Numerical Stochastic Perturbation Theory and The Gradient Flow

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Motivations

**Goal:** The running coupling of QCD

**Finite-size scaling** techniques provide a general solution to scale-dependent renormalization problems.

- The finite-volume scheme i.e. the fields' boundary conditions
  $\rightarrow$ **Schrödinger functional**
  (K. Symanzik '81; M. Lüscher et. al. '92)
- The non-perturbative definition of the coupling
  $\rightarrow$ **gradient flow coupling**
  (M. Lüscher '10)

**Start:**
- We consider pure $SU(3)$ Yang-Mills theory
- From PT we can obtain important insights into this new tool
  $\rightarrow$ NSPT is a natural framework for the gradient flow!
The gradient flow coupling

- The **gradient flow** evolves the gauge field as a function of the flow time parameter \( t \geq 0 \) according to,

\[
\partial_t B_\mu = D_\nu G_{\nu\mu} + \alpha_0 D_\mu \partial_\nu B_\nu, \quad B_\mu|_{t=0} = A_\mu,
\]

where

\[
G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu], \quad D_\mu = \partial_\mu + [B_\mu, \cdot].
\]

- Correlation functions of the field \( B \) are **automatically finite** for flow times \( t > 0 \), once the theory in 4d is renormalized in the usual way.  

(M. Lüscher, P. Weisz '11)

**Energy density**

\[
\langle E(t) \rangle = -1/2 \langle \text{Tr} G_{\mu\nu}(t) G_{\mu\nu}(t) \rangle.
\]

- From flow observables one can define a **renormalized coupling**, e.g.,

\[
\bar{g}^2(\mu) \equiv \mathcal{N}^{-1} \langle t^2 E(t) \rangle, \quad \mu = \sqrt{1/8t},
\]

where \( \mathcal{N} \) is such that \( \bar{g}^2 = g_0^2 + O(g_0^4) \).  

(M. Lüscher '10)
The Schrödinger Functional and $\bar{g}_{GF}$

- We consider SF boundary conditions with zero boundary fields, which have to be maintained at all flow times $t$.

- To apply finite-volume scaling, one has to run the renormalization scale with the size of the finite volume box given by $L$,

$$\mu = 1/L,$$

and rescale with $L$ all dimensionful parameters, e.g.,

$$c = \sqrt{8t}/L, \quad T = L.$$  

(Z. Fodor et. al. '12; P. Fritzsch, A. Ramos '13)

- A c-family of running couplings can be introduced as,

$$\bar{g}_{GF}^2(L) \equiv \mathcal{N}^{-1} \langle t^2 E(t, T/2) \rangle \bigg|_{t = c^2 L^2 / 8},$$

where $\mathcal{N}$ depends on the specific scheme.  

(P. Fritzsch, A. Ramos '13)
The gradient flow on the lattice

- The **gradient flow** can be studied on the lattice as,

\[ \partial_t V_{x\mu}(t) = -\left\{ g_0^2 \nabla_{x\mu} S_G(V(t)) \right\} V_{x\mu}(t), \quad V_{x\mu}|_{t=0} = U_{x\mu}, \]

where \( \nabla \) is the Lie-derivative on the gauge group, and \( S_G \) is, e.g., the Wilson gauge action \( \Rightarrow \text{Wilson flow!} \) (M. Lüscher '10)

- The **SF boundary conditions** for zero boundary fields, are realized on the lattice as,

\[ V_\mu(x + \hat{k}L, t) = V_\mu(x, t), \quad V_k(x, t)|_{x_0=0, \tau = I} = I, \quad \forall t \geq 0. \]

- We consider the regularized energy density,

\[ \langle \hat{E}(t, x_0) \rangle = -1/2 \langle \text{Tr} \, \hat{G}_{\mu\nu}(t, x_0) \hat{G}_{\mu\nu}(t, x_0) \rangle, \]

where \( \hat{G} \) is the **clover** definition of the field strength tensor corresponding to the lattice flow \( V \).
Numerical Stochastic Perturbation Theory (D. Hesse’s talk)

- Stochastic Quantization introduces a “stochastic time” $t_s$, in which the fundamental fields evolve according to the **Langevin equation**, 

$$\partial_{t_s} U_{x\mu}(t_s) = -\left\{ \nabla_{x\mu} S_G(U(t_s)) + \eta_{x\mu}(t_s) \right\} U_{x\mu}(t_s),$$

where $\eta$ is a Gaussian distributed noise field. (G. Parisi, Y.S. Wu '81)

- Considering the formal **perturbative expansion**, 

$$U(t_s) \rightarrow V + \sum_{k>0} g_0^k U^{(k)}(t_s),$$

in the Langevin equation, one can obtain an approximate solution by solving the resulting hierarchy of equations order-by-order in $g_0$.

- **Stochastic Perturbation Theory (SPT)** 

$$\lim_{t_s \rightarrow \infty} \langle \mathcal{O} \left[ \sum_k g_0^k U^{(k)}(t_s) \right] \rangle_\eta = \sum_k g_0^k \mathcal{O}_k[U] = \langle \mathcal{O}[U] \rangle.$$

- **NSPT** considers a **discrete approximation** of the Langevin equation, and performs this program **numerically**! (F. Di Renzo et. al. '94)
NSPT and The Gradient Flow

- In the gradient flow, the noise field is not present and the initial distribution of the fundamental gauge field is taken into account,

\[ \partial_t V_{x\mu}(t) = -\left\{ g_0^2 \nabla_{x\mu} S_G(V(t)) \right\} V_{x\mu}(t), \quad V_{x\mu}|_{t=0} = U_{x\mu}(t_s). \]

- Analogously to the Langevin equation, considering the formal perturbative expansion,

\[ V(t; t_s) \to V + \sum_{k>0} g_0^k V^{(k)}(t; t_s), \quad V^{(k)}|_{t=0} = U^{(k)}(t_s), \quad \forall k, \]

one can obtain an approximate solution for the gradient flow!

- **SPT for The Gradient Flow**

\[ \lim_{t_s \to \infty} \langle O \left[ \sum_k g_0^k V^{(k)}(t; t_s) \right] \rangle_\eta = \sum_k g_0^k O_k[V(t)] = \langle O[V(t)] \rangle. \]

- Using the machinery of NSPT this program can be implemented numerically!

- No gauge fixing step is needed along the flow.
Determination of $\langle t^2 \hat{E}(t, T/2) \rangle = \hat{\xi}^{(0)} g_0^2 + \hat{\xi}^{(1)} g_0^4 + \hat{\xi}^{(2)} g_0^6 + \ldots$

(P. Fritzsch, A. Ramos '13)
Determination of $\langle t^2 \hat{E}(t, T/2) \rangle = \check{\xi}^{(0)} g_0^2 + \check{\xi}^{(1)} g_0^4 + \check{\xi}^{(2)} g_0^6 + \ldots$

(P. Fritzsch, A. Ramos '13)
Determination of $\langle t^2 \hat{E}(t, T/2) \rangle = \hat{\xi}^{(0)} g_0^2 + \hat{\xi}^{(1)} g_0^4 + \hat{\xi}^{(2)} g_0^6 + \ldots$

\begin{align*}
\hat{\xi}^{(1)} s_{L/a} = 12 & \\
L/a = 12 & \\
\hat{\xi}^{(1)} & \\
\epsilon^2
\end{align*}

<table>
<thead>
<tr>
<th>$c$</th>
<th>0.075</th>
<th>0.269</th>
<th>0.373</th>
<th>0.453</th>
<th>0.522</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon^2$</td>
<td>0.0000</td>
<td>0.0005</td>
<td>0.0010</td>
<td>0.0015</td>
<td>0.0020</td>
</tr>
</tbody>
</table>
Determination of $\langle t^2 \hat{E}(t, T/2) \rangle = \xi^{(0)} g_0^2 + \xi^{(1)} g_0^4 + \xi^{(2)} g_0^6 + \ldots$
Comparison with Monte Carlo data

\[ E_s - g_s^2 E_s(0) \times 10^5 \]

- \( c = 0.2958 \)
- \( c = 0.5000 \)
- \( c = 0.4031 \)
- \( c = 0.1936 \)
Comparison with Monte Carlo data

<table>
<thead>
<tr>
<th>c</th>
<th>\langle t^2 \hat{E}_s \rangle</th>
<th>\langle t^2 \hat{E}_m \rangle</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>\text{MC}</td>
<td>\text{NSPT}</td>
</tr>
<tr>
<td>0.1936</td>
<td>0.004780(86)</td>
<td>0.004631(22)</td>
</tr>
<tr>
<td>0.2958</td>
<td>0.00552(15)</td>
<td>0.005464(49)</td>
</tr>
<tr>
<td>0.4031</td>
<td>0.00483(18)</td>
<td>0.004776(64)</td>
</tr>
<tr>
<td>0.5000</td>
<td>0.00355(14)</td>
<td>0.003489(64)</td>
</tr>
</tbody>
</table>

MC data obtained with a customized MILC code, results are for \( L/a = 8 \).
Noise to signal ratio vs $c$

\[
\sqrt{N_{\text{meas}}} \sigma(\varepsilon^0_s) / (\varepsilon_s^0), \quad \epsilon = 0.0125
\]

$L/a = 6$
$L/a = 8$
$L/a = 10$
$L/a = 12$
$L/a = 14$
Autocorrelation time vs $c$

$\tau_{\text{int}} \left[ \tilde{\xi}_m \right] / \tau_{\text{meas}}, \epsilon = 0.05, L/a = 8$

$O(g_0^2)$
$O(g_0^4)$
$O(g_0^6)$
Conclusions

- Mild extrapolations, and good statistical behavior for the flow observables we have considered.
- NPST provides a natural setup for a (numerical) perturbative solution of the gradient flow.
- The setup is flexible: different action regularizations, boundary conditions, and observables can be implemented easily.

Outlook

- Continuum limit extrapolations
  - Cut-off effects in the step-scaling function
  - $\Lambda_{GF}$ and PT relation to other schemes
    $\rightarrow$ require bigger lattices (n.b. cost $\propto (L/a)^6$)
- Inclusion of fermions and QCD
Numerical precision

The most expensive simulations were performed at $L/a = 12$. The results of the extrapolations are,

<table>
<thead>
<tr>
<th>$c$</th>
<th>$\xi_s^{(0)}$</th>
<th>$\delta\xi_s^{(0)}/\xi_s^{(0)}$</th>
<th>$\xi_s^{(1)}$</th>
<th>$\delta\xi_s^{(1)}/\xi_s^{(1)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.008656(38)</td>
<td>0.5%</td>
<td>0.005827(37)</td>
<td>0.6%</td>
</tr>
<tr>
<td>0.3</td>
<td>0.008231(66)</td>
<td>0.8%</td>
<td>0.005958(45)</td>
<td>0.8%</td>
</tr>
<tr>
<td>0.4</td>
<td>0.006413(78)</td>
<td>1.2%</td>
<td>0.005004(85)</td>
<td>1.7%</td>
</tr>
<tr>
<td>0.5</td>
<td>0.004026(62)</td>
<td>1.5%</td>
<td>0.00345(11)</td>
<td>3.2%</td>
</tr>
</tbody>
</table>

Autocorrelation $\tau_{\text{int}}$ ($\tau_{\text{int}}/10\text{ LDU}$) and $N_{\text{eff}} = N_{\text{meas}}/(2\tau_{\text{int}})$,

<table>
<thead>
<tr>
<th>$\xi_s^{(0)}$</th>
<th>$\epsilon$</th>
<th>0.0125</th>
<th>0.025</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{\text{int}}</td>
<td>_{c=0.22}$</td>
<td>4.43(94)</td>
<td>4.10(87)</td>
<td>2.07(24)</td>
</tr>
<tr>
<td>$\tau_{\text{int}}</td>
<td>_{c=0.50}$</td>
<td>8.2(22)</td>
<td>5.1(12)</td>
<td>2.66(33)</td>
</tr>
<tr>
<td>$N_{\text{eff}}</td>
<td>_{c=0.22}$</td>
<td>109(24)</td>
<td>112(24)</td>
<td>550(63)</td>
</tr>
<tr>
<td>$N_{\text{eff}}</td>
<td>_{c=0.50}$</td>
<td>61(16)</td>
<td>89(21)</td>
<td>429(53)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\xi_s^{(1)}$</th>
<th>$\epsilon$</th>
<th>0.0125</th>
<th>0.025</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{\text{int}}</td>
<td>_{c=0.22}$</td>
<td>5.8(14)</td>
<td>3.54(70)</td>
<td>2.54(32)</td>
</tr>
<tr>
<td>$\tau_{\text{int}}</td>
<td>_{c=0.50}$</td>
<td>9.9(28)</td>
<td>21.3(75)</td>
<td>4.85(78)</td>
</tr>
<tr>
<td>$N_{\text{eff}}</td>
<td>_{c=0.22}$</td>
<td>87(20)</td>
<td>130(26)</td>
<td>448(56)</td>
</tr>
<tr>
<td>$N_{\text{eff}}</td>
<td>_{c=0.50}$</td>
<td>51(14)</td>
<td>21.6(76)</td>
<td>235(38)</td>
</tr>
</tbody>
</table>
**Numerical effort**

<table>
<thead>
<tr>
<th>( \bar{\xi}_s^{(0)} )</th>
<th>( \epsilon )</th>
<th>0.0125</th>
<th>0.025</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau_{\text{int}}</td>
<td>c = 0.22 )</td>
<td>1.117(28)</td>
<td>0.677(19)</td>
<td>0.541(14)</td>
</tr>
<tr>
<td>( \tau_{\text{int}}</td>
<td>c = 0.50 )</td>
<td>1.567(48)</td>
<td>0.837(25)</td>
<td>0.567(14)</td>
</tr>
<tr>
<td>( N_{\text{eff}}</td>
<td>c = 0.22 )</td>
<td>17880(45)</td>
<td>24980</td>
<td>24980</td>
</tr>
<tr>
<td>( N_{\text{eff}}</td>
<td>c = 0.50 )</td>
<td>12750(38)</td>
<td>24980</td>
<td>24980</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \bar{\xi}_s^{(1)} )</th>
<th>( \epsilon )</th>
<th>0.0125</th>
<th>0.025</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau_{\text{int}}</td>
<td>c = 0.22 )</td>
<td>1.717(54)</td>
<td>0.921(28)</td>
<td>0.636(16)</td>
</tr>
<tr>
<td>( \tau_{\text{int}}</td>
<td>c = 0.50 )</td>
<td>4.00(17)</td>
<td>2.030(83)</td>
<td>1.144(37)</td>
</tr>
<tr>
<td>( N_{\text{eff}}</td>
<td>c = 0.22 )</td>
<td>11630(36)</td>
<td>24980</td>
<td>24980</td>
</tr>
<tr>
<td>( N_{\text{eff}}</td>
<td>c = 0.50 )</td>
<td>5000(22)</td>
<td>6150(25)</td>
<td>10910(35)</td>
</tr>
</tbody>
</table>

\[
N_{\text{eff}} = \frac{N_{\text{meas}}}{2 \tau_{\text{int}}}
\]
Determination of \( \langle t^2 \hat{E}(t, T/2) \rangle = \tilde{\mathcal{E}}^{(0)} g_0^2 + \tilde{\mathcal{E}}^{(1)} g_0^4 + \tilde{\mathcal{E}}^{(2)} g_0^6 + \ldots \)

(P. Fritzsch, A. Ramos '13)

<table>
<thead>
<tr>
<th>( L = 4 )</th>
<th>( c )</th>
<th>0.1581</th>
<th>0.3162</th>
<th>0.4183</th>
<th>0.5000</th>
<th>0.5701</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_s )</td>
<td>0.0001(23)</td>
<td>0.0004(26)</td>
<td>0.0002(31)</td>
<td>0.0000(30)</td>
<td>0.0002(28)</td>
<td></td>
</tr>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_m )</td>
<td>0.0001(23)</td>
<td>0.0006(25)</td>
<td>0.0006(30)</td>
<td>0.0005(28)</td>
<td>0.0005(26)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( L = 6 )</th>
<th>( c )</th>
<th>0.1054</th>
<th>0.2981</th>
<th>0.4082</th>
<th>0.4944</th>
<th>0.5676</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_s )</td>
<td>0.0003(22)</td>
<td>0.0007(18)</td>
<td>0.0018(14)</td>
<td>0.0025(17)</td>
<td>0.0029(20)</td>
<td></td>
</tr>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_m )</td>
<td>0.0002(19)</td>
<td>0.0010(24)</td>
<td>0.0012(22)</td>
<td>0.0014(22)</td>
<td>0.0015(23)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( L = 8 )</th>
<th>( c )</th>
<th>0.1118</th>
<th>0.2958</th>
<th>0.4031</th>
<th>0.4873</th>
<th>0.5590</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_s )</td>
<td>0.00056(63)</td>
<td>0.0016(27)</td>
<td>0.0023(36)</td>
<td>0.0028(43)</td>
<td>0.0031(48)</td>
<td></td>
</tr>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_m )</td>
<td>0.00003(59)</td>
<td>0.0032(23)</td>
<td>0.0051(45)</td>
<td>0.0057(57)</td>
<td>0.0057(64)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( L = 12 )</th>
<th>( c )</th>
<th>0.0745</th>
<th>0.2687</th>
<th>0.3727</th>
<th>0.4534</th>
<th>0.5217</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_s )</td>
<td>0.00021(68)</td>
<td>0.0083(68)</td>
<td>0.011(11)</td>
<td>0.014(14)</td>
<td>0.015(16)</td>
<td></td>
</tr>
<tr>
<td>( \delta \tilde{\mathcal{E}}^{(0)}_m )</td>
<td>0.00045(80)</td>
<td>0.0062(87)</td>
<td>0.007(14)</td>
<td>0.009(18)</td>
<td>0.011(21)</td>
<td></td>
</tr>
</tbody>
</table>

\[
\delta \tilde{\mathcal{E}}^{(0)}_{s,m} = \frac{\hat{\mathcal{E}}^{(0)}_{s,m}}{\hat{\mathcal{N}}_{s,m}} - 1
\]
Autocorrelation time vs $c$

$\tau_{\text{int}}\left[\mathcal{E}_s^{(0)}\right]/\tau_{\text{meas}}, \epsilon = 0.05$

$L/a = 8$
$L/a = 12$
$L/a = 4$
$L/a = 6$
Autocorrelation time vs $L$

\[
\frac{(a/L)^2 \tau_{\text{int}}}{\tau_{\text{meas}}, \epsilon = 0.05}
\]

- $c = 0.3$
- $c = 0.4$
- $c = 0.5$