## PEBBL 2.0 User Guide

Jonathan Eckstein\* Cynthia A. Phillips<sup>†</sup>

January 2019

#### Abstract

PEBBL is a C++ framework for implementing general parallel branch-and-bound optimization algorithms, providing a mechanism for the efficient implementation of a wide range of branch-and-bound methods on an large variety of parallel computing platforms. This document describes:

- The history, goals, and general properties of PEBBL
- How to download and compile PEBBL
- PEBBL's special search capabilities, including enumeration, early output, and checkpointing
- PEBBL's ability to enumerate multiple solutions meeting various criteria
- PEBBL's basic architecture, including its serial and parallel layers
- The design of the serial layer and the notion of manipulating subproblem states
- The design and capabilities of the parallel layer
- How to build a simple serial branch-and-bound algorithm using PEBBL
- How to extend a serial implementation into a parallel one
- Many of the numerous parameters that can be used to control PEBBL's behavior.

<sup>\*</sup>Management Science and Information Systems and RUTCOR, Rutgers University, 100 Rockafeller Road, Piscataway, NJ 08854

<sup>&</sup>lt;sup>†</sup>Sandia National Laboratories, Mail Stop 1318, Albuqurque, NM 87123

# Contents

1	Introduction									
	1.1	What	is PEBBL?	4						
	1.2	Chang	ges in this release	4						
	1.3	The G	enealogy of PEBBL	5						
2	Dov	Downloading and Compiling PEBBL 5								
	2.1	Systen	n requirements	5						
	2.2	Downl	oading PEBBL	6						
	2.3	Struct	ure of the pebbl directory	6						
	2.4	Config	guration	6						
		2.4.1	Configuring with cmake-gui	7						
		2.4.2	Configuring with ccmake	9						
	2.5	Compi		2						
	2.6			13						
0		1 • 4								
3				4						
	3.1		V	15						
		3.1.1	9,	15						
		3.1.2		17						
		3.1.3	, , , , , , , , , , , , , , , , , , ,	19						
	3.2		O .	21						
		3.2.1		21						
		3.2.2	1	21						
		3.2.3		22						
		3.2.4	, I	22						
	3.3		v	23						
		3.3.1	1	23						
		3.3.2	9	25						
		3.3.3		26						
		3.3.4	Work distribution between clusters	28						
		3.3.5	Ramp-up: starting the parallel search	31						
		3.3.6	Enumeration in parallel	32						
		3.3.7	On-processor multitasking: threads and the scheduler	32						
4	$\operatorname{Cre}$	ating I	PEBBL Applications 3	5						
1	4.1	_		35						
	4.2			36						
	<b>-</b>	4.2.1		36						
		4.2.2	v S	39						
		4.2.3		12						
		4.2.4		15						
		1.4. I		٠,						

		4.2.5	Selected additional methods	46
		4.2.6	Creating your own parameters	47
		4.2.7	Serial main programs: drivers	49
		4.2.8	"Quiet" operation	51
		4.2.9	Retrieving solutions to C++ code	51
		4.2.10	Debugging outputs	51
	4.3	Definir	ng a parallel application	52
		4.3.1	Methods you should create — parallelBranching-derived class	54
		4.3.2	Methods you should create — parallelBranchSub-derived class	56
		4.3.3	Standard disambiguations	57
		4.3.4	Parallel solution management and parallel reset	58
		4.3.5	Incumbent heuristics in parallel	60
		4.3.6	The ramp-up phase and parallel preprocessing	62
		4.3.7	Providing for checkpoints	63
		4.3.8	The main program: serial/parallel drivers	64
		4.3.9	Running in communicators other than MPI_COMM_WORLD	65
		4.3.10	Retrieving solutions to C++ code	65
_	ъ			<b>~</b> =
5	Para		67	
	5.1			67
	5.2	_	0 0 1	68
	5.3		eration	70
	5.4	Genera		71
	5.5		bent	71
	5.6		t	71
	5.7		el work distribution	73
	5.8		el thread control	76
	5.9		up (standard implementation)	77
	5.10		order and protocol	78
	5.11	Termir	nation	80
6	Pvt	hon-Rs	ased Utilities	82
-	6.1			82
	6.2			82
	0.2	- 1110 PC		02

## 1 Introduction

### 1.1 What is PEBBL?

PEBBL (Parallel Enumeration and Branch-and-Bound Library) is a C++ class library for constructing serial and parallel branch-and-bound optimization algorithms. It is a framework, shell, or skeleton that handles the generic aspects of branch and bound, allowing the developer to focus primarily on the unique aspects of their particular branch-and-bound algorithm. It is thus similar to other software projects such as PUBB [18, 17], BoB [12], PPBB-Lib [20], and ALPS [15] (PEBBL's development has significantly influenced the architecture of ALPS). PEBBL has a number of unique features, including very flexible parallelization strategies and the ability to enumerate near-optimal solutions.

In principle, one can build an arbitrary branch-and-bound method atop PEBBL by defining a relatively small number of abstract methods. By defining a few more methods, the algorithm can be immediately parallelized. PEBBL contains numerous tuning parameters that can adapt the resulting parallel implementation to any parallel architecture that supports an MPI message passing library [19].

## 1.2 Changes in this release

The principal changes in PEBBL since the prior release (version 1.6) are:

- 1. The ability to run within a user-specified MPI communicator, as opposed to only within MPI\_COM\_WORLD.
- 2. Support for multi-level parallelism throughout the search process for example having clusters of 100 MPI processes to process each subproblem, but using many such clusters in parallel to explore different parts of the search tree simultaneously **Still have to do this!**
- 3. Distribution through github.com using git, rather than through a Sandia labs server using subversion (svn).
- 4. Adoption of the cmake build system in place of autoconf.
- 5. Separation from the ACRO family of packages. PEBBL now consists of just one package and has no external dependencies. Some parts of the old UTILIB package are now embedded with PEBBL.
- 6. As part of the separation from ACRO, the directory structure of PEBBL has been completely reworked and greatly simplified, as described in Section 2.3 below. Related changes include
  - C++ #include directives for PEBBL are now naturally self-documenting in that header file names starting with pebbl/. There is no longer a "flattened" copy of

the include files structure, so subdirectories such as pebbl/bb or pebbl/pbb must be explicitly specified.

- The file names for the included Python scripts now end in .py.
- 7. Miscellaneous bug fixes.

## 1.3 The Genealogy of PEBBL

Most of the development work on PEBBL has been carried out by

- Jonathan Eckstein, Rutgers University
- William Hart, Sandia National Laboratories
- Cynthia A. Phillips, Sandia National Laboratories.

PEBBL was originally the "core" layer of the PICO (Parallel Integer and Combinatorial Optimization) package. PICO was designed to solve mixed integer programming problems, but included a "core" layer supporting implementation of arbitrary branch and bound algorithms. In the Spring of 2006, the development team decided to distribute this core layer as a software package in its own right, changing its name from "the PICO core" to PEBBL. Much of PEBBL's basic design is thus described in preliminary publications concerning PICO [6, 8, 7]. In fact, significant portions of this user guide are derived from Eckstein et al. [7, 8].

PEBBL's parallelization strategies are partially patterned after CMMIP [4, 5], a parallel mixed integer programming solver developed for the Thinking Machines CM-5 parallel supercomputer. CMMIP, however, was specifically designed for mixed integer programming, and to take advantage of particular features of the CM-5 architecture. PEBBL is more generic in two senses: it is a framework that one can use to implement any branch-and-bound algorithm, and it is designed to run in a generic message-passing environment. The ABACUS package [10] also influenced some of PEBBL's design.

## 2 Downloading and Compiling PEBBL

## 2.1 System requirements

- A Unix-like operating systems (including Linux, Mac OS X, or some version of the Linux subsystem for Microsoft Windows). This guide assumes basic familiarity with the command-line interface to such environments.
- The git version management system (required for initial download only)
- The cmake configuration and build system (including GNU make)
- A C++ compiler, such as g++
- For parallel execution, some form of MPI, such as OpenMPI or MPICH.

These packages should be readily installable in most Unix-like systems.

The PEBBL distribution also includes some Python scripts, for which a Python interpreter is needed. These scripts perform auxiliary functions and are not required to run PEBBL.

## 2.2 Downloading PEBBL

To download the latest version of PEBBL, issue the following git command:

git clone https://github.com/PEBBL/pebbl.git

This command will create a directory called pebbl.

## 2.3 Structure of the pebbl directory

PEBBL's directory structure has been greatly simplified from prior releases. The subdirectories of pebbl are:

- src Contains the source code. Nearly all the contents of this directory is within a subdirectory pebbl (which allows PEBBL C++ #include statements to naturally self documenting). Within pebbl/src/pebbl, header and .cpp files are mixed in seven further directories pebbl/src/pebbl/bb (for "branch-and-bound"), pebbl/src/pebbl/comm (for "communication"), and so forth.
- data Contains data files for the example application programs. Its subdirectories are pebbl/data/knapsack for the simple knapsack solver and pebbl/data/monomial for the maximum monomial agreement solver.
- doc Contains documentation, include the PDF of this document. Currently, the only sub-directory in this location is pebbl/doc/uguide, which contains the LaTeX source and other files necessary to produce this document.

scripts contains some useful Python scripts related to PEBBL.

## 2.4 Configuration

PEBBL now uses cmake and an "out-of-source" build scheme. To configure PEBBL for your system, create another directory at the same level as the pebbl directory created by git; this directory will hold your compiled version of PEBBL. From here on, this document will assume that this directory is called buildpebbl, but the name can be anything you wish.

Before compiling, you must configure PEBBL. To do so, first descend into the buildpebbl directory. If you are in an environment with usable X graphics, then give the command

If your system does not have usable X graphics (for example, if running over a slow remote connection) then instead give the command

ccmake ../pebbl

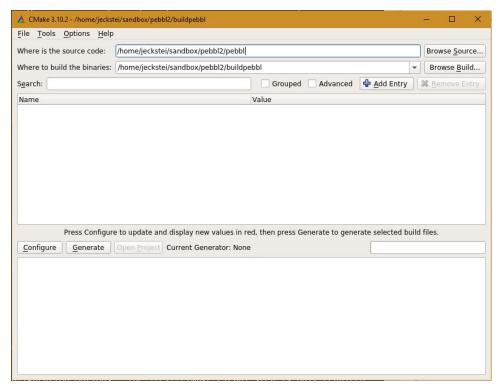


Figure 1: Initial display from cmake-gui.

#### 2.4.1 Configuring with cmake-gui

After you start cmake-gui, a window like the one shown in Figure 1 should appear. Start the configuration process by pressing the "Configure" button on the lower left, after which a window like that in Figure 2 should pop up.

For ordinary applications, it is sufficient to press the "Finish" button in this pop-up window, which selects the default native compilers. If you wish to specify a non-default C++ compiler or use a cross-configuration environment, you may select one of the other options. This guide covers only the default native case.

The next display from cmake-gui should resemble Figure 3. You should now select the build options you desire by modifying the entries in the "Value" column of this display.

CMAKE\_BUILD\_TYPE: The default value "Release" builds a version of PEBBL with compiler optimization and without symbol table information. You may change this to "Debug" to build a version with symbol table information (the -g option in many compilers). A "Debug" version will be somewhat slower but allow symbolic debuggers such as gdb to view PEBBL's internal code. You may still compile your own application with debugging information, but compile PEBBL itself in "Release" mode.

CMAKE\_INSTALL\_PREFIX: Specifies where the command make install will attempt to install the PEBBL headers and library.

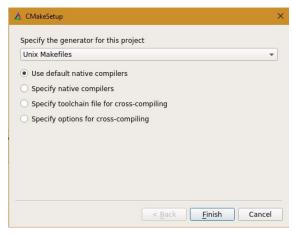


Figure 2: Generator choice pop-up from cmake-gui.

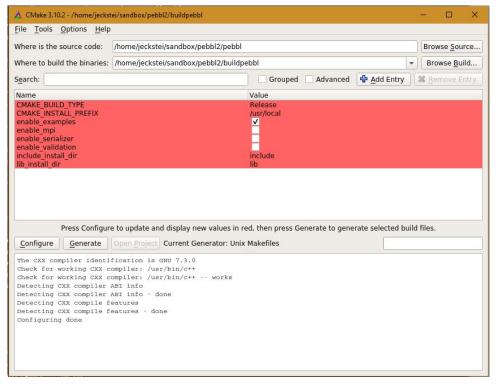


Figure 3: Appearance of cmake-gui after initial configuration step.

- enable\_examples: Leave checked to build the sample applications that come with PEBBL, or uncheck to build only the PEBBL library. The sample applications can be useful in verifying that PEBBL was built successfully.
- enable\_mpi: Check this box to build both the parallel and serial layers, which requires a version of MPI. If you leave this box unchecked, only the serial layer will be built, with the modules in the parallel layer treated as "stubs". See Section 3, page 14 for an explanation of the distinction between the serial and parallel layers.
- enable\_serializer: This option should ordinarily be left unchecked. It enables some utility functions that may slightly improve performance but are not compatible with the recent C++ compilers.
- enable\_validation: Enables some internal error-checking functions that may have a small negative impact on run-time performance.
- include\_install\_dir: This option controls the location of header files within the specified CMAKE\_INSTALL\_PREFIX directory. It should ordinarily be left unchanged.
- lib\_install\_dir: This option controls the location of the PEBBL object library within the specified CMAKE\_INSTALL\_PREFIX directory. It should ordinarily be left unchanged.

A host of additional options are available by checking the "Advanced" box above the option table. These options may be helpful if you are need to configure with specific compilation or linking flags, but are not discussed further in this document.

Figure 4 shows the appearance of cmake-gui after enabling MPI and specifying the directory installpebbl (at the same level as pebbl and buildpebbl) as the installation target directory. Press the "Configure" button again, and the message pane at the bottom of the cmake-gui window should the messages shown in Figure 5. Press the "Configure" button once more, and you should see the messages "MPI Enabled" and "Configuring done", as shown in Figure 6. This status indicates that cmake is ready to generate makefiles. Press the "Generate", after which "Generating done" should appear in the message pane. At this point, PEBBL has been configured; you may close the cmake-gui window.

#### 2.4.2 Configuring with ccmake

The cmake-gui configuration process requires an X display. If an X display connection is not available or practical, PEBBL may instead by configured using the ccmake terminal-interface tool or by issuing cmake shell commands. This section describes the ccmake configuration procedure.

You initiate ccmake configuration much as with cmake-gui: descend into the buildpebbl (or equivalent) directory and enter the command

ccmake ../pebbl

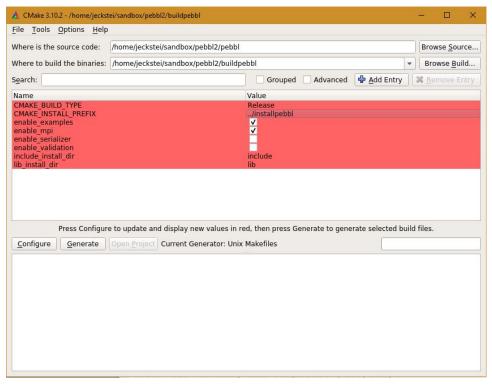


Figure 4: Appearance of cmake-gui after selecting (sample) configuration options.

```
MPI enabled.
Found MPI_CXX: /usr/lib/x86_64-linux-gnu/openmpi/lib/libmpi_cxx.so (found version "3.1")
Found MPI: TRUE (found version "3.1")
Configuring done
```

Figure 5: Appearance of lower cmake-gui pane after second configuration iteration.



Figure 6: Appearance of lower cmake-gui pane after third configuration iteration (indicating that it is ready generate makefiles).

Near the top of the terminal screen, you should now see the message EMPTY CACHE. Press the c key to initiate the first cmake configuration cycle. Shortly, the display should change to

CMAKE\_BUILD\_TYPE \*Release CMAKE\_INSTALL\_PREFIX \*/usr/local enable\_examples \*0N enable\_mpi \*OFF enable\_serializer \*OFF enable\_validation \*0FF \*include include\_install\_dir lib\_install\_dir \*lib

These options have the same interpretation as the those in the previous section of this document. You move between options with the keyboard up and down arrow keys, and pressing the enter key toggles between ON and OFF settings or allows you to enter new values. For example, to turn on debugging, validation, and the parallel layer, while setting the installation directory to be installpebbl in the same parent directory as buildpebbl, you would change the options above to

CMAKE_BUILD_TYPE	*Debug
CMAKE_INSTALL_PREFIX	*/installpebbl
enable_examples	*ON
enable_mpi	*ON
enable_serializer	*OFF
enable_validation	*ON
include_install_dir	*include
lib_install_dir	*lib

CMAKE DUTED TOOP

Press the c key again to initiate another cycle of configuration. Shortly you should see the following display:

MPI enabled.

Debug mode enabled.

Press the e key to return to the main ccmake display level. Continue pressing the c and then e keys until the option

Press [g] to generate and exit

becomes visible among the choices near the bottom of the main ccmake display screen. At this point, press the g key; ccmake should then generate the necessary makefiles and exit.

If you need access to advanced cmake options during the ccmake configuration process, press the t key to make them visible. Pressing t again hides the advanced options.

## 2.5 Compiling and installing

Once the cmake configuration process is complete (using either cmake-gui or ccmake), you compile PEBBL by simply issuing the command make in the buildpebbl directory. The resulting output should have the following appearance:

```
Scanning dependencies of target pebbl
[ 1%] Building CXX object src/pebbl/CMakeFiles/pebbl.dir/bb/branching.cpp.o
[ 2%] Building CXX object src/pebbl/CMakeFiles/pebbl.dir/bb/loadObject.cpp.o
[ 3%] Building CXX object src/pebbl/CMakeFiles/pebbl.dir/bb/pebblBase.cpp.o
[ 4%] Building CXX object src/pebbl/CMakeFiles/pebbl.dir/bb/pebblParams.cpp.o
[ 5%] Building CXX object src/pebbl/CMakeFiles/pebbl.dir/comm/MessageID.cpp.o
[ 6%] Building CXX object src/pebbl/CMakeFiles/pebbl.dir/comm/coTree.cpp.o
[ 95%] Building CXX object src/pebbl/example/CMakeFiles/commTest.dir/parKnapsack.cpp.o
[ 96%] Building CXX object src/pebbl/example/CMakeFiles/commTest.dir/serialKnapsack.cpp.o
[ 97%] Linking CXX executable commTest
[ 97%] Built target commTest
Scanning dependencies of target lipshitzian
[ 98%] Building CXX object src/pebbl/example/CMakeFiles/lipshitzian.dir/lipshitzian.cpp.o
[ 100%] Linking CXX executable lipshitzian
[ 100%] Built target lipshitzian
```

You may accelerate the compilation process by using the -j option of make to use multiple parallel threads. For example, on a system with 8 processor cores, you could issue the command

which would attempt to use 8 processes in parallel to speed up the compilation.

After compilation, the PEBBL object library, libpebbl.a may be found in the directory buildpebbl/src/pebbl, and the example application executables (if enabled) may be found in buildpebbl/src/pebbl/example.

If you wish to use the install procedure, issue the command

#### make install

after the compilation has completed successfully. If the configured install directory is a system directory such as /usr/local, you must have administrator priviledges and use the command sudo make install instead.

The make install command copies the PEBBL header files and static library to the installation directories specified during configuration. With the options shown in the previous two subsections, the header and library files would be copied to ../installpebbl/lib, respectively.

## 2.6 Testing

PEBBL provides a testing script to verify the success of the compilation process. In the same buildpebbl directory as you performed the make operation, you launch the testing script by giving the command

```
../pebbl/scripts/testScript.py
```

The script will only work correctly when run with the current working directory set to the top of the build directory tree. The test script does not require the install step described at the end of the previous section.

If you only configured with the serial layer, the testing script will only perform serial testing. In this case, the output should look like:

```
Only a serial configuration found -- maxprocs reset to 1.

Knapsack tests --
animals.1: 1
animals.2: 1
scor1k.3: 1
test-data.1000.1: 1
Monomial tests --
testdata: 1
pima-indians-diabetes.ss.33.bin: 1
Tests passed
```

If you cofigured with the parallel layer, the script defaults to running both serial tests and parallel tests using between 2 and 32 MPI processes. In this situation, its output should look like:

```
Knapsack tests --
animals.1: 1 2 4 8
animals.2: 1 2 4 8
hard24: 4 8 16 32
scor1k.3: 1 2 4 8 16 32
test-data.1000.1: 1 2 4 8
v24: 4 8 16 32
v24b: 4 8 16 32
Monomial tests --
testdata: 1 2
cmc.data.ss.bin: 16 32
pima-indians-diabetes.ss.33.bin: 1 2 4 8
Tests passed
```

For example, animals.1: 1 2 4 8 means that the knapsack test instance animals.1 was run successfully in serial and with 2, 4, and 8 MPI processes (each test instance has a range of MPI process counts in which it is tested).

The test script has a variety of command-line options, as follows:

- --minprocs=p: The smallest number of MPI processes to be tested to p (default 1)
- --maxprocs=P: The largest number of MPI processes to be tested to P (default 32 if parallel layer was compiled, and 1 if only the serial layer wascompiled)
- --add=a: The additive step between successive MPI process counts to be tested (default 0)
- --multiply=m: The multiplicative step between MPI process counts to be tested (default value 2)
- --mpicommand=command: The command used to invoke MPI; the default is mpirun; use --mpicommand=mpiexec on systems that have mpiexec but not mpirun.

An MPI process count of 1 denotes using only the serial layer. The test script starts at an MPI process count of p = minprocs and then updates it by the formula  $p \leftarrow mp + a$ ; thus, the default values of m = 2 and a = 0 cause the processor count to be successively doubled. You may also list the options by invoking the script with the single option -h or --help (in which case no testing is attempted).

## 3 Architecture and Features

PEBBL consists of two *layers*, the *serial layer* and the *parallel layer*. The serial layer provides an object-oriented means of describing branch-and-bound algorithms, with very little reference to parallel implementation. If you do not need parallelism, or are simply in the early stages of algorithm development, the serial layer allows branch-and-bound methods to be described, debugged, and run in a familiar, serial programming environment.

The parallel layer contains the core code necessary to create parallel versions of serial applications. To parallelize a branch-and-bound application developed with the serial layer, you simply define new classes derived from *both* the serial application and the parallel layer. A fully-operational parallel application only requires the definition of a few additional methods for these derived classes, principally to tell PEBBL how to pack application-specific problem and subproblem data into MPI message buffers, and later unpack them.

Any parallel PEBBL application constructed in this way inherits the full capabilities of the parallel layer, including a wide range of different parallel work distribution and load balancing strategies, and user-configurable levels of interprocessor communication. You can then add application-specific refinements to the parallelization, but are not required to. Figure 7 shows the conceptual relationship between the two layers, a serial application, and its parallelization. In the figure, the application is one of the examples distributed with PEBBL, for solving binary knapsack problems; the same basic pattern applies to all PEBBL applications. The serial layer class implementing the branch and bound algorithm is called binaryKnapsack, and the parallel application is called parallelBinaryKnapsack. The "diamond" inheritance structure shown in Figure 7 is integral to PEBBL's design — it is a powerful but sometimes problematic use of C++ multiple inheritance.

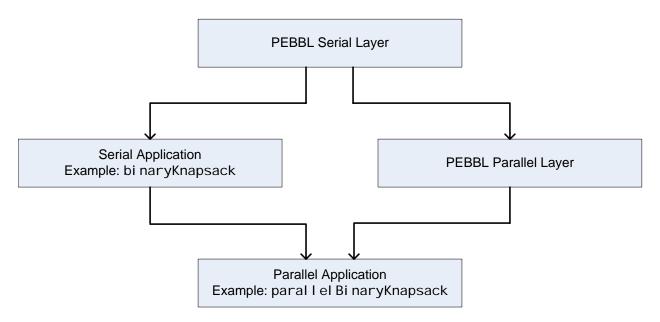


Figure 7: The conceptual relationships of PEBBL's serial layer, the parallel layer, a serial application (in this case, binaryKnapsack), and the corresponding parallel application (in this case, parallelBinaryKnapsack).

## 3.1 Serial layer architecture

#### 3.1.1 The branching, branchSub, and solution classes

To define a serial branch-and-bound algorithm, you must extend the two or three key classes in the PEBBL serial layer, branching, branchSub, and possibly solution. The branching class stores global information about a problem instance, and contains methods that implement various kinds of serial branch-and-bound algorithms, as described below. Each branchSub object stores data about a subproblem (or node) in the branch-and-bound tree, and the branchSub class contains methods that perform generic operations on subproblems. The solution class stores a description of a feasible solution to the problem. PEBBL provides some standard solution-derived template classes, essentially representing solutions as vectors of standard C++ types such as int or double; for other solution representations, users should create their own classes derived from solution. The basic branching-branchSub-solution organization of PEBBL is inspired by ABACUS [10], but is more general, since there is no assumption that cutting planes or linear programming are involved.

By way of example of PEBBL's class structure, our binary knapsack solver defines a class binaryKnapsack, derived from branching, to describe the capacity of the knapsack and the possible items to be placed in it. We also define a class binKnapSub, derived from branchSub, which describes the status of the knapsack items at nodes of the branching tree (i.e., included, excluded, or undecided); this class describes a node of the branch-and-bound tree. Each object in a subproblem class like binKnapSub contains a pointer back to the corresponding instance of the "global" problem class, in this case binaryKnapsack.

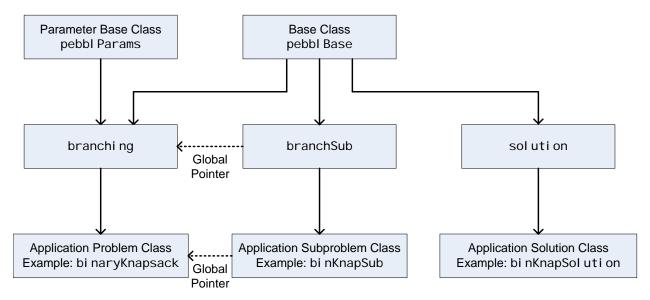


Figure 8: Basic class hierarcy for a serial PEBBL application (in this case, binaryKnapsack, with corresponding subproblem class binKnapSub and solution class binKnapSolution).

Through this pointer, each subproblem object can find global information about the problem instance and the overall branch-and-bound process. The knapsack application also defines a class binKnapSolution derived from solution, to represent solutions in a compact form that is particularly efficient for large knapsack problems.

Both branching and branchSub are derived from a common base class, pebblBase, which mainly contains common symbol definitions. The branching class also derives from pebblParams, which holds command-line-specifiable parameter objects implemented using the UTILIB class parameter package. The solution class also derives from pebblBase. Figure 8 illustrates the basic class hierarchy for a serial PEBBL application.

The class header file for the serial binary knapsack example is in acro-pebbl/packages/pebbl/src/example/pebbl/serialKnapsack.h. Note that binaryKnapsack is defined via

```
class binaryKnapsack : virtual public branching \{\ \cdots\ \} , binKnapSub is defined via class binKnapSub : virtual public branchSub \cdots\ \{\ \cdots\ \} , and binKnapSolution is defined via class binKnapSolution : public solution \cdots\ \{\ \cdots\ \} .
```

In order for subsequent parallization to work properly, you should use virtual when deriving classes from branching and branchSub. It is typically not necessary to use virtual when deriving classes from solution.

Calculations made for subproblems frequently require data stored in the problem description class, which are accessible via pointers as depicted by the two horizontal dotted arrows

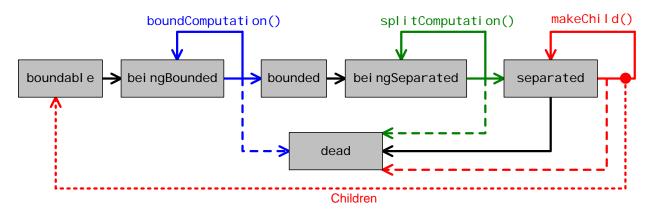


Figure 9: PEBBL's subproblem state transition diagram. It is possible that a single application of boundComputation may take a subproblem from the boundable state, through beingBounded, to bounded. Similarly, a single use of splitComputation may move a subproblem from bounded, through beingSeparated, to separated.

in Figure 8. To implement the upper arrow, the definition of the subproblem class must instantiate the abstract method bGlobal(); in binKnapSub, for example, this capability is implemented via:

```
protected:
    binaryKnapsack* globalPtr;
public:
    inline binaryKnapsack* global() const { return globalPtr; };
    branching* bGlobal() const { return global(); };
```

This pattern should be fairly typical: each object of the branchSub-derived class should contain a pointer to the branching-derived object for which it represents a subproblem. The bGlobal() method should then be implemented by casting this pointer to a branching\*.

#### 3.1.2 Manipulating subproblem states

A key feature of PEBBL, first published in Eckstein et al. [8], is that subproblems remember their *state*. Each subproblem progresses through as many as six of these states, boundable, beingBounded, bounded, beingSeparated, separated, and dead, as illustrated in Figure 9.

A subproblem always comes into existence in state boundable, meaning that little or no bounding work has been done for it, although it still has an associated bound value; typically, this bound value is simply inherited from the parent subproblem. Once PEBBL starts work on bounding a subproblem, its state becomes beingBounded, and when the bounding work is complete, the state becomes bounded.

Once a problem is in the bounded state, PEBBL may elect to split it into smaller subproblems. At this point, the subproblem's state becomes beingSeparated. Once separation is complete, the state becomes separated, at which point the subproblem's children may be created. Once the last child has been created, the subproblem's state becomes dead, and it may be deleted from memory. Subproblems may also become dead at earlier points in their existence, because they have been fathomed or represent portions of the search space containing no feasible solutions.

Class branchSub has three key abstract virtual methods, namely boundComputation, splitComputation, and makeChild, that are responsible for applying these state transitions to subproblems. PEBBL's search framework interacts with applications primarily through these methods; defining a PEBBL branch-and-bound application essentially consists of providing definitions for these three operators for the application subproblem class (e.g. binKnapSub).

The boundComputation method's job is to move the subproblem to the bounded state, updating the data member bound to reflect the computed bound value. The boundComputation method is allowed to pause an indefinite number of times, leaving the subproblem in the beingBounded state. The only requirement is that any subproblem will eventually become bounded after some finite number of applications of boundComputation. This flexibility allows PEBBL to support branch-and-bound variants where bounding is suspended on a subproblem, the subproblem is set aside, and another task or subproblem is considered. It also allows for bounding procedures that establish progressively stronger bounds through multiple stages of computation. The subproblem's bound, reflected in the data member bound, may change at each step of this process. When boundComputation decides that there is no more bounding work to be done for subproblem, it should change the subproblem state to bounded by executing setState(bounded). Changes in subproblem state should be implemented via the setState rather than by direct assignment to the data member state to ensure PEBBL can keep accurate subproblem statistics.

The splitComputation method's job is similar to boundComputation's, but it manages the process of splitting subproblems. Eventually it must execute setState(separated) to signal that the subproblem is completely separated, and then return the number of child subproblems (splitComputation has a return type of int). Before that, however, it is allowed to return an indefinite number of times with the problem left in the beingSeparated state (in which case the return value is ignored). This feature allows PEBBL to implement branch-and-bound methods where the work in separating a subproblem is substantial and might need to be paused to attend to some other subproblem or task. The subproblem's bound may be updated by splitComputation if the separation process yields additional bounding information.

Finally, makeChild returns a branchSub\* pointing to a single child of the subproblem it is applied to. This parent must be in the separated state. After its last child has been made, PEBBL automatically puts the subproblem in the dead state.

If at any point in boundComputation, splitComputation, or makeChild, it becomes evident that a subproblem does not require further investigation — for example, because it has become evident the subproblem is infeasible — one may mark the subproblem as dead by executing setState(dead).

In addition to boundComputation, splitComputation, and makeChild, some additional

virtual methods must to be defined to complete the specification of a branch-and-bound application; all these methods are described in Section 4.2.

#### 3.1.3 Pools, handlers, and the search framework

PEBBL's serial layer orchestrates branch-and-bound search through a module called the "search framework", literally, branching::searchFramework. The search framework acts as an attachment point for two user-specifiable objects, a *pool* and a *handler*, whose combination determines the exact "flavor" of branch and bound being implemented.

The pool object dictates how the currently active subproblems are stored and accessed, which effectively determines the branch-and-bound search order. Currently, there are three kinds of pool: a heap sorted by subproblem bound<sup>1</sup>, a stack, and a FIFO queue. If you specify the heap pool, then PEBBL will follow a best-first search order; specifying the stack pool results in a depth-first order, and specifying the queue results in a breadth-first order.

Critically, at any instant in time, the subproblems in the pool may in principle represent any mix of states: for example, some might be boundable, and others separated. This feature gives you flexibility in specifying the bounding protocol, which is a different aspect of the algorithm than the search order; each "handler" object implements a particular bounding protocol.

To illustrate what a bounding protocol is, consider the usual branch-and-bound method for mixed integer programming as typically described by operations researchers: one removes a subproblem from the currently active pool, and computes its linear programming relaxation bound. If the bound is strong enough to fathom the subproblem, it is discarded. Otherwise, one selects a branching variable, creates two child subproblems, and inserts them into the pool. This type of procedure is an example of what is often called "lazy" bounding (see for instance [2]), because it views the bounding procedure as something time-consuming (like solving a large linear program) that should be delayed if possible. In the PEBBL framework, lazy bounding is implemented by a handler that tries to keep all subproblems in the active pool in the boundable state.

An alternative approach, common in work originating from the computer science community, is usually called "eager" bounding (again, see [2] for an example of this terminology). Here, all subproblems in the pool have already been bounded. One picks a subproblem out of the pool, immediately separates it, and then forms and bounds each of its children. Children whose bounds do not cause them to be fathomed are returned to the pool.

Lazy and eager bounding each have their own advantages and disadvantages, and the best choice may depend on both the application and the implementation environment. Typically, implementors seek to postpone the most time-consuming operations in the hope that the discovery of a better incumbent solution will make them unnecessary. So, if the bounding

<sup>&</sup>lt;sup>1</sup>Objects of type branchSub have a member called integralityMeasure which may be used by the application to measure how far a subproblem is from being completely feasible (that is, from having candidateSolution yield true; see Section 4.2). If two subproblems have identical bounds, the one with the lower integralityMeasure will be placed higher in the heap, since it presumably is more likely to lead to an improved incumbent solution.

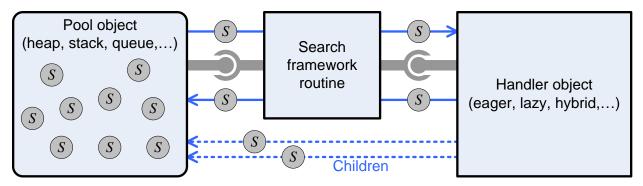


Figure 10: The search framework, pool, and handler. Each S indicates a branch-and-bound subproblem — an object of type derived from branchSub.

operation is much more time-consuming than separation, lazy bounding is most appealing. If the bounding operation is very quick, but separation more difficult, then eager bounding would be more appropriate. Eager bounding may save some memory since leaf nodes of the search tree may be processed without entering the pool, but has a larger task granularity, resulting in lower parallel communication overhead per subproblem, but also somewhat less potential for parallelism.

Because PEBBL's serial layer stores subproblem states and lets the you specify a handler object, it gives you the freedom to specify lazy bounding, eager bounding, or other protocols. The search framework routine simply extracts subproblems from the pool and passes them to the handler until the pool becomes empty. Currently, there are three possible handlers, eagerHandler, lazyHandler, and hybridHandler. The eagerHandler and lazyHandler objects respectively implement eager and lazy bounding by trying to keep as many subproblems as possible in the bounded and boundable states, respectively.

The hybridHandler object implements a strategy that is somewhere between eager and lazy bounding, and is perhaps the most simple and natural given PEBBL's concept of subproblem states. Given any subproblem, hybridHandler performs a single application of either boundComputation, splitComputation, or makeChild, to try to advance the subproblem one transition through the state diagram of Figure 9. If the subproblem's state is boundable or beingBounded, it applies boundComputation once. If the subproblem's state is bounded or beingSeparated, it applies splitComputation once. Finally, if the state is separated, the handler performs one call to makeChild, and inserts the resulting subproblem into the pool. Hybridhandler is currently PEBBL's default choice of handler.

The combination of multiple handlers, multiple pool implementations, and the freedom in implementing boundComputation and splitComputation create considerable flexibility in the kinds of branch-and-bound methods that the serial layer can implement. Figure 10 depicts the relationship of the search framework, pool, and handler.

You may choose between the existing pools and handlers by setting parameters in the branching class object; see Section 5.10. You may also in principle supply your own pools and handlers, but we consider that an advanced topic, and it is not presently covered in this guide.

## 3.2 Controlling the Search Process

#### 3.2.1 Basic tolerances

In its normal, non-enumeration mode of operation, PEBBL's optimality criteria are controlled by two parameters, absTolerance and relTolerance, with respective default values 0 and  $10^{-7}$ . PEBBL attempts to locate a single problem solution that is either within an additive distance absTolerance or a relative distance relTolerance of optimality, whichever turns out to be less restrictive. For example, setting relTolerance to 0.05 would specify a solution with 5% of optimality.

#### 3.2.2 Multiple solutions: enumeration criteria and the solution repository

PEBBL can also function in an enumeration mode in which it stores multiple feasible solutions to a problem. Enumeration mode is activated if any of the four parameters enumAbsTolerance, enumRelTolerance, enumCutoff or enumCount is set. The meaning of these parameters is as follows:

- enumAbsTolerance: Find all solutions whose objective value is within enumAbsTolerance of the best possible. For example, setting enumAbsTolerance = 6 indicates you want all solutions within 6 units of optimal.
- enumRelTolerance: Find all solutions within a relative distance enumRelTolerance of the best possible. For example, setting enumRelTolerance = 0.10 specifies that PEBBL should enumerate all solutions within 10% of optimal.
- enumCutoff: Find all solutions with an objective value better than this value. For a minimization problem, for example, setting enumCutoff = 0 instructs PEBBL to find all solutions with a negative objective value.
- enumCount: Find the best enumCount solutions; for example setting enumCount = 10 requires PEBBL to find the 10 best solutions.

If you set more than one of these parameters, PEBBL returns only solutions simultaneously meeting all the specified criteria. For example, setting enumRelTolerance = 0.05 and enumCount = 200 means that PEBBL should return only those solutions that are among the 200 best and are also within 5% of optimal.

The enumeration mechanism keeps a repository of feasible solutions represented as objects of type derived from the solution class, maintained both as a hash table and heap in reverse order of solution quality — that is, the solution on the top of the heap has the worst objective value. The hash table representation, along with hashing and comparison and methods of the solution class, prevents duplicate solutions from entering the repository. Discovery of a new best incumbent solution can cause solutions to be removed from the repository if either enumAbsTolerance or enumRelTolerance is set. If enumCount is set and the repository already contains enumCount solutions, then entry of a new solution into the repository causes the previously worst solution in the repository to be removed.

#### 3.2.3 The solution class

PEBBL represents optimization problem solutions by objects derived from the abstract class solution. PEBBL provides a template class, arraySolution < T >, which represents solutions as a one-dimensional array or vector of type T. This solution representation should be adequate for many applications; if it is not convenient or efficient for a given application, users may create their own solution-derived classes. It is even possible for a single application to use several different solution representations.

To properly maintain the hash table used to filter out duplication solutions, PEBBL needs a hash function that may be applied to solutions, and a means of comparing two solutions to see if they are duplicates. The normal means of hashing and comparison are through the sequence representation of solutions. The solution class contains abstract methods sequenceLength, sequenceData, and sequenceReset whose purpose is to convert a solution to sequence of doubles, in such a way that two solutions may be considered duplicates if and only if invoking these methods results in identical behavior. If these methods are implemented, PEBBL automatically supplies a hash function in the method computeHashValue, and comparison operator for solutions is the method duplicateOf.

It is possible to dispense with the sequence representation methods; in this case, however, users must provide their own explicit implementations of computeHashValue and duplicateOf. Even if a sequence representation is defined, users might want to override either of these methods in the interest of efficiency.

#### 3.2.4 Early output and checkpointing

Some of the calculations for which PEBBL is intended may be extremely long-running, and thus vulnerable to data loss if a system crashes or a job's time allocation is exhausted. PEBBL has two features designed to mitigate such data loss. The first, early output, tries to ensure that if a PEBBL run is interrupted, you can recover the best solution found so far. You enable this feature by setting the parameter earlyOutputMinutes to some positive value m. Each time PEBBL finds a new incumbent solution (that is, a solution better than all previously found ones) that exists for at least m minutes, PEBBL writes it to disk so that it is available if the run crashes. Early output is also useful if you wish to voluntarily terminate a run and still have access to the best feasible solution computed so far. This feature may be useful in early testing of an application for which you may not yet know appropriate tolerance values. For example, if you initiate a run with a relTolerance of 5%, but after considerable computation, the optimality gap is still 10%, you may decide you are satisfied with the 10% tolerance.

The second data loss mitigation feature is *checkpointing*, which imposes more overhead on PEBBL, but is more powerful. Checkpointing is currently available only for the parallel layer; it is not available in applications built solely on the serial layer. The key parameter controlling checkpointing is **checkPointMinutes**. If this parameter has a positive value m, PEBBL writes its complete internal state to disk approximately every m minutes. Each processor writes a separate file, and the checkpointing feature requires that all processors

have access to file I/O, although not necessarily to the same directory.

The computation can be restarted from the time of the checkpoint by specifying either of the command-line parameters restart or reconfigure.<sup>2</sup> Using restart is potentially faster, but reconfigure allows one to restart with a different parallel configuration — for example, a different total number of processors. To use reconfigure, all checkpoint files must be in (or moved to) the same directory.

Some MPI implementations provide their own checkpointing capabilities. PEBBL's checkpointing feature is independent of any such capabilities and does not require them.

The early-output mechanism and enumeration mechanisms are currently independent. When using enumeration, the early output mechanism simply outputs the best incumbent. Checkpointing, however, is fully compatible with enumerating multiple solutions: each checkpoint will save the entire state of the solution repository.

## 3.3 Parallel layer architecture

PEBBL's parallel layer attempts to accelerate the branch-and-bound process by using multiple processors, and requires some form of the MPI message passing interface. PEBBL's parallel layer will run on shared-memory (SMP) systems, but only if MPI is configured to emulate a message passing environment (which is the default on multicore systems when packages such as OpenMPI are downloaded with utilities such as the Ubuntu package manager).

PEBBL's primary mode of parallelism, as is standard in parallel branch and bound, is to explore different nodes of the search tree simultaneously on different processors. However, PEBBL has the optional capability to use different modes of parallelism during the early stages of the search; see Section 3.3.5 below.

For the most part, parallel-layer search node processing is carried out by the same boundComputation, splitComputation, and makeChild methods as in serial layer. Thus, once you have created these methods for your application, parallel execution should be available with little additional development effort.

#### 3.3.1 Inheritance pattern

The parallel layer's capabilities are embodied in the classes parallelBranching and parallelBranchSub, which have the same function as branching and branchSub, respectively, except that they perform parallel search of the branch-and-bound tree. Both are derived from a common base class parallelPebblBase, whose function is similar to pebblBase, containing mainly common symbol definitions. The class parallelBranching also derives from parallelPebblParams, which contains a large number of parameters for controlling parallel search. Furthermore, each of parallelBranching and parallelBranchSub is derived from the corresponding class in the serial layer.

<sup>&</sup>lt;sup>2</sup>As with all PEBBL command-line parameters, these parameters should be preceded by two hyphens when used on the command line, as in --restart.

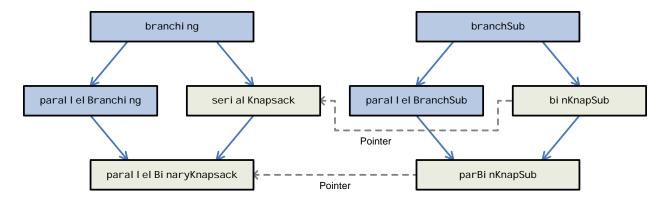


Figure 11: Partial depiction of the inheritance structure of the parallel knapsack application. Other parallel applications are similar.

To turn a serial application into a parallel application, one must define two new classes. The first is derived from parallelBranching and the serial application global class. In the knapsack example, for instance, we defined a new class parallelBinaryKnapsack which has both parallelBranching and binaryKnapsack as virtual base classes. We call this class the *global parallel class*. For each problem instance, the information in the global parallel class is replicated once on every processor.

This basic inheritance pattern is repeated for parallel subproblem objects. In the knap-sack case, we defined a parallel subproblem class parBinKnapSub to have virtual public base classes binKnapSub and parallelBranchSub. As with the serial subproblems, each instance of parBinKnapSub has a parallelBinaryKnapsack pointer that allows it to locate global problem information. Figure 11 depicts the inheritance structure for the parallel knapsack application. The classes solution and binKnapSolution are omitted from the figure since their relationship is unchanged from Figure 8, although a few additional virtual methods in solution may need to be implemented for parallel operation.

The header file acro-pebbl/packages/pebbl/src/example/pebbl/parKnapsack.h defines the inheritance structure depicted in Figure 11. It defines parallelBinaryKnapsack via

```
class parallelBinaryKnapsack :
    public parallelBranching,
    public binaryKnapsack
{
    :
}
```

and parBinKnapSub via

```
class parBinKnapSub :
        public parallelBranchSub,
        public binKnapSub
{
    private:
        parallelBinaryKnapsack* globalPtr;
    public:
        parallelBinaryKnapsack* global() const { return globalPtr; };
        parallelBranching* pGlobal() const { return globalPtr; };
        i
}
```

Once this basic inheritance pattern is established, the parallel application automatically combines the description of the application coming from the serial application (in the knapsack case, embodied in binaryKnapsack and binKnapSub) with the parallel search capabilities of the the parallel layer. For the parallel application to function, however, additional methods must be defined, as summarized in Section 4.3. The most critical of these methods are pack and unpack, which must be defined for the global parallel class, the subproblems, and solutions. These methods respectively describe how to encode and decode objects into a UTILIB Packbuffer or UnPackBuffer object (see the UTILIB documentation).

#### 3.3.2 Processor clustering

PEBBL's parallel layer employs a generalized form of the processor organization used by the later versions of CMMIP [4, 5]. Processors are organized into *clusters*, each with one *hub* processor and one or more *worker* processors. The hub processor serves as a "master" in work-allocation decisions, whereas the workers are in some sense "slaves," doing the actual work of bounding and separating subproblems. The degree of control that the hub has over the workers may be varied by a number of run-time parameters, and may not be as tight as a classic "master-slave" system. Further, the hub processor has the option of simultaneously functioning as a worker.

Three run-time parameters, all defined in parallelPebblParams, govern the partitioning of processors into clusters: clusterSize, numClusters, and hubsDontWorkSize. First PEBBL finds the size k of a "typical" cluster via the formula

$$k = \min \left\{ \text{clusterSize}, \max \left\{ \left\lfloor \frac{\overline{p}}{\text{numClusters}} \right\rfloor, 1 \right\} \right\},$$

where  $\overline{p}$  is the total number of processors. Thus, k is the smaller of the cluster sizes that would be dictated by clusterSize and numClusters. Processors are then gathered into clusters of size k, except that if k does not evenly divide  $\overline{p}$ , the last cluster will be of size  $\overline{p} \mod k$ . In clusters whose size is greater than or equal to hubsDontWorkSize, the hub processor is "pure," that is, it does not simultaneously function as a worker. In clusters smaller than hubsDontWorkSize, the hub processor is also a worker. The rationale for this arrangement

is that, in very small clusters, the hub will be lightly loaded, and its spare CPU cycles should be used to help explore the branch-and-bound tree. If a cluster is too big, however, using the hub simultaneously as a worker may unacceptably delay the hub's response to messages, slowing down the entire cluster. In such cases, a "pure" hub is preferable.

#### 3.3.3 Tokens and work distribution within a cluster

Unlike some "master-slave" implementations of branch and bound, each PEBBL worker maintains its own pool of active subproblems. This pool may be any of the kinds of pools described in Section 3.1.3, although all workers must use the same pool type. Depending on various parameter settings, however, the pool might be very small, in the most extreme case never holding more than one subproblem. Each worker processes its pool in the same general manner as the serial layer: it picks subproblems out of the pool and passes them to a search handler until the pool is empty. When running in parallel, handlers have the additional ability to release subproblems from the worker to the hub.

For the remainder of this subsection, assume for simplicity that a single cluster spans all available processors; in the next subsection, we will amend our description to cover the case of multiple clusters.

Random release of subproblems: When running in a parallel context, eagerHandler decides whether to release a subproblem as soon as it has become bounded. In parallel situations, lazyHandler and hybridHandler make the release decision when they create a subproblem. No matter which handler is used, the decision is a random one, with the probability of release controlled by run-time parameters. Released subproblems do not return to the local pool; instead, the worker cedes control over these subproblems to the hub. Eventually, the hub may send control of the subproblem back to the worker, or to another worker.

If the release probability is 100%, then every subproblem is released, and control of each subproblem is always returned to the hub at a some point in its lifetime (at creation for lazyHandler and hybridHandler, and upon reaching the bounded state for eagerHandler). In this case, the hub and its workers function like a standard "master-slave" system. When the probability is lower, the hub and its workers are less tightly coupled. The release probability is controlled by the run-time parameters minScatterProb, targetScatterProb, and maxScatterProb. The use of three different parameters, instead of a single one, allows the release probability to be sensitive to a worker's load. Basically, if the worker appears to have a fraction 1/w(c) of the total work in the cluster, w(c) denotes the total number of workers in cluster c, then the worker uses the value targetScatterProb. If it appears to have less work, then a smaller value is used, but no smaller than minScatterProb; if it appears to have more work, it uses a larger value, but no larger than maxScatterProb.

**Subproblem tokens:** When a subproblem is released, only a small portion of its data, called a *token* [16, 4], is actually sent to the hub. The subproblem itself may move to a secondary pool, called the *server pool*, that resides on the worker. A token consists of

only the information needed to identify a subproblem, locate it in the server pool, and schedule it for execution. Since the hub receives only tokens from its workers, as opposed to entire subproblems, these space savings translate into reduced storage requirements and communication load at the hub.

When making tokens to represent new, boundable subproblems, the parallel version of lazyHandler and hybidHandler take an extra shortcut. Instead of creating a new subproblem with parallelMakeChild and then making a token that points to it, they simply create a token pointing to the parent subproblem, with a special field, whichChild, set to indicate that the token is not for the subproblem itself, but for its children. Optionally, a single token can represent multiple children. If every child of a separated subproblem has been released, the subproblem is moved from the worker pool to the server pool.

**Hub operation and hub-worker interaction:** Workers that are not simultaneously functioning as hubs periodically send messages to their controlling hub processor. These messages contain blocks of released subproblem tokens, along with data about the workload in the worker's subproblem pool, and other miscellaneous status information.

The hub processor maintains a pool of subproblem tokens that it has received from workers. Again, this pool may be any one of the pools described in Section 3.1.3. Each time it learns of a change in workload status from one of its workers, the hub reevaluates the work distribution in the cluster. The hub tries to ensure that each worker has a sufficient quantity of subproblems, and optionally, that they are of sufficient quality (that is, with bounds sufficiently far from the incumbent). Quality balancing is controlled by the boolean parameter qualityBalance, which is true by default. Workload quantity evaluation is via the parameters workerSPThreshHub and hubLoadFac. A worker is judged "deserving" of work if the number of subproblems in its local pool is less than

$$\max\left\{ \texttt{workerSPThreshHub}, \left(\frac{1-\texttt{hubLoadFac}}{W}\right)Q\right\},$$

where W is the number of workers and Q is the total number of known active subproblems. The logic behind the second term in the above maximum is that hubLoadFac specifies the fraction of active subproblems that are under hub control and constitute a "working set" used by the hub to balance workloads between workers. The remaining work should be roughly even distributed among the workers. This calculation is slightly modified when the same processor is serving as both a hub and a worker, since such processors may not be able to process subproblems quite as quickly as ordinary workers. PEBBL adaptively estimates the degree of "handicap" for such colocated worker-hubs as each run progresses.

If quality balancing is activated, a worker is also judged deserving if the best bound in its pool is worse than the best bound in the hub's pool by a factor exceeding the parameter qualityBalanceFactor. Of the workers that deserve work, the hub designates the one with fewest subproblems as being most deserving, unless this number exceeds workerSPThreshHub; in that case, the workers are ranked in reverse order of the best subproblem bound in their pools.

As long as there is a deserving worker and the hub's token pool is nonempty, the hub picks a subproblem token from its pool and sends it to the most deserving worker. The message sending the subproblem may not go directly to that worker, however; instead, it goes to the worker that originally released the subproblem. When that worker receives the token, it forwards the necessary subproblem information to the target worker, much as in [4, 5, 16]. This process will be described in more detail below.

When a single activation of the hub logic results in multiple dispatch messages to be sent from the hub to the same worker, the hub attempts to pack them, subject to an overall buffer length limit, into a single MPI message, saving system overhead.

If the subproblem release probability is set to 100%, and workerSPThreshHub is set to 1, the cluster will function like a classic master-slave system. The hub will control essentially all the active subproblems, and send them to workers whenever those workers become idle. Less extreme parameter settings will reduce the communication load substantially, however, at the cost of possibly greater deviation from the search order that would have been followed by a serial implementation. Also, setting workerSPThreshHub larger than 1 helps to reduce worker idleness by giving each worker a "buffer" of subproblems to keep it busy while messages are in transit or the hub is attending to other workers.

The best setting of the parameters controlling the degree of hub-worker communication depends on both the application and the hardware, and may require some tuning, but the scheme has the advantage of being highly flexible without any need for reimplementation or recompilation.

In addition to sending subproblems, the hub periodically broadcasts overall workload information to its workers, so the workers know the approximate relation of their own workloads to other workers' loads. This information allows each worker to adjust its probability of releasing subproblems appropriately.

Rebalancing: If the probability of workers releasing their subproblems is set too low, or the search process is nearing completion, workers in a cluster may have workloads that are seriously out of balance, yet the hub's token pool may be empty. In this case, the hub has no work to send to underloaded workers. To prevent such difficulties, there is a secondary mechanism, called "rebalancing," by which workers can send subproblem tokens to the hub even if the original decision had been to keep the subproblems on the worker rather than release them. If a worker detects that it has a number of subproblems exceeding its target load in the cluster, it selects a block of subproblems in its local pool and releases them to the hub. The hub can then redistribute these subproblems to other workers.

#### 3.3.4 Work distribution between clusters

With any system-application combination, there will be a limit to the cluster size that can operate efficiently, even if its hub does not have any worker responsibilities. To be able to use all the available processors, it may then be necessary to partition the system into multiple clusters.

PEBBL's method for distributing work between clusters resembles CMMIP's [4, 5], with some additional generality: there are two mechanisms for transferring work between clusters, scattering and load balancing. Scattering comes into play when subproblems are released by workers. If there are multiple clusters, the worker makes a supplementary random decision as to whether the subproblems should be released to the worker's own hub or to a cluster chosen at random. This random decision is controlled by the apparent workload of the cluster relative to the entire system, and the parameters minNonLocalScatterProb, targetNonLocalScatterProb, and maxNonLocalScatterProb. When choosing the cluster to scatter to, the probability of picking any particular cluster is proportional to the number of workers it contains (the worker's own cluster is not excluded).

To supplement scattering, PEBBL also uses a form of "rendezvous" load balancing that resembles CMMIP's [5]; [13] and [11] also contain earlier, synchronous applications of the same basic idea. This procedure also has the important side effect of gathering and distributing global information on the amount of work in the system, which in turn facilitates control of the scattering process, and is also critical to termination detection in the multi-hub case.

Critical to the operation of the load balancing mechanism is the concept of the workload at a cluster c at time t, which we define as

$$L(c,t) = \sum_{P \in C(c,t)} |\overline{z}(c,t) - z(P,c,t)|^{\rho}.$$
(1)

Here, C(c,t) denotes the set of subproblems that c's hub knows are controlled by the cluster at time t,  $\overline{z}(c,t)$  represents the incumbent value known to cluster c's hub at time t, and z(P,c,t) is the best bound on the objective value of subproblem P known to cluster c's hub at time t. The exponent  $\rho \in \{0,1,2,3\}$  is set by the parameter loadMeasureDegree. If  $\rho = 0$ , only the number of subproblems in the cluster matters. Higher values of  $\rho$  give progressively higher "weight" to subproblems farther from the incumbent. The default value of  $\rho$  is 1.

PEBBL redistributes work between clusters using a "rendezvous" scheme that organizes all the cluster hub processors into a balanced tree whose radix (branching factor) is determined by the parameter loadBalTreeRadix, with a default value of 2. The purpose of the tree is to organize messages between cluster hubs in a way that limits the communication load on any one processor, and the tree is not related to any hierarchy of control. Note that unlike ALPS [15], PEBBL does not employ a "master of masters" or "hub of hubs" processor, and its parallelization scheme is in principle indefinitely scalable because all cluster hubs interact in a peer-to-peer manner, but one that has a bounded communication load per-sweep, independent of the number of clusters.

Load-balancing messages pass up and down the tree of cluster hubs in a pattern consisting of a *survey sweeps* followed by *balance sweeps*. The frequency of these sweeps is controlled by a timer, with the minimum spacing between survey sweeps being set by a run-time parameter. If the total workload on the system appears to be zero, then this minimum spacing is not observed and sweeps are performed as rapidly as possible, to facilitate rapid termination detection. Under certain conditions, including at least once at the end of every

run, a termination check sweep, which checks for completion of the computation, substitutes for the balance sweep.

The survey sweep gathers and distributes system-wide workload information. This sweep provides all hubs with an overall system workload estimate, essentially the sum of the L(c,t) over all clusters c. However, if the sweep detects that this calculation was based on incumbent values that differed from processor to processor, it immediately repeats itself, a situation we call a *survey restart*.

At the end of a successful survey sweep, each hub determines whether its cluster should be a potential donor of work, a potential receiver of work, or (typically) neither. Donors are clusters whose workload exceeds the average by a factor of at least loadBalDonorFac, while receivers must be below the average by at least loadBalReceiverFac. Next, the balance sweep begins. A form of parallel prefix operation [1], this single up-and-down message sweep of the tree counts the total number of donors d and receivers r, assigns each donor a unique number in the range  $0, \ldots, d-1$ , and assigns each receiver a unique number in the range  $0, \ldots, r-1$ . The first  $y = \min\{d, r\}$  donors and receivers then "pair up" via a rendezvous procedure involving 3y point-to-point messages. Specifically, donor i and receiver i each send a message to the hub for cluster i, for  $i = 0, \dots, y - 1$ . Hub i then sends a message to donor i, telling it the processor number and load information for receiver i. See [9, Section 6.3] or [3, 5] for a more detailed description of this process. Within each pair, the donor sends a single message containing subproblem tokens to the receiver. Thus, the sweep messages are followed by up to 4y additional point-to-point messages, with at most 6 messages being sent or received by any single processor — this worst case occurs when a hub is both a donor and a rendezvous point. Both the survey and balancing sweeps involve at most 2(b+1)messages being sent or received at any given hub processor, where b is the branching factor of the load-balancing tree. Thus, the total number of messages per processor per round of load balancing is bounded above by the constant 2(b+1)+2(b+1)+6=4b+10. This kind of constant upper bound on the number of messages per processor required to perform a global operation is instrumental in designing scalable parallel algorithms.

Peer-to-peer load balancing mechanisms are frequently classified as either "work stealing," that is, initiated by the receiver, or "work sharing," that is, initiated by the donor. The rendezvous method is neither; instead, donors and receivers efficiently locate one another on an equal basis, possibly across a large collection of processors.

The load balancing scheme has an important secondary function of detecting termination, which can in general be challenging in highly asynchronous parallel programs. The general approach is a varient of the "four counters" technique proposed in [14], although only three counters are actually necessary, and the pattern of messages is adapted to PEBBL's clustered processor organization. In essence, PEBBL's survey sweeps can detect the situation that no cluster in the system appears to have any active subproblems, and the total count of messages sent matches the total count of messages received. While this situation is necessary for the calculation to be truly complete, it is not sufficient, since all the constituent processors cannot typically be sampled at the exact same moment in time. Therefore, and additional check is necessary to confirm termination. When there is only one hub, the termination

procedure, while conceptually similar, is somewhat simpler.

#### 3.3.5 Ramp-up: starting the parallel search

Ramp-up refers to the initial phase of a parallel search algorithm when the number of active search nodes is of a smaller order than the available processors. In some branch-and-bound applications, particularly when the number of processors is large, poor handling of ramp-up can have significantly reduce parallel efficiency.

If only one processor at a time can work on a given search node, the vast majority of processors will be idle during the initial development of the search tree. Often, this idleness is not a major issue, because the search tree grows quickly. However, in some applications, the root node of the tree, and possibly nodes near it, may take much longer to bound or separate than "typical" nodes later in the search. In such situations, the ramp-up phase prolonged and it may be hard to make efficient use of all available processors.

To help improve ramp-up performance, PEBBL supports a special ramp-up phase in which the application may exploit parallelism within each subproblem, if it is available. During the ramp-up phase, all processors synchronously explore exactly the same search nodes near the root of the branch-and-bound tree. That is, all processors will collectively process the root node, then all processors will collectively process the same child of that root node, and so forth. Each processor will thus redundantly have in its local memory exactly the same pool of active branch-and-bound nodes as every other processor. Instead of exploring parallelism inherent in exploration of the tree, the application attempts to exploit some source of parallelism within each search node, for example in calculating the bound or deciding how to separate a subproblem. This alternate mode of parallelism, however, is entirely the responsibility of the application.

During ramp-up, the method rampingUp(), available in both parallelBranching and parallelBranchSub, returns true; otherwise, it returns false. In response to the value returned by rampingUp(), boundComputation, splitComputation, and even makeChild may then attempt to explore some form of synchronous parallelism within the processing of individual search tree nodes. These methods are free to conduct MPI communication, but should be sure to leave all processors in a uniform state upon exit.

Ramp-up execution is controlled by two virtual methods, continueRampup() and force ContinueRampUp(). When both these methods return false, PEBBL will terminate the ramp-up phase. PEBBL then automatically partitions the active search nodes, leaving each worker processor with an approximately equal number of active subproblems. PEBBL then begins its standard, asynchronous cluster/worker/hub search phase.

The default implementation of continueRampup() is controlled by two parameters, ramp UpPoolLimit and rampUpPoolLimitFac. It returns true as long as the number of active subproblems does not exceed max{rampUpPoolLimit,  $\bar{p}$  · rampUpPoolLimitFac}, where  $\bar{p}$  is the total number of processors. The default implementation of forceContinueRampUp() is to return true whenever the total number of subproblems created is does not exceed the parameter minRampUpSubprobsCreated. You may override these rudimentary implementations with implementations more specific to your application.

When the ramp-up phase ends, PEBBL evenly distributes the current active subproblems among the worker processors. Since all processors have the same tree in local memory at the end of the ramp-up phase, this distribution can be efficiently performed without any interprocessor communication. This process is called *crossover*.

#### 3.3.6 Enumeration in parallel

PEBBL's parallel layer now supports the same multiple-solution enumeration criteria as its serial layer. For scalability, storage of the repository is partitioned approximately equally among all processors through a mapping based on the solution hash value — every solution s has a unique "owning" processor based on its hash value. Each processor has a local repository segment using the same hash-table-and-heap representation as the serial layer's single repository.

When enumeration is active and a solution s is passed to foundSolution on processor  $p_0$ , foundSolution immediately uses s's hash value to compute its owning processor p(s). Unless  $p(s) = p_0$ , foundSolution immediately sends the s to processor p(s). Using the hash table representation of the local portion of the repository and the duplicateOf method, processor p(s) then checks if s is a duplicate of a solution already in its local segment of the repository. If so, it simply discards s. Otherwise, it enters s into the local repository. At the end of the run, PEBBL uses a synchronous parallel sort/merge algorithm to output a sorted list of all solutions found, ordered from best objective value to worst.

Unless enumCount is in use, this logic is essentially all that is needed. If enumCount is set, however, the implementation becomes more complicated. In that case, for proper pruning, PEBBL maintains an estimate of the enumCount<sup>th</sup>-best solution in the union of the repository segments of all processors, called the *cutoff solution*. To keep track of the cutoff solution, PEBBL organizes all processors into a balanced tree. By periodically sending sorted arrays of solution values up this three, PEBBL computes the current cutoff solution value, which it then broadcasts down the tree. This technique is not totally scalable with respect to the value of enumCount, in that each processor potentially needs sufficient storage to hold enumCount solution values and identifier codes (but not entire solutions).

#### 3.3.7 On-processor multitasking: threads and the scheduler

Once the ramp-up phase is over, the PEBBL parallel layer requires each processor to perform a certain degree of multitasking. PEBBL handles the multitasking through what it calls "threads", although they are not true threads, for example, in the POSIX sense: such true multithreading would be incompatible with some older MPI implementations and some specialized supercomputer node operating systems. Instead, PEBBL uses non-preemptive threads, essentially coroutines that voluntarily and periodically return control to a central scheduler module.

The PEBBL scheduler module recognizes two main types of threads: *message-triggered* and *compute* threads. Each message-triggered thread effectively "listens" for MPI messages with a specific tag value. If the scheduler detects a complete received message with the

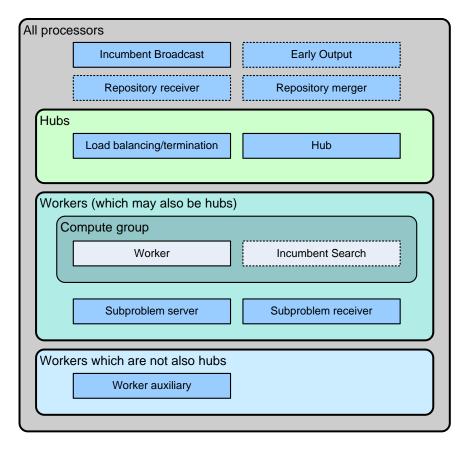


Figure 12: PEBBL's standard threads. A dashed outline indicates that the thread may not exist in some cases.

specified tag, it activates the thread to process the message (which may involve sending messages to other processors). The thread then returns to a dormant state until the scheduler detects the next message with its specified tag.

If there are no messages pending processing, the scheduler instead tries to activate the compute threads. Each compute thread has a bias which may be considered as a kind of priority. Among all compute threads that have declared themselves "ready", the scheduler tries to allocate CPU resources in proportion to the threads' bias values. Threads can adjust their bias values over time.

Figure 12 depicts PEBBL's standard threads. You may add additional threads of your own, but that is an advanced topic not currently covered in this guide. The standard threads are as follows:

**Incumbent broadcast thread:** This message-triggered thread is active on all processors. Its job is to make sure that all processors become aware, as soon as possible, of the objective value used to prune the search tree. It implements a form of asynchronous broadcast using a tree with an adjustable branching factor.

Early output thread: This message-triggered thread is active on all processors if the pa-

rameter earlyOutputMinutes is positive; otherwise it is absent. This thread coordinates the process of writing solution files, making sure the file is written by a processor that is priviledged to do I/O (the MPI standard specifies that not all processors, and perhaps only one processor, must have file and console output capabilities).

- **Repository receiver thread.** This thread is active on all processors if PEBBL is enumerating multiple solutions. It handles the receipt of most messages involved in coordinating the individual repository segments on each processor into a global asynchronous repository.
- Repository merger thread. This thread active is on all processors whenever the parameter enumCount is greater than 1. When enumCount is in use, certain messages required to maintain a global estimate of the cutoff solution may be sent on a time-delayed basis to limit peak message volumes; the repository merger thread handles this "throttled" message sending process.
- **Hub thread:** This thread is active on all hub processors, and responds to messages from workers; these messages contain acknowledgements of received subproblems, tokens for released subproblem, and worker load information. Note that a hub processor's work distribution functions may also be activated in other situations besides receipt of one of these messages, via the parallelBranching::activateHub() method.
- Load balancing/termination thread: This thread is active on all hub processors, and manages termination detection. It also controls checkpointing if checkPointMinutes is positive. When there is more than one cluster, it also manages the balancing of workload between clusters. It is generally message-triggered, but in multi-cluster situations it may also self-activate on some processors via the ready() predicate called by the scheduler.
- Worker thread: This compute thread is active on all worker processors, and manages the processing of subproblems.
- Incumbent heuristic thread: This optional compute thread may be active only on workers, and is controlled by the parameter useIncumbentThread. Its purpose is to heuristically search for improved incumbent solutions. Packaging this function into a compute thread allows PEBBL to directly control the fraction of CPU resources being dedicated to heuristic incumbent construction; the bias of this thread automatically adjusts based on the relative gap, the relative difference between the incumbent value and the best known bound among active search tree nodes. However, if the worker thread becomes idle (because it has no subproblems to process), the incumbent search thread will attempt to use all available CPU resources on the worker. This behavior can be useful near the beginning of a run if the number of subproblems at the end of the ramp-up phase is less than the total number of worker processors: instead of being totally idle, worker processors attempt to heuristically find incumbents until their worker threads receive subproblems.

**Subproblem server thread:** This message-triggered thread is active on all worker processors. It receives messages from the hub processors, and may in response send subproblems to other workers for processing.

**Subproblem receiver thread:** This message-triggered thread is active on all worker processors, receiving subproblems for processing.

Worker auxiliary thread: This message-triggered thread is active on workers that are not also functioning as hubs. The hubs send this thread various instructions, such as to write a checkpoint, check for termination, or terminate the search process. The worker auxiliary thread also periodially receives information relevant to the load balancing algorithms.

## 4 Creating PEBBL Applications

When using PEBBL, you should generally first create a serial PEBBL application and debug it using whatever C++ development tools you are most comfortable with. Then you should extend it to a parallel application using MPI.

## 4.1 Compiling and linking your application

To build a PEBBL application, you must indicate the proper include path to the compiler and the proper library location to the linker. There are two choices for the include directory root:

- path/pebbl/src, where path is the location where you downloaded PEBBL
- If you performed the make install step after compiling, you may also use include file location specified in the install step, <code>CMAKE\_INSTALL\_PREFIX/include\_install\_dir</code>, where <code>CMAKE\_INSTALL\_PREFIX</code> and <code>include\_install\_dir</code> are as selected in the <code>cmake</code> configuration process. With the configuration settings shown in Section 2.4, this directory would be <code>path/installpebbl/include</code>.

PEBBL is compiled to a static library libpebbl.a. After compilation, this library file is located in path/buildpebbl/src/pebbl, where buildpebbl is the cmake build directory. The make install step copies this library to CMAKE\_INSTALL\_PREFIX/lib\_install\_dir, where CMAKE\_INSTALL\_PREFIX and lib\_install\_dir are as selected in the cmake configuration process. With the configuration settings shown in Section 2.4, this directory would be path/installpebbl/lib.

In a standard unix/Linux environment the compiler directives needed if you did not perform the make install step would be

-I[path/]pebbl/src -L[path/]buildpebbl/src/pebbl -lpebbl

where path is the directory where you downloaded PEBBL, assuming that the cmake build directory is named buildpebbl.

If you did perform the make install step, you may specify the install locations instead. Assuming that lib\_install\_dir and include\_install\_dir were left at their default values of include and lib, respectively, the required compiler/linker directives would be

-ICMAKE\_INSTALL\_DIR/include -LCMAKE\_INSTALL\_DIR/lib -lpebbl

If PEBBL was downloaded to location path and the configuration options are as shown in Section 2.4, these directives would be

-I[path/]installpebbl/include -L[path/]installpebbl/lib -lpebbl

## 4.2 Defining a serial application

To create a basic serial PEBBL application, you need to:

- Define a class extending branching
- Define a class extending branchSub
- If necessary, create a class extending solution
- Create a "driver" program that runs your algorithm.

You may concentrate your code for all these purposes in a single C++ file. Conventionally, however, you would use a header (.h or .hpp) file to define your new classes, one or more additional C++ source files containing code to implement methods for those classes, and a separate C++ source file containing the driver.

To load the basic definitions of branching, branchSub, and solution into the compiler, you should #include the file <pebbl/bb/branching.h>. Supposing your classes are called myBranching and myBranchSub, and you are using a single header file, it should take the general form shown in Figure 13.

We now describe how to construct these classes; in the course of this description, you may also refer to the files serialCore.h, and serialKnapsack.{h,cpp} in the directory acro-pebbl/packages/pebbl/src/example/pebbl.

### 4.2.1 Methods you should create — branching-derived class

In your branching-derived derived class, for example myBranching, you should define the following methods:

### Constructor

Classes derived from branching should have a constructor with no arguments; the diamond inheritance pattern used by PEBBL means that constructors with arguments are in general not advisable for branching- and branchSub-derived classes. The constructor should contain

```
#include <pebbl/bb/branching.h>
using namespace pebbl;
class myBranchSub; // Forward declaration
class myBranching : virtual public branching
    friend class myBranchSub;
public:
    myBranching methods and data here
}
class myBranchSub : virtual public branchSub
    friend class myBranching;
protected:
    // A pointer to the global branching object
    myBranching* globalPtr;
public:
    // Return a pointer to the global branching object
    myBranching* global() const { return globalPtr; }
    // Return a pointer to the base class of the global branching object
    branching* bGlobal() const { return global(); }
    myBranchSub methods and data here
}
```

Figure 13: Standard code pattern for creating a serial PEBBL application.

a call to branching::branchingInit(···). If you want to maximize the objective function, you should supply branchingInit an argument of maximization; if you want to minimize, you can leave the argument list blank, or supply the argument minimization. Thus, one might have something like

```
myBranching()
{
    branchingInit(minimization);
    :
};
```

The direction of minimization is stored in the data member branching::sense. The values minimization and maximization are C++ enum values, equal to +1 and -1, respectively.

#### Destructor

Naturally, you should also have a destructor for your branching-derived class, for example:  $\sim myBranching() \{ \cdots \};$ 

## branchSub\* blankSub()

You must provide a blankSub() method of return type branchSub\* that returns an empty subproblem specific to your application. To avoid circularity, the class declaration for myBranching should declare this method, but not include its code, as in:

```
branchSub* blankSub();
```

Once myBranching and myBranchSub are both declared, you should have the actual code, for example:

```
branchSub* myBranching::blankSub()
{
    myBranchSub* newSP = new myBranchSub;
    newSP->setGlobalInfo(this);
    return newSP;
};
```

Here, myBranchSub::setGlobalInfo is a method that is required to be a member of the subproblem class (see Section 4.2.2 below), and copies any necessary information from the myBranching object into a myBranchSub object. At a minimum, it should set the subproblem's globalPtr member.

```
bool setupProblem(int& argc,char**& argv)
```

This method is responsible for reading in any input data describing the problem instance. Its arguments argc and argv are standard unix-style command line descriptors. However, by the time setupProblem is called, these arguments will be "cleaned" of any MPI-related information and parameter settings recognized by PEBBL. Typically, setupProblem should

simply read a problem description from the file whose name is pointed to by argv[1]. The setupProblem method should return true is problem setup was successful.

```
void reset(bool resetVB = true)
```

Perform any initializations needed after setupProblem and before solving the actual problem. For some applications, the default implementation branching::reset may suffice. The optional argument resetVB indicates whether virtual base classes should be reset as well; it is present to allow one to avoid multiple redundant initializations of such bases classes. Typically, it can be ignored, although there may be a minor performance penalty. If you override the reset method, make sure your implementation invokes branching::reset in addition to any application-specific initializations it performs.

#### 4.2.2 Methods you should create — branchSub-derived class

#### Constructor

As with the branching-derived class, you should have an empty-argument constructor for your branchSub-derived class, for example:

```
myBranchSub() { ··· };
```

#### Destructor

A destructor is naturally required, for example:

```
\simmyBranchSub() { \cdots };
```

## branching\* bGlobal() const

This method is required for methods in branchSub to locate the corresponding problem-wide information in the corresponding branching object. Presuming you have declared a data member myBranching\* globalPtr as in Figure 13, then Figure 13's definition should suffice:

```
branching* bGlobal() const { return global(); };
```

Your implementations of methods such as boundComputation() will almost certainly require access to problem-wide but application-specific information. In the implementation above, this may be obtained directly through globalPtr or slightly more elegantly via

```
myBranching* global() const { return globalPtr; };
```

## void setGlobalInfo(myBranching\* global\_)

The purpose of this routine should be to "bind" a particular subproblem object to the problem description embodied in the object \*global\_. At a minimum, this requires setting globalPtr. For example:

```
void setGlobalInfo(myBranching* global_)
{
   globalPtr = global_;
   (Copy any other desired information from *global_)
}
```

#### void setRootComputation()

A call to this method indicates that a *myBranchSub* object should be made into a root subproblem. Information on the problem instance should be obtained, for example, via global() or globalPtr.

## void boundComputation()

This method should attempt to bound the subproblem. When the bound computation is complete, it should execute setState(bounded). If the method exits without calling setState(bounded) to declare the subproblem bounded, PEBBL will assume that the bounding operation is incomplete: it will call boundComputation() repeatedly (but perhaps not immediately) until the subproblem is fathomed or declared bounded. To indicate the value of the bound, you set the double data member bound; you may update bound as many times as you like, and PEBBL will use the information immediately, even before the problem state becomes bounded — for example, a sequence of calls to boundComputation() may gradually improve the bound. To indicate infeasibility of a subproblem, or that it cannot possibly improve upon the current solution stored in bGlobal()->incumbentValue, you may execute setState(dead).

## bool candidateSolution()

PEBBL will only invoke this method for subproblems in the bounded state. Returning true means that the just-computed bound is exact: not only is it a bound on all solutions in the region of the search space corresponding to the subproblem, but that bound is also attained by at least one feasible solution in that region. Unless one is enumerating multiple solutions, such a subproblem is considered a terminal node of the branch-and-bound tree, and will not be separated. In integer programming, for example, you would want candidateSolution() to return true whenever the linear programming relaxation produces a solution that has all integer values. Returning true also indicates to PEBBL that you have computed a feasible solution to the overall optimization problem, as opposed to just a bound. PEBBL will most likely invoke extractSolution() (see below) to retrieve this solution.

## solution\* extractSolution()

PEBBL will only call this method for bounded subproblems for which candidateSolution

has returned true. The method should return a pointer to a solution-derived object containing a solution corresponding to the subproblem bound. See Section 4.2.3 for more information on solution objects. Ownership of the returned object is ceded to PEBBL.

## int splitComputation()

This method should attempt to separate the subproblem. Similarly to boundComputation(), it will be invoked repeatedly until it calls setState(separated). The value returned is the number k of child problems generated (simply 2 for many applications). The number of children can vary between subproblems. If you return without declaring the problem separated, PEBBL will ignore the return value and invoke splitComputation() again later. In the course of separating the problem, you may update bound at any time to reflect any further information gained in the course of separation; PEBBL will use this information immediately. This routine may also execute setState(dead), in which case PEBBL will immediately prune the subproblem.

If PEBBL is not in enumeration mode, it will call splitComputation() only for nodes for which candidateSolution has returned false. On the other hand, if PEBBL is enumerating multiple solutions, it is possible that splitComputation() may be called for nodes for which candidateSolution has returned true. If you need your application to be compatible with enumeration, it should be able to handle this case of separating an otherwise "terminal" subproblem. In some applications, such nodes may require a completely different separation technique than other nodes, and possibly a different number of children. Ideally, when separating a subproblem P for which candidateSolution has returned true, you should create one or more children corresponding to search-space regions which are disjoint and contain all solutions corresponding to P except the one just returned by P.extractSolution(). This latter solution will already be known to PEBBL and need not be examined again. If a node is "truly terminal" in that it corresponds to a subset of the search space containing only a single distinct feasible solution, then splitComputation() should call setState(dead) and return 0.

#### branchSub\* makeChild(int whichChild)

This method should create a child problem and return a pointer to it. The argument whichChild may take any value between 0 and k-1, where k was the value returned by splitComputation() for this subproblem. A value of 0 indicates you should create the first child, a value of 1 indicates you should create the second child, and so forth.

When you create a child problem, you should make sure that its globalPtr is set as in the parent problem, and all local data are initialized correctly. In order for PEBBL to correctly track subproblem depth and counts of created subproblems, it is also necessary to correctly set up various data members of the branchSub class. PEBBL provides a method called branchSubAsChildOf to perform this operation. Specifically, the child problem should invoke branchSubAsChildOf(parent) soon after it is created, where parent is a pointer to the parent subproblem. Alternatively, the parent subproblem may call

child->branchSubAsChildOf(this);

where *child* is a pointer to the child subproblem just created.

#### 4.2.3 The solution class and related methods

PEBBL manipulates feasible problem solutions via objects whose type is derived from solution. For example, the extractSolution() method should return a solution\*, as should the initialGuess method; see Section 4.2.5 below. The solution class itself contains (among others) the following members:

```
double value: the solution's objective value.
int serial: a serial number (assigned automatically by PEBBL).
size_type hashValue: a value for use in hash tables
```

It is possible to represent solutions via the solution base class; however, such a representation will essentially contain only the solution's objective value, and no other information. To construct such an object, use the constructor solution(branching\*), and then set the value of the resulting object. For example, for the code in the myBranchSub class of Figure 13, one would use

```
s = new solution(global());
s.value = objective value;
```

Far more likely, however, you will want a true solution representation that contains more information than just the objective value. In this case, you should use another class derived from solution. Here, there are two choices: use the template class arraySolution < T >, or derive your own solution-based class.

Note that each instance of the solution class contains its own sense member which must be set to maximization or minimization consistently with branching-derived object describing the problem instance (for example, myBranching). Typically, this is handled by passing a branching\* pointer to the solution constructor.

Starting with PEBBL 1.6, the solution class includes a reference counter, and its destructor will throw an exception if activated when this counter is nonzero. One should not directly invoke the destructors of solution-derived objects by using the delete operator, but instead use the dispose() method of the solution class. This method decrements the reference counter and then call the destructor if the counter is zero. The reference counter may also be incremented or decremented by the incrementRefs() and decrementRefs() methods, respectively. If a solution-derived object is allocated on the stack by direct declaration, rather than by using the new operator, one should call its decrementRefs() method before it passes out of scope; otherwise its destructor will trigger an exception.

The template arraySolution<T> is a ready-made PEBBL-supplied class that represents a solution as a one-dimensional array (that is, a vector) of some type T which may be implicitly converted to a double without loss of information. To create such a solution object, invoke a constructor (supplied by PEBBL) of the form arraySolution< $T>(z,v,b,t,\nu)$ , where:

- z denotes the objective value of the solution
- v is either a UTILIB array object of type BasicArray<T>, an STL vector of type vector<T>, or some object derived from either of those possibilities (for example, the UTILIB IntVector type derives from BasicArray<int>, and may thus be used to create an arraySolution<int>). This information is copied into the new arraySolution object.
- b is a pointer to the branching-derived object describing the problem instance; within the class myBranchSub of Figure 13, you would set b = global(), and within the myBranching of Figure 13, you would set b = this. One function of this argument is to make sure that the maximization / minimization sense of the arraySolution is set correctly.
- t is optional, and is simply a const char\* pointing to a description of the type of solution, for example, "Vector of integers".
- $\nu$  is also optional, and is a pointer to a BasicArray<br/><br/>CharString> object containing names of the decision variables. It should be at least as long as v.<br/> These names are used when printing the solution contents.

For descriptions of the types BasicArray and CharString, see the UTILIB documentation. If arraySolution does not apply to your problem, is inconvenient, or will be inefficient, you should derive your own class of objects from solution, as in:

class 
$$\textit{mySolution}$$
 : virtual public solution  $\{\ \cdots\ \}$  .

You may use more than one kind of solution class in a single application.

To facilitate hashing and comparison, solutions normally have a "sequence representation", as described in Section 3.2.3. This representation is essentially a one-dimensional array of doubles, although it need not be (and probably should not be) explicitly stored. By default, PEBBL uses this sequence representation to compute a solution's hashValue and to compare two solutions to detect duplicates. The solutions are considered duplicates if and only if their sequence representations are identical in both length and contents.

In addition to application-specific data members describing a solution, a customized solution class like *mySolution* should typically define the following **virtual** methods:

#### Constructor

To create the underlying solution object, your solution constructor should invoke the solution(branching\*) constructor. It should also set the value member to reflect the solution's objective value. For the <code>myBranching</code>, <code>myBranchSub</code>, classes, for example, the standard constructor pattern would be

Note that in the invocation of solution(global\_), the myBranching\* pointer global\_ is automatically cast to a base class pointer of type branching\*.

## Destructor

A destructor should be provided. However, as noted above, it should not be invoked directly through delete, but through the solution class' dispose() method.

```
const char* typeDescription() const
```

Returns a const char\* describing the type of solution, for example "Knapsack solution".

```
virtual void printContents(std::ostream& s)
```

Write the solution contents (for example the decision variable values) to the stream s. You do not need to write the objective value; it is printed by another method. The default implementation is a stub.

```
virtual size_type sequenceLength()
```

Return the number of elements in the sequence representation of the solution.

```
virtual double sequenceData()
```

Return the next element of the sequence representation.

The following method is related to sequenceData() and sequenceLength(), but may not have to be overridden:

```
virtual void sequenceReset()
```

Cause the next call to sequenceData() to return the first element in the sequence. The default implementation is simply to set the data member sequenceCursor (built into the solution class) to zero.

Note that PEBBL will call sequenceData() at most sequenceLength() times between calls to sequenceReset(). Typically, the default implementation of sequenceReset() will suffice, and each call to sequenceData() should return the sequenceCursor<sup>th</sup> element of the sequence and then increment sequenceCursor.

It is not absolutely necessary that a solution have a sequence representation, and thus not absolutely required that you define sequenceLength() and sequenceData(). If you do

not define those methods, however, you must define two other methods:

```
size_type computeHashValue()
```

Return the hash value of the solution.

```
bool duplicateOf(solution& other)
```

Return true if other is an identical solution, and otherwise false.

Normally, it is recommended that you simply retain the default implementations of these methods, and define application-specific versions of sequenceLength(), sequenceData(), and possibly sequenceReset(). The default implementations of computeHashValue() and duplicateOf are based on the sequence representation. Even if you have defined a sequence representation, you may elect to override computeHashValue() and/or duplicateOf to improve efficiency.

#### 4.2.4 The foundSolution method

So far, the only means we have discussed for providing solutions to PEBBL is the method extractSolution (see Section 4.2.2), which PEBBL calls between boundComputation and splitComputation for subproblems whose bounds are known to be exact. Many branch-and-bound algorithms encounter feasible solutions at other points in the search process. When this occurs, you may call the method branching::foundSolution(solution\* sol), where sol is a pointer to a solution-derived object. You need not first ascertain whether \*sol is a better solution than the incumbent, or, when enumerating multiple solutions, whether it is eligible to enter the repository. PEBBL will determine whether the solution is useful, and otherwise delete it. Note that calling foundSolution(sol) cedes memory ownership of one reference to \*sol to PEBBL. If the caller would like to continue using \*sol after calling foundSolution(sol), the following apply:

- The caller should invoke sol->incrementRefs() before calling foundSolution(sol)
- The caller should not alter the contents of \*sol solution after invoking the method foundSolution(sol), since doing so could cause internal errors or unpredictable behavior in PEBBL
- Once it no longer needs \*sol, the caller should invoke sol->dispose().

If the caller does not have further need of \*sol after calling foundSolution(sol), no action is necessary.

It is safe to call foundSolution at any point within the branch-and-bound tree exploration, for example, from within the methods boundComputation, splitComputation and makeChild. For example, from the boundComputation method of the hypothetical myBranchSub class, you could invoke foundSolution via global()->foundSolution(sol). You should not call foundSolution at points before the branch-and-bound search has begun

(for example, in the setupProblem method or the preprocess method described immediately below), or after the search has concluded. To provide a rough initial solution before the tree exploration process has started, use the initialGuess method described immediately below.

#### 4.2.5 Selected additional methods

We now present an inexhaustive list of additional methods that you may wish to override for particular applications.

## void branching::preprocess()

This method is intended for "preprocessing" of the problem prior to commencing the branch-and-bound search; the default implementation is an empty stub. In principle, its functions could be combined with  $setupProblem(\cdots)$ , but it is provided for clarity and to ease migration to the parallel layer.

## solution\* branching::initialGuess()

PEBBL calls this method between preprocessing and the start of the branch and bound search. Its intention is allow computation of a "quick and dirty" initial guess at the solution. In a knapsack problem, for example, this routine could run a simple greedy heuristic. Your implementation need not be guaranteed to find a usable solution; if it does not, it should just return a NULL pointer. The default implementation is a stub that simply returns NULL.

## |bool branching::haveIncumbentHeuristic()

The default implementation of this method just returns false. You should change it to return true if your application has a way of trying to obtain a feasible solution from a non-terminal bounded subproblem.

## void branchSub::incumbentHeuristic()

This method applies only to the serial layer, and PEBBL will only call it directly if the method haveIncumbentHeuristic() returns true. PEBBL calls it at two points, once a solution has become bounded, and once it has become separated. The intention is to allow the heuristic calculation of feasible solutions. Whenever your implementation finds a feasible solution, it should communicate it to PEBBL by calling foundSolution. The default implementation is a stub.

You may wish to check the subproblem state at the beginning of your implementation of incumbentHeuristic. For example, if you wish your heuristic to be invoked only when subproblems become bounded, and not when then become separated, you could begin your implementation with

#### if (state != bounded) return;

If you wish to construct heuristic solutions at other points besides when subproblems become bounded or separated, you can create your own heuristic method and invoke it at other times, having it call foundSolution to send new solutions to PEBBL.

Note that the parallel layer treats incumbent heuristics somewhat differently, and parallel-layer runs will not explicitly call incumbentHeuristic; see Section 4.3 below.

```
void branchSub::makeCurrentEffect()
```

PEBBL has the notion of a "current subproblem" – the one presently being bounded or separated. The method makeCurrentEffect() provides a "hook" that is called whenever a subproblem is made "current". In a branch-and-cut algorithm, for example, this method could load the subproblem's cuts into the linear programming solver. Its default implementation is a stub.

```
void branchSub::noLongerCurrentEffect()
```

PEBBL calls this "hook" whenever a subproblem ceases to be "current". Again, its default implementation is a stub.

```
bool branchSub::forceStayCurrent()
```

PEBL calls this method when it is considering replacing the current subproblem with a different one. Returning true indicates that the current subproblem should be kept current if at all possible. The default implementation always returns false, meaning that PEBBL is free to "unload" the current subproblem, and replace it with a different one.

```
bool branching::checkParameters()
```

PEBBL calls this method to make sure that its runtime parameters are set correctly and consistently. You may override this method to perform additional checks specific to your application, and then call branching::checkParameters() to make sure PEBBL's internal checks are invoked. You are most likely to need this routine if you have defined your own application-specific runtime parameters; see the section immediately below.

#### 4.2.6 Creating your own parameters

In addition to PEBBL's existing parameters, you may create your own command-line parameters. The simplest place to do so is in the constructor of your branching-derived class. Alternately, you can define a underlying base class to hold your parameters: you could create a class <code>myParams</code> to hold your parameters, and then derive <code>myBranching</code> from both branching and <code>myParams</code>. Parameter creation statements should usually reside in constructors and have the general form

```
create\_categorized\_parameter("commandLineName",\\ internalName,\\ "< datatype>",\\ "defaultValue",\\ "text description",\\ "category"[,]\\ [error check object])
```

Here,

- commandLineName is the name to be recognized on the command line. For example, fooBar will cause the option --fooBar=value to be recognized on the command line.
- internalName is a reference to a class data member in which to store the value of the parameter; usually, internalName and commandLineName should be identical for clarity.
- datatype is the C++ datatype of internalName. Common choices are bool, int, double, and string.
- default Value is a text representation of the default value for the parameter. It should match the initial value stored in the data member internalName. Note that the specification of default Value does not automatically initialize the value of internalName; its initial value should be set by the class constructor and reset methods.
- text description is a parameter description printed in response to --help. For descriptions longer than one line, embed newline-tab character sequences (" $\n$ ") in this text.
- category The category header to be used when printing the parameter description in response to --help. You may invent new categories.
- error check object is optional and specifies simple constraints on the value of the parameter. For example,

#### ParameterNonnegative<int>()

specifies that an integer parameter must be nonnegative, while

#### ParameterBounds<double>(0.0,1.0)

specifies that a double-datatype parameter must have values between 0 and 1, inclusive. Other common forms for error-check objects are

ParameterLowerBound<datatype>(minimum value)
or ParameterUpperBound<datatype>(maximum value)

For more details, refer to the UTILIB Parameter and related class documentation.

For error checks that are more elaborate, or involve interactions between multiple parameters, you may specify parameter error checks by overloading the checkParameters boolean method in the branching class, for example with *myBranching*::checkParameters; if this routine detects an error, it should print a diagnostic message and return false. If it does not, it should execute return branching::checkParameters() to invoke the standard checks on PEBBL's built-in parameters.

Note that for parameters of type bool, you may omit =value on the command line, in which case the value is set to true. That is, --fooBar is equivalent to --fooBar=true

Figure 14: Code equivalent to the serial driver<myBranching>(argc,argv) template.

#### 4.2.7 Serial main programs: drivers

PEBBL is structured as a callable library, and can thus be incorporated directly into other C++ applications. If you want your PEBBL application to function as a simple "solver" executable that simply reads in a problem instance data file and solves it, you need to create a "driver" main program. A simple template function called driver is available for this purpose. Using this template, you can construct the driver for the hypothetical example application myBranching as follows:

```
Header file #includes, including myBranching class and class and cpebbl/branching.h>
int main(int argc, char** argv)
{
    return driver<myBranching>(argc,argv);
}
```

Invoking driver<myBranching>(argc,argv) is equivalent to the code shown in Figure 14. Note that the main PEBBL header file <pebbl/branching.h> automatically includes the necessary UTILIB header files to define the method InitializeTiming(). Note also that setup(···), reset(), and solve() are all methods of the branching class that you typically do not override. Calling setup(argc,argv) parses the command line, extracting and processing all command line arguments recognizable as PEBBL parameters, including any application-specific parameters created as described in Section 4.2.6. It then calls your implementation of setupProblem, with argc and argv adjusted so that parameter-setting arguments are removed; setup's returning true indicates both that all command line parameters were processed correctly, and that your setupProblem implementation returned true, indicating it was successful. The method solve() invokes the branch-and-bound search engine, and prints subproblem count and timing statistics upon termination. It also uses your solution-derived class' printContents implementation to write the final solution(s) to a file whose name is derived from the first command line argument not recognizable as a

parameter setting, typically by appending sol.txt; if no such parameter can be found, the file is called sol.txt). If you instead wish to specify your own choice for the solution file, use the --output=filename command-line option. Here, filename may contain path information, and thus need not be in the current directory.

The setup method manages parsing of the command line including option specifications and a problem instance data file name. Supposing your driver were called myDriver, the command line myDriver datafile would call myBranching::setupProblem(argc,argv) with argv[1] containing the null-terminated string datafile — with a typical implementation of setupProblem, this would cause your application to read in the problem instance description in datafile. In parsing the command line, setup will also recognize all PEBBL command-line parameters (see Section 5 for a partial catalog) along with any parameters defined for myBranching, as described in Section 4.2.6. For example, in the command line

myDriver --relTolerance=0.05 --earlyOutputMinutes=2 datafile

the PEBBL parameters relTolerance and earlyOutputMinutes would be set to 0.05 and 2, respectively. In this example, myBranching::setupProblem(argc,argv) would still be called with argv[1] containing the null-terminated string datafile, presumably reading the problem instance in datafile. The setup method also automatically recognizes several special command-line arguments:

- --help Causes setup to print a usage line followed by a description of all available parameters, and then return false (so that the driver above would not attempt to solve a problem). If you want to control the form of the usage line, override the method void branching::write\_usage\_info(char\* progName,std::ostream& os). When PEBBL calls this method, the argument progName is set equal to argv[0].
- --version must be the first argument if present. It causes setup to print the value of the static std::string data member branching::version\_info and return false (so that the driver above would then immediately exit). You may alter the contents of version\_info, for example, in the constructor for your branching-derived class.
- --param-file=file allows multiple parameter settings to be read from the file file see the UTILIB Parameter class documentation for a description of the file format.

The reset() method invoked by the driver template performs all necessary initializations prior to the solution process, which is performed by solve(). The solve() method in turn invokes several lower-level methods, principally:

search() to perform the actual branch-and-bound search.

printAllStatistics() to print information about the number of search nodes and run time.

solutionToFile() to write the solution file.

#### 4.2.8 "Quiet" operation

If PEBBL is embedded within another application, it may be desirable to have it run "quietly", without any configuration, status, or performance-statistics printouts. In this case, you should use the search() routine instead of solve() and make sure that solution status printouts are disabled by setting both branching::statusPrintCount and statusPrintSeconds to zero (see Section 5.6 for discussion of the corresponding runtime parameters).

#### 4.2.9 Retrieving solutions to C++ code

Note that PEBBL applications can be invoked in ways other than the simple driver above; for example, they could be embedded in more complicated C++ programs, in which case you would probably use the search() method to perform the branch-and-bound search, and avoid command-line-oriented methods like driver, setupProblem, and solve().

Various approaches are available to retrieve solutions computed by running the search() method; note that all the methods described in this subsection are members of the branching class. If you are not enumerating multiple solutions, you should simply use the method getSolution(), which returns a solution\* pointer to the incumbent solution. This method returns NULL if no solution was found. Within your application, the solution\* pointer returned by getSolution() will most likely need to be cast "up" the inheritance hierarchy so that its contents may be accessed, preferably using the C++ dynamic\_cast operator.

For retrieving multiple solutions from a run enumerating multiple solutions, the simplest technique is to define an object <code>solArray</code> of type <code>BasicArray<solution\*></code> and then call the method <code>getAllSolutions(solArray)</code>. This method will redimension <code>solArray</code> to the size of the repository and fill it with <code>solution\*</code> pointers to the repository members, in objective-value order, starting with the best value.

For compatibility with the parallel layer, a second, iterator-like technique is also possible. In this approach, one first calls  $\mathtt{startRepositoryScan}()$ , which returns the size n of the repository. One may then call  $\mathtt{nextRepositoryMember}()$  up to n times: each time, it will return a different member of the repository. Again, solutions are returned in objective value order, starting with the best values.

For any solution pointer sol returned by getSolution, getAllSolutions, or next-RepositoryMember, the application should call sol->dispose() when it no longer needs the corresponding solution object. As discussed in Section 4.2.3, one should never directly use delete on solution-derived objects, because they are reference-counted.

#### 4.2.10 Debugging outputs

In the process of debugging a PEBBL application, it may be necessary to print diagnostic outputs. Through the companion UTILIB package that it automatically includes, PEBBL provides special mechanisms for such output. The most frequently used is the DEBUGPR macro, which takes the form

DEBUGPR(level, action);

Inside a class derived from branching, such a statement indicates that the code given by action be executed if the PEBBL debug output level specified by the run-time parameter debug in Section 5.2 has a value of level or higher. Typically, action should involve writing text to the specialized stream ucout. For example, the statement

```
DEBUGPR(10,ucout << "Value of n is " << n << endl);</pre>
```

will print the value of the variable n whenever the debug output level is at 10 or higher. While it makes not difference in the serial layer, using the special stream ucout is preferable to using the standard stream cout because ucout has special features that make it more convenient in a parallel setting. In particular, when used in parallel, each line of text sent to ucout will be prefixed by a tag indicating which processor wrote the information.

A slightly different form of debug printing is used in subproblem classes derived from branchSub, as opposed to problem classes derived from branching. In this setting, the diagnostic output above would instead be expressed as

```
DEBUGPRX(10,global(),ucout << "Value of n is " << n << endl);</pre>
```

The reason for this difference is that, for efficiency reasons, branchSub does not derive from the same UTILIB CommonIO utility class that branching does.

The CommonIO class from UTILIB makes several other variations on the DEBUGPR available for specialized situations. Consult the UTILIB documentation for more information.

An advantage of using the DEBUGPR and related facilities instead of *ad hoc* print statements is that the diagnostic output may be left in the code indefinitely and triggered whenever needed by using the debug runtime parameter. For example, running a PEBBL application with the command-line option --debug=10 would set the debugging level to 10.

# 4.3 Defining a parallel application

Now suppose that your serial layer applications runs acceptably, and you wish to parallelize it. If you want to use parallelism, be sure that you have configured PEBBL with the enable\_mpi option; see Section 2.4.

When Acro is compiled with MPI, the preprocessor symbol ACRO\_HAVE\_MPI is defined; otherwise it is not defined (the "ACRO" in this symbol refers to a larger package within which PEBBL used to be distributed). When ACRO\_HAVE\_MPI is undefined, only the serial portions of PEBBL are compiled; the parallel portions are omitted or become stubs. You may wish to follow this same pattern within your own application source code.

Figure 15 outlines the recommended inheritance and pointer pattern for creating parallel layer classes from a serial application. Here, the serial layer classes are <code>myBranching</code> and <code>myBranchSub</code>, and the corresponding respective parallel layer classes are <code>myParBranching</code> and <code>myParSub</code>. Note that the header file <pebbl/pbb/parBranching.h> defines all the classes in both the serial and parallel layers.

Note that PEBBL uses parallelBranchSub::pGlobal() to find the parBranching object associated with a subproblem object. The method global() in Figure 15 would be

```
#include <pebbl/pbb/parBranching.h>
using namespace pebbl;
class myParSub; // Forward declaration
class myParBranching :
   virtual public parallelBranching,
   virtual public myBranching
public:
   myParBranching methods and data here
};
class myParSub :
   virtual public parallelBranchSub,
   virtual public myBranchSub
protected:
   // A pointer to the global parallel branching object
   myParBranching* globalPtr;
public:
   // Return a pointer to the global branching object
   myParBranching* global() const { return globalPtr; }
   // Return a pointer to the parallel global base class object
   parallelBranching* pGlobal() const { return global(); }
   myParSub methods and data here
};
```

Figure 15: Standard code pattern for creating a parallel PEBBL application.

for your own use and might not be necessary if your parBranching-derived class does not encapsulate significantly more data than your branching-derived class.

Your parBranching-derived class may also contain additional parameters not present in your branching-derived class. The method for the creating such additional parameters is identical to that of Section 4.2.6, but the corresponding data members should be in your parBranching-derived class, for example *myParBranching*, and the necessary matching calls to create\_categorized\_parameter should be in that class' constructor.

#### 4.3.1 Methods you should create — parallelBranching-derived class

#### Constructor

It is advised that you create a constructor with a single argument, the MPI communicator under which the search will be run, with a default value of MPI\_COMM\_WORLD. This constructor should set the MPI communicator member mpiComm of the parBranching class and call the no-argument constructor for your serial application class, such as myBranching.

```
myParBranching(MPI_Comm comm_ = MPI_COMM_WORLD) :
myBranching(),
mpiComm(comm_)
{ ··· };
```

#### Destructor

You should also have a destructor:

```
\simmyParBranching() { \cdots };
```

```
void reset(bool VBflag = true)
```

Perform all needed initializations subsequent to reading in the problem instance. This process consists of the following steps (not necessarily in the given order):

- Invoke the underlying serial problem-instance class reset method, for example by *myBranching*::reset.
- Register at least one reference solution; see Section 4.3.4.
- Invoke the parBranching::reset method.
- Perform any additional application-specific initializations that are needed only by parallel runs.

The VBflag argument has the same purpose as the resetVB argument in serial reset methods. See Section 4.3.4 below for an example implementation of the parallel reset method.

### parallelBranchSub\* blankParallelSub()

This method is similar to blankSub, but should return a parallel subproblem with correctly initialized global pointers, as in the following code; see Section 4.3.2 below for a possible implementation of myParSub::setGlobalInfo.

```
parallelBranchSub* myBranching::blankParallelSub()
{
    myParSub* newSP = new myParSub;
    newSP->setGlobalInfo(this);
    return newSP;
};
```

#### void pack(utilib::PackBuffer& outBuffer)

PEBBL uses this method when broadcasting the problem description. It should write all the the information describing a problem instance (i.e. everything read by  $setupProblem(\cdots)$ ) into the UTILIB PackBuffer supplied in the argument outBuffer. Writing to a PackBuffer is very similar to writing to an unformatted stream: for most native C++ datatypes, the << operator, that is, "outBuffer << data" will write scalar data. Entire UTILIB arrays, for example of datatype BasicArray<T>, IntVector or DoubleVector, may also be written with <<<, as can STL sets or vectors of standard C++ base types. See the UTILIB documentation for the details of PackBuffers.

```
void unpack(utilib::UnPackBuffer& inBuffer)
```

Again, PEBBL uses this method when broadcasting the problem description. Its job is to read from inBuffer the information written by pack. Most native C++ datatypes, along with many UTILIB-supplied containers and STL sets or vectors of simple types, may be read via the the >> operator, applied in exactly the same order as you used << in pack. For example, data written by

```
outBuffer << time << money;</pre>
```

in pack might be read via

```
inBuffer >> time >> money;
```

in unpack.

```
int spPackSize()
```

This method should return an upper bound on the number of bytes needed to pack all the information to describe  $a \ subproblem$  — that is, the maximum amount of space needed by the method  $myParSub::pack(\cdots)$  described below. It does not refer to the amount of space needed by myParBranching::pack, which PEBBL is able to detect automatically. In PackBuffers and UnPackBuffers, most C++ native datatypes require the same amount of space as their machine representations: i.e a data member of type x requires sizeof(x)

bytes. You should use  $\mathtt{sizeof}(\cdot)$  in your implementation to make sure it is portable between 32- and 64-bit architectures and varying compilers. For standard container datatypes such as UTILIB arrays, STL sets, or STL vectors of type T, the space required is a single  $\mathtt{sizeof}(\mathtt{size\_t})$  to hold the size of the container, plus  $m \cdot \mathtt{sizeof}(T)$ , where m is the maximum container size possible for the given problem instance.

The spPackSize() method is called after the problem has been read and broadcast, so all information set by myBranching::setupProblem and myParBranching::unpack should be available to it in all processors.

Instead of direct calculation, one possible approach to implementing spPackSize() is to create a "dummy" subproblem of the largest size you anticipate needing, invoke your  $myParSub::pack(\cdots)$  method to write it to a dummy buffer dumBuf, and finally measure the size of that buffer with dumBuf.size().

#### 4.3.2 Methods you should create — parallelBranchSub-derived class

#### Constructor

Again, you need an empty-argument constructor, for example:

```
myParSub() \{ \cdots \};
```

## Destructor

You also need a destructor:

```
\simmyParSub() { \cdots };
```

## parallelBranching\* pGlobal() const

This method is similar to bGlobal, but returns a pointer of type parallelBranching\*, implementing the third dashed arrow in Figure 11. Given globalPtr as defined in Figure 15, it could be implemented via

```
myParBranching* global() const { return globalPtr; }
parallelBranching* pGlobal() const { return global(); }
```

## void setGlobalInfo(myParBranching\* global\_)

As in the serial, case, the purpose of this routine should be to "bind" a particular subproblem object to the problem instance description embodied in the object global. It should also make sure that the corresponding serial-layer binding is also performed. For example:

```
void setGlobalInfo(myParBranching* global_)
{
    globalPtr = global_;
    myBranching::setGlobalInfo(global_); // Sets serial layer pointer etc.
    :
}
```

```
void pack(utilib::PackBuffer& outBuffer)
```

This method should pack the application-specific portion of the description of the subproblem into the PackBuffer object outBuffer, typically using the << operator. For more details about writing to UnPackBuffer objects, see the description of branching::unpack above.

```
void unpack(utilib::UnPackBuffer& inBuffer)
```

This method should unpack the application-specific portion of the description of the subproblem from the UnPackBuffer object inBuffer, typically using the >> operator. For more details about reading from PackBuffer objects, see the description of branching::pack above.

```
virtual parallelBranchSub* makeParallelChild(int whichChild)
```

This method is similar to makeChild, but returns a parallelBranchSub\*. It should create the whichChild'th child of the present subproblem, counting from 0 to k-1, where k is the number of children. PEBBL only calls this method for subproblems in the separated state.

Note: p->makeParallelChild(whichChild) should *not* have the side-effect of changing the bound of \*p, or memory errors may occur. This restriction may be removed in subsequent PEBBL releases.

### 4.3.3 Standard disambiguations

While the "diamond" inheritance pattern shown in Figure 7 is powerful, it may also lead to some ambiguities. When an inherited method is defined in several different base classes, the C++ compiler may be unsure which implementation to use. If such ambiguity occurs when compiling a parallel PEBBL application, the general rule is to use the implementation in either parallelBranching or parallelBranchSub, which will in turn automatically call the appropriate serial layer routine. In a class such as *myParBranching*, for example, it may be necessary to define

```
bool setup(int& argc,char**& argv)
{
    return parallelBranching::setup(argc,argv);
}
```

and similarly for a few other routines.

#### 4.3.4 Parallel solution management and parallel reset

PEBBL does not need distinct serial and parallel versions of the class representing problem solutions; the same solution class fulfills this role in both serial and parallel settings. To function in a parallel settings, however, user-defined solution-derived classes require a few additional methods beyond those mentioned in Section 4.2.3. Specifically, you should define implementations of the following virtual methods:

#### solution\* blankClone()

This method should return a new "blank" version of the current solution, that is, a (derived) solution object of the same type and dimensions. The blank copy should contain all information obtained or copied from your branching-derived class (for example, from the myBranching class). This information should include any pointers to the problem instance class, and the correct setting of sense. For all such information embedded in the solution base class, the constructor solution(solution\*) can be useful; a standard implementation pattern might be

```
solution* blankClone() { return new mySolution(this); };
mySolution(mySolution* toCopy) :
    solution(toCopy),
    ...other initializations ...
{ ... };
```

It is not necessary for the object returned by blankClone() to contain any valid information about a particular solution to your problem instance.

## void packContents(PackBuffer& outBuf)

Pack the application-specific information in the current solution into the PackBuffer object outBuf, typically using the >> operator. For more details about writing to PackBuffer objects, see the description of branching::pack above.

# void unpackContents(UnPackBuffer& inBuf)

Unpack application-specific solution information from the UnPackBuffer object inBuf, typically using the << operator. The order of unpacking should be identical to the order of packing in packContents. For more details about reading from UnPackBuffer objects, see the description of branching::unpack above.

## int maxContentsBufSize()

This method should return an upper bound on the maximum number of bytes that calls to packContents(outBuf) might write to the buffer outBuf for a solution to the current problem instance. For more information about how to calculate this buffer size, see the discussion of the parallelBranching::spPackSize() method above.

PEBBL has its own methods for packing and unpacking information contained in the

solution base class; packContents unpackContents, and maxContentsBufSize() do not need to take such information into account.

The interprocessor communication mechanism for solutions requires that you "register" a pointer to a "reference" object for each solution-derived class used by your application. It is recommended that you perform this operation in your parallel reset method, for example, myParBranching::reset. Reference solutions have three purposes:

- To calculate the maximum buffer size needed to receive a solution object: for each reference solution, PEBBL will call the method maxContentsBufferSize, and incorporate the results into its buffer sizing calculations.
- To create new solutions from messages: when a processor receives a message containing a solution, PEBBL calls the blankClone method for one of the reference solutions producing a new object s. PEBBL then reads the solution message into s by invoking s.unpack.
- To keep track of multiple solutions types: each kind of solution is assigned a typeId value, which is stored in the reference solution. When a processor receives a message containing a solution, this typeId value allows PEBBL to determine what kind of solution object it encodes.

Usually, a given application uses only one kind of solution, in which case the registration process is simple. You need only create a single solution object and pass it to the method parallelBranching::registerFirstSolution(solution\*). This object should be configured so that its maxContentsBufSize() method will return the correct value for the current problem instance. For example, if your application uses the arraySolution<int> solution representation and the maximum length of a solution is n, your myParBranching::reset would contain

#### registerFirstSolution(new arraySolution<int>(n,this));

The constructor arraySolution < int>(n,this) creates an array solution object of length n (of indeterminant contents); it can also accept optional arguments for a type name (e.g. "My application solution"), and an array of variable names. Constructing the reference solution with the maximum possible length n ensures that PEBBL's internal message buffers will be long enough for any message encountered.

If you use an application-specific solution-derived class, make sure your reference solution's maxContentsBufferSize method will return the maximum necessary space necessary to pack the solution's contents for the current problem instance, and its blankClone method will create properly formed solutions ready to have their unpack methods called on the results of any message pack operation. Assuming the mySolution (myBranching\*) constructor of Section 4.2.3 behaves in the manner, a typical form for the parallel reset method is

```
void myParBranching::reset(bool vbFlag=true)
{
    myBranching::reset();
    registerFirstSolution(new mySolution(this));
    parallelBranching::reset();
     :
    Any additional application-specific parallel-only initializations
     :
}
```

If your application uses more than one type of solution representation, you must register a reference solution for each type. You should register the first with registerFirstSolution, and the rest with registerSolution, which also takes a single solution\* argument. Equivalently, you can call clearRegisteredSolutions(), and then invoke registerSolution for each reference solution. Each solution type will be assigned an identifier of C++ type size\_type, which is returned from the registerFirstSolution or registerSolution call, and is also stored in the corresponding reference solution's typeId member. Whenever you create a new solution, make sure its typeId member is set to the identifier corresponding to its type (this should happen automatically, for instance, if you create all new solutions by applying blankClone to the corresponding reference solution).

Note that calling registerFirstSolution or registerSolution cedes ownership of one reference to the argument to PEBBL. Therefore it is not typically necessary to call the dispose() method of the registered solutions. PEBBL will do this automatically upon descruction or reset of a branching-derived object, or a call to clearRegisteredSolutions().

In the parallel setting, you still make PEBBL aware of new solutions using the same initialGuess, extractSolution, and foundSolution methods as in serial applications. However, these methods have more complex behavior in the parallel layer and may now trigger various forms of interprocessor communication. If you are not using enumeration, the communication is typically a simple broadcast of a possible new incumbent value. If enumeration is active, then new solutions may be "hashed" to other processor to check for duplication and for incorporation into the global solution repository. The foundSolution method also has special behavior during the ramp-up phase, see Section 4.3.6 below.

#### 4.3.5 Incumbent heuristics in parallel

PEBBL's parallel layer provides facilities allowing careful control over how much CPU time per processor is spent on incumbent heuristics. In the parallel setting, there are two possible levels of incumbent heuristic: a "quick" incumbent heuristic that is run for each bounded or separated subproblem, much as in the serial layer, and a separate incumbent thread whose CPU usage is controlled by the thread scheduler. We now consider the methods that implement this functionality. As in the serial layer, incumbent heuristics communicate solutions to PEBBL by calling foundSolution.

## void parallelBranchSub::quickIncumbentHeuristic()

The heuristic to be run for every bounded or separated subproblem, similarly to the method branching::incumbentHeuristic in the serial layer. The default implementation is a stub. You need not attempt to truly run your heuristic every time quickIncumbentHeuristic() is called. For example, your implementation could immediately return if the subproblem has the wrong state, or does not look particularly "attractive". If you do run your heuristic and find an improved incumbent, you should call updateIncumbent() or perform a similar sequence of operations. The process of calling quickIncumbentHeuristic() is separate from the heuristic thread and does not require existence of the heuristic thread. If you wish the incumbent heuristic calculations to be identical in the serial and parallel layers, make sure hasParallelIncumbentHeuristic() (see immediately below) returns false, and implement quickIncumbentHeuristic as follows:

```
void myParSub::quickIncumbentHeuristic()
{ myBranchSub::incumbentHeuristic(); };
```

## bool parallelBranching::hasParallelIncumbentHeuristic()

Returns false by default. Return true if your implementation has the capability to run a heuristic thread. PEBBL will create a heuristic thread if this method returns true and the parameter useIncumbentThread is true.

## void parallelBranchSub::feedToIncumbentThread()

This method is a "hook" called for each bounded subproblem. It is intended to examine a subproblem, and if it seems sufficiently attractive, copy some representation of it to the data structures used by the routine parallelIncumbentHeuristic. In creating these data structures, you may want to make them able to store representations of more than one subproblem.

# void parallelIncumbentHeuristic(double\* controlParam)

This is the method invoked by the incumbent thread. The argument controlParam is set by the scheduler to try to control the amount of CPU time each call uses. If you wish, you may ignore the value of this argument, and simply set \*controlParam = 1 upon exit. If you wish to be more responsive to the scheduler, try to do an amount of work roughly proportional (in some sense of your own choosing) to \*controlParam, and then set \*controlParam equal to the amount of work performed.

# ThreadObj::ThreadState incumbentHeuristicState()

This method indicates whether the incumbent thread is ready to run. The default implementation is to always return ThreadObj::ThreadBlocked, indicating the thread is unable to run. As soon as your thread has some data upon which to operate, you should return ThreadObj::ThreadReady instead.

#### double incumbentThreadBias()

This method indicates the importance of running the incumbent heuristic relative to the regular branch-and-bound worker process. The default implementation uses a formula involving various standard parameters and the current relative gap between the best known search node and the incumbent; see Section 5.8. You are free to override this method with something more specific to your application, but the details are omitted here.

#### 4.3.6 The ramp-up phase and parallel preprocessing

Section 3.3.5 describes how PEBBL can take advantage of non-tree parallelism during the early growth of the search tree. During the ramp-up phase, the methods boundComputation, splitComputation, and makeChild are called synchronously on identical subproblems for all processors. In your myParSub class, you may further override the implementations of these methods in your myBranchSub class, so they can exploit synchronous parallelism during ramp-up. The method parallelBranchSub::rampingUp() will return true during the ramp-up phase, and false otherwise.

Just before the ramp-up phase starts, but after the problem description has been broadcast, all processors invoke preprocess() and initialGuess(). The default behavior of preprocess is to just have all processors redundantly call the serial preprocess() method for the application. If you override preprocess() in your parallel-layer classes, however, you may substitute a different computation, perhaps parallelizing your preprocessing calculations.

A common source of errors during the ramp-up phase is processors not being sufficiently synchronized. If, for example, two processors do not agree on the value of the incumbent, they may start following different computational paths, eventually resulting in an MPI deadlock. At any point in your implementation of ramp-up that you could change the incumbent in a way that might not be identical for all processors, you should call

#### parallelBranchSub::rampUpIncumbentSync()

before taking any action that could lead to a different pattern of search tree exploration or any variations in MPI routine calls. This method forcibly synchronizes the incumbent and (if enumeration is active) the solution repository. In parallel settings, PEBBL automatically calls rampUpIncumbentSync() immediately after initialGuess, so your initialGuess routine may return different solutions in different processors without any special subsequent action. PEBBL will select one of the best solutions as the incumbent; if enumeration is active, other solutions may be retained in the repository.

The foundSolution method has a second, optional argument sync which is relevant only during the ramp-up phase, and only if enumeration is active. Its default value is the enum constant notSynchronous. Instead supplying the value synchronous indicates to PEBBL that you are guaranteeing that all processors are calling the routine at the same time, with the first argument set to identical solutions. This information allows PEBBL to reduce the overhead associated with maintaining the solution repository.

The following methods are useful in controlling the ramp-up phase.

```
void parallelBranchSub::rampUpIncumbentHeuristic()
```

This method substitutes for the usual quickIncumbentHeuristic() during the ramp-up phase. The default implementation of rampUpIncumbentHeuristic() is:

```
if (bGlobal()->haveIncumbentHeuristic())
    {
        incumbentHeuristic();
        pGlobal()->rampUpIncumbentSync();
    }
```

The effect of this code is to run the *serial* incumbent heuristic and then synchronize across processors. If you like, you may have your implementation of rampUpIncumbentHeuristic() call feedToIncumbentThread(), even though the incumbent heuristic thread will not be running yet. This practice allows the incumbent thread on each processor to be "primed" with information found during the ramp-up phase, so it may immediately begin doing useful work once ramp up ends.

```
bool parallelBranching::continueRampUp()
```

Ramp up will continue as long as either this method or forceContinueRampUp() return true. The default implementation is described in Section 3.3.5, but you are free to override it.

```
bool forceContinueRampUp()
```

Ramp up will continue as long as either this method or continueRampUp() return true. The default implementation is described in Section 3.3.5, but you are free to override it.

```
void rampUpCleanUp()
```

PEBBL calls this method on all processors when the ramp-up phase is over. The default implementation is a stub.

## 4.3.7 Providing for checkpoints

If your application maintains data structures not written and read by your implementations of the methods myParBranching::pack, myParBranching::unpack, myParSub::pack, and <math>myParSub::unpack, then PEBBL's checkpointing feature will neither save nor restore them. To make sure any such information is saved with each checkpoint and restored whenever restarting from a checkpoint, you need to define a few extra methods:

```
void myParBranching::appCheckpointWrite(PackBuffer& outBuf)
```

Write application-specific data to the PackBuffer outBuf, typically using the << operator. This method will be called separately for each processor and for each checkpoint. The default implementation is a stub.

```
void myParBranching::appCheckpointRead(UnPackBuffer& inBuf)
```

Read the information written by appCheckpointWrite from inBuf, typically using the >>

operator. This routine will be called on each processor when a checkpoint is read using the restart option. The default implementation is a stub.

## $\verb|void| \textit{myParBranching}:: \verb|appMergeGlobalData(UnPackBuffer& inBuf)| \\$

This method is similar to the appCheckpointRead routine, but invoked when restarting with --reconfigure. It will be called on every processor, but multiple times — once for each dataset written by appCheckpointWrite when the checkpoint was created. When restarting with --reconfigure, the numbers of worker and hub processors may be different from when the checkpoint was written.

#### 4.3.8 The main program: serial/parallel drivers

PEBBL provides a template that constructs a driver program similar to that of Section 4.2.7, but able to sense and use available parallelism. If PEBBL senses that more than one MPI processor is available or if the command-line option --forceParallel is present, it invokes the parallel-layer version of your application; otherwise, it invokes the serial-layer version. If it invokes the serial-layer version, only the command-line parameters defined for that version will be recognized; if you have defined additional parameters in your parallel-layer classes, they will only be recognized if that layer is invoked.

The serial/parallel driver template is also called driver, and its syntax is nearly identical to the serial driver template, but with two template arguments <*B*, *PB*>. *B* refers to your serial branching-derived problem-instance class, and *PB* refers to your parallelBranching-derived class. For example, you could the template invoke via

#### driver<myBranchinq,myParBranchinq>(argc,argv)

If you have configured PEBBL without MPI, then the two-argument form of driver is still defined, but the second template argument *PB* is ignored. Thus, you can use a single driver program for your application whether or not you have configured PEBBL to use MPI. Once it has detected whether multiple MPI processors are available and whether —-forceParallel was used, the driver template invokes, in both the serial and parallel cases, essentially the same setup-reset-solve code pattern as described in Section 4.2.7.

The standard code pattern for creating a serial/parallel driver is shown in Figure 16. The #ifndef block is needed if you have enclosed the definition of myParBranching within an #ifdef ACRO\_HAVE\_MPI block. In this case, even though the second template argument myParBranching will be ignored in the instantiation of driver, one must make myParBranching a defined type to guard against possible compiler errors; with some compilers, this safeguard may not be needed.

Depending on your MPI environment, your serial/parallel driver may have to be invoked in a particular way in order to detect the availability of parallelism. The most common such invocation procedure involves the mpirun command, as specified in the MPI standard. For example,

mpirun -np 4 myParDriver --useIncumbentThread=false datafile

```
Include application-specific header files, for instance myParBranching.h
Include <pebbl/parBranching.h>, unless already included in preceding headers

#ifndef ACRO_HAVE_MPI
typedef void myParBranching;
#endif

int main(int argc, char* argv[])
{
   return driver<myBranching,myParBranching>(argc,argv);
}
```

Figure 16: Standard code pattern for creating a serial/parallel driver program.

would run *myParDriver* on four processors, without an incumbent heuristic thread, and with the input file *datafile*. See Section 5.8 for a description of the useIncumbentThread option.

Note, however, that some installations may use different, nonstandard commands for running MPI programs.

## 4.3.9 Running in communicators other than MPI\_COMM\_WORLD

The provided drivers will run PEBBL within the communicator MPI\_COMM\_WORLD. For an example of how to invoke PEBBL within a different communicator, please refer to the program commTest.cpp in the src/pebbl/example directory. This program runs the example knapsack application in a communicator consisting of MPI ranks  $\lfloor P/2 \rfloor, \ldots, P-1$ , where P is the total number of MPI processes. The other MPI processes remain idle, which makes the program somewhat pointless, other than to illustrate how to run within a specific communicator. Doing so is quite straightforward: you simply pass the desired communicator as an argument to the constructor for your parallelBranching-derived class, assuming that this constructor is set up as specified at the beginning of Section 4.3.1. For example, if the parallelBranching-derived class is called myParBranching and you wish to run within the (already declared and constructed) communicator specialCommunicator, you would simply declare your problem instance by

myParBranching instance(specialCommunicator);

#### 4.3.10 Retrieving solutions to C++ code

As in the serial case, you may invoke PEBBL search as a subroutine from your own parallel C++ applications. The methods available for retrieving solutions are identical to the

Figure 17: Example of scanning the solution repository in the parallel layer.

serial layer methods described is Section 4.2.9 — that is, getSolution, getAllSolutions, startRepositoryScan, and nextRepositoryMember — but the parallel layer redefines them to work properly in parallel. It is critical that these routines be called synchronously on all processors, or the PEBBL application will probably hang.

The solution-retrieval methods getSolution, getAllSolutions, startRepositoryScan, and nextRepositoryMember have an optional argument that is ignored in the serial layer, specifying which processor(s) the result(s) should be returned to. The default for this argument is the special value pebblBase::allProcessors, specifying that results be returned to all processors through a broadcast operation. Otherwise, the argument should be set to an integer k in the range  $0 \le k < \text{uMPI::rank specifying the particular processor that is to receive the solution(s). On other processors, getAllSolutions will leave its argument unmodified, and getSolution and nextRepositoryMember will return NULL.$ 

If the repository is very large, it is possible that it will fit in the memory of the entire processor ensemble, but not in the memory of a single processor. In this case, using getAllSolutions will cause out-of-memory errors, and it is preferable to use the iterator-like methods startRepositoryScan and nextRepositoryMember, so that the entire repository need not reside simultaneously within a single processor.

As in the serial case, when a solution returned by getSolution, getAllSolutions, or nextRepositoryMember is no longer needed, one should call its dispose() method in order to enable proper reference counting and avoid memory leaks.

As an example, assuming that *instance* is an object whose type is derived from the parallelBranching class, and that the search() method has already run to completion, the code in Figure 17 sends every solution in the repository to processor 0, which prints their objective values.

## 5 Parameters

This section describes various command line parameters that PEBBL recognizes. The listing is not exhaustive, but contains the parameters you should typically find most useful. A complete listing is produced by specifying the help parameter to driver programs constructed in the manner described in this guide. You may add your own application parameters as described in Section 4.2.5.

## 5.1 Checkpointing

### abortCheckpointCount

Layer: Parallel only

Datatype: int Default value: 0

Constraints: Nonnegative

Primarily for debugging purposes. Causes an abort after writing this many checkpoints. A zero value, which is the default, disables this feature.

#### checkpointDir

Layer: Parallel only Datatype: string

Default value: Current directory, or from environment variable

Directory to place checkpoint files. The environment variable PEBBL\_CHECKPOINT\_DIR, if defined, provides a default value. If this variable is undefined, the default is the process current directory.

#### checkpointMinInterval

Layer: Parallel only

Datatype: double

Default value: 0

Constraints: Nonnegative

Minimum minutes of CPU time per processor between writing checkpoints.

### ${\tt checkpointMinutes}$

Layer: Parallel only

Datatype: double

Default value: 0

Constraints: Nonnegative

Desired minutes between starting to write successive checkpoints; the default value of 0 disables checkpointing.

#### reconfigure

Layer: Parallel only

Datatype: bool
Default value: false

Resume from a previously written checkpoint, reading the checkpoint files serially. The configuration of worker and hub processors need not be identical to the run that wrote the checkpoint.

#### restart

Layer: Parallel only

Datatype: bool
Default value: false

Restart from a previously saved checkpoint, attempting to read the checkpoint files in parallel. The configuration of worker and hub processors must be identical to the run that wrote the checkpoint.

## 5.2 Debugging and performance tuning aids

## debug

Layer: Serial and parallel

Datatype: int Default value: 0

Constraints Nonnegative

Debugging diagnostic output level. To add diagnostic output controlled by this parameter to your application, you may use the DEBUGPR and related macros.

#### debug-solver-params

Layer: Serial and parallel

Datatype: bool Default value: false

If true, print the value of all parameters.

## ${\tt debugSeqDigits}$

Layer: Parallel only

Datatype: int Default value: 0

Constraints: Lower bound: 0, Upper bound: 10

Number of sequence digits prepended to output lines. This feature allows you to run debug output through the unix **sort** utility to obtain output grouped by processor. Another way to separate debugging output by processor is to use the **dumpSplit** utility described below in Section 6.1.

#### forceParallel

Layer: Parallel only

Datatype: bool
Default value: false

Force the use of a parallel PEBBL solver, even if there is only one processor.

#### hubDebug

Layer: Parallel only

Datatype: bool
Default value: false

Supplies a specific debug level for hub operations.

## ${\tt loadLogSeconds}$

Layer: Parallel only

Datatype: double

Default value: 0

If positive, triggers output of load logging information suitable for visualization with the pebblLoadGraph utility described in Section 6.2. A positive value indicates the approximate number of seconds that should elapse between load information samples on each processor. For example, a value of 0.1 indicates that each processor should record load information 10 times per second.

#### printDepth

Layer: Serial and parallel

Datatype: bool
Default value: false

Include subproblem depth in debugging output.

#### printIntMeasure

Layer: Serial and parallel

Datatype: bool Default value: false

Include subproblem "integrality measures" in debugging output.

#### workerDebug

Layer: Parallel only

Datatype: bool
Default value: false

Supplies a specific debug level for the worker thread and related operations.

#### 5.3 Enumeration

### ${\tt enumAbsTolerance}$

Layer: Serial and parallel

Datatype: double Default value: -1.0

Constraints Lower bound: -1

Absolute tolerance for enumeration. Find solutions that are within this additive distance of optimality. The default value means the feature should not be used.

#### enumCutoff

Layer: Serial and parallel

Datatype: double Default value: (none)

If set, specifies an absolute threshold on enumerated solutions. Only solutions with values strictly better than enumCutoff will be retained.

#### enumCount

Layer: Serial and parallel

Datatype: int Default value: 0

Constraints Nonnegative

If positive, indicates that only the best enumCount solutions (that meet other enumeration criteria, if any) should be retained.

#### enumRelTolerance

Layer: Serial and parallel

Datatype: double
Default value: -1.0

Constraints Lower bound: -1

Relative tolerance for enumeration. Find solutions that are within this multiplicative factor of being optimal. For example, a value of 0.1 requests solutions within 10% of optimality. The default value means the feature is disabled.

#### enumFlowControl

Layer: Parallel only

Datatype: bool
Default value: false

Enables a hypercube flow control scheme for solution objects when enumeration is being used in parallel. This scheme is designed to prevent MPI errors resulting from too many messages converging simultaneously at a single receiving processor. This mode should only be needed if there is very high solution transmission volume, and only with certain MPI

implementations. In serial or without enumeration, it has no effect.

### 5.4 General

## help

Layer: Serial and parallel

Datatype: bool
Default value: false

If true, print usage information and parameter definitions, and then exit.

#### randomSeed

Layer: Serial and parallel

Datatype: int Default value: 1

Constraints nonnegative

Global seed for random number generation.

### version

Layer: Serial and parallel

Datatype: bool
Default value: false

If true, print version information and exit. Should be used on the command line only, and as the first parameter specified.

#### 5.5 Incumbent

#### startIncumbent

Layer: Serial and parallel

Datatype: double Default value: (none)

Value of some known feasible solution.

# 5.6 Output

## $\verb"earlyOutputMinutes"$

Layer: Serial and parallel

Datatype: double

Default value: 0

Constraints Nonnegative

If this many minutes have elapsed since its creation, output the current incumbent to a file in case of a crash or timeout. The default value disables this feature.

#### output

Layer: Serial and parallel

Datatype: CharString
Default value: See Section 4.2.7

File in which to write the final solution(s). If omitted, output is written in the current directory, using a filename constructed as described in Section 4.2.7.

#### printFullSolution

Layer: Serial and parallel

Datatype: bool
Default value: false

Print full solution(s) to standard output as well as writing it to a file.

#### printSolutionSynch

Layer: Parallel only

Datatype: bool
Default value: true

Indicates that only MPI's designated I/O processor (typically processor 0) is allowed to write the solution. If false, some communication overhead may be saved in the solution output process.

#### statusPrintCount

Layer: Serial and parallel

Datatype: int
Default value: 100,000
Constraints Nonnegative

The maximum number of subproblems bounded between status printouts. Status printouts are triggered by thresholds on wall clock time and the total number of subproblems bounded since the last status printout. Since the default value is large, the default behavior will typically be to trigger status printouts based on wall clock time.

#### statusPrintSeconds

Layer: Serial and parallel

Datatype: double Default value: 10.0

Constraints Nonnegative

The maximum number of seconds elapsing between status printouts.

## suppressWarnings

Layer: Serial and parallel

Datatype: bool Default value: false

Suppress warning messages.

## trackIncumbent

Layer: Parallel only

Datatype: bool
Default value: false

Print a message whenever there is a new incumbent.

# 5.7 Parallel work distribution

# clusterSize

Layer: Parallel only

Datatype: int Default value: 64

Constraints: Lower bound: 1

Maximum number of processors controlled by a single hub (including the hub itself). Unless numClusters is set, this will be the size of all but the last cluster.

# $\verb+hubsDontWorkSize+$

Layer: Parallel only

Datatype: int Default value: 10

Constraints: Lower bound: 2

Size of cluster at or above which hubs do not also function as workers.

# hubLoadFac

Layer: Parallel only
Datatype: double
Default value: 0.10

Constraints: Lower bound: 0, Upper bound: 1

The target fraction of subproblems to be controlled by hub processors at any given time. See Section 3.3.3 for a detailed discussion of the function of this parameter.

## loadMeasureDegree

Layer: Serial and parallel

Datatype: int Default value: 1

Constraints Must be 0, 1, 2, or 3

Used to measure the "weight" of a subproblem used to calculate worker and cluster workloads. Specifically, if a subproblem has bound b and the current incumbent value is z, its weight is  $|z-b|^{\text{loadMeasureDegree}}$ . Note that subproblem weight is used primarily by the load balancing algorithms in the parallel layer, but LoadMeasureDegree also exists in the serial layer for technical reasons. Its value should not materially affect the operation of the serial layer. In the parallel layer, larger values put more load balancing stress on the quality of subproblems, and lower values more stress on quantity of subproblems; a value of zero sets a processor's workload equal to the number of subproblems it controls. The parameter qualityBalance specifies additional attention to subproblem quality in load balancing, beyond that specified in loadMeasureDegree.

#### numClusters

Layer: Parallel only

Datatype: int Default value: 1

Constraints: Lower bound: 1

Forces a minimum number of processor clusters, even if all are smaller than clusterSize.

#### qualityBalance

Layer: Parallel only

Datatype: bool Default value: true

If true, hubs shift work between workers based on each worker's best subproblem bound, as well as the total workload as measured by (1) in Section 3.3.4. Note that this workload metric may already take some measure of quality into account if loadMeasureDegree is positive.

#### minScatterProb

Layer: Parallel only
Datatype: double
Default value: 0.05

Constraints: Lower bound: 0, Upper bound: 1

#### targetScatterProb

Layer: Parallel only
Datatype: double

Default value: 0.25

Constraints: Lower bound: 0, Upper bound: 1

#### maxScatterProb

Layer: Parallel only
Datatype: double
Default value: 0.90

Constraints: Lower bound: 0, Upper bound: 1

These parameters control how frequently subproblems are released from workers. Generally, you should observe the ordering

## $minScatterProb \le targetScatterProb \le maxScatterProb.$

The release decision scheme uses the notion of a worker having its "fair share" of work, as described in Section 3.3.3. If a worker has exactly its fair share of work, then it releases subproblems with probability targetScatterProb. If it has more than its fair share, it uses a higher probability, linearly increasing up to maxScatterProb if it has 100% of the work in the system. Similarly, if it has less than its fair share, it uses a lower probability, linearly decreasing down to minScatterProb if appears to have no work.

#### minNonLocalScatterProb

Layer: Parallel only
Datatype: double
Default value: 0.0

Constraints: Lower bound: 0, Upper bound: 1

## targetNonLocalScatterProb

Layer: Parallel only
Datatype: double
Default value: 0.33

Constraints: Lower bound: 0, Upper bound: 1

#### maxNonLocalScatterProb

Layer: Parallel only
Datatype: double
Default value: default: 0.9

Constraints: Lower bound: 0, Upper bound: 1

When there is more than one cluster, these parameters control the decision, once a worker has decided to release a subproblem, of whether it should be released to the worker controlling hub, or to a randomly chosen hub (which could also be the worker's own hub). This decision

is based on whether the worker's cluster has its "fair share" of the total workload: a fraction w(c)/W of the total work, where w(c) is the number of workers in the worker's cluster, and W is the total number of workers. When the worker's cluster has its fair share, random scattering is performed with probability targetNonLocalScatterProb. If the cluster has more than its fair share, a larger probability is used, increasing linearly to maxNonLocalScatterProb if the cluster has all the work in the system. If the cluster has less work, a smaller probability is used, decreasing linearly to minNonLocalScatterProb if the cluster has no work.

# 5.8 Parallel thread control

# incThreadBiasFactor

Layer: Parallel only
Datatype: double

Default value: 100.0

Constraints: Nonnegative

#### incThreadBiasPower

Layer: Parallel only
Datatype: double
Default value: 1.0

Constraints: Nonnegative

## incThreadMaxBias

Layer: Parallel only
Datatype: double
Default value: 20.0

Constraints: Nonnegative

# $\verb"incThreadMinBias"$

Layer: Parallel only
Datatype: double
Default value: 1.0

Constraints: Nonnegative

These parameters are used in computing the bias (priority) of the incumbent heuristic thread, if it is present. If we represent the above parameters by  $\phi$ ,  $\pi$ ,  $\bar{b}$ , and  $\underline{b}$ , respectively, the formula for the incumbent thread bias b is

$$b = \max \left\{ \underline{b}, \min \left\{ \overline{b}, \phi r^{\pi} \right\} \right\},\,$$

where r is the current relative gap, that is, the relative difference between the incumbent value and the best known bound in the pool of active subproblems.

# timeSlice

Layer: Parallel only
Datatype: double

Default value: 0.01

Constraints: Lower bound:  $10^{-7}$ 

Target thread timeslice in seconds. This is the typical run time or "granularity" that the scheduler tries to acheive for each invocation of a compute thread.

## useIncumbentThread

Layer: Parallel only

Datatype: bool
Default value: true

Controls whether each worker dedicates a thread to incumbent search. If false, the only source of new incumbents will be terminal subproblems and quickIncumbentHeuristic(). This parameter is ignored if haveParallelIncumbentHeuristic() returns false.

## workerThreadBias

Layer: Parallel only

Datatype: double Default value: 100.0

Constraints: Nonnegative

Scheduling priority for main worker thread.

# 5.9 Ramp-up (standard implementation)

The following parameters control the default implementation of the ramp-up crossover mechanism, that is, the transition from ramp-up to "regular" parallel execution. Your application may override parallelBranching's default implementations of continueRampUp() or forceContinueRampUp() to ignore these parameters or interpret them differently.

#### minRampUpSubprobsCreated

Layer: Parallel only

Datatype: int Default value: 0

Constraints: Nonnegative

Force this many subproblem creations before ramp up ends.

## rampUpPoolLimit

Layer: Parallel only

Datatype: int Default value: 0

Constraints: Nonnegative

Total subproblem pool size beyond which the ramp-up phase may end.

# rampUpPoolLimitFac

Layer: Parallel only Datatype: double

Default value: 1

Constraints: Nonnegative

Desired average number of subproblems per worker processor immediately after ramp-up.

# 5.10 Search order and protocol

## breadthFirst

Layer: Serial and parallel

Datatype: bool Default value: false

In serial, use breadth-first search; in parallel, use an approximation of breadth-first search based on treating all subproblem pools as FIFO queues. Ignored if depthFirst is also specified.

# depthFirst

Layer: Serial and parallel

Datatype: bool
Default value: false

In serial, use depth-first search; in parallel, use an approximation based on treating all subproblem pools as stacks. Overrides breadthFirst if both are specified.

Note that if neither breadthFirst nor depthFirst is specified, then PEBBL uses best-first search. That is, it tries to select the subproblem with the lowest possible bound for minimization problems, and the highest possible bound for maximization problems. In parallel, conformance to the best-first search order is only approximate.

#### initialDive

Layer: Serial and parallel

Datatype: bool
Default value: false

# integralityDive

Layer: Serial and parallel

Datatype: bool
Default value: true

These options are useful for applications that do not have a good incumbent heuristic.

Setting initialDive is incompatible with the breadthFirst and depthFirst options, and integralityDive is only meaningful if initialDive is true. InitialDive specifies that the best-first search order should only be followed after the first incumbent is found. Beforehand, PEBBL should "dive" in the tree to try to identify a feasible solution. If integralityDive is true, then "diving" means giving priority to processing subproblems with the lowest value of the data member branchSub::integralityMeasure (a value of zero is interpreted as meaning a subproblem is "integer feasible"). If integralityDive is false, it means selecting the subproblem with the highest possible depth. Both these techniques tend to produce initial search trees similar to classical depth-first search. Once an incumbent is found, PEBBL reverts to best-first search.

# eagerBounding

Layer: Serial and parallel

Datatype: bool
Default value: false

Specifies the search protocol implemented by the "eager" handler, as described in Section 3.1.3. This handler tries to bound subproblems as soon as they are created and keep all subproblems in the pool in either the bounded or possibly beingBounded or beingSeparated states. This handler is recommended for applications in which subproblem bounds are typically computed very quickly. This parameter is ignored if lazyBounding is also specified.

# lazyBounding

Layer: Serial and parallel

Datatype: bool
Default value: false

Specifies the search protocol implemented by the "lazy" handler, as described in Section 3.1.3. This handler attempts to delay bounding subproblems as long as possible, and fill all subproblem pools with boundable and possibly beingBounded or beingSeparated problems. Once a problem is separated, its children are created as soon as possible. This option takes precedence over eagerBounding.

If both eagerBounding and lazyBounding are false, which is the default, PEBBL uses the "hybrid" handler described in Section 3.1.3. This handler simply chooses problems from the subproblem pool, attempts to advance them one state in Figure 9, and replaces them. With this handler, the subproblem pools may contain a mix of all the possible states except dead.

# 5.11 Termination

# absTolerance

Layer: Serial and parallel

Datatype: double

Default value: 0

Constraints Nonnegative

When enumeration is not active, the absolute tolerance for optimal objective value. Subproblems are fathomed when their bounds are within absTolerance of the incumbent value. The final solution reported should be within this distance of the true optimum. This parameter is used to set the branching class member absTol. However, applications may adjust the value of absTol. For example, in a linear pure integer program with all objective function coefficients integer, you may want to set absTol to at least 1. In this situation, you could alternatively design your branching-derived class to round up the value of branchSub::bound to the next integer.

# relTolerance

Layer: Serial and parallel

Datatype: double Default value:  $10^{-7}$ 

Constraints Nonnegative

When enumeration is not in use, the relative tolerance for optimal objective value. If the incumbent value is z and the subproblem bound is b, a subproblem can be fathomed if  $|(z-b)/z| \leq \texttt{relTolerance}$ . This parameter essentially controls the number of digits of precision of the final solution. A value of zero is possible, but not recommended unless your bound calculations use only integer arithmetic, and there is no possibility of round-off error. This parameter is used to set the data member relTol in the branching class.

### integerTolerance

Layer: Serial and parallel

Datatype: double Default value:  $10^{-5}$ 

Constraints Lower bound: 0, Upper bound: 1

Tolerance for determining whether numbers are integers. Note that this parameter does not affect PEBBL itself, but only applications that use the methods <code>isInteger(double)</code> or <code>isZero(double)</code> provided for convenience in class <code>pebblBase</code>, from which <code>branching</code> and <code>branchSub</code> are both derived.

#### maxCPUMinutes

Layer: Serial and parallel

Datatype: double

Default value: 0

Constraints Nonnegative

# maxSPBounds

Layer: Serial and parallel

Datatype: double

Default value: 0

Constraints Nonnegative

# ${\tt maxWallMinutes}$

Layer: Serial and parallel

Datatype: double

Default value: 0

Constraints Nonnegative

These parameters control PEBBL's built-in abort function. A PEBBL run will abort if the CPU time (per processor) exceeds maxCPUMinutes, the total number of subproblems bounded exceeds maxSPBounds, or the total wall clock time spent in the search exceeds maxWallMinutes. In each case, a zero value, which is the default, means there is no limit.

# printAbortMessage

Layer: Serial and parallel

Datatype: bool Default value: true

Instructs PEBBL to print an explanatory message when aborting due to the maxCPUMinutes, maxSPBounds, or maxWallMinutes limits.

# rampUpOnly

Layer: Serial and parallel

Datatype: bool
Default value: false

Forces PEBBL runs to terminate immediately after ramp-up. This parameter is provided primarily for debugging or evaluating the performance of your application's ramp-up phase.

#### useAbort

Layer: Serial and parallel

Datatype: bool
Default value: false

If true, force an abort when an error occurs.

# 6 Python-Based Utilities

PEBBL provides some utility programs written in Python, residing in pebbl/scripts. The testScript.py utility is for verifying that PEBBL has been compiled correctly, and is described in Section 2.6. This section describes the remaining utilities, dumpSplit.py and pebblLoadGraph.py.

# 6.1 The dumpSplit.py utility

The dumpSplit.py utility is helpful for separating logs produced by setting the debug command-line parameter. For parallel runs, PEBBL prefixes each line of output with the MPI process number enclosed in square brackets. For example, output lines from processor 0 start with [0], output lines from processor 1 start with [1], and so forth. These lines typically appear intermixed in the output. The .py utility is meant to assist in forming a clearer picture of what is happening on each individual processor. Its usage is through a command line of the form

Here, path is the location of the utility and logFile is the pathname of the file containing the PEBBL debug output. For each processor p that dumpsplit.py detects in logFile, it writes a file of the form logFile.p containing just the output flagged as coming from processor p. For example if dumpsplit.py were to be run on a file called dump.log containing debug log output from three processors, its output would be the files dump.log.0, dump.log.1, and dump.log.2.

# 6.2 The pebblLoadGraph.py utility

The pebblLoadGraph.py allows you to visualize parallel performance-tracking data produced by invoking the loadLogSeconds parameter described in Section 5.2. To use this utility, your Python installation must contain the matplotlib package available at http://matplotlib.org. When PEBBL is run with loadLogSeconds set to a positive value, performance data are placed in a file called problemName.loadLog in the current directory, where problemName is the name of the current problem instance, typically derived from the problem instance filename. The pebblLoadGraph.py utility processes such files to produce either screen or PDF-file graphics. You invoke this utility by a command of the form

$$path/pebblLoadGraph.py\ [options]\ file$$

where *file* denotes the load-log file produced by the PEBBL runs. By default, graphical output is placed in a file whose name is derived from *file* but ends in .pdf. The options available in the optional clauses *options* are extensive and may be viewed in their entirety by the command

The most common options are

- --noworkers Do not graph subproblem loads at worker processors. The opposite of this option, --workers, is the default.
- --nohubs Do not graph subproblem loads at hub processors. The opposite of this option, --hubs, is the default.
- --proc=p Only graph loads for processor p. The argument p may also take the value hubs, workers or all, which is the default. This parameter may be specified multiple times: for example, --proc=0 --proc=2 will show only information for processors 0 and 2.
- --bounds=p Show the known solution bounds (lower bound for a minimization problem, upper bound for a maximization problem) known at processor p. The p argument is interpreted the same way as for the --proc option.
- --incumbent=p Show the incumbent values known at processor p. The p argument is interpreted the same way as for the --proc option.
- --show Show the graphical output on-screen in addition to producing the default PDF file. Requires an active X display connection.
- --startseconds= $s_1$  Only show information after  $s_1$  seconds of PEBBL runtime.
- --endseconds= $s_2$  Only show information before  $s_2$  seconds of PEBBL runtime elapsed.

Note that separate loads may be displayed for a single processor if it is both a worker and a hub — one display indicates subproblems under control of the worker process and the other indicates subproblems under control of the hub process.

Figure 18 shows the result of running pebblLoadGraph.py with its default settings on a logfile produced by running PEBBL on a difficult knapsack problem using 8 MPI processors, two of which were designaged as combined worker-hubs, and the rest as workers.

# Acknowledgements

This work was performed in part at Sandia National Laboratories. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energys National Nuclear Security Administration under contract DE-NA0003525.

# References

[1] G. E. Blelloch. Scans as primitive parallel operations. *IEEE Trans. Comput.*, 38(11):1526–1538, 1989.

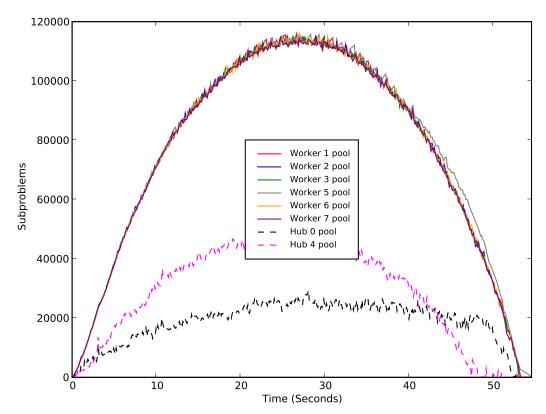


Figure 18: Sample graphical output from pebblLoadGraph.py

- [2] J. Clausen and M. Perregaard. On the best search strategy in parallel branch-and-bound: best-first search versus lazy depth-first search. Ann. Oper. Res., 90:1–17, 1999.
- [3] J. Eckstein. Control strategies for parallel mixed integer branch and bound. In Supercomputing '94: Proceedings of the 1994 ACM/IEEE conference on Supercomputing, pages 41–48, New York, NY, USA, 1994. ACM.
- [4] J. Eckstein. Parallel branch-and-bound algorithms for general mixed integer programming on the CM-5. SIAM J. Optim., 4(4):794–814, 1994.
- [5] J. Eckstein. Distributed versus centralized storage and control for parallel branch and bound: mixed integer programming on the CM-5. *Comput. Optim. Appl.*, 7(2):199–220, 1997.
- [6] J. Eckstein, W. E. Hart, and C. A. Phillips. Resource management in a parallel mixed integer programming package. In *Proceedings of Intel Supercomputer Users Group*, 1997.
- [7] J. Eckstein, C. A. Phillips, and W. E. Hart. PICO: an object-oriented framework for parallel branch and bound. RUTCOR Research Report RRR 40-2000, Rutgers University, 2000.

- [8] J. Eckstein, C. A. Phillips, and W. E. Hart. PICO: an object-oriented framework for parallel branch and bound. In *Inherently parallel algorithms in feasibility and optimization and their applications (Haifa, 2000)*, volume 8 of *Stud. Comput. Math.*, pages 219–265. North-Holland, Amsterdam, 2001.
- [9] W. D. Hillis. The Connection Machine. MIT Press, 1985.
- [10] M. Jünger and S. Thienel. Introduction to ABACUS a branch-and-cut system. *Oper. Res. Lett.*, 22(2-3):83–95, 1998.
- [11] G. Karypis and V. Kumar. Unstructured tree search on simd parallel computers: a summary of results. In *Supercomputing '92: Proceedings of the 1992 ACM/IEEE conference on Supercomputing*, pages 453–462, Los Alamitos, CA, USA, 1992. IEEE Computer Society Press.
- [12] B. Le Cun and C. Roucairol. BOB: a unified platform for implementing branch-and-bound like algorithms, 1995. http://citeseer.ist.psu.edu/cun95bob.html.
- [13] A. Mahanti and C. J. Daniel. A SIMD approach to parallel heuristic search. *Artif. Intel.*, 60:243–282, 1993.
- [14] F. Mattern. Algorithms for distributed termination detection. *Distrib. Comput.*, 2:161–175, 1987.
- [15] T. K. Ralphs, L. Ládanyi, and M. J. Saltzman. A library hierarchy for implementing scalable parallel search algorithms. *J. Supercomput.*, 28(2):215–234, 2004.
- [16] V. J. Rayward-Smith, S. A. Rush, and G. P. McKeown. Efficiency considerations in the implementation of parallel branch-and-bound. *Ann. Oper. Res.*, 43(1-4):123–145, 1993.
- [17] Y. Shinano, K. Harada, and R. Hirabayashi. Control schemes in a generalized utility for parallel branch-and-bound algorithms. In *IPPS: 11th International Parallel Processing Symposium*. IEEE Computer Society Press, 1997. http://citeseer.ist.psu.edu/shinano97control.html.
- [18] Y. Shinano, M. Higaki, and R. Hirabayashi. A generalized utility for parallel branch and bound algorithms. In SPDP '95: Proceedings of the 7th IEEE Symposium on Parallel and Distributeed Processing, page 392, Washington, DC, USA, 1995. IEEE Computer Society.
- [19] M. Snir, S. W. Otto, S. Huss-Lederman, D. W. Walker, and J. Dongarra. *MPI: The Complete Reference*. MIT Press, 1996.
- [20] S. Tschöke and T. Polzer. Portable parallel branch-and-bound library PPBB-Lib user manual, 1996. http://citeseer.ist.psu.edu/tsch96portable.html.