Lattice Field Theory

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Lattice Field Theory

- Numerical simulation of gauge (field) theories with fermions using Feynman's path integral

- Field theory is defined in terms of a Lagrangian
  $\rightarrow$ Term describing the gauge field $\rightarrow$ gauge action
  $\rightarrow$ Term describing the fermions $\rightarrow$ fermion action

- Simulations possible at weak coupling (perturbative) and strong coupling (nonperturbative)

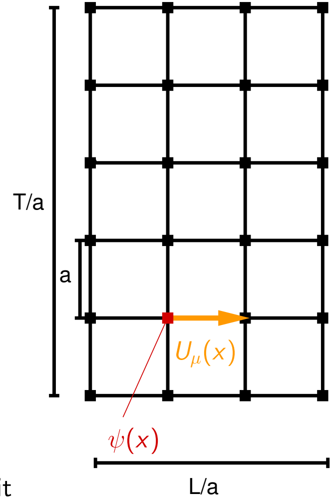
- Most prominent example: QCD
  $\rightarrow$ SU(3) gauge theory with 2 light flavors (up/down) plus strange plus charm (plus bottom, top)

- Path integral requires a probability interpretaion
  $\rightarrow$ Wick-rotate to Euclidean time $t \rightarrow i\tau$

$$\langle \mathcal{O} \rangle_E = \frac{1}{Z} \int \mathcal{D}[\psi, \overline{\psi}]\, \mathcal{D}[U]\, \mathcal{O}[\psi, \overline{\psi}, U]\, e^{-S_E[\psi, \overline{\psi}, U]}$$

Lattice Field Theory

- Discretize space-time and set up a hypercube of finite extent $(L/a)^3 \times T/a$ and spacing a
- Path integral is now a huge but finite dimensional integral
  $\rightarrow$ Finite lattice spacing $a \rightarrow$ UV regulator
  $\rightarrow$ Finite volume of length $L \rightarrow$ IR regulator
  (Physics in a finite box of volume $(aL)^3$ plus limit $L \rightarrow \infty$)
- Stochastic procedure requiring statistical data analysis
- Different discretizations for gauge and fermion actions possible
  $\rightarrow$ Wilson, Symanzik gauge; Wilson, staggered, domain-wall fermion
  $\rightarrow$ Discretization effects disappear after taking $a \rightarrow 0$ continuum limit



Lattice Simulations

- Typically a two (three) step process
  1. Generate ensembles of gauge field configurations
     → Sea-sector or QCD vacuum (gluons, fermion bubbles)
     → Dynamical simulations: gluons and fermions 2f, 2+1f, 2+1+1f, ...
  2. Valence-sector "measurements"
     → Read-in gauge field to calculate matrix elements of operators describing the process of interest
  3. Data processing, statistical data analysis

- Required resources differ

- Costs of the simulation however always dominated by inverting the Dirac operator

- Dirac operator is always a diagonally dominant sparse matrix
  → Implementation depends on chosen discretization
  → Size proportional to $L^3 \times T \times (4\ \textit{dimensions}) \times (4\ \textit{spinor}) \times (3\ \textit{color})$

Key Algorithms

- Hybrid Monte Carlo update algrotihmn for generating gauge field configurations
  → “Workhorse” for generating dynamical gauge field configurations
- Conjugate Gradient (CG) (and its variants)
  → Inverting the Dirac operator (large sparse matrices)
- Accelerating algorithms (Deflation, multi-grid, . . .)
  → Calculate low-modes, eigenvectors of the Dirac operator and re-use
- Satistical data analysis
  → Jackknife, Bootstrap resampling
  → χ^2 fits, model-averaging
  → Machine-learning

Resources

- Large sparse matrix operations allow for parallelization
  → MPI (message passing interface): subdivide matrix into blocks
  each block is assigned to a node
  → OpenMP (threading): is used on a node taking advantage of shared memory
  ⇝ Hybrid OpenMP + MPI parallelization
  → Use GPU's for acceleration

- Balance of compute power (CPU or GPU) and network favored (infibiband)
  → Development of communication avoided algorithms

- Generation of gauge fields is expensive but gauge fields can be reused in many calculations
  → 10's of TB storage needed
  → Accelerating calculations with eigenvectors requries 100's of TB
  → Postprocessing data for analysis requires 10's of TB

Software

- HMC and measurements for Wilson or domain-wall fermions: Grid
  - → Highly optimized `c++` code (c++17), templated, ...
  - → Compilers: `g++`, `clang++` plus `openmpi` or `mvapich2`, ...
  - → NVIDIA GPU: nvcc; AMD GPU: rocm, sycl; ...
  - → Libraries: hdf5, gmp, mpfr, fftw, mkl, ...

- Analysis
  - → `python` with `numpy` and `matplotlib` or `matlab`

[Boyle et al. NPB Proc.Suppl. 29(2004)838]

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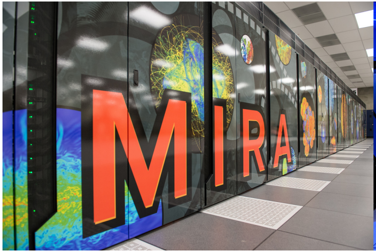

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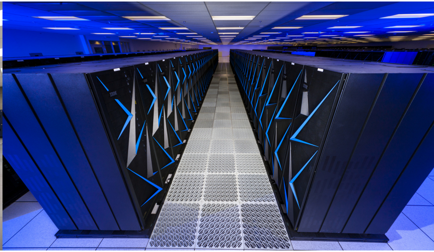

[Sierra/Lassen LLNL] (#3 Top 500 11/2021)

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