ACM/CS 114 Parallel algorithms for scientific applications

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► the preamble

```
#include <getopt.h> // for getopt and friends
#include <pthread.h>

#include <cstdio>
#include <cstdlib> // for atof
#include <cmath>

#include <map>
#include <iostream>
#include <iomanip>
```

private and shared data structures

```
12 // shared information
13 struct problem {
    int workers: // total number of threads
14
    double dz;
                     // the width of each subdivision
16
     double sum; // storage for the partial computations
     pthread mutex t lock; // mutex to control access to the sum
19
  };
20
  // thread specific information
22 struct context {
    // thread info
24
    int id;
     pthread t descriptor:
    // the workload for this thread
26
     long subdivisions; // number of subdivisions
     double z_low; // the lower limit of integration
28
     double partial; // record the partial sum computed by this thread
29
     // the shared problem information
30
     problem* info;
31
32 };
```

▶ the coarse grain task

```
33 // worker
34 void* worker(void* arg) {
     context* ctxt = (context *) arg;
35
     // pull the problem information from the thread context
36
     double dz = ctxt->info->dz:
     double z = ctxt -> z low + dz/2;
38
     // loop over the subdivisions assigned to this thread
     double sum = 0.0:
40
     for (long i=0; i < ctxt->subdivisions; i++) {
41
         sum += std::log(1-z)/z;
42
        z += dz;
43
44
     // multiply by the width of each subdivision and adjust the sign
45
     sum *= -dz:
46
     // grab the lock
48
     pthread mutex lock(&(ctxt->info->lock));
     // store the result
50
     ctxt->info->sum += sum;
51
     // and release the lock
52.
     pthread_mutex_unlock(&(ctxt->info->lock));
53
54
     // all done
55
     return 0:
56
57
```

▶ the task master – interface and allocation of storage

```
// driver
  double dilog(double z, long N, int threads) {
60
     // the width of each interval subdivision
     const double dz = z/N;
     // setup the problem context
     problem info;
64
     info.workers = threads;
     info.dz = dz;
     info.sum = 0.0;
67
     pthread mutex init(&info.lock, 0);
68
69
     // and an array to hold the thread contexts
70
     context thr info[threads];
     // partition the number of subdivisions
     long nominal load = N/threads;
```

► the task master – spawning the threads

```
// spawn the workers
74
     for (int tid=0; tid<threads; tid++) {
        // store the thread id
76
        thr info[tid].id = tid;
        // point to the shared problem info
78
        thr info[tid].info = &info;
79
80
        // compute the starting point of the partial integral
81
        thr_info[tid].z_low = tid*nominal_load*dz;
        // compute the number of subdivisions for this thread
83
        if (tid == threads - 1) {
84
            // the last thread gets the leftovers
            thr info[tid].subdivisions = N - tid*nominal load;
86
         } else {
87
            thr_info[tid].subdivisions = nominal_load;
         }
89
90
        // create the thread
        int status = pthread create(
92
            &(thr_info[tid].descriptor), 0, worker, &thr_info[tid]);
        if (status) {
94
           printf("error %d in pthread create\n", status);
96
97
```

▶ the task master – harvesting the threads and returning the result

```
// harvest the threads
for (int tid=0; tid<threads; tid++) {
    pthread_join(thr_info[tid].descriptor, 0);
}

// all done
return info.sum;
}</pre>
```

▶ the main program – reading the command line

```
106 // main program
   int main(int argc, char* argv[]) {
      // default values for the command line options
108
      long N = 1000:
     double z = 1.0;
110
     int threads = 8;
      // read the command line
      int command;
      while ((command = getopt(argc, argv, "z:N:t:")) != -1) {
         switch (command) {
116
         case 'z':
            // get the argument of the dilogarithm
118
            z = atof(optarg);
            break:
         case 'N':
            // get the number of subdivisions
            N = (long) atof(optarg);
            break;
124
         case 't':
            // get the number of threads
126
            threads = atoi(optarg);
            break:
130
```

error checking and the invocation of the task master

```
// error checking
      // abort if N < 1
      if (N < 1) {
         std::cout
134
             << "the number of subdivisions must be positive"
            << std::endl:
136
         return 0;
      }
139
140
      // abort for z > 1 to avoid dealing with the imaginary part
      if (z > 1.0) {
141
         std::cout << "math domain error: z > 1" << std::endl;</pre>
142
         return 0;
143
144
      // compute
146
      double value = dilog(z, N, threads);
147
```

► the task master – printing out the answers

```
// build a database of the known dilogarithm values
      const double pi = M_PI;
149
      std::map<double, double> answers;
150
      answers[1.0] = pi*pi/6;
      answers[-1.0] = -pi*pi/12;
154
      // print out the value
      std::cout << "Li2(" << z << ")="
          << std::setprecision(17) << std::endl
156
          << " computed: " << value << std::endl;</pre>
      // check whether we know the right answer
158
      std::map<double,double>::const iterator lookup = answers.find(z);
159
      if (lookup != answers.end()) {
160
         // and if we do, print it out
161
         double exact = lookup->second:
162
         std::cout << " exact: " << exact << std::endl:
163
         // compute the approximation error and print it out
         double error = std::abs(exact-value)/exact;
         std::cout
166
            << std::setiosflags(std::ios base::scientific)
            << " error: " << error << std::endl;
      return 0:
```

Building and running the threaded driver

```
1 #> g++ dilog-threads.cc -o dilog-threads -pthread
2 #> dilog-threads -N 1e7 -z 1.0 -t 4
  Li2(1) =
   computed: 1.6449340301295035
     exact: 1.6449340668482264
     error: 2.23223068274304058e-08
  #> time dilog-threads -N 1e9 -z 1.0 -t 8
  Li2(1) =
  computed: 1.6449340044883614
     exact: 1.6449340668482264
10
     error: 3.79102520315773892e-08
13 real 0m2 803s
14 user 0m20.693s
15 sys 0m0.006s
16 #>
```

▶ the preamble

```
#include <getopt.h> // for getopt and friends
#include <mpi.h>

#include <cstdio>
#include <cstdlib> // for atof
#include <cmath>

#include <map>
#include <iostream>
#include <iomanip>
#include <iomanip>
```

coarse grain task

```
12 double dilog(double zprime, long N, int id, int processes) {
     // the width of each interval subdivision
     const double dz = zprime/N;
     // compute the starting point of the partial integral
     const double z low = id*zprime/processes;
16
     // partition the number of subdivisions
     long nominal load = N/processes;
18
     // the last process gets the leftovers
19
     if (id == processes - 1) {
20
        nominal load = N - id*nominal load;
     }
     // initialize the partial sum
     double sum = 0.0:
24
     double z = z low + dz/2:
     // loop over the subdivisions assigned to this thread
26
     for (long i=0; i < nominal_load; i++) {
        sum += std::log(1-z)/z;
28
29
        z += dz;
30
     // collect the partial answers from all the processes
31
     double value;
32
     MPI Allreduce (
        &sum, &value, 1, MPI DOUBLE, MPI SUM, MPI COMM WORLD);
34
     // multiply by the width of each subdivision and adjust the sign
35
     return -dz*value;
36
37
```

▶ the main program – setting up MPI

```
38 // main program
39 int main(int argc, char* argv[]) {
   // initialize MPI
    int status = MPI_Init(&argc, &argv);
     if (status != MPI SUCCESS) {
42.
        std::cout << "error in MPI Init; aborting..." << std::endl;</pre>
        return status:
44
     1
     // get process information from the world communicator
46
     int id, processes;
47
     MPI Comm rank (MPI COMM WORLD, &id);
48
     MPI Comm size (MPI_COMM_WORLD, &processes);
49
```

► reading the command line

```
// default values for the command line options
51
52.
     long N = 1000;
     double z = 1.0;
     // read the command line
54
     int command;
55
     while ((command = getopt(argc, argv, "z:N:")) != -1) {
        switch (command) {
57
        case 'z':
58
            // get the argument of the dilogarithm
59
            z = atof(optarg);
60
           break:
        case 'N':
            // get the number of subdivisions
            N = (long) atof(optarg);
            break;
66
```

error checking and computation

```
// error checking
     // abort if N < 1
     if (N < 1) {
         if (id == 0) {
            std::cout
               << "the number of subdivisions must be positive"
               << std::endl:
74
        MPI_Finalize();
76
         return 0;
78
      }
     // abort for z > 1 to avoid dealing with the imaginary part
79
     if (z > 1.0) {
80
         if (id == 0) {
81
            std::cout << "math domain error: z > 1" << std::endl;</pre>
82
83
        MPI_Finalize();
84
85
        return 0;
86
     // compute
87
     double value = dilog(z, N, id, processes);
88
     if (id != 0) { // let all but processor 0 die
20
        // shut down MPI
90
        MPI Finalize();
91
        return 0:
92
```

printing out the results

```
// build a database of the known dilogarithm values
95
      const double pi = M PI;
      std::map<double, double> answers;
96
      answers[1.0] = pi*pi/6;
      answers[-1.0] = -pi*pi/12;
98
99
      // print out the value
100
      std::cout << "Li2(" << z << ")=" << std::setprecision(17) << std::endl;
      std::cout << " computed: " << value << std::endl:
102
103
      // check whether we know the right answer
      std::map<double,double>::const_iterator lookup = answers.find(z);
104
      if (lookup != answers.end()) {
105
         // and if we do, print it out
106
         double exact = lookup->second;
         std::cout << " exact: " << exact << std::endl:
108
         // compute the approximation error and print it out
109
         double error = std::abs(exact-value)/exact;
         std::cout
            << std::setiosflags(std::ios_base::scientific)
            << " error: " << error << std::endl;
      }
      // shut down MPI
116
      MPI Finalize();
      return 0:
118
119
```

Building and running the MPI driver

- ▶ on my desktop, or mind-meld.cacr.caltech.edu
 - where there is no queue manager

```
#> mpic++ dilog-mpi.cc -o dilog-mpi -lmpi cxx -lmpi
2 #> mpirun -np 4 dilog-mpi -N 1e7 -z 1.0
  Li2(1) =
   computed: 1.6449340301295035
     exact: 1.6449340668482264
     error: 2.23223068274304058e-08
  #> time mpirun -np 8 dilog-mpi -N 1e9 -z 1.0
  Li2(1) =
   computed: 1.6449340044883614
     exact: 1.6449340668482264
10
     error: 3.79102520315773892e-08
13 real 0m3 697s
  user 0m0.018s
  sys 0m0.015s
  #>
```

Running the MPI driver on a shared resource

- ▶ on shc.cacr.caltech.edu there is a queue manager
 - don't use mpirun: you are running on the head node
 - instead, request a dedicated node

```
# shc-a> mpic++ dilog-mpi.cc -o dilog-mpi
2 # shc-a> qsub -I -1 nodes=1:core8 -1 walltime=0:15:00
  gsub: waiting for job 105059.mistress to start
4 qsub: job 105059.mistress ready
5 Logging in as aivazis on shc168, a linux.x86 system
    setting up: (environment) (aliases) (machines) (tools: Linux-2.x x86 64)
7 # shc168> time mpirun -np 8 dilog-mpi -N 1e9 -z 1.0
8 Li2(1)=
  computed: 1.6449340044883614
     exact: 1.6449340668482264
10
     error: 3.79102520315773892e-08
13 real 0m10.501s
14 user 1m14.642s
15 sys 0m0.273s
16 # shc168> exit
17 logout
  qsub: job 105059.mistress completed
19 # shc-a>
```