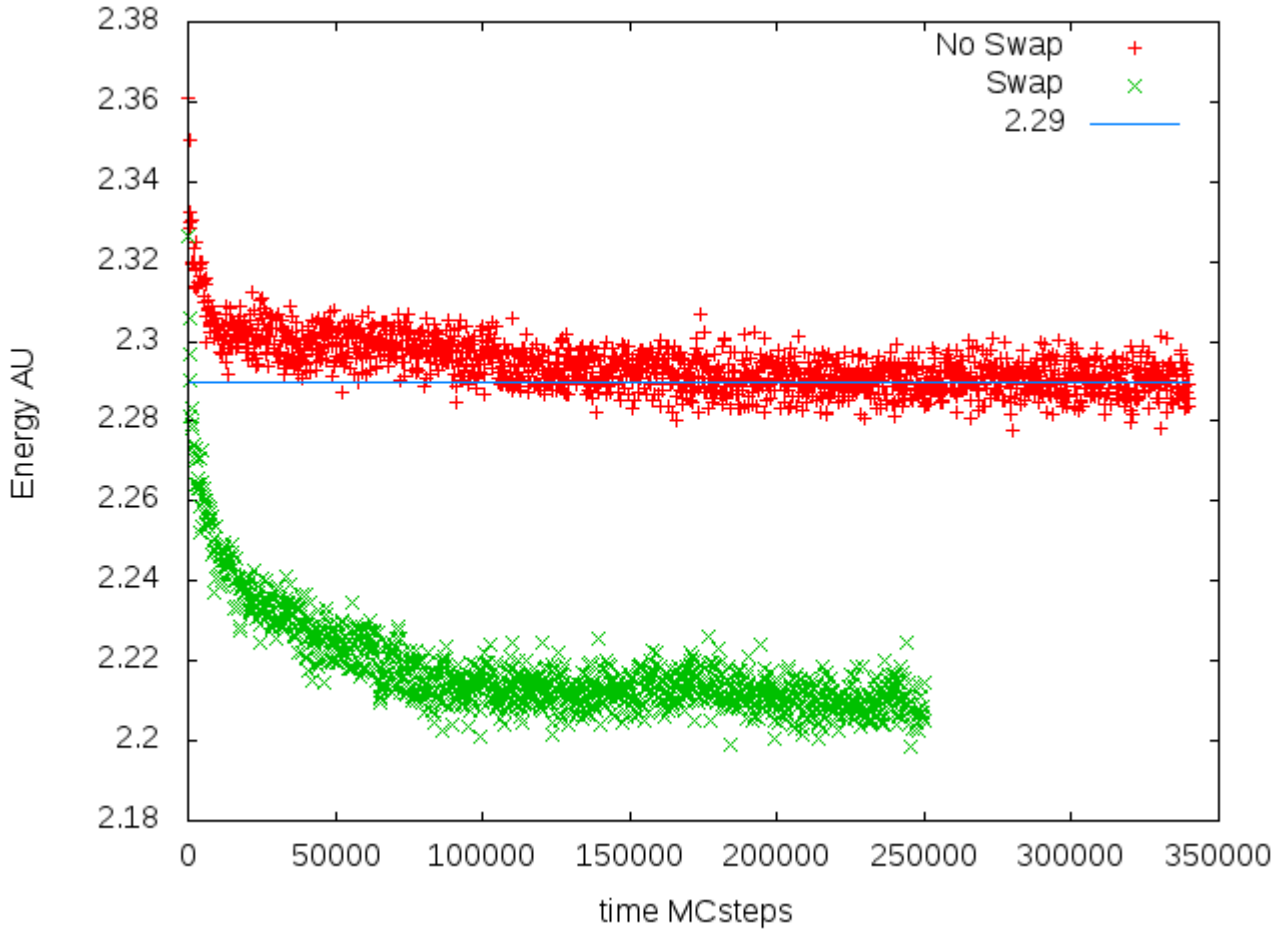
In short range potential, reduces the problem **from O(N^2) to O(N)**.

- Cannot get rid of BOXES!

- **We can have smaller boxes so its more parallelizable.**
- I sent boxes to different OpenMP processes. **Litle Improvement.**

Swap

- 100 times faster or more (unavoidable if available)



Still too slow

at lowest

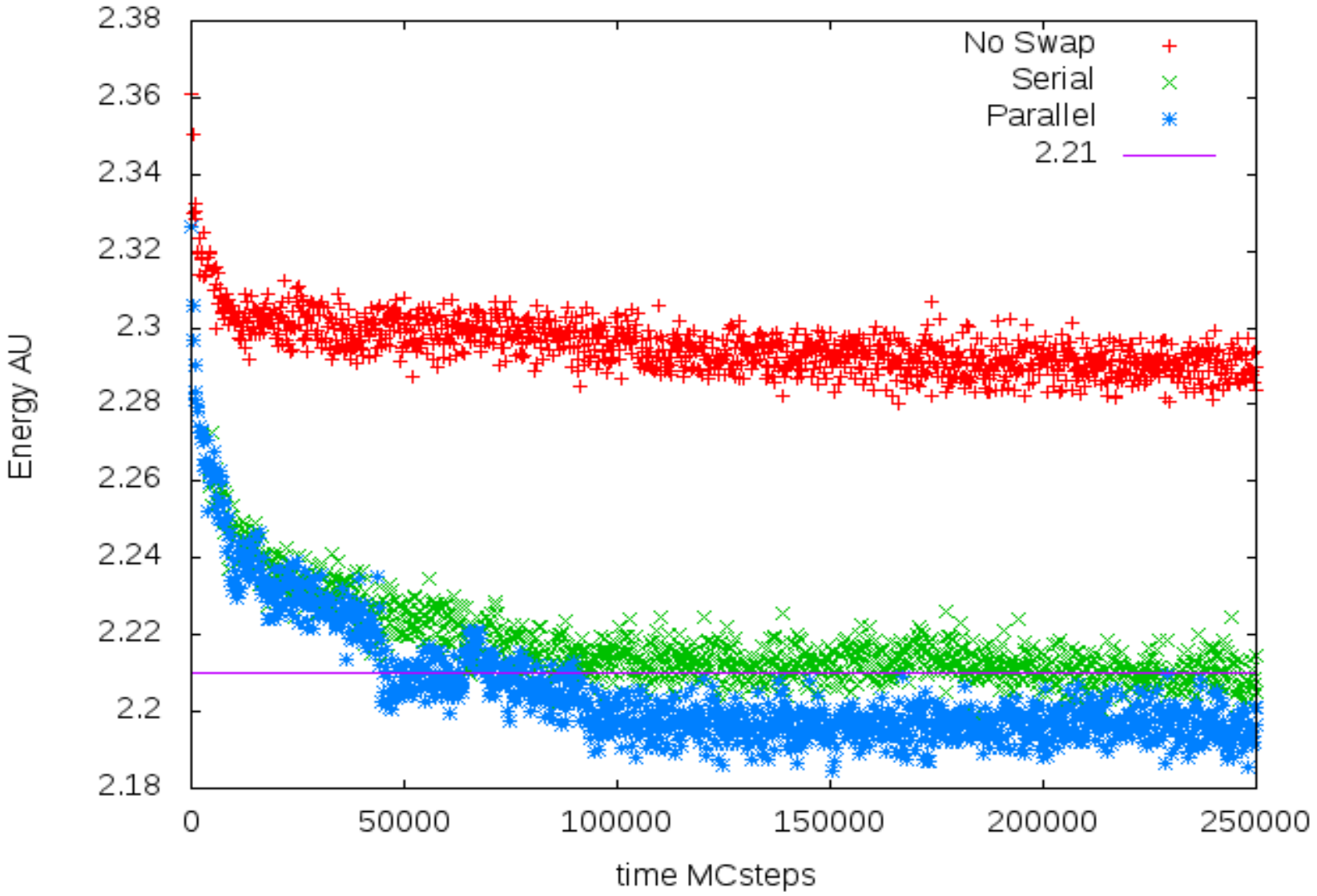
temperatures !!!

Parallel Tempering

- Try to equilibrate systems at (slightly) different temperatures.
- Periodically, try to exchange their configuration, with Boltzmann Weight.
- So a wider region of the space phase is visited!

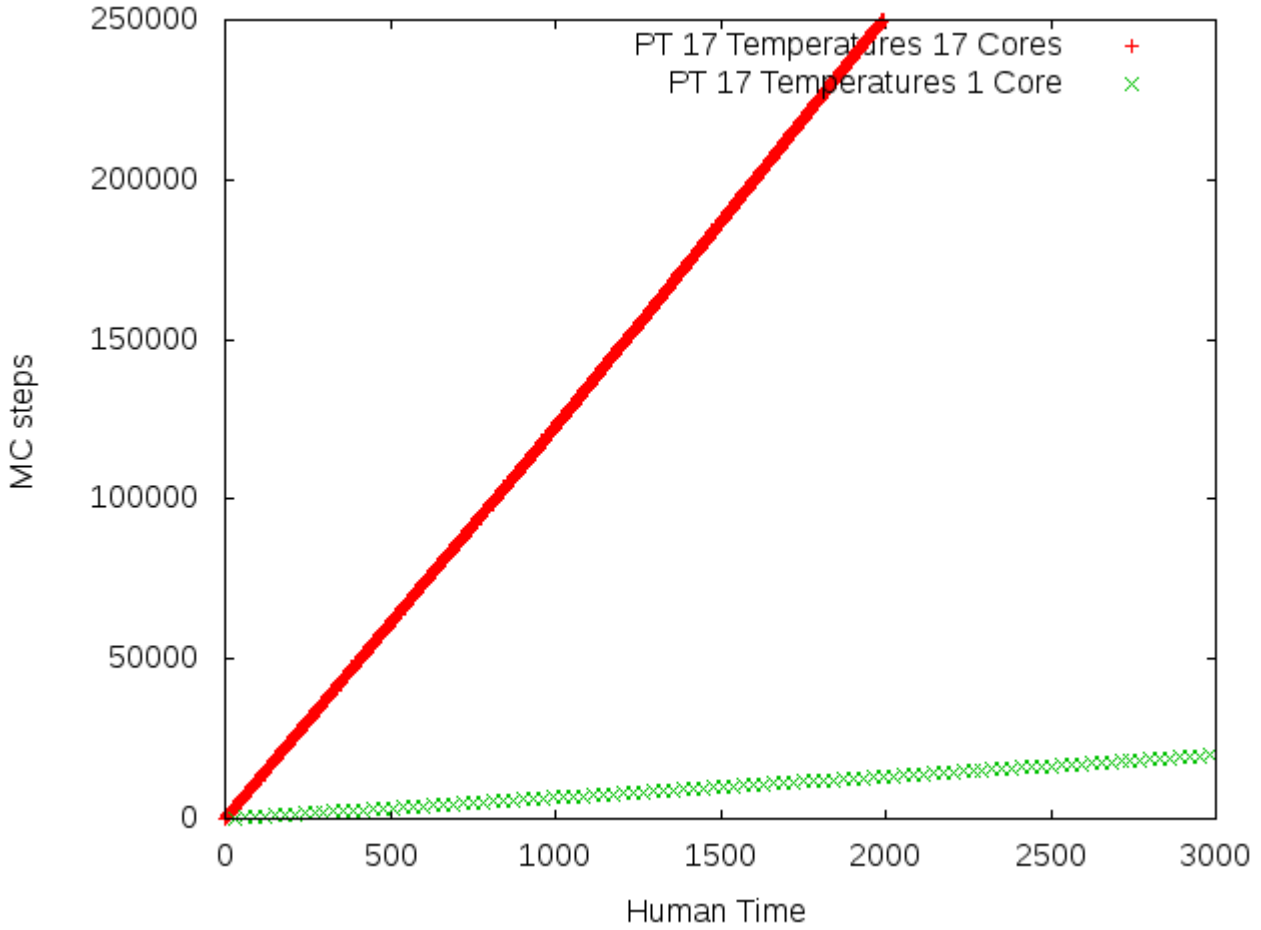
- **Systems have to be very close in energy to have successful PT ($E \sim N$, but $\Delta E \sim N^{0.5}$)**
- **Often you equilibrate temperatures you don't need.**

PT equilibrates in less MC steps



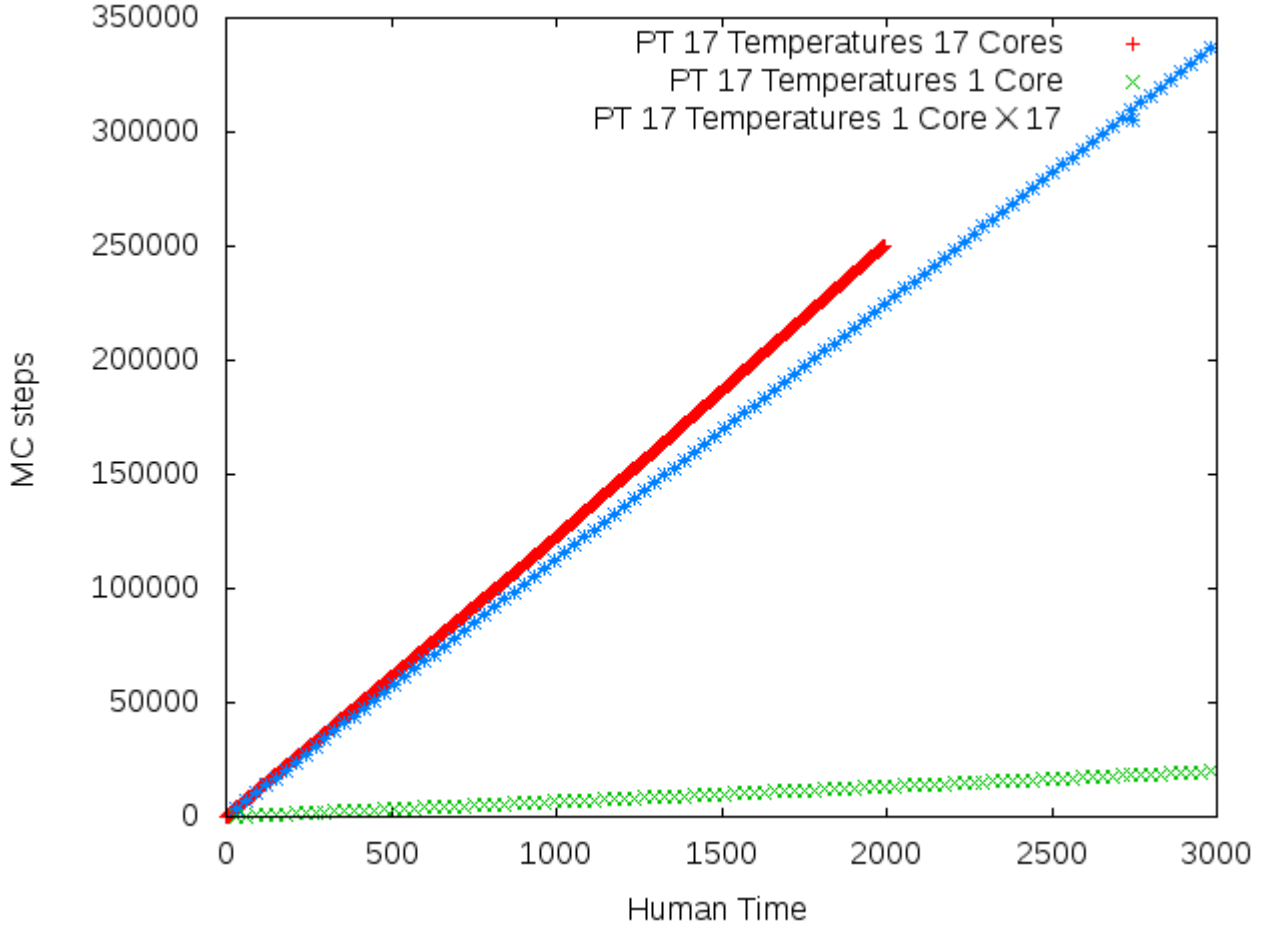
PT and Parallel Computing

- It is too slow in a **single core**



PT and Parallel Computing

- And (Slightly) less efficient than MPI!! (More cache misses?)



Some things I learned

- -O4 !!
- PT with MPI
- INDENTATION: Emacs does it for you (now my code is 2000+ lines)
- OpenMP: Easy and inefficient
- Use libraries.
- Be cache Friendly, test it with **perf stat**

220407112 cache-references:u (+- 0.26%)

8829667 cache-misses:u # 4.006 % of all cache refs (+- 1.48%)