Clustering Jets at the Exascale

Steven Ko, Salvatore Rappoccio, Lukasz Ziarek

Overview : In the past, particle physics has relied upon improvements in processing speed of single computing cores in order to improve data acquisition rates. This feature will be critical to the proposed "High Luminosity Large Hadron Collider" (HL-LHC) and other colliders, where the computational challenges move from the petascale to the exascale. Unfortunately, since the mid-2000's, this improvement in single-core processing speed has hit a limit, and improvements in processing time must now come from concurrent processing. However, the current reconstruction techniques are not enabled for concurrent processing. In order to continue improving the processing capabilities of particle physics experiments in the HL-LHC era, it will be necessary to explore cutting-edge techniques in parallel processing.

There are several general classes of problems in particle physics event reconstruction that could be modified in order to achieve concurrent processing. One such opportunity that has not yet been explored is in "jet clustering," a nearest-neighbor type of algorithm used to cluster hadronically-fragmented jets into a single object.

Intellectual Merit : This proposal focuses on parallelizing the existing jet clustering algorithms in use at the LHC experiments. The proposed improvements will be to use this as a test case for deployment of cutting-edge parallelization techniques such as lightweight concurrency extraction, speculative computing, and smarter distribution. Some recent experience shows that the nearest-neighbor type of algorithm used by the jet clustering is amenable to such improvements.

Broader Impacts : The benefits of this proposal are twofold : firstly, there will be an immediate improvement of the jet clustering algorithms themselves that will lead to higher data acquisition rates at the LHC. Secondly, the computing techniques developed could be used in other applications, inside of particle physics and elsewhere. Since nearest-neighbor algorithms are ubiquitous in scientific computing, it is expected that techniques developed to parallelize this particular problem will be applicable to a wide variety of others in academia and industry.

In addition, these core developments can train students in the newest computing techniques, giving them cutting-edge experience that is highly relevant in academia and private industry.

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1 Introduction

The research proposed here will focus on deploying advanced techniques in parallelization to improve algorithms involved in particle physics research at the Large Hadron Collider (LHC) and beyond. As a specific test case, this research focuses on immediate improvements to one particular algorithm, jet clustering, although the principles developed could be deployed in other areas of particle physics reconstruction and elsewhere.

With the discovery of the Higgs boson by the Large Hadron Collider (LHC) experiments ATLAS and CMS [1, 2], the standard model (SM) of particle physics is now complete. This model unifies the electromagnetic force (carried by the *photon*) with the weak force, responsible for radioactive decay (carried by the *W and Z bosons*). At long last, physicists now understand that via interactions with the Higgs field, the W and Z bosons acquire a mass, but the photon does not. This is referred to as "electroweak symmetry breaking".

A new phase of particle physics has therefore begun. The questions have shifted from the cause of electroweak symmetry breaking, to the study of the Higgs boson and its interactions in detail. To understand the larger picture of the fundamental forces in nature, it will be imperative that high-luminosity colliders be built to study the Higgs in detail, requiring exascale computing tools (in speed and throughput) to reach the goals.

One of the major technical challenges that lies ahead in exascale-level computing for these high-luminosity colliders is the continuation of the scaling of computational power year by year, known colloquially as "Moore's Law". To set the scale, at the CMS experiment with the LHC collision flux ("luminosity") reaching $7 \times 10^{33}\,\mathrm{cm^{-2}s^{-1}}$, the processing time to reconstruct each collision event by CMS was approximately 20 seconds per event. However, as the luminosity is increased, the computational time currently scales quadratically. The luminosity at the HL-LHC is expected to reach as high as $> 1 \times 10^{34}\,\mathrm{cm^{-2}s^{-1}}$, which would correspond (naively) to enormous processing times, on the order of many minutes to several hours per event! Clearly, it is necessary for the computing power to scale in order to compensate for this dramatic increase in CPU time with increasing luminosity.

Unfortunately, the expected end of the historic scaling of single-core processing capability [3] can adversely affect the long-term processing capability for particle physics experiments. Without improvements in single-core computational speed, the only avenues left are algorithmic improvements, and parallelization. Algorithm development is being undertaken at the LHC experiments to reduce the computational time of the software for data acquisition and reconstruction, using both single-core and multi-core approaches. However, long-term improvements will require fundamental improvements in processing capabilities using parallelization.

The currently proposed exploratory research will deploy new and innovative computer science techniques to particle physics. One algorithm that is particularly amenable to improvement using these techniques is the clustering of final-state particles produced in collisions into groups called "jets". Jets are produced via quantum chromodynamic (QCD) interactions of quarks and gluons that hadronize. These "jet clustering" algorithms group the particles into jets based on nearest-neighbor clustering (NN). This algorithm can become computationally expensive as the number of particles that are produced in a collision grows, scaling as $N^2 \log N$ or $N \log N$. Techniques that

leverage and combine speculative computing, lightweight concurrency, and smarter distribution can strongly impact these types of NN algorithms [4, 5, 6, 7, 8]. Thus, this research will serve as a real-world test case for the deployment of these algorithms, with both immediate and long-term benefits.

2 Prior Work

2.1 Results from Prior Support

Results from prior NSF support : None.

2.2 Overview of Activities

The investigators of this proposal have a widely-varied and applicable skill set to accomplish the goals of extending LHC computing to the exascale.

Salvatore Rappoccio (tenure-track Assistant Professor) joined the Faculty at the University at Buffalo, SUNY (UB) in 2012. He has 15 years of experience programming in a high-energy physics environment, as well as other numerical software design for the private sector.

Since 2007, Rappoccio has been a member of the Compact Muon Solenoid (CMS) experiment at CERN. From 2008-2010, he was the co-leader of the Analysis Tools group of the CMS Software Project. He was responsible for deployment of jet reconstruction algorithms as well as other tools for data analysis of LHC collision data during the startup phase of the LHC. His primary responsibilities included managing deployment of highly-performing software (including visualization) tools in a team consisting of ∼15 people. He has been instrumental in improving the single-core computational speed for jet clustering at CMS since 2008.

His research interests include utilizing jet clustering algorithms in new and innovative ways to search for signals of physics beyond the standard model of particle physics. His pioneering efforts resulted in the first measurements and searches for new phenomena with advanced jet clustering algorithms at CMS, outlined in Refs. [9, 10, 11]. These techniques have become hugely popular in the LHC experiments and in the theoretical community. Prof. Rappoccio is a leader in the jet reconstruction community, contributing to and editing seminal reports on the subject in Refs. [12, 13, 14]. In addition to this academic work, he has also been involved in numerical software design for MIT's Lincoln Laboratories (the details of which are classified).

Currently, Rappoccio is mentoring two students (one graduate student, Jaba Chelidze, and one undergraduate student, Jonathan Goodrum) in achieving parallelization of the jet clustering algorithms. The latter is working under the "Collegiate Science and Technology Entry Program" (CSTEP) [15]. As described by the program, CSTEP exists "to support talented underrepresented students pursuing science, technology, engineering and mathematics".

Lukasz Ziarek has 9 years of experience in language, compiler, and runtime design targeted at improving multicore performance. He has worked on 5 compilers and 3 Java VMs. He is an expert at speculative and transactional computation focusing on the extraction of parallelism and lightweight concurrency.

Steven Ko has 10 years of experience in distributed systems. His recent focus has been large-scale data processing in the cloud using MapReduce and other technologies built on top of it. He also has 5 years of experience in large-scale storage and data management in data centers.

3　Proposed Program of Research

The "jet clustering" technique is employed by many different particle physics experiments and theorists worldwide, and is implemented in a common software framework called `fastjet` [16]. The mathematical problem is analogous to the "K-nearest neighbors algorithm" [17] (kNN). The single-core optimization of jet clustering is outlined in Ref. [18]. In a single core, the computational time scales as $O(N^2)$ or $O(N \ln N)$, where N is the number of inputs to the algorithm, which scales linearly with luminosity. Since the luminosity of future colliders is expected to drastically increase over existing machines, it will be critical to develop parallelization strategies to maintain scalability of the jet clustering algorithms that exist to future machines.

We now discuss specific strategies that can be developed to optimize performance in this algorithm.

3.1　Technical Challenges

To achieve the necessary improvements in performance required for scalability of jet clustering, we propose to examine parallelization opportunities across the entire software stack, including three specific areas : (1) the use of lightweight concurrency extraction to mask high-latency computations or I/O actions, (2) extraction of parallelization from the computation itself in the form of optimistic speculation and specialized transform, and (3) new methods for distributing the computation to maximize parallelization on each node.

Lightweight Concurrency for Latency Masking

Many mathematical kernels contain opportunities for extracting "micro parallelism," usually on the order of tens of instructions, from their computational components. Unfortunately, it is very difficult to parallelize this computation profitably as the overhead of thread creation, scheduling, synchronization, and migration outweigh the gains in parallelism. Instead of extracting explicit parallelism from such computations, we propose to explore methods of lightweight asynchrony to allow for computation to proceed while waiting on high latency I/O operations to complete or the results of other computations. Since the creation of threads and associated schedule and synchronization costs are typically prohibitive, we will explore new threading models that allow for logically-distinct computations to execute within a given construct. The PIs previous research has indicated that such schemes can profitably boost overall performance in the context of ML code [19, 20]. The salient research challenges in applying this strategy are as follows: 1) identifying what computation can be executed safely during high latency operations at compile time, 2) providing a lightweight threading runtime and programming model in the context of an imperative language, 3) specializing the approach to numeric kernels, and 4) building support for computation in a distributed setting.

Speculative Computation

In addition to exploring explicit parallelization of the numeric kernels in jet clustering, we propose to explore extraction of parallelism via speculative computation. At its core, speculative computation breaks apart sequential or parallel tasks into smaller tasks to be run in parallel. Once the speculation has completed, the runtime system validates the computation. If the computation is incorrect (*i.e.* a "datarace" is detected, the computation cannot be serialized, *etc.*), the incorrect computation is re-executed in a non-speculative manner. If the rate of mis-speculation is low, such techniques can be leveraged to extract additional parallelism. There have been many different

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proposals, including large efforts on transactional memory [], lock elision [], thread level specula-tion and speculative multithreading [], for integrating speculative computation into programming languages and their associated runtimes []. The PIs have extensive experience with transactional memory [21], lightweight rollback methods [22], leveraging memoization to reduce re-computation costs [23, 24], and deterministic speculation [25]. We propose to explore a specialized speculation framework leveraging different speculation strategies, including speculation extracted by the pro-grammer via programming language primitives, library level speculation, and compiler extracted speculation. The salient research challenges in applying this strategy are as follows: 1) identifi-cation the appropriate speculation model and discovering speculation points at compile time, 2) providing a speculative runtime specialized for jet clustering and capable of realizing user, library, and compiler injected speculation, and 3) exploring new and specialized lightweight validation and re-execution mechanisms, including validation across multiple speculation strategies.

Smart Distribution

In order to increase parallelism, we will explore the use of the MapReduce execution frame-work [26, 27]. MapReduce is a runtime system recently developed for large-scale parallel data processing. It enables programmers to easily deploy their applications on a cluster of machines. Programmers only need to write two functions, Map and Reduce, and submit these two functions as a job to the system. Then the MapReduce framework takes care of all the aspects of the execution of the job. For example, the framework packages and distributes the two functions over the cluster so that the whole cluster can be utilized to execute the job; it also takes care of fault-tolerance by monitoring the cluster during the execution of the job and redistributes the job if some machine fails.

Due to this simplicity and power, it is quickly gaining popularity in industry for large-scale data processing. Many applications in scientific computing have not yet explored the use of MapReduce in depth, however previous research has explored implementing similar kNN-style algorithms with MapReduce [7, 8]. We intend to explore this question in the context of jet clustering for the LHC.

3.2 Research Plan

Preliminary studies of naive parallelization of a few specific algorithms in the `fastjet` package reduced processing times by factors of 2-3 by moving to concurrent processing with 8 cores, with no increase in memory cost. By further deploying the advanced strategies described above, this factor of 2-3 improvement is expected to grow significantly.

These preliminary studies were performed by Rappoccio and Mr. Goodrum (undergrad student) over the summer of 2013. Having a postdoctoral fellow to work on this project will greatly increase the likelihood of success.

The postdoctoral fellow requested in this proposal is envisioned to have a computer science background. There will be two graduate students, one with a physics background (but with strong computational skills), and one with a computer science background. Furthermore, it is expected that Mr. Goodrum will continue to work with the group under his CSTEP Fellowship. This team, under the guidance of Rappoccio, Ziarek, and Ko, will perform the implementation and study of these algorithms in the real-world `fastjet` software environment, testing the improvements at the extensive cluster at the **Center for Computational Research** here at UB.

4   Broader impacts

The broader impacts of this research are many fold. The jet-clustering algorithm is very similar to the "kNN" algorithm, which is widely applicable throughout research and industry. The improvements that are developed here at the cutting edge of scientific inquiry will possibly be adaptable to other real-life applications.

In addition to the core physics developments enabled by improved scalability of the `fastjet` software environment, this award will also serve as a validation mechanism for core computer science research in programming languages and distributed systems. The development of the system will require core systems research in expanding and applying the technological advances made previously by the PIs.

5   Outreach and Education

While it is critical to pursue a rigorous research program, a large part of the responsibility of scientists is to educate the next generation effectively. There is already extensive work being done to educate high school-level students and teachers about particle physics via the *QuarkNet* program at UB, however there is very little in the way of educating the general public. In addition to participating in the existing *QuarkNet* activities, the plan outlined in this proposal will extend the coverage of the outreach program at UB to engage the broader public in discussions of major results in particle physics, as well as to enliven particle physics for young students. This will be implemented based on similar events as the "HiggsFest" [28] that Prof. Rappoccio organized at UB.

5.1   Higgsfest and other public events

The "Higgsfest" that was organized here at UB in 2012 is highlighted in Ref. [28]. The aim of the event was to invite the general public for "plain English" summaries and hands-on demonstrations that were geared for a multitude of age and knowledge levels. This was attended by over 100 people, including children, high-school students, physics and non-physics undergraduates, and interested members of the community.

Some of the hands-on demonstrations included building models of Feynman diagrams from craft material (for young children), a fully-functional four-layer coincidental muon scintillator detector, a cloud chamber made out of tupperware, felt, and dry ice, and the actual Higgs events from the CMS collaboration in an interactive event display. The event was covered by the "UB Reporter" here at UB [29].

Two more such events are proposed, the first to coincide with the LHC turn-on sometime in 2015, and the second to coincide with the newest results from the LHC after data-taking commences. These are events that should generate high media coverage, and will be a good opportunity to capitalize on public interest in this field. In the event of a major new discovery at the LHC during Run 2, the public interest will be very high, so having the experience of what works and what does not work in such events is extremely valuable to maximize the public impact.

In addition, this removes the stigma associated with science and technology fields at an early age. When young children can attend an event with their parents and take something away from it, this shows them that science is an integral part of life, and nothing to be particularly nervous about pursuing. It may even convince younger people to pursue a scientific career.

One of the major points learned during the last "Higgsfest" is that it is often difficult to have economically-disadvantaged students attend the lectures because of a lack of transportation

possibilities. This is something to rectify for future projects along these lines. Therefore, in addition to holding the event directly at the UB North Campus (which is difficult for inner-city Buffalo schools to reach), a duplicated event is also proposed closer to the inner city that is easier to attend, or possibly to visit these schools directly. Some possible locations are the UB South Campus, or at "Babeville" [30], where the UB Physics Department routinely organizes the "Science and Art Cabaret" [31]. Both locations provide the infrastructure needed for the event, and access for disadvantaged schools and students in the inner city of Buffalo.

5.2 Undergraduate research

As discussed above, Mr. Goodrum is participating in the "Collegiate Science and Technology Entry Program" (CSTEP) here at UB while working on this project. This program focuses on disadvantaged or minority students who would otherwise have a difficult time pursuing STEM-related fields. Prof. Rappoccio is a strong believer in the principles and practice of this program, and intends to continue this work in the future. There are also numerous opportunities for Independent Study and Honors' Theses for undergraduates in the Physics department.

5.3 Summary

In summary, the problem of expanding LHC computing to the exascale is a difficult, but tractable one. This proposal investigates the possibility of applying cutting-edge parallelization techniques such as lightweight concurrency extraction, speculative computation, and smarter distribution, to the real-world application of LHC data processing. The overall goal is to reduce the computational time for k-nearest-neighbor-like numerical kernels used for jet clustering. The investigators of this proposal have extensive experience in the various aspects of the problem, and the synergistic application of this experience is expected to attain considerable improvements in this area, which are absolutely critical to the success of the future LHC physics program.

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BUDGET JUSTIFICATION

Institution : The State University of New York at Buffalo (UB)
PI : Salvatore Rappoccio
Co-I : Lukasz Ziarek, Steven Ko

Personnel

The requested funds of $915,569 USD (for 3 years starting in 2014) would cover two (2) months of summer salary for Profs. Rappoccio, Ziarek and Ko per year for three (3) years ($172,062), the full salary for one (1) postdoctoral fellow for three (3) years ($154,224), and salary plus tuition for two (2) graduate students, totaling $91,812 in salary and $33,432 in tuition.

If awarded, efforts for Profs. Rappoccio, Ziarek and Ko will be reduced to be in compliance with NSF 2 month policy.

Fringe

Fringe benefit rates are based on the applicable federally negotiated rates published at http://www.research.buffalo.edu/sps/about/rates.cfm.

Travel

This research will require regular travel to conferences and CERN. Hence, the proposal requests $12,486 in travel funds for the three years of activity.

Facilities and Administration Indirect Costs

Indirect cost rates are based on the applicable federally negotiated rates published at http://www.research.buffalo.edu/sps/about/rates.cfm

Facilities, Equipment and Other Resources

Center For Computational Research
UB has a large computational research center, CCR, which is a Linux-based cluster on the Open Science Grid, and also has a large GPU cluster for possible parallel processing developments.

Office
The faculty, postdoctoral fellows and graduate students all have office space at UB.

Postdoctoral Fellow Mentoring

One postdoctoral fellow will be funded on this project. There are extensive postdoctoral fellowship mentoring activities at UB, as well as via the CMS Experiment at CERN. These include guidance in career paths, work/life balance discussions, and technical skill development such as writing grant proposals, etc. Specific elements are highlighted below.

- **University at Buffalo (UB)**

  - The UB Office of Postdoctoral Scholars offers diverse services for postdoctoral fellows, including the *"Postdoc Survival Skills Workshops"*, targeted seminars and symposia for postdoctoral fellows, social functions, and logistical assistance.
  - The UB Physics Department offers several services to our postdoctoral fellows, including a biweekly Journal Club for particle physics and cosmology, weekly seminars and colloquia, and weekly social functions inside the department.

- **CERN**

  - The opportunities for a postdoctoral fellow at CERN are extensive. There are also a plethora of workshops, seminars, conferences, etc, at CERN. There are also smaller weekly avenues for networking possibilities, as well as seminars for postdoctoral fellows to gain visibility for their work.
  - It is also worth pointing out that, because of the world-class nature of CERN, it often attracts very high-level members of the particle physics community on a regular basis. Such opportunities for visibility among the top-tier scientists in the world (including Nobel and Milner Prize winners, etc) are hard to understate.

In all, the postdoctoral fellow that will be supported by this proposal will have ample opportunities for professional advancement and development, as well as a myriad of opportunities for a community of peers in both professional and social settings.

Data Management Plan

The algorithms that are developed with this research plan will be integrated into the main `fastjet` software framework for distribution among collaborators (both experimental and theoretical) worldwide [1].

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[1] http://fastjet.fr