Fourier Accelerated HMC in the Chiral Model

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The Principal Chiral Model

In the continuum, the 2D $SU(N) \times SU(N)$ model is defined via the Euclidean Lagrangian:

$$\mathcal{L} = \frac{1}{T} Tr\, \partial_\mu U \partial_\mu U^\dagger \tag{1}$$

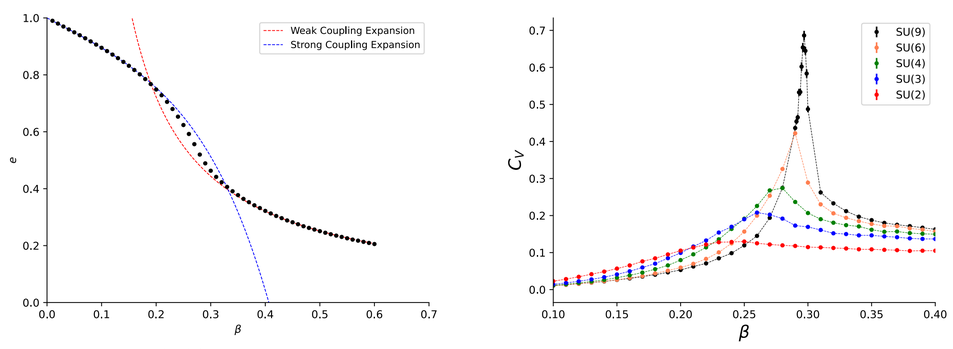
On the lattice, the model is defined via the action:

$$S = -\beta N \sum_{x,\mu>0} Tr\{U_x^\dagger U_{x+\mu} + U_{x+\mu}^\dagger U_x\} \tag{2}$$

- Shares properties with QCD (asymptotic freedom and dynamical mass generation).
- $SU(N) \times SU(N)$ global symmetry but not locally gauge invariant.
- Possible to obtain analytical predictions $\rightarrow$ exact solution through Bethe ansatz.

By studying the effect of Fourier acceleration in this model, we aim to establish a foundation for investigating more complex theories and, ultimately, QCD.

We now present a small subset of the properties of the model analysed with our lattice simulations. We show the $SU(4)$ energy density and the heat capacity for different N.



(a) $SU(4)$ Energy Density **(b)** Heat Capacity for Different N

Figure 1: Properties of the model: energy density and heat capacity

1 The energy density results agree with predictions $\rightarrow$ model validation.

2 Peak in heat capacity $\rightarrow$ suggests a phase transition in the $N \rightarrow \infty$ limit.

HMC & Fourier Acceleration

In HMC the configurations that build up the Markov chain are obtained by introducing a conjugate field π and evolving both fields using a Hamiltonian:

$$H = \frac{1}{2}\pi \cdot \pi + S(U) \tag{3}$$

In turn, this means that the molecular dynamics evolution of the fields is determined by:

$$\dot{\pi}_x = -2i\beta N \sum_{\mu>0} \left((U_{x+\mu} + U_{x-\mu})\, U_x^\dagger - h.c \right) - \frac{1}{N} Tr\{...\} I \tag{4}$$

$$\dot{U}_x = i\pi_x U_x \tag{5}$$

In HMC, higher momentum modes evolve faster than those with lower momentum and impose a strict upper bound on the integration step size. This means the more physical low-energy modes barely evolve $\rightarrow$ high autocorrelations between the configurations. Taking the limit $a \rightarrow 0$ only accentuates this (more high energy modes are included in the simulation), causing the Integrated Autocorrelation Time (IAT) to diverge as $\tau_{IAT} \approx a^{-z} \approx \xi^z$

Fourier acceleration (FA) aims to solve the problem of critical slowing down by speeding up the evolution of low momentum modes and slowing down the high ones. The goal is to make the evolution rate independent of the mode's momentum, removing critical slowing down. The idea behind FA is to modify the dynamics of the system by adding a momentum-dependent mass in the Hamiltonian which can differentiate between the different modes. In particular, this is done by introducing the inverse kernel of the action in the conjugate field term:

$$H = \frac{1}{2}\pi \cdot K^{-1} \cdot \pi + S(U) \tag{6}$$

$$S = U \cdot K \cdot U \tag{7}$$

The name Fourier acceleration comes from the fact that the kernel K is diagonal in Fourier space, which greatly simplifies its inversion. In the case of the principal chiral model, the inverse kernel in Fourier space is given by:

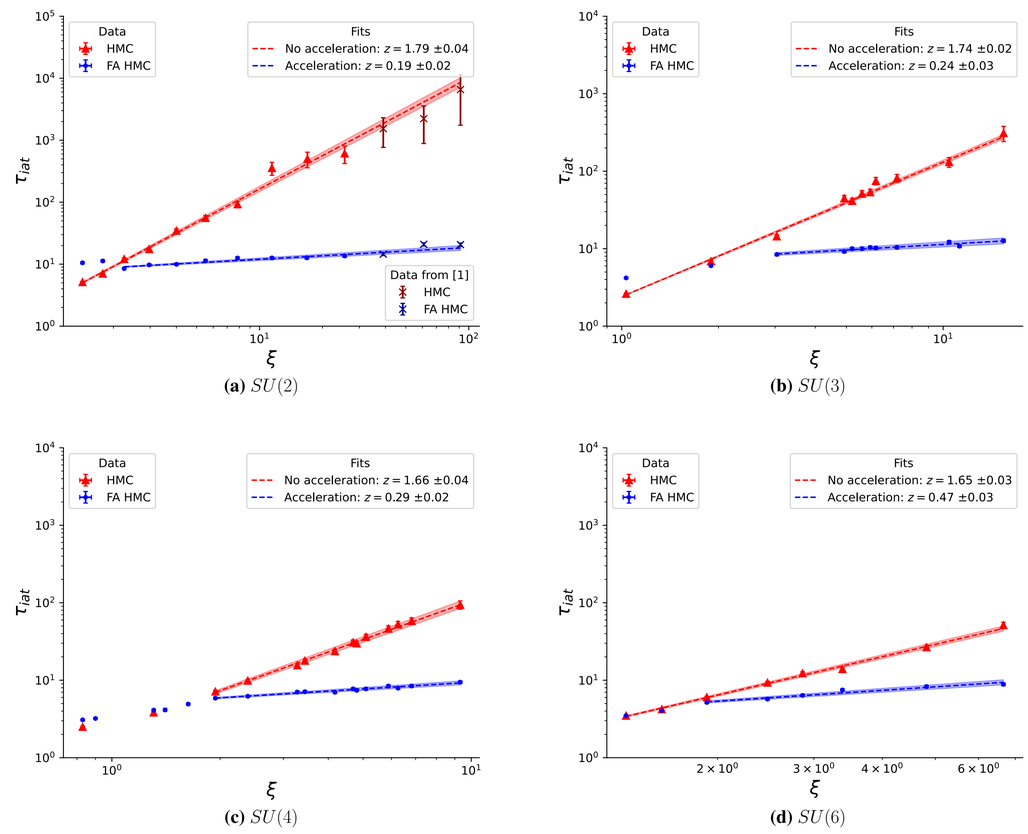
$$\tilde{K}_k^{-1}(M) = \frac{1}{\sum_\mu 4\sin^2(\frac{\pi k \cdot \mu}{L}) + M^2} \tag{8}$$

where M^2 is a tuneable parameter. The modification of the Hamiltonian induces a change in the discrete-time update of the field U:

$$U_x(t+dt) = \exp\{i\mathcal{F}^{-1}[\tilde{K}_k^{-1}(M)\tilde{\pi}_k(t)]_x dt\}\, U_x(t) \tag{9}$$

Acceleration Results

To test the algorithm's efficiency we measured the integrated autocorrelation time of the susceptibility (prone to critical slowing down). The IAT for different correlation lengths ξ and $SU(N)$ groups are presented below for both HMC and FA HMC. This work is a continuation and generalisation of [1] in which $SU(2)$ was examined, therefore we include some of its data for large correlations in our $SU(2)$ plot.



(a) $SU(2)$ **(b)** $SU(3)$ **(c)** $SU(4)$ **(d)** $SU(6)$

Figure 2: Autocorrelation time τ_{IAT} as a function of the correlation length for several $SU(N)$ choices in accelerated and non-accelerated algorithm versions.

The following conclusions can be extracted from our results:

1 FA does not completely eliminate critical slowing down $\rightarrow$ it mitigates it.

2 One order of magnitude speedup at small correlation lengths.

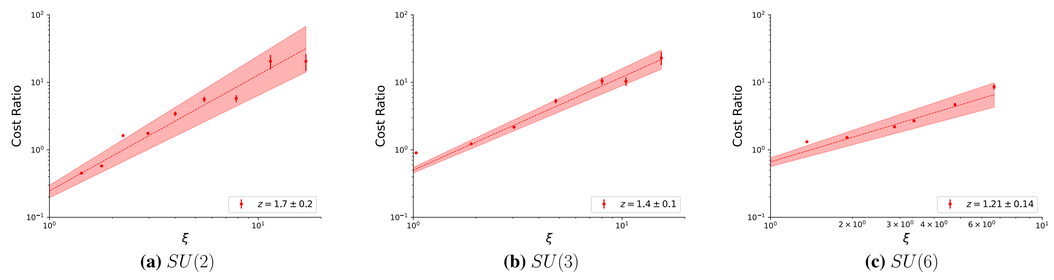
3 Two orders of magnitude improvement at high correlation lengths.

4 The relative advantage of FA HMC over HMC decreases as N increases $\rightarrow$ larger group space associated with higher N?

FA HMC reduces the impact of critical slowing down but also introduces a more complex molecular dynamics evolution. Therefore, it is essential to ensure that the reduction in IAT compensates for any increase in run time. We define the algorithmic cost as:

$$\text{Cost} = \frac{\text{Time}}{\text{Nº Configurations}}\, \tau_{IAT} \tag{10}$$

The plots below show the cost ratio between traditional HMC and FA HMC for various ξ and N values.



(a) $SU(2)$ **(b)** $SU(3)$ **(c)** $SU(6)$

Figure 3: Cost ratio as a function of the correlation length for several $SU(N)$.

1. Results confirm that FA HMC outperforms HMC $\rightarrow$ order of magnitude speed-up for moderate $\xi \sim 10$ even when accounting for run-time.
2. Once more, the advantage of FA HMC diminishes as N increases $\rightarrow$ several elements contribute to the algorithm's cost, all of which could vary as N is increased.

Conclusion & Further Research

- **Generalised FA for general N in the 2D principal chiral model.**
- **Achieved order of magnitude speed-up even at modest correlation lengths.**
- **Verified physical results (exact mass spectra, continuum limit) for the model, exceeding precision of previous studies.**
- **Next step $\rightarrow$ Gauge Theories.**

References

[1] Roger Horsley, Brian Pendleton, and Julian Wack. Hybrid Monte Carlo simulation with Fourier acceleration of the N=2 principal chiral model in two dimensions. *Phys. Lett. B*, 849:138429, 2024.

[2] Pablo Morandé. Mphys Code. https://github.com/pmorande27/MPhysProject, 2024.