

ACM/CS 114

Parallel algorithms for scientific applications

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Improving the update loop

- ▶ the plan is to keep the workers alive and updating the grid while either we converge or `max_iterations` is reached
- ▶ the main thread
 - ▶ loops to spawn all the threads
 - ▶ and immediately enters a loop to harvest them
- ▶ the workers use a condition variable to synchronize among themselves
 - ▶ they iterate, updating the grid
 - ▶ grab a mutex, deposit their local maximum deviation from the last iterations, update a counter that records how many workers have completed their update, and release the lock
 - ▶ enter another critical section with the termination logic
 - ▶ everybody uses a condition variable to wait for the slowest worker
 - ▶ the slowest worker checks the convergence criterion and updates the termination flag, swaps the grid blocks and signals everybody else
 - ▶ if the termination flag is set, or if the maximum number of iterations has been reached, all threads exit

Threaded Jacobi: the updated master thread

```
1 void Jacobi::_solve(Problem & problem) {
2     Grid & current = problem.solution();
3
4     // create and initialize temporary storage
5     Grid next(current.size());
6     problem.initialize(next);
7
8     // shared thread info
9     Task task(_workers, current, next);
10    // per-thread information
11    Context context[_workers];
12
13    // let's get going
14    std::cout << "jacobi: spawning " << _workers << " threads" << std::endl;
15    for (size_t tid=0; tid < _workers; tid++) {
16        context[tid].id = tid;
17        context[tid].task = &task;
18
19        int status = pthread_create(&context[tid].descriptor, 0, _update, &context[tid]);
20        if (status) {
21            throw ("error in pthread_create");
22        }
23    }
24    // harvest the threads
25    std::cout << "jacobi: harvesting " << _workers << " threads" << std::endl;
26    for (size_t tid = 0; tid < _workers; tid++) {
27        std::cout << "jacobi: waiting for thread " << tid << " to finish" << std::endl;
28        pthread_join(context[tid].descriptor, 0);
29        std::cout << "jacobi: thread " << tid << " done" << std::endl;
30    }
31    // done
32    std::cout << "jacobi: done." << std::endl;
33    return;
34 }
```

Threaded Jacobi: updated thread data

```
35 struct Task {
36     // shared information
37     size_t workers; // the number of threads
38     double tolerance; // the convergence tolerance
39     Grid & current;
40     Grid & next;
41
42     bool done; // is there more work?
43     double maxDeviation; // the value
44     size_t contributions; // the number of threads that have deposited contributions
45     pthread_mutex_t gridUpdate_lock; //the mutex
46     pthread_cond_t gridUpdate_check;
47
48     Task(size_t workers, double tolerance, Grid & current, Grid & next) :
49         workers(workers), tolerance(tolerance), current(current), next(next),
50         done(false), maxDeviation(0.0), contributions(0),
51         gridUpdate_lock(), gridUpdate_check() {
52         // initialize the grid update lock
53         pthread_mutex_init(&gridUpdate_lock, 0);
54         pthread_cond_init(&gridUpdate_check, 0);
55     }
56
57     ~Task() {
58         pthread_mutex_destroy(&gridUpdate_lock);
59         pthread_cond_destroy(&gridUpdate_check);
60     }
61 };
```

Threaded Jacobi: the main thread

```
1 void Jacobi::_solve(Problem & problem) {
2     Grid & current = problem.solution();
3
4     // create and initialize temporary storage
5     Grid next(current.size());
6     problem.initialize(next);
7
8     // shared thread info
9     Task task(_workers, _tolerance, current, next);
10    // per-thread information
11    Context context[_workers];
12    // spawn the threads
13    std::cout << "jacobi: spawning " << _workers << " workers" << std::endl;
14    for (size_t tid=0; tid < _workers; tid++) {
15        context[tid].id = tid;
16        context[tid].task = &task;
17
18        int status = pthread_create(&context[tid].descriptor, 0, _update, &context[tid]);
19        if (status) {
20            throw ("error in pthread_create");
21        }
22    }
23    // harvest the threads
24    for (size_t tid = 0; tid < _workers; tid++) {
25        pthread_join(context[tid].descriptor, 0);
26    }
27    // done
28    std::cout << "jacobi: done." << std::endl;
29    return;
30 }
```

Threaded Jacobi: workers, part 1

```
31 // the threaded update
32 void * Jacobi::_update(void * arg) {
33     Context * context = static_cast<Context *>(arg);
34
35     size_t id = context->id;
36     Task * task = context->task;
37
38     const size_t workers = task->workers;
39     Grid & current = task->current;
40     Grid & next = task->next;
41
42     size_t maxIterations = (size_t) 1e4;
43     // iterate, updating the grid until done
44     for (size_t iteration = 0; iteration < maxIterations; iteration++) {
45         // thread 0: print an update
46         if (id == 0 && iteration % 100 == 0) {
47             std::cout << " " << iteration << std::endl;
48         }
49
50         double max_dev = 0.0;
51         // do an iteration step
52         // leave the boundary alone
53         // iterate over the interior of the grid
54         for (size_t j=id+1; j < current.size()-1; j+=workers) {
55             for (size_t i=1; i < current.size()-1; i++) {
56                 next(i,j) = 0.25*(current(i+1,j)+current(i-1,j)+current(i,j+1)+current(i,j-1));
57                 // compute the deviation from the last generation
58                 double dev = std::abs(next(i,j) - current(i,j));
59                 // and update the maximum deviation
60                 if (dev > max_dev) {
61                     max_dev = dev;
62                 }
63             }
64         }
65         // done with the grid update
```

Threaded Jacobi: workers, part 2

```
66 // grab the grid update lock
67 pthread_mutex_lock(&task->gridUpdate_lock);
68 // update the global maximum deviation
69 if (task->maxDeviation < max_dev) {
70     task->maxDeviation = max_dev;
71 }
72 // leave a mark
73 task->contributions++;
74 // bookkeeping at the end of the update
75 if (task->contributions == workers) {
76     // if i am the slowest worker
77     // swap the blocks between the two grids
78     Grid::swapBlocks(current, next);
79     // check convergence
80     if (task->maxDeviation < task->tolerance) {
81         std::cout
82             << " +++ thread " << id << ": convergence in " << iteration << " iterations"
83             <<std::endl;
84         task->done = true;
85     }
86     // reset our accounting and signal everybody
87     task->contributions = 0;
88     task->maxDeviation = 0;
89     pthread_cond_broadcast(&task->gridUpdate_check);
90 } else {
91     // all but the slowest wait here
92     pthread_cond_wait(&task->gridUpdate_check, &task->gridUpdate_lock);
93 }
94 // release
95 pthread_mutex_unlock(&task->gridUpdate_lock);
96 // check whether we are done
97 if (task->done) {
98     break;
99 }
100 }
101 return 0;
102 }
```

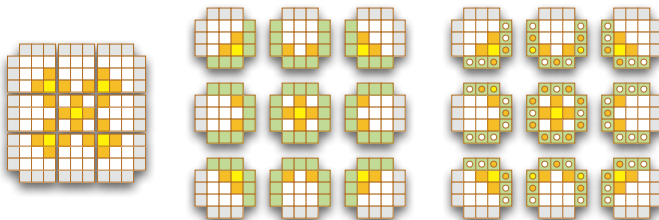
Assessing the improved implementation

- ▶ the improved threading scheme is not much more complex
 - ▶ we keep track of how many threads have computed their grid update
 - ▶ the slowest worker check the convergence criterion and performs all the necessary bookkeeping
 - ▶ while everybody else waits
 - ▶ use `pthread_cond_broadcast` to wake the other workers
- ▶ here is the performance comparison for 10,000 iterations on a 1000×1000 grid on the same 8-core MacPro

threads	1	2	4	8	16
previous(s)	413.306	211.050	109.509	98.279	74.087
updated(s)	408.636	208.832	107.015	59.043	61.481

Parallelization with MPI

- ▶ the MPI implementation will require careful data management
 - ▶ we must partition the mesh among processes
 - ▶ each process work on its own subgrid
 - ▶ it will allocate its own memory, for both actual data and the guard zones
 - ▶ it must locate its patch in physical space
 - ▶ communication is required every iteration
 - ▶ so that neighbors can synchronize their boundaries
 - ▶ think of the synchronization as a kind of boundary condition!
 - ▶ parallel convergence testing involves a collective operation



A little bit of help

- ▶ MPI supports this common use case through a Cartesian *virtual topology*
 - ▶ a special communicator with a map from a d -dimensional virtual process grid to the normal linear process ranks
 - ▶ and local operations that enable you to discover the ranks of your virtual neighbors
 - ▶ there is even a special form of send/receive so that you don't have to worry about contention and race conditions during the boundary synchronization
- ▶ to create a Cartesian communicator

```
1 int MPI_Cart_create(MPI_Comm old,  
2     int ndims, int* layout, int* periods, MPI_Comm* new);
```

- ▶ to find out the coordinates of a process in the virtual grid given its rank

```
1 int MPI_Cart_coords(MPI_Comm cartesian,  
2     int rank, int ndims, int* coords);
```

- ▶ you can also find out the ranks of your neighbors

```
1 int MPI_Cart_shift(MPI_Comm cartesian,  
2     int dimension, int shift, int* origin, int* neighbor);
```

The MPI driver, part 1

```
26 int main(int argc, char* argv[]) {
27     int status;
28     // initialize mpi
29     status = MPI_Init(&argc, &argv);
30     if (status) {
31         throw("error in MPI_Init");
32     }
33     // get my rank in the world communicator
34     int worldRank, worldSize;
35     MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);
36     MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
37     size_t processors = static_cast<size_t>(std::sqrt(worldSize));
38
39     // default values for our user configurable settings
40     size_t n = 9; // points per processor
41     size_t threads = 1;
42     double tolerance = 1.0e-3;
43
44     // read the command line
45     int command;
46     while ((command = getopt(argc, argv, "n:e:t:")) != -1) {
47         switch (command) {
48             // get the convergence tolerance
49             case 'e':
50                 tolerance = atof(optarg);
51                 break;
52             // get the grid size
53             case 'n':
54                 n = (size_t) atof(optarg);
55                 break;
56             // get the number of threads
57             case 't':
58                 threads = (size_t) atoi(optarg);
59                 break;
60         }
61     }
```

The MPI driver, part 2

```
62 // print out the chosen options
63 if (worldRank == 0) {
64     for (int arg = 0; arg < argc; ++arg) {
65         std::cout << argv[arg] << " ";
66     }
67     std::cout
68         << std::endl
69         << "  grid size: " << n << std::endl
70         << "  workers: " << threads << std::endl
71         << "  tolerance: " << tolerance << std::endl;
72 }
73
74 // instantiate a problem
75 Example problem("cliche", 1.0, processors, n);
76
77 // instantiate a solver
78 Jacobi solver(tolerance, threads);
79 // solve
80 solver.solve(problem);
81 // save the results
82 Visualizer vis;
83 vis.csv(problem);
84
85 // initialize mpi
86 status = MPI_Finalize();
87 if (status) {
88     throw("error in MPI_Finalize");
89 }
90
91 // all done
92 return 0;
93 }
```

The Jacobi declaration

```
1 class acm114::laplace::Jacobi : public acm114::laplace::Solver {
2     // interface
3 public:
4     virtual void solve(Problem &);
5
6     // meta methods
7 public:
8     inline Jacobi(double tolerance, size_t workers);
9     virtual ~Jacobi();
10
11     // data members
12 private:
13     double _tolerance;
14     size_t _workers;
15
16     // disable these
17 private:
18     Jacobi(const Jacobi &);
19     const Jacobi & operator= (const Jacobi &);
20 };
```

The Problem declaration

```
1 class acml14::laplace::Problem {
2     //typedefs
3 public:
4     typedef std::string string_t;
5     // interface
6 public:
7     string_t name() const;
8     inline MPI_Comm communicator() const;
9     inline int rank() const;
10    // access to my grid
11    inline Grid & solution();
12    inline const Grid & solution() const;
13    // interface used by the solver
14    virtual void initialize();
15    virtual void applyBoundaryConditions() = 0;
16    // meta methods
17 public:
18     Problem(string_t name, double interval, int processors, size_t points);
19     virtual ~Problem();
20    // data members
21 protected:
22     string_t _name;
23     double _delta, _x0, _y0;
24     int _rank, _size, _processors;
25     int _place[2];
26     MPI_Comm _cartesian;
27     Grid _solution;
28    // disable these
29 private:
30     Problem(const Problem &);
31     const Problem & operator= (const Problem &);
32 };
```

The Problem constructor

```
94 Problem::Problem(  
95     string_t name, double interval, int processors, size_t points) :  
96     _name(name),  
97     _delta(interval/((points-2)*processors+1)),  
98     _x0(0.0), _y0(0.0),  
99     _rank(0), _size(0), _processors(processors), _place(),  
100     _cartesian(),  
101     _solution(points) {  
102  
103     // build the intended layout  
104     int layout[] = { processors, processors };  
105     // find my rank in the world communicator  
106     int worldRank;  
107     MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);  
108     // build a Cartesian communicator  
109     int periods[] = { 0, 0 };  
110     MPI_Cart_create(MPI_COMM_WORLD, 2, &layout[0], periods, 1, &_cartesian);  
111     // check whether i can participate  
112     if (_cartesian != MPI_COMM_NULL) {  
113         // get my rank in the cartesian communicator  
114         MPI_Comm_rank(_cartesian, &_rank);  
115         MPI_Comm_size(_cartesian, &_size);  
116         // get my logical position on the process grid  
117         MPI_Cart_coords(_cartesian, _rank, 2, &_place[0]);  
118         // now compute my offset in physical space  
119         _x0 = 0.0 + (points-2)*_place[0]*_delta;  
120         _y0 = 0.0 + (points-2)*_place[1]*_delta;  
121     } else {  
122         // i was left out because the total number of processors is not a square  
123         std::cout  
124             << "world rank " << worldRank << ": not a member of the cartesian communicator "  
125             << std::endl;  
126     }  
127 }
```

The Example declaration

```
1 class acml14::laplace::Example : public acml14::laplace::Problem {
2     // interface
3 public:
4     virtual void applyBoundaryConditions();
5
6     // meta methods
7 public:
8     inline Example(
9         string_t name, double interval, int processors, size_t points);
10    virtual ~Example();
11
12    // disable these
13 private:
14     Example(const Example &);
15     const Example & operator= (const Example &);
16 };
```


The implementation of Jacobi::solve, part 1

```
1 void Jacobi::solve(Problem & problem) {
2     // initialize the problem
3     problem.initialize();
4
5     // get a reference to the solution grid
6     Grid & current = problem.solution();
7     // build temporary storage for the next iterant
8     Grid next(current.size());
9
10    // put an upper limit on the number of iterations
11    size_t maxIterations = (size_t) 1e4;
12    for (size_t iteration = 0; iteration < maxIterations; iteration++) {
13        // print out a progress repot
14        if ((problem.rank() == 0) && (iteration % 100 == 0)) {
15            std::cout
16                << "jacobi: iteration " << iteration
17                << std::endl;
18        }
19        // enforce the boundary conditions
20        problem.applyBoundaryConditions();
21        // reset the local maximum change
22        double localMax = 0.0;
23        // update the interior of the grid
24        for (size_t j=1; j < next.size()-1; j++) {
25            for (size_t i=1; i < next.size()-1; i++) {
26                // the cell update
27                next(i, j) = .25*(current(i+1, j)+current(i-1, j)+current(i, j+1)+current(i, j-1));
28                // compute the change from the current cell value
29                double dev = std::abs(next(i, j) - current(i, j));
30                // and update the local maximum
31                if (dev > localMax) {
32                    localMax = dev;
33                }
34            }
35        } // done with the grid update
```

The implementation of `Jacobi::solve`, part 2

```
36 // swap the blocks of the two grids, leaving the solution in current
37 Grid::swapBlocks(current, next);
38 // compute global maximum deviation
39 double globalMax;
40 MPI_Allreduce(&localMax, &globalMax, 1, MPI_DOUBLE, MPI_MAX, problem.communicator());
41 // convergence check
42 if (globalMax < _tolerance) {
43     if (problem.rank() == 0) {
44         std::cout
45             << "jacobi: convergence in " << iteration << " iterations"
46             << std::endl;
47     }
48     break;
49 }
50 // otherwise
51 }
52 // when we get here, either we have converged or ran out of iterations
53 // update the fringe of the current grid
54 problem.applyBoundaryConditions();
55 // all done
56 return;
57 }
```

Boundary conditions and data exchanges, part 1

```
1 void Example::applyBoundaryConditions() {  
2     // a reference to my grid  
3     Grid & g = _solution;  
4     // my rank;  
5     int rank = _rank;  
6     // the ranks of my four neighbors  
7     int top, right, bottom, left;  
8     // get them  
9     MPI_Cart_shift(_cartesian, 1, 1, &rank, &top);  
10    MPI_Cart_shift(_cartesian, 0, 1, &rank, &right);  
11    MPI_Cart_shift(_cartesian, 1, -1, &rank, &bottom);  
12    MPI_Cart_shift(_cartesian, 0, -1, &rank, &left);  
13  
14    // allocate send and receive buffers  
15    double * sendbuf = new double[g.size()];  
16    double * recvbuf = new double[g.size()];
```

Boundary conditions and data exchanges, part 2

```
17 // shift to the right
18 // fill my sendbuf with my RIGHT DATA BORDER
19 for (size_t cell=0; cell < g.size(); cell++) {
20     sendbuf[cell] = g(g.size()-2, cell);
21 }
22 // do the shift
23 MPI_Sendrecv(
24     sendbuf, g.size(), MPI_DOUBLE, right, 17,
25     recvbuf, g.size(), MPI_DOUBLE, left, 17,
26     _cartesian, MPI_STATUS_IGNORE
27 );
28 if (left == MPI_PROC_NULL) {
29     // if i am on the boundary, paint the dirichlet conditions
30     for (size_t cell=0; cell < g.size(); cell++) {
31         g(0, cell) = 0;
32     }
33 } else {
34     // fill my LEFT FRINGE with the received data
35     for (size_t cell=0; cell < g.size(); cell++) {
36         g(0, cell) = recvbuf[cell];
37     }
38 }
```

Boundary conditions and data exchanges, part 4

```
39 // shift to the left
40 // fill my sendbuf with my LEFT DATA BORDER
41 for (size_t cell=0; cell < g.size(); cell++) {
42     sendbuf[cell] = g(1, cell);
43 }
44 // do the shift
45 MPI_Sendrecv(
46     sendbuf, g.size(), MPI_DOUBLE, left, 17,
47     recvbuf, g.size(), MPI_DOUBLE, right, 17,
48     _cartesian, MPI_STATUS_IGNORE
49 );
50 if (right == MPI_PROC_NULL) {
51     // if i am on the boundary, paint the dirichlet conditions
52     for (size_t cell=0; cell < g.size(); cell++) {
53         g(g.size()-1, cell) = 0;
54     }
55 } else {
56     // fill my RIGHT FRINGE with the received data
57     for (size_t cell=0; cell < g.size(); cell++) {
58         g(g.size()-1, cell) = recvbuf[cell];
59     }
60 }
```

Boundary conditions and data exchanges, part 5

```
62 // shift up
63 // fill my sendbuf with my TOP DATA BORDER
64 for (size_t cell=0; cell < g.size(); cell++) {
65     sendbuf[cell] = g(cell, g.size()-2);
66 }
67 // do the shift
68 MPI_Sendrecv(
69     sendbuf, g.size(), MPI_DOUBLE, top, 17,
70     recvbuf, g.size(), MPI_DOUBLE, bottom, 17,
71     _cartesian, MPI_STATUS_IGNORE
72 );
73 if (bottom == MPI_PROC_NULL) {
74     // if i am on the boundary, paint the dirichlet conditions
75     for (size_t cell=0; cell < g.size(); cell++) {
76         g(cell, 0) = std::sin((_x0 + cell*_delta)*pi);
77     }
78 } else {
79     // fill my BOTTOM FRINGE with the received data
80     for (size_t cell=0; cell < g.size(); cell++) {
81         g(cell, 0) = recvbuf[cell];
82     }
83 }
```

Boundary conditions and data exchanges, part 6

```
84 // shift down
85 // fill my sendbuf with my BOTTOM DATA BORDER
86 for (size_t cell=0; cell < g.size(); cell++) {
87     sendbuf[cell] = g(cell, 1);
88 }
89 // do the shift
90 MPI_Sendrecv(
91     sendbuf, g.size(), MPI_DOUBLE, bottom, 17,
92     recvbuf, g.size(), MPI_DOUBLE, top, 17,
93     _cartesian, MPI_STATUS_IGNORE
94 );
95 if (top == MPI_PROC_NULL) {
96     // if i am on the boundary, paint the dirichlet conditions
97     for (size_t cell=0; cell < g.size(); cell++) {
98         g(cell, g.size()-1) =
99             std::sin((_x0 + cell*_delta)*pi) * std::exp(-pi);
100     }
101 } else {
102     // fill my TOP FRINGE with the received data
103     for (size_t cell=0; cell < g.size(); cell++) {
104         g(cell, g.size()-1) = recvbuf[cell];
105     }
106 }
107
108 return;
109 }
```