Implementation of cohort parallelisation in the SEAPODYM code

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Abstract

This report describes NeSI/REANNZ's consultancy project entitled "SEAPODYM cohort parallelisation" whose work was performed from May to September 2025. The outcome of this work is a C++ library, seapodym-parallel, which can be leveraged by the SEAPODYM code to parallelize the spatio-temporal evolution of tuna fish densities in the Pacific. The seapodym-parallel library implements a variation of the manager/worker setup whereby workers create new fish age cohorts and advances these in time. The manager distributes tasks to the workers and stores results. The implemented manager/worker design differs from traditional implementations in that tasks can only be started when other tasks have completed specific internal steps.

1 Introduction

SEAPODYM is a quantitative spatio-temporal model of population dynamics that solves partial differential equations with initial and boundary conditions in C++. The model is parameterized using a maximum likelihood estimation approach that integrates georeferenced datasets obtained from industrial fishing and scientific campaigns.

The objective of this work is to parallelise the SEAPODYM code to achieve higher performance. This was achieved by designing and implementing the sepodym-parallel library (github.com/PacificCommunity/seapodym-parallel.git), a collection of C++ classes that abstract parallelization. The library comes with a CMake build system, unit tests and continuous integration via GitHub actions. The documentation of the API can be found at https://pacificcommunity.github.io/seapodym-parallel/.

2 What is a cohort?

A cohort is a group of fish that are born at the same time. Each cohort can be integrated forward in time independently of other cohorts, until the cohort reaches a certain age and dies. At the next time step, a new cohort is born and integrated forward in time until it, too, dies. Except at the first time step, the initial condition of each cohort depends on the density of the other cohorts at the previous time step. Thus, the integration of each cohort must take into account the state of the other cohorts and this requires careful consideration when parallelising the code.

An example of cohort time integration is shown below:

Here, the vertical axis represents time increasing from top to bottom ($N_t = 6$). The horizontal axis represents the tasks than can be performed concurrently. Each row represents different age groups (here $N_a = 3$). Each cohort is identified by an integer $(0, 1, \dots, 7)$. Cohort 1 is one unit time older than cohort 2. Therefore cohort 1 dies one time step before cohort 2. The number of time steps a cohort is integrated is $i = i_{beg} \dots i_{end} - 1$ where $i_{beg} \ge 0$ and $i_{end} \le N_a$. When a cohort dies, it is replaced by a new cohort at the next

Table 1: Start and end integration indices for each cohort of example (1)

cohort Id	$ i_{beg} $	i_{end}
0	2	3
1	1	3
2	0	3
3	0	3
4	0	3
5	0	3
6	0	2
7	0	1

time step.

3 Cohort task dependencies

To instantiate the new cohort, data will need to be communicated from the cohorts at the previous time step. Figure 1 shows the dependency of the new cohorts on the older cohorts at different steps of example (1).

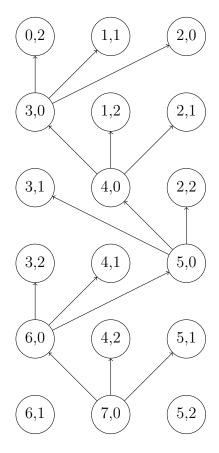


Figure 1: Dependency of cohort tasks on other cohort, step tuples. The first digit is the cohort Id and the second the step.

4 Parallel task farming with dependencies

We opted for a task farming approach, which involves creating a pool of tasks that can be executed concurrently, and a manager that assigns the tasks to the workers. Each task consists of advancing a cohort in time.

In classical task farming, the manager starts by assigning tasks to the workers. The manager sends a message to each worker, along with some input parameters. Each worker then executes the task and reports the results

back to the manager, who then assigns a new task to the worker. When no more tasks are available, the manager sends a message to the workers to shut down. The advantage of task farming over other approaches is that resources (workers) and tasks are dynamically matched, often allowing for better load balancing. A possible drawback of task farming is the additional complexity of coordinating the assignment of tasks, additional communication and the need to reserve an MPI rank for the manager.

Clearly, the dependencies between tasks and sub-tasks shown in Fig. 1 prevent us from using a naive task farming approach. since tasks can only be started when other tasks' particular steps have completed (as indicated by the arrows). This requires the manager to keep track of task-step dependencies.

We start by describing a worker's task. A task has a identification number taskid that fully describes the task to accomplish. A worker waits for a task to be assigned by the manager. The worker reports back the status of the execution of each task to the manager. The corresponding pseudo-code is shown in Algorithm 2.

Algorithm 1 A worker's pseudo-code.

- 1: while true do
 - taskid = G(e)tTaskIdFromManager
- 2: **if** taskid < 0 **then** Break
- 3: end if
- ▶ Perform the task, stepping from stepBeg to stepEnd 1
- 4: TASKFUNC(taskid, stepBeg, stepEnd)
 - ▶ Notify the manager that this worker is available again

▶ Advance a cohort

- 5: SENDSIGNALTOMANAGER(DONE)
- 6: end while

The task function defined in Algorithm 2 is responsible for advancing the cohort associated with taskid from stepBeg to stepEnd - 1. Note the call

Algorithm 2 The task function executed by the worker.

- 1: **function** MyFunction(taskid, stepBeg, stepEnd)
- 2: data = GETDATAFROMMANAGER(taskid)
- 3: cohort = CREATECOHORT(taskid)
- 4: $\mathbf{for} \text{ step} = \text{stepBeg to stepEnd 1 } \mathbf{do}$
- 5: STEPFORWARD(cohort)
- 6: SENDSTEPCOMPLETEMESSAGETOMANAGER(taskid, step)
- 7: end for
- 8: end function

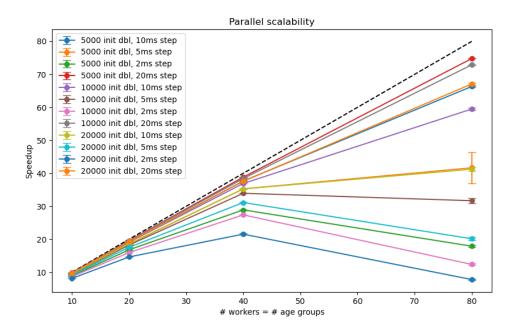


Figure 2: Parallel scaling as a function of the number of workers, for different step execution times and number of doubles initially fetched from the manager. The number of age groups matches the number of workers. These results assume no initialisation setup time.

to sendStepCompleteMessageToManager which informs the manager that a specific step for a task has been completed.

The manager code orchestrates the work. It maintains a list of all active workers, a task queue, a list of completed tasks and stores the results. Since workers will be sending various types of messages ("worker is available" or "result of task-step X"), the manager needs to be able to distinguish between these. This is done by using message tags. The manager's pseudo-code is shown in Algorithm 3.

5 Scalability

Figure 2 shows the parallel scalability of the cohort parallelisation approach described above as the number of workers is increased (see code testTaskStepFarmingCohort). The speedup numbers were obtained for an idealized scenario, assuming a fixed cost of communication to initialize a new cohort and a constant cost

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Algorithm 3 The manager's pseudo-code.
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1: while not taskQueue.empty() or not assigned.empty() do

    ▶ Look for messages "task-step complete"

 2:
       while true do
                                        ▶ Probe for messages from workers
          msg = getMessageFromAnyWorker
 3:
          if msg.type != "task-step complete" then
 4:
              break
 5:
          end if
 6:
                              ▷ Store the result R(e)sults.insertmsg.output
          taskid = output[0]
 7:
          step = output[1]
 8:
 9:
          completed.insert(taskid, step)
          if step == stepEnd - 1 then
10:
              assigned.erase(taskid)
11:
12:
          end if
       end while
13:
                              ▶ Assign ready tasks to any available worker
14:
       for taskid in taskQueue do
15:
          taskDependencies = getTaskStepDependencies(taskid)
16:
          bool ready = true
          for dep in taskDependencies do
17:
              if completed.find(dep) == completed.end() then
18:
                 readv = false
19:
                 break
20:
              end if
21:
          end for
22:
23:
          if ready and not activeWorkers.empty() then
              worker = activeWorkers.begin()
24:
25:
              activeWorkers.erase(worker)
              SENDTASKTOWORKER(taskid, worker)
26:
              assigned.insert(taskid)
27:
28:
              taskQueue.erase(taskid)
29:
          end if
       end for
30:
                                      ▶ Drain all worker-available messages
       for worker in workers do
31:
          msg = getMessageFromAnyWorker
32:
          if msg.type == "worker is available" then
33:
              activeWorkers.insert(worker)
34:
          end if
35:
       end for
36:
37: end while
                                     6
                                              ▶ Send stop signal to workers
38: stop = -1
39: for worker in workers do
40:
       sendStopSignalToWorker(worker)
41: end for
```

of executing a step on the NeSI/REANNZ AMD Milan node cluster. In all cases the number of workers was chosen to match the number of age groups N_a .

Perfect parallel scaling is shown as the black dashed line. Good scalability depends on the time taken to execute each step and the amount of data fetched from the manager at the start of each task. Parallel efficiency > 50% is achieved for time step times ≥ 10 ms and initial data sizes ≤ 10000 doubles. For instance, a time step taking 10ms and an initial data size of 10000 doubles yields a speedup of 60 when using 80 workers, i.e. 75% parallel efficiency.

At every step, the worker sends data to the manager, as well as a message to inform the manager that the step has been completed. This introduces a communication overhead that limits parallel scalability. Taking the example of 20,000 doubles sent by 80 workers to the manager at a cadence of 10 ms, we get a data transfer rate of 1.3 GB/s = 100 Gb/s, which is close to the bandwidth of the Infiniband communication fabric. To further improve parallel scalability, one would need to either increase the computational load per step, reduce the amount of data to be transferred or apply some form of data compression. For instance, one could send floats instead of double and this would improve the speedup from 40 to 60.

6 The cost of initialization

Scalability can be affected by load imbalance. Some concurrently executing tasks may take longer than others to complete. When synchronization occurs, which is the case at every time step in SEAPODYM, then workers whose task has finished need to wait for the slowest worker to finish their task. While the solution of the reaction-diffusion equations takes the same time for all cohorts, the initialization of a new cohort can lead to severe load imbalance and can thus affect the parallel speedup. Fig. 3 shows the the ratio of the compute time over the initialization time, the higher the better. Initialization involves reading data from file and other one off operations.

Let us estimate the effect of a high initialization time on parallel scalability. Let I denote the time it takes to initialize a cohort, C the compute time required to advance the density one time step and N the number of workers. The parallel speedup, defined as the ratio of single worker execution over the parallel execution, is

$$S = \frac{I + NC}{I + C} = N \frac{I/(NC) + 1}{I/C + 1}$$
 (2)

Note that for large numbers of workers $S \approx N \frac{1}{I/C+1}$ and thus the impact of

Time to compute / time to initialize ratio

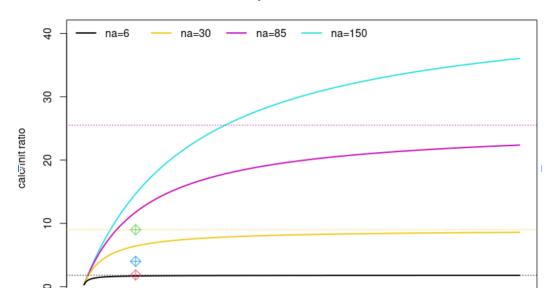


Figure 3: Ratio of compute over initialization time for SEAPODYM.

initialization is to reduce the speedup slope (I/C > 0). Figure 3 shows the ratio $(I/C)^{-1}$ for our initial implementation. This ratio, though increasing for large Ns, was close to 1 for moderate N values.

To mitigate the initialization effect on parallel scalability, the cohort initialization step was split into cohort independent and dependent steps. The cohort independent initialization can be performed for all cohorts at the start of the simulation. Since there are $\sim N$ cohorts, this has the effect of amortizing the initialization cost. Only the final stage of cohort construction, which involves reading forcing and spawning data, is executed when launching a new cohort.

7 Comparing blocking and non-blocking get operations

A significant part of initialing a cohort is spent *fetching* data from the manager. Assuming the number of age groups to match the number of workers

N, the speedup becomes

$$S = N \frac{I/(NC) + 1}{I/C + DN/C + 1}$$
 (3)

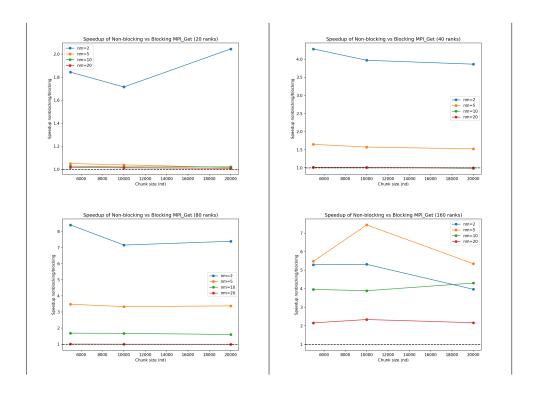
where the term D represents the time it takes to gather spawning data from a previous time cohort. The term DN/C is the relative cost of communicating the spawning data of the N previous cohorts relative to the compute time of a step. Clearly, communication flattens the speedup curve as N increases. In contrast to the initialization effect, the flattening gets more pronounced with a large number of workers.

One way to lessen the impact of communication is to allow communication and computation to overlap. Our library supports both synchronous and asynchronous get operations. The default mode to get data is blocking and in this case the retrieved data is ready when the call completes. Alternatively, the programmer may rely on getAsync calls in which case the programmer indicates his/her desire to fetch the data to be used sometimes in the future. Upon completion of getAsync, the data is not immediately available. startEpoch and endEpoch calls before, respectively after getAsync, determine the earliest moment the data can be requested and the latest time data must be available. The retrieved data are guaranteed to be available only when endEpoch is called. (An additional "flush" medthod can be invoked to synchronize operations within a period.)

In Fig. 7 we compare the execution time of MPI get operations using the blocking and non-blocking variants. Each test (implemented in testAsyncPutGet) involves reading N chunks (= number of workers) of nd values from rank 0 and summing the result. In the blocking test, the chunks are read one at a time, followed by a sleep operation lasting nm milliseconds and a sum operation over the chunk. In the nonblocking test, a big array is filled by reading the chunks asynchronously, followed by the sleep operation – these two operations are within a single epoch. The final step then involves summing up the values of the big array. The benefit of using non-blocking get calls is particularly apparent for large chunks nd and small amount of work (low nm).

8 Parallel Scaling for SEAPODYM

The parallelization strategies presented in the previous sections have been implemented into the SEAPODYM code. Below we describe a first scalibility test, involving 36 age groups (96 cohorts) advanced over the period 1979-1983



(60 time steps). All the runs (Fig. 4) were performed on REANNZ AMD Milan platform using a single node.

Note the better than linear scalability between 3-18 workers. Possible reasons for this behaviour are: (1) with more workers processes handle smaller amounts of data which may fit better in cache, (2) with more workers the scheduling overhead distributes work more evenly (reduction of load imbalance), (3) MPI may pipeline messages more efficiently with additional ranks and (4) disk and I/O contention may be decreased.

9 Summary and future work

A parallel library (seapodym-parallel) has been developed to parallelize the SEAPODYM code. While the library has been tested independently and a version of SEAPODYM now runs with this library, more checks are warranted. The SEAPODYM code comes in different flavours, parallelization has been added at present only to the version that evolves the fish densities in time. Extending parallelization to other SEAPODYM versions, including one that maximizes the likelihood function remains to be done.

The parallelization is based on a task farming approach with additional features: (1) tasks have sub-tasks (steps), (2) tasks can be started only when

seapodym_cohort speedup on AMD Milan CPU (36 age groups)

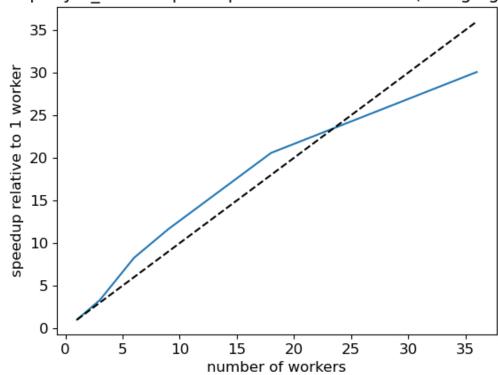


Figure 4: Parallel speedup relative to a single worker run for a SEAPODYM test.

other tasks' specific steps have completed and (3) data is sent to the manager at the end of each step. The manager stores and distributes the data to workers on request using one-sided MPI communication with passive targets. As such, the manager does not actively contribute to the data exchange, it is the workers who decide when to fetch and send data.

A conscious choice in the design of the task farming implementation is to have all data exchanges channeled through the manager. This means that the (spawning) data required by workers at the start of a new cohort cannot be directly received from other cohorts (or worers) but must go through the manager first. The rationale for this choice is to facilitate the implementation of parallelism in other versions of SEAPODYM.

Nevertheless, we demonstrated that parallel efficiency of 84 % can be achieved for 36 age groups and one worker per age group using blocking communication. The corresponding reduction of manager execution time was from 60 to 2 seconds, a \approx 30x speed improvement. Additional gains can potentially be attained by using non-blocking communication, a feature supported by seapodym-parallel. However, care should be taken to ensure correct synchronization. A common type of error is to consume the fetched data before the "get" operation has completed. Another pitfall is to fetch data from the manager that has not yet been filled in. Therefore, we recommend careful profiling, and replacing blocking by non-blocking calls only in the regions that are known to be performance intensive.