CAA: Covariant Approximation Averaging

a new class of error reduction techniques

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with T. Blum E. Shintani,

C. Lehner, T. Kawanai, T. Ishikawa, J.Yu,
R. Arthur, P. Bolye, ….
RBC/UKQCD in preparation

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INT Lattice QCD Summer School, August 21 will be posted just after this lecture !

RBRC-967

A new class of variance reduction techniques using lattice symmetries

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We present a general class of unbiased improved estimators for physical observables in lattice gauge theory computations which significantly reduces statistical errors at modest computational cost. The error reduction techniques, referred to as covariant approximation averaging, utilize approximations which are covariant under lattice symmetry transformations. We observed cost reductions from the new method compared to the traditional one, for fixed statistical error, of 16 times for the nucleon mass at $M_\pi \sim 330$ MeV (Domain-Wall quark) and 2.6-20 times for the hadronic vacuum polarization at $M_\pi \sim 480$ MeV (Asqtad quark). These cost reductions should improve with decreasing quark mass and increasing lattice sizes.

PACS numbers: 11.15.Ha,12.38.Gc,07.05.Tp

As non-perturbative computations using lattice gauge theory are applied to a wider range of physically interest-

In lattice gauge theory simulations an ensemble of gauge field configurations $\{U_1, \cdots, U_{N_{\rm conf}}\}$ is generated

- Precise theoretical calculation becomes even more important to confirm or reject the standard model More than half of CPU cycles of lattice QCD are for valence calculations
  - on physics point QCD simulation
  - multi hadron simulation

It's shame to be limited by statistical error

statistical noise reduction techniques

- LMA

  L. Giusti, P. Hernandez, M. Laine, P. Weisz and H. Wittig, JHEP 0404, 013 (2004)
  see also H. Neff, N. Eicker, T. Lippert, J. W. Negele and K. Schilling, Phys. Rev. D 64 (2001) 114509 and T. DeGrand and S. Schaefer, Comput. Phys. Commun. 159 (2004) 185

  works for low mode dominant quantities

- Truncated Solver Method (TSM)

  G. Bali, S. Collins, A. Schaefer, Comput. Phys. Commun. 181 (2010) 1570

  uses stochastic noise to avoid systematic error

- All-to-all propagator [S. Ryan's lecture]

  J.Foley, K.Juge, A. O'Cais, M. Peardon, S. Ryan, J-I. Skullerud, Comput.Phys.Commun. 172 (2005) 145

  uses stochastic noise
  could use CAA as a part of A2A

- Also closely related to the improved solvers

  Deflations, EigCG, Domain decomposition, MultiGrid, …..

- Other application specific reductions
  multi-hit (pure Gauge)
  multi level: Luscher, M. and Weisz, P. (2001). J. High Energy Phys., 09, 010

Multiple timestep in HMC

- Multiple time steps in MD integrators

- Sexton & Weingarten trick

- Hasenbusch trick : introduce intermediate mass

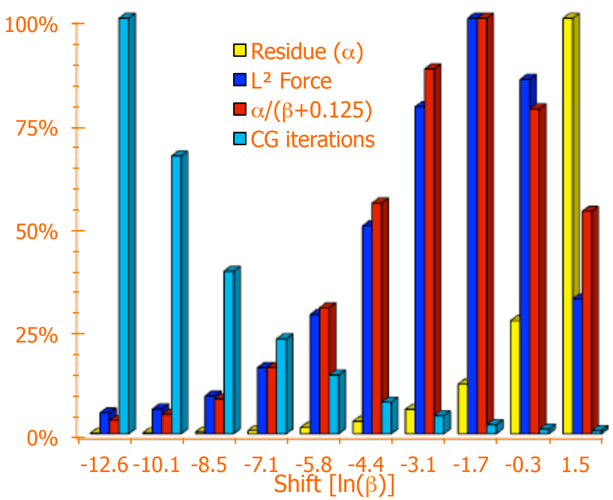
$$\det[D(m)] = \overbrace{\det[D(m_I)]}^{\text{cheap mode}} \times \overbrace{\det\left[D(m)D(m_I)^{-1}\right]}^{\text{expensive mode}}$$

- Clark & Kennedy RHMC (quotient force term)

Berlin Wall was torn down
by Smart Work Sharings

Similar tricks for valence ?

A. Kennedy 06



State of Obvious

- Many interesting physics are limited by statistical error

$$\mathrm{err} \approx C \times \frac{1}{\sqrt{N_{\mathrm{meas}}}}$$

- Do more number of measurements, N_{meas}
- Change to observable with smaller fluctuation, C
- Covariant Approximation Averaging (CAA)
  Combine the above using
  - symmetries of the lattice action
  - (crude) approximations

Covariant Approximation Averaging (CAA)

- Original observable $\mathcal{O}$

- Covariant approximation of the observable $\mathcal{O}^{(\mathrm{appx})}$ under a lattice symmetry $g \in G$

$$\langle \mathcal{O}^{(\mathrm{appx})} \rangle = \langle \mathcal{O}^{(\mathrm{appx}),g} \rangle$$

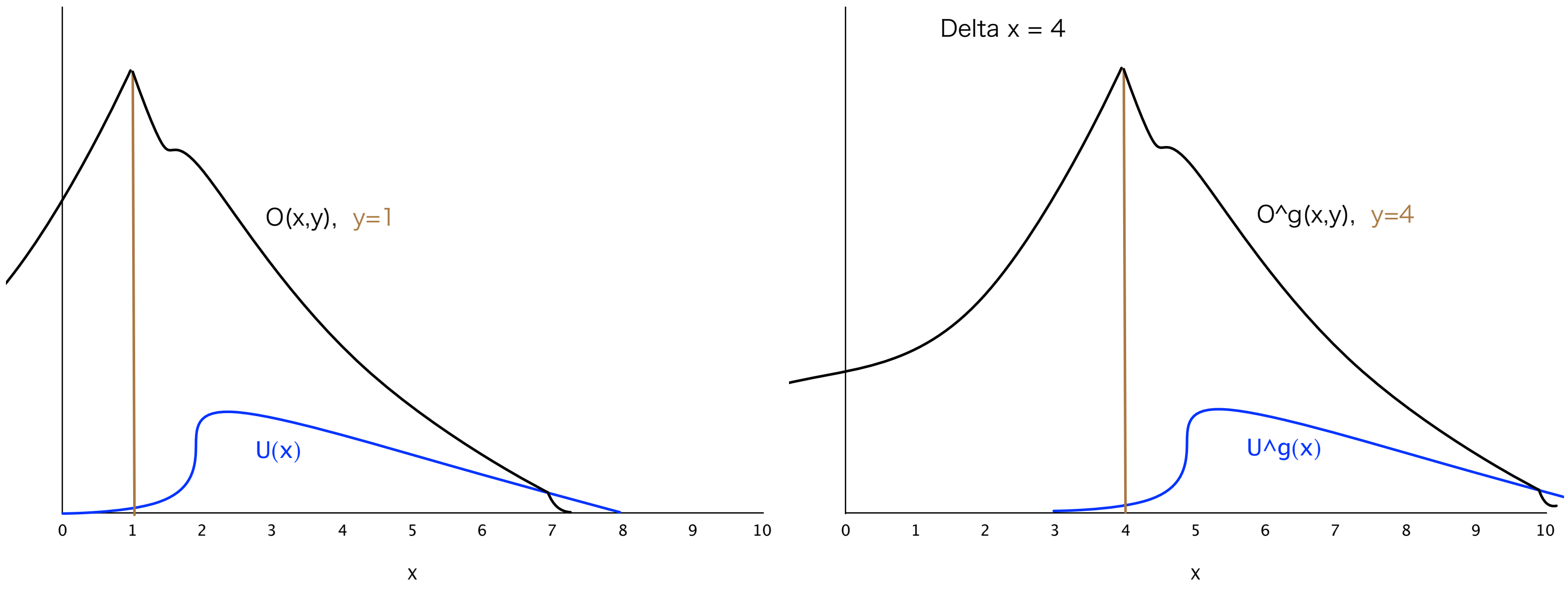
- Unbiased improved estimator

$$\mathcal{O}^{(\mathrm{rest})} = \mathcal{O} - \mathcal{O}^{(\mathrm{appx})}$$

$$\mathcal{O}^{(\mathrm{imp})} = \mathcal{O}^{(\mathrm{rest})} + \frac{1}{N_G} \sum_{g \in G} \mathcal{O}^{(\mathrm{appx}),g}$$

Covariant approximation

- $O^{(appx)}$ needs to be precisely (to the numerical accuracy required) covariant under the symmetry of lattice action to avoid systematic errors.



One should check in the code using explicitly shifted gauge configuration

Unbiasness proof

- Consider a element g of lattice symmetry G e.g. $x_\mu \to x + \Delta x_\mu^{(g)}$
- transformation of fields

$$U_\mu(x) \to U_\mu^g(x) = U_\mu(x - \Delta x^{(g)})$$

$$\begin{aligned}\mathcal{O}[U_\mu] \to & \mathcal{O}^g[U_\mu^g](x_1, x_2, \cdots, x_n) \\ & = \mathcal{O}[U_\mu^g](x_1 - \Delta x^{(g)}x, x_2 - \Delta x^{(g)}x, \cdots, x_n - \Delta x^{(g)}x),\end{aligned}$$

- Observable (and its approximation) is called to have covariance under g iff

$$\mathcal{O}^g[U_\mu^g](x_1, x_2, \cdots, x_n) = \mathcal{O}[U_\mu](x_1, x_2, \cdots, x_n)$$

or, more explicitly,

$$\mathcal{O}[U_\mu^g](x_1 - \Delta x^{(g)}, x_2 - \Delta x^{(g)}, \cdots, x_n - \Delta x^{(g)}) = \mathcal{O}[U_\mu](x_1, x_2, \cdots, x_n) \quad .$$

- When g is a symmetry of lattice, and $O^{(appx)}$ is covariant $\langle \mathcal{O}^g \rangle = \langle \mathcal{O} \rangle$

$$\mathcal{O}^{(\mathrm{rest})} = \mathcal{O} - \mathcal{O}^{(\mathrm{appx})}$$

$$\mathcal{O}^{(\mathrm{imp})} = \mathcal{O}^{(\mathrm{rest})} + \frac{1}{N_G} \sum_{g \in G} \mathcal{O}^{(\mathrm{appx}),g}$$

$$\langle \mathcal{O}^{\mathrm{imp}} \rangle = \langle \mathcal{O} \rangle$$

Why expect improvements ?

$$\mathcal{O}^{(\mathrm{rest})} = \mathcal{O} - \mathcal{O}^{(\mathrm{appx})}$$

$$\mathcal{O}^{(\mathrm{imp})} = \mathcal{O}^{(\mathrm{rest})} + \frac{1}{N_G} \sum_{g \in G} \mathcal{O}^{(\mathrm{appx}),g}$$

- $O^{(\mathrm{imp})}$ has smaller error, smaller C
  <= accuracy of approximation controls error,
  need not to be too accurate (0.1% is good enough)

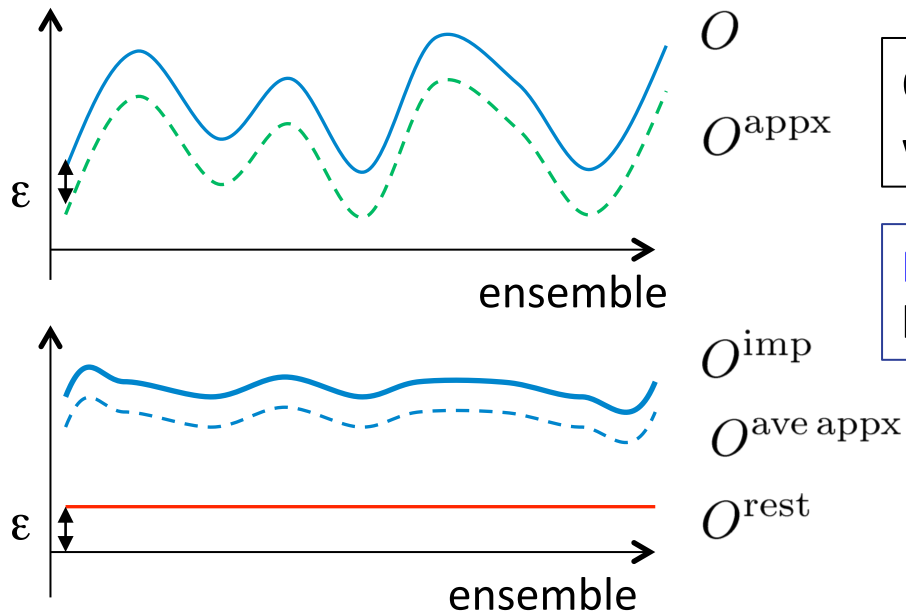
- N_G suppresses the bulk part of noise cheaply

$$\mathrm{err} \approx C \times \frac{1}{\sqrt{N_{\mathrm{meas}}}}$$

Valence version of Hasenbushing in HMC

AMA : a smart work sharing

- Ideal approximation



$O^{\rm appx}$ is <u>*strongly correlated*</u> with original one.

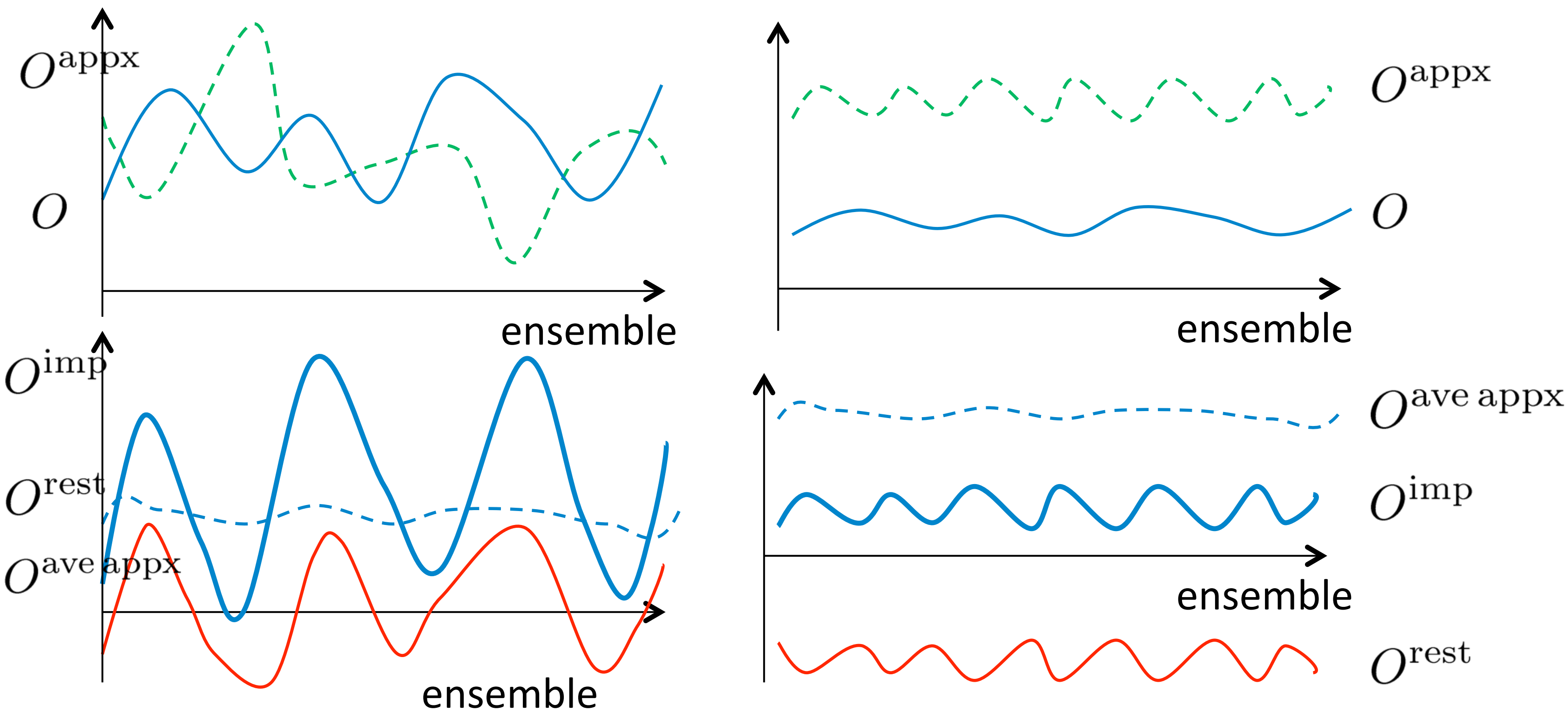
R(corr) b/w O and $O^{\rm (appx)}$ needs to be larger than 0.5 [C. Lehner]

$$\mathrm{err}^{\mathrm{imp}} \simeq \mathrm{err}/\sqrt{N_g}$$

- ε, accuracy of approximation should be smaller than $O^{\rm ave\ appx}$
- $\Delta O^{\rm rest}$ which is statistical error of $O^{\rm rest}$ depends on the strength of correlation.
- The computational cost of $O^{\rm appx}$ should be much smaller than original.

AMA : not working

- Nightmare case
  - Anti-correlated or bad approximation



$$\text{err}^{\text{imp}} \gg \text{err}$$

Examples of covariant approximations

- Low mode approximation used in the Low Mode Averaging (**LMA**)

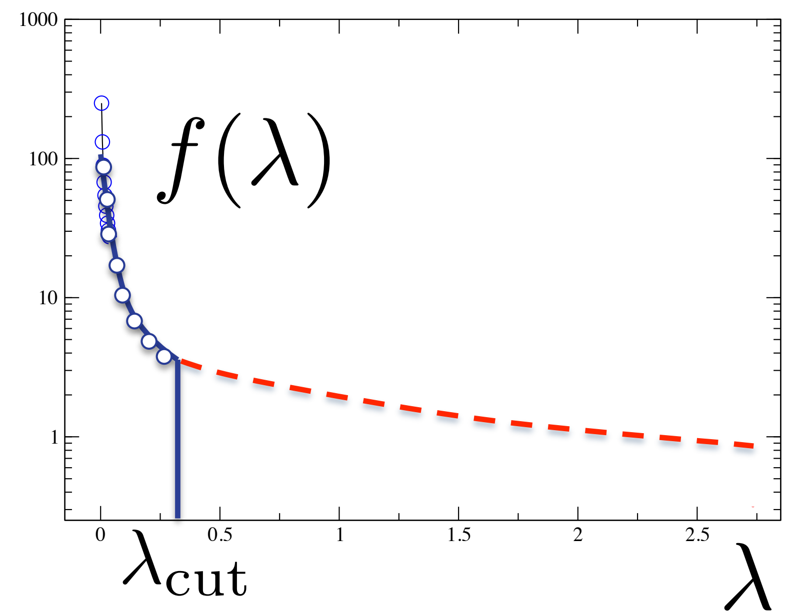
L. Giusti et al (2004), see also T. DeGrand et al. (2004)

accuracy control : # of eigen mode

$$\mathcal{O}^{(\mathrm{appx})} = \mathcal{O}[S_l],$$

$$S_l = \sum_{\lambda} v_\lambda f(\lambda) v_\lambda^\dagger,$$

$$f(\lambda) = \frac{1}{\lambda}\theta(\lambda_{\mathrm{cut}} - |\lambda|)$$



Deflation using low eigenmodes from Lanczos [Neff et al, JLQCD]

- 4D even/odd preconditioning

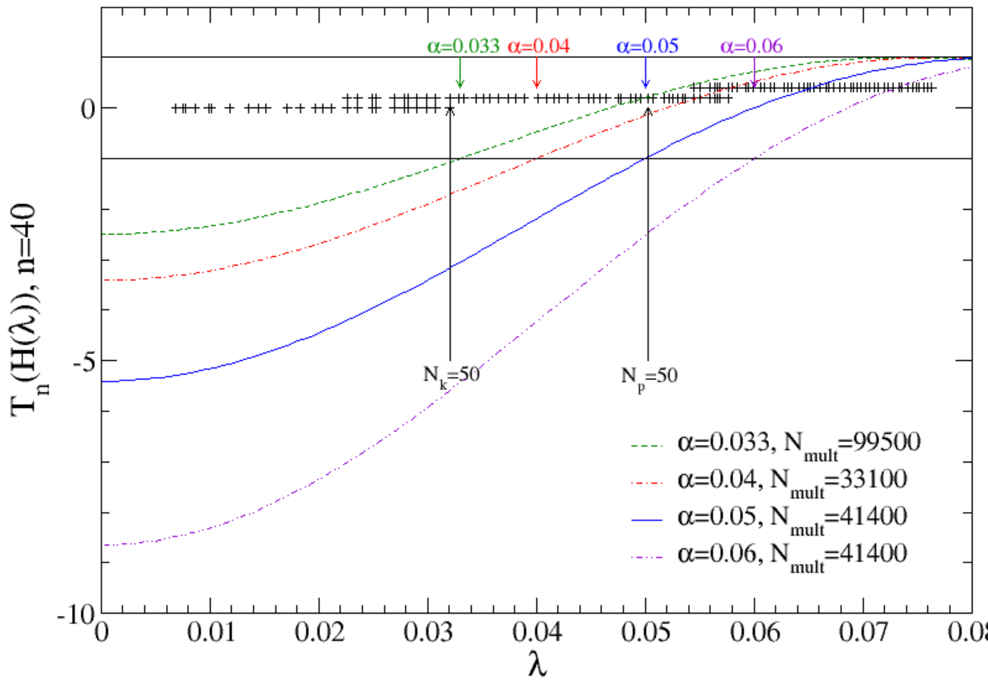
  [R. Arthur]

$$D_{DW} = \begin{pmatrix} M_5 & K(M_4)_{eo} \\ K(M_4)_{oe} & M_5 \end{pmatrix}$$

$$\begin{aligned} D_{DW}^{-1} &= \begin{pmatrix} 1 & 0 \\ -KM_5^{-1}(M_4)_{oe} & M_5^{-1} \end{pmatrix} \begin{pmatrix} D_{ee}^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -K(M_4)_{eo}M_5^{-1} \\ 0 & 1 \end{pmatrix} \\ D_{ee} &= M_5 - K^2(M_4)_{eo}M_5^{-1}(M_4)_{oe} \end{aligned}$$

- Polynomial accelerated
  P_n(H_DWF)
- With shift
  H-> H-c
- eigen Compression
  / decompression

$$\psi = v_1 + v_2$$
$$H(\psi) = \lambda_1 v_1 + \lambda_2 v_2$$



Low-mode decomposition

- 4D even-odd decomposition

$$D_{DW} = \begin{pmatrix} M_{5\,ee} & KM_{4\,eo} \\ KM_{4\,oe} & M_{5\,oo} \end{pmatrix}$$

M_5 : with 5D differential, 4D diagonal
M_4 : with 4D differential, 5D diagonal

$$= \begin{pmatrix} 1 & KM_{4\,eo}M_{5\,oo}^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} D_{ee} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ KM_{4\,oe} & M_{5\,oo} \end{pmatrix}$$

$$D_{ee} = M_5 - K^2 M_{4\,eo} M_{5\,oo}^{-1} M_{4\,oe}$$

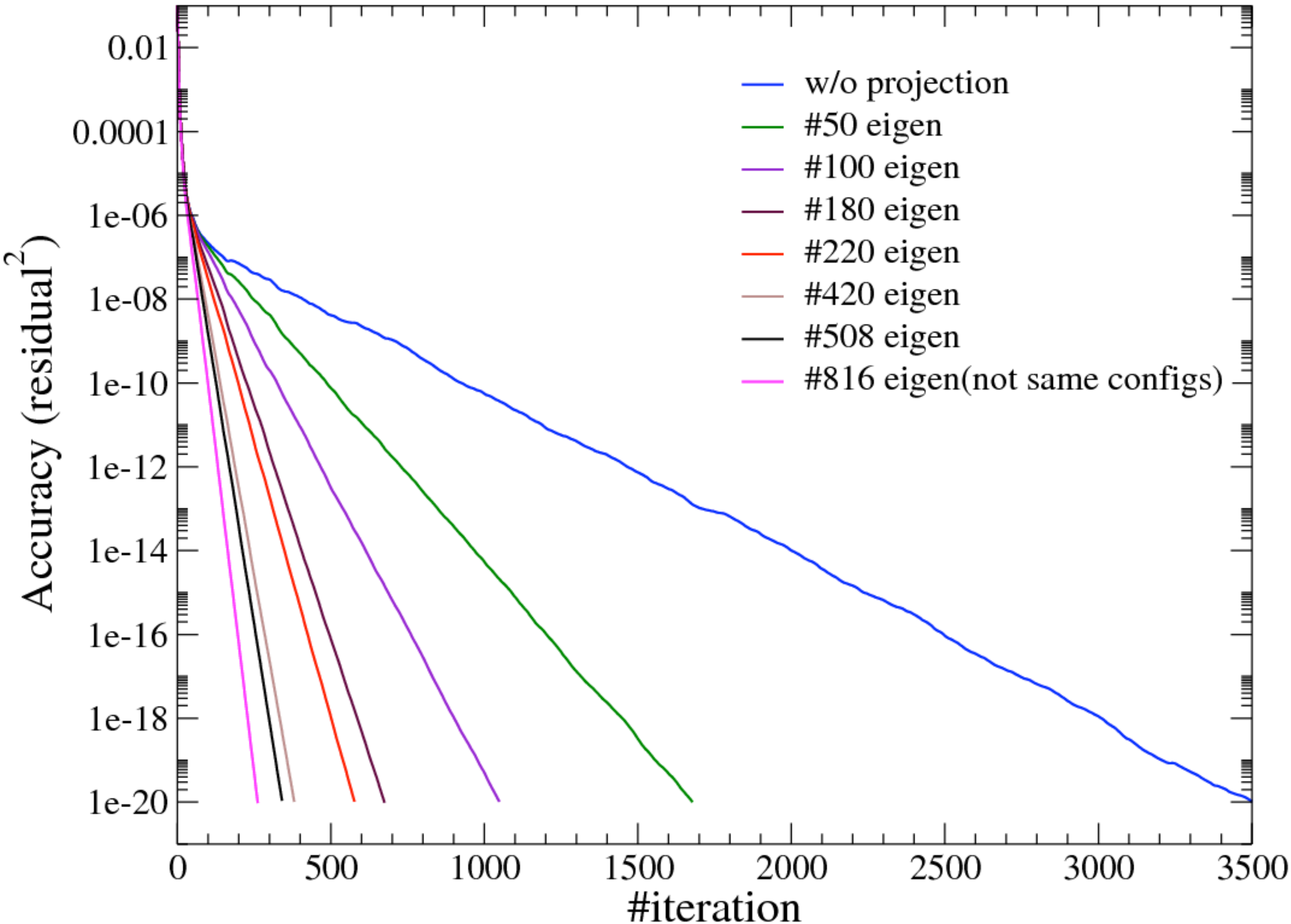
$$D_{DW}^{-1} = \begin{pmatrix} 1 & 0 \\ -KM_{5\,oo}^{-1}M_{4\,oe} & M_{5\,oo}^{-1} \end{pmatrix} \begin{pmatrix} D_{ee}^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -KM_{4\,eo}M_{5\,oo}^{-1} \\ 0 & 1 \end{pmatrix}$$

- Low mode decomposition

$$D_{ee}^{-1} = D_{\mathrm{low}\,ee}^{-1} + D_{\mathrm{high}\,ee}^{-1}$$

$$D_{\mathrm{low}\,ee}^{-1} = H_{\mathrm{low}\,ee}^{-2} D_{ee}^{\dagger} = \sum_k \frac{1}{\lambda_k^2} \psi_k (D_{ee}\psi_k)^{\dagger}, \quad H_{ee}\psi_k = \lambda_k \psi_k, \quad H_{ee} = \Gamma_5 D_{ee}$$

$$D_{\mathrm{low}\,DW}^{-1} = \begin{pmatrix} 1 & 0 \\ -KM_{5\,oo}^{-1}M_{4\,oe} & M_{5\,oo}^{-1} \end{pmatrix} \begin{pmatrix} D_{\mathrm{low}\,ee}^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -KM_{4\,eo}M_{5\,oo}^{-1} \\ 0 & 1 \end{pmatrix}$$



Accuracy (residual^2)
#iteration
0.01
0.0001
1e-06
1e-08
1e-10
1e-12
1e-14
1e-16
1e-18
1e-20
0
500
1000
1500
2000
2500
3000
3500
w/o projection
#50 eigen
#100 eigen
#180 eigen
#220 eigen
#420 eigen
#508 eigen
#816 eigen(not same configs)

Examples of Covariant Approximations (contd.)

- All Mode Averaging **AMA**

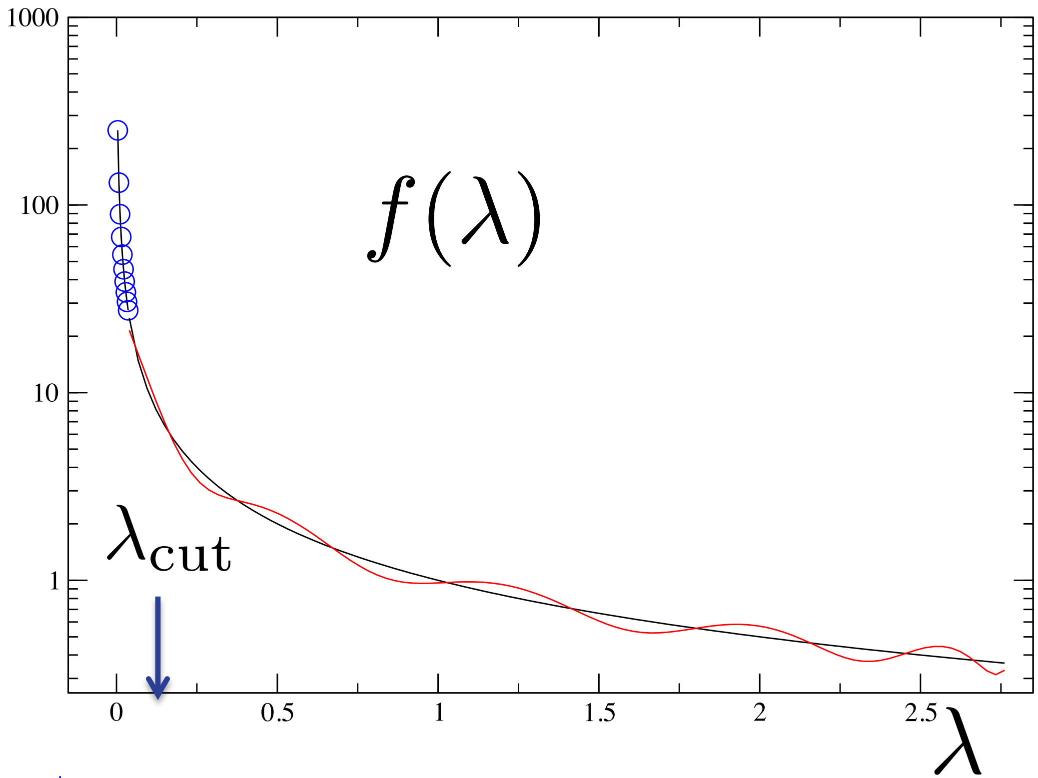
  Sloppy CG or Polynomial approximations

$$\mathcal{O}^{(\mathrm{appx})} = \mathcal{O}[S_l],$$

$$S_l = \sum_\lambda v_\lambda f(\lambda) v_\lambda^\dagger,$$

$$f(\lambda) = \begin{cases} \frac{1}{\lambda}, & |\lambda| < \lambda_{\mathrm{cut}} \\ P_n(\lambda) & |\lambda| > \lambda_{\mathrm{cut}} \end{cases}$$

$$P_n(\lambda) \approx \frac{1}{\lambda}$$

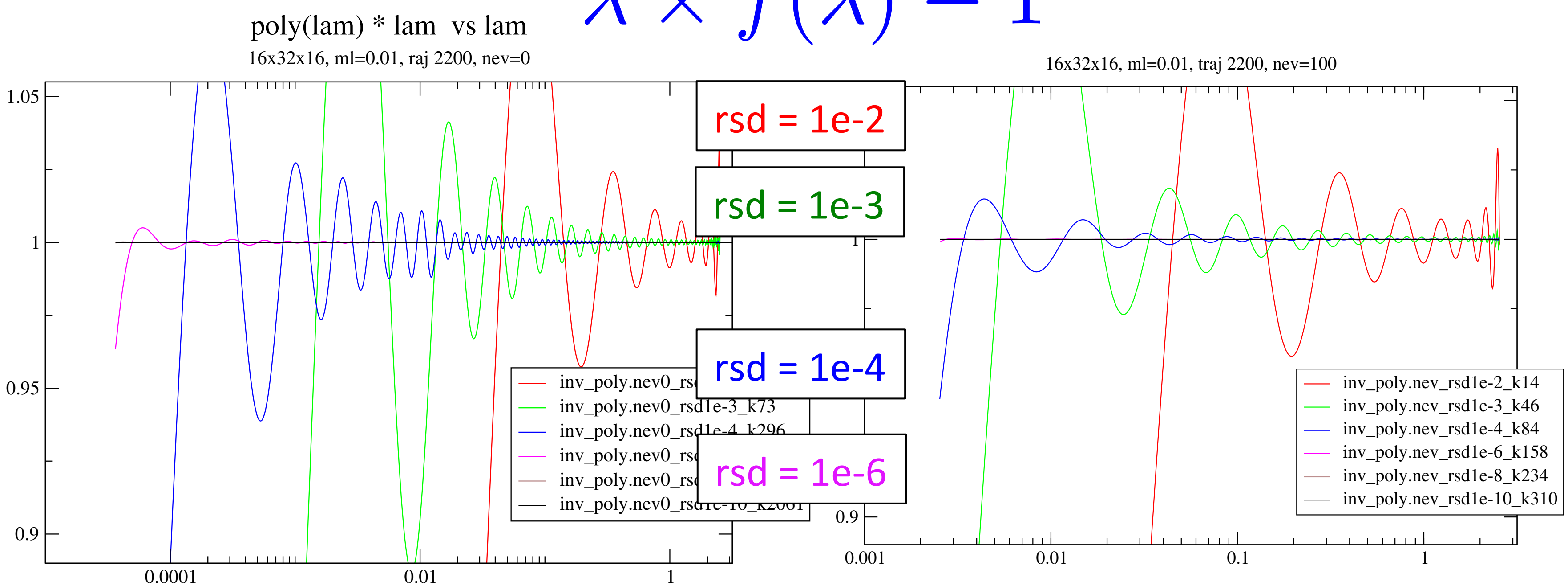


accuracy control :

- low mode part : # of eig-mode
- mid-high mode : degree of poly.

All mode approximation via sloppy CG

$$\lambda \times f(\lambda) - 1$$

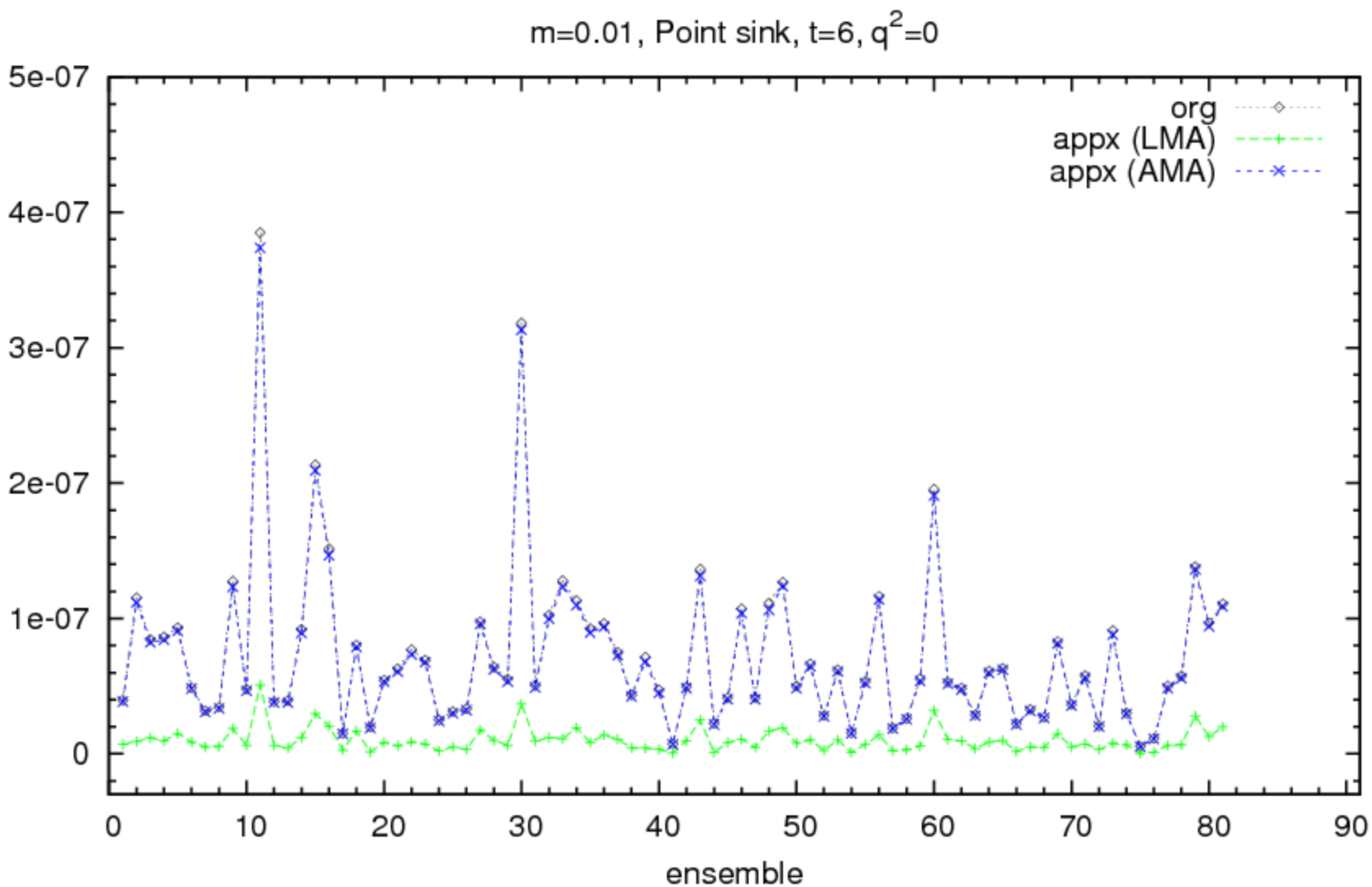


no eigenvector assists | 100 eigenvector assists

- Conjugate residual with sloppy convergence criteria, which is equivalent to construct a polynomial approximating 1/λ
- The starting vector needs to be translation invariant to be a covariant approx.
- low eigenvectors reduces the size of the dynamic range of 1/λ
  - → Better approximation with smaller polynomial degrees
- low λ region has larger relative errors
- One could employ other construction of polynomial approximation for 1/λ, such as min-max, conjugate rasidual

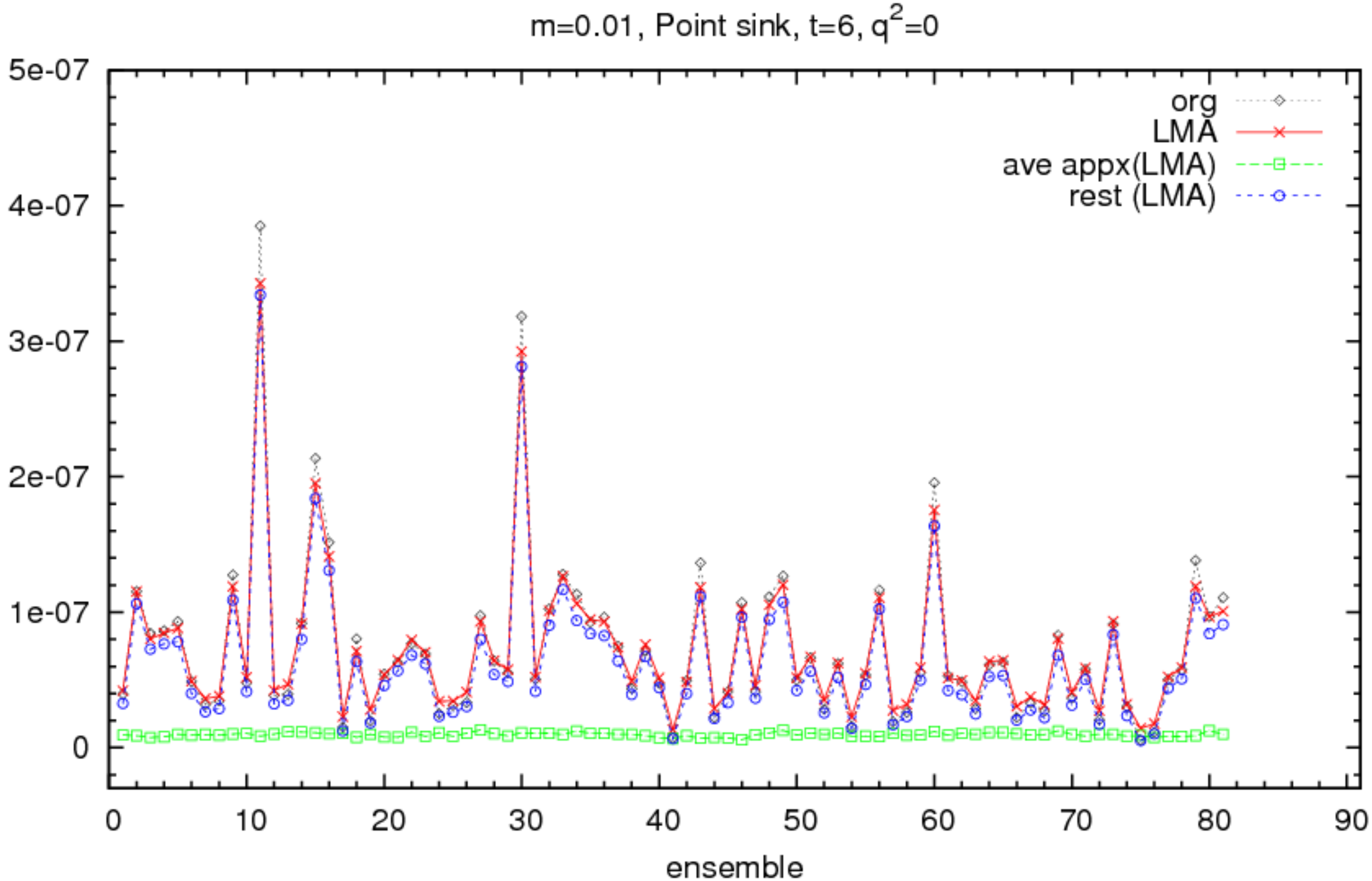
Correlation

- NN propagator at short time-slice



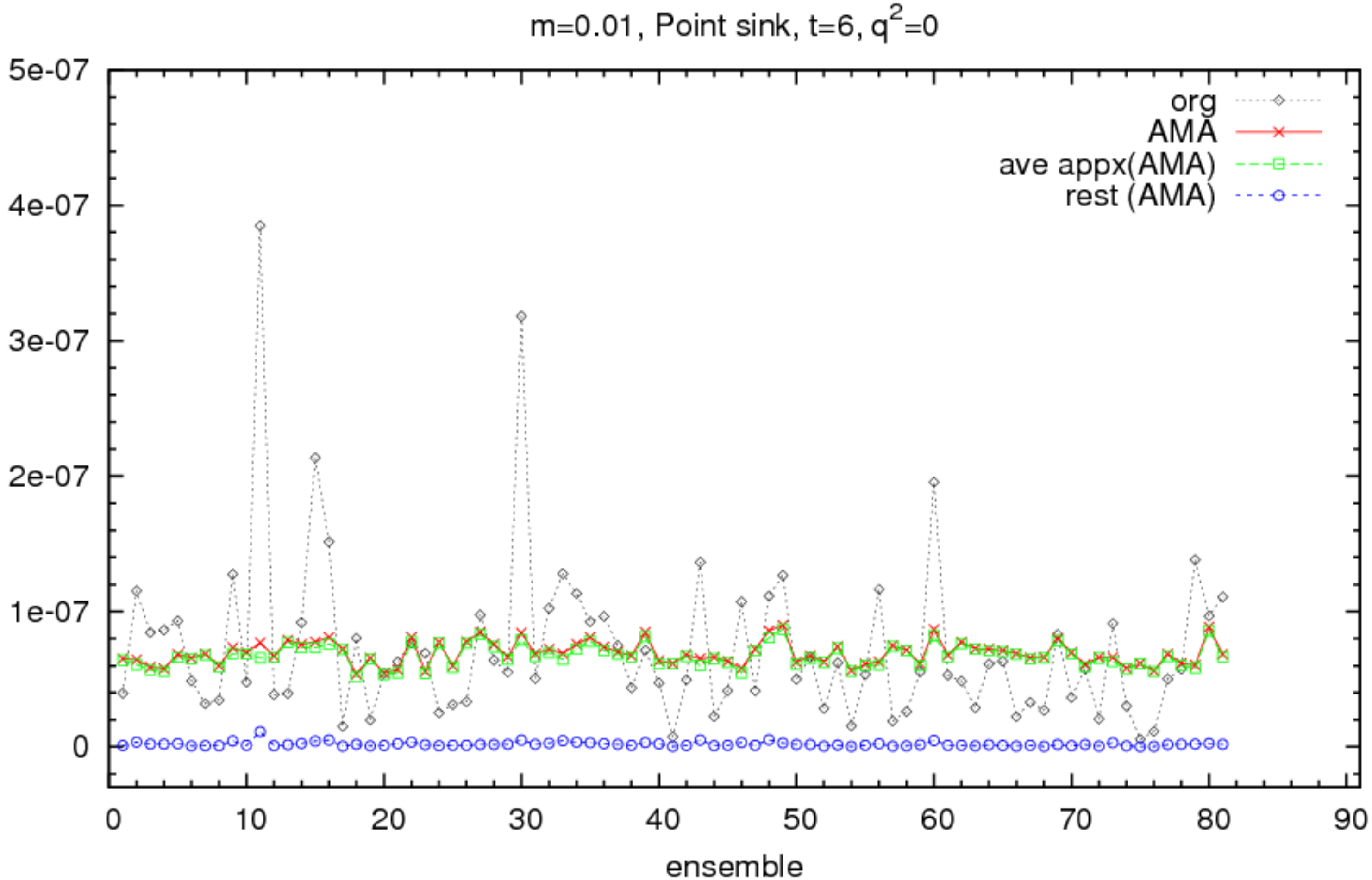
Correlation

- NN propagator (LMA) at short time-slice

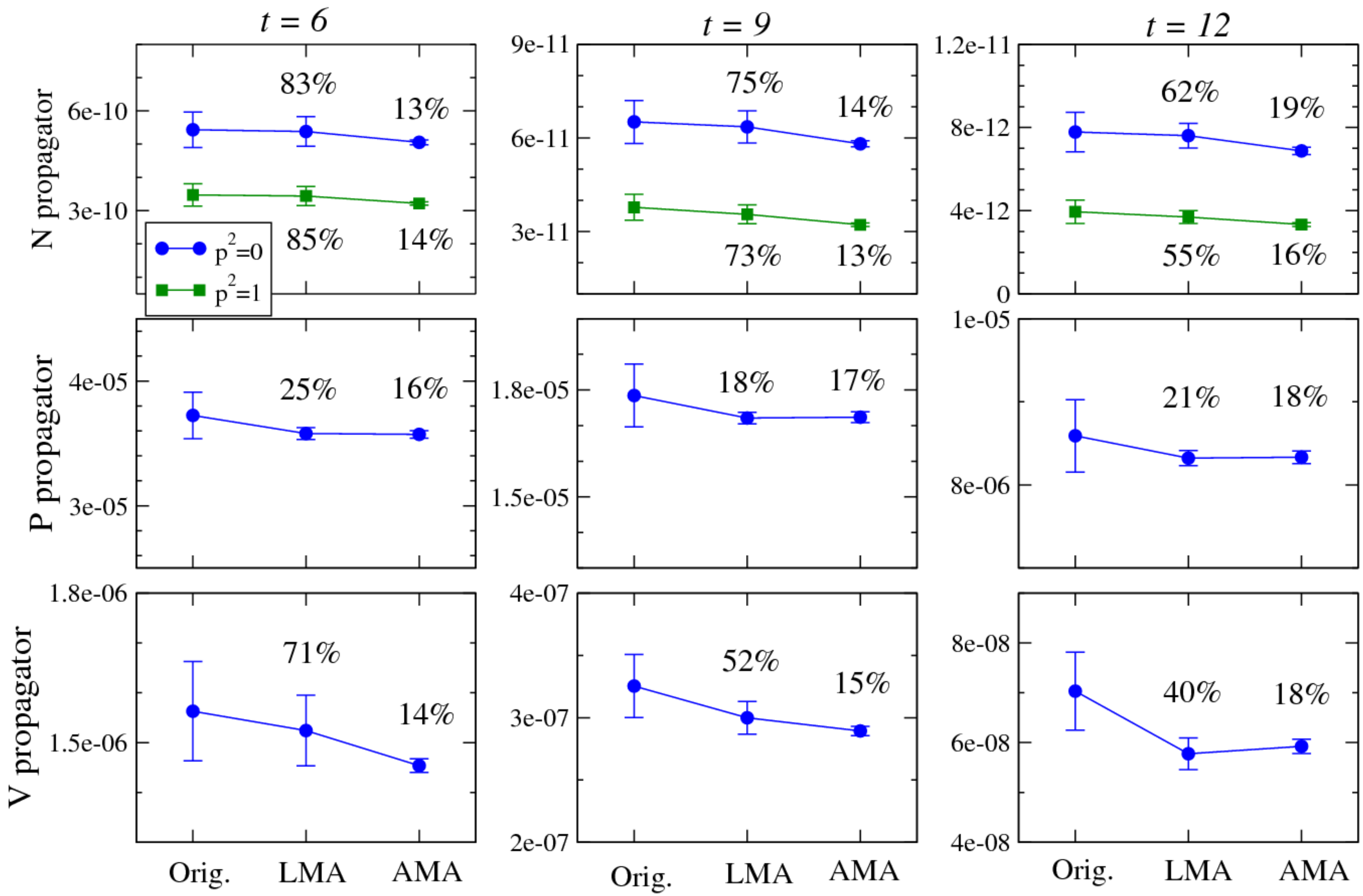


Correlation

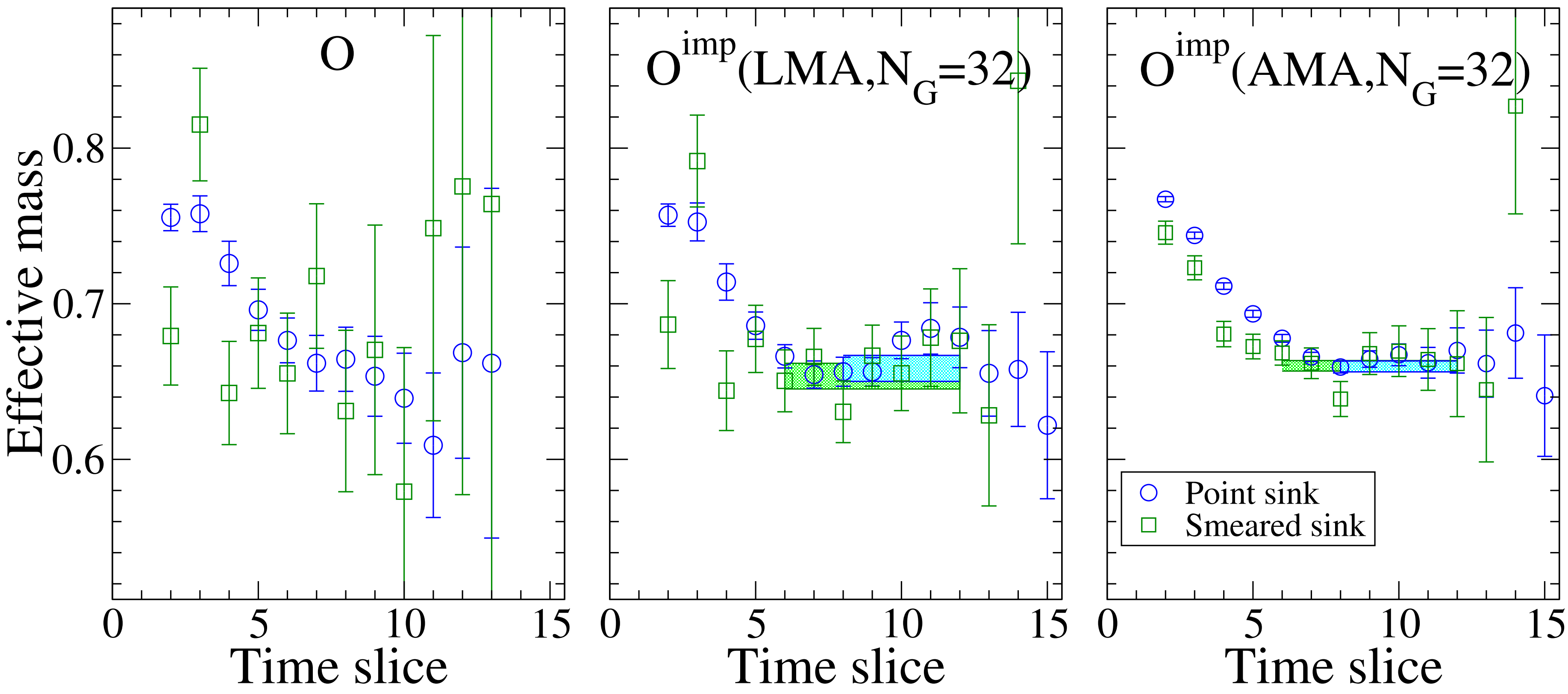
- NN propagator (AMA) at short time-slice



AMA results for hadron 2pt functions [E. Shintani]

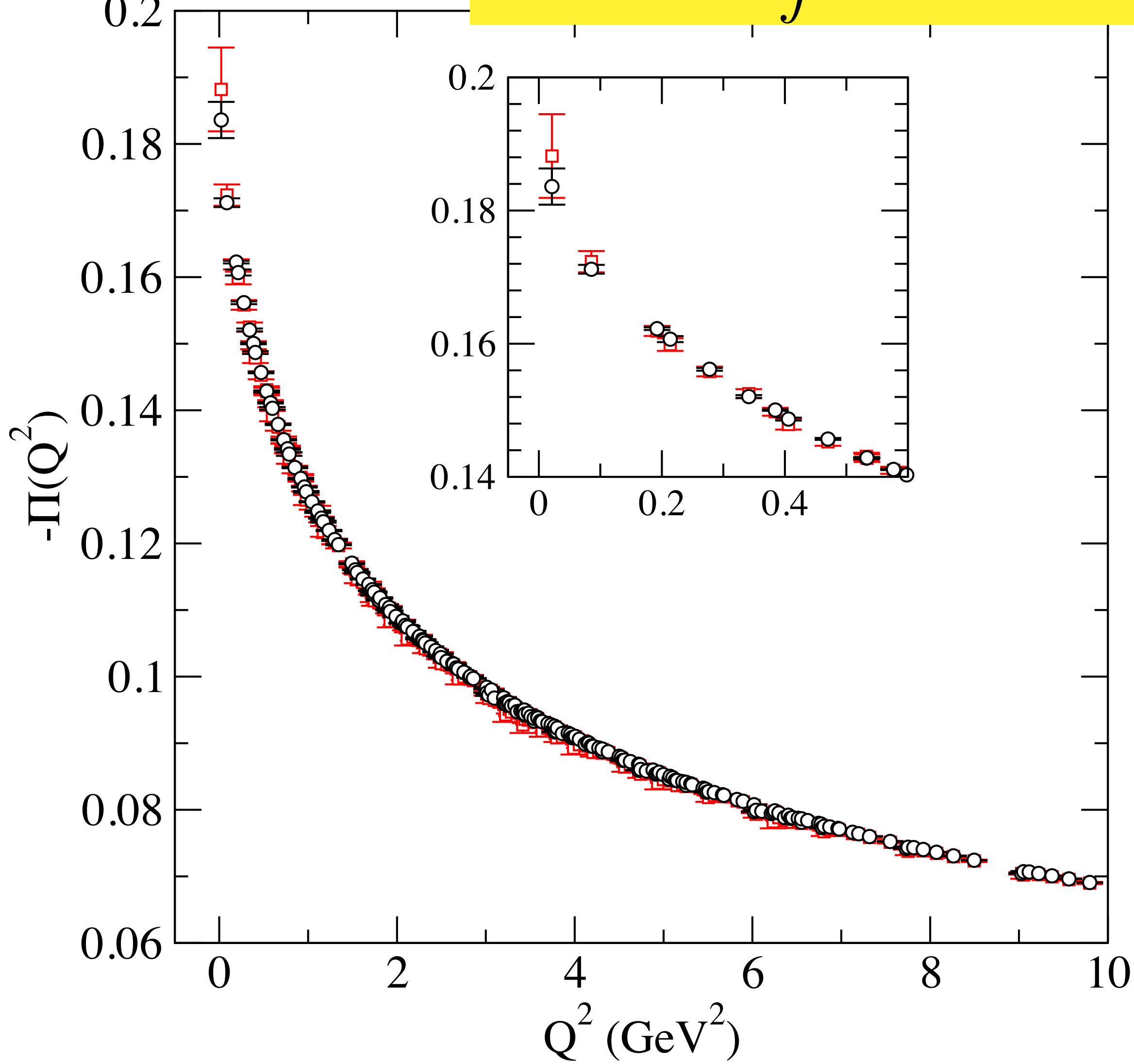


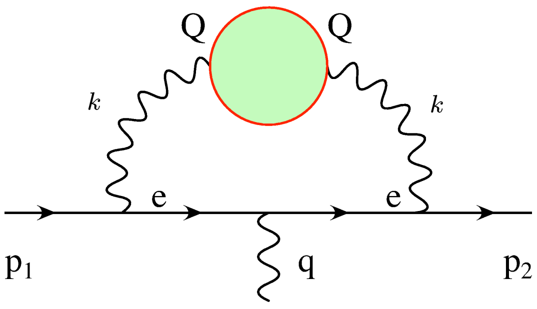
Nucleon effective mass using DWF



Hadronic vacuum polarization(AsqTad)

$$\Pi_{\mu\nu}(Q^2) = \int dx \langle V_\mu(x) V_\nu(0) \rangle e^{-q(x-y)}$$





Cost comparison for test cases

- x 16 for DWF Nucleon mass (M_{PS}=330MeV, 3fm)
- x 20 for AsqTad HVP (MPS=470 MeV, 5 fm)
- should be better for lighter mass & larger volume ?

	$N_{\rm conf}$	$N_{\rm meas}$	LM	$\mathcal{O}$	$\mathcal{O}_G^{(\rm appx)}$	Tot.	scaled cost	
m_N			$m = 0.005$, 400 LM				gauss	pt
AMA	110	1	213	18	91+23	350	0.063	0.065
LMA	110	1	213	18	23	254	0.279	0.265
Ref. [2]	932	4	-	3728	-	3728[a]	1	1
			$m = 0.01$, 180 LM					
AMA	158	1	297	74	300+22	693	0.203	0.214
LMA	158	1	297	74	22	393	0.699	0.937
Ref. [2]	356	4	-	1424	-	1424	1	1
HVP			$m = 0.0036$, 1400 LM				max	min
AMA	20	1	96	11	504+420	1031	0.387	0.050
LMA	20	1	96	11	420	527	10.3	3.56
Ref. [1]	292	2	-	584	-	584	1	1

Variants of CAA

- CAA (Covariant Approximation Averaging)
  - Name
    approximation,
    approximation accuracy control
  - LMA (Low Mode Averaging)
    low mode approx of propagator,
    # of eigen vectors
  - AMA (All Mode Averaging),
    low mode (optional)+Polynomial approx,
    (# of eigenV) Polynomial degree
    (also other type of minimization)
  - Heavy quark averaging [T. Kawanai]
    heavier mass quark prop as an approx of light prop
    quark mass
  - ?????

Other Examples of Covariant Approximations

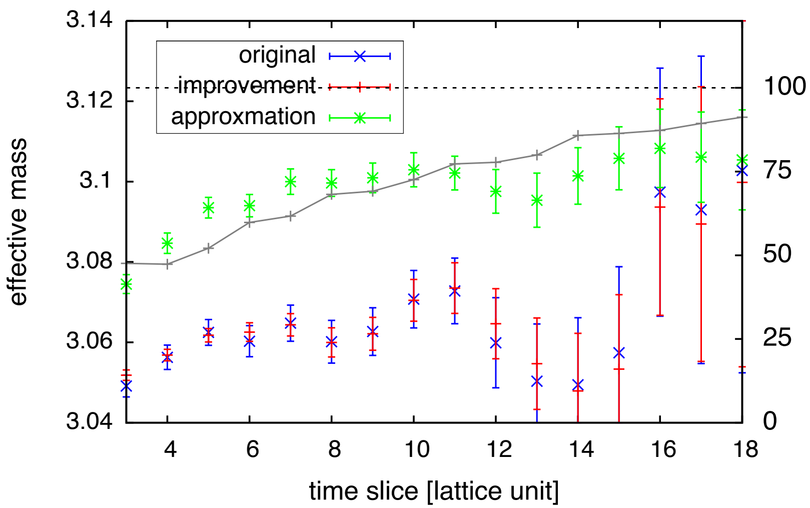
- Less expensive (parameters of) fermions :
  - Larger mf
  - Smaller Ls DWF
  - Mobius
  - even staggered or Wilson .....
- Different boundary conditions
- More than one kinds of approximation (c.f. multi mass Hasenbushing)

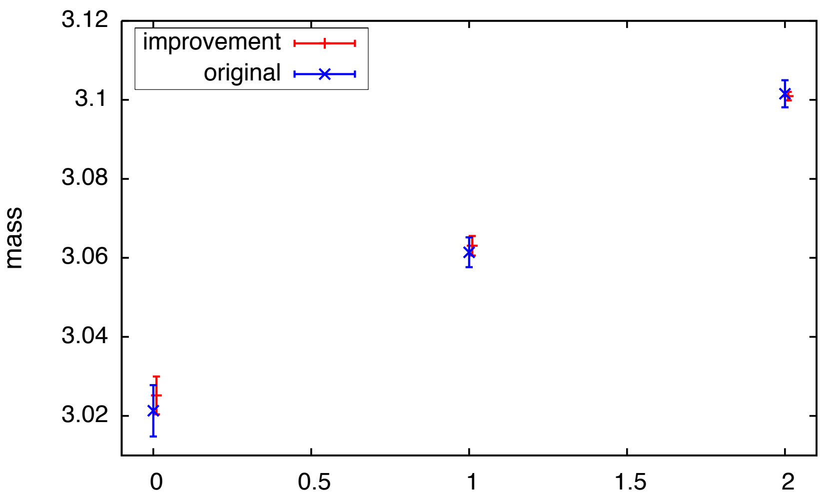
Strongly depends on Observables / Physics (YMMV)

Would work better for EXPENSIVE observables and/or fermion, potentially a game changer ?

Larger mass as CAA
[Taichi Kawanai]

24^3x64x16, 20 config ,
mf=0.01 (target) mf=0.04 “approximation”





Summary

- CAA , LMA, AMA, …. : Class of Statistical error reduction technique
  - AMA is a valence version of the Hasenbush trick
  - AMA could improve existing data easily

1. Do Full CG for selected config / source
   (existing data : This expensive part is already done)
2. Find a good approximation (accuracy of sloppiness / number of eigenvalue) that reproduce your exact CG result by, say, 95%
   (mathematically find a strongly correlated approximation, R(corr) > 0.5)
3. Subtract the approx obs with same source location as full CG
4. Perform many s $\mathcal{O}^{(\mathrm{rest})} = \mathcal{O} - \mathcal{O}^{(\mathrm{appx})}$ add back

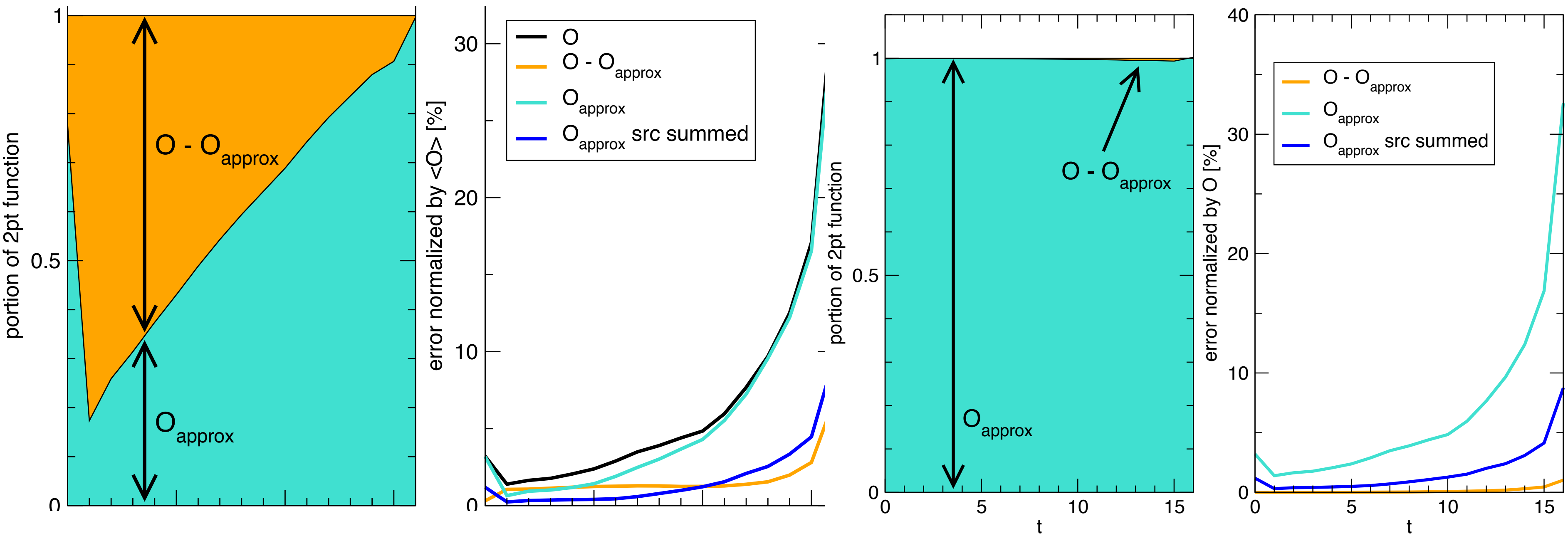
You could use other config.

$$\mathcal{O}^{(\mathrm{imp})} = \mathcal{O}^{(\mathrm{rest})} + \frac{1}{N_G} \sum_{g \in G} \mathcal{O}^{(\mathrm{appx}),g}$$

- Your Millage May Varies….
- Home Work : find a good / cheap / funny approximations

AMA in USQCD Static-light
[PI Tomomi Ishikawa]

16^3x64x16, 20 conf, 100 eigenvectors



LMA

AMA

3pt function [E. Shintani]

- Application to the form factor measurement
  - CP-even and CP-odd nucleon EM form factor

$$\langle n(P_1)|J_\mu^{\rm EM}|n(P_2)\rangle_\theta = \bar{u}_N^\theta \Big[\underbrace{\frac{F_3^\theta(Q^2)}{2m_N}\gamma_5\sigma_{\mu\nu}Q_\nu}_{\rm P,T\text{-}odd} + \underbrace{F_1\gamma_\mu + \frac{F_2}{2m_N}\sigma_{\mu\nu}Q_\nu}_{\rm P,T\text{-}even} + \cdots \Big] u_N^\theta$$

  - Complicated structure in the ratio method

Cf. Yamazaki et al., PRD79, 114505 (2009)

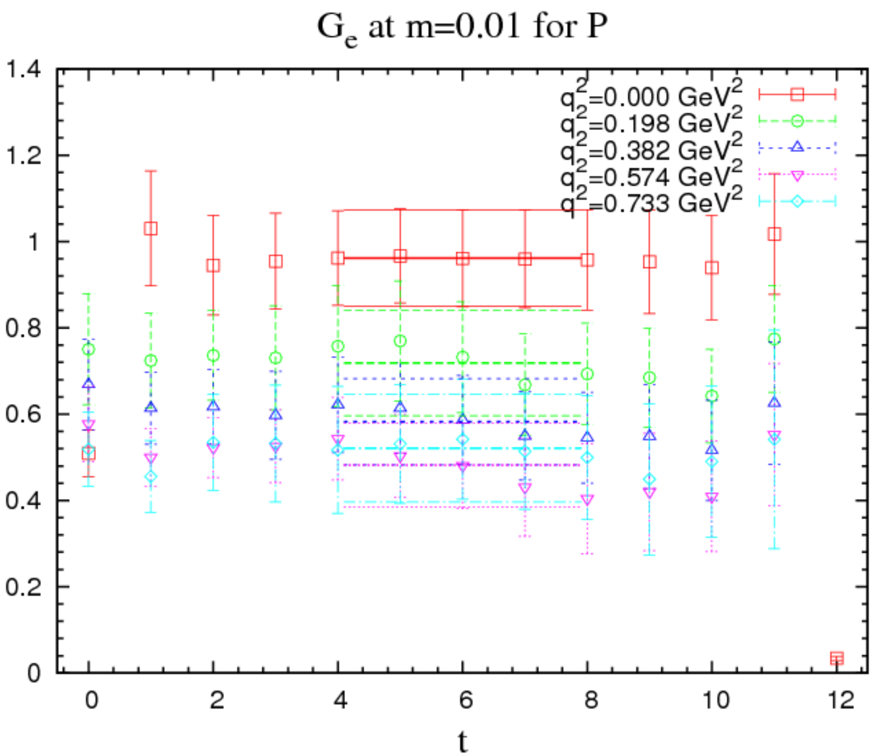
$$R_{J_\mu}(t,\vec{q}) = \sqrt{\frac{m_N}{2(E_N+m_N)}}\frac{\langle \eta_N^g J_\mu \bar{\eta}_N^g\rangle(t,\vec{q})}{\langle \eta_N^l \bar{\eta}_N^g\rangle(t_{\rm snk}-t_{\rm src},0)} R(t,\vec{q}),$$

$$R(t,\vec{q}) = \left[\frac{\langle \eta_N^l \bar{\eta}_N^g\rangle(t_{\rm snk}-t,\vec{q})\langle \eta_N^g \bar{\eta}_N^g\rangle(t-t_{\rm src},0)\langle \eta_N^l \bar{\eta}_N^g\rangle(t_{\rm snk}-t_{\rm src},0)}{\langle \eta_N^l \bar{\eta}_N^g\rangle(t_{\rm snk}-t,0)\langle \eta_N^g \bar{\eta}_N^g\rangle(t-t_{\rm src},\vec{q})\langle \eta_N^l \bar{\eta}_N^g\rangle(t_{\rm snk}-t_{\rm src},\vec{q})}\right]^{1/2}$$

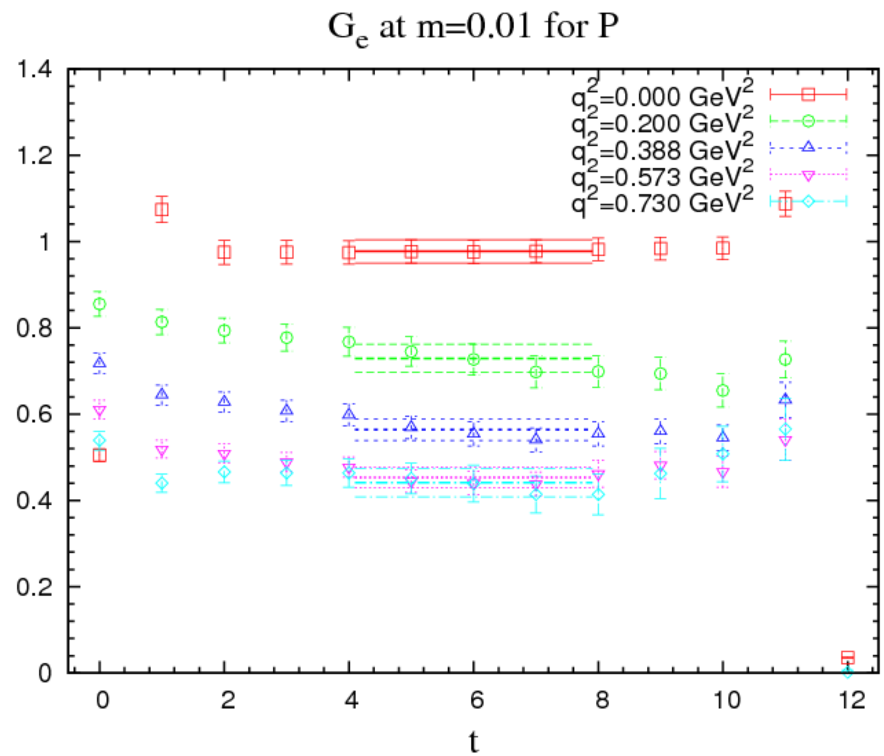
Ratio has complicated combination of both low and high mode,

so AMA has more advantage than LMA even if AMA need larger cost.

LMA



AMA

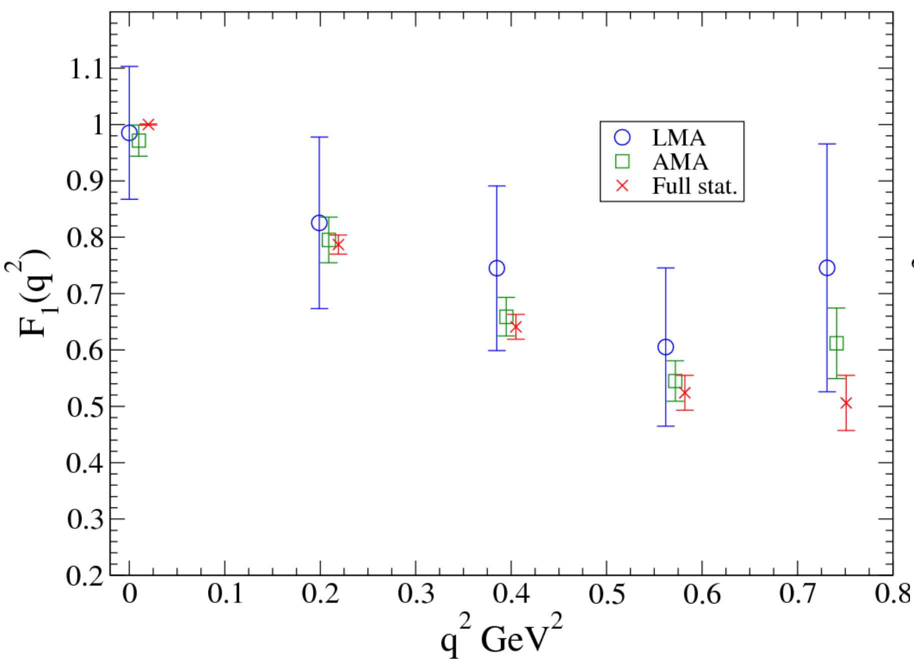


q^2 GeV^2	G_e (LMA)	G_e (AMA)
0.0	0.96(11)	0.98(3)
0.198	0.72(12)	0.73(3)
0.382	0.58(10)	0.56(3)
0.574	0.48(10)	0.45(2)
0.733	0.52(12)	0.44(3)

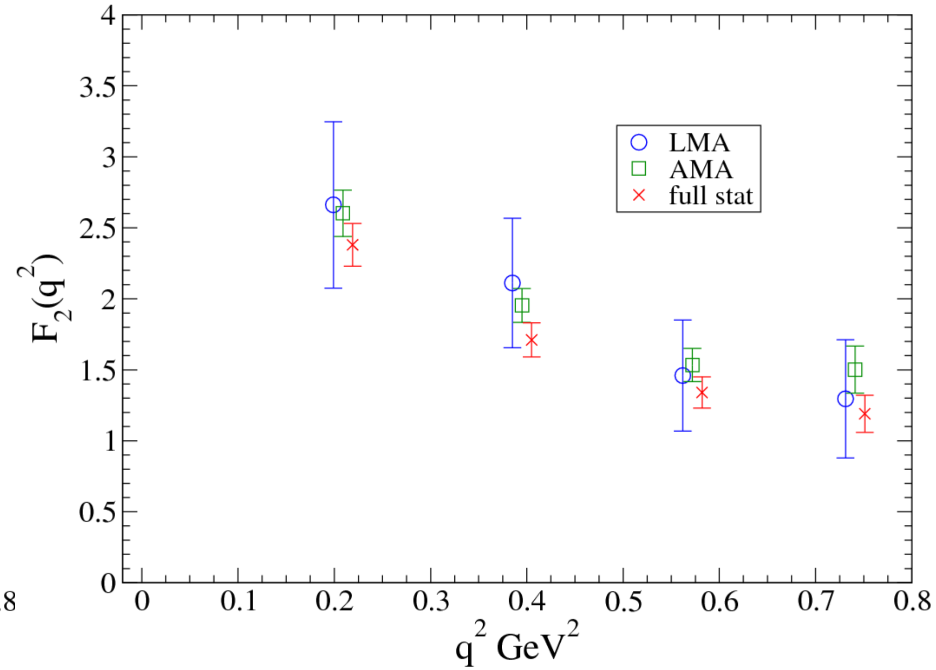
Statistical error of AMA is about 3--5 times smaller than LMA.

Comparison of isovector $F_{1,2}$ [E. Shintani]

m=0.01



m=0.01



- Results are well consistent with full statistics.
- Statistical error is much reduced in AMA rather than LMA.
- Compared to full statistics, AMA results (m=0.01) have still 1.2 -- 1.5 times larger statistical error (except for $F_1(0)$).
- This may be due to correlation between different source points.

CP-odd part

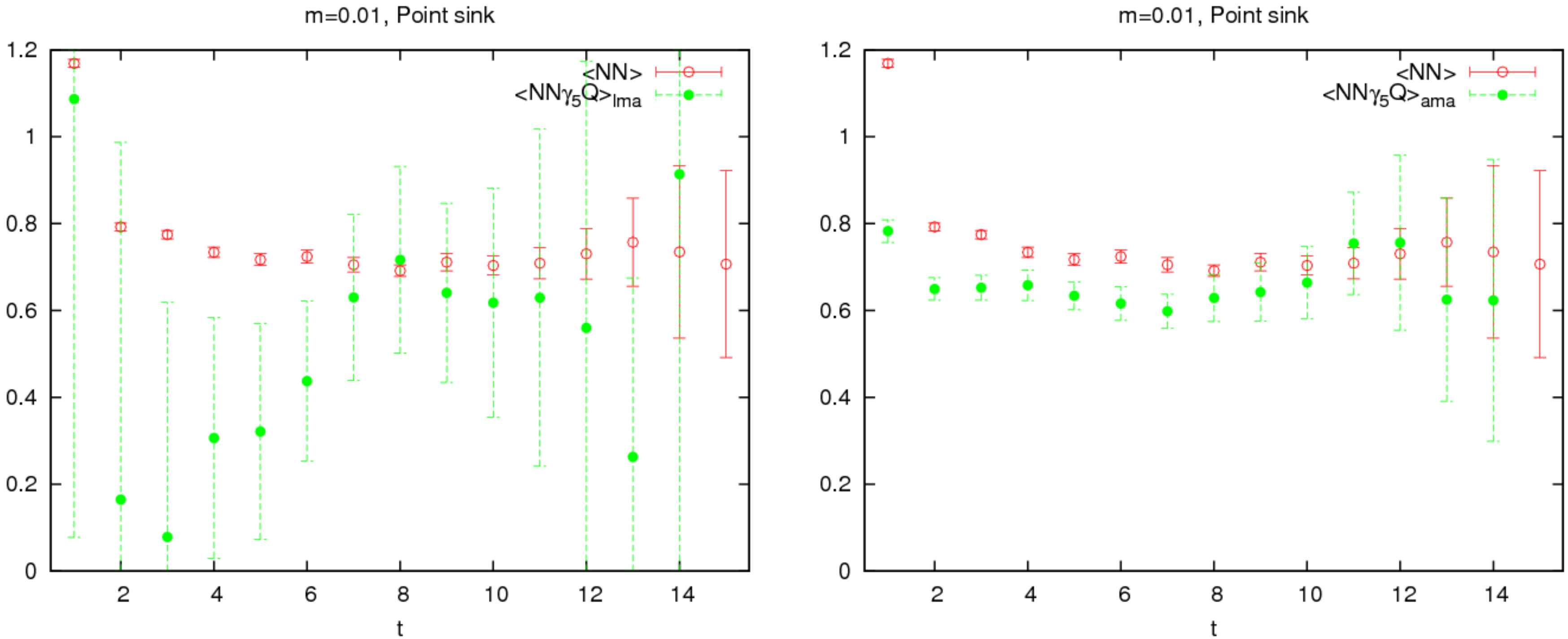
- Nucleon 2pt function with θ reweighting

$$\langle \eta_N \bar{\eta}_N \rangle_\theta (\vec{p}) = Z_N^2 \frac{ip \cdot \gamma + m_N e^{i\alpha(\theta)\gamma_5}}{2E_N}$$

$$\mathrm{tr}\left[\gamma_5 \langle Q \eta_N \bar{\eta}_N \rangle (\vec{p})\right] \simeq Z_N^2 \frac{2m_N}{E_N} \alpha e^{-E_N t}$$

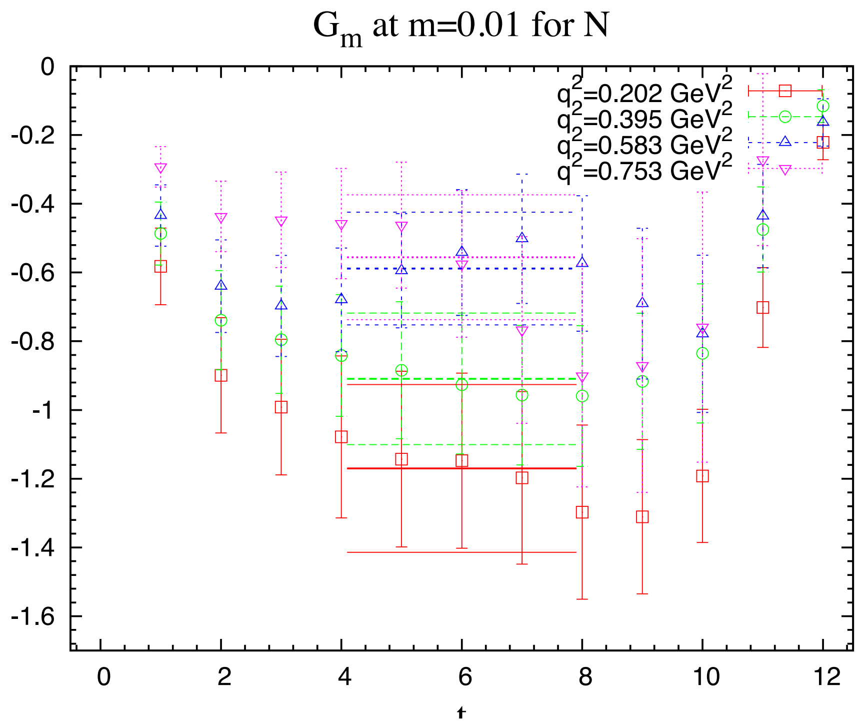
  - Q is topological charge.
  - α which is CP-odd phase is necessary to extract EDM form factor.
  - It is good check of applicability of LMA/AMA to CP-odd sector.
  - Effective mass plot shows the consistency of the above formula

CP-odd part [E. Shintani]

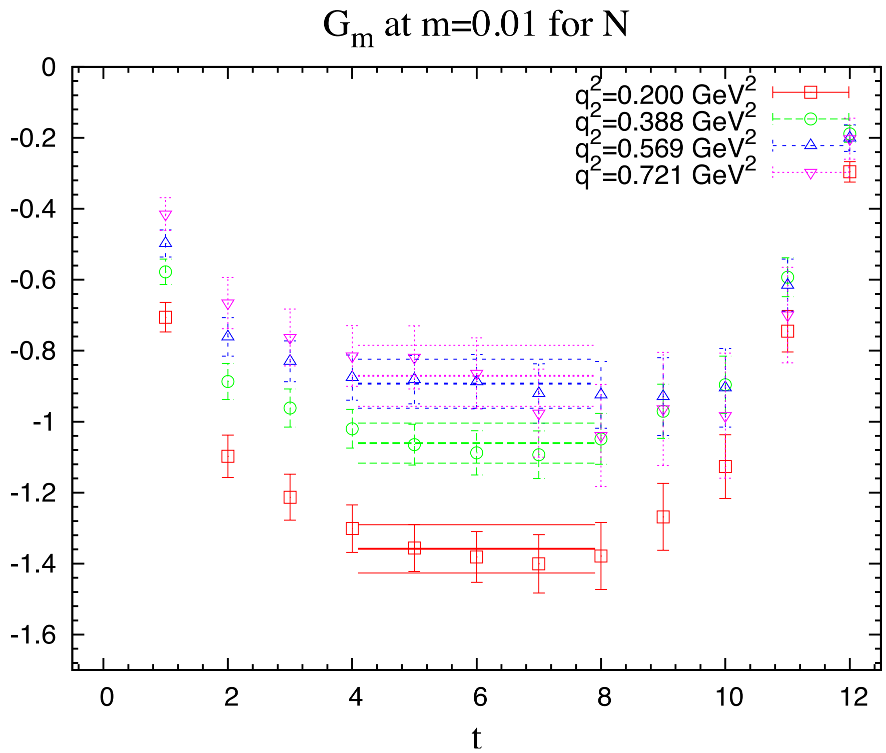


- There is good plateau in AMA, and this figure actually shows CP-odd part has consistent exponent with CP-even(nucleon mass) part as expected.
- CP-odd part has both contribution from high and low lying mode.
- AMA works well even in CP-odd sector !

Nucleon Magnetic formfactor

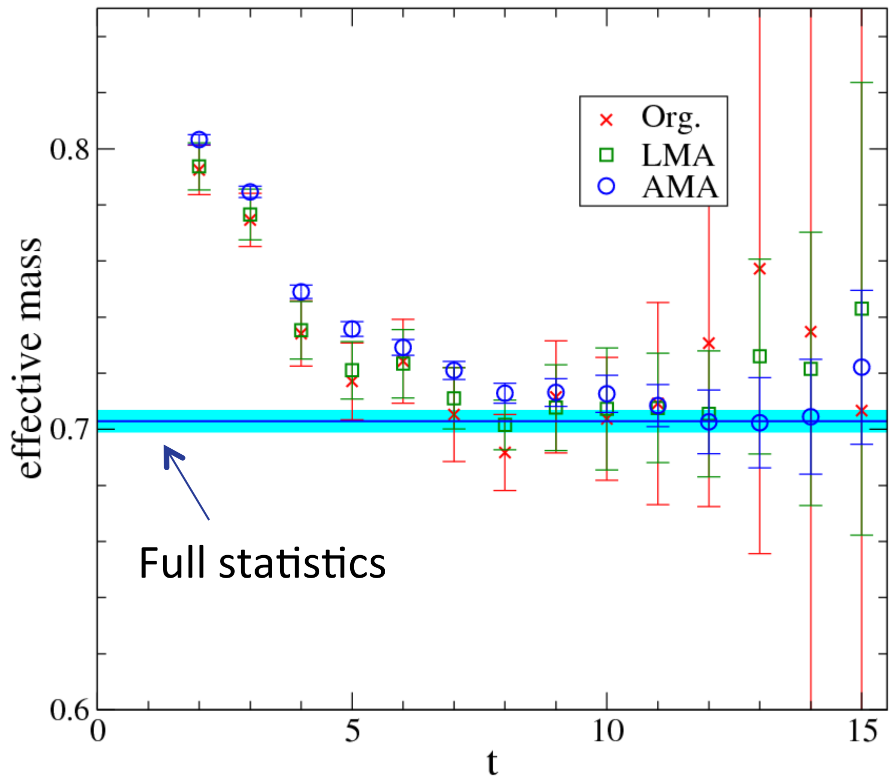


Original CG

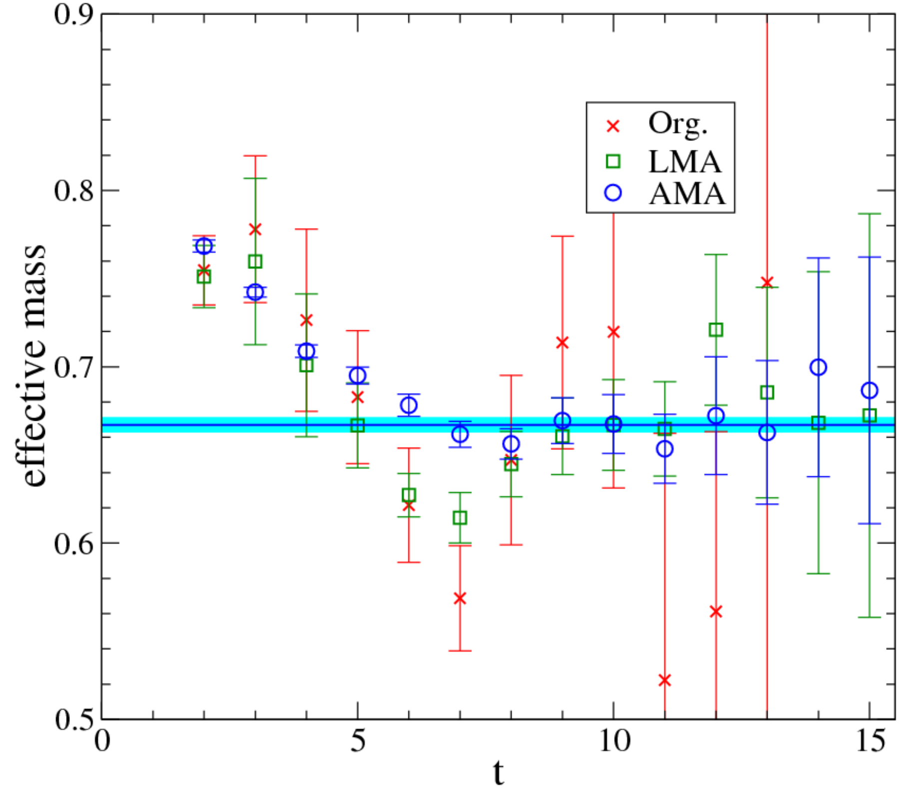


AMA

N, m=0.01, point sink



N, m=0.005, point sink



	LMA [7,15]	AMA [7,15]	statistics	Full statistics (Gaussian sink)
m = 0.01	0.712(16)	0.710(5)	N_{conf}=80, N'_{mes}=32	0.703(4), N_{conf} = 356, N_{mes}=4
m = 0.005	0.673(22)	0.666(13)	N_{conf}=26, N'_{mes}=32	0.663(4), N_{conf} = 932, N_{mes}=4

Yamazaki et al., PRD79, 114505 (2009)

Cost (in the case of 24cube m=0.01)

Use of unit of quark propagator "prop" in full CG w/o deflation

Yamazaki et al., PRD79, 114505 (2009)

- Case of full statistics

  In N_{conf} = 356, N_{mes}=4,

  Total： 356×4 = 1424 prop

- Case of AMA w/o deflation

  Since calculation of O^{appx} need 1/50 prop, then in N_{conf}=81, N'_{mes}=32

  Total： 80 + 80×32/50 = 131 prop ⇒ 10 times fast

- Case of AMA w/ deflation

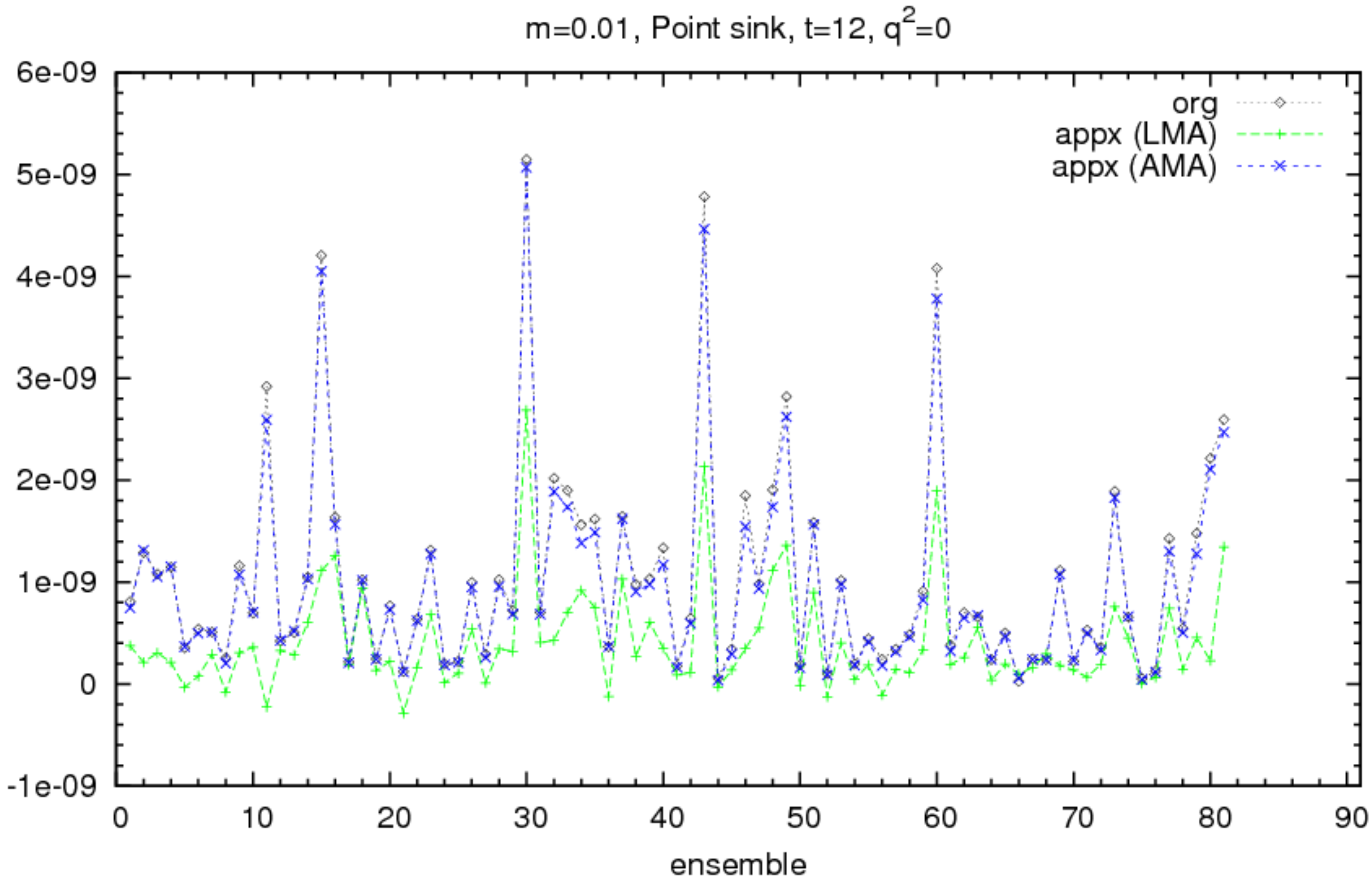
  When using 180 eigenmode, calculation of O^{appx} need 1/80 prop, but in this case the calculation of lowmode is ~1 prop/configs. Deflated CG makes reduction of full CG to 1/3 prop, then

  Total： 80/3 + 80×32/80 + 80 = 138 prop ⇒ 10 times fast

  <u>Note that stored eigehmode is useful for other works.</u>

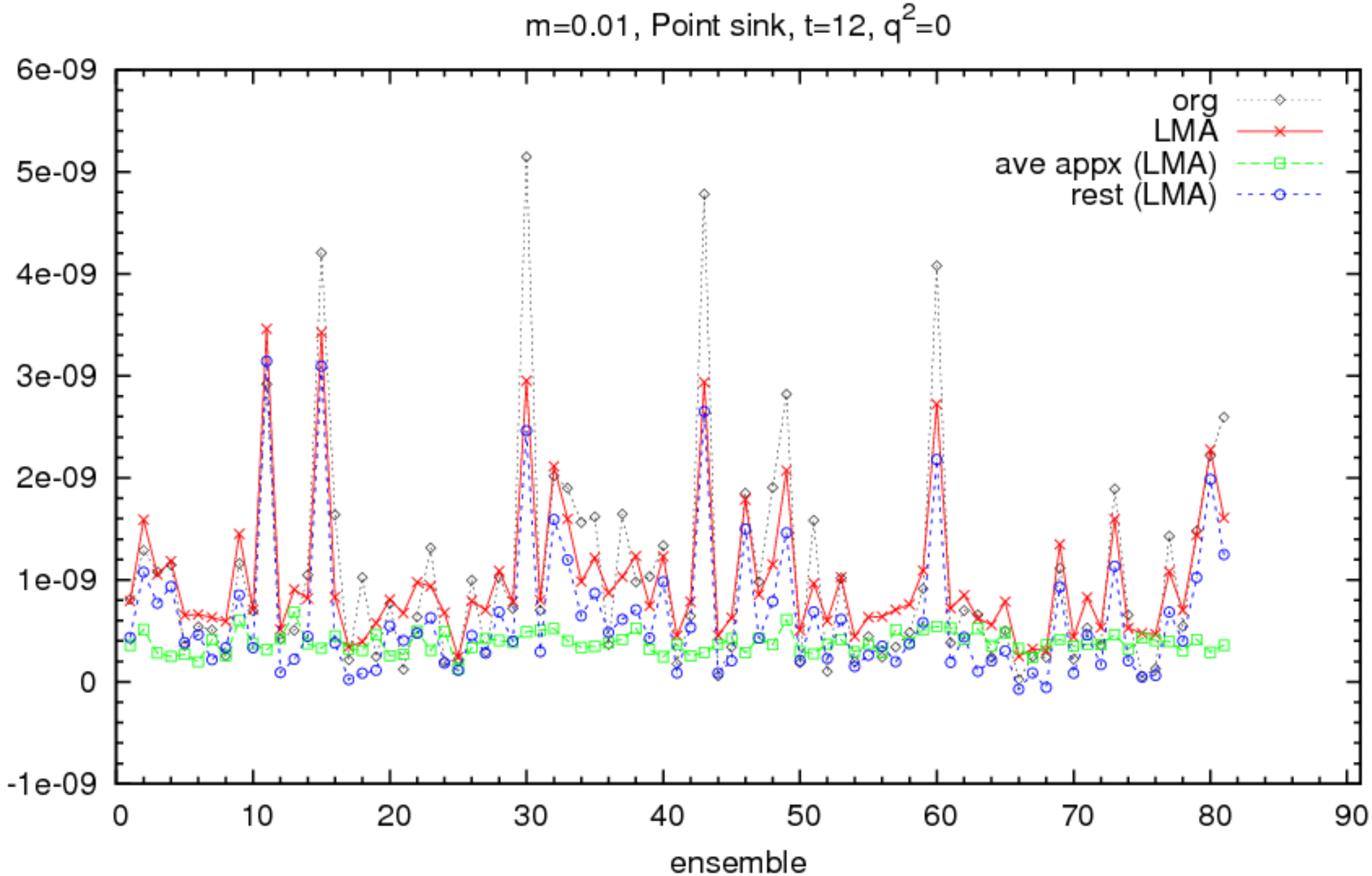
Correlation

- NN propagator at long time-slice



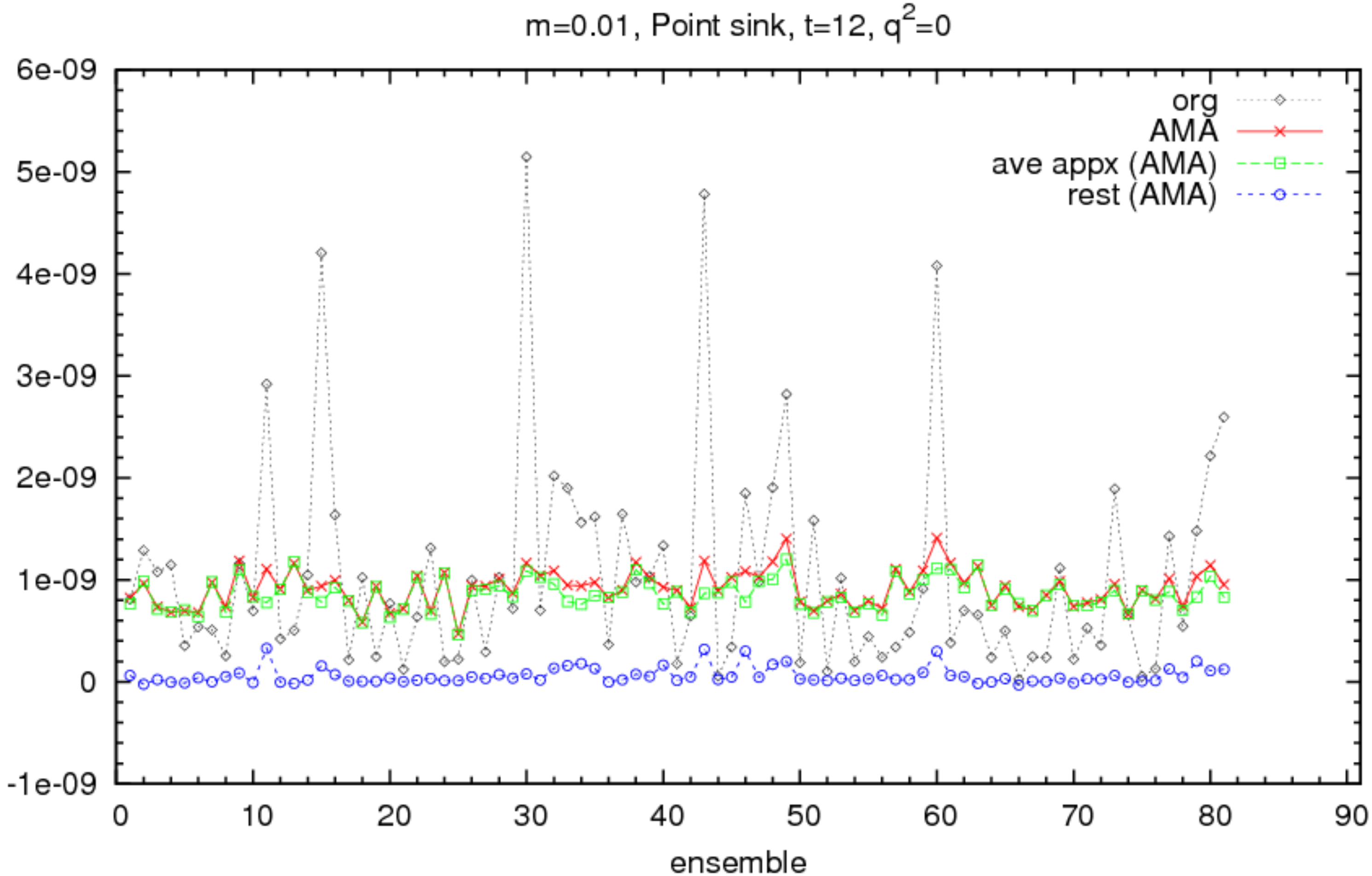
Correlation

- NN propagator (LMA) at long time-slice



Correlation

- NN propagator (AMA) at long time-slice



Other technical details

- Implicitly Restarted Lanczos with Polynomial acceleration and spectrum shifts for DWF and staggered in CPS++ [E. Shintani, T. Blum, TI].
- Eigen Vector compression / decompression

- Sea Electric Charge is now controlled by QED reweighting
  [T. Ishikawa et. al. arXiv:1202.6018]
- Aslash-SeqSrc method