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State of the Art in Parallel Computing with R

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Abstract

R is a mature open-source programming language for statistical computing and graphics. Many areas of statistical research are experiencing rapid growth in the size of data sets. Methodological advances drive increased use of simulations. A common approach is to use parallel computing.

This paper presents an overview of techniques for parallel computing with R on computer clusters, on multi-core systems, and in grid computing. It reviews sixteen different packages, comparing them on their state of development, the parallel technology used, as well as on usability, acceptance, and performance.

Two packages (**snow**, **Rmpi**) stand out as particularly suited to general use on computer clusters. Packages for grid computing are still in development, with only one package currently available to the end user. For multi-core systems five different packages exist, but a number of issues pose challenges to early adopters. The paper concludes with ideas for further developments in high performance computing with R. Example code is available in the appendix.

Keywords: R, high performance computing, parallel computing, computer cluster, multi-core systems, grid computing, benchmark.

1. Introduction

R ([R Development Core Team 2008a](#)) is an open-source programming language and software environment for statistical computing and graphics. The core R installation provides the language interpreter and many statistical and modeling functions. R was originally created

by R. Ihaka and R. Gentleman in 1993 and is now being developed by the R Development Core Team.

R is highly extensible through the use of packages. Packages are libraries for specific functions or specific areas of study, frequently created by R users and distributed under suitable licenses. A large number of packages are available at the Comprehensive R Archive Network (CRAN) at <http://CRAN.R-project.org/> or the **Bioconductor** repository (Gentleman *et al.* 2004) at <http://www.Bioconductor.org/>. The R language provides a powerful and extensible environment for statistical and graphical techniques. Providing software for parallel or high performance computing (HPC) with R was not a development goal.

Nonetheless, research during the last decade has explored using parallel computing techniques with R. The first available package was **rpvm** by Li and Rossini. This package provides a wrapper to the Parallel Virtual Machine (PVM) software. Early papers describing parallel computing with R are Li and Rossini (2001), Yu (2002), Sevcikova (2003) and Rossini *et al.* (2003). There is increasing interest in high performance computing with R, particularly in the last two years. The R mailing lists (<http://www.R-project.org/mail.html>) now frequently host discussions about using R for parallel computing, and the useR! 2008 Conference (Ligges *et al.* 2008) contained a tutorial (Eddelbuettel 2008) and three sessions on HPC with R where several new packages were presented.

Two primary drivers for the increased focus on high performance computing include larger data sets (Berman *et al.* 2003), and increased computational requirements stemming from more sophisticated methodologies.

Bioinformatics provides a good illustration for the “growing data” problem. Consider that just a few years ago, experimentally-generated data sets often fit on a single CD-ROM. Today, data sets from high-throughput data sources—as for examples “next generation” DNA sequencing (Shaffer 2007)—no longer fit on a single DVD-ROM. In genome research, data sets appear to be growing at a rate that is faster than the corresponding performance increases in hardware.

At the same time, methodological advances have led to more computationally demanding solutions. A common thread among these recent methods is the use of simulation and resampling techniques. Markov chain Monte Carlo (MCMC) and Gibbs sampling, bootstrapping, and Monte Carlo simulation are examples of increasingly popular methods that are important in diverse areas of statistical analysis investigating geographic, econometric, and biological data.

Both increased data size and increased simulation demands have been approached by researchers via parallel computing. Data sets can frequently be subdivided into “chunks” that can undergo analysis in parallel. This is particularly the case when the analysis of a given data “chunk” does not depend on other chunks. Similarly, simulation runs that are independent of other simulations can be executed in parallel. Hence, both drivers for increased interest in high performance and parallel computing with R can be seen as so-called “embarrassingly parallel” problems that are suitable for execution in parallel.

This paper reviews the state of parallel computing with R, and provides a starting point for researchers interested in adopting parallel computing methods. The paper is organized as follows. Section 2 discusses code analysis with R, and introduces parallel computing concepts at the hardware and software level. Section 3 presents R packages for computer cluster and grid computing, multi-core systems and resource management. Section 4 provides a discussion of these different packages. The next section focuses on application packages and general tips for parallel computing. Section 6 concludes with a summary and outlook.

2. Overview

2.1. Code analysis for R

Adapting code for parallel evaluation requires extra effort on the part of the researcher. For this reason it is important to ensure that parallelization is necessary. Important considerations include use of appropriate serial algorithms, adoption of “best practices” for efficient R programming, and knowledge of packages tailored to processing of large data sets.

A number of tools are available to profile R code for memory use and evaluation time. How to use these tools and how to detect probable bottlenecks is described in [R Development Core Team \(2008b\)](#), [Venables \(2001\)](#), [Gentleman \(2008\)](#), and in the R help page `?Rprof`. The CRAN packages **proftools** ([Tierney 2007](#)) and **profr** ([Wickham 2008](#)) provide more extensive profiling tools, an overview is available in Table 1 in the appendix.

There are a lot of different ways to solve performance issues, with the appropriate solution often depending on the specific problem. Common techniques to improve R code ([Gentleman 2008](#); [Chambers 2008](#)) include:

Vectorized computation: Vectorized computation means any function call that, when applied to a vector, automatically operates directly on all elements of the vector. Many functions in R are vectorized. These are often implemented in C (see below), and hence very fast. This greatly reduces the need for loops and similar constructs that are prevalent in other languages. Vectorized computations should be used when possible.

apply()-functions: There are a number of functions that can be used to apply a function, iteratively, to a set of inputs. Appropriately implemented **apply()**-like functions help to recognize vectorized structure of code, and are often very readily adopted to parallel computation.

Foreign language interfaces: R provides a powerful interface to functions and libraries written in other languages. The main reason for using foreign languages is efficiency, since R is not compiled. In some situations the performance of R can be substantially improved by writing code in a compiled language. The most widely used interfaces are the `.C()` and `.Call()` functions which provide linkage to C and compiled code. R itself is largely written in C and it is easy to make use of the internal data structures, macros and code from routines written in C (see [R Development Core Team 2008b](#)).

There are many code optimization solutions for special problems. This paper will focus on techniques for improving R code with parallel computing.

2.2. Parallel computing

To understand and to evaluate the different packages that are available, it is important to have an overview of existing technologies for parallel computing. Detailed introductions can be found in various books for parallel computing or computer clusters ([Sloan 2004](#); [Dongarra et al. 2003](#)).

In general, parallel computing deals with hardware and software for computation in which many calculations are carried out simultaneously. The main goal of parallel computing is the improvement in calculating capacity.

Hardware

We provide only a brief high-level review of hardware types which support parallelism. Multiprocessor and multi-core computers have multiple processing elements within a single machine. In computers available to the general statistical computing community, the main memory is usually shared between all processing elements (shared memory). The idea of multicomputers—often called distributed computers—is the use of multiple computers to work on the same task. Operation gets more difficult on heterogeneous multicomputers where nodes may differ in terms of the architecture, operating system or key component libraries (e.g., installed R versions). But in most cases multicomputer environments are homogeneous. A distributed computer is a computer system in which the computers (processing elements with their own memory) are connected by a network. If the computers are located in a local area network (LAN) they may be called a computing cluster. In grid computing, machines are connected in a wide area network (WAN) such as the Internet. Grid computing faces challenges in addition to parallelization, including heterogeneous environments, resource allocation, and resource management.

Software

Several programming languages and libraries have been created for programming parallel computers. Kernel-level facilities targeted for high performance computing (e.g., BProc, MOSIX) are well-developed on Linux operating systems, with additional implementations for Windows or Mac OS X. System-level tools focus especially on the management and monitoring of parallel tasks. Section 3.4 provides a list and short description of such resource management systems. User-level libraries are most important for the end user and parallel code designer. They can be classified based on the underlying memory architecture.

Shared memory: Shared memory programming languages communicate by manipulating shared memory variables. Widely used shared memory application programming interfaces (APIs) include OpenMP ([Dagum and Menon 1998](#)) and POSIX Threads (Pthreads, [Butenhof 1997](#)). These are implementations of multithreading, a method of parallelization whereby the manager (master) thread forks a specified number of worker (slave) threads, with tasks divided among threads. Each thread executes parallelized sections of code independently.

OpenMP: Open Multi-Processing is an API that supports multi-platform shared memory multiprocessing programming in C/C++ and Fortran. Commercial and open source compilers for many architectures including Windows are available. OpenMP is a portable, scalable model that gives programmers a simple and flexible interface for developing parallel applications. The section of code that is meant to run in parallel is marked accordingly by using a preprocessor directive that will cause the threads to form before the section is executed.

Pthreads: POSIX Threads is a POSIX standard for threads. Libraries implementing the standard are often named Pthreads. Open source implementations exist for many architectures, including Windows. Pthreads defines a set of C programming language types, functions and constants. Programmers can use Pthreads to create, manipulate and manage threads, as well as to synchronize thread evaluation.

OpenMP is under active development. Recent work indicates that is easier to program with OpenMP than Pthreads and that OpenMP delivers faster execution times ([Breshears and Luong 2000](#); [Binstock 2008](#)).

Distributed memory: Message-passing APIs are widely used in distributed memory systems. Message passing involves sending messages between participants. A manager-worker architecture—often called master-slave—is most common. In this model of communication one device or process (manager) controls one or more other devices or processes (workers). Once a manager-worker relationship between devices or processes is established (spawned), the direction of control is always from the manager to the workers. Well known message passing implementations are MPI (Message-Passing Interface, [Message Passing Interface Forum 1998](#)) and PVM (Parallel Virtual Machine, [Geist et al. 1994](#)).

MPI: Message-Passing Interface is a standardized and portable message-passing system designed to function on a wide variety of parallel computers. The MPI interface is meant to provide essential virtual topology, synchronization, and communication functionality between a set of processes in a language-independent way. Open source implementations for many architectures, including Windows, exist. MPICH2 ([Buntinas et al. 2007](#)) and DeinoMPI ([Deino Software 2006](#)) currently provide a Windows implementation and OpenMPI ([Gabriel et al. 2004](#)) and MPICH2 are popular on Unix. OpenMPI is a project combining technologies and resources from several other projects (e.g., LAM/MPI) with the stated aim of building the best MPI library available.

PVM: The Parallel Virtual Machine is designed to allow a network of heterogeneous Unix and/or Windows machines to be used as a single distributed parallel computer. Open source implementations for many architectures including Windows exist.

A comparison of MPI and PVM approaches is available in [Gropp and Lusk \(2002\)](#). For computer clusters PVM is still widely used, but MPI appears to be emerging as a de-facto standard for parallel computing.

3. Packages for parallel computing with R

This section discusses a number of different packages and technologies for parallel computing with R. The packages are compared using specific software engineering criteria in [Section 4](#). [Appendix A](#) contains short code examples for all packages mentioned here. An overview is available in [Table 1](#) and in [Appendix Table 2](#) and [3](#).

This section is divided into four parts: Packages for computer clusters, for grid computing, for multi-core systems, and technologies for resource management.

3.1. R packages for computer clusters

Nine different R packages for cluster-based parallel computing are available at CRAN (see [Table 1](#)). [Figure 1](#) visualizes a family tree of these R packages. At the top of the figure are communication layers, and on the bottom are high-level R packages. Most of the packages are based on technologies described in [Section 2.2](#). It is also possible to compile R with external libraries to support computer clusters.

Rmpi

The package **Rmpi** (Yu 2002) is an wrapper to MPI, providing an R interface to low-level MPI functions. In this way, the R user does not need to know details of the MPI implementations. It requires that MPI is installed, and runs under popular MPI implementations: LAM/MPI, OpenMPI, MPICH, MPICH2 and DeinoMPI. **Rmpi** runs on clusters with Linux, Windows or Mac OS X.

The **Rmpi** package includes scripts to launch R instances at the slaves from the master (`mpi.spawn.Rslaves()`). The instances run until closed, with `mpi.close.Rslaves()`. The package provides several R-specific functions, in addition to wrapping the MPI API. For example, parallel versions of the R `apply()`-like functions are provided by, e.g., `mpi.parApply()`. R objects can be efficiently sent to slaves using `mpi.bcast.Robj2slave()`. **Rmpi** includes some error-handling to report errors from the workers to the manager.

rpvm

The **rpvm** package (Li and Rossini 2001) is an interface to PVM. It supports low-level PVM functions from R. There are no additional R functions, so the user has to provide all communication and parallel execution directives. There is no command to launch R instances at the slaves from the master. Instead, the command `.PVM.spawnR()` can be used to execute an R script file (read by `source()`) at the slaves; after running the script the R instance will be closed automatically.

The package requires a running PVM installation on clusters with Linux, Windows or Mac OS X.

nws

The package **nws** (Bjornson *et al.* 2007) provides functions to store data in a so-called “NetWorkSpace” (NWS), and uses the ‘sleigh’ mechanism for parallel execution. NetWorkSpaces runs on Linux and Windows platforms. It requires a running NetWorkSpace server. **nws** is implemented in the widely-available Python language, using the Twisted framework for network programming. NetWorkSpaces currently supports the Python, Matlab, and R languages, and allows limited cross-language data exchange.

There are two basic functions for executing tasks in parallel (`eachElem()`, `eachWorker()`). The package uses the manager-worker paradigm, and automatically load-balances R function evaluations. To enable the manager to communicate with workers, sleigh supports several mechanisms to launch R instances at workers to run jobs: local, secure shell (SSH), remote shell (RSH), load sharing facilities (lsf), web launch.

The **nws** package and the NetWorkSpace Server are available as an open source and commercial product from REvolution Computing (and had previously been marketed as LindaSpaces by Scientific Computing Associates).

snow

The package **snow** (Simple Network of Workstations, Rossini *et al.* 2007) supports simple parallel computing in R. The R interface supports several different low-level communication mechanisms, including: PVM (via the **rpvm** package), MPI (via **Rmpi**), NetWorkSpaces (via **nws**), and raw sockets (useful if PVM, MPI or NWS are not available). This means it is

possible to run the same code at a cluster with PVM, MPI or NWS, or on single multi-core computer.

The **snow** package includes scripts to launch R instances on the slaves (`cl <- makeCluster()`). The instances run until they are closed explicitly via the command `stopCluster(cl)`. The package provides support for high-level parallel functions like `apply()` and simple error-handling to report errors from the workers to the manager.

snowFT

The **snowFT** package is an extension of the **snow** package supporting fault tolerance, reproducibility and additional management features. The interface is very similar to the **snow** interface. The heart of the package is the function `performParallel()`, which is a wrapper function for `clusterApplyFT()`. Additional management features are functions for repairing a cluster, e.g., to add, remove and restart slaves of a cluster. The package only supports the PVM communication layer.

snowfall

The **snowfall** package (Knaus 2008) supports simple parallel computing in R. It is a top-level wrapper around the package **snow**, meant to ease development of parallel R programs. The interface strives to be as simple as the **snow** interface, yet differs in some aspects. For example it does not require handling of the R cluster object by the user. The package supports the same low-level communication mechanisms as **snow**. Additionally, all functions also work in sequential mode. This can be useful for debugging or when no cluster is present.

The package is designed as a connector to the cluster management tool **sfCluster** (see Section 3.4), but can be used without **sfCluster**.

papply

The package **papply** was developed to augment the parallel `apply()`-functionality of the **Rmpi** package. Similar to the serial `apply()` function, `papply()` applies a function to all items of a list, and returns a list with the results. It uses the **Rmpi** package to distribute the processing evenly across a cluster. If **Rmpi** is not available, it implements this as a non-parallel algorithm. This package is an add-on package to **Rmpi**, contains the function `papply()` and additional debugging support, and is no longer actively maintained.

biopara

The package **biopara** allows the user to distribute execution of parallel problems over multiple machines. It uses raw socket connections (SSH). The package contains only one function: `biopara()`. Every parallel run requires the TCP/IP port numbers and computer hostnames, and all computers have to be in a trusted environment. An R instance has to be started at every worker, or a custom start script has to be executed, in order to spawn the workers manually.

The **biopara** package provides limited fault tolerance and load balancing, and is no longer actively maintained.

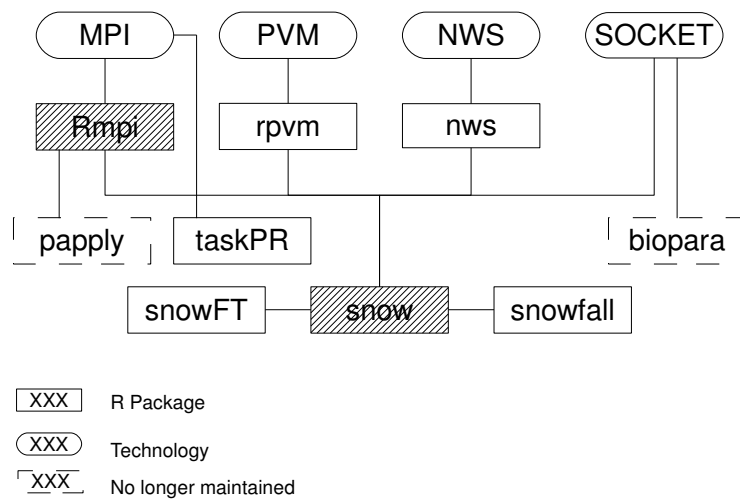


Figure 1: The family tree of R packages for computer clusters. Particularly useful packages are shaded.

taskPR

The **taskPR** package is an interface that uses the MPI implementation LAM/MPI for parallel computing. If there is no available LAM universe, tasks will be executed serially on the manager. A function that needs to be run in parallel has to be enclosed within the function `PE()` and will be executed at the first slave. The next `PE()` call will be executed at the next slave, and so on. There is no support of high-level parallel functions like `apply()`.

Using external libraries: BLAS and PBLAS

R relies on third-party BLAS libraries for common linear algebra and matrix operations. Optimized and parallelized shared-memory implementations of these libraries exist, and can be used for parallel computing on multicomputers and multi-core systems with R (R Development Core Team 2008a).

The Basic Linear Algebra Subprograms (BLAS) is the de-facto application programming interface standard for libraries to perform basic linear algebra operations such as vector and matrix multiplication. The linear algebra routines in R can make use of enhanced BLAS implementations (e.g., ATLAS, Intel MKL) and of parallel BLAS routines: PBLAS (NETLIB 2007) is a collection of software for performing linear algebra operations on any system for which MPI or PVM is available. The library has to be integrated into R when R itself is compiled, using the configuration option `-with-blas` (R Development Core Team 2008a).

3.2. R packages for grid computing

At present, two R packages and one Java-based software collection exist for grid computing in R. These solutions are very new and were presented at the useR! 2008 conference in August 2008.

GridR

The **GridR** package (Wegener *et al.* 2007) submits R functions for execution in a grid environment (on a single computer or a cluster) and provides an interface to share functions and variables with other users (`grid.share()`). Job submission is available via a web service, ssh or locally. Execution modes are from Condor (Tannenbaum *et al.* 2001), Globus (Foster 2005), or single server. The grid infrastructure uses R as interface and client. The server side implementation of **GridR** uses several external software components: Globus Toolkit 4 grid middleware, an installation of the R environment on the grid machines, and a GRMS-Server installation from the Gridge toolkit (Pukacki *et al.* 2006) on a central machine in the grid environment.

The grid configuration can be performed with XML configuration files or at runtime by passing parameters. The main functions are `grid.init()` to initialize the grid and `grid.apply()` to submit a function into the grid environment. This function is different from the R `apply()`-like functions, it does not apply a function to different data. Additionally there are functions to facilitate the management of running grid jobs (e.g., `grid.check()`).

The R package is available at CRAN and the maintainer website (see Table 1).

multiR

The **multiR** package (Grose 2008) is not yet available, but this package was presented at the useR! 2008 conference. The implementation has some similarity with **snow** and **GridR**, but is meant to be independent of the many different types of hardware and software systems. It requires additional software components to be installed before it can be used.

Main differences between **multiR** and **snow** involve job submission (via Grid middleware) and security (certificates). This is implemented with a 3 tier client/server architecture provided by GROWL (Hayes *et al.* 2005). In this architecture, the server component communicates with Grid nodes on behalf of the client. The implementation will extend the `apply()` family of functions, and allows multiple function invocations in a distributed environment.

Biocep-R

The Biocep-R project (Chine 2007) is an open source Java solution for integrating and virtualizing access to servers with R. Tools make it possible to use R as a Java object-oriented toolkit or as a Remote Method Invocation (RMI) server. The Biocep-R virtual workbench provides a framework enabling the connection of all the elements of a computational environment: Computational resources (local machine, a cluster, a grid or a cloud server) via a simple URL, computational components via the import of R packages, GUIs via the import of plug-ins from repositories, or the design of new views with a drag-and-drop GUI editor.

Software and further information is available at the maintainer website (see Table 1). It requires an installed Java 5 run-time and R. The project is under active development. User manuals and tutorials are not yet available.

3.3. R Packages for multi-core systems

There are five different packages using multi-core systems to accelerate computations in R. Four of the implementations are relatively new, they were all developed and presented in the last two years.

pnmath and pnmath0

These two packages (Tierney 2009) offer a parallel implementation of most of the basic R numerical math routines (most of the non-random number, non-BLAS routines) for multi-core architectures. The package **pnmath** uses OpenMP; **pnmath0** uses Pthreads.

On loading, the packages replace built-in math functions with hand-crafted parallel versions. Once loaded, the package provides access to parallel functions with no further changes to user code. The packages use timing estimates (determined at install-time, if possible) to calibrate when the benefits of parallel evaluation outweigh the costs of thread initialization. With numerically intensive code, these packages yield a speed-up of up to a factor given by the number of available processors. The packages work on most platforms, including Windows, but require compiler and library support as detailed in the package README files. Both packages are available at the maintainers website (see Table 1).

fork

The package **fork** (Warnes 2007) provides simple wrappers around the Unix process management API calls: **fork**, **signal**, **wait**, **waitpid**, **kill**, and **exit**. This enables construction of programs that utilize and manage multiple concurrent processes.

The main function of the package is **fork(slave_function)**. This creates a new R instance that is an exact copy of the current R process, including open files, sockets, etc. Communication between the instances uses socket connections **socketConnection()**. There is no support of high-level parallel functions like **apply()** or any error handling.

The R package is available at CRAN and works only in a Unix environment. Commercial support for this package is available from Random Technologies, LLC (<http://www.random-technologies-llc.com/>).

R/parallel

The package **rparallel** (Vera *et al.* 2008) enables automatic parallelization of loops without data dependencies by adding a single function: **runParallel()**. A data dependency occurs when the calculation of a value depends on the result of a previous iteration (e.g., $a[n] = a[n - 1] + 1$). For efficient R programming (see Section 2.1) an **apply()**-like implementation of loops without data dependencies is preferred.

The package uses a master-slave architecture. The implementation is based on C++, and combines low level operating system calls to manage processes, threads and inter-process communications. The package is able to locate loops and automate their parallelization by requiring that the user enclose the **runParallel()** function and the target loop within an **if/else** control structure.

The R package is available at the maintainer website (see Table 1).

romp

The package **romp** (Jamitzky 2008) is only available as a presentation from the useR! 2008 conference; some example code (version 01a) without documentation is available at the maintainers website. The package transforms R code to Fortran, inserts OpenMP directives, and compiles the Fortran code (**compile.mp()**). The compiled code is then executed in R. The example code includes functions **apply.mp()** and **sum.mp()**.

multicore

The **multicore** package provides functions for parallel execution of R code on machines with multiple cores or CPUs. Unlike most other packages, all jobs share the full state of R when parallel instances are spawned, so no data or code needs to be copied or initialized. Spawning uses the “fork” system call or operating system-specific equivalent, and is fast. Spawning establishes a pipe between the master and child process. The pipe can be used to send data from the child process to the master. The package provides high-level parallel functions like `mclapply()` and simple error-handling to report errors from the workers to the manager. The package works on Unix systems, with experimental support for Windows available.

This promising package was released after the body of this review was complete, and is not included in subsequent comparison and discussion.

3.4. Resource manager systems

Deploying parallel computing application becomes increasingly challenging as the number of jobs, users or compute nodes increases. A resource management tool can alleviate such issues. Resource manager systems are software applications to submit, control and monitor jobs in computing environments. Synonyms are job scheduler or batch system. These applications work on the operating system level and mostly directly monitor the communication protocols. Therefore they are independent from the R language. They make the parallel computing environment manageable for administrators, especially if several people work in the same environment and need to avoid resource or scheduling conflicts.

Commonly used resource management systems used with R are described here; an overview is available in Table 2 in the appendix.

SLURM: A highly scalable resource manager

SLURM (Jette *et al.* 2003), the Simple Linux Utility for Resource Management, is an open-source resource manager. **SLURM** is powerful enough to be deployed on clusters containing over 100k processors, yet simple enough to be used for small personal clusters.

SLURM works particularly well with OpenMPI, but can be built for use with different message passing libraries. **SLURM** can be deployed over different high-end fabrics (such as Quadrics or Federation) as well as Myrinet or Ethernet. **SLURM** can also use external batch processing systems such as Maui or Moab.

SLURM provides several key functions. The `salloc` command allocates exclusive and/or non-exclusive access to resources (such as computing nodes) to users for some duration of time. The `sbatch` or `srun` commands provide a framework for starting and executing work (typically a parallel job) on a set of allocated nodes. Job state can be monitored using the `sinfo` and `squeue` commands as well as the `sview` graphical user interface. **SLURM** can also arbitrate contention for resources by managing a queue of pending work. Lastly, job accounting functionality, including record-keeping in SQL backends, is also available.

SLURM is under active development, and is being released under the standard GNU GPL. It is also available as a component of commercial clusters such as IBM’s BlueGene.

SGE: Sun Grid Engine

SGE is an open source batch-queuing system, supported by Sun Microsystems ([Sun Microsystems, Inc. 2002](#)). It is available as an open source or commercial product. **SGE** is responsible for accepting, scheduling, dispatching, and managing the remote execution of large numbers of standalone, parallel or interactive user jobs. It also manages and schedules the allocation of distributed resources such as processors, memory, disk space, and software licenses.

SGE is a very powerful and complex system to manage computer environments ranging from small computer clusters and compute farms up to grid computing networks. It is optimized to manage large environments. There is a large command line user interface to communicate with the **SGE**. The main functions are `qsub` to submit jobs and `qstat` to get a status listing of all jobs and queues. There is also a X-window command interface and monitoring facility.

An R package, called **Rsg**, as interface to the **SGE** queuing system exists and provides functions for using R with the **SGE** environment via the `qsub` command. The package requires an installed and configured **SGE**, a shared network device, and R with an installed **snow** package. It is optimized for the use on computer clusters and not in grid environments.

The package offers functions to get information from the **SGE** (`sge.job.status()`) and to submit work (R code) to an R cluster started from the **SGE** (`sge.apply()`, `sge.submit()`). At the manager the data object is split as specified by the number of jobs. Each data segment along with the function and argument list are saved to a shared network location. Each R instance loads the saved file, executes it, and saves the results to the shared network location. Finally the master script merges the results together and returns the result.

At the time of review the first version of the package was available. The code is not yet complete, and proper documentation is missing. The package does not support any of the parallel computing technologies described in Section 2.2. For the commercial LSF Queuing System a very similar package **Rlsf** ([Smith et al. 2007](#)) exists on CRAN.

sfCluster

sfCluster ([Knaus 2008](#)) is a small resource manager optimized for cluster solutions with R. It is a Unix tool written in Perl for managing and observing R instances running on clusters. Parallel R code has to be written with the **snowfall** package.

sfCluster automatically sets up the cluster for the user, and terminates all running R sessions after execution has finished. It allows multiple clusters per user and offers four execution modes: batch mode (`-b`), interactive R shell (`-i`), monitoring mode (`-m`) and sequential mode (`-s`). For developing parallel code the sequential mode and the `parallel=FALSE` option in the **snowfall** package can be used for developing on a single machine.

The software is available in a beta version at the maintainer website (see Table 2 in the appendix). At the time of review **sfCluster** was only available for Unix systems, and was based on LAM/MPI. The scheduler does not support queue mode and is optimized for the requirements of the maintainers institute.

Further resource manager

There are a lot of other possibilities for resource managers. The choice of an appropriate tool can be difficult, and the decision will likely depend on the architecture used and the specific requirements.

Package	Version	Websites	Technology
<i>Computer cluster</i>			
Rmpi	0.5-6	http://CRAN.R-project.org/package=Rmpi http://www.stats.uwo.ca/faculty/yu/Rmpi	MPI
rpvm	1.0.2	http://CRAN.R-project.org/package=rpvm http://www.biostat.umn.edu/~nali/SoftwareListing.html	PVM
nws	1.7.0.0	http://CRAN.R-project.org/package=nws http://nws-r.sourceforge.net	NWS and socket
snow	0.3-3	http://CRAN.R-project.org/package=snow http://www.cs.uiowa.edu/~luke/R/cluster	Rmpi , rpvm , nws , socket
snowFT	0.0-2	http://CRAN.R-project.org/package=snowFT	rpvm , snow
snowfall	1.60	http://CRAN.R-project.org/package=snowfall http://www.imbi.uni-freiburg.de/parallel/	snow
papply	0.1	http://CRAN.R-project.org/package=papply http://math.acadiau.ca/ACWMac/software/papply.html	Rmpi
biopara	1.5	http://CRAN.R-project.org/package=biopara http://hedwig.mgh.harvard.edu/biostatistics/node/20	socket
taskPR	0.31	http://CRAN.R-project.org/package=taskPR http://users.ece.gatech.edu/~gte810u/Parallel-R	MPI (only LAM/MPI)
<i>Grid computing</i>			
GridR	0.8.4	http://CRAN.R-project.org/package=GridR http://www.stefan-rueping.de/	web service, ssh, Condor, Globus
multiR	-	http://e-science.lancs.ac.uk/multiR/	3 tier client/server architecture
Biocep-R	NA	http://biocep-distrib.R-Forge.R-project.org/	Java 5
<i>Multi-core system</i>			
pnmath(0)	0.2	http://www.cs.uiowa.edu/~luke/R/experimental/	openMP, Pthreads
fork	1.2.1	http://CRAN.R-project.org/package=fork	Unix: fork
rparallel	0.6-20	http://www.rparallel.org/	C++, file
romp	0.1a	http://code.google.com/p/romp	openMP
multicore	0.1-3	http://CRAN.R-project.org/package=multicore	fork

Table 1: Overview of parallel R packages for computer clusters, grid computing and multi-core machines, including the latest version numbers (as of December 2008), the corresponding URLs and technologies.

Package	Version	Releases	First Version	Last Version	Development
<i>Computer cluster</i>					
Rmpi	0.5-6	12	2002-05-10	2007-10-24	++
rpvm	1.0.2	12	2001-09-04	2007-05-09	++
nws	1.7.0.0	8	2006-01-28	2008-08-08	+
snow	0.3-3	9	2003-03-10	2008-07-04	++
snowFT	0.0-2	2	2004-09-11	2005-11-29	0
snowfall	1.60	5	2008-01-19	2008-10-22	+
papply	0.1	1	2005-06-23	2005-06-23	0
biopara	1.5	3	2005-04-22	2007-10-22	--
taskPR	0.31	3	2005-05-12	2008-03-12	-
<i>Grid computing</i>					
GridR	0.8.4	1	2008-12-04	2008-12-04	-
<i>Multi-core system</i>					
fork	1.2.1	6	2003-12-19	2007-03-24	+

Table 2: Versions (in December 2008) of R parallel computing packages available at CRAN, characterized by state of development (++: highly developed, stable; --: in development, unstable).

4. Comparison and discussion

This section provides a discussion and critical comparison of packages for parallel computing with R.

4.1. State of development

It is important to have stable software whose basic functionality changes in a structured fashion. New features need to be introduced to allow leading-edge research. Legacy code might be deprecated and then removed in an orderly fashion, and over several release cycles, to minimize unnecessary disruption of user work flows. With these considerations in mind, we characterize the state of development of R packages in Table 2 (as of December 2008). The characterization is based on the number of released versions, the release frequency and the results from the performance analysis tests shown in Section 4.6 and Appendix B. The table shows only packages for parallel computing which are available via CRAN.

Packages for basic communication protocols MPI and PVM are very well developed, having been available and in wide use for close to a decade. The code and functionality are stable over recent releases. The higher-level wrapper package **snow** is also mature and stable. On the other hand, the package **snowfall** is still being developed, with recent addition of functionality. The **nws** (NetWorkSpaces) package is a relatively recent addition based on previous work; it is mature, while also still being extended. The packages **biopara** and **papply** are no longer actively maintained. The **biopara** package contains many comments and preliminary “debugging” output, and has seen only yearly releases; it is classified as “under development”. Packages assessed as ‘0’, ‘-’ or ‘--’, require or have the opportunity for major code and functionality changes.

4.2. Technology

Table 1 provides an overview of the different technologies employed by the various parallel computing packages. Differences among technologies were described in Section 2.2. For future developments and wide adoption, it is important for all packages to use standardized communication protocols, and to establish platform-independent solutions.

For computer clusters, PVM is still widely used. However, MPI appears to be emerging as a de-facto standard for parallel computing. For parallel computing with R, MPI is the best-supported communication protocol. Different MPI implementations exist and cover many different computer architectures. Most of them are supported by the package **Rmpi**. The higher-level package **snow** can then deploy **Rmpi** (as well as **rpvm**, **nws** or sockets) whereas the package **taskPR** only supports the LAM/MPI implementation. NWS and sleigh represent a slightly different approach to parallel computing with R. The shared global workspace model of these approaches could be very useful for special tasks. A visualization of the technical relation between the packages for computer clusters is available in the family tree in Figure 1.

For grid computing the only available package **GridR** uses the Globus Toolkit. Globus, developed by the Globus Alliance, is probably the most standardized and most widely used middleware for grid computing.

Early interfaces and integration of multi-core technology into R exist as research projects that are under active development. The OpenMP standard for multi-core systems and multiprocessors provides an established technology for parallelization at the compiler level. The package **pnmath** is a promising integration of this technology.

Several packages use coarse-grained processes to evaluate R expressions in parallel. The package **rparallel** uses a master-slave architecture to launch several R instances on the same machine using system-level commands. Every R instance requires its own main memory, and the amount of main memory will frequently limit scalability. The same problem appears for the package **fork**, which is limited to Unix environments.

Installation

In general, installation of packages in the R environment is simple, with the user invoking the `install.packages()` function. This function takes a vector of package names, downloads these packages from on-line repositories, and installs them in user- or system-wide R libraries. However, packages for parallel computing are often based on underlying communications technology (e.g., MPI, PVM) and the packages have to be linked to libraries providing the corresponding technology. The underlying communication libraries have to be installed and configured on the computer cluster. In many cases the communication libraries will be installed by a system administrator, and the R packages must be customized (e.g., using the `configure.args` argument to `install.packages()` function, or in extreme cases by altering the R package configuration files) to find the appropriate communication library.

In order to use some external libraries (such as PBLAS) the R program itself has to be recompiled and reinstalled.

4.3. Fault tolerance and load balancing

Fault tolerance for parallel algorithms provides continued operations in the event of failure of some slaves. On the other hand, load balancing is a technique to spread processes between

	Learnability	Efficiency	Memorability	Errors	Satisfaction
RmpiR	+	--	++	+	+
rpvm	--	--	+	-	--
nws	+	+	++	+	+
snow	+	++	++	+	++
snowFT	+	++	++	+	++
snowfall	++	++	++	+	++
papply	+	+	++	+	0
biopara	--	--	0	0	--
taskPR	+	-	++	0	-

Table 3: Assessment of the usability of the R packages for computer clusters (ranging from ++ to --).

resources in order to get optimal resource utilization. Both aspects are very important in the field of parallel computing.

Only the packages **snowFT** and **biopara** have integrated solutions for fault tolerance. Thus for many common use cases the users must accommodate the possibility of failure during lengthy calculations.

The packages **Rmpi**, **snow**, **snowFT**, **snowfall** and **biopara** support load balancing for the `apply()` functions. Resource managers (discussed below) can help with load balancing.

4.4. Usability

Usability describes how easily software can be deployed to achieve a particular goal. Given the focus of R on statistical computing, this section stresses use cases that can arise in a variety of statistical analyses.

For computer clusters, the basic communication packages **Rmpi** and **rpvm** cover the full functionality of both communication standards and provide an essentially complete API to these standards. The complexity of the full API makes these packages somewhat more difficult for researchers with primarily statistical interests to become familiar with. The other R packages for computer clusters were developed to improve usability by providing a somewhat higher level of abstraction. Table 3 shows an estimation of the components of usability (Shneiderman and Plaisant 2004) for R packages for computer clusters. “Learnability” describes how easy it is for first-time users to learn functionality. “Efficiency” describes how quickly users can perform tasks. “Memorability” is the assessment of how easily users can reestablish details required for use. How to avoid errors and to fix them is reviewed in “Errors”. “Satisfaction” describes how pleasant it is to use a package.

To assess the learnability of R packages the quality of the vignettes and help files were reviewed. Only the package **snowfall** integrates a vignette into the R package. The existence of online tutorials for the packages **Rmpi** and **snow** improves their learnability score.

To get good efficiency for an R package it is important to provide functions that facilitate writing simple code. Code based directly on the **Rmpi** and **rpvm** packages can become complex, because the user must interact with the communication API at a relatively low level. **biopara** and **taskPR** only have functions for sending commands to workers, so a lot of additional code

	Learnability	Efficiency	Memorability	Errors	Satisfaction
<i>Grid computing</i>					
GridR	+	–	+	–	–
rparallel	0	+	+	–	0
<i>Multi-core system</i>					
pnmath(0)	++	++	++	++	+
fork	+	–	+	–	–

Table 4: Assessment of the usability of the available R packages for grid computing and multi-core systems. (ranging from ++ to --).

for basic functionality has to be implemented by the user.

R’s package structure provides for help files, and allows optional vignettes, so the memorability score for every R package is elevated. However, some packages provide incomplete, complex, or difficult to navigate help files. This leads to lower scores.

In order to correct and fix errors, it is important that functions provided by a package help the user to identify sources of error. For example, parameters should be checked for correctness before use. The scoring criteria for “Errors” was determined based on experiences during creation of test code in the appendix.

For satisfaction, the functionality provided by the different packages was compared. The packages **rpvm**, **biopara** and **taskPR** provide only very basic functions for parallel computing. The packages **snow**, **nws** and **Rmpi** have scripts to launch R instances at the workers. The packages **snowFT** and **snowfall** use scripts from the package **snow**.

The usability assessment of packages for grid computing is very difficult to determine, due to lack of mature and stable packages. Table 4 shows an estimation of the components of usability for available R packages for grid computing and multi-core systems.

In the **GridR** package the user has to deal with intricate configuration and connection to the grid system. Once the configuration is finished, the parameters can be reused in subsequent runs. Complex jobs require the user to implement a lot of additional code.

The usability of the packages **pnmath** is excellent. Once the package is loaded, parallelization runs without further code modification; the user employs familiar R functions. The package **rparallel** is still in development and adequate documentation is missing, but the usability of the code is promising. Implementing R’s **apply()**-like functions for loops without data dependencies would be a valuable addition to this package (see Section 2.1).

4.5. Acceptance

To evaluate the acceptance of parallel computing packages, the number of links from the DESCRIPTION files of other packages was counted. We used the **Bioconductor** (Gentleman *et al.* 2004) repository as a reference set of packages. This repository comprises about 294 R packages oriented towards research in bioinformatics and computational biology. Four packages use **snow**, three **Rmpi** and one package carries an additional references to **rpvm**. Therefore about 2% of the bioinformatic packages use parallel computing technologies, the packages **snow** and **Rmpi** are used exclusively.

Similar results can be found in the Comprehensive R Archive Network (CRAN) with more than 1700 R packages. The **snow** package is used by 21 (1.2%) packages and **Rmpi** by 10 (0.5%) packages. All other packages are used at the most two times.

The packages for grid computing and multi-core systems are in active development and not yet used in any other package. Only example code and applications exist for proof of principle and functionality.

4.6. Performance

Performance of the different parallel computing packages can differ due to a number of reasons. Among these reasons, design and efficiency of the implementation as well the technology and hardware are likely the dominant factors.

A benchmark was designed to evaluate the performance of the cluster packages. A performance evaluation of the packages for grid computing and multi-core systems was not possible, mainly due to unavailability or complex system requirements of the packages. The package **rparallel** was excluded from the benchmark, because the benchmark does not include a component for loops without data dependencies. The package **pnmath** was excluded because in the benchmark no NMATH routines were used.

The benchmark analysis was further restricted by focusing on packages providing functionality that allows all benchmark code to be run in a meaningful fashion. The packages **snowFT**, **papply**, **biopara**, **taskPR** and **rpvm** were excluded from the benchmark. The package **biopara** only supports socket connections, the package **taskPR** only supports the LAM/MPI implementation and both packages are unstable. The package **rpvm** does not have scripts to launch R instances at the slaves. There is only a function (`.PVM.spawnR()`) to run a R script file at the workers, therefore data can not be stored in R worker instances. The packages **snowFT** and **papply** are add-on packages which use the same communication mechanism as **snow** and **Rmpi**. They include additional functionality for better usability or error handling. Therefore they execute additional checks that reduce performance. The same behavior can be found for the **snowfall** package. For these packages all time measurements for the three components tests are about 10% slower than the computations with the **snow** package.

The benchmark comprises three different components: Sending data from the manager to all workers, distributing a list of data from the manager to the workers and a classic parallel computation example from the numerical analysis literature, the integration of a three-dimensional function. Details and code are provided in Appendix B. The computation times for each package and scenarios are summarized in Table 5.

Component test 1 sends a lot of data to all workers. Data transmission is relatively expensive in terms of time. In the **Rmpi** package the `mpi.bcast()` command is used for sending data to the workers. This uses a very efficient tree-like algorithm to broadcast the data. All other packages send the data in a serial loop over all slaves from the manager to the workers. One data sending operation must finish before the next starts (the `snow.time()` function in **snow** helps to visualize this process; see Figure 2).

The package **nws** sends every communication through the NetWorkSpace server. Component 1 and 2 show a bottleneck due to this communication model. Even in component 3 the **nws** implementations are the slowest solutions.

	Component 1	Component 2	Component 3
Rmpi	0.91	1.83	3.00
nws	14.87	3.49	3.03
snow			
MPI	10.33	2.00	2.96
PVM	4.13	1.01	2.93
NWS	8.68	1.58	2.98
socket	3.47	0.93	2.90
snowfall			
MPI	13.99	2.07	2.93
PVM	4.29	0.94	2.93
NWS	8.82	1.62	2.99
socket	3.77	1.00	2.91

Table 5: Computing time in seconds of the performance evaluation of R packages for computer clusters.

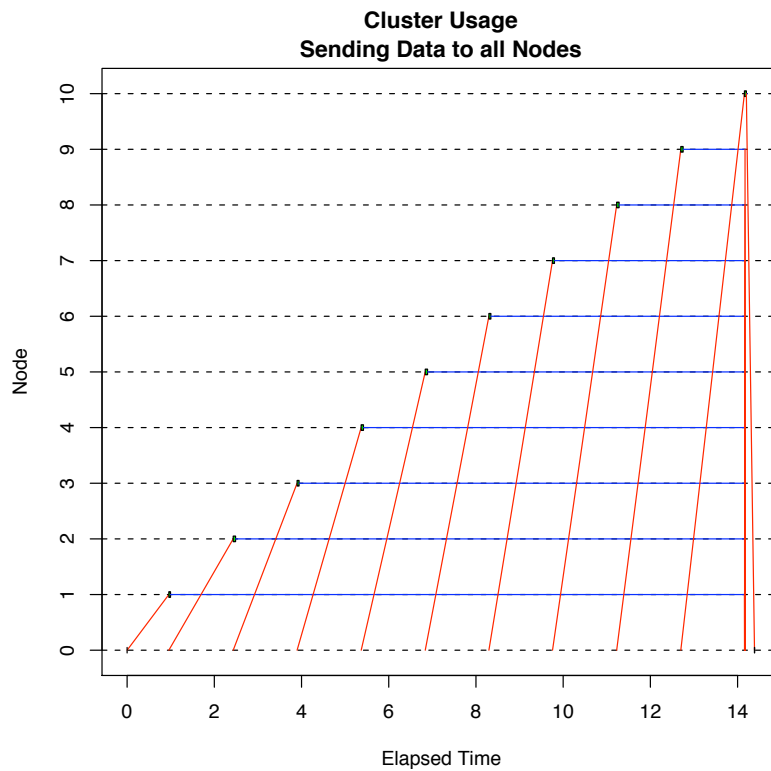


Figure 2: Visualization of timing information for cluster usage for component test 1 with the **snow** package using MPI. Green rectangles (near the diagonal) representing active computation (in this case very small), blue horizontal lines representing a worker waiting to return a result, and red lines representing master-slave communications.

For component 3 there are three different ways for a serial implementation: using nested for-loops (75.6 sec), using vectorization (0.01 sec) and using the `apply()` function (21.1 sec). As mentioned in Section 2.1, improvements in the serial version of the code are of great importance. For the parallel implementation an `apply()`-like implementation was used (see Appendix B). This implementation is comparable to the serial `apply()` function. The parallelization achieves an improvement of a factor 10 compared to the serial `apply()` function.

The package **snow** (when using sockets) is the fastest solutions for parallel computing with R. If the ratio of communication and calculation time is good (see component test 3 and Figure 2 in the appendix), all packages have similar performance.

5. Application examples and tips for parallel computing

In this section we briefly describe two application packages which use the technologies that were discussed above. The section ends with some general tips for parallel computing in R.

5.1. Application examples

These application examples serve as concrete illustration for the increased efficiency of parallel computing with R. Both packages are available via the **Bioconductor** repository (<http://www.Bioconductor.org/>).

affyPara

The package **affyPara** (Schmidberger and Mansmann 2008) contains parallelized functions for preprocessing of exploratory oligonucleotide microarray analysis. The package is designed for large numbers (>200) of microarrays. It distributes arrays to different workers and accelerates the standard preprocessing methods by up to a factor of 15. The package is based on the cluster package **snow** and extends the package **affy**. Users switching from **affy** to **affyPara** must make only minor code changes. One limitation in the design of **affyPara** is that it re-implements rather than reuses **affy**; changes in **affy** require implementation of corresponding changes in **affyPara**.

ShortRead

The package **ShortRead** (Morgan *et al.* 2008) implements base classes, functions, and methods for representation of high-throughput, short-read sequencing data. Raw data from single experiments is very large (e.g., 10's of GB). Considerable computational processing can be required to summarize this data for down-stream analysis. If a running **Rmpi** cluster is available, **ShortRead** distributes the data processing across available workers. The only user-level requirement for accessing this performance benefit is to load the **Rmpi** package. **ShortRead** illustrates how parallel processing can be integrated into R packages without requiring extensive user participation.

A number of other application packages have similar integration of parallel computing in R. All of these offer good performance improvements using parallel computing techniques. In general, the integration of serial and parallel code into one package is preferred as it provides the possibility of using the packages on both a single-processor machine and in parallel environments, without requiring duplicate code development.

5.2. Tips for parallel computing with R

In closing this section, it is appropriate to reiterate some generally-accepted best practices from parallel computing:

- Communication is much slower than computation; care should be taken to minimize unnecessary data transfer to and from workers, and to maximize the amount of computation performed in each remote evaluation.
 - Some functions produce large results, so it pays to reduce these on the workers before returning.
 - Very large objects, e.g., provided as additional `apply()`-like function parameters, might in some cases be more efficiently constructed on each worker, rather than being forwarded from the manager to each worker.
- Random number generators require extra care. It is important to avoid producing the same random number stream on each worker, and to facilitate reproducible research. Special-purpose packages (**rsprng**, **rlecuyer**) are available; the **snow** package provides an integrated interface to these packages. An overview of random number generator packages is available in Table 3 in the appendix. Reproducible research requires the ability to partition and schedule jobs across the same number of workers, and in a reproducible order. The `apply.seq` argument of `apply()`-like functions in the **Rmpi** package provides facilities for achieving this scheduling.
- R's rules for lexical scoping, its serializing functions and the environments they are defined in all require some care to avoid transmitting unnecessary data to workers. Functions used in `apply()`-like calls should be defined in the global environment, or in a package name space.

The enthusiasm for high performance computing in R has lead the user community to create a new mailing list, starting in October 2008 (<https://stat.ethz.ch/mailman/listinfo/R-sig-hpc>). The list is the recommended place for asking questions about parallel computing with R.

6. Summary and outlook

In this section, we provide a brief summary of the “state of the art” of parallel programming with R. We also provide an outlook about possible future developments.

6.1. State of the art

As we discussed in Section 4, two well developed R packages stand out for use in high-performance multicomputer environments: **Rmpi** and **snow**. Both have acceptable usability, support a spectrum of functionality for parallel computing with R, and deliver good performance. Other packages try to improve usability, but so far usability gains have usually been achieved at the expense of lower functionality.

Facilities to harness multi-core architectures exist. External and architecture optimized libraries (e.g., PBLAS) represent one solution. However, linear algebra is not always a substantial bottleneck in general statistical computation. The packages **Rmpi** and **snow** can use

several R instances started at one machine, using sockets or MPI for communication. However, every R instance requires its own main memory, and the amount of main memory will frequently limit scalability.

Early-stage packages for grid computing are available. Further developments hinge on a clearer understanding of how grid infrastructure can be leveraged for statistical applications.

6.2. Further developments

R packages for multicomputer environments are well developed and very useful. There is room for minor improvements in documentation (e.g., adding vignettes to aid new users in establishing simple clusters) and performance optimization. The most exciting prospects for new development are in areas other than the multicomputer environment covered so well by **snw** and **Rmpi**.

Multi-core systems are now very common, and the number of processors per chip is growing. There is a compelling need for integration of R code into multi-core environments. The **pnmath** packages are a first step in this direction. This approach has the potential to speed up numerically intensive code, yielding a factor of improvement given by the number of available processors. Enabling multi-core functionality as implemented in **pnmath** required manual adjustment of all C-level functions. To design a package to support a more abstract use of multi-core systems for package development seems to be a very difficult task; the interactive nature of R and existing multi-core technology implies runtime compilation. The **multicore** package, first released after this review was complete, represents a very promising approach to processing on multicore chips.

From an end-user perspective, computer clusters are often unavailable, the physical costs (acquisition, maintenance, etc.) are high, and effective use requires a diverse skill set (e.g., advanced user-level system configuration, mastery of batch job submission, careful formulation of problems to effectively manage communication costs). Therefore it is difficult to use this technology. Cloud computing (Vouk 2008) allows users to access services from the Internet without knowledge of the technology infrastructure that supports them. These web services provide resizable computer capacity in the cloud. There are several companies which offer computing services for relatively modest costs. Cloud computing usually offers pre-defined “machine images” that contain OpenMPI support, and that can be extended with the latest R version and packages. An exciting prospect would be the development of a new R package for communication with the cloud, a web portal to control access, and an appropriate business model for managing costs. Such a cloud computing package could provide cost-effective cluster-based computing to end users.

In terms of hardware, the (parallel) computing power of graphic processing units (GPUs) might provide significant performance benefits to R users. Following on the earlier releases of vendor-specific APIs (e.g., nVidia (2007) proposed CUDA), standards for programming GPUs in a vendor-independent fashion are beginning to emerge (Khronos Group 2008). They offer a programming model that is designed to allow direct access to the specific graphics hardware, with the graphics hardware running a very high number of threads in parallel. A bioinformatics application for sequence alignment with GPUs (C code, no R integration) has been published by Manavski and Valle (2008) and illustrates the usability of GPUs for acceleration and management of large amounts of biological data.

The flexibility of the R package system allows integration of many different technologies to address practical statistical questions. This provides an excellent opportunity to explore and prototype how different approaches can be effectively integrated into end-user software. This leads us to expect that whichever technologies emerge, R should be well-positioned to take advantage of them.

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