Intervals and OpenMP: Towards an Efficient Parallel Result-Verifying Nonlinear Solver*

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Abstract. Nonlinear systems occur in diverse applications, i.e., in the steady state analysis of chemical processes. If safety concerns require the results to be provably correct then result-verifying algorithms relying on interval arithmetic should be used for solving these systems. Since such algorithms are very computationally intensive, parallelism must be exploited to make them feasible in practice. We describe our framework for the verified solution of nonlinear systems and our approach to parallelizing it with OpenMP. First numerical results show that the parallelization scheme is indeed successful but that the attainable speedup is limited for some unknown reason.

1 Introduction

Solving nonlinear systems is a recurring task in a variety of areas including robot motion planning, computer graphics, and steady state analysis of time-dependent phenomena, to name just a few. In this note we will consider an example from the latter class of problems, namely the search for singularities in a chemical process.

Let $\mathbf{p} \in \mathbb{R}^k$ denote the adjustable *parameters* controlling the process (such as heating, inflow concentrations, etc.), and let $\mathbf{x} \in \mathbb{R}^\ell$ describe its internal *state* (reaction rates, current temperature, etc.). Then the steady states of the process are described by a set of nonlinear equations, $\mathbf{f}(\mathbf{p}, \mathbf{x}) = \mathbf{0}$. Singularities mark those parameter values $\mathbf{p}^*$ where transitions from unique steady states $\mathbf{x} = \mathbf{x}(\mathbf{p})$ to multiple steady states occur. As multiple steady states can lead to fluctuations in the quality of the resulting product or can even cause severe damage to the facility, being able to *guarantee* the absence of singularities in the parameter range $[\mathbf{p}] = [\underline{p_1}, \overline{p_1}] \times \cdots \times [\underline{p_k}, \overline{p_k}]$ intended for operating the process is an important goal during process analysis and design.

One approach to determining the singularities first creates a larger system, $\mathbf{F}(\mathbf{z}) = \mathbf{0}$, by augmenting the system $\mathbf{f}(\mathbf{p}, \mathbf{x}) = \mathbf{0}$ with equations characterizing a

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specific type of singularity [1]. Here, $\mathbf{z} \in \mathrm{I\!R}^n$ comprises the variables $\mathbf{p}$ and $\mathbf{x}$, as well as auxiliary variables introduced during the augmentation, and $\mathbf{F}$ consists of the functions $\mathbf{f}$ and additional functions involving derivatives such as $\partial \mathbf{f} / \partial \mathbf{x}$; see [2] for more details.

In a second step, a result-verifying nonlinear solver is applied to the augmented system; see, e.g., [3]. These solvers are based on interval arithmetic [4] and are able to either *guarantee* that the system has no solution (i.e., there are no singularities of a specified type in the process), or to yield sharp bounds for the parameter combinations that might lead to singular behavior and therefore must be avoided.

Even if the result-verifying algorithms have been improved substantially during the last years, the solution of nonlinear systems remains a computationally intensive task, in particular for realistic problems with several dozens of parameters. Therefore, exploiting parallelism is essential for the successful solution of such problems.

In the following section we briefly describe some key features of our framework for the verified solution of nonlinear systems. Then we discuss how the solver's inherent coarse-grained parallelism can be exploited with OpenMP. In Sect. 4 we report on numerical experiments.

2 The Result-Verifying Solver

Our framework for the solution of nonlinear systems consists of three modules. The central **solver** module implements an interval–based branch–and–bound nonlinear solver. The augmented system to be solved is set up in a symbolic **preprocessing** step, and the function and derivative values needed in the **solver** are provided in a third **evaluation** module.

The basic branch–and–bound algorithm works as follows. Given some "box" $[\mathbf{z}] = [\underline{z_1}, \overline{z_1}] \times \ldots \times [\underline{z_n}, \overline{z_n}] \subset \mathrm{I\!R}^n$, evaluating the components F_i of the function $\mathbf{F}$ with appropriate interval-based methods yields intervals $[F_i]$ that are *guaranteed* to enclose the ranges of the F_i over the box $[\mathbf{z}]$, even in the presence of rounding errors. Therefore, if $0 \notin [F_i]$ for some i, then the system $\mathbf{F}(\mathbf{z})$ cannot have a zero in $[\mathbf{z}]$, and the box can be excluded from further consideration. If $0 \in [F_i]$ for all i then the system may, but need not, have a zero in $[\mathbf{z}]$. In this case the box is split into two (or more) subboxes, and the above test is applied recursively to these until the size of the boxes drops below a specified threshold.

Starting with an initial box corresponding to the intended ranges of the process parameters, this procedure results in a list of small boxes, which are guaranteed to contain all singularities that might be contained in the initial box. Several acceleration techniques are available $[2, 3, 5, 6]$ that, added to the basic branch–and–bound algorithm, enhance its efficiency. These techniques rely on Taylor expansions of the functions F_i and therefore require the (interval) evaluation of derivatives such as $\partial F_i / \partial \mathbf{z}$. Some of these techniques are also able to *prove* that the resulting boxes indeed do contain singularities.

The branch–and–bound algorithm lends itself naturally to a recursive implementation, as summarized in the following pseudocode.

```
function Check( [z] )   /* checks if the box [z] may contain a solution */
if 0 ∈ [F_i] for each i = 1,...,n   /* [F_i]: enclosure of the range of F_i over [z] */
        and none of the more sophisticated tests allows discarding [z]
then
    if [z] is "small enough"
        add [z] to the list of possible solutions
    else
        split [z] into two subboxes [z^(1)], [z^(2)]
        call Check( [z^(1)] )
        call Check( [z^(2)] )
```

Considering the dynamic call-tree as a whole, however, reveals a large amount of coarse-grained parallelism: All subboxes occurring at some fixed recursion depth can be handled independently from each other.

In addition to the coarse-grained inter-box parallelism, the work done for each box can also be spread over multiple processors. Here, medium-to-fine-grained parallelism is obtained by distributing the evaluation of the n functions F_i and the n^2 partial derivatives $\partial F_i/\partial z_j$, as well as the solution of linear systems occurring in the acceleration techniques, etc. Finally, the evaluation of each function bears limited potential for a third level of very fine-grained parallelism.

3 Exploiting the Coarse-Grained Parallelism with OpenMP

To exploit the inter-box parallelism, the dynamic call-tree is traversed in breadth-first order. Let L_k be a list containing the boxes at recursion depth k. Then, working on the boxes in L_k one-by-one (or in parallel), subboxes resulting from splitting a box are not handled immediately but placed in the list L_{k+1}, which is read only when the work on L_k is completed; see the following pseudocode.

```
L_0 = { the box [z] to be searched for singularities }
for k = 0, 1, ..., until L_k = ∅
    L_{k+1} = ∅
    for all boxes [z] in L_k (in parallel)
        if 0 ∈ [F_i] for each i = 1,...,n
                and none of the more sophisticated tests allows discarding [z]
        then
            if [z] is "small enough"
                add [z] to the list of possible solutions
            else
                split [z] into two subboxes [z^(1)], [z^(2)]
                add [z^(1)] and [z^(2)] to L_{k+1}
```

In a distributed memory environment with message passing [7, 8], the lists L_k may either be managed by a single processor using a standard master–slave approach, or the processors may work on private sub-lists following some "mediated" scheme [9]. Since the amount of work spent for a box can vary significantly, simply assigning the same number of boxes to each processor is not sufficient to keep the workload roughly balanced. The best strategy depends on the number of processors and on the relative speeds of communication and computation.

With shared memory and OpenMP [10, 11], the situation is much simpler. Distributing the work on L_k over several processors requires just parallelizing the "for all boxes $[\mathbf{z}] \in L_k$" loop and one additional synchronization to prevent the same L_{k+1} entry being written to by different processors. To account for the different amount of work associated with the boxes, we mimic the behavior of the master–slave approach by using scheduling with chunk size 1, i.e., the boxes are distributed one-by-one, and as soon as a thread has finished its work on a box it is assigned the next box.

As the OpenMP parallelization requires fewer changes to the code than an MPI-based version and in addition can be done incrementally, we have decided to first use OpenMP for the inter-box parallelism. If this approach cannot provide sufficient speedup we may switch to a hybrid parallelization scheme later, using MPI for the inter-box parallelism and OpenMP for distributing the work associated with a single box.

4 Numerical Results

The numerical experiments were performed on a Sun Fire 6800 server with 24 processors (900MHz) and 24GB of main memory running Solaris 9. The programs were written in C++ and compiled with version 5.5 of the Sun C++ compiler. This compiler provides support for interval arithmetic and allows intervals to be used together with OpenMP constructs.

Table 1 gives the timings for several versions of the code and different numbers of processors. The data refer to solving a system with 29 equations and 29 unknowns. This system results from augmenting the model of a hydration reactor with additional equations characterizing a saddle–node singularity; cf. [2] for details.

First, we note that compiling the same *serial* code with the `-xopenmp` flag slows down its execution by roughly 20%, due to some aggressive optimizations being disabled by this flag. Parallelizing the code requires some restructuring and in particular introduces additional data movements and constructor calls. Taking both effects together, the parallel code—run on a single processor—is about 1.3 times slower than the optimized serial code.

This performance loss is compensated when the parallel code is run on $p > 1$ processors. The data indicate that the scheduling scheme (`static, 1`) is superior to the standard scheme, which partitions the list L_k into p equally-sized chunks and assigns one chunk to each processor.

Table 1. Timings (minutes:seconds) for solving a system with $n = 29$ unknowns.

Program version	#Procs	Time	Speedup
Serial	1	17:32	
Serial, compiled with `-xopenmp`	1	21:18	
Parallel	1	22:55	1.00
Parallel, `schedule( static, 1 )`	2	13:52	1.65
Parallel, `schedule( static, 1 )`	3	11:20	2.02
Parallel, `schedule( static, 1 )`	4	10:46	2.13
Parallel, standard scheduling	4	11:41	1.96
Parallel, `schedule( dynamic, 1 )`	4	12:00	1.91

Surprisingly, `( static, 1 )` scheduling (i.e., thread j is assigned the tasks ℓ where $\ell \equiv j \bmod p$) seems at least competitive to `dynamic` scheduling, which in theory should adapt better to the different complexity of the parallel tasks. This indicates that the average complexity of each thread's tasks is approximately equal, so that the lower administrative overhead of `static` scheduling is dominating in the case $p = 4$. (For $p = 2$, `dynamic` scheduling is slightly better than the `static` scheme.)

Up to now, we cannot explain why the speedup seems limited to about 2, even if more than four processors are used. We are, however, confident that two of the obvious limiting factors do not apply in this case.

1. *Granularity too small.* For the hydration reactor, a total of 195 381 boxes was considered, yielding an average of more than 5 milliseconds per box. Thus, the granularity is indeed rather coarse-grained.
2. *Load imbalance.* Starting with the one-box list L_0, the lists L_k remain short throughout the first recursion levels. Thus, only a few processors can participate in the work, and as the work per box may vary significantly, there is the danger of severe load imbalance among the active processors.
   To assess these effects, the lengths of the lists L_k have been monitored. As can be seen from Fig. 1, the vast majority of the boxes (193 964 out of 195 381, or 99.3%) are handled at recursion levels $18, \ldots, 45$ in lists containing at least 400 boxes, and 90.1% of the boxes occur at levels $25, \ldots, 42$, where the list length even exceeds 4 000. Therefore it is *very* unlikely that load imbalance is a limiting factor for $p = 4$ processors.
   For this reason we have not yet employed loop-free scheduling mechanisms such as `taskq` available with KAI's Guide++ [12] and Intel's C++ 7.1 [13] compilers or a stack mechanism described by D. an Mey [14], but for higher numbers of processors these techniques may help reducing the speedup-limiting effects of the startup phase since they allow to exploit parallelism between independent boxes at *different* recursion depths. Then, we might also skip the first recursion steps and start with multiple boxes.

Experiments with simpler programs indicate that constructor calls for creating thread-local objects might be responsible for a large part of the inefficiency.

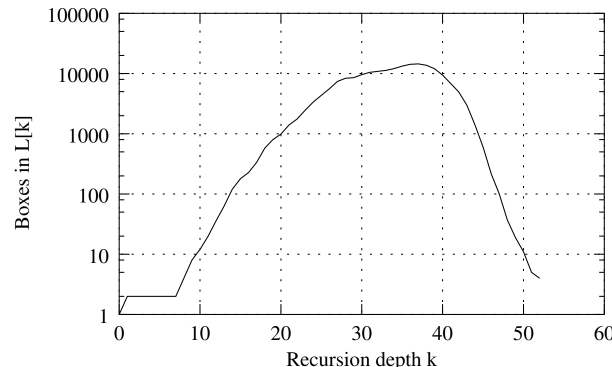

Fig. 1. Lengths of the lists L_k at different recursion depths k.

To further investigate this issue we are currently building another implementation of our framework relying on the KAI compiler for the OpenMP parallelization and on the freely available C-XSC library [15] for the interval operations.

5 Concluding Remarks

We have described a framework for the result-verifying solution of nonlinear systems arising in the analysis and design of chemical processes. An approach for coarse-grained OpenMP parallelization has been proposed, which in theory—due to rather long loops being distributed—is expected to yield almost perfect speedup on moderate numbers of processors. The approach also bears potential for additional levels of smaller-grained parallelism.

For reasons that are not yet fully understood, the speedups obtained in the experiments do not meet the theoretical predictions. We expect to obtain significantly better results with deeper insight into the behavior of the parallel code.

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