Avoiding Serialization Effects in Data / Dependency aware Task Parallel Algorithms for Spatial Decomposition.

Christoph Niethammer
and Colin W. Glass
and José Gracia
High performance computing center Stuttgart
University of Stuttgart
Email: {niethammer,glass,gracia}@hlrs.de

Abstract—Spatial decomposition is a popular basis for parallelising code. Cast in the frame of task parallelism, calculations on a spatial domain can be treated as a task. If neighbouring domains interact and share results, access to the specific data needs to be synchronized to avoid race conditions. This is the case for a variety of applications, like most molecular dynamics and many computational fluid dynamics codes. Here we present an unexpected problem which can occur in dependency-driven task parallelization models like StarSs: the tasks accessing a specific spatial domain are treated as interdependent, as dependencies are detected automatically via memory addresses. Thus, the order in which tasks are generated will have a severe impact on the dependency tree. In the worst case, a complete serialization is reached and no two tasks can be calculated in parallel. We present the problem in detail based on an example from molecular dynamics, and introduce a theoretical framework to calculate the degree of serialization. Furthermore, we present strategies to avoid this unnecessary problem. We recommend treating these strategies as best practice when using dependency-driven task parallel programming models like StarSs on such scenarios.

I. INTRODUCTION

Parallel programming is the key to modern day computing. A variety of new parallel programming models have come up in recent years, facilitating the often difficult task of parallelizing code. One of them is StarSs, a dependency-aware task based programming model which automatically extracts program parallelisation at the task level [1]. This is achieved by comparing memory addresses of input and output variables – thereby detecting data dependencies between tasks. Thus, the programmer need not deal with the actual parallelisation, but simply specifies chunks of work to be treated as tasks. The StarSs programming model is described in section [III].

In this paper, we present a scenario from everyday HPC computing – spatial decomposition with result sharing between neighbouring areas – where this elegant approach is led astray, resulting in a catastrophic failure of the intended parallelisation. Section [II] outlines the scope of applications, where this problem can occur, while section [IV] describes the actual case studied. In section [V] a theoretical framework on the speedup of a basic implementation as found in literature is introduced and section [VI] presents strategies to achieve the best possible parallelization by adhering to simple rules regarding the chronological ordering of task creation. The theoretical speedup and the improved strategies are both verified experimentally in section [VII].

II. SCOPE OF THE ADDRESSED PROBLEM

Many codes make use of spatial decomposition to achieve parallelism. In some cases, data of neighbouring areas is on a read-only basis. Since no data is written to neighbouring areas, all areas are independent from each other and therefore the risk of unwarranted dependencies not given. However, there are many cases where results are partly equivalent for neighbouring areas. To avoid calculating the same values twice, they are written to both areas. Examples herefor are e.g. Molecular Dynamics (MD) (Newton’s third law) and finite volume methods (flux across boundaries). These are examples of cases relevant to this paper. In both the abovementioned cases, force on a molecule and flux to/from a cell, only the net total is relevant. Therefore, the contributions of different neighbours are summed up, hereby avoiding unnecessary memory consumption. Thus, different neighbours will write to the same memory. Race conditions need to be avoided by preventing simultaneous write access. If we assume we treat the calculation of one area as one task in StarSs, different neighbours wanting to write to the same memory address will lead to the automatic detection of dependencies between these neighbours. Obviously, it is sufficient to avoid simultaneous write access. However, StarSs does not know that. Therefore, not only all neighbours wanting to write to one area need to wait, but all their neighbours have to wait on them in turn and so on. This leads to unnecessary serialization. The degree of serialization depends on the exact nature of the areas, definition of tasks and most important, on the order of task generation. As we will show on the case of the link-cell algorithm for MD, the standard implementation from literature leads in the worst case to complete serialization, or in other words, a maximum speedup of 1. By adhering
to simple strategies, the maximum speedup can be increased significantly.

III. THE STARSS PROGRAMMING MODEL

StarSs is a dependency aware task based parallel programming model. The basic idea is the extraction of parallelism out of a serial program using input and output dependencies. This frees the programmer from the difficult task of identifying parallel parts in his program, leaving it to the StarSs runtime. Currently StarSs implementations are available for C/C++ (Ompss) and Fortran (SMPSs).

In StarSs tasks are generated from functions or methods. To declare a function or method as a task, code annotations in form of pragmas (C/C++) or comments (Fortran) similar to OpenMP [2] are used. For each task the input and output parameters have to be defined. In C/C++ this requires additional pragma parameters, while in Fortran the parameters’ intent clauses are used. During runtime the actual dependencies between tasks are determined by the memory addresses of the passed parameters. In figure [1] an example C program is shown.

```c
#include <stdio.h>

int main() {
    int N;
    double *a, *b, *c, *d;
    ...
    #pragma css start
    unit_vec(N, 0, a);
    unit_vec(N, 1, b);
    unit_vec(N, 2, c);
    vec_add(N, c, b, c);
    vec_add(N, a, b, d);
    scalar_product(N, c, d, &s);
    #pragma css finish
    ...
}
```

Fig. 1. Simple C program calculating $s = \langle \vec{e}_2 \cdot \vec{e}_1, \vec{e}_3 \cdot \vec{e}_1 \rangle$ for the N dimensional unit vectors $\vec{e}_i$ with StarSs.

The StarSs runtime starts the program in a master thread. Every call to a function or method with a task annotation results in the creation of a task with the respective dependencies. This task is added to the task execution list and the master thread continues. Worker threads created by the runtime look through this list and search for tasks which have no unmet input dependencies. These tasks are ready to be executed.

The dependencies between the tasks can be represented by a directed acyclic graph (DAG) which is shown in figure 2. Tasks are the vertices of the DAG and edges are the dependencies. The direction of an edge is from output to input parameters and is always oriented downwards in the DAG. Numbers inside the vertices denote the chronological order of task creation in the program.

The StarSs model includes additional statements for runtime initialization/finalization and for the synchronization between the master and worker threads. For a detailed description we refer to the SMPSs manual [3].

IV. EXAMPLE: MOLECULAR DYNAMICS

A standard method to speed up Molecular Dynamics calculations for short range potentials is the link-cell (LC) method [4]. It allows to reduce the complexity of the search for interaction partners from $O(N^2)$ to $O(N)$ for $N$ particles [1]. The basic idea behind the LC method is to decompose the simulation area into smaller cells, which are of the size of the cutoff radius ($r_c$). Therefore, while searching for the interaction partners of one particle, only particles within the same and the neighbouring cells need to be considered. All other particles are beyond the cutoff radius $r_c$.

The number of required computations can be reduced further by considering Newton’s third law (action = reactio). For a given particle, only half the interactions need to be calculated. When the interaction of a particle A with another particle B is calculated, the result of the respective interaction of particle B with particle A is already known, so the second calculation can be omitted. Clearly, this requires writing to the own memory and to the memory of the interaction partner at the time of force calculation. But by this only half of the neighbouring cells have to be considered during calculation. The stencils for the 2D and 3D case are shown in Fig. 3.

In the following we consider the algorithm on the cell level. We define the term cell-cell interaction as the calculation of all interactions of the particles in one cell with all particles in another cell. A cell interacting with itself also qualifies as a cell-cell interaction. Where we need to distinguish explicitly between the interaction within one cell and between two differing cells, we denote this by the terms intra- and inter-cell interaction respectively.

1 A particle is small localized object with properties, e.g. an atom or a molecule.

2 A stencil is a geometric pattern, relative to the point of interest.
Although in principal it does not make any difference, in which order the interactions are calculated, the LC algorithm as described in literature follows a given procedure\[4\]: it starts with a cell and calculates the intra-cell interaction, followed by the inter-cell interactions, before moving on to the next cell.

Bringing this algorithm to the StarSs programming model is straightforward: every cell-cell interaction is a task. This provides sufficient work load for each task, while delivering a lot of tasks compared to treating all cell-cell interactions of one cell as a single task.

As we update both cells involved in a task, they are specified as inout dependency. This will protect the particle data from being updated by multiple tasks/threads simultaneously. The StarSs runtime will then create a directed acyclic graph (DAG) of the specified tasks taking into account the given dependencies and execute the program with the extracted parallelism.

As we will show in the following sections, the degree of parallelism will depend on the order of task creation and therefore on the way the stencil is evaluated for all elements.

V. EXAMINATION OF THE STRAIGHTFORWARD IMPLEMENTATION

In the StarSs task DAG the critical path length is the longest path from the start to the end of a program. The critical path length \( t_{cp} \) determines the maximal possible speedup \( S \) of a program, as the tasks in the path have to be executed in sequential order:

\[
S = \frac{t_s}{t_{cp}}
\]

where \( t_s \) is the sequential execution time of the program.

For the following considerations we assume that all tasks have equal execution time. Under this assumption, the critical path length can be given by the number of executed tasks instead of the overall duration of their execution. Looking at the DAG, we further neglect some of the dependencies as the static nature and periodicity of the stencil allows it.

As discussed earlier, the link-cell as described in literature calculates the intra-cell and then the inter-cell interactions. The stencil is moved over the cells first in x, then y and last in z direction. We will refer to this as the basic implementation. As we have four inter-cell interactions there exist in total \( 4! = 24 \) different permutations of the execution order of the tasks.

The achievable speedup can be expressed using three numbers: The number of stencil executions for the whole domain \( k \), the number of tasks in the single stencil \( n \) and the stencil displacement, \( \Delta \), which is the number of interactions to be calculated before the interaction with the next neighbour can be done:

\[
S(\Delta, k, n) = \frac{n k}{n + \Delta (k - 1)}.
\]

In the limit \( k \to \infty \) we get a speedup of

\[
S_{\text{max}}(\Delta, n) = \lim_{k \to \infty} S(\Delta, k, n) = \frac{n}{\Delta}.
\]

For the basic implementation, \( \Delta \) for the 2D stencil varies (depending on the permutation) between 2 and 5. It is 2 if the neighbour in x direction follows the intra-cell evaluation and 5 if it is the last interaction evaluated. For the 3D case \( \Delta \) is within \([2, 14]\) respectively.

Therefore, in both cases the worst case is thus \( \Delta = n \) and so by (3) no speedup is achieved at all! The best case is \( S_{\text{max}}(2, 5) = 2.5 \) for 2D and \( S_{\text{max}}(2, 14) = 7 \) for 3D.

Figure 4 shows a part of the real and simplified DAG for a suboptimal basic 2D stencil, which we refer to as the "naïve" version (see Fig 5(a)), applied to a \( 5 \times 5 \) cell domain with periodic boundary conditions. The real DAG was extracted with Temanejo[5].

\^Naïve because it is the geometrically most appealing stencil, but has a pretty terrible speedup.
However, if we disregard the basic stencil implementation and evaluate the cell-cell interaction with the neighbor in x direction first (see Fig. 5(c)), then $\Delta = 1$ and we get a DAG which can be seen as a stencil pipeline and which becomes the formula for the speedup of a pipeline

$$S = \frac{nk}{n + k - 1}$$

(4)

where now $n$ is the number of operations and $k$ is the pipeline depth. Here $k$ corresponds to the number of stencils which will be executed concurrently until the first stencil finishes. This is the optimal version for the stencil implementation and will at most result in a speedup of $k$. In 2D $k$ equals 5, in 3D 14, therefore even the optimal stencil implementation cannot be parallelized across an entire many-core node with 16 cores or more.

![Fig. 5. Different possible execution orders for cell interactions in the 2DStencil and their theoretical speedups: (a) naive: $S_{\text{max}} = 1.25$, (b) bad/worst case: $S_{\text{max}} = 1$, (c) optimal stencil: $S_{\text{max}} = 5$](image)

VI. IMPROVED STRATEGIES

As we have seen, the stencil implementation, with an outer loop over the cells and an inner loop over the stencil, runs into often severe speedup limitations, due to the unnecessarily generated dependencies. To overcome these limitations, different strategies can be applied:

1) The first way to improve the scalability is parallelizing the stencil execution by changing loop ordering. We will refer to this as “loop exchanged” (loopex) version later on. Instead of using an outer loop over all cells and an inner loop over the stencil pattern, the loops are exchanged and therefore the outer loop is over the stencil pattern and the inner loop over the cells. This strategy will reduce the dependencies between the tasks dramatically and allows the parallel execution of at least one row at once.

A smaller pitfall of this method is the direct dependencies in the loop directions (x,y and z) which can introduce again a serialization when it comes to neighbour dependencies. To circumvent this, a coloring scheme is used: Two-strided loops go over the domain preventing locks due to dependencies in the forward cell interaction steps for each of the directions x, y and z. For the coloring scheme used in the 2D example see Fig. 6. Note that a simple coloring scheme without loop reordering cannot extract the same amount of parallelism. This can be trivially seen by looking at figure 6.

The implementation of this optimization strategy clearly requires a bit of code overhead compared to the original implementation and especially the coloring scheme is an error prone part.

2) The second approach is a stencil with task nesting (currently only supported by Ompss [6]). In this version a loop over all intra-cell interactions is used. But instead of using a static loop to start the inter-cell interaction tasks recursion is used. After completed execution, each intra-cell interaction task calls a inter-cell task with one of its neighbours. This again calls the next inter-cell task, until all neighbours (whole stencil) are evaluated. By this dynamic approach, the DAG will be dynamically built during execution, which reduces the number of dependencies at runtime, allowing more tasks to be executed in parallel.

3) The last method is buffering the data from every neighbor and using a “reduce” step after the calculation to obtain the final result. Therefore, different tasks no longer write to the same memory and are independent from each other. This is a well known solution, but may lead to a dramatic increase in the overall memory consumption of the application. So it is very important to figure out if the application will become memory bound.

VII. EVALUATION

The evaluation of our theoretical prediction was done with a test kernel implementing the feature of the link-cell algorithm from MD as described in sections V and VI. The measurements were done on the HLRS systems Laki and Hermit using SMPSs 2.4 and the current Ompss version. While Laki is a NEC cluster with 8 core dual socket Xeon X5560 nodes, Hermit is a Cray XE6 system with 32 core dual socket Opteron 6276 nodes.

Before the actual evaluation, we measured the influence of the runtime scheduling system overhead. This is important, as we are only interested in the limitation caused by the structure of the task DAG. For this, we varied the execution time of the single tasks from 100ns to 100ms (see Fig. 7). Based on the

The used versions from the git developer repository were Nano 5eaf9dc11133365124927ee599fe84b283d8392 and Mercurium d41a4f63ac76881fa21200dd617a23a7f6689c.
results, a single task durations of 5ms was selected for the 3D and 10ms for the 2D examples. These lie well within the region where the runtime overhead can be neglected.

To prevent influences from boundary effects resulting in circular dependencies within the task DAG a $50 \times 50$ cell domain was used for the 2D and a $30 \times 10 \times 10$ cell domain for the 3D experiments.

First we implemented the basic algorithm of the 2D and 3D stencil with different interaction orderings and by this resulting in different displacements $\Delta$. As the results in Figure 8 show, the theoretical values from equation (2) are in excellent agreement with the experimental values.

![Fig. 7. Effect of the single task duration on the overall program runtime using Ompss.](image)

To evaluate our optimization strategies we implemented the loop exchange and nested versions for the 2D and 3D stencil. The results are shown in Figure 9.

![Fig. 8. Scaling for different displacements in the 2D stencil obtained with the SMPSs-2.4 runtime on a single HLRS Laki node.](image)

Figure 9 shows again perfect agreement with the predicted speedups for the stencil implementations (bad,opt), loop reordered (loopex) and nested for 2D and 3D on a single Hermit node.

VIII. CONCLUSION

In this paper we discussed serialization effects in data dependency driven task parallel algorithms for spatial decomposition. As an example, we showed that the implementation of the link-cell algorithm described in literature, with concurrent cell updates, results in a limited speedup. In this algorithm, the order in which the cells in the neighbour stencil are evaluated has a direct effect on the speedup. Starting from the task DAG and the critical path we derived the theoretical upper limit for the speedup and verified it experimentally. The cause for this limitation was identified to be the lack of a mutual exclusion or concurrent execution for tasks which do update the same data but do not depend on a specific execution order.

In general it can be seen that the stencil implementation has a major impact on parallelism and the programmer should pay attention to this. For a 3D simulation, the maximal speedup varies between 1 and 14 depending on the order in which the stencil is evaluated.

To achieve speedups beyond the theoretical limited given by (3), we implemented two other kernels resulting in a wider DAG: a loop and displacement based version as well as a version using nested tasks. Both versions are not limited in their theoretical speedup as long as the number of tasks is large enough. The applicability of those two techniques was again proven by experiments. The results show pretty good
scalability. The loop exchanged + coloring version scales perfectly up to 32 threads. The nested version scales up to 23 threads but shows weird behavior with more threads, which is probably caused by the runtime and under investigation.

As we have shown, dependency driven parallelization of codes based on spatial decomposition with data sharing, may easily result in severe and unnecessary speedup limitations. In the worst case, the attempted parallelization results in complete serialization. This can easily be avoided by adhering to simple rules, as put forth in this paper. Taking this advice into account the StarSs approach for dependency aware task based programming delivers good performance with little effort for the programmer. After discussing the results presented in this paper with the StarSs developers, the integration of a mutual exclusion clause is now planned.

ACKNOWLEDGMENTS

This work was supported by the European Community’s Seventh Framework Programme [FP7-INFRASTRUCTURES-2010-2] project TEXT under grant agreement number 261580 and project APOS under 277481.

REFERENCES

[1] J. Planas, R. M. Badia, E. Ayguadé, and J. Labarta, “Hierarchical task based programming with StarSs,” Int. J. of High Performance Computing Applications, vol. 23, no. 3, pp. 284–299, 2009.
[2] [Online]. Available: [http://openmp.org/wp/openmp-specifications/](http://openmp.org/wp/openmp-specifications/)
[3] “Smp superscalar (smpps) user’s manual version 2.4,” 2011.
[4] M. Griebel, T. Dornseifer, and T. Neunhoeffer, Numerical Simulation in Fluid Dynamics, a Practical Introduction. Philadelphia: SIAM, 1998.
[5] S. Brinkmann, C. Niethammer, J. Gracia, and R. Keller, “Temanejo - a debugger for task based parallel programming models,” in ParCo2011: Proceeding of the International Conference on Parallel Computing, 2011.
[6] A. Duran, E. Ayguadé, R. M. Badia, J. Labarta, L. Martinell, X. Martorell, and J. Planas, “Ompss: a proposal for programming heterogeneous multi-core architectures,” Parallel Processing Letters, vol. 21, no. 2, pp. 173–193, 2011.