Numerical Stochastic Perturbation Theory
and
The Gradient Flow

Mattia Dalla Brida*
Trinity College Dublin, Ireland

Dirk Hesse
Università degli Studi di Parma, Italia

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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
  \[\rightarrow\textit{Schrödinger functional}\]
  \[\text{(K. Symanzik '81; M. Lüscher et. al. '92)}\]

- The non-perturbative definition of the coupling
  \[\rightarrow\textit{gradient flow coupling}\]
  \[\text{(M. Lüscher '10)}\]

**Start:**

- We consider pure $SU(3)$ Yang-Mills theory
- From PT we can obtain important insights into this new tool
  \[\rightarrow\text{NSPT is a natural framework for the gradient flow!}\]
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.

**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, P. Weisz '11)

(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 $L$,
  \[ \mu = \frac{1}{L}, \]
  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,
  \[ \bar{g}^2_{GF}(L) \equiv \mathcal{N}^{-1} \langle t^2 E(t, T/2) \rangle \big|_{t=c^2L^2/8}, \]
  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,
  \[
  \frac{\partial_t}{t} V_{x\mu}(t) = - \left\{ g_0^2 \nabla_{x\mu} S_G (V(t)) \right\} V_{x\mu}(t), \quad V_{x\mu} |_{t=0} = U_{x\mu},
  \]
  where \( \nabla \) is the Lie-derivative on the gauge group, and \( S_G \) is, e.g., the Wilson gauge action \( \Rightarrow \) **Wilson flow!** (M. Lüscher '10)

- The **SF boundary conditions** for zero boundary fields, are realized on the lattice as,
  \[
  V_{\mu}(x + \hat{k}L, t) = V_{\mu}(x, t), \quad V_k(x, t) |_{x_0=0, \tau = \Pi}, \quad \forall t \geq 0.
  \]

- We consider the regularized energy density,
  \[
  \left\langle \hat{E}(t, x_0) \right\rangle = -1/2 \left\langle \text{Tr} \hat{G}_{\mu\nu}(t, x_0) \hat{G}_{\mu\nu}(t, x_0) \right\rangle,
  \]
  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**, 

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

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)**

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

- **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,

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

- 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**

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

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

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

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

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

\begin{tabular}{|c|c|c|c|c|c|}
\hline
$c$ & 0.075 & 0.269 & 0.373 & 0.453 & 0.522 \\
\hline
\end{tabular}

\begin{align*}
\check{\xi}^{(2)}_{L/a = 12} & = 0.0000 \\
 & \quad \quad \quad 0.0005 \\
 & \quad \quad \quad 0.0010 \\
 & \quad \quad \quad 0.0015 \\
 & \quad \quad \quad 0.0020 \\
 & \quad \quad \quad 0.0025 \\
 & \quad \quad \quad 0.0030 \\
 & \quad \quad \quad 0.0035 \\
 & \quad \quad \quad 0.0040 \\
 & \quad \quad \quad 0.0045 \\
\end{align*}
Comparison with Monte Carlo data

\[ E_s - g_0^2 E_s^{(0)} \times 10^5 \]

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

| $c$   | $\langle t^2 \hat{E}_s \rangle$ | $\langle t^2 \hat{E}_m \rangle$ |
|-------|---------------------------------|---------------------------------|
|       | $O(g_0^4)$                       | $O(g_0^6)$                       |
|       | MC     | NSPT     | MC     | NSPT     |
| 0.1936 | 0.004780(86)  | 0.004631(22)  | 0.0034(11)  | 0.0031669(96) |
| 0.2958 | 0.00552(15)  | 0.005464(49)  | 0.0054(19)  | 0.004095(29)  |
| 0.4031 | 0.00483(18)  | 0.004776(64)  | 0.0050(21)  | 0.003744(44)  |
| 0.5000 | 0.00355(14)  | 0.003489(64)  | 0.0037(17)  | 0.002785(44)  |

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

\[ \sqrt{N_{\text{meas}}} \frac{\sigma(E_s^{(0)})}{(E_s^{(0)})}, \epsilon = 0.0125 \]

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

$\tau_{\text{int}} = \frac{\hat{\xi}_m}{\tau_{\text{meas}}}$, $\epsilon = 0.05$, $L/a = 8$

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

| $c$  | $\tilde{\xi}_s^{(0)}$     | $\delta \tilde{\xi}_s^{(0)}/\tilde{\xi}_s^{(0)}$ | $\tilde{\xi}_s^{(1)}$      | $\delta \tilde{\xi}_s^{(1)}/\tilde{\xi}_s^{(1)}$ |
|------|-----------------------------|-----------------------------------------------|-----------------------------|-----------------------------------------------|
| 0.2  | 0.008656(38)                | 0.5%                                         | 0.005827(37)                | 0.6%                                         |
| 0.3  | 0.008231(66)                | 0.8%                                         | 0.005958(45)                | 0.8%                                         |
| 0.4  | 0.006413(78)                | 1.2%                                         | 0.005004(85)                | 1.7%                                         |
| 0.5  | 0.004026(62)                | 1.5%                                         | 0.00345(11)                 | 3.2%                                         |

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

| $c$  | $\tilde{\xi}_s^{(0)}$     | $\delta \tilde{\xi}_s^{(0)}/\tilde{\xi}_s^{(0)}$ | $\tilde{\xi}_s^{(1)}$      | $\delta \tilde{\xi}_s^{(1)}/\tilde{\xi}_s^{(1)}$ |
|------|-----------------------------|-----------------------------------------------|-----------------------------|-----------------------------------------------|
| 0.2  | $\tau_{\text{int}}|c=0.22$  | 4.43(94)                                      | 4.10(87)                    | 2.07(24)                                      |
|      | $\tau_{\text{int}}|c=0.50$  | 8.2(22)                                       | 5.1(12)                     | 2.66(33)                                      |
| 0.3  | $N_{\text{eff}}|c=0.22$    | 109(24)                                       | 112(24)                     | 550(63)                                       |
|      | $N_{\text{eff}}|c=0.50$    | 61(16)                                        | 89(21)                      | 429(53)                                       |
| 0.4  | $\tau_{\text{int}}|c=0.22$  | 5.8(14)                                       | 3.54(70)                    | 2.54(32)                                      |
|      | $\tau_{\text{int}}|c=0.50$  | 9.9(28)                                       | 21.3(75)                    | 4.85(78)                                      |
| 0.5  | $N_{\text{eff}}|c=0.22$    | 87(20)                                        | 130(26)                     | 448(56)                                       |
|      | $N_{\text{eff}}|c=0.50$    | 51(14)                                        | 21.6(76)                    | 235(38)                                       |
## Numerical effort

| $\tilde{E}^{(0)}$ | $\epsilon$ | 0.0125 | 0.025 | 0.05 |
|------------------|------------|--------|--------|------|
| $\tau_{\text{int}}|c=0.22$ | 1.117(28) | 0.677(19) | 0.541(14) |
| $\tau_{\text{int}}|c=0.50$ | 1.567(48) | 0.837(25) | 0.567(14) |
| $N_{\text{eff}}|c=0.22$ | 17880(45) | 24980 | 24980 |
| $N_{\text{eff}}|c=0.50$ | 12750(38) | 24980 | 24980 |

| $\tilde{E}^{(1)}$ | $\epsilon$ | 0.0125 | 0.025 | 0.05 |
|------------------|------------|--------|--------|------|
| $\tau_{\text{int}}|c=0.22$ | 1.717(54) | 0.921(28) | 0.636(16) |
| $\tau_{\text{int}}|c=0.50$ | 4.00(17) | 2.030(83) | 1.144(37) |

| $N_{\text{eff}}|c=0.22$ | 11630(36) | 24980 | 24980 |
| $N_{\text{eff}}|c=0.50$ | 5000(22) | 6150(25) | 10910(35) |

$N_{\text{eff}} = \frac{N_{\text{meas}}}{2 \tau_{\text{int}}}$
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)

| $L$ | $c$ | $0.1581$ | $0.3162$ | $0.4183$ | $0.5000$ | $0.5701$ |
|-----|-----|----------|----------|----------|----------|----------|
| $L = 4$ | $\delta \tilde{\mathcal{E}}^{(0)}_s$ | $0.0001(23)$ | $0.0004(26)$ | $0.0002(31)$ | $0.0000(30)$ | $0.0002(28)$ |
| | $\delta \tilde{\mathcal{E}}^{(0)}_m$ | $0.0001(23)$ | $0.0006(25)$ | $0.0006(30)$ | $0.0005(28)$ | $0.0005(26)$ |
| $L/a = 6$ | $c$ | $0.1054$ | $0.2981$ | $0.4082$ | $0.4944$ | $0.5676$ |
| | $\delta \tilde{\mathcal{E}}^{(0)}_s$ | $0.0003(22)$ | $0.0007(18)$ | $0.0018(14)$ | $0.0025(17)$ | $0.0029(20)$ |
| | $\delta \tilde{\mathcal{E}}^{(0)}_m$ | $0.0002(19)$ | $0.0010(24)$ | $0.0012(22)$ | $0.0014(22)$ | $0.0015(23)$ |
| $L/a = 8$ | $c$ | $0.1118$ | $0.2958$ | $0.4031$ | $0.4873$ | $0.5590$ |
| | $\delta \tilde{\mathcal{E}}^{(0)}_s$ | $0.00056(63)$ | $0.0016(27)$ | $0.0023(36)$ | $0.0028(43)$ | $0.0031(48)$ |
| | $\delta \tilde{\mathcal{E}}^{(0)}_m$ | $0.00003(59)$ | $0.0032(23)$ | $0.0051(45)$ | $0.0057(57)$ | $0.0057(64)$ |
| $L/a = 12$ | $c$ | $0.0745$ | $0.2687$ | $0.3727$ | $0.4534$ | $0.5217$ |
| | $\delta \tilde{\mathcal{E}}^{(0)}_s$ | $0.00021(68)$ | $0.0083(68)$ | $0.011(11)$ | $0.014(14)$ | $0.015(16)$ |
| | $\delta \tilde{\mathcal{E}}^{(0)}_m$ | $0.00045(80)$ | $0.0062(87)$ | $0.007(14)$ | $0.009(18)$ | $0.011(21)$ |

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

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

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

The graph shows the autocorrelation time $\tau_{int}$ normalized by the measured time $\tau_{meas}$ for different values of $c$ and $\epsilon$. The data points are represented for $c = 0.3$, $c = 0.4$, and $c = 0.5$, each with error bars indicating the variability.

The equation used is $(a/L)^2 \tau_{int} / \tau_{meas}$, where $\epsilon = 0.05$. The x-axis represents $L/a$, while the y-axis shows the normalized autocorrelation time.