Simulation methods in physics

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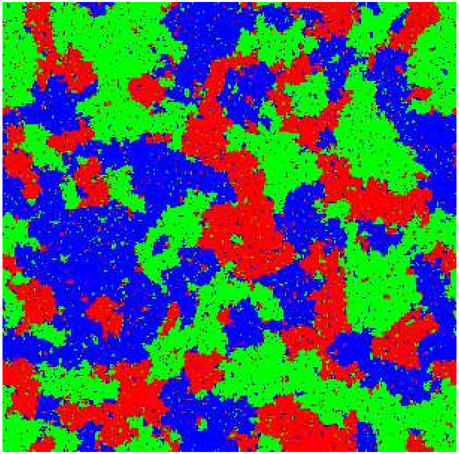


Intro

- This course covers (mostly) basic + somewhat more advanced Monte Carlo methods – *lattice MC simulations*.
- Monte Carlo is an extremely broad term – many (not necessarily computer!) simulation methods involving random numbers are called Monte Carlo such-and-such.
- In these lectures, we shall mostly concentrate on solving *partition functions* on a (usually) regular *lattice*:

$$Z = \int \left[\prod_{\mathbf{x}} d\phi(\mathbf{x}) \right] \exp[-\frac{1}{k_B T} H(\phi)]$$

Here $H(\phi)$ is the Hamiltonian (energy) of the system, k_B the Boltzmann constant and T temperature.

The coordinates are

$$\mathbf{x}_i = a n_i, \qquad n_i = 0 \ldots N_i$$

where a is the *lattice spacing* (physical length), and the lattice has

$$N = \prod_{i=1}^{d} N_i$$

discrete points (i.e. the box is d -dimensional).

- The integral is $N \times$ dim(ϕ) -dimensional – well-defined, in principle computable! However, the dimensionality is huge – typically $10^6 - 10^9 \rightarrow$ Monte Carlo integration is needed.

- Example: Ising model

$$Z = \sum_{\{s_i=\pm 1\}} \exp[-\beta/2 \sum_{<ij>} (1 - s_i s_j)]$$

Here the sum in the exponent goes over the nearest-neighbour sites of the lattice. (Note: dimensionless, “lattice” units!)

- Lots of applications within statistical physics and condensed matter physics (crystalline structure, spin models, superconductivity, surface physics, glassy systems . . .)

Lattice field theory

- The Feynman path integral (in Euclidean spacetime):

$$Z = \int \left[\prod_x d\phi(x) \right] \exp[-S(\phi)]$$

- Discretize space $\rightarrow$ the path integral becomes mathematically well-defined. However, our space-time is not discrete $\rightarrow$ the results have to be extrapolated to the continuum limit, where the lattice spacing a goes to zero.

- *Field theory on the lattice:*

  – provides an explicit ultraviolet cutoff, removing the UV divergences so common in field theories. These have to be renormalized before the continuum limit is taken.

  – allows the use of (almost all of) the analytical tools used for continuum field theories – especially, the lattice perturbation theory is equivalent to the standard one (but more cumbersome to use).

– provides new analytical methods and tools, not possible for continuum field theories (strong coupling/"high temperature" expansions, duality relations etc.).

– emphasizes the connection between *field theory and statistical mechanics*: Feynman path integral $\equiv$ partition function. All of the tools developed for statistical mechanics are at our disposal!

– permits the evaluation of the path integral numerically, using *Monte Carlo calculations*. The integral is evaluated as-is, without expanding it in any small parameter ($\equiv$ *non-perturbative*).

Models studied in HEP context:

- *Lattice QCD:*

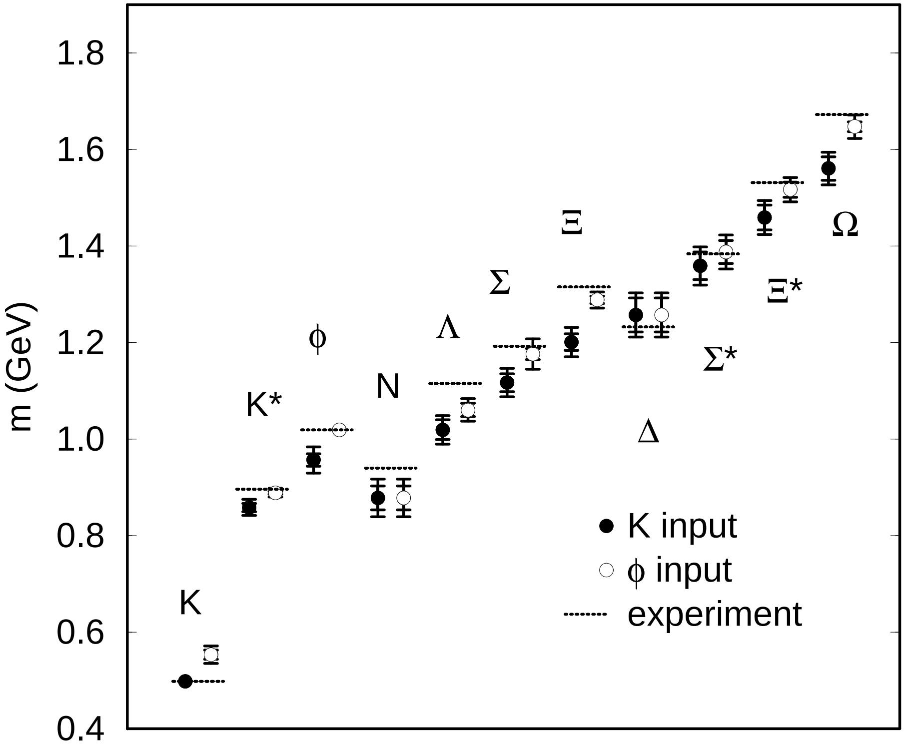
  Almost all interesting QCD physics non-perturbative!

  Since around 1980 Quantum Chromodynamics (QCD) has been studied extensively on the lattice. The results have given invaluable *qualitative* insights (confinement); and, during the last $\sim$ 5 years the results have also been *quantitatively* comparable to experiments.

  • Confinement mechanism, hadronic mass spectrum, matrix elements . . .

  • QCD phase transition at $T \approx 150$ GeV

Light hadron masses (CP-PACS collaboration, 2002).



- *Electroweak phase transition:*

  Electroweak theory at $T = 0$ is perturbative: coupling constants are small, and the gauge bosons W, Z are massive. However, as T increases, the "broken SU(2) symmetry" is restored: gauge bosons become massless, and IR singularites make the theory non-perturbative.

  Since $\sim$ 1994 EW theory (theories) have been studied extensively on the lattice, with very solid results $\Rightarrow$ we know how the EW phase transition behaves. Applied also to MSSM (Minimal Supersymmetric Standard Model)

- *Many other models . . .*

  - QED
  - Ginzburg-Landau theory (superconductivity)
  - Quantum gravity

Textbooks about MC methods:

- Gould, Tobochnik: An introduction to Computer Simulation Methods: Applications to Physical Systems. Pretty elementary.
- K. Binder und D.W. Heermann, Monte Carlo Simulation in Statistical Physics, Springer Series in Solid-State Sciences 80, Springer 1988. More condensed and advanced.

Books about lattice field theory:

- M. Creutz, *Quarks, Gluons and Lattices*, Cambridge University Press 1983
- I. Montvay and G. Münster, *Quantum Fields on a Lattice*, Cambridge University Press 1994
- H.J. Rothe. *Lattice Gauge Theories: an Introduction*, World Scientific 1992
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