Parton Distribution Functions and Amplitudes of the Pseudoscalar Mesons and the Nucleon from Lattice QCD

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Abstract

A long-standing challenge in lattice QCD is the direct computation of key measures of hadron structure, including parton distribution functions, quark distribution amplitudes, and three-dimensional measures such as the transverse-momentum-dependent distributions, and generalized parton distributions. Recently, new approaches have been proposed that enable their direct computation, and these are characterized by a requirement that the hadron of interest be increasingly relativistic. The ~~aim of this~~ **Class A Continuation** proposal ~~is~~ aims to capitalize on recent developments, and our previous USQCD allocation, to compute the structure functions of the pion and nucleon using the pseudo-PDF and current-current matrix element formulation using the distillation framework, and to extend the calculation to that of the gluon contribution to hadron structure, and to embark on calculations of three-dimensional imaging through the calculation of GPDs in the pseudo-PDF approach. This project is relevant to the hadron structure experimental programs at JLab, and at RHIC-spin. With the recent CD0 and site selection of the EIC, the extension to the gluon distributions is particularly timely. **We request an allocation of 58 KNL-core-hours, 0.88M GeForge GPU-Hours, 6M SKX-core-hours, together with an addition 100 TByte tape storage, and 60 Tbyte of disk storage.**

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1 Goals and Milestones

Nuclear physics is a vast, rich field, whose phenomenology has been explored for decades through intense experimental and theoretical efforts. However, it is only now that direct connections to quantum chromodynamics (QCD), the underlying theory of the strong interactions, and the basic building blocks of nature, quarks and gluons, are solidifying. The phenomena of confinement and chiral symmetry breaking are jointly responsible for the intervening forty years of research and development between the discovery of QCD [1, 2, 3], the formulation of QCD on a discretized space-time [4] and recent numerical solutions of simple systems at the physical values of the quark masses along with the inclusion of electromagnetism. This new-found ability is changing nuclear physics. It is permitting us to address key questions that define the field, such as how the observed particles emerge from QCD, how gluons manifest themselves in the spectrum and structure of hadrons, and how the spin and other attributes of the pion and proton are partitioned between the quarks and gluons. The target for this proposal is to refine critical aspects of the nature of strongly interacting particles composed of quarks and gluons and their dynamics by direct calculations at the physical light quarks masses using the numerical technique of lattice QCD.

One of the great challenges posed by QCD is to understand how protons and neutrons, the basic building blocks of most of the observed matter in the universe, are made from quarks and glue. First principles calculations in this area are directly relevant to the experimental programs at JLab 12 GeV and LHC, and the future electron-ion collider (EIC), to be sited at BNL and which has now received CD0. Our knowledge of hadron structure is encapsulated in a variety of measures. From the earliest observations of Bjorken scaling in Deep Inelastic Scattering, a one-dimensional longitudinal description of the nucleon has been provided through the unpolarized and polarized *Parton Distribution Functions* (PDFs). In contrast, the transverse distribution of charge and currents was probed in elastic scattering, encapsulated in the electric and magnetic form factors. More recently, new measures have been discovered correlating both the longitudinal and transverse structures: the *Generalized Parton Distributions* (GPDs) describing hadrons in longitudinal fractional momentum x and impact-parameter space, and the *Transverse-Momentum-Dependent Distributions* (TMDs) providing a description in x and transverse momentum space. These new descriptions have opened new vistas on the nucleon, in particular enabling orbital angular momenta to be discerned.

From the inception of these new measures, the lattice community has attempted to calculate them from first principles. However, the formulation of lattice QCD in Euclidean space provides a formidable restriction: the x dependence could not be computed directly, but only the x moments of the distributions. Furthermore, the breaking of rotational symmetry on the lattice in practice restricted such calculations to only the first few moments. Recently, new ideas have been proposed that aim to circumvent one or more of these restrictions[5, 6, 7, 8, 9, 10, 11, 12].

The work proposed here will be to further exploit these new methods to investigate the properties of the pion, the lightest hadron composed of the light u, and d, and of the nucleon through calculation of so-called good "Lattice Cross Sections" identified in ref. [12], and through the calculation of pseudo-PDFs[11]. In particular, we will calculate the collinear one-dimensional x-dependent parton distribution function of the pion and nucleon, notably at large x. The calculations proposed here can also be used to compute the moments of the parton distributions for comparison with earlier works [13]. The determination of large-x part of the pion PDF is the goal of the approved experiment C12-15-006 at Jefferson Lab, whilst the determination of the kaon structure function is the goal of the approved run-group C12-15-006A. Furthermore, the approved experiments E-03-012, E-00-002, at Jefferson Lab (12 GeV) are targeting the determination of the nucleon structure functions at large-x. x The large-x region is precisely the region our computational methods are more effective and therefore our work is in close synergy with the already approved experimental efforts at Jefferson Lab. In

addition to the experimental program at Jefferson Lab, at the Theory Center, the JAM collaboration aims towards the determination of PDFs from experimental data. Our future plans include a close collaboration with JAM using our lattice QCD results to further enhance the fidelity of the pion and nucleon PDFs.

Our proposed program of work for the coming year capitalizes on the progress during the current allocation period in both computational efficiency and physics reach. Firstly, we have clearly shown the advantage of the distillation framework for the calculation of hadron structure using the pseudo-PDF approach; we will exploit this to refine our current calculations of the parton distribution functions of the nucleon and pion, and to calculate at near-to-physical light-quark masses. Secondly, we will use the high statistical precision and sampling of the gauge configurations facilitated through the use of distillation to perform calculations of the gluon contributions to nucleon structure. Finally, we will perform exploratory studies of Generalized Parton Distributions (GPDs) within the pseudo-PDF framework.

already introduced above

The framework for the calculation of Bjorken-x-dependent PDFs using the pseudo-distribution and "lattice cross section" approaches has been described in the introduction to our 2019 proposal. We will repeat that description here, but emphasise that it provides a framework that permits collinear factorization with a well-defined short-distance scale. However, there are two theoretical developments by our group over the past year that we will exploit in our proposed work for 2020-2021. The first is the development of the framework to calculate gluon pseudodistributions[14] for forward scattering, and the second is the formalism for the calculation of Generalized Parton Distributions in the pseudodistribution approach[15].

emphasize

GPDs

Recent Progress

Pion Parton Distribution Function

In ref. [16], we computed, for the first time, the valence PDF of the pion using Ioffe-time pseudo-distribution functions, using the ensembles $a127m415$ and $a127m415L$ of Table 1. The resulting Ioffe-time distribution (ITD) is shown as the left-hand panel of Figure 1. A comparison of our calculation of $xf_V^\pi(x)$ with other approaches is shown as the right-hand panel

We have recently used USQCD resources to extend our prior calculation[17] of the pion PDF through the LCS approach in two important ways. Firstly, we have now computed the kernel relating the computed lattice matrix elements to the parton distribution functions at $\mathcal{O}(\alpha_s)$, enabling us to associate scale with the extracted parton distribution functions. Secondly, we have performed the calculation on four different ensembles of Table 1, enabling to investigate the finite lattice spacing, volume and quark-mass dependencies. A comparison between this new lattice calculation[20], and pheneomenological determinations, is show in Figure 2. Our results suggest a softer $(1-x)^2$ behavior at large x, rather than a harder $(1-x)$ behavior, and our future research will aim to provide a more definitive answer to this question.

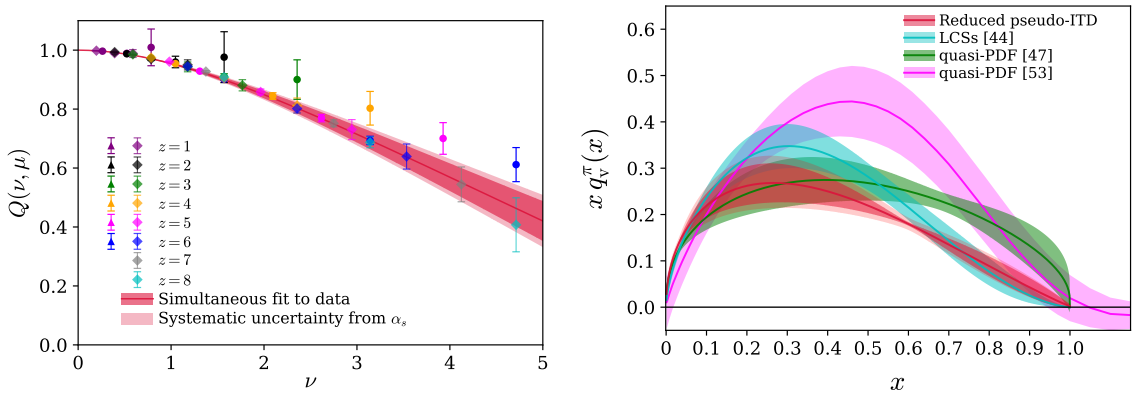
phenomenological

shown

Nucleon Pseudo-PDF

The exploratory, first calculation of PDF of the nucleon through the pseudo-PDF approached[9], performed in the quenched approximation to QCD has been extended to calculations using the USQCD Wilson-clover lattices on the ensembles $a127m415, a127m415L$ and $a094m390$ of Table 1 allowing for the first time some understanding of finite-volume and discretisation effects[23]. The ITD and resulting nucleon PDF at on the $a127m415L$ ensemble is shown as the left- and right-hand panels of Figure 3; note that a further calculation including the $a091m170L$ ensemble is in preparation.

discretization



distribution

Figure 1: The left-hand panel shows the reduced $\overline{\text{MS}}$ Ioffe-Time Distribution matched to a scale of $\mu = 2$ GeV; the circle and diamonds show the reduced Ioffe-time matrix elements obtained on the smaller 24^3 and larger 32^3 ensembles, respectively. The band is obtained from a simultaneous fit to the matched ITDs in the limit of infinite volume. The right-hand panel shows the resulting PDF $xq_V^\pi(x)$, at a scale $\mu = 4$ GeV,together with other lattice results: our calculation using the LCS approach[17], and two calculations using the quasi-PDF approach[18, 19].

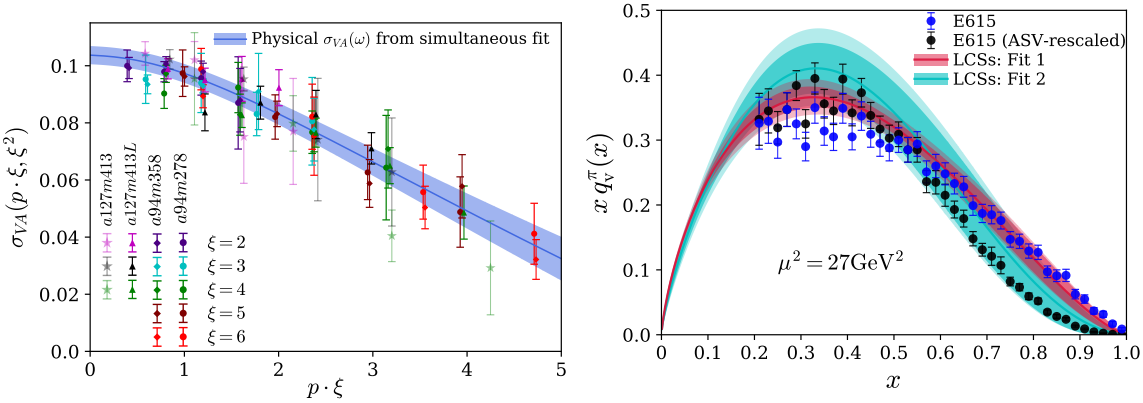


Figure 2: The left-hand plot shows the current-current matrix elements determined on our four ensembles against Ioffe time $\nu = p \cdot \xi$, where ξ is the spatial separation between the currents; the band is the Ioffe-time distribution at the physical limit. The right-hand plot shows the resulting valence PDF of the pion in comparison with phenomenological determinations[21, 22].

PDF obtained from fit to experimental data

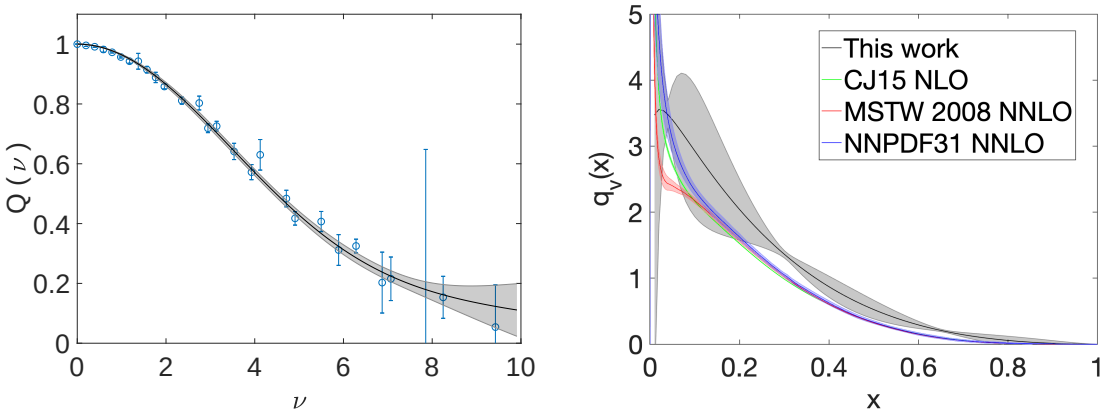


Figure 3: The left- and right-hand panels show the nucleon ITD and PDF at a scale $\mu = 2$ GeV on the larger of our two lattices at the coarser lattice spacing. The grey bands denote a fit to the phenomenological form $f(x) \simeq x^a(1-x)^b(1 + c\sqrt{x} + dx)$, ~~as used by the JAM collaboration.~~ Phenomenological PDF bands are from refs. [24, 25, 26], evolved to the same scale.

Momentum smearing in Distillation Framework

An important requirement to reliably determine the x-dependent parton distribution functions from the ITD is a sufficient range and resolution in the Ioffe time $\omega = p \cdot \xi$, thereby requiring that we be able to boost the hadron to high momentum. Unfortunately, the signal-to-noise ratio rapidly degrades at large momentum, and therefore we have been investigating a new approach whereby we combine distillation with so-called "momentum smearing". The success of this method is illustrated in Figure 4, where we show the extracted energy of the nucleon as we boost its spatial momentum using both standard "distillation", and its boosted version; momentum smearing is essential to reach the high energies needed for this study.

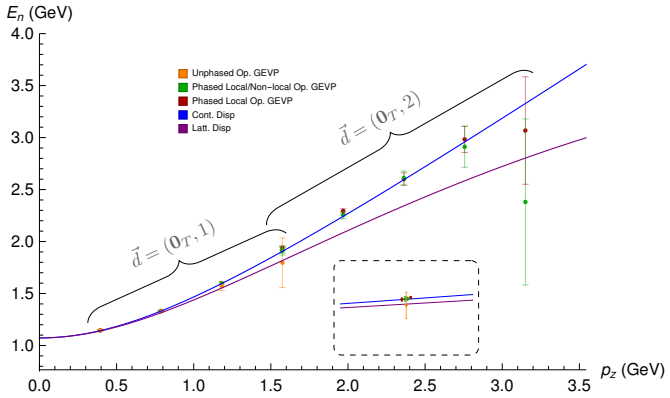


Figure 4: The figure shows the energy, E_n, of the ground-state nucleon as a function of the spatial momentum, using standard "distillation" at lower values of the momenta, labelled by *unphased-op*, together with energy obtained using momentum smearing, labelled by *phased-op*, for two different operator bases. The lines denote the expected energies according to the continuum dispersion relation, and to a discretised version for free-meson particles.

labeled

discretized

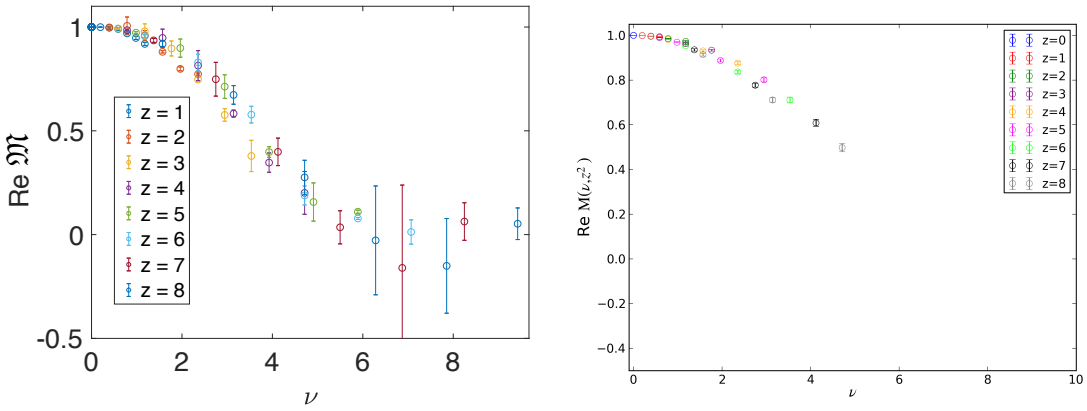


Figure 5: The left- and right-hand plots so the unevolved, reduced pseudo-ITD $\mathcal{M}(\nu, z^2)$ from ref. [23], and using the distillation framework, using the $a094m390$ ensemble.

Work for 2020-2021 Allocation Year

Our program of work for the 2020-2021 will focus on three broad areas, which we now discuss.

PROJECT I: Isovector PDF of the Nucleon and Pion with "distillation"

Our aim is to extend the calculation of both the nucleon and kaon/pion Parton Distribution Functions to lighter pion masses, and within the distillation framework to allow a better sampling of our lattices. We discuss the advantages of the distillation framework in further detail in the next section, but using the current allocation we have already demonstrated the efficacy of our approach through the more complete sampling of the lattice for the nucleon pseudo-PDF, as we illustrate in Fig. 5.

PROJECT II: Gluonic degrees of freedom in hadrons

In the manner of the isovector PDFs computed in the Ioffe-time framework, the parton distribution functions of the gluon can be related to the matrix elements of field-strength tensors separated along a spatial direction z:

$$M_{\mu\alpha;\lambda\beta}(z,p) \equiv \langle p|\mathrm{Tr}[F_{\mu\alpha}(z)U(z,0)F_{\lambda\beta})0)U(0,z)]|p\rangle \tag{1}$$

where U's are gauge links inserted to ensure gauge invariance. The necessary formalism to relate the resulting pseudo-ITD to the gluon PDF has recently been developed[14], and we will exploit this to obtain, for the first time, the gluon distribution within the pseudo-PDF framework, using the Wilson-flow procedure[27]. Example results showing the quality of the data is shwon in Figure 6. We are also pursuing, in parallel, its calculation using the LCS approach[12]. shown

PROJECT III: Exploratory calculation of Generalized Parton Distributions

The Generalized Parton Distributions provide a three-dimensional image of the nucleon and pion in the longitudinal momentum fraction x and the impact parameter b_T. The one-loop matching coefficients relating Ioffe-time distributions to the GPDs within the pseudo-PDF approach have recently been computed[15], and the distillation framework provides a straight-forward framework in which

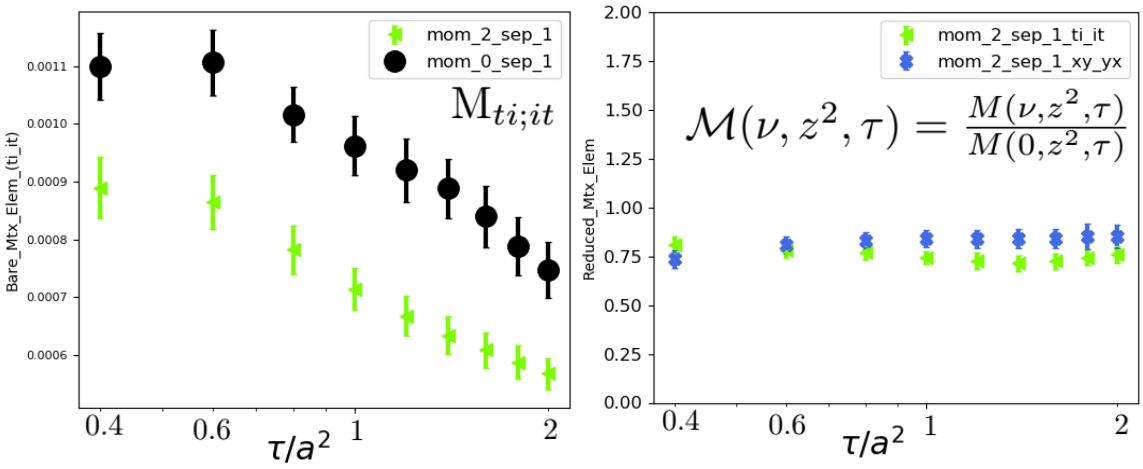


Figure 6: The left-hand panel shows the gluon matrix element $M_{it;it}(z = 2)$ for both zero and two units of momentum in the z direction vs the Wilson-flow evolution time; the right-hand panel shows the corresponding reduced matrix element

to implement it. Finally, we note that in our calculation of the gluonic contributions to hadron structure, we will use the gradient-flow method[27]

Computational Strategy

Our strategy will be to use an already generated gauge ensembles, with a clover-fermion action, a lattice spacing $a \simeq 0.09$ fm, with pion masses down to 170 MeV. The framework for our calculations will be *distillation*, which was described in detail in our 2019-2020 proposal. Thus we will only outline the salient points of the method for our program of calculations in this document.

In summary, distillation is a method of smearing in which the smearing $\Box(t)$ is expressed as a truncated outer product of eigenvectors $v^{(i)}(t)$ of the three-dimensional Laplacian

$$\Box(t) = \sum_{i=1}^{N_{\rm vec}} v^{(i)}(t) v^{(i)\dagger}(t).. \tag{2}$$

For compactness, we will discuss the case of mesons, where we write a "smeared" two-point correlation function as

$$C_{AB}(t_f, t_i; \vec{p}) = \langle \Phi^A_{ijk}(\vec{p}, t_f) \tau^{ii'}(t_f, t_i) \tau^{ii'}(t_f, t_i) \tau^{jj'}(t_f, t_i) \tau^{kk'}(t_f, t_i) \bar{\Phi}^B_{i'j'k'}(\vec{p}, t_i) \tau^\dagger(t_f, t_i) \rangle, \tag{3}$$

where

$$\Phi^{A,ij}_{\alpha\beta}(\vec{p}, t) = \sum_{\vec{x}} v^{*(i)}(\vec{x}, t) e^{-i\vec{p}\cdot\vec{x}} [\Gamma^A(t)\gamma_5]_{\alpha\beta} v^{(j)}(\vec{x}, t) \tag{4}$$

$$\tau^{ij}_{\alpha\beta}(t_f, t_i) = v^{*(i)}(t_f) M^{-1}_{\alpha\beta}(t_f, t_i) v^{(j)}(t_i). \tag{5}$$

Here $i, j = 1, \ldots, N_{\rm vec}$, α, β are spinor indices, and t_i, t_f the source and sink timeslices respectively, and Γ is an operator that may include derivatives. The crucial observation in the above construction is that the Φ's of eqn. 4, denoted "elementals", encode the structure of the operator, with, for

example, derivatives now acting on the (quark-mass-independent) ξ's, whilst the parallel transport of the quark fields is encoded in the "perambulators" of eqn. 5. The advantages of the method are three-fold. Firstly, the factorization between the perambulators and elementals enables operators of essentially unrestricted spatial structure to be used at both source and sink, without the calculation of additional perambulators. Secondly, correlator of eqn. 3 involves spatial sums both at the source and at the sink, thus providing a more complete sampling of the lattice. Finally, the form of eqn. 3 can straightforwardly be extended to baryons, with only the need for the calculation of an appropriate set of baryon "elementals". The implementation of momentum smearing within the distillation framework requires the computation of boosted perambulators, obtained from the boosted eigenvectors

$$\tilde{v}^{(i)}(\vec{x},t) = e^{i\vec{\zeta}\cdot\vec{x}} v^{(i)}(\vec{x},t) \tag{6}$$

where ζ is a three-momentum allowed on our lattice.

The calculation of three-point functions proceeds likewise, and it involves the introduction of so-called "generalized perambulators",

$$S^{ij}_{\rm LCS}(t_f,t_i,t;x_0,\xi) = v^{(i)\dagger}(t_f) M^{-1}(t_f;x_0+\xi,t)\Gamma_1 G_Q(x_0+\xi;x_0,t)\Gamma_2 M^{-1}(x_0,t;t_i) v^{(j)}(t_i) \tag{7}$$

$$S^{ij}_{\rm pPDF}(t_f,t_i,t;\vec{q},\xi,) = \sum_{x_0} v^{(i)\dagger}(t_f) M^{-1}(t_f;x_0+\xi,t)\Gamma W(x_0+\xi;x_0,t) e^{-i\vec{q}\cdot\vec{x_0}} M^{-1}(x_0,t;t_i) v^{(j)}(t_i) \tag{8}$$

where G_Q is a spectator quark propagator for the case of the LCS approach, and W is a Wilson line in the pseudo-PDF approach. The resulting three-point function can then be written

$$C^{\rm 3pt}_{AB}(t_f,t_i,t;x_0,\xi,\vec{p}) = {\rm Tr}\langle \phi^A(\vec{p},t_f) S(t_f,t_i,t;x_0,\xi)\Phi^B(\vec{p},t)\tau^\dagger(t_f,t_i)\rangle,. \tag{9}$$

for the case of mesons, where S corresponds to $S_{\rm LCS}$ or to $S_{\rm pPDF}$ for the case of the LCS and pseudo-PDF approaches, respectively. $C^{\rm 3pt}_{\rm AB}$ is of the same form as $C_{\rm AB}$ of eqn. 3, with one of the perambulators replaced by a generalized perambulator. Note that in the pseudo-PDF calculation of eqn 8, there is an additional time-sliced sum at t. This has two important consequences. Firstly, for the pseudo-PDF calculation of the nucleon, we are able to perform momentum projections at each time location in a three-point function, something we have not been able to achieve using our previous methods. Secondly, the ability to insert momentum at t enables us to explicitly introduce a momentum transfer thus facilitating the calculations of the off-forward matix elements describing GPDs. Note the same set of *perambulators* and *generalized perambulators* are employed for baryon and meson structure calculations.

Software

We will use the *Chroma* software framework, which now supports multigrid on the GPUs, KNLs and the Skylake nodes. for the computation of the elements, we use *harom*, running on top of the three-dimensional `qdp++` code. We have made considerable advances to our software since our last submission. Firstly, the construction of the generalized perambulators of eqn. 8 has been implemented and verified within *Chroma* in a way that obviates the need to write solution vectors to disk, and enabled the results presented in Figure 5. Secondly, the software framework for the construction of the baryons elements and their contraction to form the two- and three-point functions has now been optimized both in terms of computational performance, and in terms of memory usage such that we are now able to use 128 eigevectors, needed on our larger lattices, rather than the 64 we have used in our previous work.

A remaining task is to implement the calculation of the generalized perambulator in the LCS approach, eqn. 7; the computational cost will not add signficantly to that provided in Table 2, but requires integration into our framework.

Ensemble ID	a (fm)	M_π (MeV)	β	$L^3 \times T$
$a127m415$	0.127(2)	415(23)	6.1	$24^3 \times 64$
$a127m415L$	0.127(2)	415(3)	6.1	$32^3 \times 96$
$a094m390$	0.094(1)	390(3)	6.3	$32^3 \times 64$
$a094m270$	0.094(1)	270(3)	6.3	$32^3 \times 64$
$a091m170$	0.091(1)	170(2)	6.3	$48^3 \times 96$

Table 1: Table of Wilson-clover lattices referenced in this proposal.

Ens	Task	N_{eigen}	N_{src}	N_{sep}	N_{mom}	Node	Cost/cfg	N_{cfg}	**TOTAL**
$a094m170$	Genprop	128	4	4	3	KNL	140,000	350	49M
	Prop		4		3	KNL	26,000		9M
	Baryon					SKX	1,300		0.41M

Table 2: PROJECT I: The cost of the isovector calculation, as described in the text, expressed in core-hours on the specified resource, where N_{src} and N_{sep} are the number of source locations and source-sink separations respectively, and N_{mom} is the number of momenta used in eqn. 6

Resource Request

We now describe the resources for each of our projects in turn.

PROJECT I: Isovector PDFs

Here we will use lattice $a091m170$ of Table 1. The tasks comprise the calculation of the perambulators and generalized perambulators, the calculation of the baryon elementals, and the calculation of the two-point and three-point functions using those elementals. For the solution of the perambulators and generalized perambulators, the calculation is dominated by the solution of the Dirac equation, which we perform using the multigrid inverter within *Chroma*. For our target lattice, this can be performed efficiently on 6 nodes, where we are able to exploit the factors of three in the spatial directions to use 48 of the 64 cores on the KNLs at JLab; a single inversion requires 40 seconds. As noted earlier, momentum smearing within the distillation framework requires that we compute an additional set of *boosted* perambulators, and here we will use two different boost momenta. Finally we need to compute the *elementals*. Total resources for this project are listed in Table 2.

PROJECT II: Gluon Distributions

This calculation involves only the calculation of the two-point correlators, the computation of any gluonic operators being negligible. However, it is characterised by the need for very high statistics, and from our experience with the calculation of the gluon distribution on the $a094m270$ ensemble, this requires the calculation of the two-point functions from a large number of source locations on the lattice. We are currently performing this calculation on the GPUs for each time slice, and we propose to calculate the additional perambulators on the $a094m170$ lattice on every other time slice. We base our estimate on the cost of performing the calculation on the KNLs used in Table 3, scaled by the USQCD conversion factor of 1 RTX2080-GPU-hour = 38 KNL core-hours; we note that we could use the KNLs likewise.

Ens	Task	$N_{\rm eigen}$	$N_{\rm src}$	$N_{\rm mom}$	Node	Cost/cfg	$N_{\rm cfg}$	**TOTAL**
$a094m170$	Prop	128	44	1	RTX	2,500	350	0.88M

Table 3: PROJECT II: The cost of the gluon structure calculation, as described in the text, expressed in RTX GPU hours.

Ens	Task	$N_{\rm eigen}$	$N_{\rm src}$	$N_{\rm sep}$	$N_{\rm trans}$	Node	Cost/cfg	$N_{\rm cfg}$	**TOTAL**
$a094m170$	GPD Genprop	64	4	4	11	SKX	16,000	350	5.6M

Table 4: PROJECT III: The cost of the GPD calculation calculation, as described in the text, expressed in core-hours on Skylake/cascade nodes, where $N_{\rm src}$ and $N_{\rm sep}$ are the number of source locations and source-sink separations respectively, and $N_{\rm trans}$ is the number of momentum transfers in eqn. 8. Note that we assume the use of all 36/40 cores of a Sky/Cascade, though in practice we can only use 32.

PROJECT III: Generalized Parton Distributions

The methodology of the computation of the GPDs is that of the calculation of the PDFs in Project I above. However, it is distinguished by the need to include many momenta in the calculation of the generalized perambulator of eqn 8 which both imposes additional computational and memory requirements. This for this exploratory calculation we will use the $a094m390$ ensemble. Our timings are based on the observed performance to compute a set of generalized perambulators on Skylake nodes, where an efficient implementation of the multigrid algorithm restricts us to only 32 cores per two Skylake nodes on the target ensemble. The cost is listed in Table 4.
0.5cm

Summary: We request **58M KNL-core-hours, 6M Skylake-core-hours** and **0.88M RTX-GPU-hours**

Storage: The baryon elementals are the are ~~the~~ most expensive element of our calculation in terms of storage. Per configuration of the $a094m170$ lattice they require 250 GByte of storage, or 88 TByte for the full ensemble. We therefore request another 100 TByte of Tape storage, and 30 TByte of disk storage to facilitate 100 configurations of data of the largest ensemble to be ~~on~~ on disk.

Readiness and Run Schedule

The software used in this proposal is that of USQCD, and in particular *Chroma*. We are investigating workflow as to whether there are more optimal ways of avoiding storage, such as computing elementals "on the fly", and the extent to which we can exploit either KNLs or SKX nodes.

Data sharing and exclusive rights

We note that most of the data generated as part of this proposal comprises the correlators, the "perambulators", "generalized perambulators", and elementals. These are available for projects not in competition with ours.

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