Numerical Aspects of LQCD

The goal of numerical calculations of Lattice QCD is to solve the Feynman Path integral.

$$\langle O \rangle = \frac{1}{Z} \int DU D\psi D\bar{\psi}\, e^{-S}\, O[U,\psi,\bar{\psi}]$$

This integral is highly dimensional. This poses a problem because even with largest computers, resources are limited.
To perform any calculation on any computer, the computer needs to:
- retrieve data/information (communication)
- compute cycles
- Memory to store input/output.

From a computational perspective, to solve this integral we require two resources: memory and compute cycles.
An efficient calculation needs to balance the use of these resources.
Communications can become a limiting factor as well.
We can look at the fermion action to get a sense of the numerical problem.

$$S_F^0[\psi,\overline{\psi}] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})}{2a} + m\,\psi(n) \right)$$

The above form of the action shows that for a position n, only the nearest neighborgs are involve.

Exercise 1.
Write the above equation as $\bar{\Psi} D \Psi$ and find the form of D. Usen $n=0,1,2,3$.

$$\Psi_a D_{ab} \Psi_b$$

$$(\bar{\psi}_1\ \bar{\psi}_2\ \bar{\psi}_3\ \bar{\psi}_4)\, a^4\sum_\mu \gamma_\mu \begin{pmatrix} m & 1 & 0 & 0 \\ 1 & m & 1 & 0 \\ 0 & 1 & m & 1 \\ 0 & 0 & 1 & m \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} =$$

$$a^4 \sum_\mu \gamma_\mu \,(\bar{\psi}_1 m + \bar{\psi}_2,\ \bar{\psi}_1 + m\bar{\psi}_2 + \bar{\psi}_3,\ \bar{\psi}_2 + \bar{\psi}_3 m + \bar{\psi}_4,\ \bar{\psi}_3 + m\psi_4) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

$$= \bar{\psi}_1\psi_1 m + \bar{\psi}_2\psi_1 + \bar{\psi}_1\psi_2 + m\bar{\psi}_2\psi_2 + \bar{\psi}_2\psi_3 + \bar{\psi}_3\psi m + \bar{\psi}_4\psi_3$$
$$+ \bar{\psi}_3\psi_4 + m\bar{\psi}_4\psi_4$$

The above exercise shows that the Dirac operator is a sparse matrix. In practice, it makes more sense to define the action of D on ψ as a function instead of an operation

$$
\begin{aligned}
&T(U'|U)\exp(-S[U]) \\
&\qquad = T_0(U'|U)\,\min\left(1,\ \frac{T_0(U|U')\exp(-S[U'])}{T_0(U'|U)\exp(-S[U])}\right)\exp(-S[U]) \\
&\qquad = \min\left(T_0(U'|U)\,\exp(-S[U])\,,\ T_0(U|U')\,\exp(-S[U'])\right) \\
&\qquad = T(U|U')\exp(-S[U'])
\end{aligned}
\tag{4.17}
$$

Prove that detailed balance is satisfied.

$$T(U'|U)\,e^{-S[U]} = T_0(U'|U)\min\left(1,\ \frac{T_0(U,U')}{T_0(U'|U)}\,\frac{e^{-SU'}}{e^{-SU}}\right)e^{-SU}$$

$$= \min\left(T_0(U'|U)\,e^{-SU},\ T_0(U,U')\,e^{-SU'}\right)$$

$$T(U|U')\,e^{-SU'} = T_0(U|U')\min\left(1,\ \frac{T_0(U',U)}{T_0(U|U')}\,\frac{e^{-SU}}{e^{-SU'}}\right)e^{-SU'}$$

$$= \min\left(T_0(U|U')\,e^{-SU'},\ T_0(U',U)\,e^{-SU}\right)$$

$$\Rightarrow T(U|U')\,e^{-SU} = T(U|U')\,e^{-SU'}$$