MPI profiling with Allinea MAP

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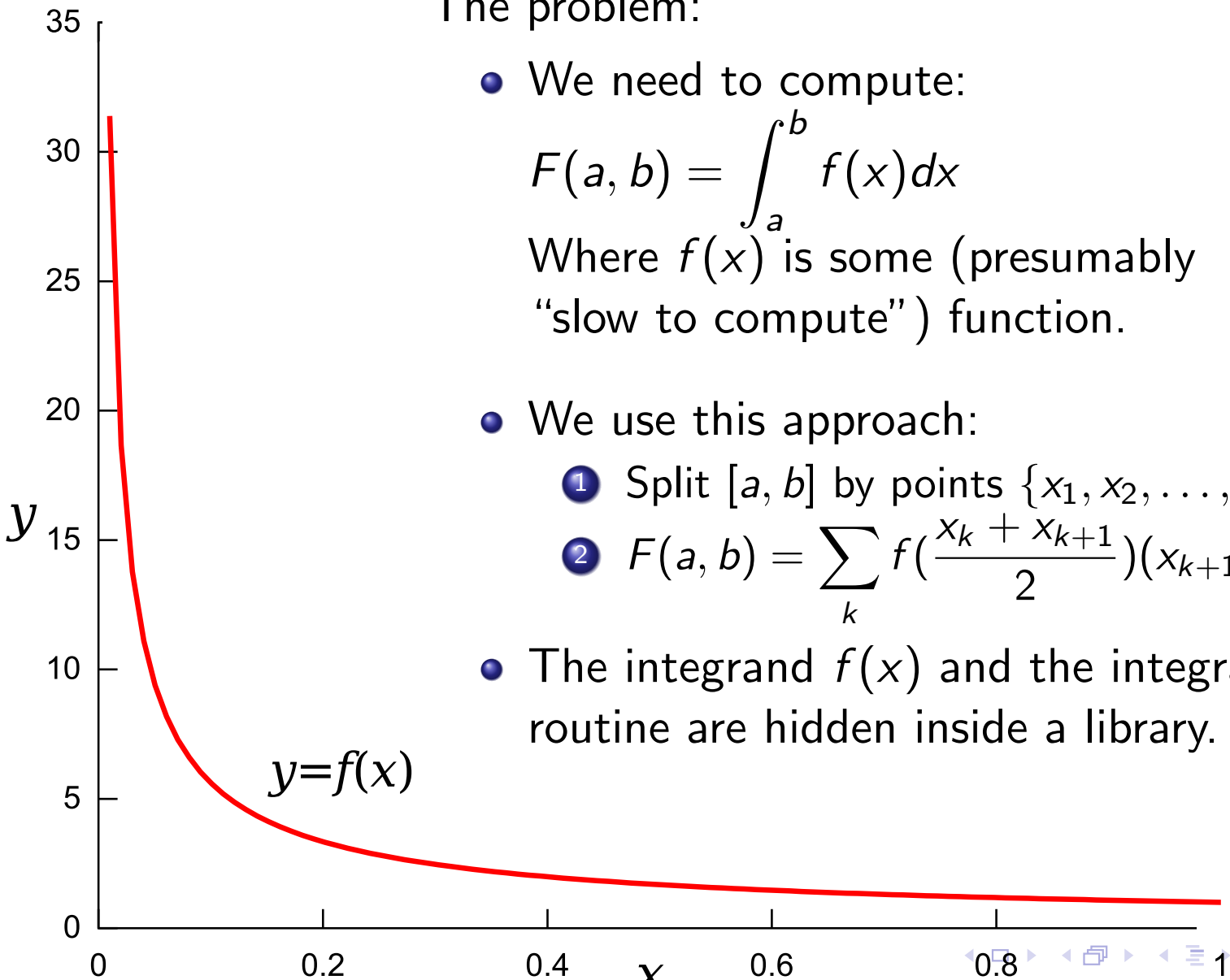
Problem: Calculation of a definite integral.



The problem:

- We need to compute:

  $$F(a,b) = \int_a^b f(x)dx$$

  Where $f(x)$ is some (presumably "slow to compute") function.

- We use this approach:
  1. Split $[a,b]$ by points $\{x_1, x_2, \ldots, x_k\}$
  2. $F(a,b) = \sum_k f(\frac{x_k + x_{k+1}}{2})(x_{k+1} - x_k)$
- The integrand $f(x)$ and the integration routine are hidden inside a library.

Sequential program code

```
1  #include <stdio.h>
2  #include <math.h>
3
4  // Declare integrand() and integral() from ``mymath'' library
5  #include "mylib/mymath.hpp"
6
7  int main(int argc, char** argv)
8  {
9    unsigned long int n;
10   if (argc!=2 || sscanf(argv[1],"%lu",&n)!=1) {
11     fprintf(stderr,"Usage:\n%s integration_steps\n\n\n",argv[0]);
12     return 1;
13   }
14
15   // Integration limits.
16   const double global_a=1E-5;
17   const double global_b=1;
18
19   // Perform integration
20   const double y=integral(integrand, n, global_a, global_b);
21
22   const double y_exact=4*(pow(global_b,0.25)-pow(global_a,0.25));
23   printf("Result=%lf Exact=%lf Difference=%lf\n", y, y_exact, y-y_exact);
24
25   return 0;
26 }
```

Problem size behavior: how to measure.

Do we even need to parallelize?

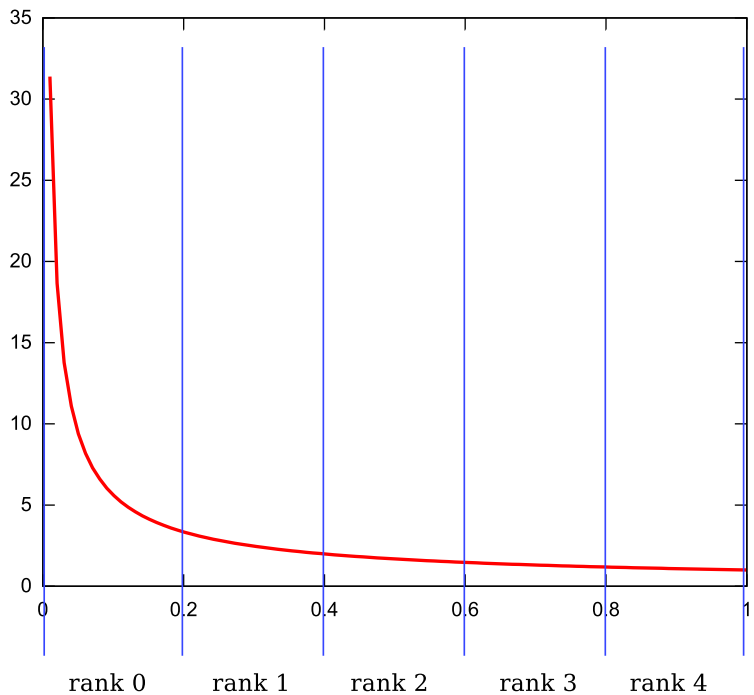
```
# Compilation:
$ gcc -O3 -o integral_seq.x integral_seq.cxx\
      -L./mylib -lmymath
# Timed runs:
$ time -p ./integral_seq.x 1000000
Result=3.775045 Exact=3.775063 Difference=-0.000019
real 2.12
$ time -p ./integral_seq.x 2000000
Result=3.775058 Exact=3.775063 Difference=-0.000005
real 4.28
$ time -p ./integral_seq.x 8000000
Result=3.775062 Exact=3.775063 Difference=-0.000001
real 17.61
```

The time grows linearly with the problems size. Acceptable accuracy at 8M points. Can we speed it up?

Parallellization: domain decomposition.

Approach:

- Split $[a, b]$ into several domains;
- Compute integrals independently.



$$F(a, b) = \int_a^b f(x)dx$$

1. Assign a process to each domain $[x_k, x_{k+1}]$
2. Let each process compute $F(x_k, x_{k+1})$
3. $F(a, b) = \sum_k F(x_k, x_{k+1})$

"Embarassingly parallel" problem, high speedup is expected.

A sketch of the parallel code

```
1   MPI_Init(&argc, &argv);
2
3   int rank, nprocs;
4   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
5   MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
6
7   // ...Get total number of steps, broadcast it...
8   // ...
9
10  // Each rank figures out its integration limits and number of steps
11  unsigned long my_stepbase, my_nsteps;
12  get_steps(nsteps_all, nprocs, rank,  &my_stepbase, &my_nsteps);
13
14  const double per_step=(global_b-global_a)/nsteps_all;
15  const double x1=global_a + my_stepbase*per_step;
16  const double x2=x1 + my_nsteps*per_step;
17
18  // Compute my own part of the integral
19  double my_y=integral(integrand, my_nsteps, x1, x2);
20
21  // Sum all numbers on master
22  double y=0;
23  MPI_Reduce(&my_y, &y, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
24
25  // ... print results ...
26  // ...
27
28  MPI_Barrier(MPI_COMM_WORLD);
29  // Here we could start another computation.
30  MPI_Finalize();
```

Parallel performance: how to measure.

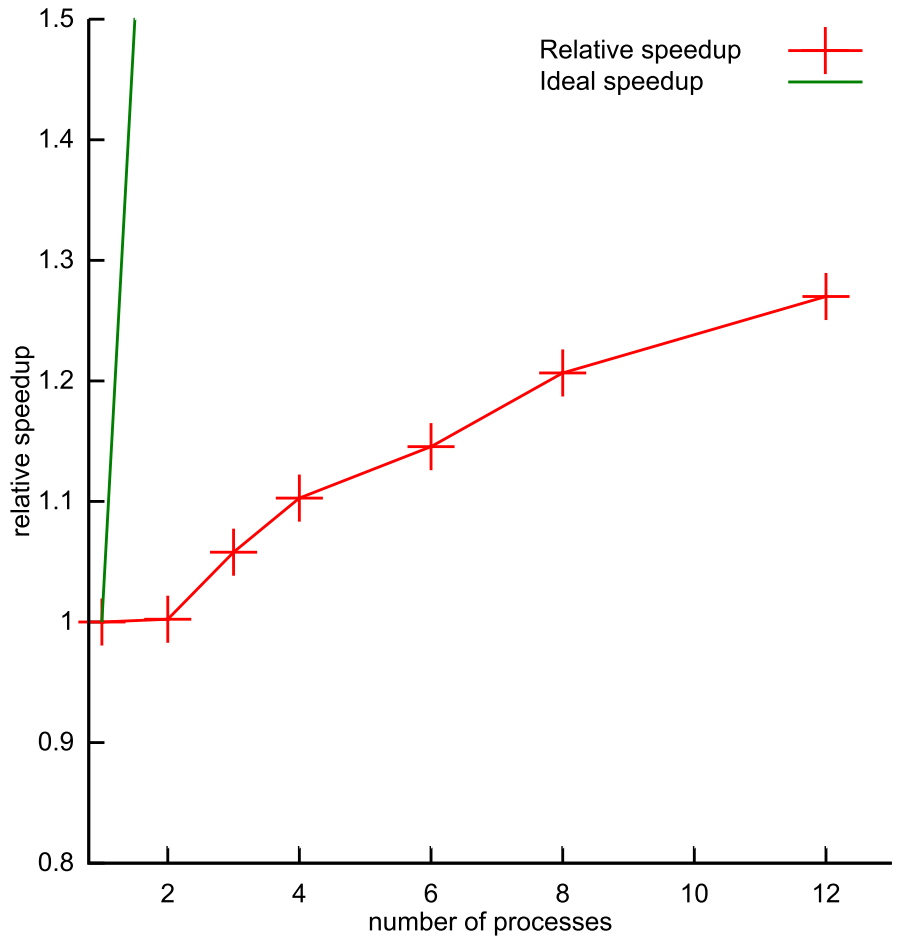
Now let's see how much we achieved...

- Strong scaling: as we add processes, how do we fare?
- Weak scaling: as we add *both* processes and work?

```
$ mpicc -O3 -o integral_par.x integral_par.cxx \
        -L./mylib -lmymath
$ time -p mpirun -np 1 ./integral_par.x 8000000
Result=3.775062 Exact=3.775063 Difference=-0.000001
real 17.23
user 17.08
sys 0.02
$ time -p mpirun -np 2 ./integral_par.x 8000000
Result=3.775062 Exact=3.775063 Difference=-0.000001
real 17.24
user 31.98
sys 0.05
```

Parallel performance: results

Is there a performance problem?



- Relative speedup:
  $s(p) = \frac{(\text{time with 1 process})}{(\text{time with } p \text{ processes})}$
- Ideal relative speedup:
  $s_{\text{ideal}}(p) = p$
- Our speedup is
  25% on 12 nodes!
- I'd call it "*dismal*".
  We **do** have a problem!
- Why? How to figure it out?

How does performance analysis work?

How to collect data?

- Instrumentation:
  - Insert timers & counters in the code
  - Requires source or binary processing
- Sampling:
  - Interrupt & check the program at regular intervals
  - Introduces statistical error

What kind of data?

- Profile:
  - Summary information only
  - Relatively small file
- Trace:
  - Detailed recording during the run
  - Potentially huge file
  - Profile can be recovered

Allinea MAP does tracing by sampling.

Prepare for profiling

To prepare for profiling/tracing, one needs to:

- Compile with full optimization
- Generate debugging symbols
- Link with system libs dynamically
  - Usually the default
  - Notable exception: Cray
- On Flux: load `ddt` module

```
$ mpicc -g -O3 -o integral_par.x \
        integral_par.cxx -L ./mylib -lmymath
$ module add ddt
```

Running Map: simple way (demo)

1. Get interactive access to a compute node
2. Change to your working directory
3. Optionally, set *sampling interval*
4. Run as you would, prefixed by `map`

```
$ qsub -V -I -X -q flux -l qos=flux,nproc=12 \
       -l walltime=10:0:0 -A account_flux
$ cd $PBS_O_WORKDIR
$ export ALLINEA_SAMPLER_INTERVAL=5
$ map mpirun -np 12 ./integral_par.x 10000
```

Caution:

- Too small interval: large overhead!
- Too large interval: not enough samples!
- *Allinea* recommends at least 1000 samples/process

Running Map: other options

What if you can not or would not run a GUI?

- Have slow or non-existing X connection to compute nodes.
- Do not want to wait for interactive session.

Use `-profile` option.

```
1 #PBS -V
2 #PBS -q flux -l qos=flux -A account_flux
3 #PBS -l nproc=12,walltime=10:0:0
4 cd $PBS_O_WORKDIR
5 export ALLINEA_SAMPLER_INTERVAL=5
6 map -profile mpirun -np 12 ./integral_par.x 8000000
```

This will create a `*.map` file. Then run from the login node:

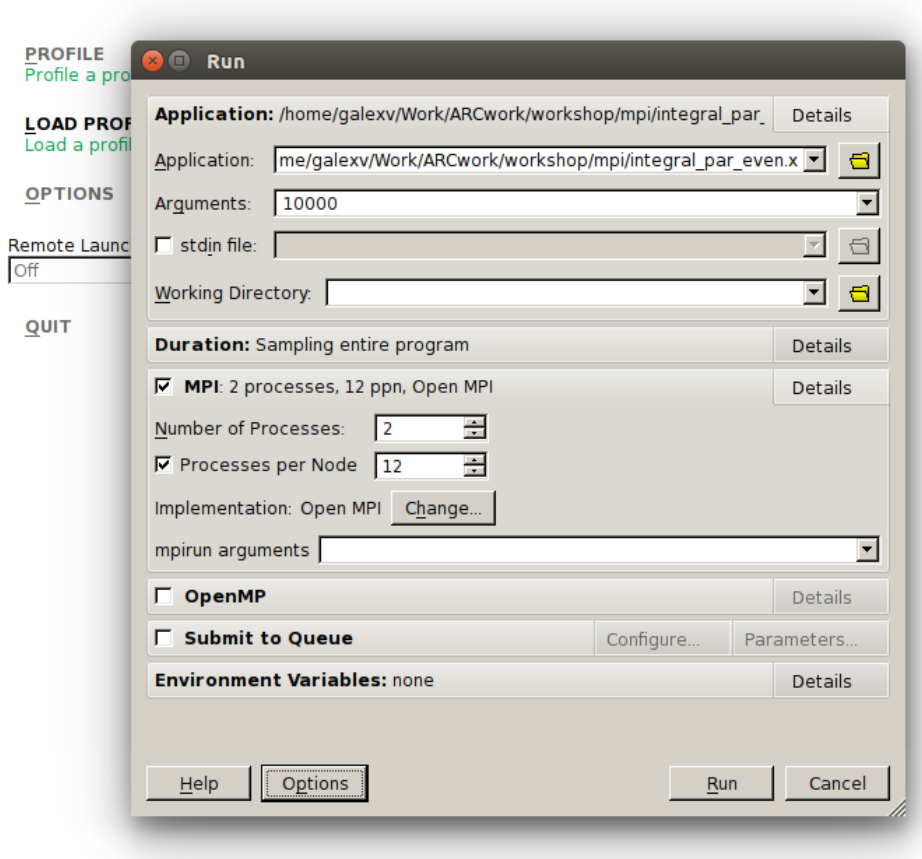
```
1 $ map integral_par_even_12p_*.map
```

If you are submitting to a Flux queue...

1. Run `map` from the login node:

```
$ map ./integral_par.x 8000000
```

2. Set number of processes
3. Check **Submit to queue**
4. Click **Configure...**
5. Load a proper *submission template file* (see next page)
6. Click **OK**
7. Click **Run**

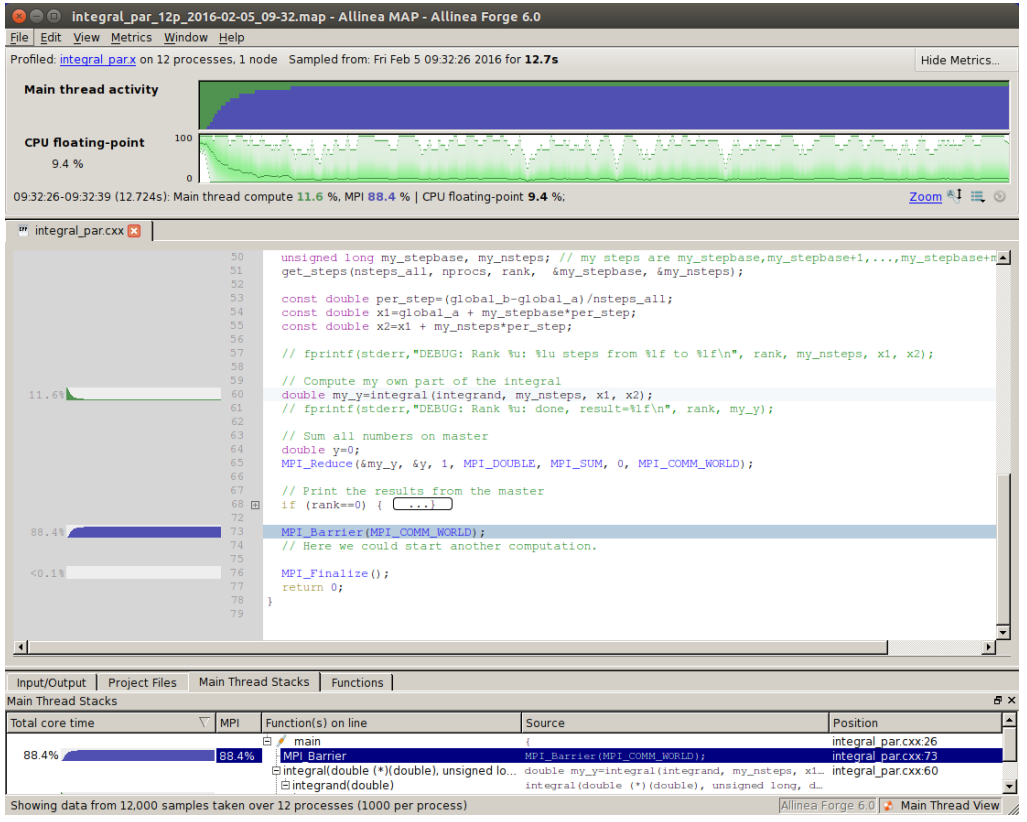


Submission template for Flux

```
1  #PBS -V
2  #PBS -l walltime=WALL_CLOCK_LIMIT_TAG
3  #PBS -l nodes=NUM_NODES_TAG:ppn=PROCS_PER_NODE_TAG
4  #PBS -q QUEUE_TAG -l qos=flux -A account_flux
5  #PBS -o PROGRAM_TAG-allinea.stdout
6  #PBS -e PROGRAM_TAG-allinea.stderr
7
8  cd $PBS_O_WORKDIR
9  AUTO_LAUNCH_TAG
```

Time for a live demo!

- Most of the time is spent in `MPI`;
- As run progresses, *even more* time is spent in `MPI`;
- Problem: some processes spend more time computing $f(x)$ then others!
- It's called "Load Imbalance".



Possible solutions:

- Distribute work unevenly (but how?)
- Implement *Dynamic Load Balancing*.

Dynamic load balancing

Idea: If a process has nothing to do, make it to do something.

Manager-Workers approach:

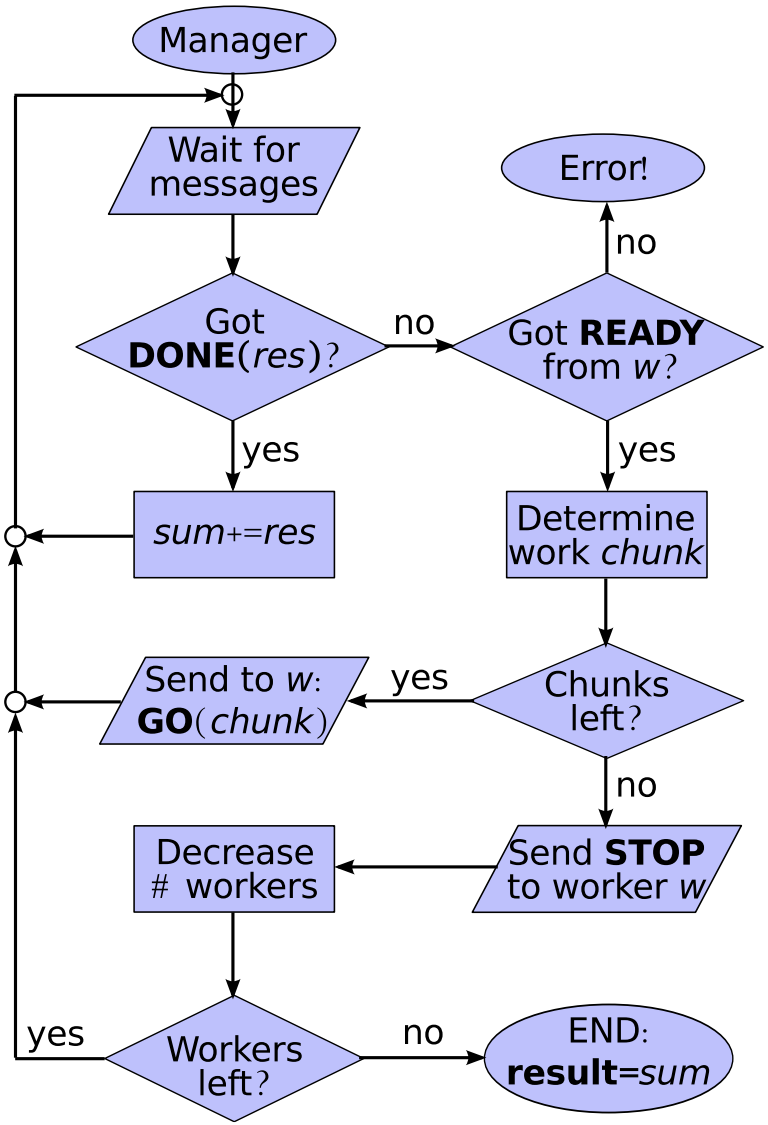
Manager

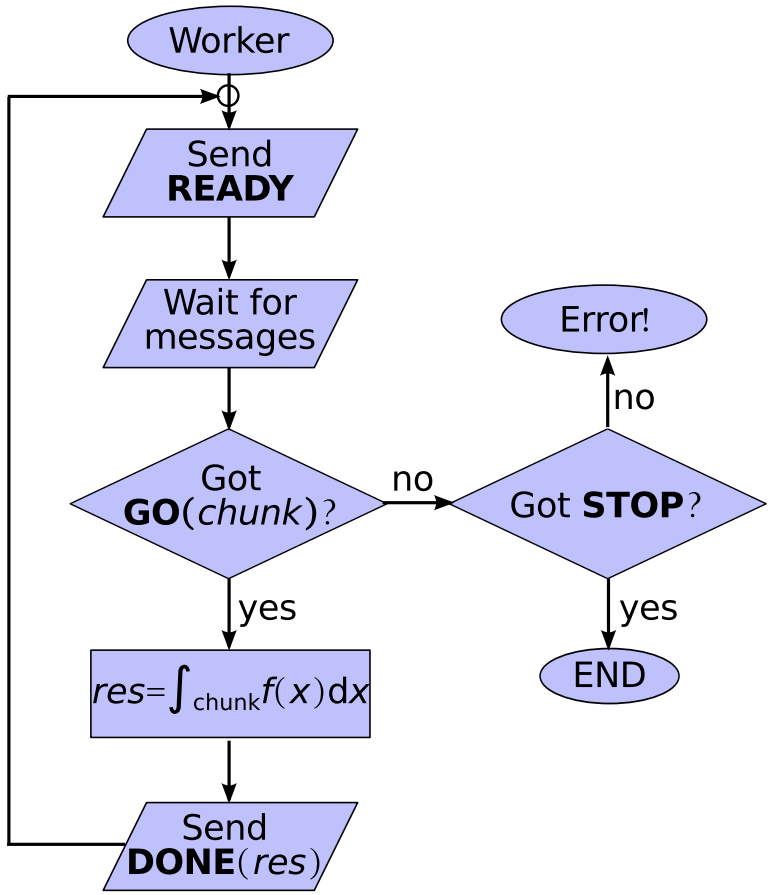
1. Listen to all workers
2. Worker sent `READY` ?
   - send `GO` with a job chunk
3. Worker sent `DONE`?
   - add result to the sum
4. No more job chunks?
   - send `STOP` to the worker
5. No more workers?
   - we are done!
   - Otherwise, go to (1)

Worker

1. Send `READY` to the Manager
2. Listen to the Manager
3. Manager sent `GO` ?
   - Get job chunk
   - Do the calculation
   - Send `DONE` with result to the Manager
   - Go to (1)
4. Manager sent `STOP`?
   - exit.

Dynamic load balancing





Dynamic Load Balancing: Worker code

```
1  void do_worker(int manager, int rank)
2  {
3    for (;;) {
4      // Inform manager that i am ready:
5      MPI_Send(NULL,0, MPI_DOUBLE, manager, TAG_READY, MPI_COMM_WORLD);
6      // ...and wait for the task.
7      double range_data[3]; // expect x1, x2 and the number of steps (as double!)
8      MPI_Status stat;
9      MPI_Recv(range_data,3,MPI_DOUBLE, manager, MPI_ANY_TAG, MPI_COMM_WORLD, &stat);
10     switch (stat.MPI_TAG) {
11     case TAG_GO:
12       break; // do normal work
13     case TAG_STOP:
14       return;
15     default:
16       fprintf(stderr,"Rank %d: Got unexpected tag=%d, aborting.\n",rank,stat.MPI_TAG);
17       MPI_Abort(MPI_COMM_WORLD, 2);
18     }
19     // we are here on TAG_GO.
20     const double x1=range_data[0];
21     const double x2=range_data[1];
22     const unsigned long my_nsteps=range_data[2];
23     // Compute my own part of the integral
24     double my_y=integral(integrand, my_nsteps, x1, x2);
25
26     // Send the result to manager
27     MPI_Send(&my_y,1,MPI_DOUBLE, manager, TAG_DONE, MPI_COMM_WORLD);
28   }
29 }
```

Dynamic Load Balancing: Manager code

```
1  double do_manager(const double global_a, const double global_b,
2                    const unsigned long nsteps_all, const unsigned long points_per_block,
3                    const int nprocs, const int rank)
4  {
5    const double per_step=(global_b-global_a)/nsteps_all;
6
7    int nworkers_left=nprocs-1;
8    unsigned long ipoint=0; // next point to be processed
9    double y=0;
10   for (;;) {
11     // Get a tagged message and possibly a result from any worker
12     double y_worker=0;
13     MPI_Status stat;
14     MPI_Recv(&y_worker,1,MPI_DOUBLE, MPI_ANY_SOURCE,MPI_ANY_TAG, MPI_COMM_WORLD, &stat);
15     const int rank_worker=stat.MPI_SOURCE;
16     switch (stat.MPI_TAG) {
17     case TAG_READY:
18       // Do we have any work for this worker?
19       if (ipoint>=nsteps_all) {
20         // if not, stop the worker
21         MPI_Send(NULL,0,MPI_DOUBLE, rank_worker, TAG_STOP, MPI_COMM_WORLD);
22         --nworkers_left;
23         break;
24       }
```

Dynamic Load Balancing: Manager code (cont.)

```
1       { // Prepare chunk of work for the worker
2         const unsigned long ns_worker=
3            (ipoint+points_per_block > nsteps_all)? (nsteps_all - ipoint) : points_per_block;
4         const double x1=global_a+ipoint*per_step;
5         const double x2=x1+ns_worker*per_step;
6         double range_data[3];
7         range_data[0]=x1;
8         range_data[1]=x2;
9         range_data[2]=ns_worker;
10        // Send the chunk
11        MPI_Send(range_data,3,MPI_DOUBLE, rank_worker, TAG_GO, MPI_COMM_WORLD);
12        // adjust the amount of points
13        ipoint += ns_worker;
14      }
15      break;
16    case TAG_DONE:
17      y += y_worker;
18      break;
19    default:
20      fprintf(stderr,"Rank %d (manager): Got unexpected tag=%d from %d,"
21                     " aborting.\n",rank,rank_worker,stat.MPI_TAG);
22      MPI_Abort(MPI_COMM_WORLD,1);
23    }
24    if (nworkers_left<=0) { // Any active workers left?
25      return y;
26    }
27  }
28 }
```

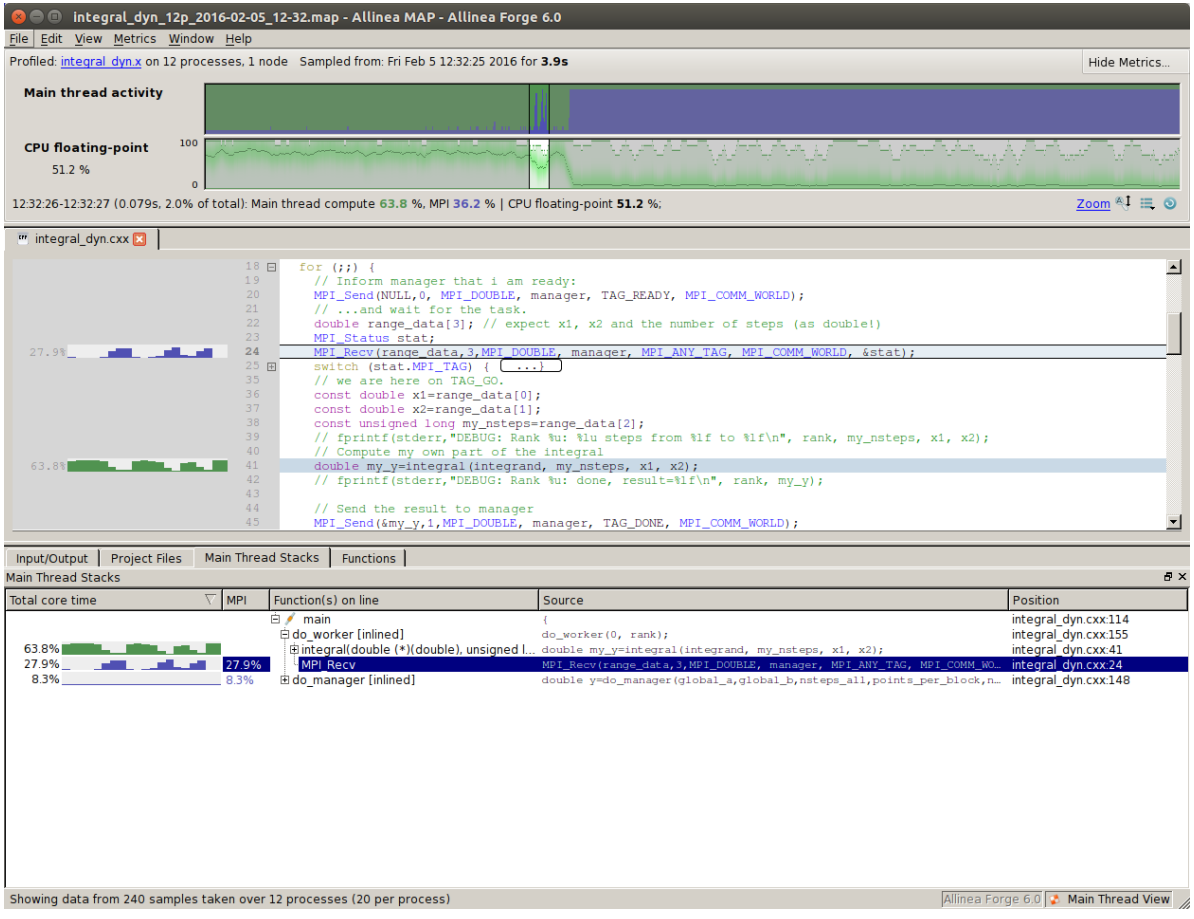
Dynamic Load Balancing: main

```
1  int main(int argc, char** argv)
2  {
3    MPI_Init(&argc, &argv);
4
5    int rank, nprocs;
6    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
7    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
8
9    // Get command line arguments, broadcast
10   unsigned long int nsteps_all, points_per_block;
11   // ....
12
13   // Global integration limits.
14   const double global_a=1E-5;
15   const double global_b=1;
16
17   // Split into workers and manager:
18   if (rank==0) { // Run as the manager and get the result:
19     double y=do_manager(global_a,global_b,nsteps_all,points_per_block,nprocs,rank);
20
21     const double y_exact=4*(pow(global_b,0.25)-pow(global_a,0.25));
22     printf("Result=%lf Exact=%lf Difference=%lf\n", y, y_exact, y-y_exact);
23   } else { // Run as a worker
24     do_worker(0, rank);
25   }
26
27   MPI_Barrier(MPI_COMM_WORLD);
28   // Here we could start another computation.
29   MPI_Finalize();
30   return 0;
31 }
```

Dynamic Load Balancing: large block size (2500)

Run with:

```
$ map mpirun -np 12 ./dyn_integral.x 8000000 2500
```

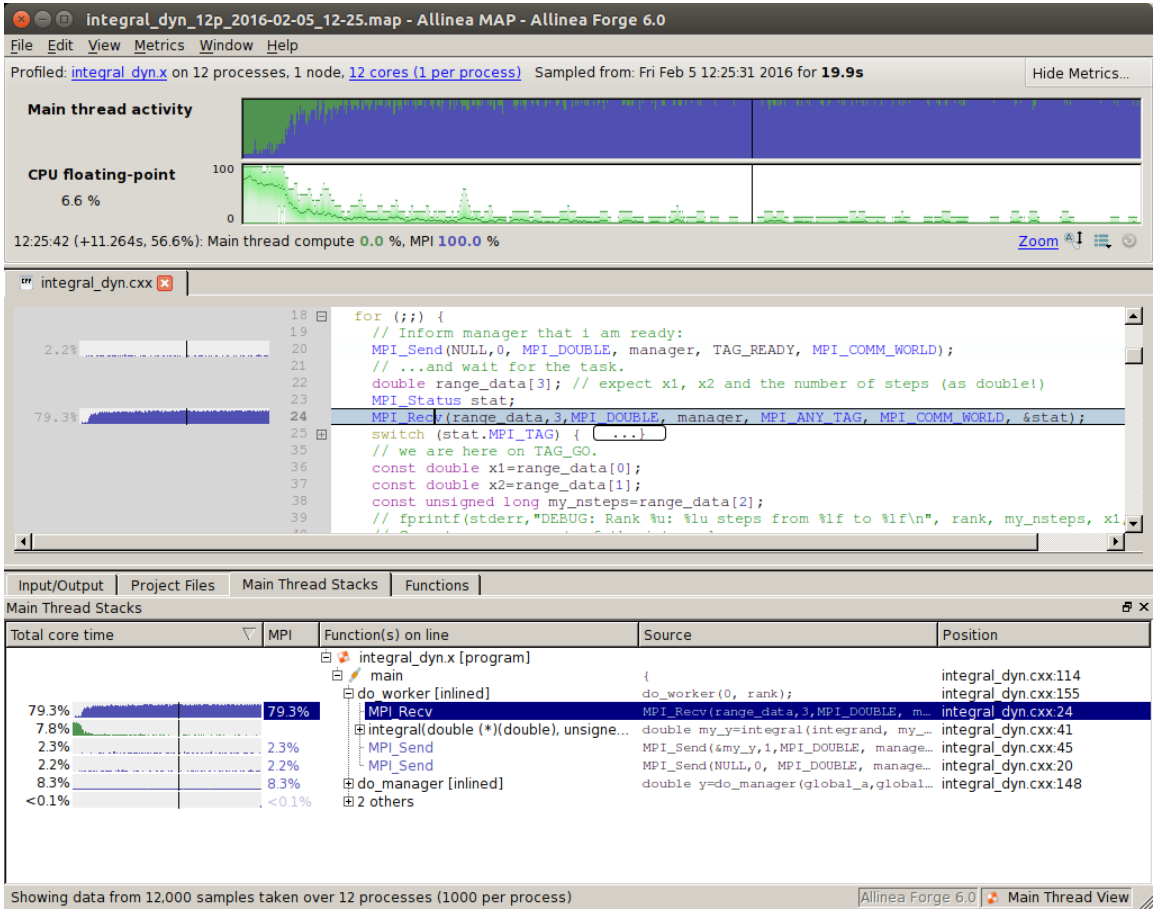


- CPU occupied till half-way
- Spikes in MPI use: Manager receiving data
- Looks like the last worker was holding everyone
- Other workers: *worker starvation* (no work to do)

Dynamic Load Balancing: small block size (2)

Run with:

```
$ map mpirun -np 12 ./dyn_integral.x 8000000 2
```

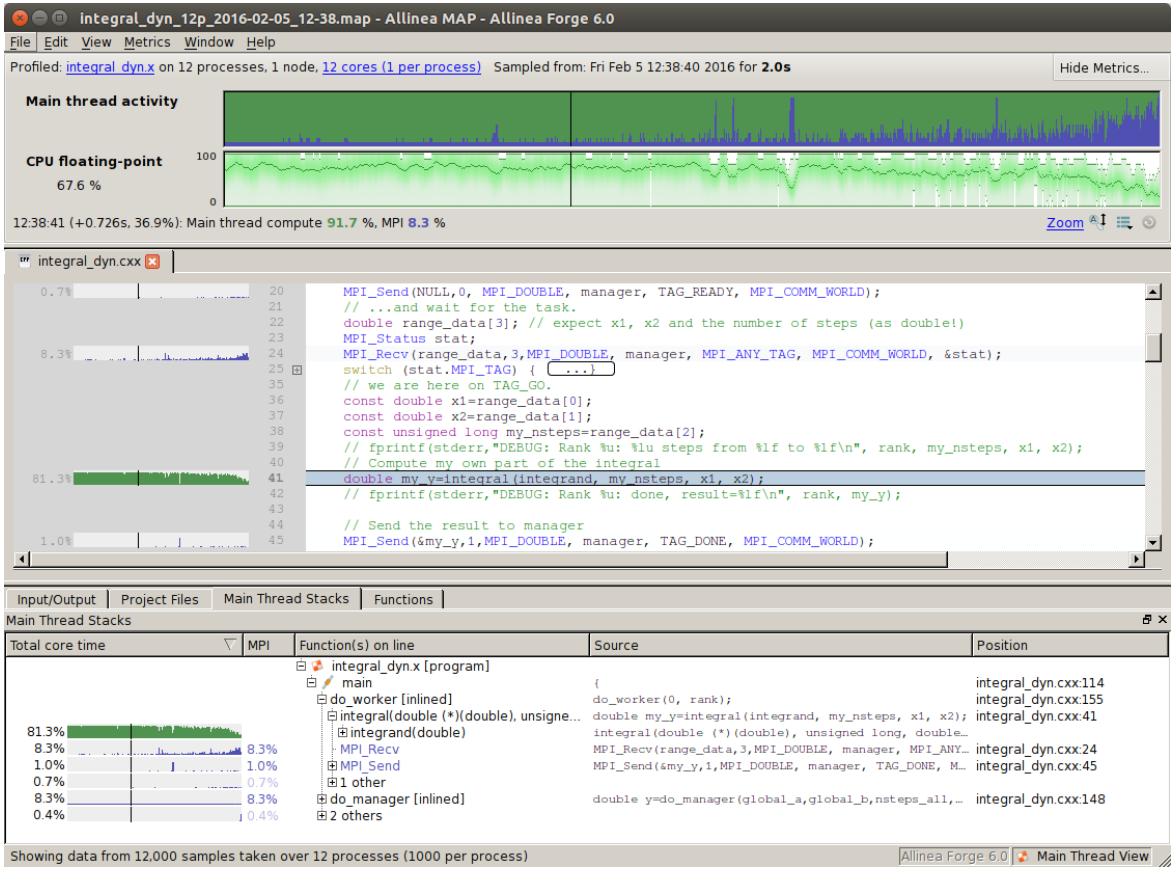


- Brief useful CPU work, then all time is in `MPI`
- Just moving data around:
  - Workers receiving data
  - 8% (1/12) of time: Manager sending data.
- Very low *computation/communication ratio*.

Dynamic Load Balancing: good block size (100)

Run with:

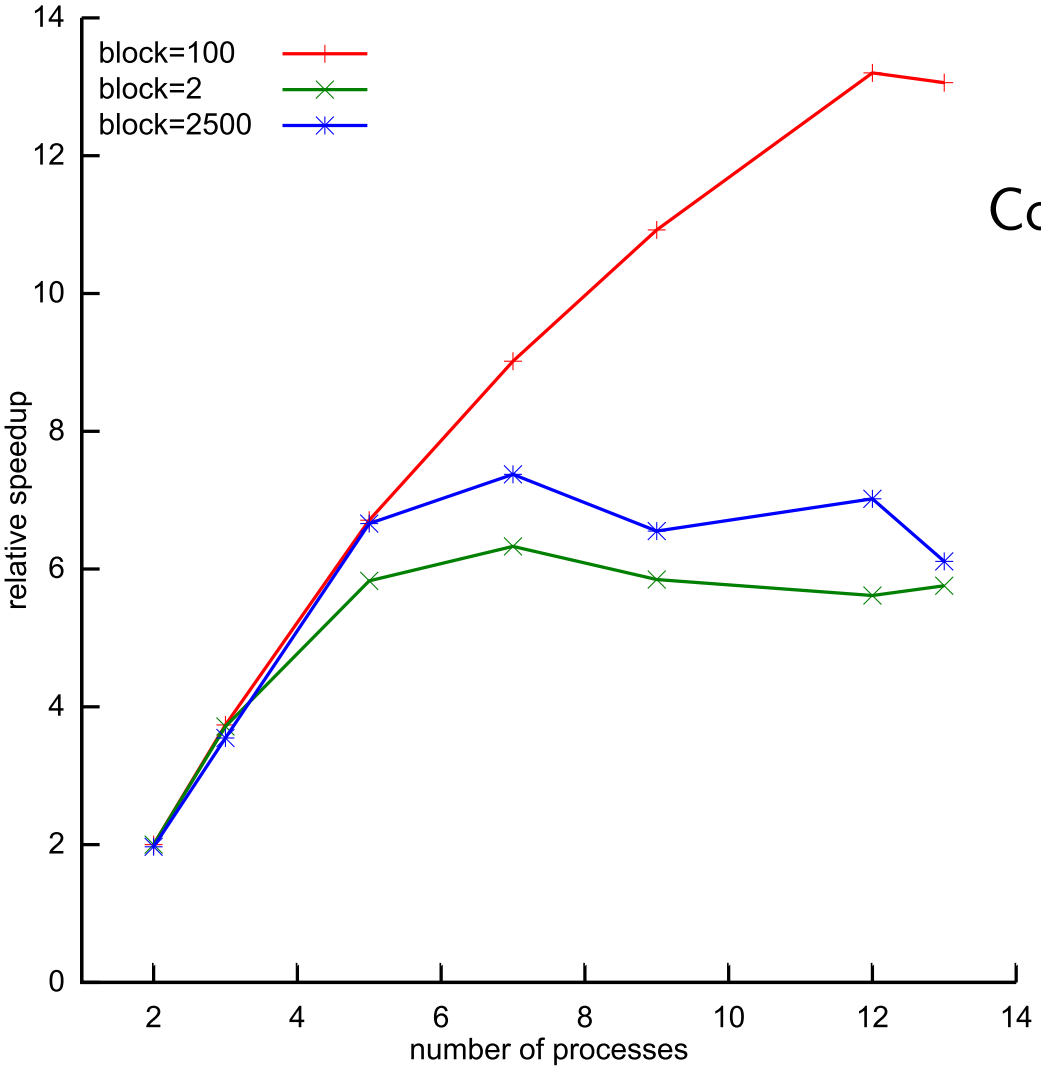
```
$ map mpirun -np 12 ./dyn_integral.x 8000000 100
```



- 80% time CPU is busy!
- 8% (1/12) of time: Manager work.
- Mostly `MPI` by the end of the run.
- OK computation/ communication ratio.
- Still room for improvement!

Dynamic Load Balancing: Strong scaling graph.

How does it look now?



Conclusions:

- Block size does affect performance.
- Block size 100 grows up to node size (12).
- Too small block: `MPI` communication overhead.
- Too large block: workers starvation.

Concluding slide

Take-home message

- Once you made your program parallel,
  do simple scaling experiments.
- If scaling is bad, use profiling tools to understand why.
- *Allinea Map* is available for all Flux users.
- *Map* can analyze not only parallel, but single-node
  and `OpenMP` performance. (Can show something if time permits!)
- If you need any advise and/or help with your parallel programming,
  ARC provides free consulting service
  - Just send a mail to HPC support...
  - ...or directly to: `"Alexander Gaenko" <galexv@umich.edu>`

Thank you for your attention!