AN MPI IMPLEMENTATION OF A SELF-SUBMITTING PARALLEL JOB QUEUE

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Abstract. We present a simple and easy to apply methodology for using high-level self-submitting parallel job queues in an MPI environment. Using C++, we implemented a library of functions, MPQueue, both for testing our concepts and for use in real applications. In particular, we have applied our ideas toward solving computational combinatorics problems and for finding bifurcation diagrams of solutions of partial differential equations (PDE). Our method is general and can be applied in many situations without a lot of programming effort. The key idea is that workers themselves can easily submit new jobs to the currently running job queue. Our applications involve complicated data structures, so we employ serialization to allow data to be effortlessly passed between nodes. Using our library, one can solve large problems in parallel without being an expert in MPI. We demonstrate our methodology and the features of the library with several example programs, and give some results from our current PDE research. We show that our techniques are efficient and effective via overhead and scaling experiments.

1. Introduction

Our methodology is mainly motivated by our work in computational combinatorics [27] and partial differential equations (PDE) [22, 23, 24]. In combinatorial applications, we have the needs and methods to follow trees. The bifurcation diagrams we study in PDE are similar in structure to these trees, and so we can supervise their generation using similar ideas. Traditional approaches to parallel PDE solvers obtain speed up by distributing operations on large matrices across nodes. Our methodology instead uses job queues to solve such problems at a higher level. Our parallel implementation for creating bifurcation diagrams for PDE is suggested by the nature of a bifurcation diagram itself. Such a diagram contains branches and bifurcation points. These objects spawn each other in a tree hierarchy, so we treat the computation of these objects as stand-alone jobs. For PDE, this is a new and effective approach. Processing a single job for one of these applications may create several new jobs, thus a worker node needs to be able to submit new jobs to the boss node. These jobs require and produce a lot of complicated data. For our proof of concept tests and real applications, we have implemented our ideas in a library of C++ functions, in part to take advantage of that language’s facility with complicated data structures. In this article, we refer to our library as MPQueue.

The Message Passing Interface (MPI) [12] is a well-known portable and efficient communication protocol which has seen extensive use. In spite of its advantages, MPI is difficult to use because it does not have a high-level functionality. MPQueue is small, lightweight, and remedies some of these shortcomings. It uses MPI behind the scenes, is easy to use, and is Standard Template Library (STL) friendly. MPQueue has a high-level functionality allowing for the rapid development of parallel code using our self-submitting job queue technique. In order to easily pass our data structures between nodes, our library uses the Boost Serialization Library (BSL) [25]. It was a design goal of ours to make everything as simple as possible, so that one does not have to worry

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about the details of MPI or serialization when applying our methods. MPQueue is freely available from this paper’s companion website [21].

Section 2 contains a brief overview of some popular software packages that facilitate parallel programming. These fall into roughly three categories, threaded applications for shared memory multi-core processing, message passing for multi-node, distributed memory clusters, and single-system image clusters. Our library uses message passing and is intended for use on distributed memory clusters. Sections 3 and 4 explain line-by-line two simple example programs, one for factoring an integer, and the other for squaring a matrix. The purpose of these examples is not to provide efficient solutions for these demonstration applications, but to present our methodology and describe the key features of MPQueue in full detail. In Section 5 we give a more serious example, namely that of finding placements of non-attacking queens on a chessboard. This code is more complicated, and while not optimal, it does solve the problem on a $20 \times 20$ board, which would not be possible in a timely manner using serial code. We also investigate efficiency, scaling, and speedup for this example. A computationally intensive and mathematically complex example result for PDE can be found in Section 6. The full mathematical details of the particular PDE we are interested in can be found in [24], along with our state of the art numerical results which use MPQueue. In Section 7 we give an overview of the implementation of MPQueue. This section also includes an overhead experiment and summarizes the evidence of our implementation’s solid performance. Section 8 contains some concluding remarks, including possible future refinements to MPQueue.

The companion website [21] for this paper contains: the MPQueue source code, the library reference guide (see also Table 7.1), all the files needed to compile and execute the three example programs, and for the less initiated, line-by-line descriptions of the three example programs.

2. Related work

In this section we give a short description of some existing systems offering parallel computing solutions.

2.1. Shared memory multithreading systems on multicore processors. Many existing libraries share some features with MPQueue, but unlike MPQueue, use a shared memory model with multithreading. These systems are not designed for use with a distributed memory cluster. They could conceivably be effectively used with some single-system image cluster software (see Section 2.3).

- Intel’s Cilk++ language [17] is a linguistic extension of C++. It is built on the MIT Cilk system [5], which is an extension of C. In both of these extensions, programs are ordinary programs with a few additional keywords: cilk_spawn, cilk_synk and silk_for. A program running on a single processor runs like the original code without the additional keywords. The Cilk system contains a work-stealing scheduler.
- Fastflow [1] is based on lock-free queues explicitly designed for programming streaming applications on multi-cores. The authors report that Fastflow exhibits a substantial speedup against the state-of-the-art multi-threaded implementation.
- OpenMP [9] is presented as a set of compiler directives and callable runtime library routines that extend Fortran (and separately, C and C++) to express shared memory parallelism. It can support pointers and allocatables, and coarse grain parallelism. It also includes a callable runtime library with accompanying environment variables.
- Intel Threading Building Blocks (TBB) [26] is a portable C++ template library for multicore processors. The library simplifies the use of lower level threading packages like Pthreads. The library allocates tasks to cores dynamically using a run-time engine.
- Pthreads [6] is a POSIX standard for the C programming language that defines a large number of functions to manage threads. It uses mutual exclusion (mutex) algorithms to avoid the simultaneous use of a common resource.
2.2. Message Passing Interface systems. There are a few existing libraries that are built on top of MPI. These are C++ interfaces for MPI, without job queues, and mostly without higher level functionality. It would have been possible to implement MPQueue on top of some of these packages, in particular, on top of Boost.MPI.

- The Boost.MPI library [14, 16] is a comprehensive and convenient C++ interface to MPI with some similarity to our library. Like MPQueue, Boost.MPI uses the BSL to serialize messages.
- MPI++ [2] is one of the earliest C++ interfaces to MPI. The interface is consistent with the C interface.
- mpi++ [15] is another C++ interface to MPI. The interface does not try to be consistent with the C++ interface.
- Object Oriented MPI (OOMPI) [19] is a C++ class library for MPI. It provides MPI functionality though member functions of objects.
- Para++ is a generic C++ interface for message passing applications. Like our interface, it is a high level interface built on top of MPI and is meant to allow for the quick design of parallel applications without a significant drop in performance. The article [8] describes the package and includes an example application for PDE. Para++ uses task hierarchies but does not implement job queues.

2.3. Single-System Image (SSI) Cluster software. A single-system image cluster [7, 18] appears to be a single system by hiding the distributed nature of resources. Processes can migrate between nodes for resource balancing purposes. In some of its implementations, it may be possible to run shared memory applications.

- Kerrighed [20] is an extension of the Linux operating system. It allows for applications using OpenMP and Posix multithreading, presenting an alternative to using MPI on a cluster with distributed resources. This approach is seemingly simpler than message passing, but the memory states of the separate nodes must be synchronized during the execution of a shared memory program. This probably is not as efficient as a carefully designed message passing solution.
- OpenSSI is another SSI clustering system based on Linux. It facilitates process migration and provides a single process space. OpenSSI can be used to build a robust, high availability cluster with no single point of failure. It is a general purpose system that is not specifically designed for parallel computing.
- The Linux Process Migration Infrastructure (LinuxPMI) is a Linux Kernel extension for single-system image clustering. The project is a continuation of the abandoned openMosix clustering project which is a fork of MOSIX [3].

2.4. Summary of Alternatives to MPQueue. As researchers in PDE and combinatorics, we have a need for the computational power only obtainable through parallel programming. To be practical, we need a method that uses the distributed memory clusters available to us. Our key, proven effective programming idea is to use self-submitting job queues. We did not find an existing package that completely satisfied all of our requirements, and so wrote our own, MPQueue. Our main design goal was to make a simple library that is easy to use, allowing effortless, rapid development of scientific experiments requiring parallel execution, without sacrificing performance.

Existing shared memory model software for multicore systems have some similar functionality as MPQueue, but they do not suit all needs because of the limitations on the number of cores on currently available hardware. It may be a possibility to use some such systems on top of SSI cluster software to implement techniques similar to ours over a distributed memory cluster, but we do not believe that this would be any simpler than or have as good performance as our simple, more direct message passing approach.
Figure 3.1. A possible order of jobs in the job queue during the factorization of 120. The arrows represent the job submission process. The circled jobs are the prime number outputs and so they do not produce new submissions.

Other message passing systems are mainly concerned with lower level tasks. They offer a large variety of ways to send and receive messages efficiently, but generally do not offer higher level constructs. It would probably be a reasonable programming alternative to implement our key idea of the self-submitting job queue on top of some of these existing systems, but we do not think the result would be as simple to use or have better performance than our implementation. In the sequel, we demonstrate with examples how our simple message passing system handles low level details automatically and offers an easy to use yet powerful and efficient programming methodology based on the self-submitting job queue.

3. Factoring example

Listing 3.1 shows an example program using the MPQueue library for factoring an integer. This example demonstrates many of the features of the library. In particular, it shows the general structure of a program, including the creation, supervision, and post-processing of job queues. It also shows the mechanism by which workers themselves can submit new jobs. The main idea of the algorithm is to split the input as a product of two integers that are as large as possible, and then submit these factors to the job queue for further splitting. These submissions are done by the workers. The job submission process is visualized in Figure 3.1. Note that the order of job submissions is not fully determined.

The companion website [21] contains not only the source code for this and the other examples, but a more detailed line-by-line explanation of the code. See also Table 7.1 for a complete list of the commands found in the MPQueue library, together with a brief description of their function. Here, we include an overview of this example program, in particular the lines of code which implement key MPQueue features. The MPQueue header file included in all our examples contains our new definitions as well as all header files needed to use MPI and the required parts of the BSL [25]. In each example, we define a finite list of job types as positive integers, although in this first simple example there is only one type of job.

In each of our example programs, the main function (found here on line 21) is executed by every node. First, the MPI is initialized and nodes are split into one boss and several workers. Only the boss returns from the \texttt{MPQstart} function call (line 23). The workers are then ready to accept jobs. The boss creates two job queues, one for storing jobs to do, and another for storing results. This program computes the prime factorization of the example integer found on line 25. The boss places the first splitting job into the job queue and starts the supervision of the workers via a call to the \texttt{MPQrunjobs} function (line 27), where it will spend the vast majority of its running time.

In this example, the workers split numbers into factors and submit these factors (see lines 14–15) to \texttt{inqueue} for further splitting. The workers return the prime factors, which the boss collects in the \texttt{outqueue}. When there are no more jobs, the boss enters a loop (line 29) and retrieves all the prime factors from the output queue.

The user-coded \texttt{MPQSwitch} function is called every time a new job needs to be processed. There typically are more than the one job type found in this first most simple example. Here, the workers (and only the workers) spend all their productive time in \texttt{MPQSwitch}, recursively finding pairs of factors of an input integer and submitting two new factor jobs for each pair of factors found. The \texttt{job.data} variable initially contains the serialized input of the job at the time the function is called.
# include "MPQueue.h"
# include "math.h"
using namespace std;

const int SPLIT = 1; // only one job type, so no cases in MPQswitch

void MPQswitch (Tjob & job) {
    int x;
    from_string (x, job.data);
    int sqrt = int (sqrt (double (x)));
    for (int y = sqrt; y > 1; y--)
        if (0 == x % y) {
            // found a divisor
            MPQsubmit (Tjob (SPLIT, x/y)); // submit two new jobs
            MPQsubmit (Tjob (SPLIT, y));
            job.data = ""; // no output to return
            return;
        }
}

int main (int argc, char *argv[]) {
    MPQinit (argc, argv);
    MPQstart (); // only the boss returns
    Tjobqueue inqueue, outqueue;
    int x = 1120581000; // factor this number
    inqueue.push (Tjob (SPLIT, x)); // add one job to the job queue
    MPQrunjobs (inqueue, outqueue); // supervise queue processing
    cout << x << "_factors_as:\n";
    while (!outqueue.empty ()) {
        int factor; // one factor
        from_string (factor, outqueue.front().data);
        cout << factor << "\n";
        outqueue.pop();
    }
    MPQstop ();
}

LISTING 3.1. Prime factorization example program.

This variable is replaced by the serialized output of the job. It is a key feature for the ease of doing high-level programming with our library that the input and output data can contain arbitrarily complicated data structures. In this simple example, the output is the same as the input if no factors were found in the loop initiated on line 12, whence the input is a prime, otherwise the output is empty.

4. Matrix square example

Listing 4.1 shows an example program for calculating the square of a matrix. The example demonstrates several new features of the MPQueue library. Namely, it shows how to efficiently share a large amount of data with all the workers using MPQsharedata, how to serialize struct data types using a template function, and how to use MPQtask to return results to the boss for immediate processing rather than using the output job queue. Unlike the first example, this program uses three job types so that a switch statement is required in the MPQswitch function. Here, we want the job types to be positive integers, so NONE is added to take the unused value of zero.

The variable matrix contains the input matrix (initialized in lines 43–44), while the variable square contains the result of the program, the square of the input matrix. The boss uses our


```cpp
#include "MPQueue.h"
using namespace std;

enum { NONE, DATA, MULTIPLY, RESULT };
type< vector< int > > Trow;
v vector< Trow > matrix, square;
type struct {
  int pos;      // row index
  Trow result;  // output row
} Tdata;

template< class Archive > void serialize(Archive & ar, Tdata & data, const unsigned int version) {
  ar & data.pos;
  ar & data.result;
}

void MPQswitch ( Tjob & job ) {
  Tdata data;
  switch ( job.type ) {
    case DATA:               // receive the input matrix
      from_string ( matrix, job.data );
      break;
    case MULTIPLY:           // calculate one row
      from_string ( data.pos, job.data );
      data.result = Trow ( matrix.size (), 0);
      for ( int j = 0; j < matrix.size (); j++ )
        for ( int k = 0; k < matrix.size (); k++ )
          data.result [ j ] += matrix [ data.pos ] [ k ] * matrix [ k ] [ j ];
      job = Tjob ( RESULT, data );             // prepare the result
      MPQtask ( job );                        // send result to boss
      break;
    case RESULT:              // receive one output row
      from_string ( data, job.data );
      square [ data.pos ] = data.result;
      job.data = "";                  // nothing to return
  }
}

int main ( int argc, char * argv[] ) {
  MPQinit ( argc, argv );
  MPQstart ();
  Trow row ( 10, 1 );               // input matrix containing
  v vector< Trow > mat ( row.size (), row ); // 1 at every entry
  square.resize ( row.size () );    // container for the output
  MPQsharedata ( Tjob ( DATA, mat ) ); // input matrix sent to workers
  Tjobqueue inqueue, outqueue;
  for ( int i = 0; i < mat.size (); i++ ) // every row is a separate job
    inqueue.push ( Tjob ( MULTIPLY, i ) );
  MPQrunjobs ( inqueue, outqueue );  // run the jobs
  for ( int i = 0; i < row.size (); i++ )
    for ( int j = 0; j < row.size (); j++ )
      cout << square [ i ] [ j ] << " ";
  cout << "\n";
  MPQstop ();
}
```

Listing 4.1. Matrix square example program.
function \textit{MPQsharedata} on line 46 to painlessly share an STL structure with the nodes. In lines 48–49 the job queue is filled with \textit{MULTIPLY} jobs, each requesting the calculation of one row of the goal matrix. The boss then starts the supervision of the workers, again spending the bulk of its time in \textit{MPQrunjobs}.

As in the previous example, the workers execute \textit{MPQswitch} and spend all their productive time in that function. Their work, however, this time depends on the job type. Also different from the factor example, the \textit{MPQswitch} function can be executed by the boss, in this case with \textit{job.type} set to \textit{RESULT}, as the result of a \textit{MPQtask} call by a worker. The variable \textit{data} contains one row of the result produced by a worker. When the input matrix is shared by all the workers, each worker receives the matrix as a \textit{DATA} job. They deserialize the data and store it locally in the variable \textit{matrix}. Lines 24–29 are where a worker calculates one row of the goal matrix. The input (position within the matrix) is deserialized into \textit{data.pos}, and the calculated row is stored in \textit{data.result}.

Workers circumvent the output queue by using \textit{MPQtask} (line 31) to send their calculated row results to the boss. Here, the boss receives and deserializes a row and puts it into the appropriate row of the result matrix \textit{square}. Thus, in lines 33–36, the boss does some actual work, not just supervising workers. The boss is usually idle during most of the supervision process. Thus it can be more efficient for the boss to do tasks such as post-processing during supervision, rather than waiting until the workers are all done.

5. \textsc{Non-attacking Queens example}

We now present an application that illustrates how to avoid the \textit{too many jobs} obstacle to scalability. The example uses local job queues to avoid excessive communication costs. This technique enhances the flexibility of our methodology, allowing for the efficient use of the library in somewhat unexpected situations.

The \textit{n}-queen puzzle is a well-known problem in mathematics. It concerns the placement of \textit{n} non-attacking queens on an \textit{n} × \textit{n} chess board. Figure 5.1 shows a valid partial placement with one missing queen. For a survey of results on the generalizations of this problem see [1]. Listing 5.1 shows an example program which counts the number of solutions on an \textit{n} × \textit{n} board. Figure 5.2 shows the serial pseudo code. We were able to run this code for \textit{n} ≤ 20 on a cluster containing 24 Intel(R) Xeon(TM) 2.80GHz dual CPUs with hyper-threading. For \textit{n} = 20, it took 9.0 hours (see Figure 5.3) using the 96 = 24 × 2 × 2 cores to find the 39,029,188,884 solutions. Note that the state of the art is \textit{n} = 26, that is, the number of solutions for \textit{n} = 27 is not known.

Our code uses a parallel version of a standard backtracking algorithm. A worker keeps a local job queue containing possible search branches, i.e., valid partial placements. If this queue grows large enough, then the worker submits one of the partial placements to the boss node as a job so that another worker can process it. Submitting jobs to the boss node too early may result in a very large global job queue and a lot of unnecessary communication between the nodes. Submitting jobs too late can starve the workers for jobs. The decision depends on the number of nodes, the speed of the nodes, and the branching factor of the search tree. Our code uses a simple heuristic that depends on an overflow value that we have adjusted experimentally. Figures 5.3 and 5.4 show the effect of different choices of the value. This very simple submission process could be fine tuned using the \textit{MPQinfo} command (see Table 7.1), the only MPQueue command not demonstrated in any of our three examples. Many of the task distribution schemes discussed in the survey paper [13] could be implemented using the \textit{MPQinfo} command.

In the sequel of this section we provide a description of the more important aspects of the algorithm as they are specifically implemented in the lines of code found in Listing 5.1. The \textit{size} of the board is set to some positive integer, 20 in this example (line 9). A partial placement of queens is a vector of type \textit{Trow} of length between 0 and \textit{size}, whose integer value \textit{j} in the \textit{i}-th entry denotes a valid (non-conflicting) placement of a queen in the \textit{j}-th row of the \textit{i}-th column of the board. When the length of a partial placement row equals \textit{size}, it is in fact a full placement and a
```cpp
#include "MPQueue.h"
#include <deque>
using namespace std;

enum { NONE, PLACE, RESULT };
typedef vector< int > Trow;
unsigned long int allsolutions = 0; // total number solutions
int overflow = 70; // controls local queue size
const int size = 20; // size of the board

bool inline fits ( const Trow & row ) {
    int j = row.size () - 1;
    for ( int i = 0; i < j; i++ )
        if ( ( row[ i ] == row.back () ) || ( abs ( row[ i ] - row[ j ] ) == j - i ) )
            return false; // queens interfere
    return true; // last queen fits
}

void MPQswitch ( Tjob & job ) {
    Trow row; // a partial placement
deque < Trow > rows; // local job queue
    unsigned int solutions = 0; // local number of solutions
    switch ( job.type ) {
    case PLACE: // add queen in next column
        from_string ( row, job.data );
        rows.push_back ( row ); // populate a local job queue
        while (!rows.empty () ) {
            row = rows.back ();
            rows.pop_back ();
            for ( row.push_back ( 0 ); row.back () < size; row.back ()++ )
                if ( fits ( row ) ) { // does the new queen fit?
                    if ( row.size () == size ) // all queens added
                        solutions++; // found a new solution
                }
                else {
                    rows.push_back ( row ); // add to local job queue
                    if ( rows.size () > overflow ) { // if too many local jobs
                        MPQsubmit ( Tjob(PLACE, rows.front ()) ); // send one to the boss
                        rows.pop_front ();
                    }
                }
        }
    job = Tjob(RESULT, solutions); // prepare the result
    MPQtask ( job ); // send result to the boss
    break;
    case RESULT: // update total solutions
        from_string ( solutions, job.data );
        allsolutions += solutions;
        job.data = ""; // no result to return
    }
}

int main ( int argc, char * argv[]) {
    MPQinit ( argc, argv );
    MPQstart ();
    TJob queue inqueue, outqueue;
inqueue.push ( Tjob(PLACE, Trow ()) ); // initial empty placement
    MPQrunjobs ( inqueue, outqueue );
cout << allsolutions << ", solutions\n";
    MPQstop ();
}
```

Listing 5.1. Non-attacking queens example program.
A partial placement of queens on a $5 \times 5$ board. In the example code, this placement is encoded as the vector $(0, 3, 1, 4)$. This partial placement can be extended to the full placement $(0, 3, 1, 4, 2)$. There are 10 distinct placements on the $5 \times 5$ board.

**Figure 5.1.**

| Input: size |
| Output: solutions |

1. add empty row to the queue of partial placements // no queens placed yet
2. while queue is not empty do
3. move the last job from queue into row
4. increase the size of row // add room for the next column
5. for $i \in \{0, \ldots, size\}$ do
6. set the last coordinate of row to $i$ // place the next queen into the $i$-th row
7. if row is a good partial placement then
8. if row is a full placement then
9. increment solutions
10. else
11. add row to queue

**Figure 5.2.** Pseudo code for the serial non-attacking queens placement program. The algorithm uses simple backtracking.

A solution has been found. After the usual initialization where the boss and worker nodes are created, the boss puts an empty placement job on the queue and begins supervision by entering `MPQrunjobs` (line 57), where it will stay until the counting is done and its global variable `allsolutions` is output with the final result. In the algorithm’s counting of numbers of solutions at the ends of branches of partial placements, workers return partial sums counting some valid placements to the boss by submitting a `RESULTS` task to the boss via a call to `MPQtask` (line 43). This causes the boss to update its global variable of the master count (line 47).

In order to control communication costs (and in fact fine-tune performance), workers use local job queues named `rows` (line 27) containing up to `overflow` (line 8) number of partial placement row vectors. Until the queue is empty, workers pop off local partial placement jobs, repeatedly calling the function `fits` (lines 11 and 31) with a row vector containing an attempt to extend to a valid placement to the next column. A valid extension causes the worker to either increment the number of solutions found (line 33) if the edge of the board was reached, or otherwise add it as a partial placement job to the local queue for another round of extending by itself (line 35). Before the next local job is started, the worker checks if the local queue has reached `overflow`, and if so pops a partial placement job off of the local queue and sends it to the boss to be placed on the global queue (lines...
Figure 5.3. Load diagrams of the 20-queen placement example code for two different values of the overflow variable. In both cases there were 95 available workers. The shaded region shows the number of workers actively working on jobs. The solid curve shows the number of jobs available in the global job queue together with the number of active workers. The unshaded region below 95 represents idle workers. The pictures show that the choice of 85 for overflow is too large, since with this choice there are not enough available jobs and so the program takes longer to finish. The optimal value of 70 was determined experimentally. From Figures 5.4 and 5.5 it appears that the optimal overflow value is somewhat predictable and depends only on the size of the problem, not the size of the cluster.

| Nodes p | Run time $T(p)$ | Worker usage | Total usage | Efficiency $\frac{T(1)}{pT(p)}$ |
|---------|-----------------|--------------|-------------|-----------------------------|
| 1       | 94.08 sec       | 94.10 CPU sec| 94.08 CPU sec| 0.67                        |
| 3       | 47.05 sec       | 93.85 CPU sec| 112.62 CPU sec| 0.84                        |
| 6       | 18.77 sec       | 96.35 CPU sec| 98.40 CPU sec| 0.96                        |
| 24      | 4.11 sec        | 102.24 CPU sec| 103.68 CPU sec| 0.91                        |
| 48      | 2.05 sec        | 105.45 CPU sec| 106.56 CPU sec| 0.88                        |
| 72      | 1.44 sec        |              |             |                             |
| 96      | 1.11 sec        |              |             |                             |

Table 5.1. Processing times for the 15-queen placement problem using the overflow value 30. The Worker usage column is the number of workers multiplied by the run time, while Total usage includes the boss as well. A constant worker usage would indicate perfect scaling. For larger board sizes, the efficiency increases up to and beyond our maximum available 96 nodes.

When a worker’s local queue is finally empty, the worker returns the partial result via a call to \texttt{MPQtask} and then terminates (lines 43–44). The worker is of course then available for the boss to give it another partial placement job off of the global queue, until that queue is itself empty and the final count has been compiled.

Table 5.1 and Figures 5.4 and 5.5 show that our approach to the problem scales well. For the size 15 board, we could have used more than the available 96 nodes; to attempt the unknown $n = 27$ case we could make good use of a very large number of nodes.
Figure 5.4. Speedup as a function of nodes for the 12-queen placement problem. The bold numbers indicate the overflow values used for a given curve. The dashed line is the theoretical maximum speedup of $p - 1$, the number of workers. It appears that adding more than 55 nodes does not increase the speedup. This limitation is the result of the small board size. The number of solutions is only 14,200.

Figure 5.5. Speedup as a function of nodes for the 15-queen placement problem. The bold numbers indicate the overflow values used for a given curve. It appears that the optimal overflow value does not depend on the number of nodes, only on the size of the problem. The dashed line again corresponds to the theoretical maximum speedup. The number of solutions for this board size is 2,279,184.
We did not take advantage of the symmetry of the problem, which would have immediately resulted in a four-fold speedup. This could be done with minimal work, but our goal here is to present a meaningful yet simple example demonstrating the use of our library and methodology. A possible future extension to the MPQueue library that could help reduce the number of idle workers for problems like this one would be the implementation of priority job queues.

As a reminder, the companion website [21] contains the source codes and corresponding detailed line-by-line explanations for this and the previous two examples, along with the MPQueue library and the few other files needed to compile and execute the programs. Table 7.1 contains a complete list of MPQueue commands, along with a brief description of their function.

6. Application to Nonlinear Elliptic PDE

Our library has provided us with an easy way to port to a parallel environment our serial code for solving PDE. The resulting increase in computational power has enabled us to solve the computationally intensive problem

\[
\Delta u + f_s(u) = 0 \quad \text{in } \Omega \\
u = 0 \quad \text{on } \partial \Omega,
\]

where \(\Delta\) is the Laplacian, \(\Omega\) is the square or cube, and \(f_s\) is the family of nonlinearities \(f_s(u) = su + u^3\), parameterized by \(s \in \mathbb{R}\). Other regions and nonlinearities can be handled as well. We had previously developed serial C++ code for obtaining good approximations of solutions to parameterized PDE such as (6.1), provided that the dimensions involved were not too big. The reader can refer to [22, 23] (serial) and [24] (parallel) for the mathematical details of our PDE algorithms, which are based on Newton’s method operating in a coefficient space corresponding to eigenfunction expansions of solution approximations. Generally, our C++ code follows branches of solutions by starting with an initial point on a branch and an approximate tangent vector to the branch, applying Newton’s method to find a next point and corresponding tangent, and repeating until a window is exited. Each time a new bifurcation point is identified on a branch, our code seeks points on new, bifurcating branches, which can then also be followed. Processing a bifurcation point can be very quick but it can also take more time than following a branch. Thus, it is natural that following a branch and analyzing a bifurcation point are the two job types we use.

The required input for both job types is complicated. Each input is a structure with 18 different fields, containing such data as the discretized solution approximation at \(N\) grid points, the corresponding \(M\) eigenfunction expansion coefficients, the parameter \(s\), the current tangent vector, the branch history, and C++ parameter values that lead to the current state (speed, tolerances, maximum iteration counts, etc.). For large problems, the embedded vectors may be very large. The automatic serialization feature of our library makes it easy to pass such data between nodes.

Figure 6.1 shows a partial bifurcation diagram when \(\Omega\) is the square \((0, \pi)^2\). The horizontal axis is the parameter \(s\) and the vertical axis is the value of the solution at a generic point \((x^*, y^*)\) [23]. The diagram demonstrates how branch following creates a tree structure whose growth is unpredictable. Details of the size and speed for this simple example are shown in the first row of Table 6.1. Using two nodes is essentially a simulation of our serial code, since there is only one worker.

The second row of Table 6.1 shows the same summary for a problem where \(\Omega\) is the cube \((0, \pi)^3\) and we search for the branches connected to the bifurcation point on the trivial branch at \(s = 18\). Parallelization is essential since it takes about a minute to compute each of the thousands of solutions.

We conclude the section with a few details of our implementation for creating bifurcation diagrams. Solution approximations lie in a subspace spanned by the first \(M\) eigenfunctions of the Laplacian, which themselves have been previously and independently approximated by \(M\) vectors in \(\mathbb{R}^N\), obtained via calls to ARPACK if not known in closed form. For the example results included
in this section, these bases are well known in terms of sine functions. The construction of the Jacobian of the object function for Newton’s method requires order $M^2$ numerical integrations, each requiring order $N$ arithmetic operations. The number of integrations is reduced somewhat in the presence of symmetry. The search direction system is solved via a standard LAPACK subroutine. Each approximated point requires roughly 4 iterations of Newton’s method. Finding bifurcation points requires the computation of the eigenvalues of the Jacobian, computed by another LAPACK routine.

7. Implementation

7.1. Design. Passing complicated data structures between nodes requires a significant amount of work in MPI. To avoid this difficulty, we rely on the BSL. This library encodes every standard STL
data structure automatically as a string, and more complicated data types can be encoded with a minimal amount of work. The serialization is done mostly automatically using template functions. A serialized data string is sent between the nodes in two steps. In the first step, a preliminary message is sent containing the size of the string together with some additional information like the job type. In the second step, the string itself is sent. Most of this is done using point-to-point communication with \texttt{MPI\_Send} and \texttt{MPI\_Recv}. The exception is the \texttt{MPQsharedata} command, which uses point-to-point communication for the preliminary message and uses \texttt{MPI\_Bcast} for the data string.

| $\Omega$ | $M$ | $N$ | Branches | Bifurcations | Solutions | Nodes | Run time | Worker usage |
|---------|-----|-----|----------|--------------|-----------|-------|----------|--------------|
| $(0, \pi)^2$ | 323 | 41 | 7 | 5 | 165 | 2 | 8.17 min | 8.17 CPU min |
|          |     |     |           |              |           | 4 | 3.73 min | 11.19 CPU min |
| $(0, \pi)^3$ | 564 | 21 | 385 | 364 | 19724 | 26 | 22.4 hour | 560.0 CPU hour |
|          |     |     |           |              |           | 50 | 11.5 hour | 563.5 CPU hour |
|          |     |     |           |              |           | 76 | 8.98 hour | 673.5 CPU hour |

Table 6.1. Processing times for PDE examples. These results are using NCSA's IA-64 TeraGrid Linux Cluster (Mercury) with 1.3 GHz nodes \[11\]. The data for the square region corresponds to the diagrams found in Figure 6.1. The entries for the cube region are typical of the results found in \[24\]. Note that the cube problem scales well since there are many jobs.

As a result of calling \texttt{MPQstart}, all the nodes become workers except node zero, which becomes the boss. The workers go into a waiting loop, as shown in Figure 7.1 and the boss continues its own work. When the boss requires help, it builds a queue of jobs and becomes a supervisor using \texttt{MPQrunjobs}, as shown in Figure 7.2. The boss then assigns jobs in the job queue to available workers and removes these jobs from the job queue. The workers execute \texttt{MPQswitch} with the job.

When a worker finishes a job, it sends a message to the boss, letting the boss know that the result is available. The boss accepts the result from the worker and stores it in the output queue. The boss keeps track of the number of jobs sent out. If the job queue is empty or every worker is

\begin{verbatim}
Input: none
Output: none
1 repeat
2 wait for a message from the boss
3 switch the message is a
4 case data share request
5 accept the broadcast message from the boss
6 call MPQswitch to handle the broadcast message
7 case job
8 call MPQswitch to run the job
9 send the result back to the boss
10 case stop command
11 stop
\end{verbatim}

Figure 7.1. Pseudo code for the main loop of the workers. The workers get to this loop from the \texttt{MPQstart} function.
while input queue is not empty or workers are working do

if input queue is not empty and there are idle workers then

assign a job to a worker
remove the job from the input queue

else

wait for a message from a worker

switch the message is a

case job submission

add the job to the input queue

case job result

if result is not empty then

add the result to the output queue

case task

call MPQswitch to run the task

send the result back to the worker

case info request

send the info back to the worker

end switch

Figure 7.2. Pseudo code for the MPQrunjobs function. This function is run by the boss.

working already, then it only accepts messages and does not try to assign jobs. The supervision phase ends when the job queue is empty and the result of every assigned job is received.

During the supervision phase, the workers can create new jobs by sending a job to the boss using MPQsubmit. The boss puts these jobs into the currently executing job queue.

The workers can use MPQtask to ask the boss to execute a task immediately and return the result to the same worker. To satisfy this request, the boss executes MPQswitch. This feature can be used, for example, to set or get the value of a global variable like a counter. This allows for rudimentary communication between the workers. The feature can also be used for returning results to the boss. This allows the boss to post-process the results while the workers are busy with their jobs. A sequence diagram of the supervision phase is shown in Figure 7.3. At the end of the program, the boss uses MPQstop to tell the workers to quit.

See Table 7.1 for a complete list of the commands found in the MPQueue library, together with a brief description of their function. The interested reader can consult the companion website [21] to find a detailed reference guide.

7.2. Scaling and overhead. In the non-attacking queens example we presented evidence suggesting that our methodology scales well. In particular, we show with load diagrams that all workers can be kept effectively busy if the problem has very many small jobs that can be managed via a local job queue to avoid excessive communication. We show that the efficiency of our parallel solution to this typical application is very good, up to a certain number of nodes, and that this number of nodes is very large if the problem is sufficiently big. We show that the speedup for this example can be close to ideal when using the optimal overflow, that this optimal overflow value appears to be independent of the number of nodes and only dependent on the size of the problem, and that for a sufficiently large problem, an arbitrary number of nodes can be effectively used. For our PDE
Figure 7.3. An example sequence diagram for the communication between the boss and worker nodes. The boss sends out some global data to the workers using MPQsharedata. The boss creates a job queue with a single job and then becomes the supervisor by calling MPQrunjobs. The first worker takes this job and realizes that an extra job should be created. It uses MPQinfo to check if there are available workers to take this additional job. The second worker is not busy, so the first worker submits the new job. The new job is assigned to the second worker. Both workers need the value of a global variable so they use MPQtask to get it from the boss. When the workers are finished, they send the results to the boss and the supervision phase stops.
application where there are a lesser number of much larger jobs and local job queues are not needed, we have observed similarly good performance indicators (see Table 6.1 and [24]).

In a final test, we demonstrate that the overhead of our implementation is reasonable. To observe the cost of bookkeeping, data serialization, and communication, we ran two experiments where each job was an instruction to the workers to sleep for one second. In the first experiment, we sent no additional input or output data, only the type of the job. In the second experiment, each job was sent with a vector containing 1000 doubles as input, and then the same vector was returned as output. The addition of data causes some unavoidable delay on our distributed memory system due to the serialization time and inherent communication speed of the network. The results are summarized in Table 7.2. It shows that the correspondence between the overhead and the number of jobs is linear in both experiments.

8. Conclusions

We have demonstrated that parallel self-submitting job queues are a powerful computational paradigm. Job queues are high-level constructs not available in other MPI libraries. The ability of workers to submit jobs to the job queue is the key component that gives our method its flexibility and power. We implemented our ideas in a light-weight and easy to use library based on MPI. The library, MPQueue, has been used successfully in real research applications. Using our interface saves effort by avoiding low-level coding; scientists without expertise in parallel programming can rapidly develop code to obtain good results for serious research problems. Experts in parallel programming...
Table 7.2. The time in seconds to execute sleep(1) jobs on 96 nodes. We used the same cluster specified in Section 5. Since there are 95 workers, it takes at least $n/95$ seconds to do $n$ such jobs. The rest of the time is the overhead. The overhead is approximately 16 microseconds per job with no data sent, and 98 milliseconds per job with a vector of 1000 doubles serialized, deserialized and sent both ways for every job.

| Jobs n | Run time $T(p)$ | Overhead $T(p) - n/95$ | Run time $T(p)$ | Overhead $T(p) - n/95$ |
|--------|-----------------|-------------------------|-----------------|-------------------------|
| 760    | 8.02            | 0.02                    | 8.73            | 0.73                    |
| 3040   | 32.07           | 0.07                    | 24.88           | 2.88                    |
| 12160  | 128.19          | 0.19                    | 139.50          | 11.50                   |
| 48640  | 512.76          | 0.76                    | 557.90          | 45.90                   |
| 194560 | 2051.09         | 3.09                    | 2231.28         | 183.28                  |
| 778240 | 8204.51         | 12.51                   | 8964.35         | 772.35                  |

can also take advantage of our methodology for applications that can be broken into relatively large pieces. In applications such as our PDE example found in Section 6, this decomposition is obvious. We also find the approach to be effective in less obvious situations, as demonstrated in the queens example in Section 5 which uses local queues on top of the global job queue to avoid the excessive communication that would result from transmitting too many small jobs across nodes. We have supplied evidence in this same example that our approach is scalable. The overhead associated with our implementation has been demonstrated to be reasonable. Possibilities for applications are wide; we have also used MPQueue to find winning strategies in combinatorial game theory \[27\] and in simulating a critical branching random walk \[10\].

Further improvements to MPQueue could include developing algorithms for automatically adjusting the local queue size (i.e., overflow), or other more sophisticated control procedures for distributing workload, such as the implementation of priority job queues and the capability of workers to send jobs directly to workers. We could easily add to the library the ability for a subset of workers to act as sub-supervisors, each with their own pool of workers. We believe that the currently implemented features of MPQueue will suffice for most applications, and that its simplicity is in many ways an advantage.

In some communication intensive applications, efficiency could be increased by avoiding the serialization of fixed-length data. The Boost.MPI library sends fixed length data more efficiently, without sacrificing convenience. It would be possible to implement MPQueue on top of Boost.MPI or other MPI interfaces in order to take advantage of the optimizations offered by those libraries.

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