We present an overview of current academic curricula for Scientific Computing, High-Performance Computing and Data Science. After a survey of current academic and non-academic programs across the globe, we focus on Canadian programs and specifically on the education program of the SciNet HPC Consortium, using its detailed enrollment and course statistics for the past four to five years. Not only do these data display a steady and rapid increase in the demand for research-computing instruction, they also show a clear shift from traditional (high performance) computing to data-oriented methods. It is argued that this growing demand warrants specialized research computing degrees. The possible curricula of such degrees are described next, taking existing programs as an example, and adding SciNet’s experiences of student desires as well as trends in advanced research computing.

Contents

I. Introduction 1

II. The role of HPC in current research 2

III. Programs in High-Performance Computing 3
   A. Academic HPC Programs 4
   B. SciNet’s HPC Programs 5

IV. Programs in Data Science 5
   A. Academic Data Science Programs 6
   B. Non-academic Data Science training 6

V. Designing Master’s programs in HPC and Data Science 7
   A. Design of an HPC Master’s Program 7
   B. Design of a Data Science Master’s Program 8

VI. Conclusion 10

References 10

I. INTRODUCTION

The computational resources available to scientists and engineers have never been greater. The ability to conduct simulations and analyses on thousands of low-latency-connected computer processors has opened up a world of computational research which was previously inaccessible. Researchers using these resources rely on scientific-computing and high-performance-computing techniques; a good understanding of computational science is no longer optional for researchers in a variety of fields, ranging from bioinformatics to astrophysics.

Similarly, the advent of the internet has resulted in a paradigm where information can be more easily captured, transmitted, stored, and accessed than ever before. Researchers, both in academia and industry, have been actively developing technologies and approaches for dealing with data of previously-unimaginable scale. Researchers’ ability to analyze data has never been greater, and many branches of science are actively using these newly-developed techniques.

Unfortunately, the skills needed to harness these computational and data-empowered resources are not systematically taught in university courses. Some researchers, postdocs and students may find non-academic programs to fill this void, but others either do not have access to these courses or cannot commit the time to follow them. These researchers typically end up learning by trial and error, or by self-teaching, which is rarely optimal.

A number of academic programs that aim to address this issue have emerged at universities across the world (a few examples are [3, 4]). Some of these grew out of the training efforts of High Performance Computing (HPC) centres and organizations, such as those in the XSEDE partnership in the U.S., PRACE in Europe, and Compute/Calcul Canada, which have been providing local and online HPC training as part of their user support. Universities have also developed graduate programs in both Scientific and High-Performance Computing, to train scientists and engineers in the use of these computational resources.

A more-recent complement to these graduate programs is the development of the degree in Data Science (DS), that is, degrees which focus on the analysis of data, especially at scale. These degrees come in a variety of forms, from multi-year academic graduate programs to specialized private-sector training. These programs are in strong demand at present, as large companies have dis-
covered the value in thoroughly analysing the vast quantities of customer data which they collect. It is expected that this field will continue to grow, and academic programs will continue to be introduced to meet this demand.

The SciNet HPC Consortium \([7, 8]\) is the high-performance-computing consortium of the University of Toronto. SciNet provides both computational resources and specialized user support for Canadian academic researchers, and as members of its support team, we are responsible for training researchers, postdocs and graduate students at the University of Toronto in HPC techniques. In this paper we give a review of the current state of graduate-level Scientific Computing, High-Performance Computing and Data Science academic programs, and endeavour to design an ideal HPC and DS graduate program. The paper is organized as follows. In Sec. II we discuss how computation has become an essential ingredient in many academic research endeavours; in Sec. III we review the current status of education in the areas of High-Performance and Scientific Computing. In Sec. IV we present the Data Science education efforts at the academic and non-academic level. Sec. V describes what HPC and DS Master’s programs could look like. We conclude with final remarks and perspectives for the future in Sec. VI.

II. THE ROLE OF HPC IN CURRENT RESEARCH

The breadth of science being as large as it is, it is essentially impossible to give an overview of the uses of computational methods in current scientific research. We will nonetheless attempt a review of at least some computational scientific research, since the way computers are used in research (and other realms of inquiry) influences what should be taught to students.

Astrophysical computational research inherently involves large scale computing, such as the simulation of gravitational systems with many particles, magnetohydrodynamic systems, and bodies involving general relativity. Atmospheric physics requires large weather and climate models with many components to be simulated in a variety of scenarios. High-energy particle physics projects, such as the ATLAS project at CERN, require the analysis of many recorded events from large experiments, while other high-energy physics projects have a need for large scale simulations (e.g. lattice QCD investigations). Condensed matter physics, quantum chemistry and material science projects must often numerically solve quantum mechanical problems in one approximation or another; the approximations make the calculations feasible but still rely on large computing resources. Soft condensed matter and chemical biophysics research often involve molecular dynamics or Monte Carlo simulations, and frequently require sampling a large parameter space. Engineering projects can involve optimizing or analyzing complex airflow or combustion, leading to large fluid dynamics calculations. Bioinformatics often involves vast quantities of genomic input data to be compared or assembled, requiring many small computations. Research in other data-driven sciences such as social science, humanities, health care and biomedical science \([9]\), is also starting to outgrow the capacity of individual workstations and standard tools in their respective fields.

Examining these cases in more detail, one can distinguish different ways in which research relies on computational resources:

1. Research that is inherently computational, \textit{i.e.} it cannot reasonably be done without a computer, but which requires relatively minor resources (\textit{e.g.} a single workstation).

2. Research that investigates problems that do not fit on a single computer, and therefore rely on multiple computing nodes attached through a low-latency network.

3. Research that requires many relatively small computations.

4. Research that requires access to a large amount of storage, but not necessarily a lot of other resources.

5. Research that requires access to a lot of storage, on which many relatively small calculations are performed.

The distinction between the various types of research determines the appropriate systems and tools to use. Graduate students that are just starting their research often do not have enough knowledge to make the distinction (as nobody has taught them about this), let alone select and ask for the resources that they will need \([2]\).

Note that all five categories fall under “Advanced Research Computing” \((\text{ARC})\). The categories are not mutually exclusive, but research of the second and third kind are usually associated with HPC, while the fourth and fifth, and sometimes the first, are associated with Data Science \((\text{DS})\). Although there is a lot of overlap between HPC and DS, these fields require somewhat different techniques. For that reason, we will consider separate programs for HPC and DS.

III. PROGRAMS IN HIGH-PERFORMANCE COMPUTING

Much of the research presented in the previous section falls in the category \textit{Scientific Computing} \((\text{SC})\). The growth in the computational approach to research, both academic and industrial, has prompted some institutions to develop graduate-level programs designed to teach the skills needed to design, program, debug and run such calculations. These programs, having been in development for more than two decades, are now fairly wide
spread and mature, and are known by the names “Scientific Computing” or “Computational Science and Engineering”. Scientific Computing graduate degrees are offered internationally in several graduate education hubs around the world (U.S., England, Germany, Switzerland, etc., — lists of which can be found at the SIAM and HPC University [10] websites). Canada is no exception here either, with at least eight universities offering graduate-level programs in Computational Science. These programs include one-year and two-year Master’s programs, as well as Ph.D. programs. Most of these programs (e.g. the ones shown in Tables I and III) require a final thesis. The projects and theses are faculty-guided research projects and are usually one-term long, though, as with all research, these projects sometimes take longer.

A typical curriculum for a two-year Master’s program in Scientific Computing (in this case from San Diego State University) is presented in Table I. It clearly shows that Scientific Computing has its roots in research in the physical sciences; the programs heavily emphasize numerical analysis and scientific modelling. In some ways this is not surprising: computers are very apt at solving such problems, and the formalism of the physical sciences often lends itself easily to computer programming. Other topics of study which are also often encountered in these programs include finite element analysis, matrix computations, optimization, stochastic methods, differential equations and stability.

In contrast to Scientific Computing, HPC requires somewhat wider knowledge; its practitioners need to understand more than just the theoretical and numerical principles. They require skills such as serial and parallel programming (often in several languages, and on different platforms) and scripting, as well familiarity with numerics, data handling, statistics, and supercomputers and their technical bottlenecks. In addition, these practitioners are usually not computer science students, so they must cope without that background. This is somewhat unavoidable as they need to have sufficient domain knowledge as well. Much of the same holds for Data Science.

### A. Academic HPC Programs

There are not many academic programs that focus on HPC. Part of the reason may be that such programs require access to a high-performance-computing machine so that students can develop their skills on real hardware, in a real supercomputing environment. These machines require multiple computing nodes which are connected by a low-latency network. Fortunately, such systems do not need to be local: as long as the machine is accessible through the internet the machine could be used for teaching. Nonetheless, having the hardware local to the students lends advantages, since most of the administrators and analysts of the system are typically available to assist students with optimizing their codes and developing good computational strategies. Not surprisingly, the majority of the currently offered HPC graduate programs seem to have been developed in conjunction with or by supercomputer centres.

As examples of High Performance Computing programs, the University of Edinburgh (UK) offers an MSc in High Performance Computing, the Universität Politècnica de Catalunya/BarcelonaTech (Spain) offers a Master in High Performance Computing and a Master program in Data Mining and Business Intelligence, SISSA/ICTP in Italy offers a Master in High Performance Computing, while a collaboration between the University ITMO (Russia) and the University of Amsterdam (Netherlands) offers a Double-Degree Master Programs in Applied Mathematics and Informatics (Computational Science). Note that many of these programs emerged from locations with a very strong tradition and consolidated background in HPC.

### B. SciNet’s HPC Programs

Many HPC centers provide training for their users to fill the computational-skills gap for the wider scientific community, such as, SDSC, PSC, TACC, NCSA, BSC, EPCC, CSCS, SHARCNET, AceNet, Calcul Québec, among many others. In its capacity as an HPC centre based at the University of Toronto, SciNet has developed several education and training classes [12] aimed at helping students and users obtain the skills and knowledge required to get the most out of advanced-research-computing resources. SciNet’s training events and courses are currently taken by researchers, post-docs, and graduate students across many different departments and even from outside of the University of Toronto (UoT). Some of these courses are considered part of the official curricula and count as graduate level courses within the Ph.D. programs at UoT.

Initially SciNet provided training specifically oriented toward Scientific Computing, with the purpose of max-

| Course Name                                      | Type          |
|-------------------------------------------------|---------------|
| Introduction to Computational Science           | required      |
| Computational Methods for Scientists             | required      |
| Computational Modelling for Scientists           | required      |
| Computational Imaging                            | required      |
| Scientific Computing                            | required      |
| Applied Mathematics for Computational Scientists | required      |
| Seminar Problems in Computational Science       | required      |
| Computational and Applied Statistics             | elective      |
| Computational Database Fundamentals              | elective      |
| Research                                         | required      |
| Thesis                                           | required      |

**TABLE I: The curriculum for the two-year Master’s program at the Computational Science Research Center at San Diego State University** [11]: this forms a good example of a typical Scientific Computing graduate program.
imizing user productivity. These early classes focused on parallel programming (MPI and OpenMP), best coding practices, debugging, and other scientific computing needs. Over the years the breadth of classes has grown, with classes offered in Linux shell programming, parallel input/output, advanced C++ and Fortran coding, accelerator programming, and visualization. This is in addition to the annual HPC Summer School which SciNet runs in collaboration with two other HPC centres within Compute Ontario[13], i.e., CAC[13] and SHARCNET[14]. This summer school is a week-long intensive workshop on HPC topics, and more recently, also Data Science topics1.

Table II shows the training events and courses that SciNet has already been teaching in the areas of HPC and Data Science. The number and types of classes which SciNet teaches have grown significantly [16]. This can be seen in Figure 1, which presents the total student class-hours taught by SciNet over the last four years and the projection for the current year. This remarkable growth is a testament to the latent need for this material to be taught. The need for this training is supported by the enrolment statistics: our students constitute 35% of SciNet’s total users, clearly showing that even in a specialized audience this kind of training is still needed.

For several years the four-week graduate-style classes offered by SciNet have been accepted for graduate class credit by the departments of Physics, Chemistry and Astrophysics at UofT. This was possible by accepting the classes as “modular” (or “mini”) courses, one-third semester long, and bundling three such classes into a full-semester course. This arrangement has been so popular with students and faculty that the Physics Department recently listed SciNet’s winter twelve-week HPC class in the course calendar [17], allowing graduate students from other departments in the university to take the class for university credit.

The skills that SciNet aims to transfer are rare and sought-after, and complement and enhance the skills students learn in regular curricula. That is why SciNet has developed a set of Certificate Programs [15], that users and students can pursue in Scientific Computing, High Performance Computing, and/or Data Science, once they have completed enough credit-hours. As a document that proves the holder has highly competitive skills, and in lieu of graduate credit for most SciNet courses, the certificates are in high demand. In a resounding endorsement of our teaching, thus far students have completed a total of 78 certificates (52 in Scientific Computing, 19 in High-Performance Computing and 8 in Data Science). According to the current registration and trends, we are projecting to have above a 100 of certificates completed by mid-2016. Moreover, the feedback from some of our students was that their SciNet’s certificates gave them an advantage to get jobs in industry and the financial sector.

IV. PROGRAMS IN DATA SCIENCE

The wide adoption of the internet in the professional and the personal sphere ushered in the age of “Big Data”. The ease of recording of people’s online behaviour, and the ability to rapidly move data, lead to a large, diffuse, complex amount of data waiting to be mined for useful information. Because of the typically large size of the data special hardware and training are often needed. In contrast to Scientific Computing and HPC, there are many applications of Data Science in the private sector, in the medical science, banking, retail, insurance, and internet industries.

Of these industries, Bioinformatics also has a large component in the academic world. Though a more-recent addition to the HPC world, the bioinformatics field is well-populated with graduate programs, a testament to its rapid growth and latent demand. Its emergence as a major user of HPC systems has resulted in the development of “Master’s of Bioinformatics”, and related degrees. A typical Master’s program is outlined in Table III, this one from the Indiana-Purdue University at Indianapolis. While having many features in common with a more-standard SC Master’s program, such as the study of programming and algorithms, it exhibits the particular needs of the bioinformatics community, stressing the importance of genetics and biological processes, and a lesser emphasis on mathematics and programming theory.

Degrees in Data Science are relatively new, with the first Master’s program only being introduced in the U.S. (by North Carolina State University) in 2007. A sample of some of the classes offered in one such program is
| Course Name                                         | Certificate | Credits |
|---------------------------------------------------|-------------|---------|
| Data Analysis with R†                             | DS/SC       | 12      |
| Intro to Apache Spark                             | DS          | 3       |
| Machine Learning Workshop                         | DS/SC       | 6       |
| Hadoop Workshop                                   | DS          | 3       |
| Scalable Data Analysis Workshop                   | DS/SC       | 12      |
| Relational Database Basics                         | DS/SC       | 6       |
| Storage and Input/Output in Large Scale Scientific Projects | DS/SC       | 6       |
| Workflow Optimization for Large Scale Bioinformatics | DS/HPC/CS   | 6       |
| Python for High Performance Computing             | DS/HPC/SC   | 12      |
| Parallel R                                        | DS/HPC/SC   | 3       |
| Python GUIs with Tkinter                           | DS/SC       | 2       |
| Scientific Visualization                          | DS/SC       | 6       |
| Visualizing Data with Paraview                    | DS/SC       | 6       |
| Scientific Computing for Physicists†              | HPC/SC      | 36      |
| Intro to Research Computing with Python‡          | HPC/SC      | 12      |
| Intro to High Performance Computing                | HPC/SC      | 3       |
| Intro to Scientific C++                            | HPC/SC      | 6       |
| Intro to Scientific Programming with Modern FORTRAN| HPC/SC      | 7       |
| Intro to Parallel Programming                     | HPC/SC      | 7       |
| Programming Clusters with Message Passing Interface| HPC/SC      | 12      |
| Programming Shared Memory Systems with OpenMP      | HPC/SC      | 6       |
| Practical Parallel Programming Intensive           | HPC/SC      | 32      |
| Intro to GPGPU with CUDA                           | HPC/SC      | 9       |
| Programming GPUs with CUDA                         | HPC/SC      | 12      |
| SciNet/CITA CUDA GPU Minicourse                   | HPC/SC      | 12      |
| Coarray Fortran                                   | HPC/SC      | 2       |
| Parallel I/O                                      | HPC/SC      | 6       |
| Debugging, Optimization, Best Practices            | HPC/SC      | 6       |
| HPC Best Practices and Optimization               | HPC/SC      | 3       |
| HPC Debugging                                     | HPC/SC      | 3       |
| Intro to the Linux Shell                           | HPC/SC      | 2       |
| Seminars in High Performance Computing             | HPC/SC      | 4       |
| Seminars in Scientific Computing                  | HPC/SC      | 4       |

‡ denotes courses already recognized by the university as graduate level credits.

This includes 3 previously separate module courses: Scientific Software Development, Numerical Tools for Physical Scientist, and High Performance Scientific Computing.

| TABLE II: Courses taught by SciNet on Data Science (DS), High-Performance Computing (HPC), and Scientific Computing (SC). |

As can be seen, these programs have a strong focus on data, with statistics, machine learning, and databases being their standard focus. Analyzing data that are too big to fit on a standard desktop computer requires specialized equipment; such training is also part of these graduate-level programs, as indicated by the presence of the “Cloud Computing” and “Distributed Systems” classes. Like typical graduate-level programs, these degrees usually require of the student a final project or thesis.

One could argue that the novelty of methods in Data Science is due to its roots in Business Analytics (BA), where the objective is to make a decision. The field has certainly grown beyond that, and BA is now considered a sub-field of Data Science. Another more-recently developed sub-field is in the realm of health care (“Health Informatics”). Because these sub-fields are directly applicable to the private sector (and the associated revenue streams these present) these have become the most-commonly implemented post-graduate programs. The Business Analytics programs focus on using data to refine business administration, as well as develop marketing strategies. Health Informatics programs concentrate on using clinical data to optimize health care processes.

The practical focus of Data Science is reflected in the presence of an internship in the Data Science curriculum listed in Table IV. Internships in such programs are similar to other co-op-type arrangements: the student works with an employer for a semester, allowing the student to gain hands-on experience applying the skills learnt during such period.

A. Academic Data Science Programs

Graduate level programs in Data Science are not difficult to find. For instance, programs in bioinformatics (a data-driven field), can be found on the [website](#).
TABLE IV: A selection of the courses available for the Master’s of Data Science at the Indiana University.

| Course Name                                      | Type   |
|--------------------------------------------------|--------|
| Introduction to Bioinformatics                   | required |
| Seminar in Bioinformatics                         | required |
| Biological Database Management                    | required |
| Programming for Life Science                      | required |
| High Throughput Data in Biology                   | required |
| Machine Learning in Bioinformatics                | elective |
| Computational System Biology                      | elective |
| Structural Bioinformatics                         | elective |
| Transitional Bioinformatics Applications           | elective |
| Algorithms in Bioinformatics                      | elective |
| Statistical Methods in Bioinformatics             | elective |
| Computational Methods for Bioinformatics          | elective |
| Next Generation Genomic Data Analytics            | elective |
| Next Generation Sequencing                        | elective |
| Bioinformatics Project                            | required |

TABLE III: The curriculum for the “Project Track” two-year Master’s of Science in Bioinformatics at the Indiana University-Purdue University in Indianapolis; this forms a good example of a typical Bioinformatics graduate program.

of the International Society for Computational Biology. It speaks to the rapid rise of the field bioinformatics, that there are more bioinformatics programs available than Scientific Computing programs. Examples lists of other Data Science programs can be found at the NCSU analytics web site, the online business analytics programs site of predictiveanalyticstoday.com and at online.coursereport.com. They are not as common as programs in Scientific Computing, due to the fact that Data Science is relatively new field of study. Among those programs about half are offered in the fields of Business Analytics and Health Informatics, with the other half being Data Science programs proper.

B. Non-academic Data Science training

The demand for Data Science skills (or “Data Analytics” skills as they are often called in the private sector) is so high that the private sector has developed programs to meet the growing demand. A list of such companies can be found on skilledup.com, which contains a list of data science boot-camps. The format of these classes is varied, though they are all oriented toward a “bootcamp” format: some are in person, some online; some are one-week long, others twelve weeks. These programs are very applied, often with one-on-one mentorship with a seasoned Data Analytics expert. They also include direct contact with possible future employers.

Moreover, a great number of these training programs are not focused on developing analytical thinking or problem-solving skills, but rather are aimed at graduated Ph.D.s and postdocs, whose problem-solving skills are assumed to have already developed. This allows them to focus on the technical training relevant to the job market. Some of these programs are free, some of them offer fellowships, and many of them charge on the order of 10-30 thousand US-dollars for a training period of, typically, three months. These programs have acquired such a level of popularity among young and recent graduates that the companies offering these programs have started to perform evaluation tests in order to assess which candidates are more suitable to be accepted to their programs. Perhaps the most appealing part for trainees is the networking platform offered by these programs, as in most of the cases they provide the opportunity to interact with actual companies looking for new talent and avoid recruitment layers.

Institutions in the non-profit arena are also starting to offer programs on Data Science. For instance the Fields Institute, a traditional institution for mathematical research, has offered several workshops and courses, and developed a thematic program on Big Data. Other examples include the International Centre for Theoretical Physics (ICTP) and the International School for Advanced Studies (SISSA), prestigious institutions with a well known tradition in theoretical physics, now offering training in “Research Data Science”.

HPC centers are also venturing into Data Science training, offering workshops on R, Hadoop, machine learning, etc. SciNet started offering classes with greater data-oriented content (cf. Table II) in 2013, with a four-week class in scientific analysis using Python. Having now finished its third year, the class remains popular, with about twenty students taking the class each year. The 2015 fall semester also inaugurated SciNet’s first “Data Science with R” class, a class focusing on data analysis techniques using the R language. This class was very popular with over twenty-five students finishing the class, and most students requesting a second installment with more advanced material. Continuing its growth in the Data Science area, in the last year SciNet has held workshops in machine learning, scalable data analysis, and Apache Spark.

Comparing the student- and taught-hours per year shown in Fig. 2, one sees that the Data Science classes have been growing consistently, both absolutely as well
as relatively (Data Science related courses) constitute less than 2% (2012), 4% (2013), 12% (2014), 15% (2015), and we project around 31% (2016) of the total classes taught respectively in each year.

V. DESIGNING MASTER'S PROGRAMS IN HPC AND DATA SCIENCE

As mentioned above, scientific computing is used by scientists and engineers as never before, and graduate-level programs in Scientific Computing are numerous in Canada and around the world. In contrast, the development of HPC and Data Science programs is in its early stages, both in academia and the private sector. These programs are being developed to meet the continued shortfall in skill in these areas, with the McKinsey Global Institute estimating that the United States will be short 140,000 to 190,000 data analytics professionals by 2018 [20].

One may wonder whether online learning could not satisfy this need. A few examples of MOOCs (Massively Open Online Courses) in HPC and Data Science do exist. However, seeing the growth in enrolment in SciNet’s in-person courses and the summer school over the years (cf. Figs. 1 and 2) shows that many students still prefer the face-to-face format.

Similarly, one may wonder why certificate programs do not suffice for HPC and DS education. As successful as these programs are, they have a few disadvantages. Firstly, they are mostly collections of fairly specific technical training: this leaves no room for more fundamental material. Secondly, it is also hard to incorporate an internship or thesis into such a certificate. Finally, certificates tend to carry less weight than degrees, and, in line with this, the demand for for-credit courses is larger than that for not-for-credit courses, as our experience with SciNet’s Scientific Computing graduate course has shown.

A degree program in HPC or DS could offer more academic and fundamental education, which would leave the student with the analytical skills and high-level knowledge to stay on top of their field regardless of changes in computational technology.

In the following sections we propose a curriculum for graduate-level HPC and DS programs. One will notice a substantial overlap of topics with the training courses currently taught by SciNet (cf. Table II). This is no coincidence: the training program was developed on the basis of student feedback and requests, and was a primary inspiration for the curricula proposed here. The design was also influenced by the few existing examples of such programs, as described above.

It should also be emphasized that the programs in HPC and DS are both designed to allow students to follow more industrial/practically-oriented track or an academic/research-oriented track, by selecting the appropriate set of elective courses and the corresponding research project/internship. Additional advanced courses could be made available according to the interest and demand of the students.

A. Design of an HPC Master’s Program

In this section we present a comprehensive and complete curriculum for a two-year Master’s Program in High-Performance Computing. Students would complete a total of twelve courses. The five required courses, each one-term long, set the basis of HPC and ARC knowledge (including topics such as modern and professional software development, parallel techniques, performance and optimization, best practices, distributed systems and resources). The seven elective courses allow the student to specialize in a particular area. In addition, a final internship or research project would be carried out.

As in any typical Master’s program, a student entering the program will be expected to possess a Bachelor’s degree (B.Sc. or B.A.). It is desirable that students have some background in sciences and the basics of coding and programming (e.g. Fortran, C, C++); otherwise it is strongly recommended that students take introductory programming classes. Note that courses from the Data Science Master’s Program are also eligible to be taken, with consent of the graduate coordinator or adviser.

The course work for the High-Performance Computing program could consist of the following courses:

Software Development (*): The principles of creating modern, maintainable code. Special attention is given to designing modular code, and tackling scientific computational projects. Languages: C++/C/Fortran.

Best Practices (*): Introduction and discussion of techniques and methods to be considered when designing and implementing computational research projects. Topics include: version control, modularity, libraries.

Performance & Optimization (*): Principles and tools for measuring performance, finding bottlenecks, and optimizing existing code.

Basics of Parallel Programming (*): A review of homogeneous and heterogeneous architectures is
presented, followed by parallel programming paradigms such as OpenMP, MPI, and hybrid implementations.

**HPC Algorithms:** A review of commonly used algorithms in computational science, such as Monte Carlo, implicit and explicit methods to solve differential equations, timestepping techniques, finite-element and finite-volume methods.

**Machine Learning:** Theory and practice of constructing algorithms that create models from data. Topics: probabilistic foundations, linear and logistic regression, neural networks, tree models, support vector machines, density estimation, accuracy estimation, normalization, model selection.

**Numerical Methods:** A review of the commonly used numerical methods in scientific computing, such as linear solvers, fast Fourier transforms. In contrast to the HPC Algorithms, it will cover the basic principles and the theory behind the methods only briefly, and focus mostly on the implementation and utilization via libraries and specific examples.

**Scientific Computational Modeling:** This course will offer an introduction to the basics of Scientific Computing and a review of the most common algorithms and packages used in different fields of research computing and computational sciences (astrophysics, chemistry, genetics, etc.). Introduction to computing modeling, such as implementation of complex networks based on relational data sets, and the evaluation of network properties using graph theory elements, among many others.

**Programming Accelerators:** Some computational problems can be computed much more efficiently on accelerators such as graphics cards. This course will present an introduction to the use of hardware accelerators (GPUs, FPGAs, many-core systems) in HPC. Topics will include a review of the hardware, architectures, and programming languages, such as, CUDA, OpenACC, and OpenCL.

**Research Data Management:** Design strategies, storage management and I/O patterns, in order to prevent bottlenecks in massively data-driven projects. Real use cases from various fields (bioinformatics, molecular biophysics, medical physics, biochemistry, quantum-chemistry, geophysics, etc.) have shown that, quite often, approaches that work on a desktop do not perform on a larger scale. A review of the latest policies regarding scientific data availability will also be discussed and presented.

**Visualization for Scientific Computing:** A review of basic visualization concepts and methods with applications to scientific data.

**Operating System Environment:** Scientific and high performance computing is intimately linked to the hardware, OS, and application framework on which they used. This course will help students become comfortable working on *nix systems. Topics such as the command line, shell scripting and advanced OS topics will be covered.

**HPC Hardware and System Administration:** An integrated view on the technology in HPC, the machines, hardware, network, file systems, and what is involved in getting an HPC system up and running.

**Student HPC/ARC Seminar:** Weekly sessions running throughout the year, with students presenting and discussing current papers and research in the fields of HPC and ARC. Researchers and instructors will providing guidance and supervision during the sessions.

In addition to this course work, the program would include an 4-month internship or independent research project in the final year.

The program presented above is intended to be flexible. In the first year of the HPC program, students might take *HPC Algorithms, Parallel Programming, Software Development, Performance and Optimization, Best Practices*, and *Numerical Methods*, as well as attend the HPC/ARC seminar series. In year two, they might take *Research Data Management, Scientific Computational Modeling, Graph Theory Applications, Machine Learning, Visualization for Scientific Computing*, and complete the degree with a Research Project.

Eligible courses from the *Data Science* Master’s Program are also possible to take with previous consent of the graduate coordinator or adviser.

**B. Design of a Data Science Master’s Program**

Here we present a comprehensive curriculum for a two-year *Master’s Program in Data Science*. As with the HPC program, students would complete a total of twelve courses. The five required courses set the foundation of data analysis knowledge (including topics such algorithms, databases, statistics, machine learning) and seven elective courses allow the student to specialize in a particular area, such as data mining, machine learning, complex systems. In addition, a final internship or research project would be carried out, in order to obtain real-world experience.

As in any typical Master’s program, the entry level will be a bachelor’s degree (B.Sc. or B.A.). It is desirable that students have some background in sciences and the basics
of coding and programming (e.g. Python, R); otherwise it is strongly recommended that students take introductory programming classes. Notice that courses from the High Performance Computing Master’s Program may be taken with permission of the graduate coordinator or adviser (e.g. Operating System Environment).

The fundamentals of data analysis should be at the core of a program that will produce analysts capable of tackling real-life problems in Data Science. Learning theoretical and practical approaches gives students an advantage in the real world; this program proposes to combine both in a unique fashion (similar to how most SciNet courses are structured). Topics such as statistical analysis, algorithms and large data sets are at the centre of the proposed program and constitute the “core” (required) courses. Additionally, the elective courses allow students to choose a specialization path by gaining expertise in areas such as: social data mining, machine learning, and representation of complex interactions. The course work for the Data Science program could consist of the following courses:

Overview of Data Science: An overview of the field of Data Science, covering data-driven problems from several disciplines such as, astronomy, bioinformatics, digital humanities, social sciences, etc.

Basics of Programming: An introduction to programming, coding structures, and basic algorithms. This course will focus on languages with data-analytic capabilities, such as Python and R.

Data Analysis Algorithms (*): An overview of the major classes of algorithms, including comparison-based algorithms: search, sorting, hashing; information extraction algorithms (graphs, databases); graph algorithms: spanning trees, shortest paths, depth and breath-first search.

Machine Learning (*): Theory and practice of constructing algorithms that create models from data. Topics: probabilistic foundations, linear and logistic regression, neural networks, Bayesian networks, tree models, support vector machines, density estimation, accuracy estimation, normalization, model selection. Deep learning algorithms.

Database Theory (*): The mathematical foundations of databases, search and query semantics, relational, complex, object-oriented and semi-structured database models.

Database Applications: SQL, relational algebra, index, views, constraints; query complexity; data models, including I/O model, streaming model, query optimization, optimal join algorithm will be presented.

High Dimensional Data Analysis (*): Theory and methods for exploring high-dimensional data will be presented, including linear and non-linear dimension reduction, manifold learning; Euclidean representation of proximity and network data; clustering, statistical pattern recognition.

Applied Statistics (*): A review of statistical techniques, with applications to data analysis problems. Topics will include hypothesis testing, general linear models, generalized linear methods, multivariate statistics.

Best Practices: Introduction and discussion of techniques and methods to be considered when designing and implementing computational research projects. Topics include: version control, modularity, libraries.

Data Mining: Algorithmic approaches to discovering patterns in large data sets will be covered, including data exploration and cleaning; association rules, clustering, anomaly detection, and classification. Other examples will include applications to text and the web: crawling, indexing, ranking and filtering algorithms; applications to search, classification and recommendation; link analysis, significance tests. Data mining techniques applied to social media. Sentiment analysis, polarity classification; graph properties of social networks, homophily, distance, influence, spectral methods, information diffusion, probabilities models.

Data Security and Integrity: This course will cover technique on how to safely protect the integrity and privacy of sensible data, standards on data regulations (e.g. health, patient data, genomic data), privacy, encryption algorithms.

Search and Classification Algorithms: Information retrieval theory, with applications, will be explored. Examples of searching algorithms, mathematical representations and matrix applications will be covered.

Distributed Systems: Focus on distributed resources and data sets across different architectures and systems. Students will learn the skills and abilities of dealing with retrieving and screening large data sets in cloud-type based systems.

Graph Theory Applications: An introduction to graph theory and complex systems and its applications will be offered. Material will include the implementation of complex networks based on relational data sets, and the evaluation of network properties.

Visualization Techniques of Unstructured Data sets: A review of basic visualization concepts, with applications to unstructured and/or large data sets and complex and dynamical systems, in order to gain insights in the data and visually expose potential correlations.
Data Science Seminar Series: Weekly sessions running throughout the year, where students will present and discuss current papers and research in the fields of data science and analytics. Researchers and instructors will provide guidance and supervision during the sessions.

In addition to this course work, the program would include an 4-month internship or research project.

The first year of classes could consist of Overview of Data Science, Data Analysis Algorithms, Database Theory, Applied Statistics, and Visualization Techniques of Unstructured Data Sets, while the second year could contain courses in High Dimensional Data Analysis, Graph Theory Applications, Data Mining, Search and Classification Algorithms, and Distributed Systems, and would be completed by an Internship or a Research Project.

As with the HPC/ARC track, eligible courses from the HPC Master’s Program are also possible to take with previous consent of the graduate coordinator or adviser.

VI. CONCLUSION

We have demonstrated the need for programs in higher education in High-Performance Computing and Data Science. If the qualitative evidence of this seems somewhat limited, it should be understood that existing HPC and DS programs (academic and non-academic) are still relatively new. While some such programs are already in existence, in many cases students must use non-academic options, or teach the material to themselves. Academic programs would offer the benefit of not just teaching specific technical skills, but an education in the fundamentals of HPC and DS and instilling the analytical skills needed to adapt to an ever-changing technological landscape.

We have reviewed existing academic and non-academic education programs, in both HPC and DS. In light of this review, we presented a design for Master’s programs in HPC and DS, based on these examples and drawing from the experience and enrollment statistics in not-for-credit training in HPC and DS by the SciNet HPC Consortium at the University of Toronto.

To get well-founded graduate master’s programs off the ground will not be without challenges. It will likely involve partnerships and discussions with other departments and institutes in order to offer a stronger and multi-disciplinary program. Existing HPC Centers, which already operate between different disciplines, can play a fundamental role in bringing together such programs.

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