Empowering African scientists – evaluating the CD-based installer for Scubuntu

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Abstract

Open source software (OSS) is software for which the source code is made available under a software license that allows it to be used, modified and redistributed without restriction. As such, OSS is freely available for use and inspection and allows unconstrained customisation and modification for any particular need. For this reason, the South African national R&D strategy clearly identifies OSS as a vehicle for fostering local innovation and economic development. Besides these benefits, the use of OSS for scientific computing can significantly lower the barriers-to-entry for poorly funded research institutions in developing countries, while empowering scientists in those institutions to contribute and collaborate with their peers globally.

Linux, an open source operating system, can run scientific tools for almost all scientific disciplines. However, scientific computing on Linux is not widespread, despite its many advantages.

Scientific computing on Linux is hindered by a number of challenges. Probably the greatest challenge is that no Linux distribution comes pre-installed with the appropriate scientific software that a researcher may require, and it is required of the researchers to find, select, install and maintain their own software. For most researchers, this is prohibitively difficult, as it require knowledge of the OSS applications that are available as well as technical proficiency on Linux. Furthermore, the processes of selecting, installing and maintaining software can be time consuming, and the results are usually not shared, so effort is unnecessarily duplicated.

To address this problem, the Meraka Institute is developing Scubuntu, an Ubuntu-based Linux distribution designed specifically for scientists. The vision of the Meraka Institute is that Scubuntu will become the premier choice of desktop operating system for researchers and scientists.

The Scubuntu project seeks to address the problem of finding and installing appropriate software by making scientific packages part of the default distribution and providing tools to ease their discovery, installation and management. The project, with feedback from the user community, continually develops and refines profiles of scientists, based on their computing and software requirements. Based on these profiles, specifications are developed that describe the OSS scientific tools that are most appropriate for that profile.

Scubuntu 8.10, the project's first release, was completed during November 2008. It represents a proof of concept release demonstrating what the future of Scubuntu could hold. As part of Scubuntu 8.10, experimental development was undertaken to create a prototype CD-based installation program, based on the standard Ubuntu installer. This prototype installer allows users to select and install scientific software based on their field of study or profile.

This paper presents a preliminary evaluation of the Scubuntu 8.10 installation program, to determine whether it addresses the problem associated with installing scientific software on Linux.

Introduction

Scientific computing on Linux has significant benefits, but is hindered by a number of challenges. One of these is the difficulty for non-technical users of finding, selecting, installing and maintaining appropriate scientific software on Linux. Scubuntu is an initiative that seeks to address this, and other, challenges by developing an Ubuntu-based Linux distribution specifically targeted at scientific users and researchers.

As part of the development of the Scubuntu 8.10 proof of concept, released during November 2008, a prototype CD-based installation program developed. The Scubuntu 8.10 installation program is based on the standard Ubuntu installer, and allows users to easily select and install scientific software based on their field of study. This paper presents a preliminary evaluation of the Scubuntu 8.10 installation program, to determine whether it addresses the difficulties associated with finding and installing scientific software on Linux.

Section 2 provides some background on open source software (OSS), on its usage in science, as well some background information on Scubuntu itself. The Scubuntu installer is briefly discussed in section

3. Sections 4 describes the approach used in the analysis, while sections 5 and 6 summarise, present some conclusions and discuss possible future work.

Background

Open source software

Open source software (OSS) is software for which the source code is made available under a software license that allows it to be used, modified and redistributed without restriction (Open Source Software 2008). As such, OSS is freely available for use and inspection and allows unconstrained customisation and modification for any particular need. For this reason, the South African National R&D Strategy (Government of the Republic of South Africa 2002, p. 45) clearly identifies OSS as a vehicle for fostering local innovation and economic development.

Open source software is often developed collaboratively by volunteers over the internet. Studies have been conducted that show how the open nature of OSS projects, together with their open modes of communication can lead to significantly innovative solutions (Goldman and Gabriel 2005). Efforts like InnoCentive (InnoCentive Open Innovation 2008) and the work of Lakhani et al. (2007) have shown that opening up and asking for input from a wider audience can provide huge benefit and lead to more innovative solutions. This form of user participation during the production of software is a key property of most successful OSS projects.

The open source ideas of openness, sharing of ideas and collaboration aren't new. They have been employed by developers since the early days of programming and the Internet.

As described above, OSS can offer significant advantages in terms of economic development and the stimulation of innovation. It also offers a number of key benefits that affect users directly. Some of these are identified by Goldman and Gabriel (2005, p. 6, 29), and include:

- that the user and developer communities work together to improve the functionality and quality of the software
- access to high-quality, free software
- access to advice and help on software design and development
- promoting participation in the development of software
- low cost
- engaging with end-users in design and testing
- shorter time to market
- harvesting innovation
- reduced support costs
- improved integration
- avoidance of vendor lock-in

The term 'open source' and the ideas and principles behind it are being applied to diverse fields, not only software. These include art, music, education and politics, where new terms like 'open source curricula', 'open source documentary', 'open source movie productions', 'open source politics', and 'open source governance' are being used (Open Source 2008). In these new fields, open source ideas are being applied to collaboratively create works that cost less and involve input from more contributors.

This section presented a brief overview of OSS. The following section looks at the correspondence between the ideas of open source and the process of scientific discovery.

Open source software and science

There are clear similarities between the way in which open source software is created and the way in which scientific knowledge is generated. These similarities have been discussed by a number of authors. Including DiBona et al. (1999) who identify the following commonalities between the two concepts:

- the sharing of information with peers
- the opportunities for others to take existing ideas further and to apply them in different contexts
- the generation of new ideas.

In open source software, program code and ideas are openly shared. This allows the peers of the OSS developer to inspect the source code, provide ideas, critique or suggestions for improvement, provide fixes or other code contributions. It also allows others to create new projects derived from the original. This is analogous to the work of scientists, who generate new knowledge that is based on, or grounded in existing knowledge (Adler 1999).

OSS has seen increased adoption in industry and academic institutions in recent years. This is illustrated by Laird (2002), who mentions that many labs and scientists are moving away from propriety scientific applications and are beginning to use and improve open source scientific applications. Reasons for this include:

- no-cost licensing
- simpler license management
- improved large-scale programmability and flexibility
- convenience of development
- better integration
- better performance
- concerns around intellectual propriety
- better support

Besides these benefits, the use of OSS for scientific computing can significantly lower the barriers-to-entry for poorly funded research institutions in developing countries, while empowering scientists in those institutions to contribute and collaborate with their peers globally.

Linux is an example of an open source operating system, and offers a good candidate OSS platform for adoption by researchers. It is able to run a great number of scientific tools that provide support for most scientific disciplines. However, scientific computing on Linux is not widespread, despite the many potential benefits for scientists of using Linux as their desktop operating system and the existence of powerful scientific software for Linux such as SciLab (SciLab 2008), MATLAB (Matlab 2008), and the R programming language for statistics (R 2008).

Scientific computing on Linux is hindered by a number of challenges, including that:

- Few people aware of Ubuntu as platform for scientific computing
- Finding and choosing best scientific tools on Ubuntu is difficult
- OSS scientific tools are not integrated in cohesive suites
- Some OSS scientific tools provide only limited functionality
- OSS tools are not available for certain scientific tasks
- Ubuntu not certified to run all proprietary scientific software
  Software maintenance requires technical proficiency.

Probably the greatest challenge is that no Linux distribution comes pre-installed with the appropriate scientific software that a researcher may require, and it is required of the researchers to find, select, install and maintain their own software. For most researchers, this is prohibitively difficult, as it require knowledge of the OSS applications that are available as well as technical proficiency on Linux. Furthermore, the processes of selecting, installing and maintaining software can be time consuming, and the results are usually not shared, so effort is unnecessarily duplicated (Fogwill 2008).

To address this problem, the Meraka Institute (also known as the African Advanced Institute for ICT) is developing Scubuntu, an Ubuntu-based (Ubuntu 2008) Linux distribution designed specifically for scientists. The vision of the Meraka Institute is that Scubuntu will become the premier choice of desktop operating system for researchers and scientists. The Scubuntu project is discussed further in the following section.

The Scubuntu project

Overview

Scubuntu is an OSS project to develop a desktop operating system designed specifically for scientists. The Scubuntu project seeks to address the problem of finding and installing appropriate software by making scientific packages part of the default distribution and providing tools to ease their discovery, installation and management. (Scubuntu 2008) (Fogwill 2008).

The project, with feedback from the user community, continually develops and refines profiles of scientists, based on their computing and software requirements. Based on these profiles, specifications are developed that describe the OSS scientific tools that are most appropriate for that profile. The determination of these specifications represents a key design activity of the Scubuntu project, and determines the packaging and development required for each new release.

In addition to the development of scientific profiles and the identification of the associated high quality open source software, Scubuntu focuses on the packaging, integration and improvement of existing OSS scientific tools, and, eventually, on the development of new tools where no OSS alternatives exist.

Scubuntu follows the advice of Goldman and Gabriel (2005) that 'many advantages accrue when a company adopts the attitude that most innovation happens elsewhere and focuses on choosing the best outside innovations and figuring out the right distinguishing features to make its products competitive'. It is based on a popular and successful open source Linux distribution called Ubuntu, which allows Scubuntu to leverage the existing user and developer communities of Ubuntu, as well as the existing development infrastructure and technologies. Scubuntu adds value to Ubuntu by extending its reach to include the researchers and scientists, and by collaborating with its developers to package new scientific software, thereby enriching both platforms. Ubuntu, in turn, is based on Debian, and benefits from the use of Debian's highly regarded package management system (Debian 2008).

Collaboration methods

Community building is of critical importance to successful open source projects, as a sufficiently large community of contributing users and developers is required to sustain the development activity. Due to the importance of community in OSS projects, as stressed by Goldman and Gabriel (2005, p.8), a significant amount of effort will be used to create and sustain a community around Scubuntu of developers and scientists that volunteer and collaborate to continuously improve the platform. This will be accomplished by:

- aligning the Scubuntu project with Ubuntu, to leverage the large community of existing scientific users that Ubuntu already has
- raising awareness of Scubuntu through publication and exhibition at conferences and in journals
- inviting the participation of scientific users by posting on mailing lists and other online fora
- formal and informal discussions with research organisations and individual researchers to promote the adoption of Scubuntu
- handing out DVDs and promotional material at universities, Linux user group meetings and conferences
- providing good information and documentation (including information on profiles) on the project website
- publishing information about Scubuntu on sites such as freshmeat.net and slashdot.org
- responding in a timeous, friendly and helpful manner to users who interact with the team to obtain advice, assistance or information

For a community to successfully cooperate in the development of Scubuntu, effective collaboration is important. Such collaboration on open source projects is typically facilitated using a number of Internet-based technologies, including:

- on-line source code repositories for code management and sharing
- on-line mailing lists and internet relay chat for technical discussions
- on-line issue tracking tools
- on-line documentation

(Goldman and Gabriel 2005) (DiBona, Ockman and Stone 1999)

Scubuntu uses similar Internet-based technologies to facilitate collaboration, to develop and share ideas, and to coordinate development. These technologies include wikis, weblogs, on-line project collaboration websites tools such as Launchpad (Launchpad 2008) and source code revision control systems such as Bazaar (Bazaar 2008).

Licensing of scientific packages

Software licensing is means of granting specific rights to users or developers. These could include rights to copy, modify and redistribute the software. Licenses can also be used to restrict the rights that a user or developer has, as highlighted by Goldman and Gabriel (2005, p.7).

Software licensing can be complicated, and can encompass various aspects of the law, including copyright law, intellectual property law, and even, in some countries, patent law. Understanding the issues associated with software licensing is critically important for software developers. This is even more so for those involved in open source projects, where the developers seldom have a corporate legal team to support them, as would be the case with larger commercial software vendors.

For Scubuntu, the process of selecting suitable scientific software to include in the distribution needs to carefully consider the license under which that software is released. Some software packages have licenses that are 'viral', forcing derived works to be released under the same license, while other software packages have licenses that may be incompatible with those of existing packages in the distribution. These license issues must be carefully investigated and documented before any package can be added to the Scubuntu distribution.

Comparison to other initiatives

As described by van Zyl and Fogwill (2008), there are other efforts that seek to enable scientific computing on Linux, but that do not adequately address the problems of scientific computing on OSS. These include:

- Scientific Linux (Scientific Linux 2008)
- Poseidon Linux (Poseidon Linux 2008)
- Scibuntu (Scibuntu 2008)
- Bioknoppix (Bioknoppix 2008)
- Vlinux (VLinux 2008)
- Edubuntu (Edubuntu 2008)

As indicated by van Zyl and Fogwill, Scubuntu goes beyond these initiatives by:

- focusing on the development of a community of users and developers
- focusing on the development of profiles
- performing all work in the open and contributing back to Ubuntu
- packaging the appropriate tools into the core distribution to ease their installation, without compromising the users' ability to select their own preferred packages.

The Scubuntu 8.10 installer

Ubiquity overview

The Scubuntu 8.10 installer is based on a modified version of Ubiquity, the standard Ubuntu installation program. Ubiquity is a simple graphical installation program that runs from a live CD and is designed to integrate well with Debian- and Ubuntu-based systems. It is written largely in Python and uses the Debian Installer (d-i) as a back-end for many of its functions (Ubiquity 2008) (Debian Installer 2008) (Ubuntu Installer Development 2008).

The technical details of the development of the Scubuntu 8.10 installer are given by van Zyl and Fogwill (2008), and are not repeated here. Instead, the following sections present a short overview of the functionality offered by the installer.

Profiles

To understand the way in which the Scubuntu 8.10 installer installs application packages, it is necessary to understand Scubuntu's concept of profiles. Profiles in Scubuntu represent categories of packages or scientific domains (i.e. fields of study) and are associated with lists of individual application packages to form an OSS package specification for that domain.

Profiles can also be associated with sub-profiles, thus allowing more specific profiles to be nested within general profiles to form a profile hierarchy. For example, Figure 1, taken from van Zyl and Fogwill (2008), describes the situation where Scubuntu has a top-level profile called *Biology* with sub-profiles *Biochemistry* and *Molecular Biology*. Each of these sub-profiles then contain lists of software packages appropriate for Bio-Chemists and Molecular Biologists, respectively.

Profiles and sub-profiles are implemented as meta-packages in Scubuntu. *Meta-packages* are merely abstract packages that group together a set of other applications – they thus represent package sets, and do not themselves contain any application files or data. Selecting the meta-package for installation automatically selects its associated set of packages. Meta-packages thus provide a mechanism for simplifying the task of installing sets of related packages (Tille 2007). In Figure 1, *biology*, *molecular-biology*, *biochemistry* and *base-plotting-tools* would all be meta-packages, while the remaining nodes would be real application packages.

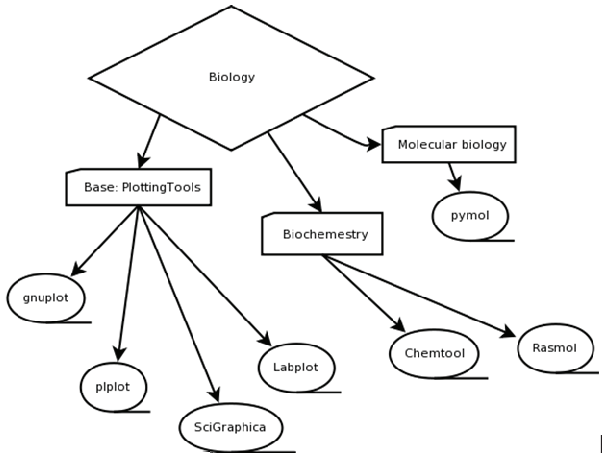

Figure 1: An example of a profile with meta-packages

Installer prototype

The hierarchy of profiles and sub-profiles serves as data to the Scubuntu installer, which presents this hierarchy as a tree (see figures 2 and 3). Each profile, sub-profile and package can be checked by the user to select it for installation. Users thus select the profiles and/or packages they wish to have installed, and the installer then takes care of the details by installing the appropriate packages and meta-packages.

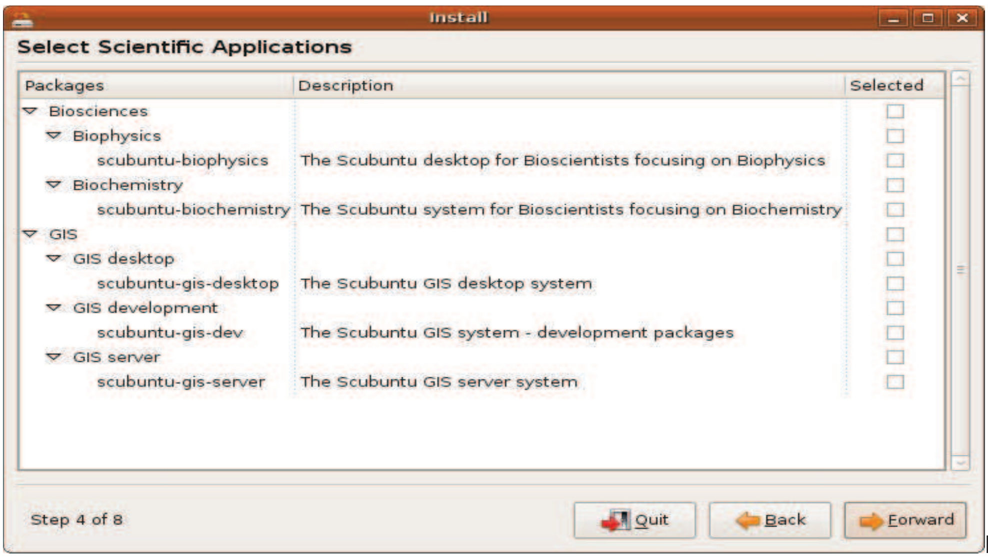

Figure 2: Scubuntu's scientific package select screen

Scubuntu 8.10 supports only two scientific fields, namely biosciences (or biological sciences) and geographic information system (GIS). These fields were selected because of the availability of expert researchers in these fields within the CSIR who were willing to assist the Scubuntu team in designing appropriate profiles.

Evaluation approach

The approach used to evaluate the Scubuntu 8.10 installer is described in this section.

The main function of the installer is to install appropriate applications for a user, based on their field of study. Thus, to evaluate the effectiveness of the installer, it is necessary to measure how well it handles the installation of software given some specific domain. For purposes of the initial evaluation described here, the BioSciences domain was selected.

The ease and effectiveness of using the installer was compared to that of using the conventional method. The conventional method (or manual approach), which assumes that no integrated scientific Linux distribution and installation tool exists, follows the follow procedure:

1. The user searches (using internet search engines and other web-based resources) for open source tools that address their needs.
2. The user reads reviews (individual or comparative) on the web in an attempt to determine the quality of the available software, filtering out software that appears to be of poor quality.
3. The user finds installation resources for the remaining software.
4. The user installs the software for which installation resources were found.
5. The user evaluates the installed software.
6. The user selects the best software for continued use.
7. (Optional) The user removes the candidates that were not selected for continued use.
8. (Optional) The user continually keeps the software up to date with bug and security fixes.

The option steps 7 and 8 above are good practice, but are not often not done.

To evaluate the Scubuntu 8.10 installer, it was used to install applications for the BioSciences profile. The user effort required to do this installation was recorded. At the same time, the steps for the conventional method above were followed, and the effort required was compared to that of using the installer. Additionally, the output of both processes were compared in terms of completeness, quality and ease of ongoing maintenance were considered.

Comparing conventional approach to the Scubuntu installer

Installing the BioSciences packages was trivially easy using the Scubuntu installer. The installer has 8 steps, some of which require user input. Selecting the BioSciences profile involved simply marking a selection from a list (see figure 3). Thereafter the installation proceeded without user intervention, and completed in under 1 hour. After installation, the following BioSciences tools and libraries were available:

- Clustal-W and Clustal-X
- DX (with documentation)
- Octave with the bioinformatics extension
- PyMol
- RasMol (with documentation)
- t-coffee (with documentation)
- BKChem
- Chemtool
- Easychem
- CERNLib
- Staden

Following the conventional method, steps 1 and 2 were eased by the existence of the scientific software list on the Scubuntu wiki (Scubuntu 2008). As an indication of the effort that would have been required had the Scubuntu list not been available, the development of the sections of that list relevant to BioSciences took over 40 hours.

Finding installation resources for software identified in steps 1 and 2 was accomplished relatively quickly for most of the candidate applications. This was largely due to the fact that much of the software was already available in Ubuntu. The most notable exception was Staden, which took a substantial amount of time (and technical know-how) to install and configure.

The evaluation of the various candidates applications (step 5) was not conducted in detail, as the evaluators were not sufficiently knowledgeable about the BioSciences domain to do so. As such, the Scubuntu BioSciences list of applications described above was assumed to be the output of such an evaluation. For real-world users, however, performing a proper evaluation will be critical, and can be expected (based on the experience of the domain experts who developed the Scubuntu list) to take several weeks of sustained effort.

Because the Scubuntu software list was used, the tools available to the user after the completion of each installation procedure were identical. The Scubuntu-installed packages were better integrated with the rest of the system, though, particularly with respect to the existence of menu items, the use of appropriate filesystem paths, and the configuration of appropriate applications to handle supported filetypes.

The cleanup of the system after evaluation (step 7) proved trivially easy, but the ongoing maintenance (step 8) presented real challenges for software not already available in Ubuntu. For instance, incorporating each new release of Staden (or each new bug/security fix) required the entire installation step to be repeated for Staden. This took a significant amount of ongoing effort, so much so that it is expected that few real-world users would continue the effort.

In contrast, keeping the Scubuntu-installed software up to date is simple using the standard Ubuntu software update tool, and requires almost no user effort whatsoever.

It is clear that the Scubuntu 8.10 installer, although still at the prototype stage, significantly improves the user experience when it comes to installing scientific applications on Linux. It greatly reduces the time and effort required to get a working scientific desktop, compared to the traditional method, while continuously providing incremental improvements in terms of quality and integration. It also eases the ongoing post-installation maintenance of the system.

Summary

Scubuntu 8.10, a proof of concept release of an Ubuntu-based Linux distribution for scientists, was released in November 2008. Scubuntu is a specific initiative of the Meraka Institute to address the challenges facing the adoption of Linux for scientific computing.

Scubuntu 8.10 includes a prototype installation program that was designed to address a key challenge for scientific users of Linux, namely that of finding and selecting the most appropriate set of packages. This paper presented a preliminary evaluation of the Scubuntu 8.10 installation program, to determine whether it addresses the difficulties associated with finding and installing scientific software on Linux.

The conclusions are presented in the next section.

Conclusion and future work

Despite the many potential benefits for scientists of using Linux as their desktop operating system, a number of challenges make this problematic:

- Few people aware of Ubuntu as platform for scientific computing
- Finding and choosing best scientific tools on Ubuntu is difficult
- OSS scientific tools are not integrated in cohesive suites
- Some OSS scientific tools provide only limited functionality
- OSS tools are not available for certain scientific tasks
- Ubuntu not certified to run all proprietary scientific software
- Software maintenance requires technical proficiency

The approach taken by Scubuntu addresses some of these problems by:

- Making all work publicly available
- Formal and informal collaboration
- The creation of user and developer communities
- Integrating scientific OSS into cohesive suites of packages
- Centralising technical management and maintenance of packages

Based on the preliminary evaluation presented here, it appears that the Scubuntu 8.10 installer does indeed address some of the challenges associated with installing scientific software on Linux. It does so by:

- Pre-selecting the best-of-breed scientific open source software and grouping these packages into profiles, freeing the user from the burden of finding, evaluating and selecting appropriate software
- Predefining profiles for supported scientific domains to ease the selection of the appropriate set of related (and integrated) applications for a user's field of study

- Providing a user friendly way for scientists to select these profiles and install the associated package sets.

The Scubuntu prototype installer will need more formal testing to verify the conclusions of the preliminary evaluation discussed in this paper. It is envisaged that formal usability testing techniques could be employed to perform such an evaluation.

Future work on the Scubuntu project will include the development of new profiles to cover additional scientific fields and the refinement of existing profiles, particularly in terms of integration between applications and the creation of default configurations on behalf of the user. There will also be continued investigation of other options for the installer program. In particular, while the Scubuntu 8.10 installer already significantly improves the experience for scientific users new to Linux, it is thought that the current design may not be optimal, as it is severely restricted by the amount of data that can be placed on a CD/DVD. There may be advantages to taking a hybrid approach, combining elements of the current design with those used by other projects. This could result in Scubuntu being comprised of a number of CD/DVDs. The first CD could include (in additional to normal packages) a set of packages commonly useful to all scientists, regardless of their field of study. Additional “add-on” CDs could then be generated for each supported scientific field – these CDs would include the domain specific packages for that particular field of study.

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Endnote

Contribution to the paper was almost equally distributed between the authors, although Pieter van Zyl did the bulk of the background reading. He also did most of the technical development and investigation required to develop the prototype installer. Thomas Fogwill did the bulk of the writing and editing, developed the framework for evaluating the installer, and conducted most of the evaluation.