Scalar Mesons on the Lattice Using Stochastic Sources on GPU Architecture.

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LATTICE 2014

June 24, 2014
Outline

1. $f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

2. Computation
   - QCD Setup
   - Stochastic Sources
   - Error Analysis on $Z_2$

3. Utilising GPU Architecture
   - Software and Hardware
   - Benchmarks
A simple system with \( I = 0 \) and \( J^{PC} = 0^{++} \).

- Our principal state of interest is the \( \sigma \) or \( f_0(500) \) due to its mysterious nature and debated partonic content. For the unphysical \( 2m_\pi > m_\sigma \), we can measure the mass of the \( \sigma \) directly.

\[
C(t) = \sum_{\bar{p}} A_{\bar{p}} e^{-E_{2\pi(\bar{p})}t} + B e^{-m_\sigma t} + \ldots
\]

In the \( 2m_\pi < m_\sigma \) regime, we will use Lüscher's approach of obtaining the scattering phase shift \( \delta(s) \) in the two-pion, flavour singlet channel.
A simple system with $I = 0$ and $J^{PC} = 0^{++}$.

- The Correlation Function

$$C(t) = \sum_{\vec{x}, \vec{y}, \vec{z}} \langle 0 | T \{ P_-(t, \vec{z}) P_+(t, \vec{y}) P_+(0, \vec{x}) P_-(0, \vec{0}) \} | 0 \rangle$$

Let:

$$P_-(t, \vec{z}), \ P_+(t, \vec{y}) \rightarrow \bar{d}(z)\gamma_5 u(z), \ \bar{u}(y)\gamma_5 d(y)$$

$$P_-(0, \vec{x}), \ P_+(0, \vec{0}) \rightarrow \bar{d}(x)\gamma_5 u(x), \ \bar{u}(0)\gamma_5 d(0)$$

and perform all possible Wick contractions on the quark operators.
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computation

Utilising GPU Architecture

Quark Propagator Diagrams

$C_{sum}(t) = C_0(t) + C_1(t) - C_2(t) - C_3(t)$

One would place a point source at 0 and one at $Z$ and use $\gamma_5$ conjugation to calculate $C_{sum}(t)$. 
\[ f_0(500) \text{ from } \pi^+ \pi^- \rightarrow \pi^+ \pi^- \text{ scattering} \]

**Quark Propagator Diagrams**

\[ C_{\text{sum}}(t) = C_0(t) + C_1(t) - 2C_2(t) \]

\( C_2(t) \) and \( C_3(t) \) are hermitian conjugate. This will save some calculation time, but not very much compared to inversions.
Disconnected Parts.

We can remove the disconnected parts when calculating the correlation function values to leave the purely connected contribution.

\[
C_0(t) \neq \sum_{\vec{x}, \vec{y}, \vec{z}} \langle \text{Tr}[S(y, 0)S^\dagger(y, 0)] \rangle \langle \text{Tr}[S(z, x)S^\dagger(z, x)] \rangle u \\
= \sum_{\vec{x}, \vec{y}, \vec{z}} \left[ \langle \text{Tr}[S(y, 0)S^\dagger(y, 0)] \rangle - \langle \text{Tr}[S(y, 0)S^\dagger(y, 0)] \rangle u \right] u \\
\times \langle \text{Tr}[S(z, x)S^\dagger(z, x)] \rangle - \langle \text{Tr}[S(z, x)S^\dagger(z, x)] \rangle u \right] u
\]

This will tend to reduce the absolute value of correlation functions and errors will become much more significant. This procedure is repeated for \( C_1(t) \).
We performed a quenched calculation using a clover improved operator on a $4^38$ lattice with periodic B.C. and the following:

| Param. | Beta  | $m_0 a$ | $a m_\pi$ | $a \text{ (GeV}^{-1})$ | $m_\pi \text{ (GeV)}$ | Therm | Skip | Config. |
|--------|-------|---------|-----------|-----------------|-----------------|-------|------|---------|
| Value  | 5.96  | -0.3    | 1.0       | 0.51            | 2.0             | 5000  | 200  | 100     |

High Beta places the system well into the deconfinement (high-temperature) phase with very unphysical pion masses. However, some studies have shown that when $m_\sigma < m_{2\pi}$, one may treat the $\sigma$ as a bound state. $^{12}$ In this regime, $m_\sigma$ is the lowest energy state.

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$^1$ T. Kunihiro et al. (2004), arXiv:hep-ph/0310312 [hep-ph].

$^2$ S. Prelovsek, T. Draper, C. B. Lang, M. Limmer, K.-F. Liu, et al. (2010), arXiv:1005.0948 [hep-lat].
Point sources are resource intensive. One must perform $N_{col} \times N_{spin} \times L^3 T$ inversions per data point for spin-colour-time dilution.

$$M_{ab}|\phi_b\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Stochastic sources can significantly reduce the number of required inversions for moderate to large lattice sizes.
Consider some set of vectors $|\eta^i_b\rangle$ such that:

$$\lim_{N_R \to \infty} \frac{1}{N_R} \sum_{i=1}^{N_R} |\eta^i_b\rangle \langle \eta^i_c | = \delta_{bc}$$

$$\lim_{N_R \to \infty} \frac{1}{N_R} \sum_{i=1}^{N_R} |\eta^i_b\rangle = 0$$

We can take advantage of this by inverting $M_{ab} |\phi_b\rangle = |\eta^i_a\rangle$ $N_R$ times for some $N_R$ number of vectors:

$$\Rightarrow \lim_{N_R \to \infty} \frac{1}{N_R} \sum_{i=1}^{N_R} M_{ab} |\phi_b\rangle \langle \eta^i_c | = \delta_{ac}$$

...but how big does $N_R$ have to be in order to get a trustworthy approximation to the true propagator?
To answer this question, we chose to investigate the Mean Square Error, Variance, and Bias of the purely stochastic contribution to the error budget for $Z_2$.

\[
M.S.E.[X_{sto}] = Var[X_{sto}] + Bias^2[X_{sto}],
\]

\[
M.S.E.[X_{sto}] = \frac{1}{n} \sum_{i=1}^{n} [X_{sto} - X_{ps}]^2
\]

\[
Bias[X_{sto}] = \frac{1}{n} \sum_{i=1}^{n} [X_{sto} - X_{ps}].
\]
M.S.E, Variance, and Bias

To answer this question, we chose to investigate the Mean Square Error, Variance, and Bias of the purely stochastic contribution to the error budget for $Z_2$ and Gaussian sources.

\[
\text{M.S.E. } \left[ \frac{X_{sto}(t)}{X_{ps}(t)} \right] = \text{Var} \left[ \frac{X_{sto}(t)}{X_{ps}(t)} \right] + \text{Bias}^2 \left[ \frac{X_{sto}(t)}{X_{ps}(t)} \right],
\]

\[
\text{M.S.E. } \left[ \frac{X_{sto}(t)}{X_{ps}(t)} \right] = \frac{1}{n} \sum_{i=1}^{n} \left[ \frac{X_{sto}(t)}{X_{ps}(t)} - 1 \right]^2
\]

\[
\text{Bias } \left[ \frac{X_{sto}(t)}{X_{ps}(t)} \right] = \frac{1}{n} \sum_{i=1}^{n} \left[ \frac{X_{sto}(t)}{X_{ps}(t)} - 1 \right].
\]
Bias is the main source of error:

\[ S^{-1}_{true} = S^{-1}_{ab} \approx \sum M^{-1}_{ab} |\eta_b\rangle \langle \eta_c| \]

\[ \text{Tr}[S^{-1}_{ab} S^{-1\dag}_{ab}] \approx \sum M^{-1}_{ab} \underbrace{|\eta_b\rangle \langle \eta_c|}_{\text{Off-diags}} \underbrace{|\eta_c\rangle \langle \eta_d|}_{\text{Off-diags}} M^{-1\dag}_{ad} \]

Solution \rightarrow \text{Tr}[S^{-1}_{ab} S^{-1\dag}_{ab}] \approx \sum M^{-1}_{ab} \underbrace{|\eta_b\rangle \langle \eta_c|}_{\text{Off-diags}} \underbrace{|\xi_c\rangle \langle \xi_d|}_{\text{Off-diags}} M^{-1\dag}_{ad} \]

N.B. This is why \( Z_2 \) out-performs other distributions. Off-diagonal terms contribute roughly the same error\(^3\) for any parent distribution, but the unit size and bimodality of \( Z_2 \) enforces the leading diagonal to be the identity.

\(^3\)S Dong, K.F Liu, (1993) hep-lat/9308015
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computation
Utilising GPU Architecture

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$

\[ C_{\text{sum}}(t) \text{ 2 source BIAS (%sum)} \]

BIAS (%sum)
Zero Plane
\(+/- 10\%
\(+/- 2\%\)

Time Slice
NRAND
BIAS (%sum)
\( f_0(500) \) from \( \pi^+ + \pi^- \rightarrow \pi^+ + \pi^- \) scattering

Computational Utilising GPU Architecture

QCD Setup
Stochastic Sources
Error Analysis on \( Z_2 \)
Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.23 +/- 0.11
N_{RAND}=100
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computaion
Utilising GPU Architecture

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computaion
Utilising GPU Architecture

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$

Effective Mass (Point Source) = $0.38 \pm 0.01$
Effective Mass (Stochastic Source) = $0.37 \pm 0.03$

$N_{\text{RAND}}=300$
$f_0(500)$ from $\pi_+\pi_- \rightarrow \pi_+\pi_-$ scattering

Computaion
Utilising GPU Architecture

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$

Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.35 +/- 0.02
$N_{\text{RAND}}=400$
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computation

Utilising GPU Architecture

QCD Setup

Stochastic Sources

Error Analysis on $Z_2$

Effective Mass (Point Source) = 0.38 +/- 0.01

Effective Mass (Stochastic Source) = 0.37 +/- 0.02

$N_{\text{RAND}}=500$
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computation
Utilising GPU Architecture

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$

$C_{\text{sum}}(t)$

Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.37 +/- 0.02

$N_{\text{RAND}}=600$
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

**Computation**

**Utilising GPU Architecture**

**QCD Setup**

**Stochastic Sources**

**Error Analysis on $Z_2$**

Effective Mass (Point Source) = 0.38 +/- 0.01

Effective Mass (Stochastic Source) = 0.38 +/- 0.02

$N_{RAND}=700$
$f_0(500)$ from $\pi^+\pi^- \to \pi^+\pi^-$ scattering

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$

Computaion
Utilising GPU Architecture

Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.38 +/- 0.02
$N_{RAND}=800$
$f_0(500)$ from $\pi^+\pi^- \to \pi^+\pi^-$ scattering

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$

Computation
Utilising GPU Architecture

Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.38 +/- 0.02
$N_{\text{RAND}}=900$
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computaion

Utilising GPU Architecture

QCD Setup

Stochastic Sources

Error Analysis on $Z_2$

Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.38 +/- 0.02
$N_{\text{RAND}}=1000$
**Error breakdown using two independent sets of 1000 random vectors from \( Z_2 \).**

| Src. | Qty.            | \( t = 1 \) | 2   | 3   | 4   | 5   | 6   | 7   |
|------|-----------------|-------------|-----|-----|-----|-----|-----|-----|
| P.S. | \( C_{sum}(t) \) | 3.84        | 2.82| 2.22| 2.21| 2.35| 2.72| 3.65|
| Sto  | \( C_{sum}(t) \) | 3.88        | 2.76| 2.32| 2.37| 2.30| 2.72| 3.67|
| P.S. | Jack-Knife      | 0.87        | 0.74| 0.58| 0.62| 0.63| 0.63| 0.70|
| Sto  | Jack-Knife      | 0.87        | 0.73| 0.60| 0.63| 0.62| 0.63| 0.71|
| -    | Rel err \( C(t)(\%) \) | 0.87        | -2.11| 4.05| 7.29| -2.24| 0.03| 0.52|
| Sto  | Bias(\%)       | 0.87        | -2.11| 4.05| 7.29| -2.24| 0.03| 0.52|
| Sto  | \( \sqrt{n} \) (stoch) | 0.06 | 0.08 | 0.08 | 0.07 | 0.07 | 0.06 | 0.06 |

Stochastic standard error calculated using,

\[
\frac{\sigma_{sto}(X_{sto})}{\sqrt{n}} = \sqrt{\frac{\text{Var}(X_{sto})}{n}} = \sqrt{\frac{\text{M.S.E.}(X_{sto}) - \text{Bias}^2(X_{sto})}{n}},
\]

for \( n \) gauge field configurations.
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computaion

Utilising GPU Architecture

QCD Setup
Stochastic Sources
Error Analysis on $Z_2$

$C_{\text{sum}}(t)$ 2 source BIAS (%sum)

BIAS (%sum)
- Zero Plane
- +/- 10%
- +/- 2%

Time Slice

$N_{\text{RAND}}$
The Disconnected Diagram is the Culprit!

\[ f_0(500) \text{ from } \pi^+\pi^- \rightarrow \pi^+\pi^- \text{ scattering} \]

Computation

Utilising GPU Architecture

QCD Setup

Stochastic Sources

Error Analysis on $Z_2$

C$_1(t)$ 2 source BIAS (%sum)

BIAS (%sum)

Zero Plane

+/- 10%

+/- 2%

Time Slice

N$_{RAND}$

BIAS (%sum)
We use the functionality of CPS and replaced its inversion function with one from QUDA. This required us to:

- Rearrange the clover matrix
- Rearrange the gauge field SU(3) matrices
- Write GPU kernels for the matrix algebra

One simply replaces the CPS file:

```
src/util/lattice/f_clover/f_clover.C
```

QUDA need not be modified. Instructions can be found at

`www.rpi.edu/~giedtj/`
Hardware

Tesla C2050
Assuming that $N_{RAND} \approx 1000$ gives acceptable results i.e. 2-5% relative error on $C_{sum}(t)$

\[
\frac{\#P.S. \text{ Inversions}}{\#Sto. \text{ Inversions}} = \frac{L^3 T}{2 \times 1000 T} = 1 \Rightarrow L \approx 12
\]

Speed-up ratios for inversions:

| Lattice (L) | 12 | 20 | 24 | 32 | 64 |
|-------------|----|----|----|----|----|
| Speed-up    | 0.87 | 4.00 | 6.91 | 16.4 | 131 |
Summary

- **Scalar States** can be investigated in the $I = 0$ flavour singlet channel using $\pi^+\pi^- \rightarrow \pi^+\pi^-$. 
- **Stochastic Sources** are a viable option to significantly reduce calculation time with acceptable error, if used judiciously.
- **GPU Architecture** is a cheap, under utilised resource, waiting to be exploited.

**Outlook**

- Other statistical techniques such as Gaussian/Stout Smearing can be investigated.
- Using **Momentum** sources could make inversion time insignificant, but one must fix to Landau gauge.
- As soon as resources are secured, we can perform the calculations on **Larger Lattices** and extract physics.
$C_0(t)$ Surface Plot (Backup)

$C_0(t)$ 2 source BIAS (%sum)

BIAS (%sum)
Zero Plane

Time Slice

NRAND

BIAS (%sum)
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computaion

Utilising GPU Architecture

$C_1(t)$ Surface Plot (Backup)

$C_1(t)$ 2 source BIAS (%sum)
$f_0(500)$ from $\pi^+\pi^- \to \pi^+\pi^-$ scattering

Computaion

Utilising GPU Architecture

**$C_3(t)$ Surface Plot (Backup)**

$C_3(t)$ 2 source BIAS (%sum)

BIAS (%sum)

Zero Plane

Time Slice

NRAND

BIAS (%sum)

$35/39$ Joel Giedt, Dean Howarth

Scalar Mesons using GPU Arch
$C_{sum}(t)$ Surface Plot (Backup)

$C_{sum}(t)$ 2 source BIAS (%sum)

BIAS (%sum)  
Zero Plane  
+/- 10%  
+/- 2%

Time Slice
NRAND
BIAS (%sum)

Scalar Mesons using GPU Arch

Joel Giedt, Dean Howarth
$C_0(t)$ Cosh Fit (Backup)

Effective Mass (Point Source) = 1.02 +/- 0.04
Effective Mass (Stochastic source) = 1.02 +/- 0.04

$N_{RAND}=1000$
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering

Computaion

Utilising GPU Architecture

Software and Hardware

Benchmarks

$C_1(t)$ Cosh Fit (Backup)

Effective Mass (Point Source) = 0.30 +/- 0.02
Effective Mass (Stochastic Source) = 0.29 +/- 0.03

$N_{\text{RAND}}=1000$
$f_0(500)$ from $\pi^+\pi^- \rightarrow \pi^+\pi^-$ scattering
Computaion
Utilising GPU Architecture

$C_2(t)$ Cosh Fit (Backup)

Effective Mass (Point Source) = 1.53 +/- 0.41
Effective Mass (Stochastic Source) = 1.55 +/- 0.41
Fitting points 2-6 inclusive only

$N_{\text{RAND}}=1000$