MOBILIZING KNOWLEDGE IN SCIENCE AND ENGINEERING:
BLENDED TRAINING FOR SCIENTIFIC SOFTWARE USERS

BY

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Dedication

This dissertation is dedicated to my children, my little companions and endless source of energy in this venture, who discovered from a young age that the love for learning is an important virtue. To my life partner, for his incomparable understanding and empathy; to every woman and mother who dares to carve her own path through life.

A special inspiration for this research undertaking in education has been my mother, a passionate philologist and teacher; as well, my maternal ancestor, Professor Aristeides Spathakis, for his research in pedagogy in the 19th century. He wrote several books on the education of women and defined education, in the widest sense, as "any action that contributes to the physical and spiritual perfection of individual" (Spathakis, 1875, p. 12).

“Our words are the children of many people.
They are sown, are born like infants,
take root, are nourished with blood”.

“Education, in the deepest sense and at whatever age it takes place, concerns the opening of identities exploring new ways of being that lie behind our current state. Whereas training aims to create an inbound trajectory targeted at competence in a specific practice, education must strive to open new dimensions for the negotiated self. It places students on an outbound trajectory toward a broad field of possible identities. Education is not merely formative - it is transformative.”
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Abstract

This research investigates training approaches followed by scientific software users whose goal is the reliable application of such software. A key issue in current literature is the requirement for a theory-substantiated scientific software user training framework that will support knowledge sharing among scientific software users, in a blended learning environment. Scientific software is used in research areas that can directly affect public safety, such as nuclear power generation computer systems, groundwater quality monitoring and engineering designs. This investigation of current software training practices employs Grounded Theory in a qualitative methodology. Snowball sampling as well as purposive sampling methods were employed. Input from 20 respondents with diverse education and experience was collected and analyzed with constant comparative analysis. The Scientific Software Training Framework that results from this study encapsulates specific aptitudes and strategies that affect the professional development of the users regarding scientific software applications, in a blended learning environment. The findings of this study indicate that scientific software developers and users should take into consideration three key parameters in the design of training techniques for successful application of scientific software: (a) Confidence in Comprehension, (b) Discipline (and Systematic Validity Procedures), and (c) Ability to Adapt.
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List of Nomenclature

blended: Onsite and online setting.

blended learning (BL): The thoughtful integration of classroom face-to-face learning experiences with online learning experiences (Garrison & Kanuka, 2004).

community of practice (CoP): It is a group of people who share a craft and/or a profession (Lave & Wenger, 1991).

distance learning: It is typically defined as structured learning that involves an instructor who is physically located in a different place from the learner, possibly providing the instruction at disparate times and by using the latest technology (Moore, Dickson-Deane & Galyen, 2011).

epistemagogy: It describes how scientists (‘epistemon’ in Greek is someone who has acquired knowledge by studying systematically a particular subject; ‘agogy’ in Greek means leading) continue to advance their knowledge in the modern learning environment.

explicit knowledge: Explicit knowledge is available in documents, laboratory manuals, databases, memos, notes etc.

hardware: It refers to the physical aspects of computers and related devices.

knowledge management: In this study, the processes that take place within a professional research environment that focus on encouraging people to make use of information more effectively by capturing and assessing their understanding and work-related practices, sharing attained knowledge with peers and seeking feedback with a view to expanding their knowledge base and improving its application.

learner: In this study, the “learner” is an adult with life responsibilities but also a researcher, who has received significant academic and, often, professional preparation.

minimalist approach to software training: In this approach software instructors guide learners towards developing basic problem solving skills. The minimalist approach was developed by John Carroll in the 1980s (Hurt, 2007).

online learning: Learning that is supported by the Internet.

peer: A colleague who may also use scientific software.

peer collaboration: A type of collaborative learning that involves users working in pairs or small groups to discuss concepts, or find solutions to problems.
risk: The product of the probability of an event occurring, that is viewed as undesirable, and an assessment of the expected harm from the event occurring (Holton, 2004).

scientific community: The community of researchers in sciences and engineering.

scientific software (SciSw): A broad spectrum of application software that has a large computational component, models physical phenomena and provides data that can be used to address gaps in scientific knowledge (Sanders, 2008; Queiroz & Spitz, 2016).

scientific software training: Training on the use of scientific software.

situated cognition: It is an adult learning theory that states that learning and the context in which the learning takes place are so closely related that they cannot be separated (Merriam & Caffarella, 1999).

social presence: The need for users of technology-based communication to perceive each other as real people (Kear, Chetwynd & Jefferis, 2014).

tacit knowledge: ‘Assumed’ knowledge (a term used for the purposes of this research); tacit knowledge is about conveying the “know-how”, i.e. knowledge that experience-based, dependent on context and personal in nature (Smith, 2001).

training: This research adopts the definition of training as defined by Dearden: “Training typically involves instruction and practice aimed at reaching a particular level of competence or operative efficiency… Often training addresses itself to improving performance in direct dealing with things … Other sorts of training are more concerned with dealing with people … Yet other kinds of training are more indirectly concerned with changing or controlling people or things. But in every case what is aimed at is improved level of performance … brought about by learning” (Dearden, 1984, p. 58-59).

user: The individual who applies the scientific software product.
CHAPTER I: INTRODUCTION

This research examines current scientific software training with a view to identifying and analyzing existing practices regarding this topic. Among the pertinent issues explored is the use of blended learning methods in current scientific software training. As there is limited research on the subject of scientific software training, this study is essential in terms of identifying current software training methodologies. The context of such methodologies is a modern, technologically innovative learning environment for researchers in the field of natural sciences and engineering that provides a wide array of learning options.

Scientific software is defined here as a broad spectrum of application software that has a large computational component, models physical phenomena and provides data that can be used to address gaps in scientific knowledge (Sanders, 2008; Queiroz & Spitz, 2016). This type of software provides scientists and engineers with results to support decisions. Scientific software is complex and difficult to use. Scientific software systems often require tens of thousands of different input parameters. The scientific and engineering models expressed in the software are the result of years of scientific work from different knowledge domains, and require specialized knowledge to understand. For example, scientific software from the discipline of environmental science could be used to show the area of contamination due to a poisonous substance released into the environment (Appendix A). The incorrect use of this software may yield an erroneous direction of travel for the poisonous substance in the groundwater, thus compromising the safety of the general public (i.e., by issuing an evacuation notice to the wrong community). Correct interpretation of data returned by the software can be
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impacted by undetected input data mistakes, incorrect choices of values for parameters, misunderstanding the limitations and constraints on models in the software, undetected hardware or software glitches, and misinterpretation of what the software output data actually means – all of which introduce a level of risk. It is essential for a scientific software user to check the validity of the data output (i.e. results) from the software.

Effective training on the use of software is necessary to ensure correct scientific decisions. Training here does not mean learning repeated, predetermined tasks, but rather it means establishing a collaborative learning environment to ensure successful problem solving using the appropriate scientific software. The effectiveness of various training methodologies is not measured in this research study; the scope of this project is to identify training techniques that are currently being employed by scientific software users for their research purposes (i.e. which training techniques are considered effective by the users who choose to follow them).

Managing the risk in making errors in scientific software applications is critical (Hannay et al., 2009). Risk here means the likelihood of unintended mistaken scientific and engineering decisions based on incorrect use and/or misinterpretation of data output from scientific software. However, despite the abundance of training literature, there is limited research that looks at successful strategies to train professionals specifically in using scientific software. Thus, the problem is that there is currently a growing need for identifying good techniques for training in order to accurately apply or interpret scientific software while there is a deficiency in the literature regarding this topic. In-depth comprehension by users of knowledge entrenched in the software is essential in order to use scientific software with accuracy and reliability.
Existing blended training methods were investigated in this study, with a view to presenting optimal adult learning methodologies for software users. Scientists participate in classroom-based as well as asynchronous or synchronous online learning activities in order to expand their knowledge (Csanyi, Reichl, & Jerlich, 2007). Online and traditional classroom instruction has been used by an increasing number of post-secondary institutions to enhance science and engineering research training (Kyriazis, Psycharis, & Korres, 2009).

This qualitative investigation employed grounded theory with an ethnographically-informed approach. It explored the community of scientific software users in their natural setting of practice and their interactions regarding scientific software training. Open-ended interviews were utilized as the primary data source so that research findings could be reported in the words of the participants. Secondary data sources included reviews of laboratory software manuals and publications as well as observations of participants using scientific software products and troubleshooting during interview sessions (Hammersley & Atkinson, 1995; Robinson, Segal, & Sharp, 2007).

Recruitment of research participants and data collection for this study took place in natural sciences and engineering computational laboratories at universities and industry sectors in Canada.

**Statement of Problem**

Software is a general term used to describe a plethora of programs used to operate computers and related devices. These programs are collections of computer instructions
or encoded information that facilitate user-computer interactions. The term *hardware* defines the physical aspects of computers and related devices.

Software is becoming increasingly important to the realms of science and engineering, as it is used as a tool in order to process data and solve models expressed mathematically in an augmenting, timelier manner. Academic researchers and industry professionals depend on such software to answer their scientific inquiries and aid in the production of state-of-the-art scientific results. Further, software provides infinite opportunities to share and collaborate. Howison & Herbsleb (2011) argued that new and important science results require the combination of evolving scientific methods, validated instruments and theory to occur; software work brings together the combined efforts of many professionals in the continuous production of new tools that can address the ever-changing needs of software users. Scientific software users are members of a knowledge-rich community of practice (i.e. scientists and engineers in academia and/or industry) who use scientific software for their work or frequently adapt the software with a view to furthering their professional goals (Sanders, 2008).

Scientific software continues to evolve as knowledge obtained through continued scientific endeavor progresses. As the software’s cognitive density increases, so does the risk of incorrect use of software or insufficient validation of software output by the user. With the advancement of scientific software products, the issue that becomes central is the effectual comprehension of the knowledge that is entrenched in the software by the users, i.e. the capabilities and limitations of the software and how these can affect the software output. If this issue is not addressed sufficiently, it could have a negative impact on reliability associated with scientific software application and trustworthiness.
of scientific results (Segal, 2007; Adams, Davies, Collins, & Rogers, 2010). Fischer (2009) has indicated that expanding on background knowledge on scientific software from the perspective of the user is not a luxury but a necessity. It is noted that, in this study, the interest lies in identifying good training practices that may enhance accurate application of scientific software and reliable interpretation of the software output data array; the latter can affect scientific decisions. Thus, users who model the migration of contaminants in the environment or predict sea level trends due to earthquakes or global climate change ought to be able to trust and confirm the output of the software in order to publish the data and inform the public opinion responsibly.

It has been reported in the literature that training practices such as review of software company-supplied manuals or classroom-based training by software company instructors have not been proven sufficient for scientific software users whose work requirements continuously generate new questions about their software tools. Thus, training of scientific software users becomes a key issue in related scientific software literature (Fischer, 2009; Hannay et al., 2009; Howison & Herbsleb, 2011). Correct use of the scientific software (which was designed for a specific purpose to solve a particular problem) is a pre-condition for correct, accurate interpretation of software output. This ensures reliable answers to scientific inquiries. For example, if medical examination results are analyzed with the help of scientific software products, we, as a society, should be able to trust the interpretation of the software output by the doctors. Equally, if residents of an area located downstream of a contaminated water source need to know about the migration of environmental contaminants towards their water sources, they are
supposed to rely with confidence on the assessment of a geochemist who uses specialized software to determine the extent of and risk associated with this situation.

Hurt (2007) conducted bibliographical searches between 1996 and 2006 and identified a gap in literature regarding the linkage between software training and adult learning. Specifically, he argued that computer software training literature contains little empirical research that specifically focuses on adults. Hurt (2007) took a grounded theory approach and explored how trainers successfully incorporated the adult learning theories of andragogy and situated cognition with the minimalist approach to software training into the software training of adults. His study showed that andragogy, which was proposed by Malcolm Knowles (1968) and is considered a prominent theory of adult education, was found to be the mediating variable across the entire training process that was examined in his study. The role of andragogy in instructional designing of computer software training materials for adult learners was also emphasized by Hughes (1998).

Scientific software users are adult learners. They have acquired knowledge and experience to construct new knowledge or to further science. Scientific software users also tend to build their own software tools, thus using their previously acquired background to construct new knowledge or to further the science (Sanders, 2008). This inclination of scientific software users to create their own software is in accordance with constructivism and its principles about individual knowledge-seeking, as described by Bednar, Cunningham, Duffy and Perry (1992). However, existing formal preparation of users on scientific software applications includes more traditional, narration-based teaching and less self-action or experimentation in technology-supported learning environments (Kyriazis et al., 2009).
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Despite the employment of various methods of educational interaction, including distance learning methods and blended forms of instruction, training of scientific software users remains a problematic undertaking (Fischer, 2009; Hannay et al., 2009; Howison & Herbsleb, 2011; Joppa et al., 2013; Queiroz & Spitz, 2016). Although there is an abundance of training literature, there is limited research that concerns itself with successful, research-supported strategies to educate users specifically on scientific software application. Bibliographic searches using the keywords “scientific software training” and “adult learner” in six databases over the last twenty years (1995-2015) have produced no legitimate results in this regard. Similar searches using the keywords “scientific software training strategy” and “blended learning” also failed to produce useful results. Thus, there is an increasing need for in-depth understanding of the scientific software training process in our modern information age and at the same time a gap in current literature regarding this topic.

Scope of Research

This exploratory research study focused on investigating the experiences of software users with respect to their training on the accurate application of scientific software. Through an ethnographically-informed grounded theory approach, this investigation looked into the needs of scientific software users as learners in their setting of practice. It also examined the interactions of users with their professional environment, in traditional and internet-supported settings. This research sought to depict “an insider’s point of view” on the training needs of users with respect to reliable
scientific software application. The results of this study are intended to produce a scientific software training framework that will help support dependable knowledge growth of users. In particular, this qualitative research study applied grounded theory methods in data collection and analysis. Research participants were recruited in universities, in the public sector, as well as private industry in Canada. This research undertaking gave emphasis on the correlation between scientific software training and the needs of users as learners. This was conducted with a view to better defining the relationship between scientific software use and in-depth learning as opposed to procedural skills transfer. Cultural factors, gender or age differences were not assessed during this research venture; however, the data exist to make correlations in future research investigations.

**Research Question**

This study examined the current state of scientific software training in a blended learning environment. The main research question was:

“What software training approaches in a blended learning environment are chosen by users whose goal is to accurately apply scientific software to questions of research?”

Certain areas were examined, including: (a) the existing training methodologies (traditional and distance learning), and (b) the feedback of scientific software users with respect to current scientific software training. As such, during this investigation, the
Chapter I Summary

This chapter presents the research study by illustrating relevant background material and stating the problem that generates interest for this investigation. A qualitative investigation based on grounded theory has been described in order to investigate existing scientific software user training. The primary research question has been included and the resulting issues from addressing that question have been presented. The following diagram (Figure 1) summarizes the relationship between the new research problem, the research question as well as the framework of this research, as presented above.

The subsequent section provides the Literature Review that supports the major themes of this investigation. This is followed by the Theoretical Framework Chapter which further elaborates on the research methodology of this study.
**Research Question**
What software training approaches in a blended learning environment are chosen by users whose goal is to accurately apply scientific software to questions of research?

**Literature Review**
- Role of Scientific Software
- Scientific Software User Training
  - Definition of Training
- Key Adult Learning Theories
- Distance Learning and Software Users

**Methodology**
- Qualitative Research, Grounded Theory
- Research Question
- Research Design
- Data collection/Data Analysis
- Limits and Constraints of Research

**Results**

**Conclusions**

Figure 1. Summary of the Research.
CHAPTER II: LITERATURE REVIEW

Introduction

In this section the role of scientific software is discussed as well as the importance of training on scientific software. Adult learning theories that have been linked with software training or adult training strategies in current literature are also included. Several issues that are related to current training strategies and may affect collaborative learning (in a traditional and online environment) regarding scientific software training are identified. It is noted here that, throughout the study, the scope of the researcher was to conduct this investigation with an open mind about the learning needs of software users; without bias towards a particular adult learning theory. The analysis of the information provided by the users has determined the essential characteristics of the training process. In addition, the following section examines the role of scientific software and its importance in accurately describing physical processes that impact decision-making with respect to the safety of the general public.

The Role of Scientific Software

Sanders (2008) defined scientific software as application software that has a large computational component, models physical phenomena and provides output for decision support. This type of software is used by researchers and professionals in natural sciences and engineering to calculate movement of rock masses in tunneling, provide predictions
for weather systems, model subsystems at nuclear generating stations, model sea level trends or analyze changing chemical compositions of oceanic sediments (Appendix A). Joppa et al. (2013) argue that users consider two primary reasons for employing scientific software: (a) the ability to ask and answer new scientific questions, and (b) the ability of other researchers to reproduce the new scientific knowledge. Certain examples of scientific software include Hydrogeochem 5.0 (http://www.scisoftware.com/environmental_software/), POLLUTEv7 Professional software (http://www.scisoftware.com) and AquaChem5.1 (http://www.scisoftware.com) for environmental/geochemical research. Scientific software plays a critical role in the acquisition of new knowledge in science and engineering. Using scientific software to help analyze, visualize, or simulate processes or data is a core element of a daily routine of a scientist. Many scientists even develop software for their own use or for a wider community. Hannay et al. (2009) conducted an empirical study using an online survey tool with 2000 working scientists. The aim of this study was to investigate how the majority of working scientists develop and use scientific software in their day-to-day work. This investigation discussed, among other issues, why there was little exchange of knowledge and results concerning scientific application software within the scientific computing community or between the latter and the general computing/engineering community. The results of this study showed that one reason for this may have been that scientific software is often exploratory i.e. the purpose of the software is usually to help with the understanding of a new problem, implying that scientists/users cannot have up-front specifications of the software requirements. This may affect collaborations and exchange of feedback between researchers. As well, selected researchers are protective
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of their methods and findings. These facts may create a challenging environment for training with regards to scientific software due to its localized development, ever-changing applications to meet the research needs and the protective nature of selected researchers (Queiroz & Spitz, 2016).

The Scientific Software User

This research study employs the term “user” to describe both the individuals who use the software product without any adaptations as well as the researchers and industry professionals who modify software to suit their needs. Hannay et al. (2009) discuss the issue of increasing importance of developing and using scientific software over time. Their study indicates the stated belief of scientists, that today, research data are generated and archived at higher rates than five and ten years ago. Scientists spend, on average, approximately 50% more of their total work time on developing scientific software than they did five or ten years ago. As well, researchers also dedicate 100% more of their total work time using scientific software than a decade ago; as such, scientific software use is increasing in frequency and significance. Pawlik, Segal, Sharp and Petre (2012) also indicate that as research evolves, “it raises new questions and challenges that the existing software may not be able to address. At the same time, advanced domain knowledge is necessary to understand what the software is supposed to do”.

Research indicates that one of the challenges of the computing community is the requirement to further explore and comprehend the needs of the user (Segal, 2007; Fischer, Nakakoji & Ye, 2009; Fischer, 2011). A critical condition for a user is to
understand what the software is designed to do in order to be able to evaluate its appropriateness and its role in the intended use and application. Further, users (who are not always computer experts) need to grasp how certain functions of the software can be adapted to their specific needs. Training methods that take into consideration the needs of users may enhance their ability to understand and aptly integrate scientific software in their work. In-depth knowledge of various characteristics of the software may potentially help with eliminating risks involving poor software usage practices and questionable research results.

Reliability Associated with Scientific Software User Practices

The following sections describe areas where risk may increase due to unreliable scientific software application and limitations in training practices. The scope of this section is to highlight the importance of training on scientific software use by describing key parameters that can influence reliability associated with scientific software user practices.

There are three major areas that may affect reliability and increase risk associated with scientific software use (Sanders, 2008; Segal, 2007; Fischer, 2009). These are:

2. User-Software Developer Communication (or customer technical support of software company).
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It is noted that this study examined assessments of users with respect to current scientific software training approaches; whether users were allowed to modify the software to address their needs or not. This research undertaking did not investigate capabilities or weaknesses of scientific software developers.

User-Scientific Software Product Interaction

Researchers in science and engineering have pointed out that scientific software products need constant adaptation in order to address their needs as users. However, there is considerable risk associated with scientific software users adapting a product in which they have received minimal training. This can result in incorrect answers to scientific inquiries as users may not be able to verify the software output (Sanders, 2008; Segal, 2007; Fischer, 2009; Fischer, Nakakoji, & Ye, 2009; Fischer, 2011). Considering that scientific software is used in a plethora of applications in modern society, i.e. medicine, meteorology, engineering or environmental science, it is evident that scientific software output needs to be thoroughly understood by users.

Letondal and Mackay (2004) investigated the issue of scientific software use within distinct groups of users and point out their significant involvement in adapting software tools in order to better address specific research requirements. Further, Sanders (2008) highlighted the lack of formal training in scientific software and identifies dependability issues associated with software use when a collaborative learning environment among software developers and software users is limited. Pawlik et al. (2012) conducted a qualitative study that included scientists who used and developed
scientific software as well as scientists who were only users of scientific software. They found that, out of 27 interviewed scientists, 24 were either almost exclusively self-taught with respect to their software development skills or combined self-teaching with one- or two-semester undergraduate courses in programming. Self-teaching of the participants was based on multiple materials; among these materials, the Internet appeared to have a prominent role as a source of information, particularly in troubleshooting situations.

User-Scientific Software Developer Communication

Scientific software developers may not be able to accurately predict the full range of user needs in every context that their software product is used (Sanders, 2008; Segal, 2005). Without formal training procedures in place and open channels of communication between software developers and the users, the efforts of the latter to develop quick solutions that address their immediate needs may actually degrade the potential of a particular software tool. Fischer (2011) discussed the need for a co-evolution of systems, communities, and individuals. In his work, software products are regarded as socio-technical systems that continuously evolve with the constructive input from software developers and users who work collaboratively in creating new knowledge. The work conducted by Fischer (2011) draws attention to the development of rich, diverse support networks where users and software designers can maintain an ongoing partnership that would foster productivity, user-centered design and an adult learning collaborative environment. Sloan, Macaulay, Forbes, Loynton and Gregor (2009) also acknowledged
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the immediate need for end-user professional development and training, which could also help with improving reliability and reducing risk regarding scientific software use.

**User-User Interaction**

Howison and Herbsleb (2011) discussed the issue of establishing a collaborative learning environment within academia with respect to scientific software use. They pointed out that, although software can be copied and distributed inexpensively, providing endless opportunities of sharing and collaborative innovation, user-user interaction is limited. They also indicated that scientific software work takes place in the context of competition amongst academic scientists for recognition and attention that focuses on publications and citations. As such, science does have a collaborative nature that is expressed in specific projects and indirectly over time as research projects build on each other, but it is not a selfless field. Howison and Herbsleb (2011) argued that collaborative learning does not occur due to competition among academic researchers and “their reputation economy”. Since substantial software contributions to existing scientific software projects are not usually rewarded through the traditional reputation economy of science, collaboration among scientific software users is not often encouraged within academia. These factors combined with the lack of current formal training of academic researchers on scientific software (as highlighted in previous citations) may substantially inhibit collaborative learning and training on scientific software. More importantly, it may affect the quality of scientific software output data interpretation, thus incurring risk, because there is limited peer collaboration in
validating software output (Fischer, 2009; Howison & Herbsleb, 2011). Pawlik et al. (2012) studied how the use of online tools can improve the collaboration between scientific software users. They found that their research participants were more inclined to work and share ideas online with colleagues who they knew in person. Further, they indicated that this parameter (i.e. the preference of the users to share information online with peers that they had previously met face-to-face) can potentially act as a limiting factor in professional collaborations and broadening of technical knowledge internationally.

The Need for Successful Scientific Software User Training

As technology advances, computer software becomes increasingly challenging to learn. The reliance of adults on software training becomes heavier in order to remain informed of current progress and learn new software skills. Research has pointed out that although training has been cited as one of the most important support functions by computer users, the adult learning aspect of computer training remains a neglected area in theory, practice and research (Mandefrot, 1997; Hurt, 2007). Hurt (2007) argued that our current knowledge of how to train the user remains elementary, due to the fact that training and support are lagging behind hardware and software development.

Regarding scientific software, Hannay et al. (2009) highlighted the value of training of practitioners in science and engineering programs on this type of software. Their study participants acknowledged a general lack of formal scientific software training among scientists. Their participants also pointed out their reliance on informal
self-study and learning from peers. The findings of this research suggested that users regard both learning at an educational institution and learning in the professional workplace as equally important to them, but only if these activities have taken place recently. However, Hannay et al. (2009) pointed out that scientists do not see the need to receive more formal scientific software training in its current form; because the formal training that scientists do receive is often supplied by a computer science department, which offers general software courses of which researchers might not see the relevance. As modern scientific software tends to become more and more complex, and as Hannay et al. (2009) argued, there is an increasing awareness among scientists of the need for improved formal training, especially for large research projects.

Joppa et al. (2013) discussed the lack of formal training in computational methods in scientists who graduate from natural science and engineering programs. They concluded that an overwhelming majority of researchers in natural sciences wish for increased computational skills, as they need to have sufficient knowledge of what the software is doing and whether it is, in fact, doing what is expected. As society’s important scientific decisions rely on accurate scientific software application, “the scientific community must ensure that the findings and recommendations put forth based on software models conform to the highest scientific expectation” (Joppa et al., 2013, p. 815).
Scientific Software Training in Modern Learning Environments

Peer collaboration, albeit in an informal fashion outside of a theoretical framework, is used extensively by researchers in science and engineering in the quest of expanding their background knowledge (Harp, Satzinger, & Taylor, 1997; Fischer, 2011). Several researchers in recent literature have indicated the need for methodical teaching of collaborative (peer) learning skills in academic programs of science and engineering. For instance, Lingard (2010) stated that employers often report that new hires typically have insufficient experience, communication skills and preparation for working (and continuing to learn) as part of a team. This is a potential result of the ineffective teaching strategies and assessment tools of collaborative learning within teams in academic curricula. Lingard (2010) wrote:

Although many universities have recognized the need to assign group projects and have begun efforts to improve engineering and computer science curricula in this regard, students seldom receive any specific training on how to function collaboratively before such assignments are given, and little attention is given to how teams are formed (p.34).

Similar concerns have been cited in literature since the 1990’s (McGinnes, 1994; Green, 1999; Hernández & Ramirez, 2008; Purzer, 2009; Purzer, 2010; Borrego, Karlin, McNair, & Beddoes, 2013). According to Vygotsky (1978), students can perform at higher intellectual levels in collaborative situations than when working individually. Collaborative learning requires “working together toward a common goal” and that “students are responsible for one another's learning as well as their own” (Dooly, 2008). This collaboration entails the whole process of learning, not only the teacher instructing
the students; it may involve students teaching one another or students working collaboratively with the teacher towards a solution. In this situation, the learners have attained their goal (to enrich their background) by helping each other understand the new concepts at hand (Dooly, 2008).

With technological advancements, tasks involving collaborative learning and completing projects in a team environment have largely moved online. This adds a new vector in the sum of the parameters that determine learning in science and engineering. Modern researchers are encouraged, and even expected by their peers, to share data in online resources and learn to incorporate distance collaboration learning technologies in their daily work routines. Although Olson & Olson (2000) determined that “distance matters”, and that interactions over distance can never replace collocated interaction, the number of scientific papers published by international collaborations doubled in the last decades (Nentwich, 2008). Miller (2009) argued that online collaboration, as a way of doing scientific research, is becoming more and more common; the work of scientific research is becoming increasingly distributed and collaborative. For example, this tendency is indicated in the formation of collaboratories, i.e. organizations of researchers that, with the help of special technological systems, conduct science in a geographically distributed manner.

The study of “complex, multidisciplinary, multiphenomena behaviours of large physical, biological, or social systems” often has researchers performing together in larger groups than those that traditionally make up a lab. For many of these projects, equipment and computing are distributed over large distances; as such, new challenges are created for collaborative learning and technological equipment (Cummings, Finholt,
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Foster, Kesselman, & Lawrence, 2008; Miller 2009). Further, this creates a new status quo, where large amounts of data with diverse characteristics are being shared and manipulated on a global scale (Hey & Trefethen, 2008). Computer science, and more specifically, software developers are presented with a new demanding task: To design software that can address the needs of the scientist/engineer in a new, distributed working environment. As expected, effective training in using scientific software in a blended, collaborative learning environment is necessary in order to ensure correct scientific decisions.

Training versus Learning

The term training has no generally accepted definition (Bramley, 1986; Mandefrot, 1997). Mandefrot (1997) argued that a precise description for learning and training is not available. Training can be a means to bring about learning and create a learning environment where people acquire new knowledge, workers learn, and help each other learn. In literature, however, training is often considered a process that only requires that one learns a specific thing by following exact directions (Bramley, 1986; Goldstein & Gessner, 1988). Often training recognizes only formal instruction, though; it does not include the chance for people to learn through observation, direct experience and from each other. Dearden (1984) gave a more holistic definition of training and links it to learning:

Training typically involves instruction and practice aimed at reaching a particular level of competence or operative efficiency...Often training addresses itself to improving performance in direct dealing with things ... Other sorts of training are more concerned with dealing with people ... Yet other kinds of training are more
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indirectly concerned with changing or controlling people or things. But in every case what is aimed at is improved level of performance ... brought about by learning (p. 58-59).

What makes Dearden's definition of training relevant for this research undertaking is that his definition clearly emphasizes a link between training and adult learning. He indicated that the purpose of training is not the narrow focus of skill acquisition but that of behavioural change, which is a characteristic of comprehensive learning. This research will adopt the definition of training by Dearden because it provides a framework for investigating how dealing with things (scientific software in this case), with people (adult learners-scientific software users), and with change (traditional and distance learning, effective collaborative learning) can influence the learning process within the community of scientific software users.

**Blended Learning**

In defining “blended learning”, Garrison & Kanuka (2004) pointed out that it is the thoughtful integration of classroom face-to-face learning experiences with online learning experiences. Garrison & Kanuka (2004) further indicated that a blended learning environment can allow for comprehensive learning to occur within scientific communities because it fosters opportunities for reflection along with independence and increased control essential to developing critical thinking. Blended instruction has been used by an increasing number of post-secondary institutions to enhance science and engineering research training (Kyriaizis, Psycharis, & Korres, 2009; Graham, 2013). What makes blended learning particularly suitable for interactions within a community
that shares scientific knowledge is its ability to facilitate a community of inquiry (Garrison & Kanuka, 2004; Graham, 2013). The social interrelations within a community of learners balance out the open communication and limitless access to information on the Internet. Therefore, blended learning can provide a suitable environment for the learner to benefit from social presence, cognitive presence and teaching presence, cultivating a vigorous community of inquiry. Garrison, Anderson and Archer (2001) argued that:

One of the characteristics of the community of inquiry is that members question one another, demand reasons for beliefs, and point out consequences of each other’s ideas—thus creating a self-judging community when adequate levels of social, cognitive, and teacher presence are evident (p. 6).

Further, as blended learning environments can afford opportunities for multiple forms of communications, critical properties associated with reliable scientific knowledge and quality higher education are strengthened through free and open dialogue, critical debate, negotiation and agreement (Garrison & Kanuka, 2004; Graham, Henrie, & Gibbons, 2014). This is especially important for the open community of scientific software users in academia who often rely on peer collaboration for obtaining feedback on scholarly work (that has societal importance in terms of water quality, engineering design, etc.). However, as literature indicates, there is a requirement for incorporating adult learning principles in blended learning design, allowing for a variety of learning pathways and resources from which the learner can choose, and a community with whom participants can interact including the instructor (Ausburn, 2004; Azizan, 2010; Roberson, 2015).

Despite the potential that blended learning has in supporting knowledge exchange within professional communities, literature has indicated that there are weak points in
blended learning that need attention. Current researchers have pointed out issues pertaining to ineffective use of learning technology tools that can waste resources. They have specifically indicated a requirement for basic technology knowledge as well as a willingness of the student to be actively involved in learning; from a didactical point of view, research has shown that blended learning can prove ineffective if presence and online phase compete, instead of complement, each other (Glogowska, Young, Lockyer, & Moule, 2011; Tayebinik & Puteh, 2012; Bueno-Alastuey & Lopez Perez, 2014; Roberson, 2015). Particular issues concerning developing countries, involve securing the required funds to purchase new technology, inadequate e-learning training for staff members, as well as student reluctance to make use of the e-learning systems (Poon, 2012; Bueno-Alastuey & Lopez Perez, 2014). Further, often stakeholders, especially administrators, view programs with an increased percentage of online learning in their structure as of lower quality as compared to on-site, traditional programs. This can have substantial impact on the successful implementation of blended learning programs (Allen & Seaman, 2013; Chawinka & Zozie, 2016).

**Adult Learning**

This section includes a literature review of training practices that have been analyzed through the lens of adult learning theory by current researchers. Merriam and Caffarella (1999) characterized behaviourism, cognitivism, social learning and constructivism as key theories that are compatible with adult learning. Hurt (2007) concluded that developing computer training methods for adults must include the theory
of andragogy. The following section will discuss the critical components of each of the theories.

**Behaviourism**

Behavioural learning theory was developed by John Watson in the early decades of the twentieth century (Lowe, 2004). There are three basic assumptions about the behavioural learning process: (a) the emphasis is on observable behaviour rather than internal thought processes, (b) environmental parameters greatly affect, even shape, behaviour, and (c) the principle of contiguity and reinforcement are central to explain the learning process (Grippin & Peters, 1983). Critics of behaviourism argue that this theory fails to show adequate generalizability in human behavior and is not able to explain the development of human language (Naik, 1998).

Several educational practices including the systematic design of instruction, programmed instruction, computer-assisted instruction, and competency-based education stem from behavioural learning theory (Lowe, 2004). Adult technical and skills training also draws from behaviourism. Training researchers often design their teaching around behavioural principles and consider observable performance as the primary indicator of training output (Bosco & Morrison, 2000). However, it was in the 1960’s and 1970’s that behavioural learning theorists started exploring the effect of cognitive processes and the internal knowledge schema of the learner on task performance (Bosco & Morrison, 2000). Behaviourist learning theory had, at that point, received heavy criticism and
cognitive learning theory trend arose to counter its dominance in the field of learning theory.

**Cognitivism**

Most contemporary cognitive psychologists consider learning as a composition of individual constructions of knowledge. Learning is a personal event that results from sustained and meaningful engagement with one’s environment (Bruner, 1986). This view also accepts that learning is an integral part of the social and cultural contexts in which it occurs (Lowe, 2004). However, cognitivism has received criticism for understanding “the mind as ‘utterly separate from the world’, as a passive receiver of empty, meaningless causal signals from the world outside, and therefore as trapped within what Heidegger calls an ‘inner sphere’” (Taylor, 2006).

Piaget and Bruner focused on the cognition and theory of instruction, which had an impact on learning theories. Piaget (1972) viewed behaviour of the human organism as starting with the organization of sensory-motor reactions and reaching higher levels of intelligence as coordination between reactions to objects becomes progressively more interwoven and complex. A basic assumption of Piaget’s theory is that a different type of assimilation and accommodation occurs at each stage of development. For example, thinking becomes possible after language develops and a new mental organization is created. Bruner (1986) focused on structuring and sequencing of knowledge in order to form a theory of instruction. He considered learning as involving three almost simultaneous processes: acquisition of new information, transformation or manipulation
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of knowledge in order to incorporate new tasks, and evaluation to see if information is adequate to the task. Gardner (1991) and his theory of Multiple Intelligences has also emerged from recent cognitive research and "documents the extent to which students possess different kinds of minds and therefore learn, remember, perform, and understand in different ways". Three features cited by Gardner generally associated with cognitive science that apply to learners interacting with computer include: (a) cognitive science is explicitly multi-disciplinary, drawing especially upon the disciplines of psychology, linguistics, anthropology, philosophy, neuroscience, and artificial intelligence, (b) a central issue for this discipline is cognitive representation, its form, structure, and embodiment at various levels, and (c) the faith that the computer will prove central to the solution of problems of cognitive science, both in the conduct of research to investigate various cognitive representations and in providing viable models of the thought process itself (Gardner, 1985, 1991; Lowe, 2004).

Previous researchers have viewed knowledge as some entity existing independent of the mind of individuals and which is transferred “inside” (Bednar et al., 1992). Consistent with this view of knowledge, the goal of instruction, from both the behavioural and cognitive information processing perspectives, is to communicate or transfer knowledge to learners in the most efficient manner possible. While behaviourist applications focus on the design of learning environments that optimize collaborative learning, cognitive information processing stresses efficient processing strategies (Bednar et al., 1992). Contemporary approaches to learning with Internet-based technology are more often rooted in cognitive learning theories (Lowe, 2004). Research on the effects of the computer on cognition investigates the cognitive development of the

Learner; the latter is viewed as a consequence of the interaction between the individual and computer, such as an increase in general problem-solving ability or mathematical reasoning. Hannafin (2006) pointed out that an intellectual partnership is formed between the individual and the technology; the resulting changes to cognition cannot be understood when the individual or the technology are considered apart. Research with technology focuses on how human processing changes in distinct, qualitative ways when an individual is engaged in an intellectual activity using the computer as a tool. Equally, scientific software users develop an intellectual partnership with their software tools as they use the latter as their vehicles in order to reach their research destinations.

Social Learning Theory

Social learning theory which combines elements from both behaviourist and cognitivist orientations suggests that people learn from observing others. Bandura (1976) stated that behaviour is learned from the environment through the process of observational learning: “Virtually all learning phenomena resulting from direct experiences can occur on a vicarious basis through observation of the people’s behaviour and its consequences for the observer” (Bandura, 1976, p. 392). However, some criticisms of social learning theory arise from this commitment to the environment as the chief influence on behavior, potentially neglecting other factors, such as genetic influences (Booth, Owen, Bauman, Clavisi & Leslie, 2000). Bandura’s theory has particular relevance to adult learning in that it accounts for both the learner and the environment in which he or she operates. Behaviour is a function of the interaction of
the person with the environment. This is a reciprocal concept in that people influence
their environment, which in turn influences the way they behave (McLeod, 2011).
Another element that connects the social learning theory to adult learning is the
importance of context and the learner’s relationship with the environment in explaining
behaviour. Mandefrot (1997) emphasized the meaning of the social aspect of computing
and how this affects the learning process. He argued that the social aspect of computing
affects motivation, individual differences, and the learning process. Motivation of
learners, for instance, may be a parameter that affects the quality of adult training
methods’ outcomes, including scientific software users’ training, especially if the
participants feel threatened by technology or overwhelmed by the learning material.

In addition, Bandura’s social learning theory has particular relevance to scientific
software training in a blended learning environment as it relates to people learning from
observing others. These observations usually take place in both traditional and online
environments in modern science and engineering laboratories (where scientific software
is applied). The social learning theory is linked to adult learning in that it accounts for
both the learner and the environment in which he or she operates; in the case of scientific
software training, this can happen in a face to-face or online setting. Behaviour is a
function of the interaction of the person with the environment. This is a reciprocal
concept in that people influence their environment, which in turn influences the way they
behave (McLeod, 2011).
Constructivism

Historically, constructivism originates from developmental psychology and social learning theories. A constructivist views learning as a process of constructing meaning. Meaning is created by the individual and is directly linked with the learner’s previous and current knowledge structure. A constructivist encourages cognitive conflict in order for new learning to occur (Bednar et al., 1992). Constructivists motivate learners to construct a viewpoint by searching for knowledge sources that may be relevant to the pre-specified core knowledge domain; the boundaries of what may be relevant cannot be defined. It is not possible to isolate units of information or make a priori assumption of how the information will be used (Bednar et al. 1992; Lowe, 2004). These principles of constructivism are directly linked to how adult learners interact with software, especially in web-based collaborative learning environments (Liao & Ho, 2008; Svensson, 2011).

In web-based collaborative learning methodologies, the center of the learning process is the student who is encouraged to develop a sense of ownership of his/her education and, thus, a passion for learning, problem solving, and understanding. In conjunction with these competencies, the constructivist learner must also be able to participate in debates and negotiate with peers as well as conduct networking, a skill that can be transferred in real life contexts and encourage collaboration among learners (Tung, Huang, Keh & Wai, 2009; Svensson, 2011). Liu & Matthews (2005) indicated that certain facets of constructivism have received criticism by advocating for individual epistemological idiosyncrasy (regarding radical constructivism) as well as for social epistemological relativism (social constructivism).
Andragogy is the art and science of teaching adults (Knowles, 1968). Adult learners are expected to be independent and capable of directing their own learning. Adults should not be seen as sponges but as a rich learning resource due to their life experiences. Their learning needs are associated with social roles. Further, adult learning is problem-centered and focused on applicability of knowledge gained. In addition, internal factors have greater impact than external factors in motivating adult learning. Adults need to relate their learning to their own life circumstances. They need to have flexibility in their learning as they usually have other “concrete” obligations to fulfill in their daily lives (Merriam, Caffarella, & Baumgartner, 2007). This is in agreement with the observations of Rachal (2002) who determined the need of adults to see the application of their learning as an investment in their professional/personal lives. Further, Knowles, Holton & Swanson (1998) argued that the goals and purposes for adult learning include societal growth, individual growth, and institutional growth. Also, the goals and purposes for which the adult learning is conducted provide a frame that puts shape to the learning experience (Knowles et al., 1998). Albright & Post (1993) stated that adults clearly prefer to seek rather than receive knowledge. They argued that this tendency increases despite adult learners’ different learning preferences or level of cognitive ability. Adults seek to learn at their own pace and to learn at the right time so that they can apply new knowledge and skills immediately. A study at the University of Georgia investigated how adults learn to use software, taking into consideration their learning preferences (degree of autonomy in the learning process), type of work and experience

with software use (Harp, Satzinger & Taylor, 1997). The study revealed that dependent learners (learners with an affinity for synchronous direct assistance) generally prefer a direct approach; self-directed learners generally prefer an autonomous approach.

Respondents reported that their best learning resources were their co-workers whereas using training manuals were the least useful learning activities. This is in agreement with andragogy principles with respect to the autonomy of the learner, the need for applicability of new knowledge, and the learner’s social role. The findings of the above-mentioned study coincide with observations made by researchers within the natural sciences field over a period of twenty years. Peer support, albeit in an informal fashion outside of a theoretical framework, is a method used extensively by professionals in the quest of expanding their background knowledge.

Andragogy, since it was introduced by Malcolm Knowles, has been the focus of continual debates. These debates concern its theoretical strength, use (whether it is learning theory, a guide to teaching or a philosophical statement) and even its applicability in today’s demanding and ever-changing knowledge requirements that adults face in their professional and personal lives (Hartree, 1984; Sandlin, 2005). The mission of adult educators is to support adults in achieving self-actualization, and andragogy is the teaching methodology used to achieve this end (Knowles, 1980). However, Davenport and Davenport (1985) showed that defining what is unique about teaching adults as opposed to children or youth is crucial for the development of the adult education research realm. This theoretical distinction has been a long-standing discussion among adult education researchers.
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Adult Learning – Summary

Figure 2 provides a summary of the theories discussed previously and their connections to adult learning and training.

<table>
<thead>
<tr>
<th>Learning Theories</th>
<th>Adult Learner Characteristics</th>
</tr>
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</table>
| Behaviourism      | •Adult Technical and Skills Training  
                   | •Observable Performance - Primary Indicator of Training |
| Cognitivism       | •Web-based Adult Learning  
                   | •Adult Learner and Technology in Intellectual Partnership |
| Social Learning Theory | •Social Aspect of Computing in Adult Learning  
                       | •Motivation and Diversity in Learning Process |
| Constructivism    | •Web-based Collaborative Adult Learning  
                   | •Adult Learners Construct Own Viewpoint  
                   | •Adult Learner is the Center of Learning Process |
| Andragogy         | •Adult Learning and Practicality of New Learning  
                   | •Peer Support and Shared Wealth of Knowledge  
                   | •Internal Motivation and Self-Directedness |

Figure 2. Adult Learning and Compatible Learning Theories.

Adult Learning and Scientific Software User Training

Scientific software training is essentially a professional development tool for software users. Researchers in the scientific software field have described software users as learners who generate new knowledge (by using and adapting software) and need to have ownership of their learning process, a characteristic that is in accordance with
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andragogy (Knowles, 1968; Fischer, 2009). A study conducted by Speck (1996) suggests a framework of theory-informed good practices with respect to adult learning and professional development activities. His findings could help with strengthening the design of a scientific software user training framework, the need of which is described in this investigation. Speck (1996) concludes the following:

1. Adults will commit to learning when the goals and objectives are considered realistic and directly relevant to the adult learners’ personal and professional needs.

2. Professional development, such as training, needs to allow participants some control over critical characteristics of their learning, such as what, why, when, and where of their learning.

3. Professional development must include opportunities for peer support so that learners participate without fear of being criticized.

4. Feedback is important for professionals receiving training, so that they can assess the results of their efforts.

5. There is rich diversity of knowledge, experiences and skills in adult learner groups. This substantial resource should be incorporated in professional development planning. Small-group training activities allow for an enhanced learning experience by providing participants with an opportunity to share, reflect, and generalize their learning experiences.

6. Follow-up support is essential for adult learners so that they can transfer and sustain new knowledge into their daily practice.
In agreement with Speck’s research findings on professional development and peer support, Tartas and Mirza (2007) indicated that collaborative practice is a core facet of professional life for both researchers and practitioners. Further, Gardner (2007) explained that the production and growth of information is exponential within an information society; thus, one of the most important tasks of scholars is that of synthesizing information from disparate sources and generating new knowledge to find solutions to problems that are increasing in complexity. As such, active participation in the learning process and peer collaboration are essential elements in creating new information, as described above. However, literature has indicated that current educational institutions often treat scientific software users as consumers, depriving them of the opportunity to decide on the course of their learning and take active roles in knowledge sharing activities with view to addressing personally meaningful and important problems (Fischer, 2009; Joppa et al., 2013). Further, research on establishing good practices in scientific software user training has not yet been performed; as a result, scientific software training is applied with questionable results (Hannay et al., 2009; Howison & Herbsleb, 2011; Joppa et al., 2013).

**Distance Learning**

Distance learning is typically defined as structured learning that involves an instructor who is physically located in a different place from the learner, possibly providing the instruction at disparate times and by using the latest technology (Moore, Dickson-Deane & Galyen, 2011). Literature indicates the pivotal role of the use of online
learning and other distance technology learning methods in lifelong education and professional development (Tung, Huang, Keh & Wai, 2009; Svensson, 2011). This is due to the fact that modern society places increasing demands on the workforce with respect to continuous upgrading of expertise. Beyond secondary and post-secondary education, lifelong education is required. This continuous learning is already making extensive use of the Information and Communication Technologies (ICT) in the form of educational technologies. Distance education, incorporating ICT, may become the norm in such lifelong education (Evans, 1997).

Literature has pointed out that researchers in natural sciences and engineering contribute to conventional as well as asynchronous or synchronous online learning activities for peer collaboration and background enhancement purposes (Csanyi, Reichl, & Jerlich, 2007). Currently, post-secondary institutions tend to incorporate blended instruction methods in science and engineering programs with a view to attracting and retaining adult learners (Kyriazis et al., 2009).

To be useful, distance learning needs to be:

1. Purposeful: The purpose and end-results of a distance learning activity should be defined clearly.

2. Structured: The structure of a distance learning activity should be coherent and well-defined as it can greatly affect a learner’s interest and engagement levels.

3. Paced: Pacing is critical in distance learning, especially to adult learners with concrete daily life obligations.
4. Engaging: Engaging the learner in a distance learning environment is as crucial as the factors described above. In the case of busy professionals enrolled in adult learning programs, the success of the program depends greatly on the distance learning material making a substantial contribution to their previously acquired background (Bissell & Endean, 2007).

O’Lawrence (2007) indicated that adult learners can benefit from online learning, enhance their background knowledge and further strengthen their andragogy-related qualities. Specifically, he argued that:

1. Having obtained a variety of background experiences through prior learning and work experience, adult learners enjoy sharing practical applications online with peers from similar backgrounds.
2. Adult learners can integrate new concepts with their prior knowledge and use the online environment to exchange ideas with colleagues with similar work experience.
3. Adult learners acquire knowledge best by having control over their learning environment; thus, online learning allows for an increased learner-centeredness, which may be preferred by scientific software users who can study tutorials on software usage at their own pace and at the appropriated time for them.

However, literature has suggested that there are adult learners who find it challenging to become familiar with software, particularly within an online environment and its new patterns of communication or to take responsibility for their own learning. This may be due to the fact that effective online learning requires adapting traditional
teaching strategies to a new learning environment (Bissell & Endean, 2007; O’Lawrence, 2007).

**Distance Learning in Scientific Software User Training**

There is limited existing research concerning the role of distance learning in scientific software user training. Anthonysamy (2005) discussed the importance of e-learning design in engineering education. Further, Bissell and Endean (2007) indicated the significance of employing distance learning methods in engineering programs, where training on scientific software applications is an essential element of the students’ academic preparation. Adams et al. (2010) investigated the benefits of incorporating mobile technologies in the field of geosciences education, which traditionally includes scientific software applications. Future research is required in order to examine how open and distance approaches to scientific software user training can provide a major resource to professionals in the fields of natural sciences and engineering.

**Chapter II Summary**

As discussed earlier, the literature indicates that there is an identified need for establishing an informed training framework for professional researchers and science or engineering practitioners who use scientific software; a framework that will address the needs of the users as adult learners. The following diagram illustrates the main elements of this research as well as how they relate to each other (Figure 3). Scientific software
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Usage is essential in addressing research questions, often with implications regarding public safety such as drinking water quality issues, earthquake modeling and predictions. However, incorrect software use may lead to erroneous research results and subsequent poor decisions.

Figure 3. Main Elements of Research Study.

The results of this study aim to contribute towards establishing a scientific software training framework that can address the associated dearth of literature, enhance the accurate use of the software, and increase dependability of scientific decisions.
CHAPTER III: THEORETICAL FRAMEWORK

Introduction

This qualitative study focused on identifying current training with respect to scientific software application. Grounded theory was applied in data collection and analysis. Grounded theory is used in order to investigate a phenomenon in its natural context and a data analysis is employed to construct a theory from empirical findings. As such, the emergent theory is ‘grounded’ in the data. Harrison (2015) pointed out that grounded theory methods allow “the researcher to ‘listen to’ the experiences of the participants as expressed freely without constraining prompts”. The data collection continues until ‘theoretical saturation’ is reached (Glaser & Strauss, 1999). In this investigation, observations in real-life settings, acquirement of “insider” accounts as well as collection of empirical data in their naturalistic setting were used from which themes emerged and conclusions extracted. Recruitment of participants and data collection for this research took place in universities and industry sectors in Canada.

In the next section, a summary of the most relevant qualitative studies is presented along with other studies that highlight the value of distance learning among science and engineering practitioners. Specifically, this new investigation was based on: (a) qualitative research studies in software engineering by Lutters and Seaman (2007) as well as Robinson, Segal and Sharp (2007), (b) adult training research on computer use by Hurt (2007), (c) research on hybrid learning experiences in geological sciences by Adams, Davies, Collins and Rogers (2010), and (d) distance learning research within the
field of engineering by Bissell and Endean (2007). The next section includes a review of the basics of qualitative research and its importance for this study.

**Qualitative Inquiry in this Study**

Literature in the field of scientific software includes a number of studies that employ qualitative methods of data collection and analysis. Software engineering researchers use qualitative approaches when they investigate complex behavioural phenomena in their field, such as exploring internal states and external environmental influences on their peers (Lutters & Seaman, 2007). Qualitative research provides a mechanism to better understand uncharted areas of inquiry or misunderstood phenomena and processes, such as scientific software related collaborative learning (Miles & Huberman, 1994; Berg, 2001; Mandefrot, 1997). The research studies by Hurt (2007) and Sanders (2008) both used qualitative methodology and open-ended interviews as their primary data collection instrument. Hurt (2007) focused on identifying how software trainers use the minimalist approach to training, as well as situated cognition, and andragogy in the software instruction of adults. His research pointed out that principles of andragogy greatly influence adult training on computer software. Sanders (2008) carried out a qualitative study on scientific software users in order to identify characteristics of current development and usage. Her research identified, among other conclusions, the need for on-going communication between scientific software developers and users; in other words, a strengthening of the culture of collaboration among researchers. Adams et al. (2010) focused their research on designing blended
scientific inquiry learning in geosciences. Their study participants conducted geological research using scientific software and collaborated in a distance learning environment. Their findings highlight the value of technology supported distributed collaboration in the field of geology. Bissell and Endean (2007) discussed the importance of distance learning approaches to engineering education. Their research highlighted the importance of team collaboration at a distance in using engineering-related software (i.e. scientific software) to address research questions. Consequently, this research study built on the findings of the aforementioned studies and further explored qualitatively current practices in scientific software training.

Qualitative inquiry was preferred due to its significant advantages in the context of this study. Qualitative research acknowledges the importance of context, allows for reconsideration of issues which are considered unreliable and subjective in quantitative research. The use of a qualitative data gathering method is highly flexible, allowing for modifications of the research hypothesis as the study progresses (Berg, 1998; Cohen et al., 2007). Qualitative inquiry is appropriate for this type of investigation: qualitative data gathering methods examine phenomena in their natural environments (Miles & Huberman, 1994; Cohen et al., 2007). This research study employed a qualitative methodology approach for the following reasons:

- It focused on providing a framework on scientific software user training that can be readily followed by peers in the field. A qualitative methodology approach would be useful in this regard: Cohen et al. (2007) discussed how qualitative research reports are typically rich with detail and insights into participants' experiences of the world. Thus, they have the capacity to holistically describe a
phenomenon, which can be more meaningful from the reader's perspective, in this case the scientific software users.

- Little has been documented regarding scientific software user training and its relationship with the learning needs of the users. Strauss & Corbin (1998) indicate that the use of grounded theory in a qualitative research approach is necessary when the researcher seeks to better understand any phenomenon that has not been adequately investigated.

However, qualitative research has shortcomings with respect to quality of data and objectivity. Although qualitative research allows for a deep understanding of phenomena, knowledge produced might not generalize to other people or other settings (Patton, 2002). The information provided and the interpretation of the information is subjective due to the human element. This is also a factor in the validity of the data, which is dependent upon the researcher (Strauss & Corbin, 1998; Patton, 2002).

This investigation employed an ethnographically-informed, grounded theory approach in a qualitative research methodology. Key elements of an ethnographic approach is the immersion of the researcher in the area under study for a long period of time (months or even years), the collection of empirical data in their naturalistic setting, and the use of constructs of the participants to structure the investigation (Miles & Huberman, 1994). Robinson, Segal and Sharp (2007) adapted classic ethnographic traditions in order to conduct shorter studies that are more applicable to software-related research. In their series of qualitative studies of software development practice as a social activity, Robinson et al. (2007) used interviews, studying of artifacts (journals notes) and serendipitous observation as data collection tools in the natural setting of
practice. Immersion in the setting of practice was not employed as a research instrument due to time considerations.

This exploration looked into the community of scientific software users in their natural setting of practice, and identified patterns in the interactions of the users with software products and peers but also various other issues that affect their training. Open-ended interviews were utilized as the primary data source so that research findings were delivered in the words of the participants. Secondary data sources included observations of participants in informal scientific software training sessions, as well as reviews of pertinent laboratory software manuals and publications (Hammersley & Atkinson, 1995; Robinson, Segal, & Sharp, 2007). Extended immersion of the researcher in the naturalistic setting of the participants was not feasible due to time considerations.
CHAPTER IV: RESEARCH DESIGN

Introduction

Scientific software training is a field with limited existing research. This qualitative investigation did not seek to test a particular hypothesis on scientific software training; it aimed to explore this field of interest. It is important to emphasize the emergent nature of qualitative research design. The researcher in qualitative research seeks to observe and interpret meanings in context (Patton, 1990; Miles & Huberman, 1994; Turner III, 2010). As such, in this study, new concepts on software training emerged from themes that were generated from the analysis of the data collected.

Grounded theory was employed in this research. Grounded theory is a systematic methodology in the social sciences involving the generation of theory from data (Glaser & Strauss, 1999; Strauss & Corbin, 1998). The strongest cases for the use of grounded theory are in studies of comparatively unexplored areas (Corbin & Strauss, 1990; Strauss & Corbin, 1998; Moghaddam, 2006). The research design of this study included coding of information and constant comparative analysis until saturation of data was achieved. Constant comparative analysis of the data is essential as it allows for the integration of the new and existing information (Bainbridge, 2013). As such, constant comparative data analysis was conducted with a view to constructing a new theoretical training framework grounded in the data collected.
Research Data Collection

This research utilized two types of data in order to attempt to answer the research goals stated above. These included primary and secondary data types. The primary data were derived from conversations with participants during the open-ended interviews. The secondary data were obtained from observations of scientific software users during training sessions, as well as from reviews of published documents and literature that were relevant to the scope of this study. The latter included (but was not limited to) software training manuals, notes kept by students, journals kept by researchers as well as course materials that were complemented by the scientific software applications at the academic institutions of interest.

As mentioned earlier, this research aimed to investigate a particular issue within the community of scientists, i.e. training on the use of scientific software. A wide definition of training was used in this study to avoid bias in the data collection process with respect to any particular type of training method or a special laboratory setting. This research adopted the definition of training by Dearden (1984) because it investigated how dealing with things (scientific software in this case), with people (adult learners-scientific software users), and with change (traditional and distance learning, effective collaborative learning) can influence the learning process within the community of scientific software users and bring about behavioural change, which is a characteristic of comprehensive learning.
Interviews

Patton (1990) stated that there are three basic types of qualitative interviewing for research or evaluation: The informal conversational interview, the interview guide approach, and the standardized open-ended interview. This study employed the informal conversational interview technique, which is an unstructured, open-ended conversation, as primary data collection source, where substantial control was given to the interviewee. The majority of the interviews were face-to-face; two of the interviews were conducted over the phone in order to accommodate the schedules of the respondents. In both cases where interviews took place over the phone, the researcher had previously visited the laboratory facility of the respondents and interviewed other colleagues of theirs. This ensured that the researcher was familiar with the work environment of the respondents prior to the phone interviews.

A general interview guide was used by the interviewer as a means to facilitate the discussions with the participants and engage their interest during the interview with a view to maximizing the outcome of the data collection process. The interview guide was not shared with the interviewee verbatim, in order to avoid influencing their feedback. Specifically, the interview guide was used by the interviewer to prompt conversations into each theme of interest and encourage the respondent to share her/his views. If new topics emerged during the interview, the interviewer freely explored these topics with the research participant’s input. McNamara (2009) and Turner III (2010) indicated that the primary advantage of the general interview guide approach, is that it allows the researcher to afford a degree of freedom and adaptability while maintaining consistency.
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regarding the areas of information that is collected from each interviewee. An example of the interview guide and the prodding questions that were used for this study is provided in Table 1.

Data collection included a focus group that provided input on the emerging results of the interviews. Recurring themes in the data and core categories emerged. The purpose of this focus group was to cross-check the interviews with critique from the target audience, i.e. the community of scientific software users, of this study. The feedback from the focus group was coded as all other pieces of information in this undertaking. As described later in this chapter, four users with various levels of experience were interviewed; two of them were new participants in the study while the two others had provided feedback earlier in the data collection phase. The interviews were open-ended, individual sessions that were arranged as all other interviews in this study; interaction between the four participants was not possible due to their different work schedules.

Hand-written notes were kept by the author during the conversations with the interviewees throughout the data collection, including the focus group interviews. Digital voice recordings were also kept when the interviewees consented to them. The researcher also inquired about secondary sources of data, such as lab journals and software training manuals. The responses of the participants on the secondary sources of data and their assessments on these documents were recorded during the interview process.

Literature in qualitative methodology indicates that even if an interview guide is prepared to ensure that essentially the same information is obtained from each person, in
an unstructured interview there are no predetermined responses (Lofland & Lofland, 1984; Strauss & Corbin, 1998; Patton, 2002; Turner III, 2010). Participants maintain the freedom to introduce the researcher to new aspects of the research topic during the interview. An interview guide for an open-ended, unstructured interview is considered a flexible tool, as the researcher may add or exclude questions, depending on the interviewees’ feedback and interest in sharing their views. In this manner, efficient use of limited interview time is ensured; also, interviewing multiple subjects can be more systematic and comprehensive; and interactions are kept relatively focused on the research topic (Berg, 1998; Lofland & Lofland, 1984). An open-ended, unstructured interview requires that the interviewer often probes for richer responses or ensures that all topics at hand are covered in the conversation (Turner III, 2010). As such, the interview guide includes prodding questions for each theme (Table 1). A potential limitation of this interview type is that there are no predetermined responses, with the result that comparing or analyzing data can be challenging.

The interview guide for this research study was divided into two main sections: a) The profile of the participant, and b) the main research question with the open-ended questions. The profile section included the socio-demographic characteristics of the participants such as education level and work experience, age, gender, and country of origin. The open-ended questions focused on the participants and their background regarding scientific software usage as well as their experiences with traditional and distance training techniques on such software.
Table 1. Interview Guide: Open-ended interview guide with prodding questions that were used by the interviewer.

<table>
<thead>
<tr>
<th><strong>Participant Profile</strong></th>
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</thead>
<tbody>
<tr>
<td><strong>Participant #:</strong></td>
</tr>
<tr>
<td><strong>Location:</strong></td>
</tr>
<tr>
<td><strong>Name:</strong></td>
</tr>
<tr>
<td><strong>Gender:</strong></td>
</tr>
<tr>
<td><strong>Age:</strong></td>
</tr>
<tr>
<td><strong>Level of Education:</strong></td>
</tr>
<tr>
<td><strong>Years of Experience:</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Research Question</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>“What software training approaches in a blended learning environment are chosen by users whose goal is to accurately apply scientific software to questions of research?”</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Guiding Themes and Prodding Questions</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Could you walk me through a typical day in your work that involves using scientific software?</td>
</tr>
<tr>
<td>b) Can you tell me about the last time you sought and obtained help with a problem regarding the software you are using?</td>
</tr>
<tr>
<td>c) Can you describe your collaboration with colleagues regarding scientific software?</td>
</tr>
<tr>
<td>d) Can you tell me about the scientific software training you have received in your career?</td>
</tr>
<tr>
<td>e) Do you use a training manual to answer your questions on the software? Is it helpful?</td>
</tr>
<tr>
<td>f) Can you give me an example of scientific software training? What would you do differently?</td>
</tr>
<tr>
<td>g) What was the most interesting issue in your training?</td>
</tr>
<tr>
<td>h) What was your best/worst training experience?</td>
</tr>
<tr>
<td>i) Have you received software training in-class or by distance? How would you describe it? Was it helpful?</td>
</tr>
<tr>
<td>j) Would you prefer in-class or distance/blended training methods? Why?</td>
</tr>
<tr>
<td>k) Describe how you exchange knowledge/ideas with your colleagues regarding software use.</td>
</tr>
<tr>
<td>l) Describe any distance learning methods that you use to collaborate with your peers with respect to scientific software.</td>
</tr>
</tbody>
</table>
Interviews - Data Collection Strategy

Snowball sampling (also referred to as chain sampling) was employed in this research study in order to establish an initial pool of potential research participants. Snowball sampling can be defined as a technique utilizing well informed people to identify other informants who have a great deal of information about a phenomenon (Strauss & Corbin, 1998). Specifically, this sampling technique is used for identifying research respondents where one respondent gives the researcher the name of another potential respondent, who in turn provides the name of a third, and so on. This technique was suitable for the purposes of this investigation which had an exploratory, ethnographic nature (Berg, 1998; Atkinson & Flint, 2001). Snowball sampling is also used to overcome the problems associated with studying concealed or hard-to-reach populations; that is, groups that are small relative to the general population, and for which no exhaustive list of population members is available (Berg, 1998). The community of scientific software users has been described in the literature as “protective” of their research ideas, laboratory practices and publication domains and, thus, it can be considered a hard-to-reach population (Hannay et al., 2009). By applying snowball sampling, the researcher in this study took advantage of the social networks of identified respondents in order to obtain a series of referrals within a circle of acquaintances to create an ever-expanding set of potential contacts.

With respect to the ethical implications associated with snowball sampling, while participants may refer others to this project, the researcher did not solicit the names of those potential participants from them. The researcher asked participants to mention this
study to others and provide the contact information of the researcher (included in the Letter of Information of the REB Application) to them. When potential participant were interested, they could then contact the researcher directly. At that time, the researcher responded to their inquiry by sending them the Letter of Information, informing them about the research participation criteria, or -if they already had that information- coordination regarding the interview details took place.

Theoretical sampling is a key feature of grounded theory (Glaser & Strauss, 1999). Theoretical sampling is linked to the purpose of generating and developing theoretical ideas and has a recurrent characteristic: at various times during the development of the study, the researcher must ask what environments, people etc. it would be meaningful to direct the research towards next, in order to develop and strengthen aspects of the emerging theory. However, Cohen et al. (2007) pointed out that occasionally the research issue governs the extent of the sampling process. In such cases, the researcher seeks to obtain information from selected people and their environment (organizations, settings, records etc.), as she is interested in exploring specific issues. Consequently, the size of the data may be fixed or the number of selected people to whom the researcher has access to may be set. This finding by Cohen et al. (2007) describes the situation of this investigation.

As such, due to the number of available respondents for this study, purposive sampling was employed in lieu of theoretical sampling (which normally requires larger sets of data) during the data collection process. Previous research studies have successfully combined purposive sampling with a grounded theory design in order to collect rich, yet sufficient data for theoretical adequacy (Frazier, 2006; Bainbridge,
The primary concern regarding employing purposive sampling is to obtain rich information from those who are in a position to provide it (Miles & Huberman, 1994; Cohen et al., 2007). This technique may be employed if the analysis of the research data reveals information about particular training issues that need further exploration during the course of this study; as such, purposive sampling was applied in order to obtain input from respondents with substantial experience in scientific software usage and specific training issues (Cohen et al., 2007).

As this was an exploratory qualitative study, the data collection ceased when it was decided that the richness of the information gathered could support the formation of main categories and themes. The participants at that time had reached twenty (20 participants in total). Mason (2010) argued that a number of issues can affect sample size in qualitative research; however, the guiding principle should be the concept of saturation. Strauss and Corbin (1998) indicated that a category is considered saturated when further data analysis does not reveal new information; in other words, when no new dimensions, actions/interactions, or consequences are seen in the data. Guest, Bunce, & Johnson (2006) suggested that, generally, 15 interviews is the smallest sample size in qualitative studies.

Further, the researcher was required to ensure that the sample size was large enough to saturate the emerging categories and themes so that new data would not cause the theory that was generated to be altered (Cohen et al., 2007). In order to sufficiently ground the results of this study in the research context, the researcher ensured theoretical adequacy and ability to check emerging themes with further data by maintaining access
to the participants and their information throughout the research study, in case further information needed to be collected.

**Interviewees-Selection Process**

The criteria for identifying the research study participants included education level and work experience in the sciences and engineering, as well as their background in using scientific software. The criteria for identifying participants for the study were:

1. Experience with scientific software usage.
2. Experience with academic research involving the usage of scientific software in science and engineering.
3. Experience with industry applications regarding scientific software usage in science and engineering.

These inclusion criteria were explicitly stipulated in the Letter of Information that was provided to potential participants, according to the Research Ethics Approval obtained for this study. Regarding the justification of the inclusion criteria, this research focused on investigating scientific software users’ experiences with respect to training for accurate application of this type of software. As such, the data collection involved open interviews where the participants would be invited to share their experiences with scientific software training and usage. Thus, the participants would have to have some knowledge about using scientific software. The distinctions “senior”, “junior” or “experienced” users were given by the respondents themselves when they were asked to comment on their own experience levels during the interviews.
The recruitment of participants was facilitated through a network of established professional links with academics and industry professionals who use scientific software as part of their daily routine. Participants in this study were initially sought within academic institutions and industry in Canada as well as internationally. Approximately 90 potential respondents were approached in total, throughout the data collection phase. Eventually, only respondents from Canadian institutions and industry were available to provide feedback to this study at the time when the data collection occurred. The participants had a range of knowledge and experience. Further, the participants were selected from various science and engineering labs; i.e. not only from fields such as geology, chemistry or environmental engineering where the researcher of this study has experience working within. This was sought in order to enhance the quality of the research (and its potential authenticity) and represent the views of various scientific software users without preconceptions.

Specifically, the recruitment of respondents for this study followed a two-layered strategy. Firstly, natural sciences and engineering computational laboratories in public university institutions, government-funded scientific research agencies and laboratories, scientific software companies, geological exploration companies, private technical consulting companies, and private scientific research laboratories were approached via e-mail with a view to identifying potential participants. The names and contact information of the institutions and companies that were contacted were found from conference websites (from the lists of sponsors and participating companies), university laboratory websites, government sites, professional networks, venues organized by professional associations and industry as well as webinars organized by scientific
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software companies, journal papers, scientific magazines, and software training manuals. The e-mails that were sent by the author to the agencies mentioned above contained the Letter of Information (and inclusion criteria) about the study.

This first snowball sampling attempt to recruit participants was successful and the first round of interviews was arranged and conducted. During each of those interviews, the author requested the respondents to share her contact details and Letter of Information with other scientific software users (either in-person or via e-mail) that the respondents may have known.

As the data collection progressed, new knowledge-rich respondents with substantial experience in scientific software application were sought; as such, purposive sampling was employed after the initial data analysis and formation of categories in order to expand on or informing the initial data gathering. During this second layer of recruitment (purposive sampling), the author contacted via e-mail several research agencies, laboratories and private industry (consulting companies and software companies) that she believed had rich knowledge about scientific software applications based on the feedback from the first group of respondents. The information about these research agencies and laboratories were found in literature and training manuals that were discussed by the participants during the first round of interviews. As well, the analysis of the initially collected feedback determined the course of action during the purposive sampling phase; techniques to strengthen the credibility of the study, such as respondent validation (discussed later in this chapter), were carried out during this stage of the data collection. The second recruitment attempt also resulted in a collection of new data; during each interview, the author continued on encouraging the respondents to
inform other potential interviewees about the study, based on the inclusion criteria mentioned above.

This study took into consideration the importance of conducting the interviews in a familiar setting where the participants would not feel restricted or uncomfortable to share information (Strauss & Corbin, 1998; Berg, 1998; Turner III, 2010). Female and male scientific software users were interviewed; the ratio was determined only by the availability and willingness of each respondent to participate in the study. The researcher of this investigation did not purposefully seek to interview equal numbers of male and female users as this was not within the scope of the study. In total, nine women and eleven men participated. Further, the age of the participants varied from 20 to over 55 years old.

As mentioned earlier, information about cultural, gender, age, ethnicity or social status differences were not taken into consideration in the data analysis in order to avoid influencing the results of the study.

Field Observations

Unstructured observation is a common ethnographic approach as a part of field research (Cohen et al., 2007; Barton, 2001). Unstructured observations are hypothesis-generating rather than hypothesis-testing (Cohen et al., 2007). In this research study, unstructured, informal observations on scientific software training took place in natural sciences and engineering computational laboratories at academic institutions and consulting companies in Canada.
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These observations were conducted during the interviews with research participants and involved the reviews of laboratory manuals and software online documentation and other training material (such as online tutorials) by the interviewees. In conjunction with coding and analyzing research data collected from the interviews and subsequent generation of categories and themes, the researcher also observed and took field notes on laboratory group activities, such as informal scientific software training sessions, in the working environment of the participants. The notes that were taken during the observations were subsequently analyzed and compared with the data collected during the open-ended interviews.

Pertinent literature has indicated that observation can lead to deeper understandings than interviews alone, because it provides knowledge of the context in which events occur, and may enable the researcher to see things of which participants are not aware, or that they are unwilling to discuss (Patton, 1990; Strauss & Corbin, 1998).

**Reliability and Validity Strategies during Data Collection**

The integration of strategies that ensure reliability and validity is required in a qualitative research design. Qualitative researchers, in general, have adhered to the list of five criteria developed by Lincoln and Guba (1985) as well as Guba and Lincoln (1989) towards evaluation for trustworthiness (a parallel concept to reliability and validity) in qualitative research. These criteria include: (a) credibility, (b) dependability, (c) transferability, (d) confirmability and (e) authenticity. However, these criteria by Guba and Lincoln (1989) referred primarily to the evaluation of a qualitative research
study after its completion – also known as post hoc evaluation (Morse, Barrett, Mayan, Olson, & Spiers, 2002). The post hoc evaluation techniques for this investigation are discussed in the following sections of this study (Data Analysis). Ensuring rigor in a qualitative research study during its development is equally crucial (Morse et al., 2002). As such, the research design of this study incorporated strategies for reliability and validity checks during the course of the investigation. It is noted here that, due to very limited literature on scientific software training methods, the author obtained theoretical background knowledge during the research, which increased the credibility of the study (Miles & Huberman, 1994). Glaser and Strauss (1999) indicate that there is no need to review any literature of the studied area before entering the field, and this is in line with this research.

A strategy to achieve reliability and validity for this investigation was the ongoing analysis of the data collected which subsequently directed the research path and specifically the application of the purposive sampling technique (selection of participants and interview themes/questions). Categorizing and comprehending (or “listening to”) the data can influence the course of the investigation and enhance the quality of the research as well as its replication and confirmation (Glaser & Strauss, 1999). A second reliability and validity strategy was to include the interview of the researcher of the study in the data collection; in this manner, the researcher confronts her opinions and preconceptions and can compare them with the views of the actual participants. A third strategy to ensure the validity of the data was to employ respondent validation; in this technique, a comparison between the accounts of different participants differently “placed” in the same lab or work environment was conducted and the emerging themes from the coding
of the data was be tested accordingly (Rajendran, 2001; Cohen, Manion, & Morrison; 2007).

Further, the ongoing development of sensitivity and flexibility of the researcher with respect to the emerging themes from the data collected was also an important parameter in the study, as this can enhance the verification process during an investigation (Berg, 1998).

**Termination of Data Collection**

The flexible nature of qualitative research requires that the researcher sets guidelines to determine when to stop the data collection process. The decision to stop sampling must take into account the research goals, the need to achieve depth through triangulation of data sources, and the possibility of greater breadth through examination of a variety of data sources. Further, the criteria for termination of data collection may include: (a) exhaustion of resources; (b) emergence of regularities, and (c) overextension, or going too far beyond the boundaries of the research (Hoepfl, 1997).

The data collection phase of this research concluded when emergence of regularities in the data became evident and the new data did not give any new information to the existing categories. As discussed earlier, termination of data collection and analysis occurs when saturation is reached. Strauss and Corbin (1998) wrote:

> Saturation is more a matter of reaching the point in the research where collecting additional data seems counterproductive; the “new” that is uncovered does not add that much more to the explanation at this time. Or, as is sometimes the situation, the researcher runs out of time, money or both” (p. 136).
Data Analysis

This section describes the analysis of the data collected during the interview process, the observations as well as the review of secondary sources of information, which included reviews of scientific software manuals, laboratory documentation, online resources on software training and training material provided by software companies in addition to manuals. During the data collection phase, an open and axial coding system of the information collected through interviews was employed. Documentation of coding and writing of memos provide a means of dependability and ability to confirm the research design because it functions as an audit trail back to the sources of the research results and conclusions (Frazier, 2006). In grounded theory, open and axial coding are two types of data analysis that allow for exploration of the data collected and identification of units of analysis to code for specific issues (open coding) as well as interconnectedness of categories and themes, i.e. axial coding (Corbin & Strauss, 1990; Saldana, 2008). Emerging trends and/or patterns in the data were identified and further illustrated in diagrams and matrices. MS Office Excel spreadsheets were used for the organization of the data. As the main categories emerged from the information provided by the participants, selective coding was used to identify overarching themes in scientific software training. Selective coding is employed after core categories and concepts have been identified in the data (Corbin and Strauss, 1990; Saldana, 2008).

This study employed a key feature of grounded theory, the constant comparative method, to identify categories and relationships that exist among the data and generate concepts. The constant comparative method requires that the researcher compares each
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piece of data with data previously analyzed in all groups that have emerged (Glaser & Strauss, 1999; Cohen et al., 2007; Frazier, 2006; Bainbridge, 2013). As categories begin to form, each piece of information falls into a specific category. This method places relevant data, which contribute to a common idea, into categories that through integration and delimitation create concepts (Glaser & Strauss, 1999). This process may allow for relationships to surface and assist in defining and understanding the new concepts as revealed by the data. The emerging concepts were therefore developed with supporting facts from interviews and documents collected throughout this investigation.

Data Analysis Examples

As discussed previously, this study explored training practices for scientific software application. This section includes two examples of how the data analysis occurred with respect to examining onsite/online learning training practices and user learning skills in respondents’ accounts:

- Onsite Learning - Data Analysis Example

In the following excerpt from the interview data, pieces of text that refer to issues associated with onsite learning are highlighted. During one of the interviews with research participants, the interviewer said, “Tell us about your experiences with respect to learning from your mentors or supervisors in university or industry”. The interviewee, a graduate student, responded:

Every lab I have seen is different. Where I worked before, the supervisor sat there with me and showed me the basics. It is easy to ask questions when somebody is near. Some people might be shy, I just ask my lab mates, but if you cannot find the answer on your own, the best way is to find someone who knows.
The following Table (Table 2) summarizes a data analysis example with linkages between the respondent’s account and onsite training.

Table 2. Data Analysis Example with respect to Onsite Training.

<table>
<thead>
<tr>
<th>Text Excerpts</th>
<th>Elements of Onsite Training</th>
</tr>
</thead>
<tbody>
<tr>
<td>“Every lab I have seen is different”</td>
<td>Emphasis on the environment in which the learner operates.</td>
</tr>
<tr>
<td>“...it is easy to ask questions when somebody is near”.</td>
<td>Learning from one another via instruction, imitation and modeling.</td>
</tr>
<tr>
<td>“Where I worked before, the supervisor sat there with me and showed me the basics”</td>
<td>Relationship of the learner with the mentor – positive learning experience.</td>
</tr>
<tr>
<td>“Some people might be shy, I ask my lab mates...”</td>
<td>Motivation of learner is enhanced due to the social aspect of the learning process.</td>
</tr>
</tbody>
</table>

- User Learning Skills Data Analysis – Example

In the following excerpt from accounts of respondents, pieces of text that may refer to the learning skills of the user are highlighted. During one of the interviews, the interviewer asked, “How do you see your role as a mentor in this lab?” The interviewee responded:

I feel it is mostly up to them, if they are motivated, they will learn. And if they want to do some research, (…) they ask, they know that they are in the driver’s seat, they want to know.

The following Table (Table 3) summarizes a data analysis example with potential linkages between the respondent’s account and learning skills.
Table 3. Data Open Coding Example with respect to User Learning Skills.

<table>
<thead>
<tr>
<th>Text Excerpts</th>
<th>Open Coding</th>
</tr>
</thead>
<tbody>
<tr>
<td>“if they are motivated, they will learn”</td>
<td>Goal oriented learner</td>
</tr>
<tr>
<td>“But if they want to do some research… they ask, they want to know”</td>
<td>Learner is internally motivated and self-directed.</td>
</tr>
<tr>
<td>“they are in the driver’s seat”</td>
<td>Self-directed learning.</td>
</tr>
<tr>
<td>&quot;If they are serious about it…”</td>
<td>Internally motivated and self-directed.</td>
</tr>
</tbody>
</table>

Figure 4 shows a summary of a coding scheme that was derived during the data analysis of this study. The first categories to be created had to do with topics related specifically to the background and academic preparation of the user (e.g., type of knowledge, ability of the user to comprehend the research problem at hand) and their training needs.
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Codes | 1st Level Categories | 2nd Level Categories
--- | --- | ---
Background of the User | Explicit Knowledge | Level of Explicit Knowledge
Adequate Resources Available | Prearranged Knowledge | Level of Explicit Knowledge
User-Software Developer Interaction | Collaborative learning | Established Access to Community of Practice
Knowledge Flow from Peers | | 
Peer Collaboration | | 
Community Knowledge Sharing | | 
Support/Collaborative Learning | | 
Face-to-Face Mentoring | | 
Online Community Sharing | Reaching out to Peers locally & internationally/Use of technology | 
Vicarious Learning | Embedded Knowledge | Level of Assumed Knowledge
Experiential Learning | | Ability to Validate Software Output
Level of trust in peer-reviewed publications | Validation of Software Output | 
Need to Test Software Output | | 
User-initiated system of “Checkpoints” | Comprehension of Research Problem at Hand | 
Familiarity with Problem at Hand | Identification and Management of Risks | Ability to Identify, Assess and Manage Risks related to Inaccurate Use of Software
Understanding of Risks related to Inaccurate Use of Software

Figure 4. Example of Coding Scheme.
Reliability and Validity Strategies during Data Analysis

As mentioned earlier, qualitative researchers, in general, have used five criteria that were developed by Lincoln and Guba (1985) as well as Guba and Lincoln (1989) towards evaluation for trustworthiness (a parallel concept to reliability and validity) in qualitative research. These criteria include: (a) credibility, (b) dependability, (c) transferability, (d) confirmability and (e) authenticity. These criteria are defined below:

- **Credibility**: The credibility criteria involve establishing confidence in the truth of the data and interpretations of them. A credibility strategy for this study involved member checking at the end of the data analysis. Member checking entailed the presentation of data, analytic categories, interpretations, and conclusions to scientific software users from whom the data were originally obtained in order to test or verify their meaning. For this credibility check to occur, the researcher ensured access to the participants and their information throughout the research study. Credibility of the study was also enhanced by ensuring that interview notes and transcripts were close to "verbatim" accounts of what transpired during the interview or observation session. In addition, the researcher of this study maintained a bank of detailed, comprehensive field notes that also supported the data analysis process and accurate, trustworthy representation of the situation at hand.

- **Dependability**: This criterion refers to the consistency of the research findings, the stability of data over time and over conditions. A dependability strategy for this study involved data triangulation, as described in detail in the following
section. This strategy allowed for the conceptual linkages in the research findings to be further refined, broadened and strengthened; it also added an elevated degree of cross-checking and validation of the data (Berg, 1998).

- **Transferability:** This criterion refers to the applicability of the research study to other contexts. A transferability strategy for this study involved maintaining detailed field notes that helped depict the context that the data collection occurred within, as well as extensive descriptions of the steps taken to enhance the quality of the study. The author in this study enhanced transferability by describing in detail the research context of this investigation.

- **Confirmability:** This criterion refers to the degree to which the results could be confirmed or corroborated by others. A confirmability strategy for this study involved other researchers (in the fields of science/engineering as well as in education) taking a "devil's advocate" role with respect to the research findings; the feedback from this process, which was repeated at least five times throughout the data analysis, was documented and incorporated in the study. This strategy involved the detailed documentation of the research procedures for checking and rechecking the data throughout the study. For this purpose, one of the two thesis supervisors were consulted routinely during the data collection and analysis processes within grounded theory methodology. Also, the researcher of this study was able to maintain access throughout the data collection phase to participants with different roles within a research laboratory or facility (mentor/supervisor, graduate student, young professional in industry) and asked each one of them, in different occasions, to comment on the emerging results of
the study during the data collection phase. All of these participants were employed in Canadian institutions/companies and were consulted at least once about the emerging themes of the study in addition to their initial open-ended interviews.

- Authenticity: This criterion is demonstrated if researchers can show that they have represented a range of different realities fairly and faithfully. Authenticity also refers to the level to which a “more sophisticated” understandings of the phenomenon being studied is developed (“ontological authenticity”), the fair representation of viewpoints of various people in different roles (“educative authenticity”), the stimulation of some form of action (“catalytic authenticity”), and the empowerment of interested parties or research participants to act (“tactical authenticity”). An authenticity strategy for this study involved audio-recording and verbatim transcribing or keeping very detailed notes of the feedback of the participants during the interviews. Additionally, reflective journaling (or memoing) was employed during the data analysis in order to accurately depict different realities and levels of understanding of the data collected. Reflective journaling or memoing was also used throughout the study as a tool to record ideas about the emerging themes and relationships between categories.
Triangulation

Triangulation is a method used by qualitative researchers to check and establish validity in their studies by analyzing a research question from multiple perspectives. As discussed previously, validity, in qualitative research, refers to whether the findings of a study are true and certain—“true” in the sense that research findings accurately reflect the situation, and “certain” in the sense that research findings are supported by the evidence (Strauss & Corbin, 1998). Triangulation can assist in eliminating biases, and it allows for a degree of cross-checking and validating the data (Berg, 1998).

In this study, data triangulation was employed as a post hoc strategy to enhance the quality and verification of the investigation. Data triangulation involved producing a set of themes and taking it across different sources of data in order to increase the validity of a study (Miles & Huberman, 1994; Berg, 1998). In this study, triangulation was conducted by using: (a) the primary source of data (data from the open-ended interviews and field notes from interview sessions with participants that included observations of scientific software usage/training activities), (b) the secondary sources of data (field notes from observations during the interviews as well as reviews of training manuals, relevant publications and laboratory manuals) and (c) the focus group feedback that were collected when reoccurring themes were identified in the research data. The realization of this particular triangulation strategy was possible during the data collection when it became apparent that there were available participants with in-depth understanding of scientific software usage that could provide feedback at the later stages of the study.
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A small group of interviewees functioned as ‘focus group’ and was used to cross-check emerging themes and research results from the data sources in this investigation. This technique is a means of listening to people's views on a specific area of inquiry in a non-threatening setting (Berg, 1998; Hendry, 2011). This practice was particularly suitable for this investigation on scientific software training; focus groups are particularly used when the subject of study is little understood (by researchers) or infrequently discussed in day-to-day life (Hendry, 2011).

For the purposes of this investigation, a focus group was conducted with available participants during the later stages of the data collection when the axial coding processes had revealed reoccurring themes in the data and core categories were being formed. Efforts were made to have a mix of new and “old” participants with a view to cross-referencing ideas without preconceptions (i.e. avoiding simply repeating opinions of previous interviewees in the study) but this also depended on the participants’ availability.

As such, four participants were asked to comment on the findings of the study; two professional users with over five years of experience in scientific software, and two graduate students. Two of them, the professional users, were new interviewees and were interviewed in-person while the two others (the graduate students) were respondents who had already contributed to the study earlier in the data collection and were willing to provide further feedback over the phone on the emerging trends of the investigation. The focus group members were interviewed individually, in an open-ended interview as all other participants of this study. The focus group members did not interact with one another, as this was not feasible due to their different schedules. The notes that were
taken during these interviews were analyzed and compared with the rest of the data in this study. The focus group was not used as the “litmus test” in order to discredit or strengthen a certain emerging theme; the participants were given the opportunity to provide their feedback on current training experiences in addition to commenting on the emerging training framework of this investigation.

The technique that was followed for the focus group in this study stemmed from the work by Reid and Reid (2005), as well as Zwaanswijk and Dulmen (2014). In these studies, the focus groups that were conducted did not involve face-to-face discussions; instead, online platforms were used, in a synchronous or asynchronous manner, where respondents were invited to post their responses and read others’ feedback. The focus group in this research was conducted in a manner similar to what is described below by Zwaanswijk and Dulmen (2014) who conducted a study on online focus groups (OFGs):

The OFGs were conducted in an asynchronous form, i.e. participants could read others’ comments and could respond at any time, not necessarily simultaneous with someone else’s participation (p. 3).

The main difference in this study was that the participants' responses were not posted on a website because the interviewees preferred not to post online their concerns about their own software training or problems about the scientific software products that they were using. As such, their individual responses were recorded in the author’s notebook; this feedback was de-identified and shared with each one of the four participants in every focus group interview. After the fourth interview, the author contacted the participants again, individually, and offered them the opportunity to comment on the contributions from all of the other focus group members.
The purpose of including the focus group in the research design was to take the results of the study back to the community of scientific software users after reaching several preliminary conclusions through systematic data analysis. In an interview setting, gathering the impressions and feedback of the focus group on the results functioned as a means of checking and cross-referencing the research findings to ensure that they make sense to the scientific software users themselves. The focus group interview data were coded, analysed and compared with the results from the primary and secondary sources of data (individual interviews, observations and software training documents).

In order to sufficiently ground the results of this study in the research context, the researcher ensured theoretical adequacy and ability to check emerging themes with further data by maintaining access to study participants and their information throughout this research undertaking, in case further information needs to be collected.

**Ethical Considerations**

As humans are the research instrument of this study, certain ethical safeguards were introduced. First and foremost, the necessary steps were taken to ensure the privacy as well as the safety of the participants. Consent and confidentiality were also taken into consideration in order to protect the participants. All necessary details about the aim and purpose of this research were available to the participants so that they saw the significance of this study, their vital role in it and, hence, felt comfortable to provide their information. The respondents were free to withdraw from the study at any time. The
confidentiality of the participants was also ensured by keeping all participants anonymous and protecting their personal information in the research. The above mentioned ethical safeguards were included in a Consent Form that was distributed to potential participants in order to inform them about the conditions of their participations and obtain their consent.

In order for this study to be realized, a Research Ethics Approval was secured by the Research Ethics Board at Athabasca University (Appendix B). The data collected were stored in the manner outlined in the Research Ethics Approval and Consent Form (Appendix C).

**Role of Researcher**

The researcher in a qualitative study is the instrument of both data collection and data interpretation. A qualitative strategy requires personal contact with the people and environments under investigation (Patton, 1990). Hoepfl (1997) identifies the characteristics that make humans the "instrument of choice" for naturalistic inquiry:

Humans are sensitive to environmental cues, and able to interact with the situation; they have the aptitude to collect information at multiple levels simultaneously; they are able to observe situations holistically; they are able to process data as soon as they become available; they can provide immediate feedback and question interpretation of research data; and they can explore unforeseen responses (p. 50).

The researcher’s role may be characterized by “theoretical sensitivity”, i.e. the ability to give meaning to the data and distinguish important contributions from participants as opposed to irrelevant ones. Strauss and Corbin (1998) suggest that a researcher may acquire theoretical sensitivity through professional experiences, personal
experiences as well as by becoming familiar with professional literature and other content-rich sources. The researcher of this investigation has experience in using scientific software within science and engineering laboratory settings in Canada and internationally. Further, she has first-hand experience on training matters and knowledge exchange techniques regarding scientific software usage, resulting in a potentially increased “theoretical sensitivity”.

Consequently, with respect to reducing the prospective of researcher bias in this study, unstructured and open-ended interviews were conducted, allowing the interviewees’ own experiences to shape the direction of the interviews. No information about the interviewees or their software was exchanged before the interviews, thus there was no means to bias the interviewees, even on a subconscious level. Further, Strauss and Corbin (1998) suggested adopting comparative thinking and obtaining multiple viewpoints of a situation as techniques for controlling intrusion of bias. As such, one of the techniques to eliminate bias in this study was to record field notes that contain reflections on the researcher’s own prejudices. Literature has indicated that consideration of self as a researcher and in relation with the topic of the study is a precondition for coping with bias (Rajendran, 2001). A second technique for the researcher was to have her notes reviewed/critiqued by the thesis supervisor and colleagues for an additional filter on bias. This technique was employed at least five times at different stages during the study. Further, as literature indicates, other practices were employed such as using a two-column field note-taking technique (one with the transcription of the audio-recording and one with comments and the researcher’s reflection on the interview information), keeping analytic notes (memoing) during the
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careful reading of the transcribed data, as well as on the training manuals or lab notes used by software users. These practices substantially helped to protect the study against researcher bias and avoiding rejection of vital data. These techniques also steered the researcher towards accepting and cross checking the new data without prejudice, doubts, and expectations.

In addition, the role of researcher included demonstrating project management skills in order to make efficient use of resources and time towards the completion of the project. Finally, it was also the responsibility of the researcher to ensure that the direction of the research remains within the framework of the research design at every stage of the investigation, and to check and cross-reference actual research findings.
CHAPTER V: RESULTS

Introduction

This section includes the findings of this study. In total, 20 research respondents participated in the study. As described in the Methodology Chapter, the data analysis commenced during the data collection and continued with selective coding after the saturation of the emerged categories. Specifically, this section presents the trail of the results, as they emerged from the investigation. The core categories pertain to the following:

1. Current training practices adopted by the community of scientific software users, based on descriptions provided by research participants as well as reviews of secondary data,

2. Knowledge sharing strategies that are employed within research laboratories for staff training on scientific software application, as well as various factors that affect these strategies, and

3. Main components that affect current scientific software training, as reported by study participants.

Each of these categories has subcategories that are analysed in their respective sections. This trail of categories (and subcategories) leads to two main themes. Firstly, the Systematic Scientific Software Training Cycle, which is based on the analysis of the information on current training approaches that constitutes each category. The Training Cycle informs a new framework, the Scientific Software Training Framework, which is
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the other main theme of this investigation and emphasizes the overarching blended learning environment of the Systematic Scientific Software Training Cycle.

Current Training Practices

This grounded theory study revealed several different ways that users satisfy their training needs on scientific software. These results stem from the analysis of the interview and focus group data as well as the reviews of secondary data sources, such as scientific software websites, their online documentation, and the laboratory manuals.

In total, 13 scientific software products were reviewed in terms of their training tools. Four of the software companies provided the scientific software manuals upon purchase of the product. Nine of them offered online video tutorials, demonstrations and resources in addition to the product manual. Six of them offered in-classroom training to users and a suite of solved, generic examples in their online libraries. Two of them had research publications using their software product on their website. Each software product had specific strengths and limitations that could be revealed only by its application on particular research problems. The online resources as well as the manuals offered by the software companies were discussed during the interviews with the respondents with respect to their usefulness and levels of updated information.

It is noted here that the respondents included users who had the ability to write code and build a numerical model as well as users who only applied the software without interfering with its code. Also, the respondents used a wide variety of software products in sciences and engineering. As such, this study focused on the training/learning needs
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of scientific software users in general, not on a specific type of software or a specific
computing skill. Various methods of training were mentioned by the participants. A
major observation from the data is illustrated in the following statement made by a
participant: “Understanding is more important than ease of use”.

Regarding current training practices, the results illustrated that there were users
who were self-taught by primarily using software company website documentation and
other relevant online asynchronous resources – without significant online/onsite peer
support and feedback. Further, there were users who had the opportunity to sit side-by-
side with a more experienced colleague and learn the basics of the software product of
their interest before they explored by themselves in order to expand their abilities as
users. In addition, there were users who were introduced to the basic principles of the
software product of interest by their work supervisor before they were expected to work
on their own. These users reported that they often felt intimidated to ask questions or
seek clarifications because of the experience gap between themselves and their
supervisor/mentor. Lastly, there were users who reported that they learned their software
in a collaborative learning environment with peers at similar levels of experience and felt
comfortable asking questions about the software freely. The following Table (Table 4)
depicts the various training techniques employed by scientific software users, as these
were described by the research participants. Table 4 also includes comments that
describe the feedback provided by the participants on each specific technique.

<table>
<thead>
<tr>
<th>Training Technique</th>
<th>Participation Rate</th>
<th>Advantages</th>
<th>Disadvantages</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Onsite Tutorials</td>
<td>4 out of 20</td>
<td>Proximity</td>
<td>Expensive, “packaged” lecture</td>
<td>No participants’ preparation beforehand.</td>
</tr>
<tr>
<td>Onsite Documents</td>
<td>20 out of 20</td>
<td>Availability</td>
<td>Outdated</td>
<td>Reiteration of ‘assumed’ knowledge</td>
</tr>
<tr>
<td>Online Documents (incl. Wikis)</td>
<td>15 out 20</td>
<td>Current Information, flexible access</td>
<td>Issues with trust and reliability of information sources</td>
<td></td>
</tr>
<tr>
<td>Online Tutorials</td>
<td>17 out of 20</td>
<td>Free, Updated</td>
<td>Inflexible, generic material</td>
<td></td>
</tr>
<tr>
<td>Onsite Mentor</td>
<td>8 out of 20</td>
<td>Proximity</td>
<td>Intimidation</td>
<td>Lack of Mentor preparation on constructive feedback techniques</td>
</tr>
<tr>
<td>Onsite Peer</td>
<td>18 out of 20</td>
<td>Immediacy, lower anxiety levels</td>
<td>Propagation of wrong information</td>
<td></td>
</tr>
<tr>
<td>Online Mentor</td>
<td>6 out of 20</td>
<td>Different perspective, Flexibility in communication</td>
<td>Trust Issues, Mentor ‘removed’ from trainee</td>
<td>Protection of ownership of ideas limits knowledge sharing and critical review of work</td>
</tr>
<tr>
<td>Online Peer</td>
<td>9 out of 20</td>
<td>Flexible Access</td>
<td>Reliability of Exchanged Information, Trust Issues</td>
<td>When exchanged information/feedback is reliable and trust in peer collaboration is established: Validity of research results is enhanced by constructive input from peers with no invested interests</td>
</tr>
</tbody>
</table>
In Table 4, an onsite mentor is someone with substantial experience on the use of scientific software products and with whom the software trainee can consult in their physical work environment. An online mentor can be a scientific software developer who offers support and advice to a new user. An onsite peer can be a colleague or fellow graduate student with equal or slightly higher experience in scientific software who works in the same physical environment with the trainee and they frequently exchange feedback on the application of the software. An online peer can be a software user who contributes to an online forum about a particular scientific software product.

As can be seen in Table 4, onsite tutorials usually offered by software companies have not been a preferred mode of training due to cost considerations as well as the “packaged” training material offered by software developers who may not be aware of the various specific applications of their software product. As Participant 02 stated: “I have not really experienced formal training. It is expensive. The software company has seminars, to promote their software, sometimes I find these seminars online, but it is not as if you had someone talking to you about specific things”.

Six respondents mentioned that if the tutorial materials had become available to them beforehand, then perhaps they would have been able to review and add their questions in order to make better use of the time with the trainee. As Participant 15 mentioned: “We were not prepared. They gave us a generic presentation on what the software does but there was not enough time for all of us to ask questions on particular problems with the software”.

Online documentation includes software website information and support tools that are available to users for troubleshooting purposes, along with wikis that are
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developed by other users and are available on the internet. From the analysis of the
references made by the respondents, the onsite peer support is crucial at the beginning
stages of the training. As training progresses, the user may explore the online resources
more independently and with a higher ability to critique the reliability of the information.
While an onsite mentor can be useful to a new scientific software user in the sense that
he/she can effectively direct the trainee, study participants commented on having high
anxiety and intimidation levels because often the mentor was also their evaluator (work
supervisor or university faculty). Participant 03 (a graduate student) mentioned: “If you
are nervous, if you feel that you do not understand the problem enough to ask a
question… if you work in a place where everyone is a senior software developer and they
do not have time to answer questions. It is difficult”. Another respondent, Participant 14
(a laboratory supervisor) said: “Everyone who comes in is expected to program in the
language they signed up for…some people look for someone to ask, some others spend a
week before they build the courage to come to us... They should not need encouragement
because we told them so (to come to ask)”.

Through onsite peer support, new users felt more at ease asking questions,
showing their work in progress and learning in a relaxed environment. Participant 02
mentioned: “For approximately one week a friend showed me the basics”. Participant 14
stated: “My group is pretty big…Very friendly people…If I talk to them, it will take me
two minutes…If I keep looking for the answer myself it will take me two weeks”.

Knowledge Sharing in the Lab

The data analysis reveals that scientific software users perceive training on this type of software as the process wherein the users inform their practices by developing their conceptual skills. This is achieved through participation in knowledge sharing activities in a blended environment (quote of Participant 11: “Everything is online, there are also some special books and a long list of tutorials and PowerPoint presentations“), cultivation of a thriving community of practice both online and conventionally (quotes of Participants: “For newcomers…We sit next to them. It happens a lot but not every day”; “But after you learn the basics on your own, there is a community of users that you can go to…”; “Here, we work with this software and we have each other, we give each other our codes…we are like a community”; “My colleague (name) is very experienced, so it was him and other members of the online (software) community who I could ask, outside of this office and around the world”) and use of risk management strategies in the application of the software and creation of new scientific information (comments made by Participants: “everyone here has to explain what they did, how they name their conversions, etc…because, I will tell you why, a new developer comes, writes a code, leaves and nobody can reproduce what he did…”; “I have seen publications where they report an error that I know might have skewed their results. It really causes doubt”).

The analysis of the collected data indicated that scientific software training is also dependent on the profile of the user; for example, their background and strengths, their motivation regarding professional development as well as willingness to share information (“if they are interested, they will ask around, they will find somehow a way
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to improve their knowledge”, “If someone has a good background, and understands the software, then I could introduce them to the software basics and show them more sophisticated things, too. But, as a last step, I would tell them to spend time on it and play by themselves. Because, by helping people and make it easy for them it does not make them learn really the software”; ”Another avenue of solution, there is an online group where I could go to and ask. The problem with this is that you make your code known a bit...”).

Knowledge sharing in this research refers to the processes that take place within a professional research environment that focuses on encouraging people to work together more effectively as well as to consolidate and share knowledge in order to make it available to members of the same community or culture; the scope of knowledge sharing is to help people become more productive. Creating tutorial documentation, course materials, providing information in online/onsite seminars and lab meetings, contributing to online discussions about technical matters, encouraging participation in blended learning “boot camps” for new users/laboratory research staff, these are all components of knowledge sharing processes as identified in this study.

The following Table of Factors (Table 5) presents the parameters that impact knowledge sharing in blended learning settings based on the results of this study. In this study, explicit knowledge refers to documenting the “know-what” in documents, laboratory manuals, databases, memos, notes etc., whereas tacit knowledge is about conveying the “know-how”, i.e. knowledge that experience-based, dependent on context and personal in nature (Smith, 2001).
Table 5. Factors influencing Knowledge Sharing in a Blended Learning Setting.

<table>
<thead>
<tr>
<th>Factor</th>
<th>Explicit Knowledge</th>
</tr>
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<tbody>
<tr>
<td></td>
<td><strong>Online/Onsite</strong></td>
</tr>
<tr>
<td><strong>Parameters</strong></td>
<td>Tutorial</td>
</tr>
<tr>
<td></td>
<td>Formal (classroom) training</td>
</tr>
<tr>
<td></td>
<td>Published paper</td>
</tr>
<tr>
<td></td>
<td>Workshop</td>
</tr>
<tr>
<td></td>
<td>Written documentation</td>
</tr>
<tr>
<td><strong>Observation</strong></td>
<td>Inadequate academic background of user may lead to misuse of time and resources in troubleshooting and problem-solving tasks. Relevant comments made by participants were the following: “Not all students have an adequate background to learn how to use the software. Some might not be familiar with computers. Some others may know about computers but without computing background”, “They do not read enough; they google stuff and look for answers there”.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Factor</th>
<th>Established Access to Community of Practice</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Parameters</strong></td>
</tr>
<tr>
<td><strong>Parameters</strong></td>
<td>Mentor</td>
</tr>
<tr>
<td></td>
<td>Peer (formal presentation)</td>
</tr>
<tr>
<td></td>
<td>Wiki</td>
</tr>
<tr>
<td></td>
<td>General Google search</td>
</tr>
<tr>
<td><strong>Observation</strong></td>
<td>Communication skills of the trainer/mentor and/or the trainee can impact the user’s ability to access the knowledge capital in her Community of Practice. Relevant comments made by participants were the following: “The mentor should tell the student that he/she should ask questions, and feel comfortable asking questions”, “For hires with computing degrees, if they come to me and say “I do not know”, I would go, “Really?”.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Factor</th>
<th>Assumed (Tacit) Knowledge</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Parameters</strong></td>
</tr>
<tr>
<td><strong>Parameters</strong></td>
<td>Published paper</td>
</tr>
<tr>
<td></td>
<td>Project retreat</td>
</tr>
<tr>
<td></td>
<td>Vicarious learning</td>
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<tr>
<td></td>
<td>Community of Practice feedback</td>
</tr>
<tr>
<td><strong>Observation</strong></td>
<td>Openness regarding research findings can be limited within the Community of Practice due to issues related to protecting ownership of ideas and publications. This can impede learning for the user and increase the propagation of wrong assumptions in research. Relevant comments made by participants were the following: “Many times, I asked to see a code and they said no, you cannot…they did not want to share the code because it was not actually working as they said in the paper”.</td>
</tr>
</tbody>
</table>
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The results of this study show that the above-mentioned parameters affect both online and onsite knowledge mobilization processes at similar degrees, without differentiation. Further, the study participants made recommendations about improving the knowledge sharing practices with respect to using scientific software accurately. Table 6 includes these comments by the participants which can be potentially of use to software companies, research laboratory directors (university faculty and/or industry) as well as new scientific software users.

Table 6. Recommendations from Participants in this Study (with Quotes of Participants).

<table>
<thead>
<tr>
<th>For Software Companies</th>
<th>“The software product has to be intuitive, with reliable and updated documentation that users can follow” (quote by Participant 05).</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Onsite Tutorials have to be designed with adult learning theory in mind, i.e. “use more questions than ‘lecturing’, allow for trainees to participate, present their views and use their experience during training sessions” (quote by Participant 16).</td>
</tr>
<tr>
<td>For Mentors</td>
<td>Bring the trainee/student in touch with industry and “encourage professionalism in training environment” (quote by Participant 15).</td>
</tr>
<tr>
<td></td>
<td>Create an environment that is based on current collaborative learning and teamwork theory.</td>
</tr>
<tr>
<td>For New Users</td>
<td>“Develop your writing/communication skills” (quote by Participant 04), as SciSw training involves extensive review and creation of documentation.</td>
</tr>
<tr>
<td></td>
<td>Be prepared for a lifelong learning journey – “accurate scientific software application is an ongoing process” (quote by Participant 11).</td>
</tr>
</tbody>
</table>
Main Components of Current Scientific Software Training

The results of this study point towards three main components that are involved in scientific software training. These include: (a) the personal skills of the user, (b) the onsite environment, and (c) the online environment.

Personal Skills of Users

The results of this study show that the usefulness and successful outcome of the training environment is impacted by the profiles of the users. In specific, the training is affected by the following sub-themes:

1. The individual learning preferences of the users.
2. The degree of responsibility and knowledge-building goals of the users.
3. The undergraduate preparation of the users.

The following describes the diversity of personal skills among scientific software users, as presented in the findings of this study; related excerpts from interview notes are included:

1. The individual learning preferences of the users: This section describes the findings of this investigation regarding the needs and/or characteristics of the scientific software users as learners in a blended training environment. As such, there were four specific findings with respect to this sub-theme:
   - The timing of the face-to-face instruction on the software impacts on the quality of the outcome with respect to training, as most respondents
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indicated that they prefer to be guided by someone more experienced than themselves during their first steps in the scientific software application. Participant 03 commented:” In another place, the supervisor sat beside me for a week, not for the whole time, gave me an introduction to the software they used there and then figured things out myself…” However, four respondents indicated that if the documentation on particular software is of high quality and updated, then new users may be able to start working independently and look for help at later stages of the training, when they need it. “There needs to be a more staged-time aspect”, Participant 13 commented. As well, Participant 02 mentioned:

Yes, after one week, I found most things that I needed by myself…When I needed something in particular, the software has good documentation, so I went there. The company has a good website. So, if you have a particular question in mind, you can look in the documentation.

- The user may not have the motivation to search for available online resources that could help him learn how to troubleshoot. Participant 04 commented:

It is not that useful to go to the online community. There is such a wide range of uses so when I try to Google stuff I did not really find anything to solve my question; there is so much out there.

- The user is able to direct her learning by using available online/onsite resources in order to improve on how to apply the software accurately.

Participant 02 commented:

An additional help is its forums, online, if a user has a problem, you can post it and someone might answer or someone else has already created an inquiry in this so I might find some answers to my problem. I have not participated in an online (synchronous) forum. But after you learn the basics, there is a community of users that you can go to.
• Face-to-face instruction is important for new users. Participant 02: “I communicate online with my colleagues overseas. But when we are face-to-face is better because we can go over the model, it is easier to make changes”. Participant 06: “If someone is interested, if they are motivated, they will learn, either from onsite or from online resources”. Participant 05 (an ‘experienced user, not senior’, according to the self-description of the participant): “When I cannot find something I just ask someone in the lab (…).I would need a day or two to go through the online tutorials (…).

There is a lot of garbage online”. Participant 04 (a ‘junior user’, based on the self-description of the participant) commented:

The online resources you assume they are right until you see that they are wrong (…). It is funny how it helps, how easy it is to ask questions when somebody is near….if they are near and you can just turn around, you can just say “hey…” It makes it very casual.

2. The degree of responsibility and knowledge-building goals of the user: This section presents the findings of this investigation with respect to the level of accountability and ownership of learning of the scientific software user. There were three findings associated with this sub-theme:

• The user is open to invest the time required in order to learn to use the software accurately. Participant 03 stated:”…it will not sink in unless I sit down and I work through it myself”. The data of this study show that systematic validation coupled with risk management practices in scientific software application are essential. As Participant 01 commented:

If I run 5 models, that is 50 days, but I do not capture the problem correctly, that’s a problem. I have to make sure that I have the parameters correctly. I
have seen publications where they report an error that I know might have skewed their results. It really causes doubt.

- The user is responsible for checking his understanding on the software default parameters, i.e. what the software is doing. As Participant 02 commented: “You have to make sure that your model functions mechanistically correct, not make assumptions in your model that cannot be true or simulate something different than what you are aiming to simulate”.

- Protecting the ownership of ideas may impact open exchange of feedback among users regarding correct application of scientific software, based on the input offered by the study respondents. As Participant 02 commented, the users are often protective of their work and/or ideas and do not share with peers outside their specific work environment:

  Other researchers are willing to share their model but not their knowledge. They describe the model they are using but not the code they are using, because they might sell it in the future. They do not give their data in order for someone else to reproduce their results.

  Participant 06 also commented on how users share information within their professional networks about their work on scientific software: “So, the projects posted in the online community are always much better quality. Because you make it public, others will see it so you want to make your model look good”. Participant 04 stated, as well:

  There is a closed group, I belong to it. But, when you post a question, you have to show a bit of your code, others will look at it, might give your ideas away...I try to show only very little code.

3. The undergraduate preparation of the users. This section describes how the respondents in this study described the role of their undergraduate academic preparation
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in their development as successful scientific software users. Of note is that nearly all study participants claimed that, in terms of actual programming and practice, they “did not get too much” during their undergrad years. Participant 12 stated: “In terms of actual programming and practice, I did not get too much during my undergrad years. I developed most of my programming skills in my grad program”. Participant 04 mentioned that during his undergraduate preparation he was introduced to some basic concepts in using scientific software but it was also in his first year as a Master’s student that he started “to work on real software”.

The following Figure (Figure 5) emerged from the data analysis of this study and depicts skills that scientific software users should develop in order to apply the software tool successfully and produce reliable scientific results. This is a finding that emerged from the grounded theory analysis and although it does not precisely describe a scientific software training approach, it indicates the required aptitudes that a user should potentially develop in order for the training to prove fruitful.
Results (Grounded in the Data)

Successful scientific software users are required to develop and maintain certain skills in an ongoing training loop:

- Ability to direct own learning onsite/online
- Ability to communicate technical inquiries to peers online/onsite
- Discipline in work routines: Methodical in recording lab work and collecting feedback
- In-depth understanding of problem at hand
- Develop trust within virtual community of practice - share reliable data, meaningful feedback: Identify and establish common ground with online peers

Figure 5. Personal Skills of Users.

Onsite Training Environment

The on-site work/training environment of the users is affected by:

1. Mentorship and pedagogical considerations.
2. Collaborative learning activities.

“The minute you walk in a lab, you know the environment, you know if the director or the professor-in-charge is approachable and the students feel welcomed to ask questions…if there are, indeed, any collaborations fostered” (Participant 18). Another participant commented: “These environments are put together on the professor’s good
intentions, but how are the professors trained to encourage teamwork?” Peer support is a traditional environment is crucial for new users, based on the amassed data. It plays an important role in their development if mentorship is conducted and feedback from peers is offered in a constructive manner. By acquiring and solidifying their technical background, new users seem more confident to search critically, analyze internet sources and to expand their knowledge spectrum in a blended environment.

Results indicated that the issue of informal learning with peers online/onsite was an important ingredient in the training process on scientific software. Participant 02, a Master’s student, stated: “The supervisor sat beside me for a week, gave me an introduction to their software and then I figured things out myself”. Participant 04, a Master of Science student close to his graduation, also indicated that”if you stumble on something, go ask someone, it is much faster… There is also an online community that shares ideas, we help each other, it speeds up the process”. Participant 09, a graduate student in his doctorate, pointed out: “With my lab mates I feel a lot more comfortable asking questions than if you work with a senior software developer, because they may not have time to answer questions at your level”. Participant 06, a Master of Science student with some experience in computing, also added: “I have not really experienced formal training like industry seminars. It is expensive (…). After you learn the basics, there is an online community of users that you can go to”. Participant 14, a faculty member, mentioned: “Group mentality, it actually produces some pretty good results”. Participant 05, an industry expert (according to her self-description during the interview) suggested:”A new software user? I would recommend they join an open community, they write to people, they ask”. Other participants mentioned that their senior undergraduate
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and graduate students start their own online chat rooms in order to share ideas about their work: “They socialize online with a common issue; the exposure that they have to their profs (professors) is minimal to the one they get through online. But they need to know how to filter the information”. Further, as Participant 08 mentioned: “We try not to lie in our papers”. Participant 20 also commented:” Pretty pics are posted now and you think you go somewhere but perhaps you may have gotten nowhere. The pace of research today moves too fast”.

The Role of the Online Environment

It is important to note that the online environment is intertwined with onsite peer support throughout the training of all interviewees. The majority of the respondents used both modes of knowledge transfer during their typical work day. A prevailing observation from the interviews was that online documentation (from software company sites) can complement onsite laboratory resources (manuals, short courses) and support the needs of the users regarding expanding their knowledge. As Participant 17, a user with over 9 years of experience in scientific software applications, stated: “The students socialize online with a common issue; the exposure that they have to their professors is minimal to the one they get through online means. But they need to know how to filter the information”.

However, 17 out of 20 participants suggested that posting questions in online discussion sites can wait until the users have confidence in their ability to critically review feedback from online peers. Also, the majority of new users that were
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Interviewed for this study claimed that lack of proper terminology, at the beginning of their training, hindered their ability to use the online community as a resource as they would not be able to accurately articulate technical questions. Figure 6 includes major references made by the respondents in all three of these factors.

The majority of the participants mentioned that building a strong background on the problem at hand should be the focus of a responsible user. Participants mentioned that often the first step that users take in their effort to learn a new scientific software product is to search online for information on how to use it. While this can prove fruitful because they can locate pertinent online documentation, the problem is that the users are not focusing on the capabilities/limitations of the software and whether this product is the best tool for their research work. The contributions made by the respondents of this
study show that investing time to read available documentation and develop sensitivity around the problem at hand is the first step towards successful use of scientific software; 17 out 20 participants supported this point. Some of their comments were: “They need to take the time to read”; “I am not sure what to ask online, I feel I do not know enough, I look in the documentation first’. Several issues were identified with this first step: (a) availability of current information, (b) learning skills and motivation of the learner, (c) background knowledge of the user. There were 15 out of 20 participants who mentioned that their undergraduate education involved little training on how to use scientific software reliably (“It was during my first course as a Master’s student, this is when I really used the software on my own”). Most participants stated that they learned on their own or in collaboration with their peers.

Comments were also made about whether this was the most effective way for them to learn taking into consideration the large amounts of time invested, troubleshooting and questioning of available documentation without adequate undergraduate preparation. Participant 13 commented:

We have a computer programming course here, it is a 1st year course, it is not very project-based, there are small projects but it is not very useful for a student. I am wondering if there was a course was in 2nd year to teach you software, I know it would have saved me lots of time.

Onsite peer support is crucial and useful to junior users, based on the interviewees’ feedback, if: (a) it takes place in a collaborative learning environment, with low anxiety levels and, (b) there is a plethora of resources available to draw information from. Experienced users mentioned that onsite peer collaboration was not an essential part of their daily routine unless they worked within a team on a joint project. The data demonstrated that protection of ideas and publication concerns come to mind before the
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users reach out to peers; their level of collaboration with colleagues depends largely on whether they are in competition with them or have developed a trusting relationship (some comments made by the participants included: “Another avenue of solution, there is a LinkedIn group where I could go to and ask. The problem with this is that you make your code known a bit”). Experienced users reported that they prefer to turn to the software developers for advice on the use and/or modification of the software product than to their colleagues in the same university.

Adapting to New Learning Environments

The findings of this research undertaking indicated that young, as well as senior, more experienced scientific software users were required to adapt their practices to include use of blended resources, i.e. online documentation as well as online forums, tutorials etc. Internet-based learning was not an option for some users when they started out their career before the 1990’s. As such, they had to develop a capability for searching for information available online, expanding their professional niche by communicating with peers online and checking the validity of resources posted on the Internet.

All interviewees agreed that a balanced approach between use of online resources and traditional interaction with peers and mentors is preferred. Participant 17 commented on this approach:

The students are given electronic copies of all the documents on fundamental papers that exist. All of the manuals are given to students as well. But they need to learn to network online. It is professional networking, if they have a problem they need to know who to contact online or here, in our lab.
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Less experienced users required more physical presence of peers, as shown in quotes of participants earlier in this chapter. Users with around 8-10 or more years of experience showed proficiency in working in either traditional, entirely online or blended environments without major concerns. The focus of these users (with around 8-10 or more years of experience) was on the topic at hand (‘Understanding is important, so that you are solving this problem and not another one’), whereas the focus of the less experienced users (1-3 years of experience) was on the mode of the delivery regarding knowledge (“It is nice to have someone near to ask questions”; “With the webinar, I did not have a full interaction with the instructor”).

The parameter ‘online learning’ appeared in the data to be useful in all facets of scientific software training but it became more and more powerful with the expansion of the understanding of the user of the problem at hand. The interview data as well as the secondary data revealed that if the users learned to interact effectively with their mentors onsite as well as online, then the quality of the software output and research results were enhanced. Participant 17 commented:

We are collaborating with people internationally. There is a communal relationship. I see that our students start their own online chat rooms to share info, technical. All students are collocated in one lab. So they can turn to their peers for help. They can ask their profs. We also send our students to conferences so that they learn from the experienced professionals. This motivates them. So a student should have a database of all of these things. Our lab has an organised database, a library for the students as a resource. Their projects are better worked through, because they receive all this feedback.
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**Blended Learning Environment**

All interviewees commented on the use of internet as a resource for their knowledge expansion. There were 15 out of 20 participants who mentioned issues of trust, familiarity with technology, not feeling sure about how to critically analyze the vast information on the web. Interviewees, who had a solid background on their subject, were much more confident in using online discussion forums to cross-check and test their ideas with online peers (“The open community we work in, you can submit your data so that they can simulate it, you can see what the reviewers have said”). Also, adequate ability to articulate technical issues/questions and communicate this to online peers was an issue that was brought up by eight participants (“They need to read enough…to know to communicate in short what they need to ask”). Also, cost of resources and training was an issue for all interviewees; comments on the time and resources required to develop online tools were made, as well (“To do video tutorials and narrate what I am doing…The problem is that it takes several days to make a tutorial video, this is why they are usually not up-to-date”).

The Internet is free (or low cost) and this can make it a popular tool. However, it is up to the users to develop the degree of sensitivity necessary to establish a solid level of understanding of the topic at hand; this can be accomplished by reading, investing time to develop their knowledge base, and critically analyzing pertinent information, so that Internet resources can be used to their full capacity. Training on science and engineering specialized software appears, from the interviewees’ perspective, to be a
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flow diagram, because the more they understand, the more they can improve the interpretation of the software output and their research results.

The usefulness of the Internet as a resource appears to be connected to the degree of responsibility of the users, to their degree of sensitivity regarding the topic at hand and their ability to direct their own learning. Figure 7 shows the parameters that influence the usefulness of blended learning (BL) in scientific software (SciSw) training.

Usefulness of BL in SciSw Training

![Flow diagram showing parameters influencing the usefulness of BL in SciSw training]

Figure 7. Parameters Influencing the Usefulness of BL in SciSw Training.

As indicated by the data analysis of this study, once the learners become familiar with the blended environment, then the mode of knowledge delivery does not affect them anymore. At this stage, they have become able to focus on the quality of the transferred knowledge, and not on the profile of the online peer or their level of familiarity of technology or the degree of social presence in their online interactions. This can
significantly enhance their ability to learn by critically analyzing the core of the information, not its delivery mode.

**The Systematic Training Cycle for Scientific Software Users**

The following Figure (Figure 8) captures the references of the majority of the scientific software users that contributed to this study, with respect to the techniques that currently address their training needs as well as the sequence of these techniques. Figure 8 presents The Systematic Training Cycle for Scientific Software Users, as it has emerged from this study. The data analysis in this investigation show that the optimal training framework is an ongoing, methodical cycle that includes, primarily, the investment of time and dedication by the user on the software and topic at hand in order to expand his or her knowledge base, followed by onsite peer support and guidance, progressive use of online resources (documentation and discussion forums) as the user becomes more and more independent, and back to the user reflecting and dedicating time to absorb new knowledge, critique available information and develop sensitivity about the research question at hand. As one of the interviewees noted: “*It is good to explore your area*”.
The study participants pointed out that the limitations of the Systematic Training Cycle for Scientific Software (SciSw) Users include issues involving different levels of collaboration, potential intimidation, reliability of resources, as well as ‘assumed’ knowledge in scientific software application environments where users receive training. For example, when asked to describe the collaborative learning design in their lab, participants responded that it really depended on the personality and background of the professor or mentor. As Participant 17 mentioned: “Well, this environment is totally built on the attitude of the professors…” This improvised situation often exists in research laboratory settings and was described as a deeper issue by respondents who were young software users. The contributions of the respondents indicated that this ad-
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Hoc situation can impede their overall learning and confidence in their research results because of the following reasons: (a) the mentor (often supervisor) has uncertain previous training on constructive feedback techniques, teamwork, teaching in a positive learning environment, (b) the student/trainee does not have adequate interaction time with mentors or colleagues, and (c) the student does not have previous formal training in working and learning within a team; overcoming personality and interpersonal issues can often impede the development of the learner.

The reliability of online resources as well as the feedback offered by the online community is an element that raised concerns among the respondents of this investigation. This is in agreement with the findings of Pawlik et al. (2012) who also raised the question of trustworthiness and reliability of the online sources from which the scientists learn about various aspects of software development. In their study, the scientists-participants did not have specific criteria with respect to assessing their online resources and whether these addressed their needs best or what type of online sources would be trustworthy and reliable for their work.

Further, the Systematic Training Cycle for Scientific Software Users is affected by the personal practices adopted by the user with respect to knowledge building on the research problem at hand and risk managing of the software application. As such, a holistic training framework that places the Systematic Training Cycle in the complete research problem-solving context is presented in the next section.
The Scientific Software Training Framework

The following Figure presents the Scientific Software Training Framework or SciSw Training Framework for users aiming to employ scientific software successfully in a modern, blended learning environment (Figure 9). This Framework is based on the Systematic Training Cycle that was presented previously and emphasizes the overarching blended learning environment that characterizes the current training practices on scientific software application. The online and onsite environments join seamlessly; the users perform in both environments and learn to communicate ideas and collaborate with their colleagues on research problems in both settings.

This framework encapsulates the observations or references made by the respondents of this study with respect to various parameters that affect each component of the Systematic Training Cycle. As such, this framework takes into consideration one of the prevailing concerns expressed by the respondents of this study, which involves the selection of the software tool in conjunction with its usefulness in the research problem-solving process, not because of its availability, ‘popularity” or “easy-to-use” type. As Participant 04 stated: “…before I use the software, I need to understand my problem”, and “…learn your problem, then be determined to learn your software”. Participant 18 also stated: “I believe there is a trade-off between understanding and ease of use”. This concern is depicted in the blue ‘bubble’ (Knowledge of Problem) as well as in the grey ‘bubble’ (Level of Sensitivity on the Problem).

The findings of this study further indicate that the development of systematic methods can enhance validation of the software output; this is an important aspect that
needs to be included in user training. This is shown in the purple ‘bubble’ of the
diagram. As Participant 03 mentioned: “The user is reliable for the results…go through
verification process so that you can check your work and you are confident that your
model will give you accurate results”. As such, it is the responsibility of the user to
check and validate the software output. Further, the quality of the online/onsite
mentorship environment as well as collaborative learning practices with peers can impact
the training process. As Participant 07, a senior user (according to the self-description
given by the respondent), stated: “As a mentor? I feel it is mostly up to the students, I do
not have a recipe, if they are interested enough they will find their way to knowledge”.
But, Participant 05 mentioned: “If you are nervous, shy and try to figure things by
yourself, it is not as productive”. Equally, the availability of resources is important in the
training process. As Participant 15 mentioned: “Have everything available, and they can
decide how they want to learn. Different learners need different things; we need to make
them available, informal and formal ways of learning”.
Figure 9. The Scientific Software (SciSw) Training Framework, based on the Systematic Training Cycle (Figure 8).
CHAPTER VI: DISCUSSION

Introduction

This chapter includes the discussion on the findings of this investigation. It elaborates on good practices associated with scientific software user (SciSw) training, based on the research data. Linkages with current theory and recommendations will be included in the following sections.

Bird’s Eye View on Scientific Software Training

The analysis of the specific elements that are included in the Systematic Scientific Software Training Framework (Figure 9) in conjunction with selective coding processes of the data collected during this exploratory study revealed that that there are three intertwined, overarching parameters in scientific software training. These parameters constitute the theoretical framework that is grounded in the data.

The results of this study, through the words of the participants, indicate that a scientific software user should consider these key parameters and include them in the design of a training technique for successful application of scientific software.

These parameters are:

1. Confidence in Comprehension,
2. Discipline (and Systematic Validity Procedures), and
3. Ability to Adapt.
The following Figure (Figure 10) illustrates the relationship between these three parameters.

![Figure 10. Three Major Parameters in SciSw User Training.](image)

The Confidence in Comprehension parameter refers to the depth of the knowledge base of the user with respect to the area of study as well as the scientific software tool, its limitations or capabilities and its usefulness in the problem solving process of the research question at hand. Confidence is defined here as a solid background in the field of the problem that a user attempts to answer by using the scientific software product; it also refers to the degree of sensitivity that the users have developed regarding the context of the research question they are attempting to solve.

 Discipline refers to the ability of the users to build in methodical ways in their work and diligently test their software programs; also, it relates to the degree of responsibility of the users to systematically invest adequate time in order to update their knowledge on current literature and software documentation that are pertinent to their research problem.

 The Ability to Adapt refers to a skill that is important to every scientific software user, as
it empowers the individual with the aptitude to conduct his/her work regardless of the type of the learning setting (traditional, online or blended). Further, with distance technologies and software engineering continuously progressing, the users are expected to keep up with new information in their field of interest. Experienced users that were interviewed during this investigation reported that they had to ‘retrain’ many times in order to stay current and understand how their field of interest continued to evolve in conjunction with their professional environment.

Through the careful analysis of all data that was available in this study, both from primary and secondary sources, it became evident that if any one of these three factors is missing, the user may not in a position to employ the software reliably. The accurate application of scientific software involves the users developing confidence both in their background of the problem at hand, and their knowledge about the software tool. While this factor is necessary, discipline in investing time to read pertinent documentation and keep up with software updates is equally crucial. By methodically keeping notes about software procedures and maintaining checkpoints to review the results during the software application, the users ensured that they were in control of the entire process, and that the software (with its capabilities and limitations) does not manipulate the research at any time. Current literature has indicated that the software product selection and usage are parameters that can influence the course of a research undertaking and, as such, there is a requirement for systematic reviews of the software output as well as careful analysis of the context within which the software product is employed (Lutters & Seaman, 2007; Joppa et al., 2013; Zacharia et al., 2015; Queiroz & Spitz, 2016).
Further, the results of this study show that as the learning environment changes continually and users are expected to keep up with information that becomes available through various modes of delivery, the ability to adapt to new learning environment and modes of interaction becomes an indispensable parameter. This parameter may be associated with the social learning theory by Bandura (1976) which accounts for both the learner and the environment in which he or she operates. Behaviour is a function of the interaction of the person with the environment. This is a reciprocal concept in that people influence their environment, which in turn influences the way they behave (McLeod, 2011). Also, social learning theory emphasizes the importance of context and the learner’s relationship with the environment in explaining behaviour. Mandefrot (1997) argued that the social aspect of computing affects motivation, individual differences, and the learning process. Software evolves and knowledge is embedded in continually updated documentation as well as in blended communications with various stakeholders, the skill to continually retrain becomes vital. Users of scientific software, who wish to apply the software correctly, need to continue to expand their ability to learn in unconventional environments and maintain their desire to enrich their knowledge base in their field of interest. However, as Harrison (2015) indicated, self-paced learning with independent use of online resources as well as onsite documentation –which is often required from scientific software users in industry and higher education, as mentioned by the research participants- can be confusing if progress indicators and structure is not in place. Online resources such as video tutorials and e-learning documentation need to be carefully designed in order to support the learner and enhance the “quality of experience” (Ljubojevic, Vaskovic, Stankovic, & Vaskovic, 2014; Hsin & Cigas, 2013).
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As mentioned earlier, all three parameters need to be considered and attained by a user in order to produce reliable scientific results. For example, a user can be highly knowledgeable and confident about the research topic at hand but they may not be prepared to use blended learning environments in order to perform in a team setting, communicate their research results and receive feedback from peers. This could substantially limit their ability to validate their work and make it useful to their scientific community. As one of the research participants stated, “...our work is meaningful if the rest of the world can see it”. Bereiter (1997) highlighted the importance of “learning how to function in a community of practice whose work is work with knowledge” (p.298). Lingard (2010) pointed out that university students seldom receive any specific training on how to function collaboratively before group assignments are given, and little attention is given to how teams are formed. Further, current research in the area of computer-supported collaborative learning emphasizes the need to structure students’ collaboration and help them to monitor and improve the state of their social engagement (Zacharia et al., 2015).

The issue of social presence in online interactions with peers appears to be a concern for most users of scientific software, both new and experienced ones. In this study, social presence is defined as the need for users of technology-based communication to perceive each other as real people (Kear, Chetwynd, & Jefferis, 2014). As such, low social presence can be a particular issue for users searching for information or solutions to software problems in online asynchronous discussion forums; this can lead to feelings of impersonality and disengagement from the training process. Consequently, developing an ability to adapt to different learning environments and
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accomplish the task at hand (for example, seek feedback on your work from the online scientific community) is vital in scientific software training and application process.

Equally, if users have background in the topic at hand but they have inadequate self-discipline in following software updates and procedures or maintaining checkpoints throughout their software analysis, the findings of this study indicate that, in such a case, the validity of the software output can be substantially affected. Parnas (2010) pointed out that teaching students how to work in disciplined ways and diligently test their software programs are critical elements in formal science and engineering education. If users are familiar with validation and accurate software application procedures and have the ability to adapt to new learning environments but their knowledge of the topic at hand is inadequate (due to possible undergraduate preparation or low degree of sensitivity in the subject), then again, the software application can be problematic because it may be used in the wrong context. For example, in a recent case study of river water pollution with mercury in Western Canada, the rates of mercury introduction to the river water were elevated, according to the laboratory (scientific software) results. However, it was eventually proven that the source of the metal was not anthropogenic, as the research results had initially implied. Careful interpretation of the software results in conjunction with the geology and precipitation levels of the area revealed that the mercury levels were elevated but within the natural limits due to the geochemical composition and weathering rates of the particular rock formations in the area around the river.

Consequently, in this case study, the scientific software user should be able to use the software tool accurately and, subsequently, be knowledgeable enough about the context of the research problem in order to correctly interpret the software output.
Andragogy or Epistemagogy?

As discussed earlier, scientific software users who participated in this study were adults with academic and, often, industry experience in a particular area of study. The analysis of both primary and secondary data of this investigation indicated that the profiles of the scientific software users as learners appear to be in agreement with the adult learner characteristics that were described by Knowles (1968) in his andragogy theory:

- Adults are internally motivated and self-directed.
- Adults bring life experiences and knowledge to learning experiences.
- Adults are goal oriented.
- Adults are relevancy oriented.
- Adult learners like to be respected.

However, certain unique qualities have become apparent with respect to the participants in this investigation and how they operate or continue to seek knowledge in their environment. This study has shown that an adult learner in the scientific software user community is a “learner” who is also a researcher; they are interested in advancing the science; they decide to learn something new in order to find the solution to a research question that they are intrinsically interested in; and, as a consequence of this, they drive their own learning. They often understand that the new information may or may not help with solving the problem they have at hand, but they still pursue it. They try various things in order to further the research; they experiment. There is not always a gain from their efforts but they still investigate, “in the dark”. This ‘thirst for exploring new
realms’ may be linked to the intrinsic motivation that adult learners have, particularly when the new learning can lead to a promotion at work, increased job satisfaction or self-esteem (Massoud, 1991; McGinnes, 1994; McGrath, 2009).

But adult-researcher learners are different than adult-employee learners who are sent by their supervisor to take a training course in order to improve on a practical aspect of their occupation, which may or may not address their personal interests (Holmes & Abington-Cooper, 2000). A researcher has developed a special sensitivity about a particular subject because of their own interest and choice. Their knowledge on the subject continues to grow through self-directed learning and peer collaborative practices, and rarely in instructor-led settings. However, adult learning, as described by Knowles (1980), focuses on environments where the students are encouraged to participate in the learning process under the direction and responsibility of the instructor. Further, adult learners in general can become more difficult to retrain as they age. Research has shown that this can be mitigated; however, the requirement for this type of studies underlines this potentially inverse relationship between age and learning (Iverson, 2005). Scientists and researchers in this study appeared to be eager to retrain even at an older age, as learning new things and experimenting is part of their personal philosophy, their raison d’être. In fact, the data analysis of this research study revealed that retraining or the ability to adapt to new ways of ‘doing’ is an essential skill for scientific software users and the scientific community, in general. Knowles (1994) wrote that ‘adults tend to be more motivated to learning that helps them solve problems in their lives’ (p. 14). Scientific software users, though, are motivated to acquire new knowledge in order to solve problems usually in the lives of others.
Further, scientific software users who offered their feedback in this study demonstrated a high desire to learn about things that they had no direct background on; they even sought to adapt to new learning ways (online/blended learning) in order to satisfy their inquisitive mind, regardless of whether they would succeed and gain something tangible or whether the new knowledge would be directly linked to their life experiences. As one of the respondents (a senior user, according to the self-description of the respondent) stated: “If they want to do some research, try something that others have never done before, then they come with questions, they drive their learning”. Adult learners in general, as they are described by Knowles (1968), need to know why they are learning new knowledge before they are willing to participate. As McGrath (2009) discussed in her review of Knowles’ andragogy, “it is important that students are informed of the benefits of covering this material and how it will benefit them when the course is finished” (p. 103). This may be a difference with the way researchers and scientific software users continue to learn, as the latter do not always have a road map and outcome reassurances for where they hope to end up with their research undertakings.

As such, this study indicates that scientific software users, as members of the scientific community, have similarities with the profile of the adult learner, as described in associated literature, with some unique characteristics. These distinctive features are presented in the Epistemagogy Assumptions in Table 7. The Epistemagogy Assumptions encapsulate the observations that were captured during the data collection phase of this investigation and refer to: (a) how scientific software users operate in their workplace, and (b) how they continue to learn and interact with peers in various learning
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environments. These new assumptions are not in contrast with andragogy; their aim is to
highlight the particular learning needs of a specific group of adult learners.

Epistemagogy is a term used for the first time; its definition is derived from the
data analysis of this study. Epistemagogy describes how scientists (‘epistemon’ in Greek
is someone who has acquired knowledge by studying systematically a particular subject;
‘agogy’ in Greek means leading) continue to advance their knowledge in the modern
learning environment. In this study, ‘epistemons’ were researchers/scientific software
users from the science and engineering community. Further research in this topic is
needed in order to explore to which extent the observations in this study may be
applicable to the scientific community.
Table 7. Andragogy and Epistemagogy Assumptions: A Comparison.

<table>
<thead>
<tr>
<th>Five Key Andragogy Assumptions (McGrath, 2009)</th>
<th>Epistemagogy Assumptions (in this study)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adults have a self-concept of being responsible for their own decisions, for their own lives.</td>
<td>Learners are adults with life responsibilities but also researchers; have received significant academic and, often, professional preparation.</td>
</tr>
<tr>
<td>Adult learners need to be made aware of the reason why they have to learn certain material.</td>
<td>Learners have a thirst for new knowledge that encompasses their life philosophy; they are research-oriented. Self-directed learning coupled with peer collaborative learning sessions are much more preferred by scientists than instructor-led lectures.</td>
</tr>
<tr>
<td>The experience of the adult learner plays a role in the classroom.</td>
<td>Learners choose to retrain and adapt to new learning environments as a result of an internal need to seek new knowledge and satisfy their research needs; old experience may or may not be transferrable to new learning environments.</td>
</tr>
<tr>
<td>Motivation plays an important part in adult learning; adults are motivated by both internal and external factors.</td>
<td>Learners are motivated primarily by internal factors; while job satisfaction plays a role, it often takes long time and lifelong efforts for scientists to receive recognition for their work (external factors).</td>
</tr>
<tr>
<td>Adult learners need to feel respected; adults need to have a safe environment before they participate in the learning experience.</td>
<td>Learners need to be able to trust colleagues and/or online peers before they engage in information sharing feedback exchange about their work and ideas.</td>
</tr>
<tr>
<td></td>
<td>Scientists and researchers appear to be eager to retrain even at an older age, as learning new things and experimenting is part of their culture, their raison d’être.</td>
</tr>
</tbody>
</table>

In summary, the study findings demonstrate that ‘epistemon’-adult learners have the following characteristics:

- Highly independent, self-directed, life-long learners.
• Willing to learn new material without necessarily knowing how this will benefit them in the end (i.e. a scientific experiment may not always give results in a meaningful and timely manner).

• Need to interact with members of their community of practice in order to exchange feedback.

• Learn best in positive, collaborative learning environments.

• Are research-oriented; strongly motivated to advance professionally.

• Are protective of the ownership of their ideas and work; this can inhibit knowledge sharing activities among colleagues and impact training of young researchers.

• Are able to adapt to new learning environments and proceed with the task at hand.

Implications for Training

Based on the above characteristics, certain inferences can be made regarding the design of training activities for adult-researcher learners or adult-epistemon learners. As such, a training facilitator for adult-epistemon learners would plan activities focusing primarily on self-directed learning tasks and/or peer collaborative learning practices rather than instructor-led sessions. The peer collaborative learning techniques would be in a relaxed, non-judgemental environment where new and experienced learners can interact in a positive manner. Also, in order to address specific questions by trainees, the
facilitator would provide the option of private one-on-one sessions rather than expect the learners to share their questions (and work/ideas) in an open forum.

**Limits and Constraints of Research Study**

As with any research venture, there were limitations associated with such an undertaking. One of the main limitations in this study was the identification and determination of participants (and educational institutions and/or organizations) willing to participate in this study. This constraint may have affected the findings as the study respondents could include primarily scientific software users with a special interest in improving their practices and expanding their professional development, and not users that neglected certain, tacit perhaps, aspects of their software training.

Engaging interviewees in rich discussions during the data collection process was a further limitation of this study as some researchers were not willing to reveal substantial amount of information about their on-going research, especially if it had not been published at the time of the interviews. This constraint may have influenced the data collection process, as there could be relevant information that was not shared with the author. Further, ensuring that the researcher’s bias was managed and incorporated in the design of the study was another constraint of this project. As the author was the key instrument of analysis and interpretation of the data, there is a risk of human error in all of its forms. The above-mentioned limitations may impact the transferability or generalizability of the findings. However, the task undertaken by the author was to provide rich data with thick descriptions and allow the readers of the study to determine
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the potential of its generalizability. Lastly, the literature that was reviewed for this study was primarily from English and French language documents.
CHAPTER VII: CONCLUSIONS

The purpose of this investigation was to explore the experiences of scientific software users with respect to current training approaches on such software. The main research question was: “What software training approaches in a blended learning environment are chosen by users whose goal is to accurately apply scientific software to questions of research?”

The results of the study identified the Systematic Training Cycle that addresses the needs of the users for accurate application of scientific software tools. The data analysis revealed that the optimal training framework is an ongoing cycle that includes the investment of time and dedication by the user on the software and topic at hand, followed by onsite peer support and guidance, progressive use of online resources as the user becomes more and more independent, and back to the user reflecting and dedicating time to absorb new knowledge and develop sensitivity about the research question at hand. This Training Cycle is the basis of the Scientific Software Training Framework that is also grounded in the data collected during this investigation and indicates the overarching blended learning environment that characterizes the current training practices on scientific software application. This framework for scientific users encapsulates the various parameters that affect the development of the users in a blended learning environment, i.e. peer collaborative learning activities, methodical practices in checking software analysis and degree of sensitivity of the users in the research question at hand.
Further, this study indicates that scientific software users exhibit similarities with the profile of the adult learner as described by pertinent literature, along with some unique characteristics as learners. These distinct features coupled with the Epistemagogy Assumptions presented earlier signify various implications with respect to training of scientific software users.

The qualitative inquiry employed in this investigation involved an ethnographically-informed approach. It explored the community of scientific software users in their natural setting of practice and their interactions regarding scientific software training. Specifically, this new investigation followed on from: (a) qualitative research studies in software engineering by Lutters and Seaman (2007) and Robinson, Segal and Sharp (2007), (b) adult training research on computer use by Hurt (2007), (c) research on hybrid learning experiences in geological sciences by Adams, Davies, Collins and Rogers (2010), and (d) Bissell and Endean (2007) on distance learning within the field of engineering. Open-ended interviews were utilized as the primary data source so that research findings were delivered in the words of the participants. Secondary data sources included observations of participants in scientific software training sessions, as well as reviews of laboratory software manuals and publications. Recruitment of research participants and data collection for this study took place in natural sciences and engineering computational laboratories at universities, public agencies and private industry sectors in Canada.
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Significance of Research

The literature has indicated that there is an identified need for establishing a scientific software training framework that encompasses the learning needs of the users, as this may contribute to the accurate use of the software within the community of scientists. This investigation focused on exploring current scientific software training practices through the eyes of the users. The results of this investigation were grounded in the data (words, notes, references) offered by the participants. The Systematic Training Cycle was identified, as an outcome of this investigation, which addresses the needs of the users for accurate application of scientific software tools. This Training Cycle is the basis for the holistic Scientific Software Training Framework that incorporates various unique environmental parameters and learning needs of the users in a blended learning setting, as they emerged from the data analysis.

The information collected from the primary and secondary data of this study illustrated that there are three intertwined parameters that scientific software users ought to consider for reliable application of scientific software. These parameters can improve the design of a successful training technique: (a) Confidence in Comprehension, (b) Discipline (and Systematic Validity Procedures), and (c) Ability to Adapt.

Through the careful analysis of all the available data, it became evident that if any one of these three factors is missing, the user may not be in a position to employ the software dependably. The accurate application of scientific software demands that the user develops confidence in her background of the problem at hand, as well as in her knowledge about the software tool. While this factor is necessary, discipline in investing
time to read pertinent documentation and keep up with software updates is equally crucial. By being methodical in keeping notes about software procedures and maintaining checkpoints to review the results during the software application, the user ensures that he is in control of the entire process, and that the software (with its capabilities and limitations) does not manipulate the research at any time. Further, as the learning environment changes continually and users are expected to keep up with information that becomes available through various modes of delivery, the ability to adapt to new learning environments and modes of interaction can be viewed as an indispensable parameter, based on the results of this study. Lastly, the Epistemagogy Assumptions, which refer to the distinct characteristics of ‘epistemon’ learners, can potentially inform the design of scientific software training methodologies.

**Recommendations for Future Research**

Future studies may seek to define how cultural backgrounds, age or gender can potentially affect scientific software collaborative learning and usage within traditional and online learning settings. Also, subsequent analysis may be carried out particularly on the indispensability of each of the parameters that comprise the Systematic Training Framework of this investigation, such as “the ability to adapt to new learning environments and modes of interaction”. In addition, with respect to particular characteristics of scientific software users as learners and the Epistemagogy Assumptions that were discussed earlier, further research in this topic is needed in order to explore at
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depth these observations and confirm their applicability within various sub-groups of the scientific community.
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APPENDIX A – Examples of Scientific Software Applications

This Appendix has been included in order to help define and describe the nature of the scientific software that is being cited within this research investigation. Three simplified scenarios have been created. The first one concerns hydrocarbon soil and groundwater contamination. The second one deals with supporting a rock formation. The third one presents an environmental problem due to mining activities.

Scenario I

Here, a scenario of scientific software use in environmental geochemistry is presented. A gasoline leak causes contamination of soil and groundwater of a municipality. The question here is how to accurately and effectively determine the extent, direction, and rate of contamination (how fast does it spread and towards which direction). A scientific software model is used to describe the affected area (Figure A.1). The user is required to take into consideration several parameters (geology, topography etc.). The user is also expected to have sufficient expertise in order to understand the various parameters that come into play in this problem and its potential solution.

Figure A.1 presents the output of the scientific software model. Consideration of several complex processes may be warranted to provide a comprehensive and reliable assessment of the natural attenuation of hydrocarbon compounds in soil and groundwater and soil; this would be a critical component of a remediation strategy design. Adequate data and a complete conceptual model of plume development and hydrogeochemical response are prerequisites for more comprehensive and realistic modeling.
**Problem at hand:** Gasoline contamination in residential area - Identification of transport rate and direction

Figure A.1. Example of a scientific software application in hydrogeology: The mathematical relationships of the contaminant transport processes are depicted within a scientific software model. The user needs to be able to trust her results so that the direction of the contamination is determined (according to the software results) towards the East, and not North or Northwest (as the question mark next to the arrow). As seen in the illustration, there is a municipality, streams running through it, neighbourhoods. The obvious question is where, how fast and at what concentrations the gasoline contamination is spreading towards – who is going to be affected by this deleterious substance and at what degree. What we don’t see in this colourful illustration are the governing equations that try to take a physical phenomenon and make it numerical.
Here, a scenario of scientific software use in structural geology and engineering is presented that concerns the stability of a natural bridge over a motorway. At the design stages of such an investigation, the group of consultants consisting of structural geologists, geoengineers, surveyors etc. is tasked with determining what the expected/anticipated rockmass displacement and settlement (i.e. movement of the ground around the natural bridge) will be. This will help determine how much steel and concrete support will be required to strengthen the bridge. As such, there are a series of options that the designer can utilize: mathematical formulations as well as sophisticated scientific software (numerical) modeling packages. The aim of scientific software of this nature is to construct a numerical model based on sound mathematical, physical and engineering principles in order to investigate a real, physical problem; its scope is to represent a physical phenomenon as closely as possible. Figure A.2 depicts the natural bridge. Superimposed on top of the photo in the figure is the geometry associated with the numerical model that has been created within a scientific software package. Consideration of several multifaceted processes may be warranted to provide a comprehensive and reliable assessment of the behavior of the material (i.e. rock) based on its properties (density, strength, internal friction, cohesion etc.) and applied stresses (forces acting on areas). The scientific software utilizes mathematical relationships that relate applied stresses (forces acting on areas) to the behaviour of the material (ground) that has been defined as the user seeks to determine what combination of stresses can cause the rock to fail.
**Problem at hand:** Rockmass stability of a natural bridge

Failure of rockmass?

Investigations on the stability of the bridge may include:

- Rockmass properties;
- Applied stresses;
- Behavior of the rock.

Figure A.2. Example of scientific software application within structural geology and Engineering: The mathematical relationships of material properties of a rock mass in supporting a natural bridge project are depicted within a scientific software model (for example, FLAC3D by Itasca Consulting Group (http://www.itascacg.com/)) that demonstrates the behaviour of the material around the bridge.
Scenario III

Groundwater can be affected by mining activities. This scenario of scientific software application involves the groundwater monitoring around mining activities, in particular in-situ leaching. In-situ leaching (ISL) refers to the process of contacting a mineral deposit with leaching fluids to dissolve the mineral without having to excavate and physically remove the ore from the subsurface (Davis & Curtis, 2007). Special chemical solutions are injected into the ore zone and the mixed leaching fluid and groundwater are then pumped out of the ground at a production well (Figure A.3). As groundwater contamination may occur during this mining procedure because radioactive constituents may be mobilized, such as uranium, arsenic, thorium and their respective daughter products, groundwater monitoring and remediation is required (Davis & Curtis, 2007). Prior to starting remediation of in-situ leach mining sites, modeling can be used to make predictions regarding the behavior of the groundwater system during and after groundwater restoration.
Problem at hand: Groundwater contamination due to mining activities.

Schematic of Uranium In-Situ Leach Mining (Davis & Curtis, 2007)

Figure A.3. Example of a scientific software application in mine remediation. The in-situ mining process is described in the diagram above. The contour lines in the graph depict dissolved Uranium concentrations (U) at various time steps (t). Here also, the software model is presented and its associated steps (HYDROGEOCHEM 5.0, http://www.scissoftware.com/environmental_software/detailed_description.php?products_id=44). Each of these steps can substantially affect the software output data (results).
APPENDIX B – Certificate of Ethics Approval

February 04, 2015

Ms. Frosyni Skordaki
Other Academic Centres/Depts\Centre for Distance Education

File No: 21657

Expiry Date: February 3, 2016

Dear Ms. Frosyni Skordaki,

The Centre for Distance Education Departmental Ethics Review Committee, acting under authority of the Athabasca University Research Ethics Board to provide an expedited process of review for minimal risk student researcher projects, has reviewed you project, ‘Scientific Knowledge Mobilization: Training Approaches for Accurate Application of Scientific Software.’.

Your application has been Approved on ethical grounds and this memorandum constitutes a Certification of Ethics Approval. It is noted that you require AU Institutional Permission to access university systems, staff or students to conduct your research project. As such, a request for this permission from the Vice-President, Academic has been initiated on your behalf.

Participant recruitment and/or data collection may not proceed until this institutional permission has been granted. You will be notified in writing of the outcome of this request for access.

AUREB approval, dated February 4, 2015, is valid for one year less a day.

As you progress with the research, all requests for changes or modifications, ethics approval renewals and serious adverse event reports must be reported to the Athabasca University Research Ethics Board via the Research Portal.

To continue your proposed research beyond February 3, 2016, you must submit an Ethics Renewal Request form before January 15, 2016.

When your research is concluded, you must submit a Project Completion (Final) Report to close out REB approval monitoring efforts.

At any time, you can login to the Research Portal to monitor the workflow status of your application.

If you encounter any issues when working in the Research Portal, please contact the system administrator at research_portal@athabascau.ca.

If you have any questions about the REB review & approval process, please contact the AUREB Office at (780) 675-6718 (780) 675-6718 FREE or rebsec@athabascau.ca.

Sincerely,
MEMORANDUM

Office of the Vice President Academic

February 22, 2015

TO: Ms. Frosyni Skordaki
    Other Academic Centres/Depts\Centre for Distance Education, Graduate Student

SUBJECT: Institutional Permission - REB File No. 21657

You have been approved to contact Athabasca University staff for your research proposal 'Scientific Knowledge Mobilization: Training Approaches for Accurate Application of Scientific Software.' subject to the following conditions:

1. Your research proposal has been approved by the Athabasca University Research Ethics Board (AUREB);
2. Staff and student information is used solely for the purpose outlined in the research proposal submitted to the AUREB;
3. Secondary uses of data or subsequent research proposal(s) will require additional approval of the AUREB, permission of the staff or former staff, students or former students and institutional permission if the individual is still an Athabasca University staff or student;
4. Staff and student participants will be provided with information about how information will be represented in documentation, reports and publications;
5. Staff and student information will not be shared with a third party;
6. The nature of communication with staff and students is that outlined in the research proposal submitted to the AUREB;
7. Staff and student demographic information will be used solely within the research project;
8. Documentation such as staff and student responses to questionnaires, interview responses (written or taped), observations of individual staff or student behaviors, etc. will not be used for any purpose other than that outlined in the research proposal submitted to the AUREB;
9. Staff and student information will be kept confidential until it is destroyed after a period not in excess of 10 years;
10. Use of personal information will be in compliance with the Freedom of Information, Protection of Privacy (FOIP) legislation of the province of Alberta, Canada.

I wish you every success with your research project.

Dr. Cindy Ives
Vice President Academic (Interim)
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APPENDIX C - Consent Form

Consent Form

“Scientific Knowledge Mobilization: Training Approaches for Accurate Application of Scientific Software”

1) I have read the Letter of Information and have had all of my questions answered to my satisfaction.

2) I understand that I am participating in the study as titled above and understand the purpose of the research as outlined in the Letter of Information.

3) I understand that I can contact Ms. Efrosyni-Maria Skordaki or a member of Athabasca University Research Ethics Board (Office of Research Ethics: 780-675-6718 or rebsec@athabascau.ca) at any time with questions or concerns, as outlined in the Letter of Information.

4) I am aware that participation is voluntary and I can withdraw data related to my company or my own participation from the analysis, at any time until the completion of data collection, without penalty. In addition, I understand that, during the interview process, my responses will be recorded in hand-written notes by the researcher of this project and digitally recorded for data analysis at a later date. Regarding the preservation of the interview content, I am provided with the option to refuse audio digital recording of the interview. In this case, the researcher will take only handwritten notes during the interview and will ask for my review and confirmation of the notes at the end of the interview process.

5) I understand that I can decide to stop being a part of the research study at any time without explanation. I am aware of my right to ask that any data I have supplied to that point be withdrawn/destroyed.

6) I understand that I have the right to omit or refuse to answer or respond to any question that is asked of me.

7) I have been assured that my name and the name of my company will be kept confidential and will not be identified in the results of this study.

8) The results of this study will be presented in theses, academic papers and academic presentations.
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9) I understand that if I wish to receive a copy of the results from this study, I may contact the Principal Researcher: Ms. Efrosyni-Maria Skordaki (Efrosyni.Skordaki@rmc.ca or emskordaki@gmail.com).

10) All names of participants and organizations will be kept confidential.

I agree that during the interview my responses can be digitally recorded for data analysis at a later date.

☐ Yes, I agree ☐ No, I do not agree

If no, the researcher will take handwritten notes during the interview and will ask for my review and confirmation of the notes at the end of the interview process.

Participant Name: ________________________________

Signature: ______________________________________

Date: __________________________________________