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

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Outline

A simple system with $I = 0$ and $J^{PC} = 0^{++}$.

- Our principal state of interest is the σ 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 σ directly.

$$C(t) = \sum_{\vec{p}} A_{\vec{p}} e^{-E_{2\pi(\vec{p})}t} + Be^{-m_\sigma t} + \dots$$

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

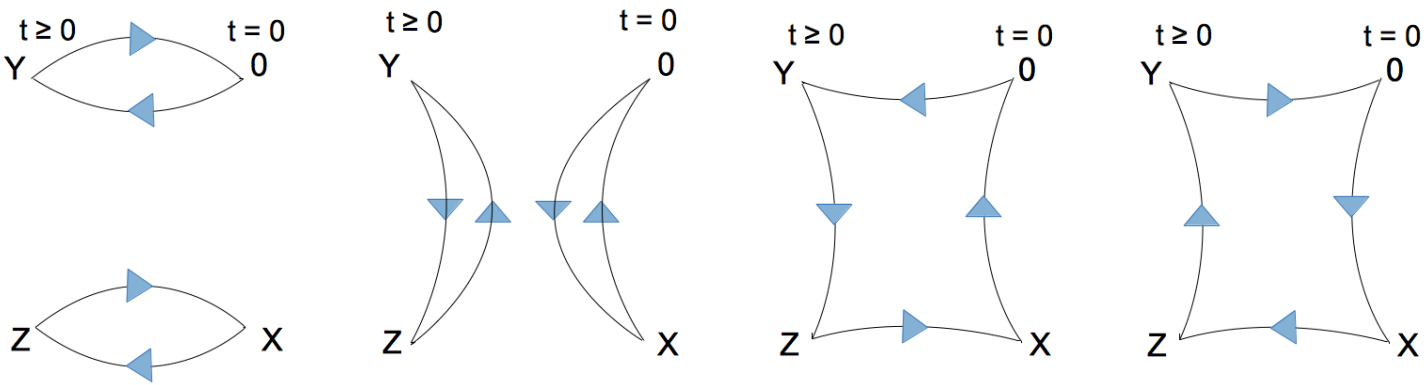
$$C(t) = \sum_{\vec{x},\vec{y},\vec{z}} \langle 0 | T\{P_-(t,\vec{z})P_+(t,\vec{y})P_+(0,\vec{x})P_-(0,\vec{0})\}|0\rangle$$

Let:

$$\begin{aligned} P_-(t,\vec{z}),\ P_+(t,\vec{y}) &\to \bar{d}(z)\gamma_5 u(z),\ \bar{u}(y)\gamma_5 d(y) \\ P_-(0,\vec{x}),\ P_+(0,\vec{0}) &\to \bar{d}(x)\gamma_5 u(x),\ \bar{u}(0)\gamma_5 d(0) \end{aligned}$$

and perform all possible Wick contractions on the quark operators.

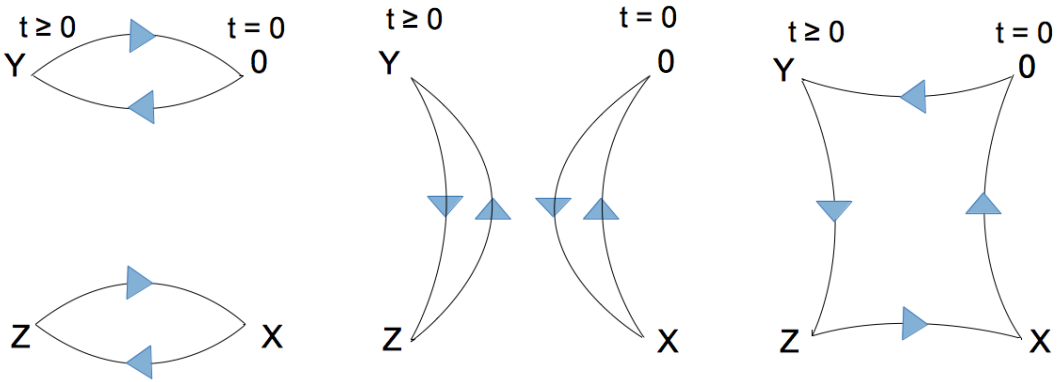
Quark Propagator Diagrams



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

One would place a point source at 0 and one at Z and use γ_5 conjugation to calculate $C_{sum}(t)$.

Quark Propagator Diagrams



$$C_{sum}(t) = C_0(t) \quad + \quad C_1(t) \quad - \quad 2C_2(t)$$

$C_2(t)$ 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.

$$C_0(t) \neq \sum_{\vec{x},\vec{y},\vec{z}} \langle \mathrm{Tr}[S(y,0)S^\dagger(y,0)]\rangle \langle \mathrm{Tr}[S(z,x)S^\dagger(z,x)]\rangle_U$$
$$= \sum_{\vec{x},\vec{y},\vec{z}} \Big[\langle \mathrm{Tr}[S(y,0)S^\dagger(y,0)] - \langle \mathrm{Tr}[S(y,0)S^\dagger(y,0)]\rangle_U \rangle_U$$
$$\times \langle \mathrm{Tr}[S(z,x)S^\dagger(z,x)] - \langle \mathrm{Tr}[S(z,x)S^\dagger(z,x)]\rangle_U \rangle_U \Big]$$

This will tend to reduce the absolute value of correlation functions and errors will become much more significant. This procedure is repeated for $C_1(t)$.

QCD Setup

We performed a quenched calculation using a clover improved operator on a $4^3 8$ lattice with periodic B.C. and the following:

Param.	Beta	$m_0 a$	am_π	$a(\text{GeV}^{-1})$	$m_\pi(\text{GeV})$	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 σ as a bound state. [1][2] In this regime, m_σ is the lowest energy state.

[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].

Stochastic Sources

- 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.

Stochastic Sources

Consider some set of vectors $|\eta_b^i\rangle$ such that:

$$\lim_{N_R\to\infty} \frac{1}{N_R} \sum_{i=1}^{N_R} |\eta_b^i\rangle\langle\eta_c^i| = \delta_{bc}$$

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

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

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

...but how big does N_R have to be in order to get a trustworthy approximation to the true propagator?

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.

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

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

$$Bias[X_{sto}] = \frac{1}{n}\sum_{i=1}^{n}[X_{sto} - X_{ps}].$$

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.

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

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

$$Bias\left[\frac{X_{sto}(t)}{X_{ps}(t)}\right] = \frac{1}{n}\sum_{i=1}^{n}\left[\frac{X_{sto}(t)}{X_{ps}(t)} - 1\right].$$

Bias Rather Than Variance

Bias is the main source of error:

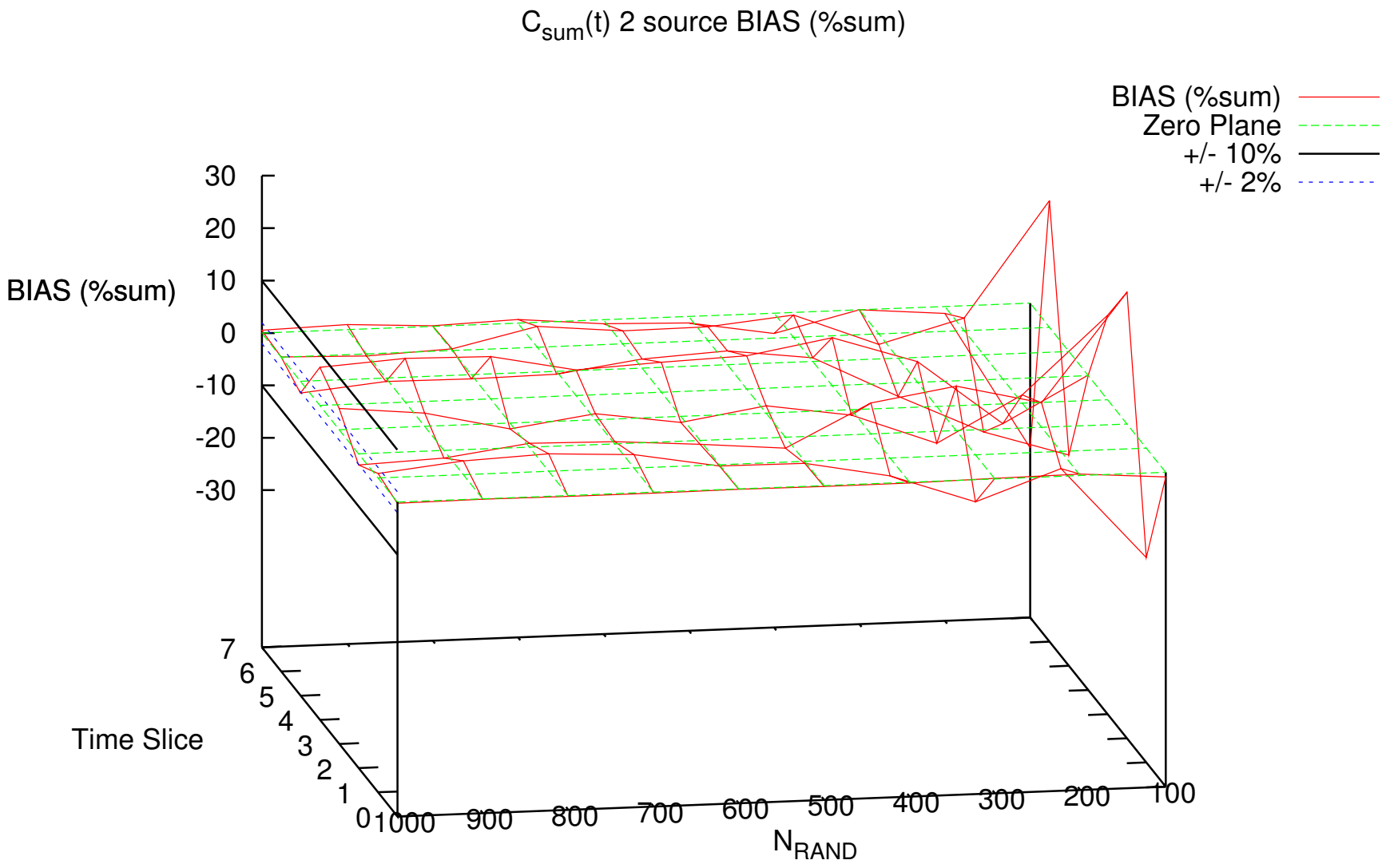
$$S_{true}^{-1} = S_{ab}^{-1} \approx \sum M_{ab}^{-1} |\eta_b\rangle\langle\eta_c|$$

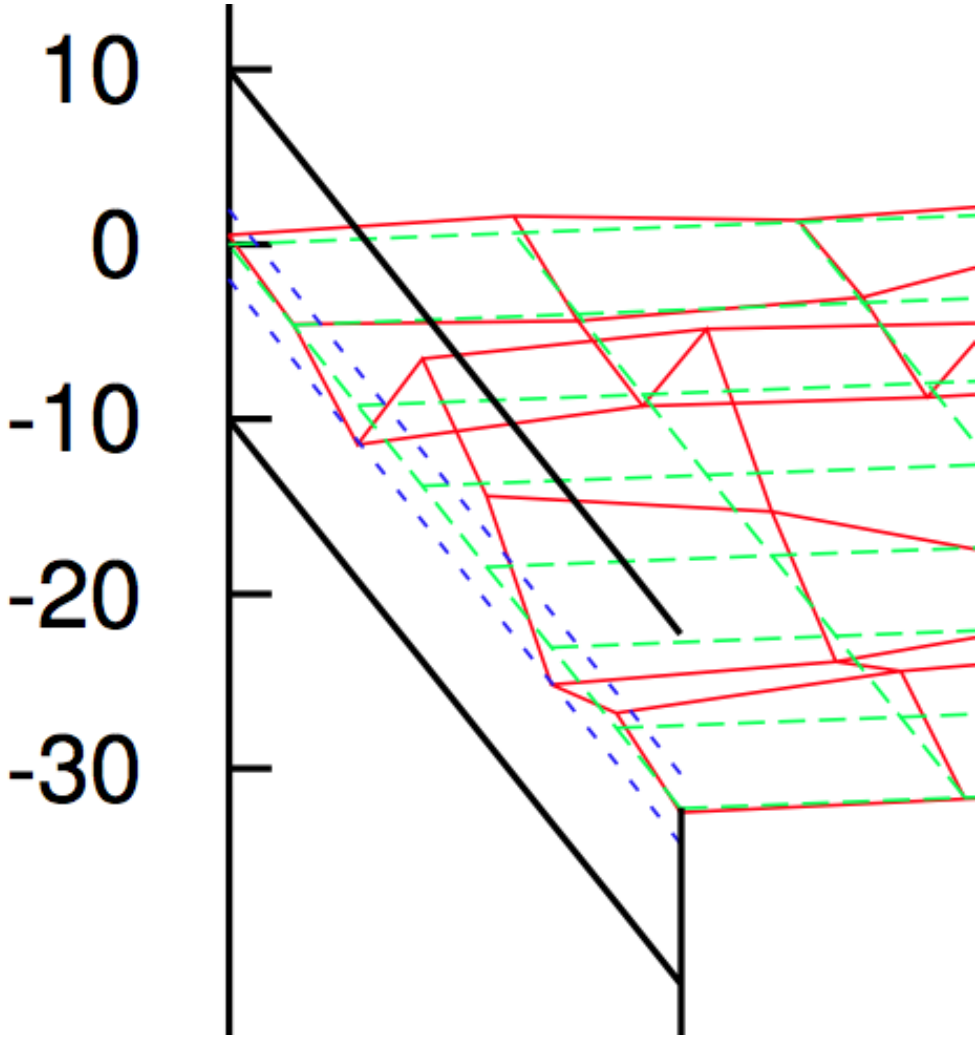
$$\mathrm{Tr}[S_{ab}^{-1} S_{ab}^{-1\dagger}] \approx \sum M_{ab}^{-1} \underbrace{|\eta_b\rangle\langle\eta_c|\eta_c\rangle\langle\eta_d|}_{\text{Off-diags} > 0} M_{ad}^{-1\dagger}$$

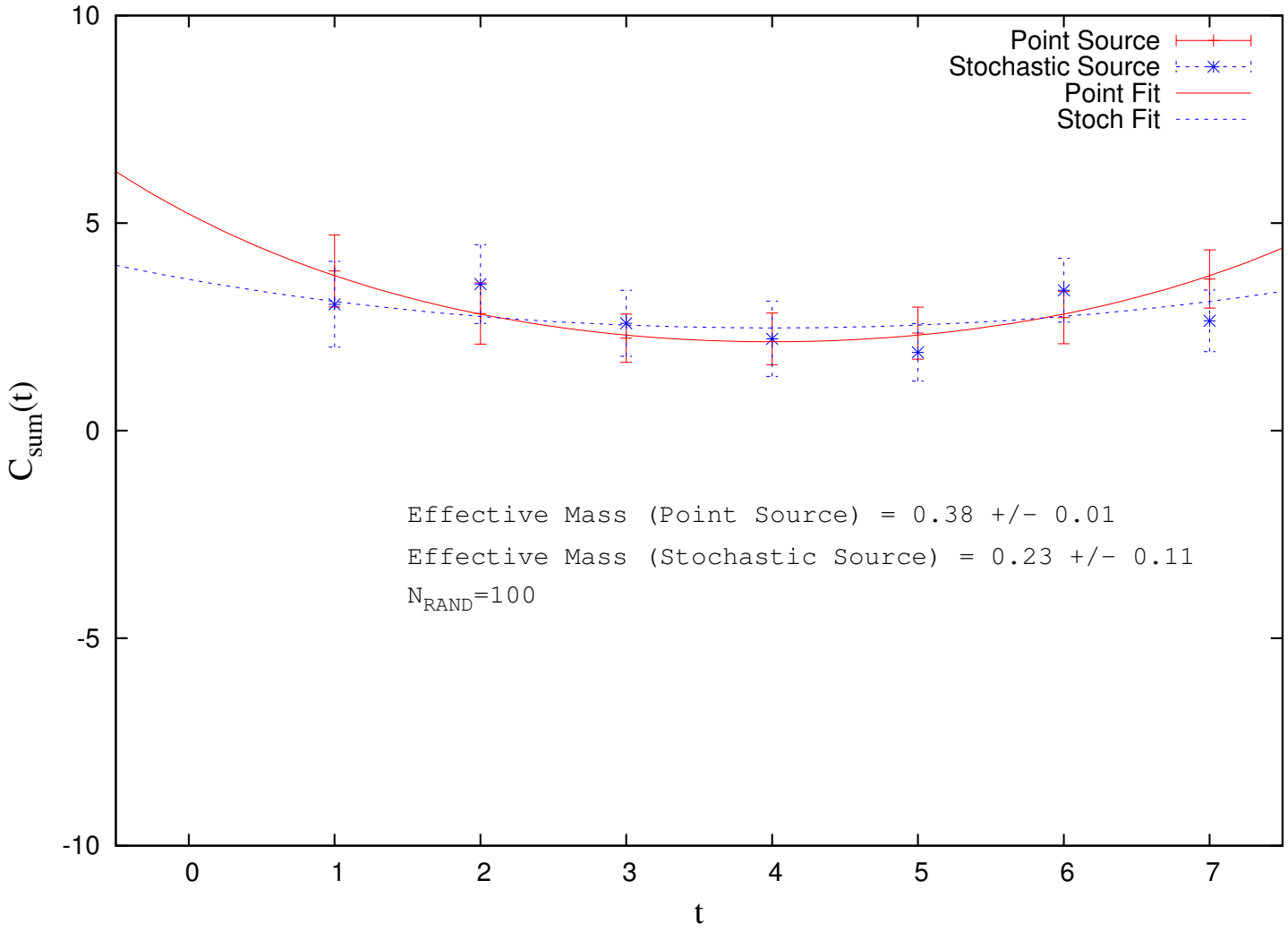
$$\text{Solution} \to \mathrm{Tr}[S_{ab}^{-1} S_{ab}^{-1\dagger}] \approx \sum M_{ab}^{-1} \underbrace{|\eta_b\rangle\langle\eta_c|\xi_c\rangle\langle\xi_d|}_{\text{Off-diags} \approx 0 \pm \epsilon} M_{ad}^{-1\dagger}$$

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


C_sum(t) 2 source BIAS (%sum)
BIAS (%sum)
Zero Plane
+/- 10%
+/- 2%
BIAS (%sum)
30
20
10
0
-10
-20
-30
Time Slice
7
6
5
4
3
2
1
0
1000
900
800
700
600
500
400
300
200
100
N_RAND


10
0
-10
-20
-30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Stochastic Source
Point Fit
Stoch Fit
Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.23 +/- 0.11
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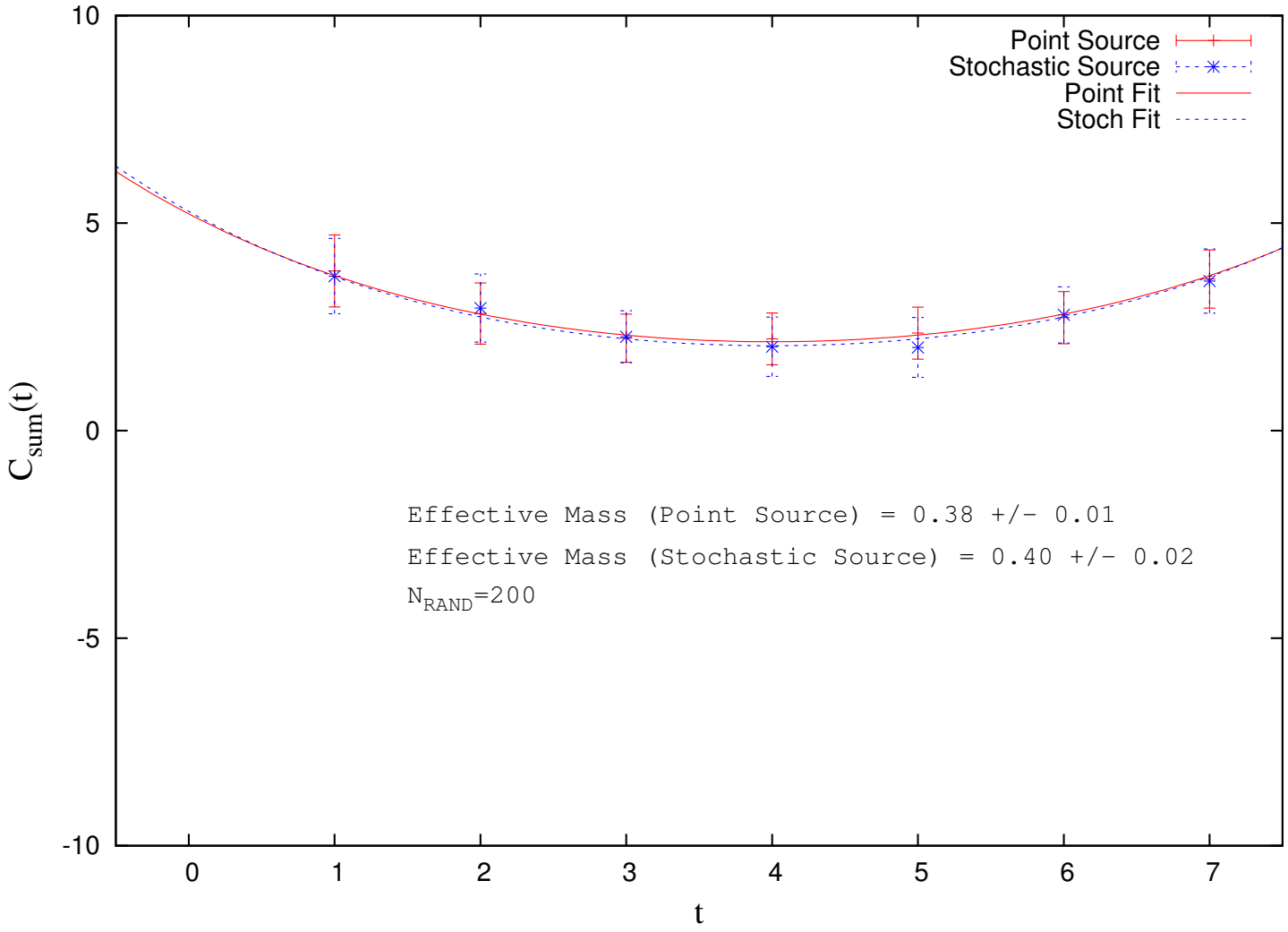
C_sum(t)
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7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Stochastic Source
Point Fit
Stoch Fit
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Effective Mass (Stochastic Source) = 0.40 +/- 0.02
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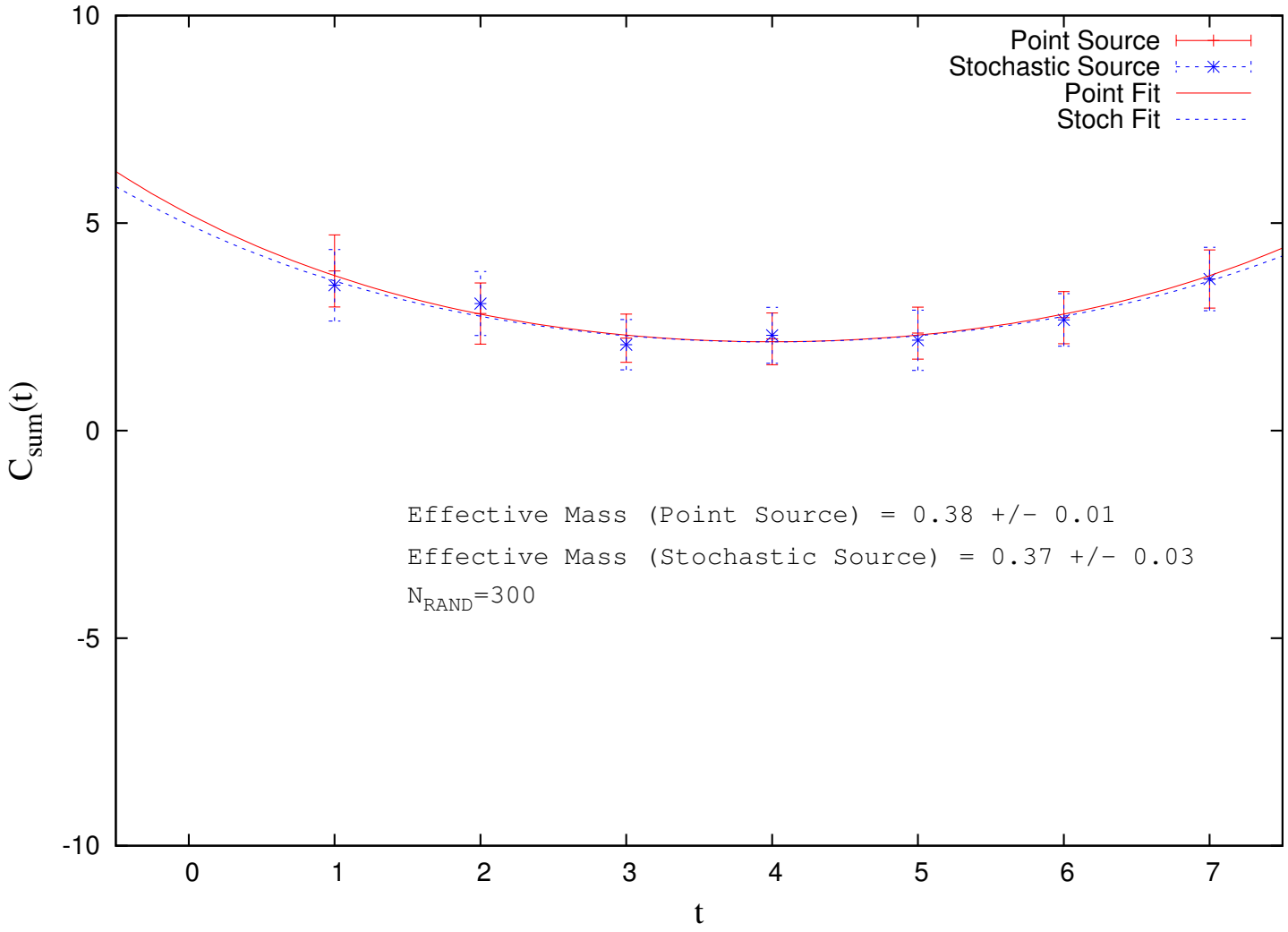
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7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Stochastic Source
Point Fit
Stoch Fit
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Effective Mass (Stochastic Source) = 0.37 +/- 0.03
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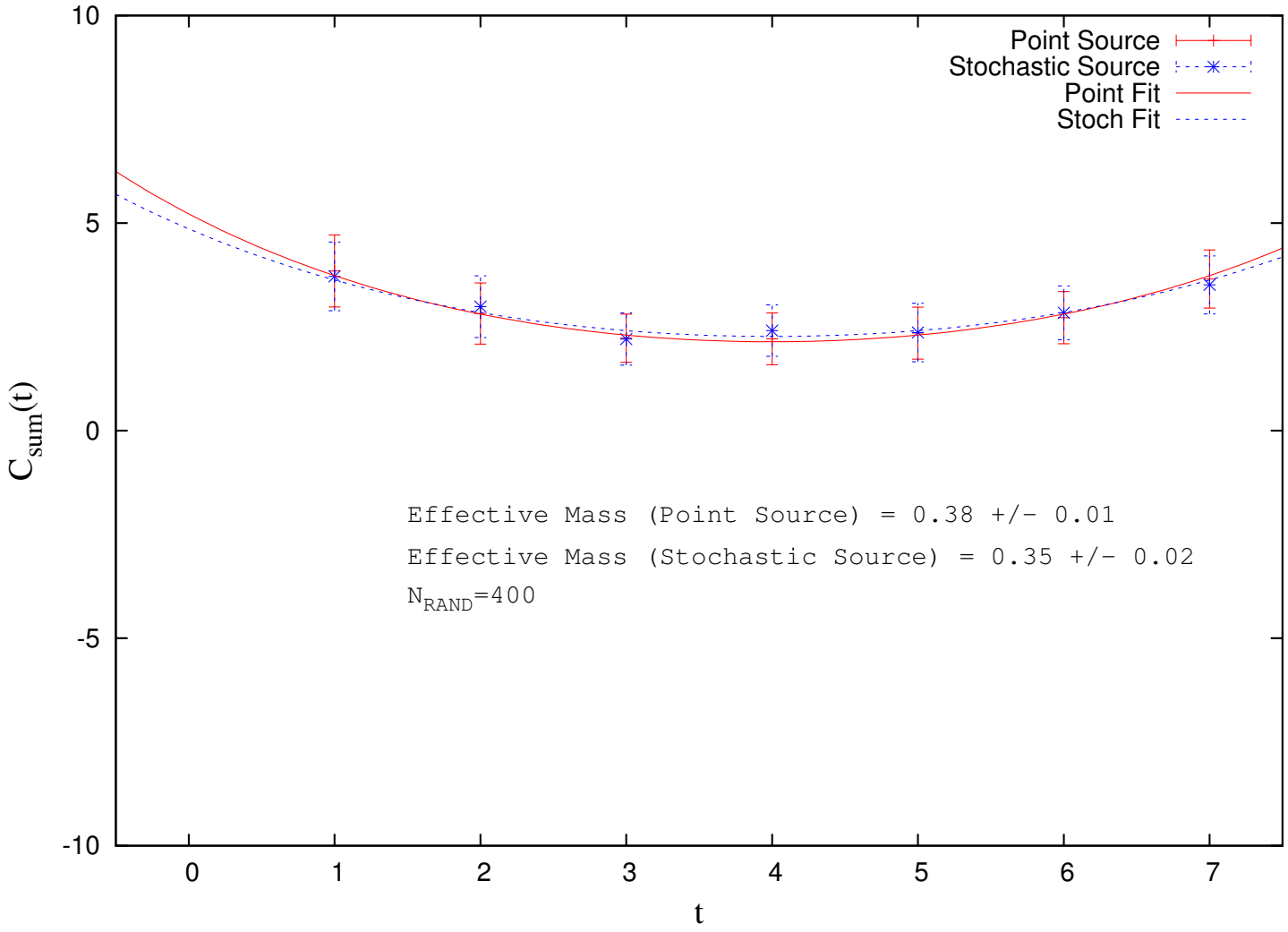
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7


Point Source
Stochastic Source
Point Fit
Stoch Fit
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Effective Mass (Stochastic Source) = 0.35 +/- 0.02
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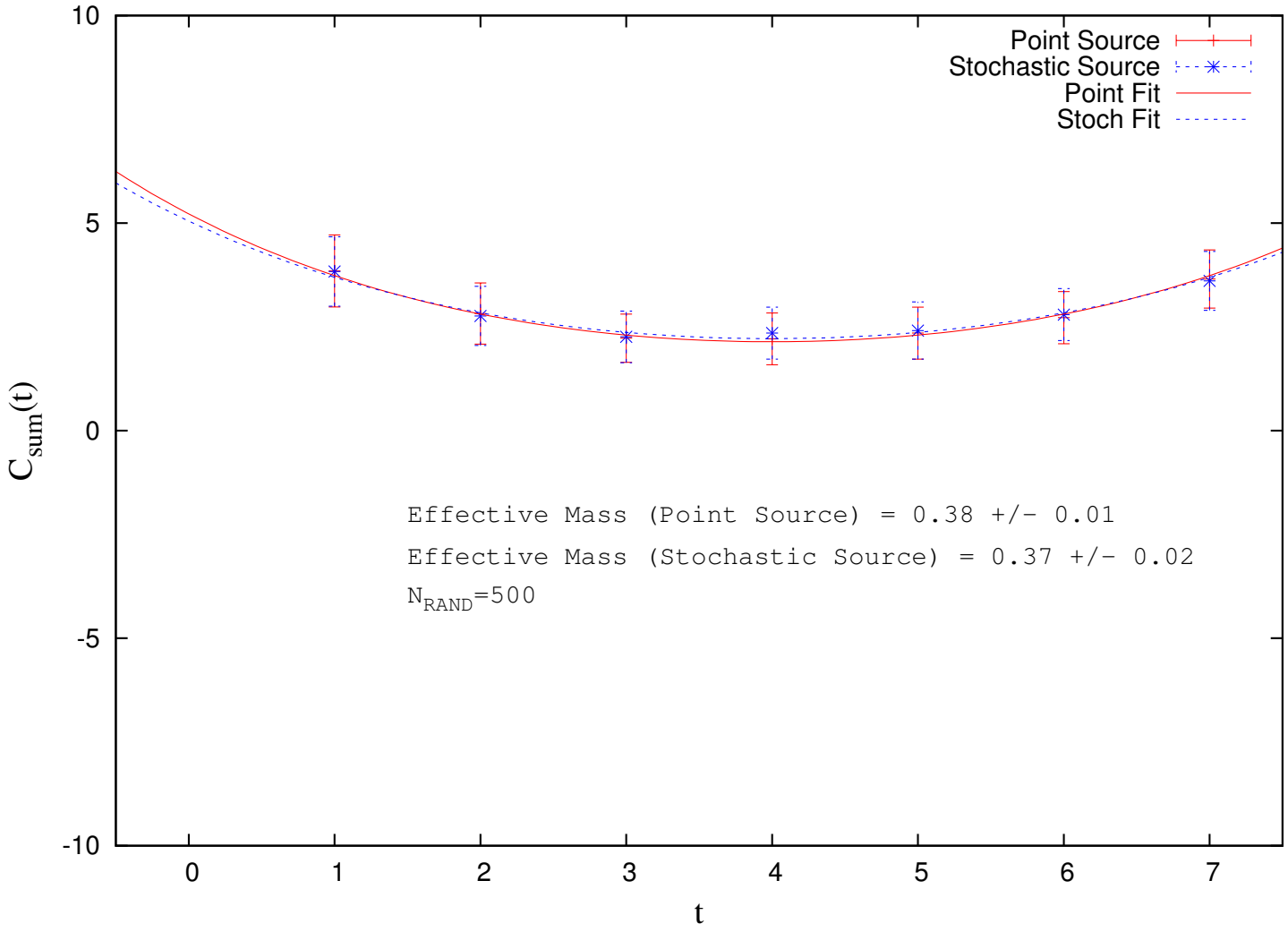
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7


Point Source
Stochastic Source
Point Fit
Stoch Fit
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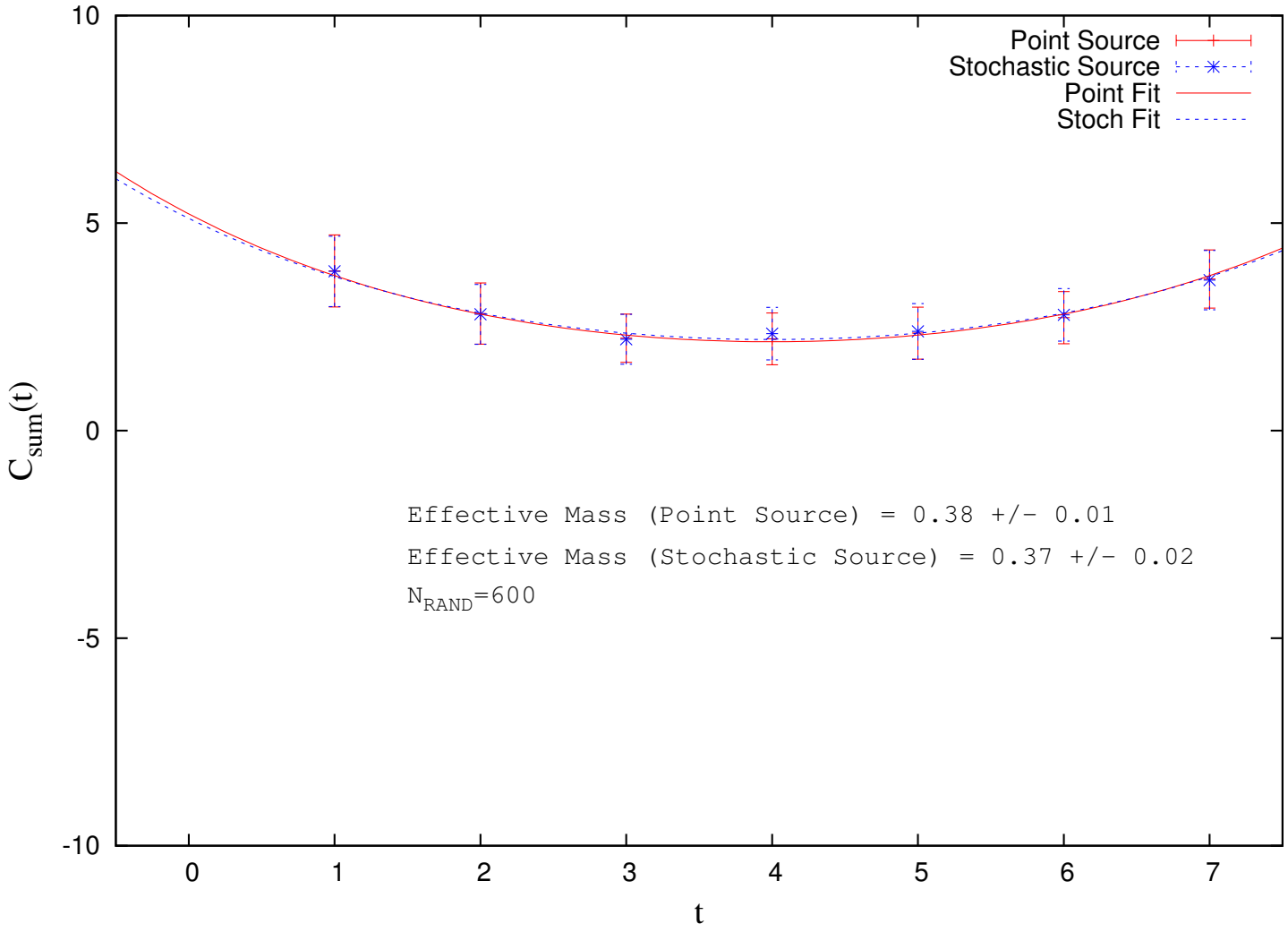
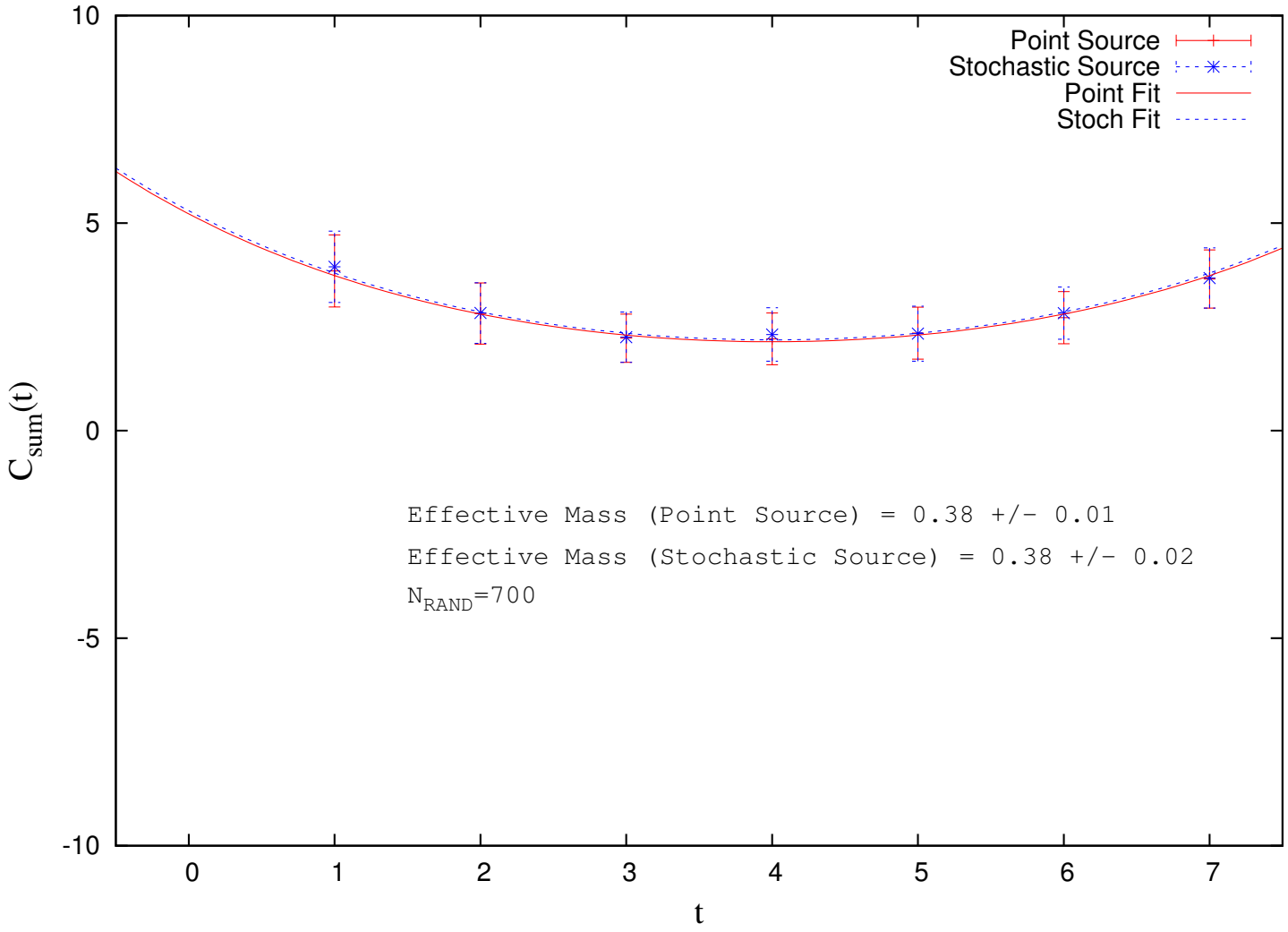
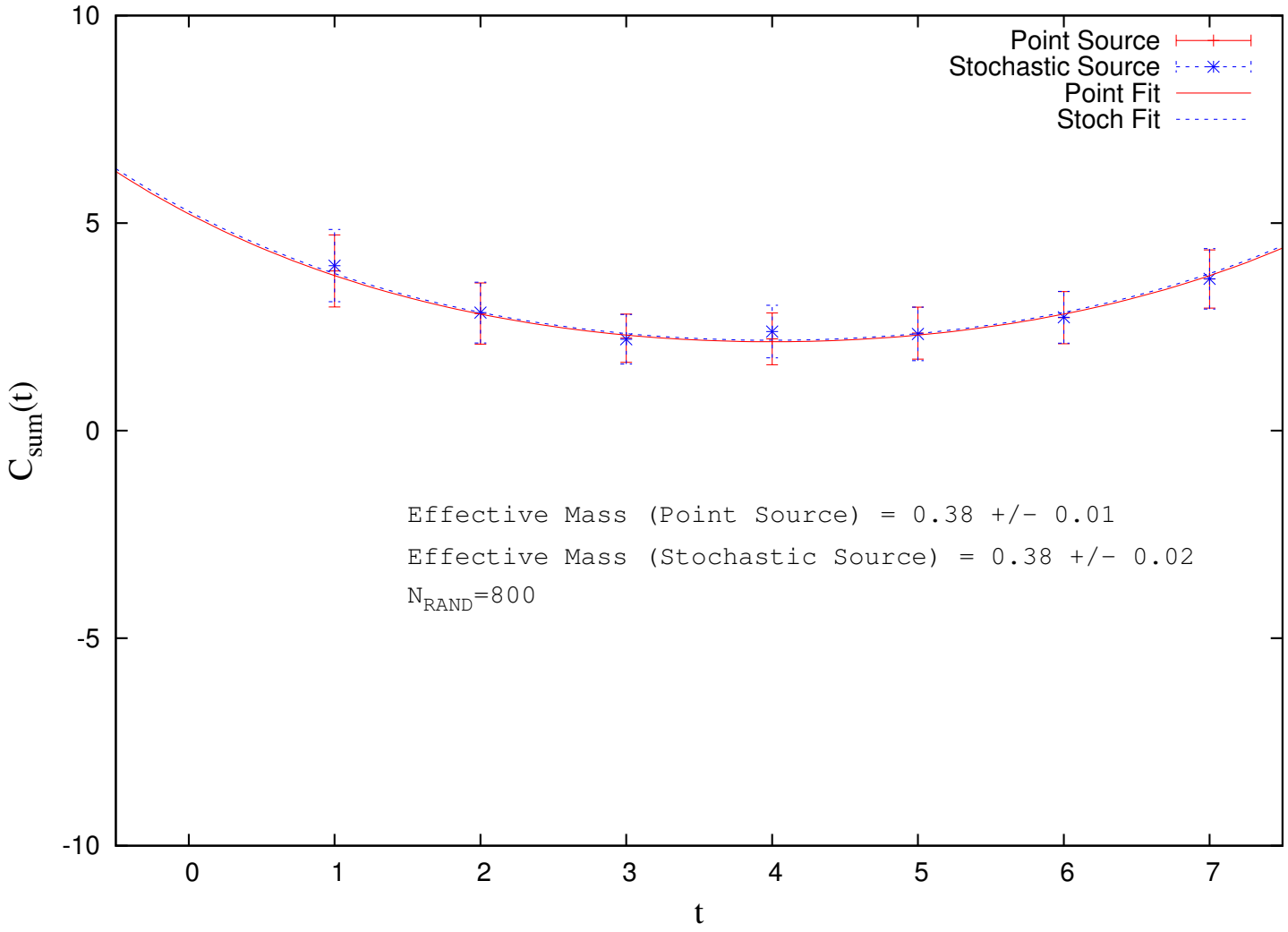
Effective Mass (Stochastic Source) = 0.37 +/- 0.02
N_RAND=500
C_sum(t)
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7


Point Source
Stochastic Source
Point Fit
Stoch Fit
Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.37 +/- 0.02
N_RAND=600
C_sum(t)
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7


Point Source
Stochastic Source
Point Fit
Stoch Fit
Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.38 +/- 0.02
N_RAND=700
C_sum(t)
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7


Point Source
Stochastic Source
Point Fit
Stoch Fit
Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.38 +/- 0.02
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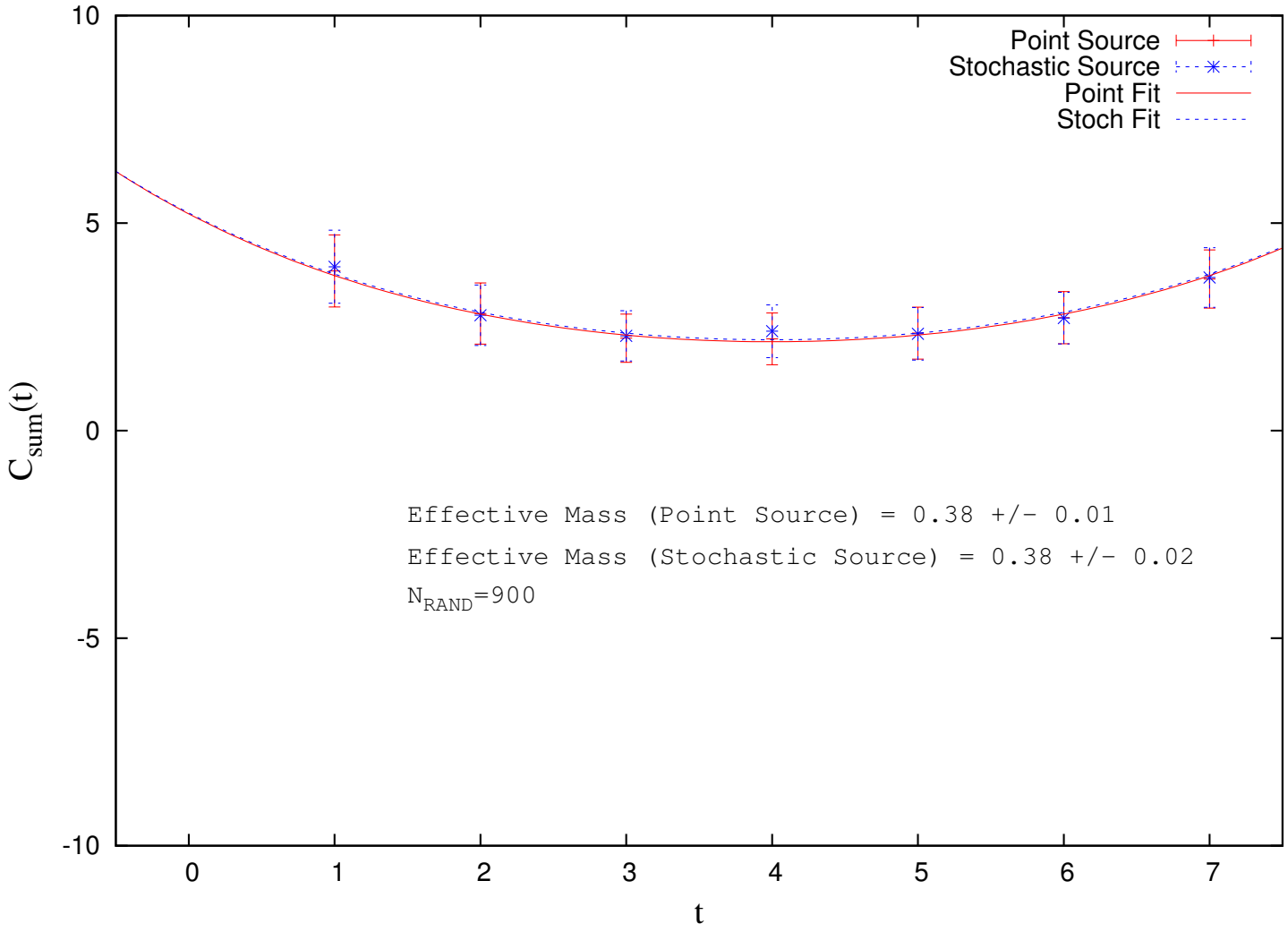
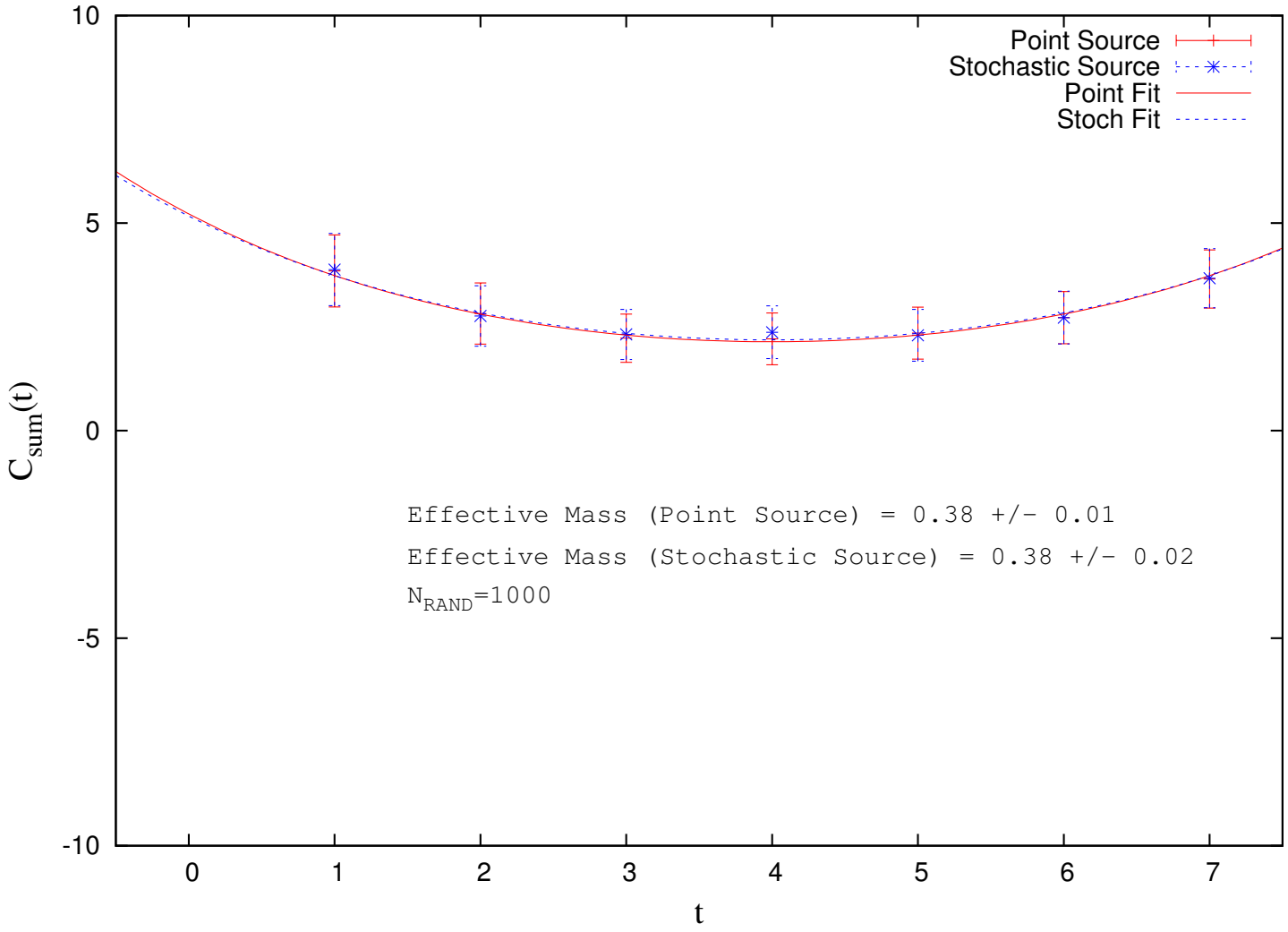
C_sum(t)
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7


Point Source
Stochastic Source
Point Fit
Stoch Fit
Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.38 +/- 0.02
N_RAND=900
C_sum(t)
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7


Point Source
Stochastic Source
Point Fit
Stoch Fit
Effective Mass (Point Source) = 0.38 +/- 0.01
Effective Mass (Stochastic Source) = 0.38 +/- 0.02
N_RAND=1000
C_sum(t)
t
10
5
0
-5
-10
0
1
2
3
4
5
6
7

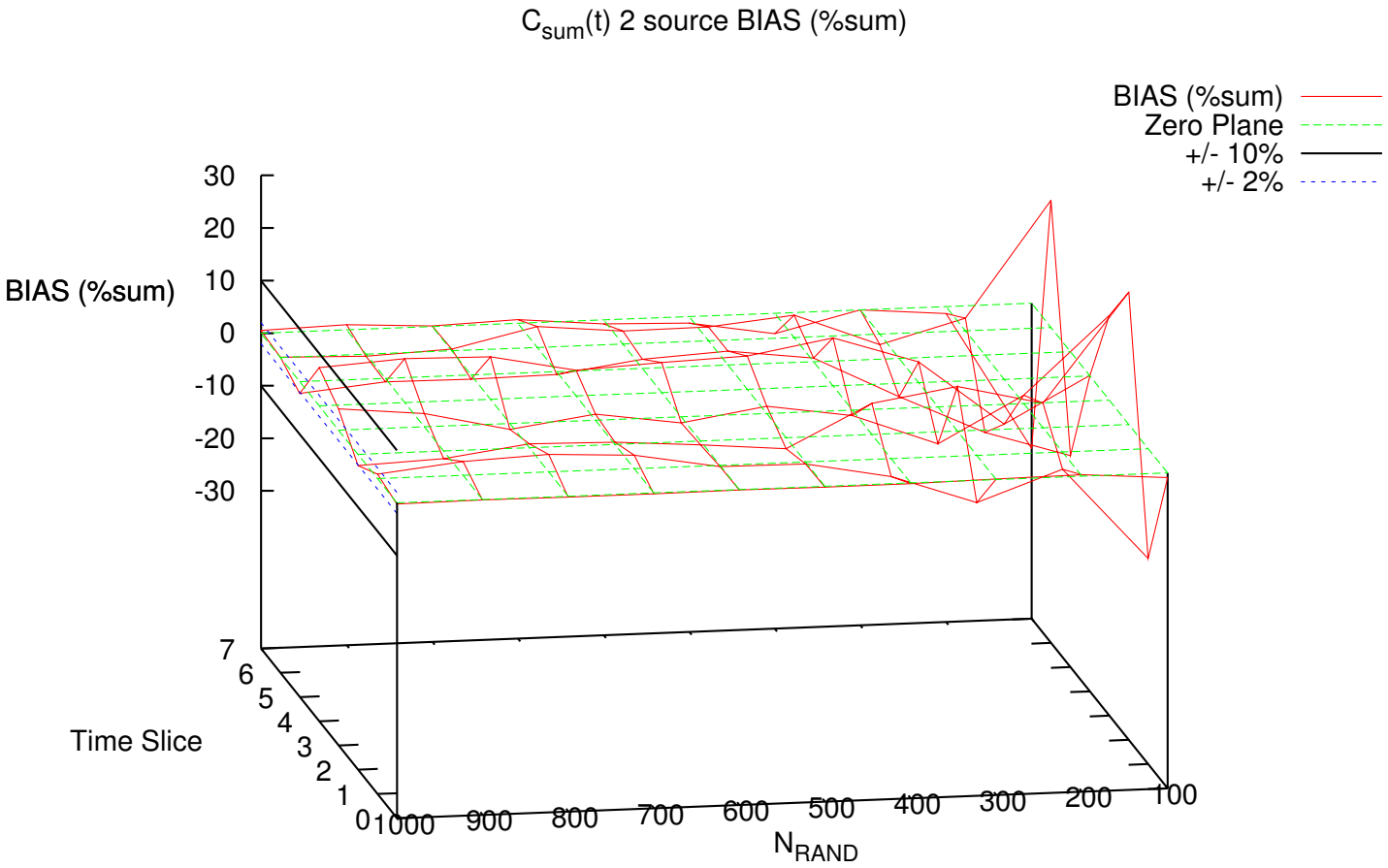
- Error breakdown using two independent sets of 1000 random vectors from Z_2.

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	$\frac{\sigma}{\sqrt{n}}$(stoch)	0.06	0.08	0.08	0.07	0.07	0.06	0.06

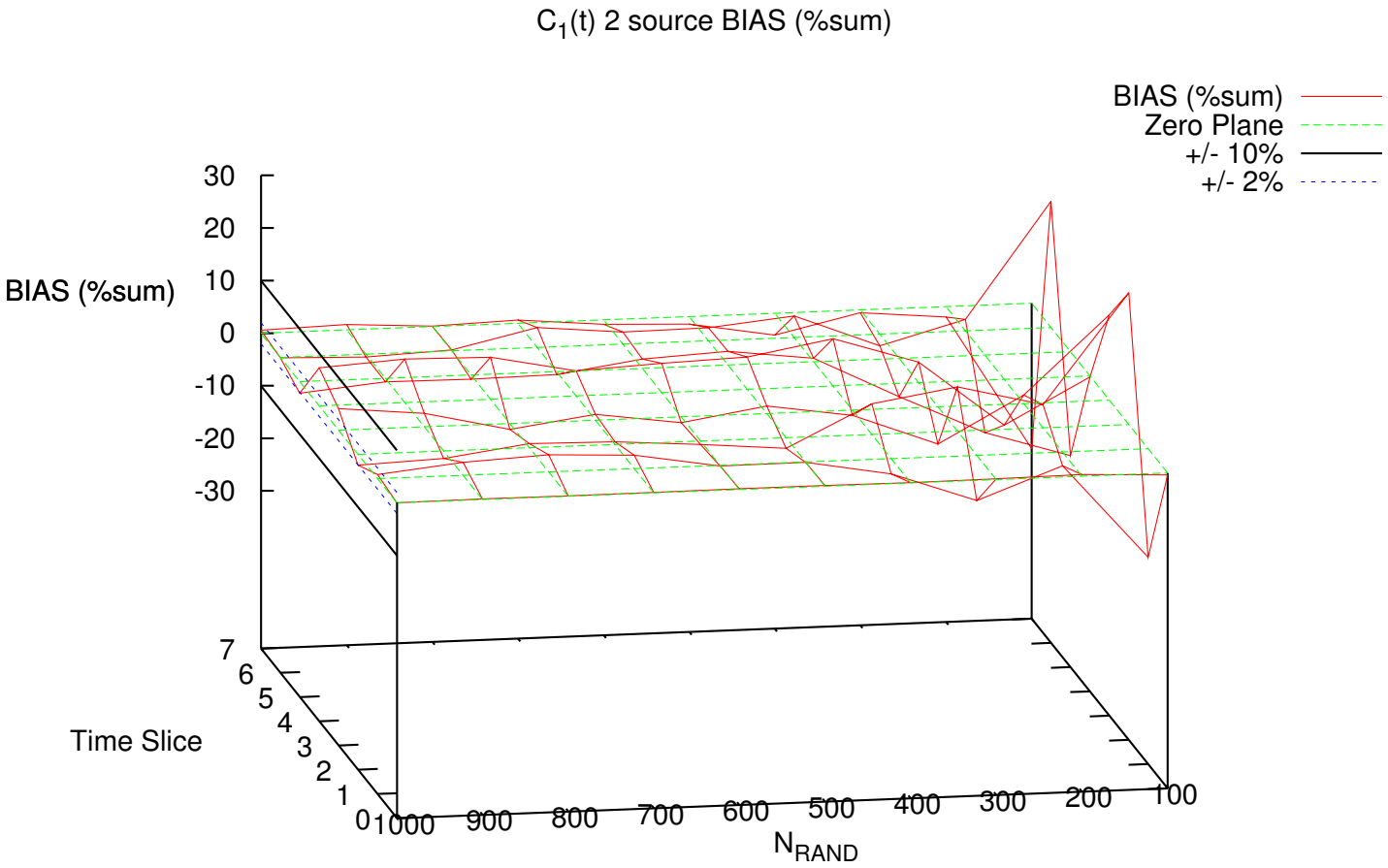
Stochastic standard error calculated using,

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

for n gauge field configurations.


C_sum(t) 2 source BIAS (%sum)
BIAS (%sum)
Zero Plane
+/- 10%
+/- 2%
BIAS (%sum)
30
20
10
0
-10
-20
-30
Time Slice
7
6
5
4
3
2
1
0
1000
900
800
700
600
500
400
300
200
100
N_RAND

The Disconnected Diagram is the Culprit!



Software

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

Benchmarks

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

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

Speed-up ratios for inversions:

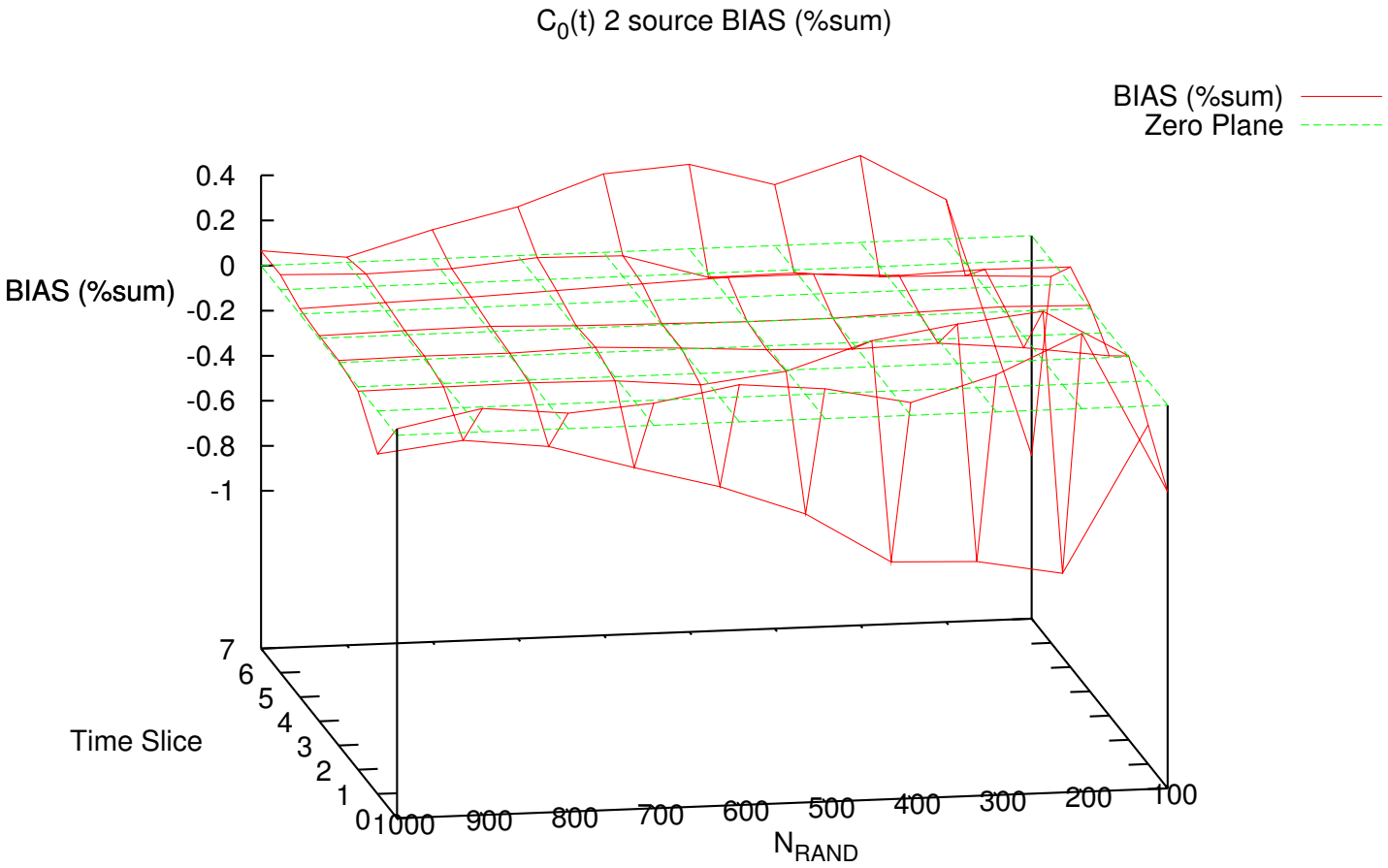
Lattice (L)	12	20	24	32	64
Speed-up	0.87	4.00	6.91	16.4	131

Summary

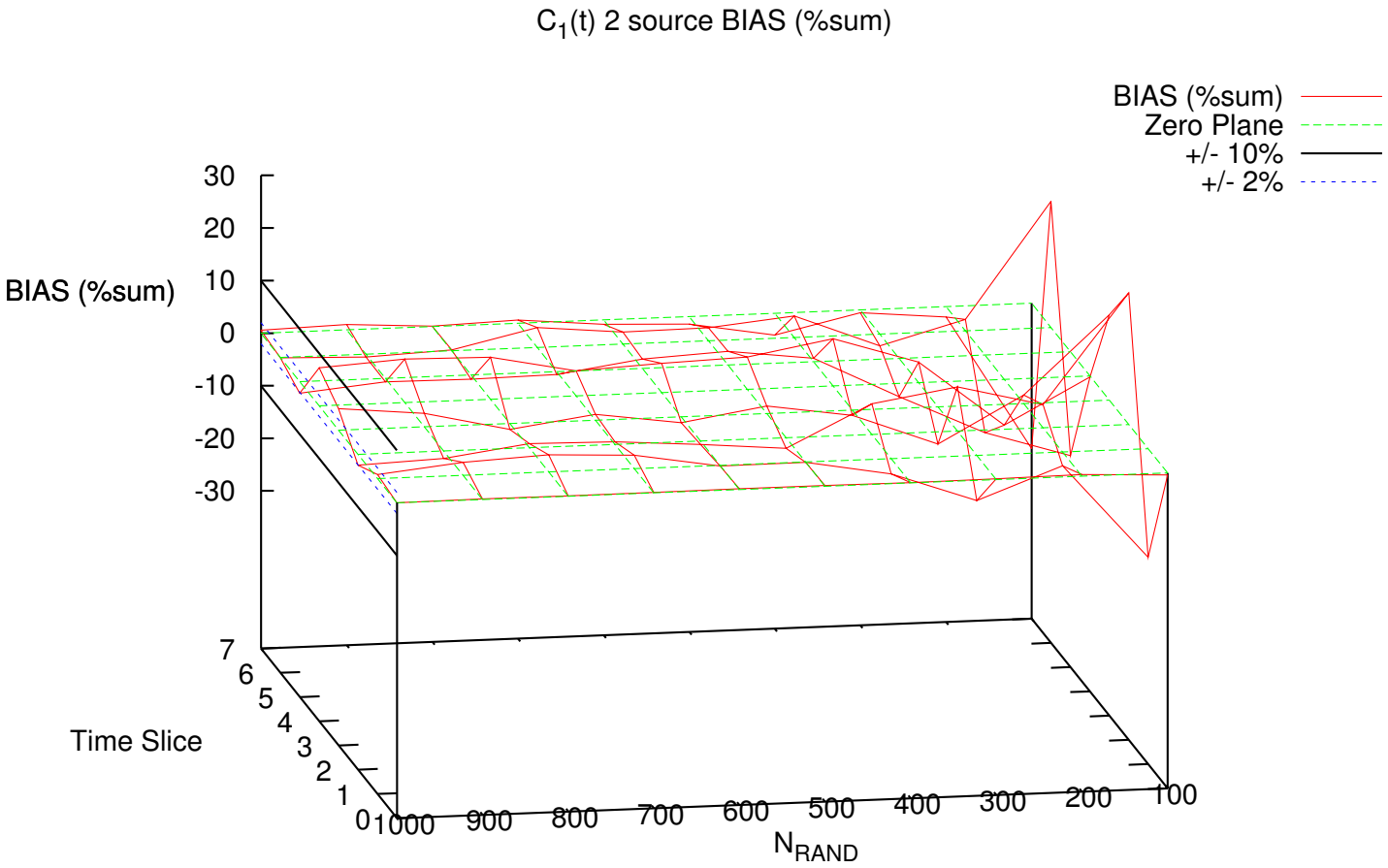
- Scalar States can be investigated in the $I = 0$ flavour singlet channel using $\pi_+\pi_- \to \pi_+\pi_-$.
- Stochastic Sources are a viable option to significanly reduce calculation time with acceptable error, if used judiciously.
- GPU Architecture is a cheap, under utilised resource, waiting to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

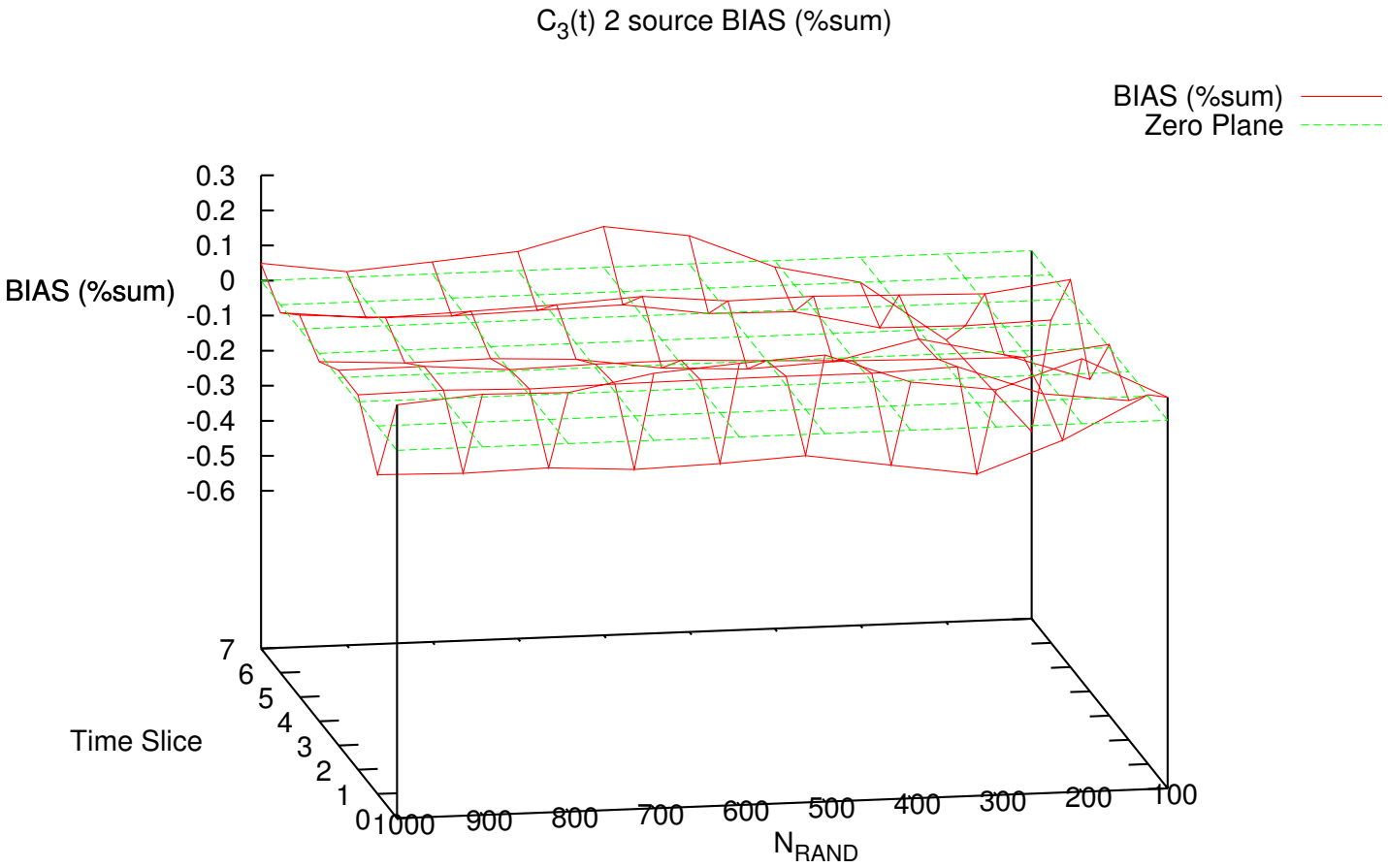
$C_0(t)$ Surface Plot (Backup)



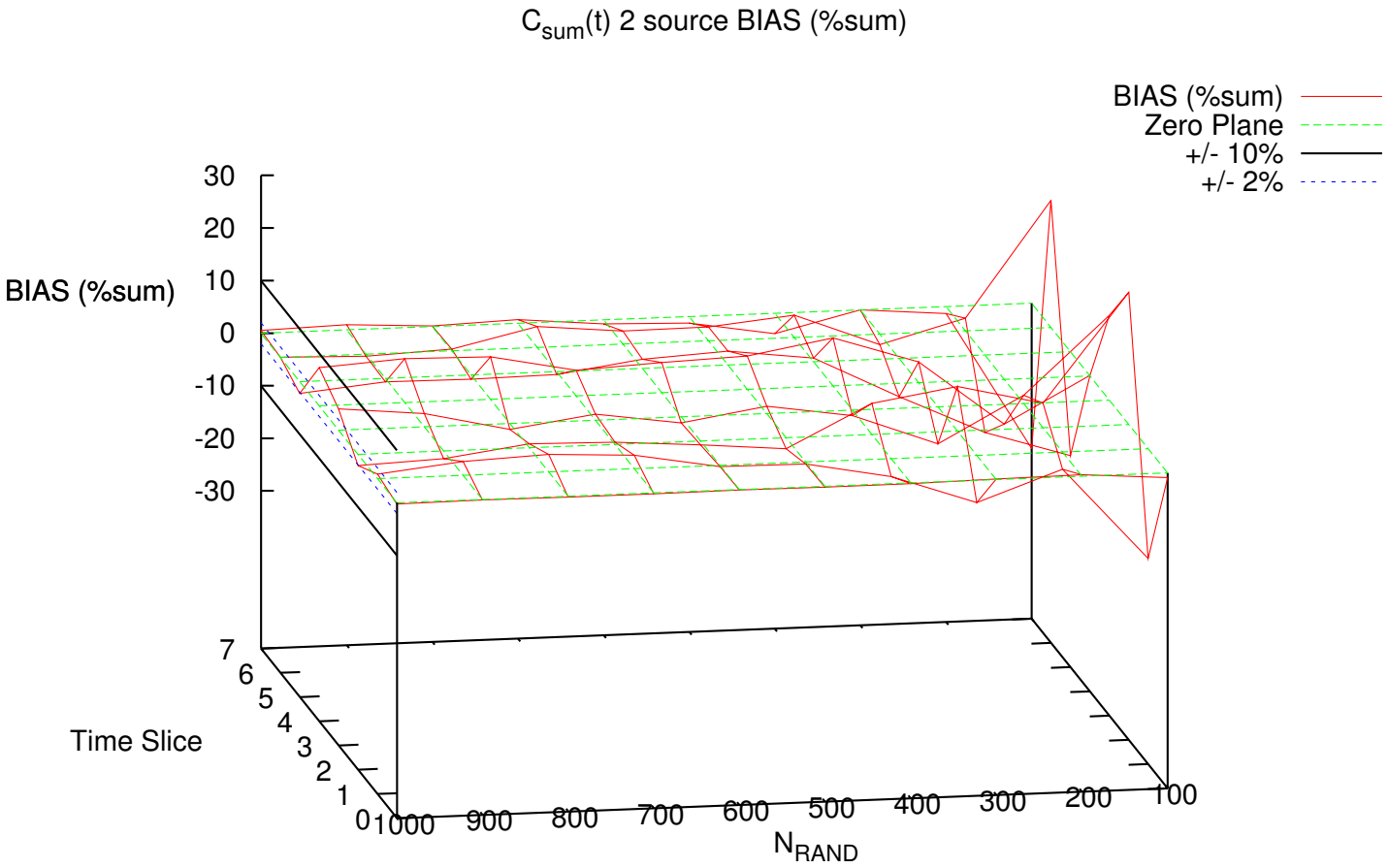
$C_1(t)$ Surface Plot (Backup)



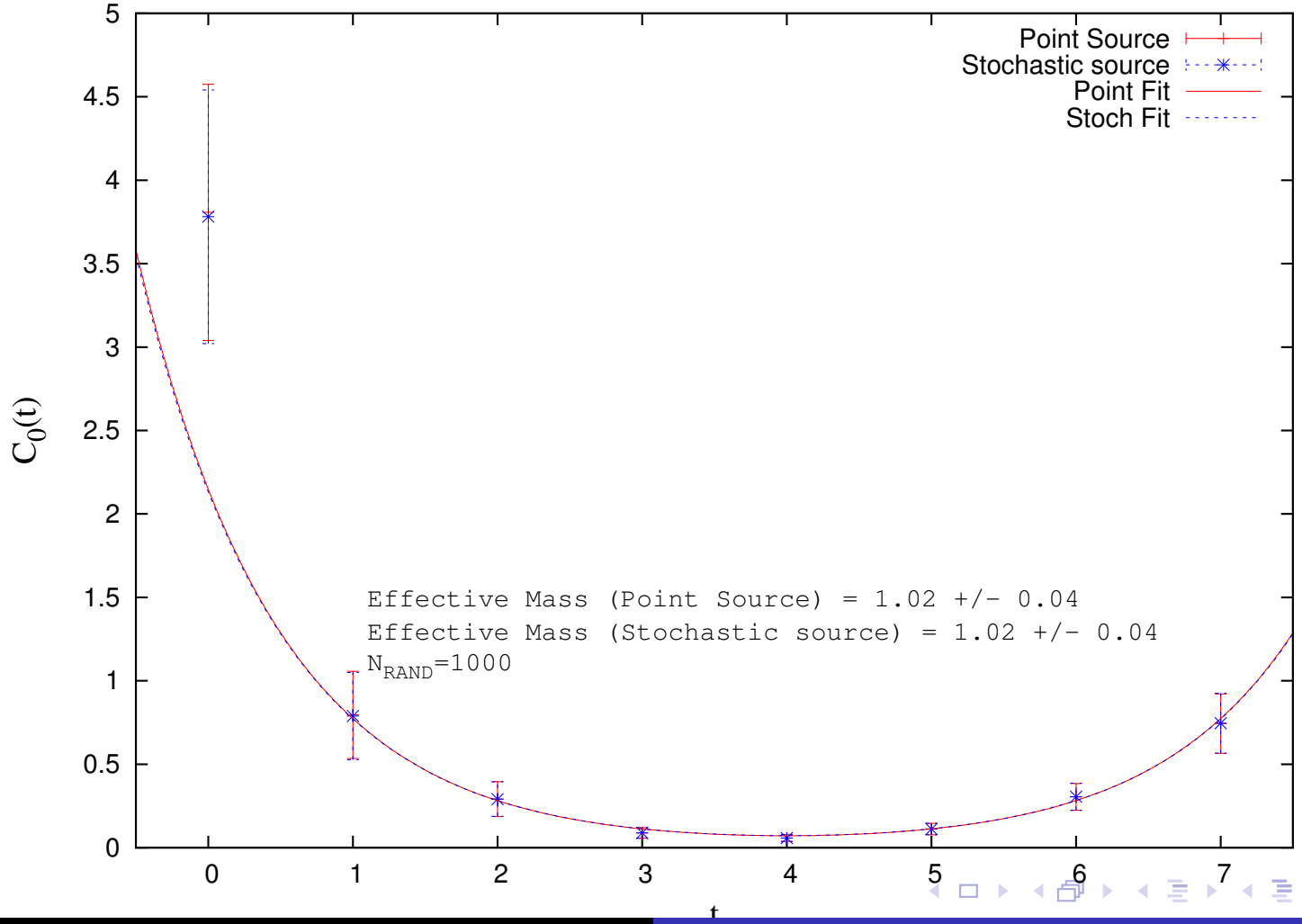
$C_3(t)$ Surface Plot (Backup)



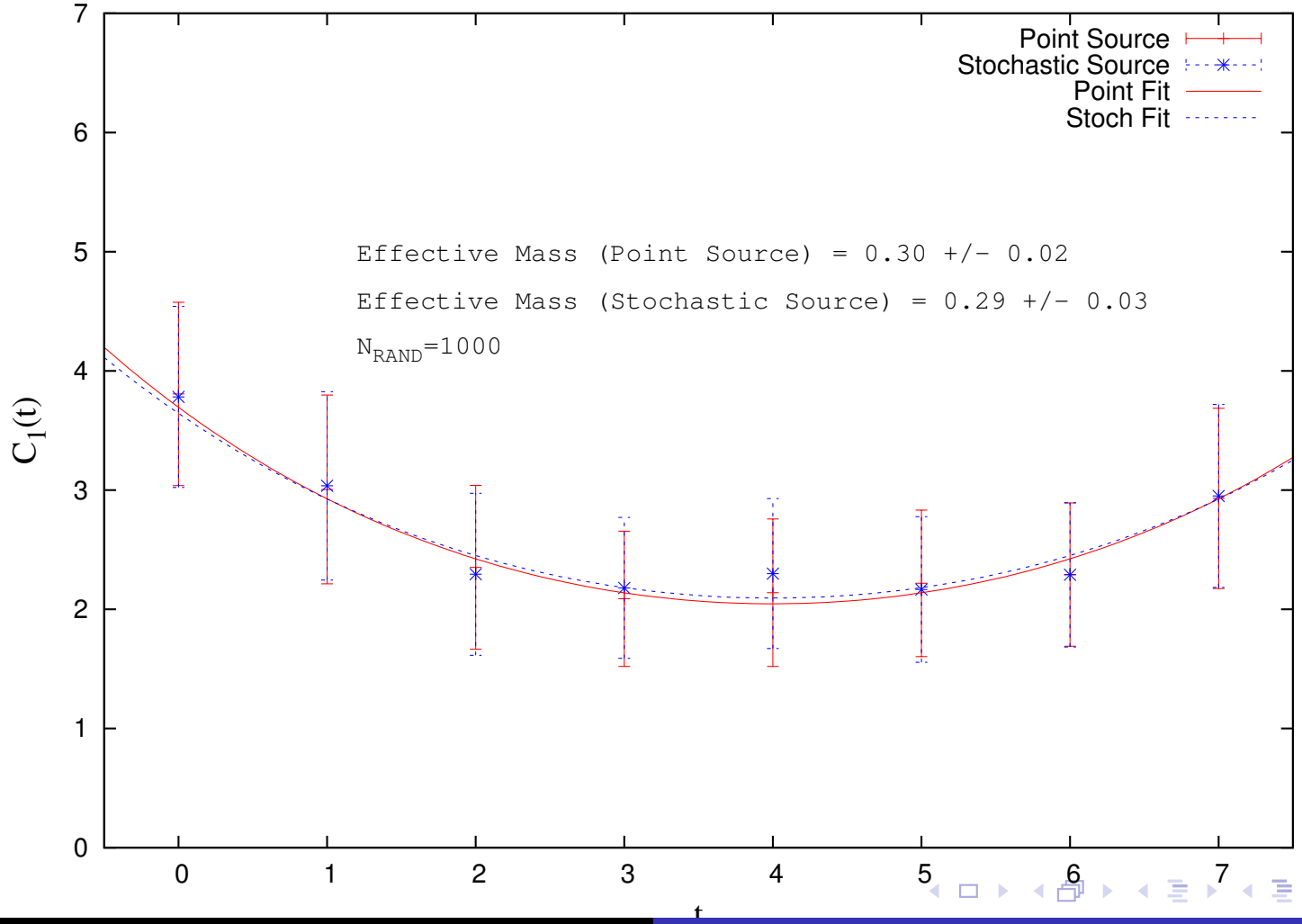
$C_{sum}(t)$ Surface Plot (Backup)



$C_0(t)$ Cosh Fit (Backup)



$C_1(t)$ Cosh Fit (Backup)



$C_2(t)$ Cosh Fit (Backup)