Using performance analysis tools for parallel-in-time integrators
Does my time-parallel code do what I think it does?

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Abstract While many ideas and proofs of concept for parallel-in-time integration methods exist, the number of large-scale, accessible time-parallel codes is rather small. This is often due to the apparent or subtle complexity of the algorithms and the many pitfalls awaiting developers of parallel numerical software. One example of such a time-parallel code is pySDC, which implements, among others, the parallel full approximation scheme in space and time (PFASST). Inspired by nonlinear multigrid ideas, PFASST allows to integrate multiple time-steps simultaneously using a space-time hierarchy of spectral deferred corrections. In this paper we demonstrate the application of performance analysis tools to the PFASST implementation pySDC. We aim to answer whether the code works as intended and whether the time-parallelization is as efficient as expected. Tracing the path we took for this work, we highlight the obstacles encountered, describe remedies and explain the sometimes surprising findings made possible by the tools. Although focusing only on a single implementation of a particular parallel-in-time integrator, we hope that our results and in particular the way we obtained them are a blueprint for other time-parallel codes.

Keywords Parallel-in-Time integration · PFASST · pySDC · Score-P · Python · Vampir · MPI · JUBE

1 Motivation

With million-way concurrency at hand, the efficient use of modern high-performance computing systems has become one of the key challenges in computational science and engineering. New mathematical concepts and algorithms are needed to fully exploit these massively parallel architectures. For the numerical solution of time-dependent processes, recent developments in the field of parallel-in-time integration have opened new ways to overcome both strong and weak scaling limit of classical, spatial parallelization techniques. In [14], many of these techniques and their properties are presented and the community website\(^1\) provides a comprehensive list of references and we refer to both sources for a detailed overview of time-parallel methods and their applications. While many ideas, algorithms and proofs of concept exist in this domain, the number of actual large-scale time-parallel application codes or even stand-alone parallel-in-time libraries showcasing performance gains is still small. In particular, codes which can deal with parallelization in time as well as in space are rare. At the time of this writing, three main, accessible projects targeting this area are xbraid, a C/C++ time-parallel multigrid solver [23], RIDC, a C++ implementation of the revisionist integral deferred correction method [27], and at least two different implementations of PFASST, the “parallel full approximation scheme in space and time”. One major PFASST implementation is written in Fortran (libpfasst), another one in Python (pySDC).

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\(^1\) https://www.parallel-in-time.org
When running parallel simulations, benchmarks or just initial tests, one key question is whether the code actually does what it is supposed to do and/or what the developer thinks it does. While this may seem obvious to the developer, complex codes (like PFASST implementations) tend to introduce complex bugs. Moreover, even if the workflow itself is correct and verified, the developer or user may wonder whether the code is as fast as it can be. Then, if all runs well, performing comprehensive parameter studies like benchmarking requires a solid workflow management and it can be quite tedious to keep track of what ran where and with what result. In order to address questions like these, advanced performance analysis tools can be used.

The performance analysis tools landscape is manifold. Tools range from node-level analysis tools using hardware counters like LIKWID [36] and PAPI [35] to tools intended for large-scale, complex applications like Scalasca [16]. There are tools developed by the hardware vendors, e.g. Intel VTune [28] or NVIDIA nvprof [5] as well as community driven open source tools and tool-sets like Score-P [22], TAU [32] or HPCToolkit [1]. Choosing the right tool depends on the task at hand and of course on the familiarity of the analyst.

It is the goal of this paper to present some of these tools and show their capabilities for performance measurements, workflows and bug detection for time-parallel codes like pySDC. Although we will, in the interest of brevity, solely focus on pySDC for this paper, our results and in particular the way we obtained them with the different tools can serve as a blueprint for many other implementations of parallel-in-time algorithms. While there are a lot of studies using these tools for classical parallelization strategies, their application in the context of parallel-in-time integration techniques is new.

Especially when different parallelization strategies are mixed, these tools can provide an invaluable help. We would like to emphasize that this paper is not about the actual results of pySDC or PFASST, like the application, the parallel speedup or the time-to-solution, but on the benefits of using performance tools and workflow managers for the development and application of a parallel-in-time integrator. One specific challenge in this regard, however, is the programming language of pySDC. Most tools focus on more standard HPC languages like Fortran or C/C++. With the new release of Score-P used for this work, Python codes can now be analyzed as well, as we will show in this paper.

In the next section we will briefly introduce the PFASST algorithm and describe its implementation in somewhat more detail. Then, Section 3 is concerned with the performance analysis tools used for this project, while Section 4 describes the endeavor of obtaining reasonable measurements from their application to pySDC, interpreting the results and learning from them. Section 5 contains a brief summary and an outlook.

2 A Parallel-in-Time Integrator

In this section we briefly review the collocation problem, being the basis for all problems the algorithm presented here tries to solve in one way or another. Then, spectral deferred corrections (SDC) are introduced, which then lead to the time-parallel integrator PFASST. This section is largely based on [4,33].

2.1 Spectral deferred corrections

For ease of notation we consider a scalar initial value problem on the interval \([t_\ell, t_{\ell+1}]\)

\[ u_\ell = f(u), \quad u(t_\ell) = u_0, \]

with \(u(t), u_0, f(u) \in \mathbb{R} \). We rewrite this in Picard formulation as

\[ u(t) = u_0 + \int_{t_\ell}^{t} f(u(s))ds, \quad t \in [t_\ell, t_{\ell+1}]. \]

Introducing \(M\) quadrature nodes \(\tau_1, \ldots, \tau_M\) with \(t_\ell \leq \tau_1 < \ldots < \tau_M = t_{\ell+1}\), we can approximate the integrals from \(t_\ell\) to these nodes \(\tau_m\) using spectral quadrature like Gauss-Radau or Gauss-Lobatto quadrature, such that

\[ u_m = u_0 + \Delta t \sum_{j=1}^{M} q_{m,j} f(u_j), \quad m = 1, \ldots, M, \]

where \(u_m \approx u(\tau_m), \Delta t \equiv t_{\ell+1} - t_\ell\) and \(q_{m,j}\) represent the quadrature weights for the interval \([t_\ell, \tau_m]\) with

\[ \Delta t \sum_{j=1}^{M} q_{m,j} f(u_j) \approx \int_{t_\ell}^{\tau_m} f(u(s))ds. \]

We can now combine these \(M\) equations into one system of linear or non-linear equations with

\[ (I_M - \Delta t Q f)(u_\ell) = u_0 \]  \hspace{1cm} (1)\]

where \(u_\ell = (u_1, \ldots, u_M)^T \approx (u(\tau_1), \ldots, u(\tau_M))^T \in \mathbb{R}^M, u_0 = (u_0, \ldots, u_0)^T \in \mathbb{R}^M, Q = (q_{i,j})_{i,j} \in \mathbb{R}^{M \times M}\) is the matrix gathering the quadrature weights, \(I_M\) is the identity matrix of dimension \(M\) and the vector function \(f\) is given by \(f(u) = (f(u_1), \ldots, f(u_M))^T \in \mathbb{R}^M\). This system of equations is called the “collocation problem” for the interval \([t_\ell, t_{\ell+1}]\) and it is equivalent to a fully implicit Runge-Kutta method, where the matrix \(Q\) contains the entries of the corresponding Butcher tableau.
We note that for \( f(u) \in \mathbb{R}^N \), we need to replace \( Q \) by \( Q \otimes I_N \).

Using SDC, this problem can be solved iteratively and we follow \[18,37,29\] to present SDC as preconditioned Picard iteration for the collocation problem (1). The standard approach to preconditioning is to define an operator which is easy to invert but also close to the operator of the system. One very effective option is the so-called "LU trick", which uses the LU decomposition of \( Q^T \) to define

\[
Q_\Delta = U^T \quad \text{for} \quad Q^T = LU,
\]

see [37] for details. With this we write

\[
(I_M - \Delta t(Q_\Delta f) (u^{k+1}_\ell) = u_0 + \Delta t((Q - Q_\Delta) f(u^k_\ell)) \tag{2}
\]
or, equivalently,

\[
u^{k+1}_\ell = u_0 + \Delta tQ_\Delta f(u^{k+1}_\ell) + \Delta t(Q - Q_\Delta) f(u^k_\ell)
\]

and the operator \( I - \Delta tQ_\Delta f \) is then called the SDC preconditioner. Writing (3) line by line recovers the classical SDC formulation found e.g. in [9].

2.2 Parallel full approximation scheme in space and time

We can assemble the collocation problem (1) for multiple time-steps, too. Let \( u_1, \ldots, u_L \) be the solution vectors at time-steps \( 1, \ldots, L \) and \( u = (u_1, \ldots, u_L)^T \) the full solution vector. We define a matrix \( H \in \mathbb{R}^{LM \times LM} \) such that \( Hu_0 \) provides the initial value for the \( \ell + 1 \)-th time-step. Note that this initial value has to be used at all nodes, see the definition of \( u_0 \) above. The matrix depends on the collocation nodes and if the last node is the right interval boundary, i.e. \( \tau_M = \ell_{\ell+1} \) as it is the case for Gauss-Radau or Gauss-Lobatto nodes, then it is simply given by

\[
H = (0, \ldots, 0, 1) \otimes (1, \ldots, 1)^T
\]

Otherwise, \( H \) would contain weights for extrapolation or the collocation formula for the full interval. Note that for \( f(u) \in \mathbb{R}^N \), we again need to replace \( H \) by \( H \otimes I_N \). With this definition, we can assemble the so-called "composite collocation problem" for \( L \) time-steps as

\[
C(u) := (I_{LM} - I_L \otimes \Delta t(QF - E \otimes H))(u) = u_0, \tag{4}
\]

with \( u_0 = (u_0, 0, \ldots, 0)^T \in \mathbb{R}^{LM} \), the vector of vector functions \( F(u) = (f(u_1), \ldots, f(u_L))^T \in \mathbb{R}^{LM} \) and where the matrix \( E \in \mathbb{R}^{L \times L} \) has ones on the lower sub-diagonal and zeros elsewhere, accounting for the transfer of the solution from one step to another.

For serial time-stepping each step can be solved after another, i.e. SDC iterations (now called "sweeps") are performed until convergence on \( u_\ell \), move to step 2 via \( H \), do SDC there and so on. In order to introduce parallelism in time, the "parallel full approximation scheme in space in time" (PFASST) makes use of an full approximation scheme (FAS) multigrid approach for solving (4). We present this idea using two levels only, but the algorithm can be easily extended to multiple levels. First, a parallel solver on the fine level and a serial solver on the coarse level are defined as

\[
P_{\text{par}}(u) := (I_{LM} - I_L \otimes \Delta t(QF - E \otimes H))(u),
\]

\[
P_{\text{ser}}(u) := (I_{LM} - I_L \otimes \Delta t(QF))(u).
\]

Omitting the term \( E \otimes H \) in \( P_{\text{par}} \) decouples the steps, allowing to perform SDC sweeps simultaneously on each step.

PFASST uses \( P_{\text{par}} \) as smoother on the fine level and \( P_{\text{ser}} \) as approximative solver on the coarse level. Restriction and prolongation operators \( I^H_{L} \) and \( I^H_{L} \) allow to transfer information between the fine level (indicated with \( h \)) and the coarse level (indicated with \( H \)). The approximate solution is then used to correct the solution of the smoother on the finer level. Typically, only two levels are used, although the method is not restricted to this choice. PFASST in its standard implementation allows coarsening in the degrees-of-freedom in space (i.e. use \( N/2 \) instead of \( N \) unknowns per spatial dimension), a reduced collocation rule (i.e. use a different \( Q \) on the coarse level), a less accurate solver in space (for solving (2) on each time-step) or even a reduced representation of the problem. The first two strategies directly influence the definition of the restriction and prolongation operators.

Since the right-hand side of the ODE can be a non-linear function, a \( \tau \)-correction stemming from the FAS is added to the coarse problem. One PFASST iteration is then comprised of the following steps:

1. Compute \( \tau \)-correction as

\[
\tau = C_H (I^H_h u^k_h) - I^H_h C_h (u^k_h).
\]

2. Compute \( u^k_{h+1} \) from

\[
P_{\text{ser}}(u_h^{k+1}) = u_{0,h} + \tau + (P_{\text{ser}} - C_H)(I^H_h u^k_h).
\]

3. Compute \( u^{k+1/2} \) from

\[
u^{k+1/2} = u^k + I^H_h (u^{k+1}_h - I^H_h u^k_h).
\]

4. Compute \( u^{k+1}_h \) from

\[
P_{\text{par}}(u_h^{k+1}) = u_{0,h} + (P_{\text{par}} - C_h)(u^{k+1/2}_h).
\]
We note that this "multigrid perspective" [3] does not represent the original idea of PFASST as described in [25, 10]. There, PFASST is presented as a coupling of SDC with the time-parallel method Parareal, augmented by the \( \tau \)-correction which allows to represent find-level information on the coarse level.

While conceptually the same, there is a key difference in the implementation of these two representations of PFASST. The workflow of the algorithm is depicted in Figure 1, showing the original approach in 1a and the multigrid perspective in 1b. They differ in the way the fine level communication is done. As described in [11], under certain conditions it is possible to introduce overlap of sending/receiving updated values on the fine level and the coarse level computation. More precisely, the "window" for finishing fine level communication is as long as two coarse level sweeps: one from the current iteration, one from the predictor which already introduces a lag of later processors (see Figure 1a). In contrast, the multigrid perspective requires updated fine level values whenever the term \( C_h(u_h^{k+1/2}) \) has to be evaluated. This is the case in step 1 and step 2 of the algorithm as presented before. Note that due to the serial nature of step 3, the evaluation of \( C_H(I_h H_h u_h^{k+1/2}) \) already uses the most recent values on the coarse level in both approaches. Therefore, overlap of communication and computation is somewhat limited: only during the time-span of a single coarse level sweep (introduced by the predictor) the fine level communication has to finish in order to avoid waiting times (see Figure 1b). However, the advantage of the multigrid perspective, besides its relative simplicity and ease of notation, is that multiple sweeps on the fine level for speeding up convergence, as shown in [4], are now effectively possible. This is one of the reasons this implementation strategy has been chosen for \texttt{pySDC}, while the original Fortran implementation \texttt{libpfasst} uses the classical workflow. Yet, while the multigrid perspective may alleviate the formal description of the PFASST algorithm, the implementation of PFASST can still be quite challenging, with PFASST are useful for the problem under consideration. Developers, on the other hand, can build on the existing infrastructure to implement new iterative methods or to improve existing methods by overriding any component of \texttt{pySDC}, from the main controller and the SDC sweeps to the transfer routines or the way the hierarchy is created. \texttt{pySDC}'s main features are [33]:

- available implementations of many variants of SDC, MLSDC and PFASST,
- many ordinary and partial differential equations already pre-implemented,
- tutorials to lower the bar for new users and developers,
- coupling to FEniCS and PETSc, including spatial parallelism for the latter
- automatic testing of new releases, including results of previous publications
- full compatibility with Python 3.6+, runs on desktops and HPC machines

The main website for \texttt{pySDC}\footnote{https://www.parallel-in-time.org/pySDC} provides all relevant information, including links to the code repository on Github, the documentation as well as test coverage reports. \texttt{pySDC} is also described in much more detail in [33].

The algorithms within \texttt{pySDC} are implemented using two "controller" classes. One only emulates parallelism in time, while the other one uses \texttt{mpi4py} [7] for parallelization in the time dimension with the Message Passing Interface (MPI). Both can run the same algorithms and yield the same results, but while the first one is primarily used for theoretical purposes and debugging, the latter makes actual performance tests and time-parallel applications possible.

We will use the MPI-based controller for this paper in order to address the questions posed at the beginning. To do that, a number of HPC tools are available which helps users and developers of HPC software to evaluate the performance of their codes and to speed up their workflows.

### 3 Performance Analysis Tools

Performance analysis is a crucial part in the development process of an HPC application. It usually starts with simply timing the computational kernels to see where the time is spent. To access more information and to determine tuning potential, more sophisticated tools are required. Several tools exist, for all kinds of measurement at all possible scales, from a desktop computer to the largest supercomputers in the world. We distinguish "profiling", which aggregates the performance
metrics at runtime and present statistical results, e.g., how often a function was called and how much time was spent there, and “event based tracing”, where each event of interest, like function enter/exit, messages sent/received etc. are stored together with a timestamp. Tracing conserves temporal and spatial relationships of events and is the more general measurement technique, as a profile can always be generated from a trace. The main disadvantage of tracing is that trace files can quickly become extremely large (in the order of terabytes) when collecting every event.

However, performance analysis tools can not only be used to identify optimization potential but also to assess the execution of the application on a given system with a specific tool-chain (compiler, MPI library, etc.), i.e. to answer the question: “Is my application doing what I think it is doing?” More often then not the answer to that question is “No”, as it was in the case we present in this work. Tools can pinpoint the issues and help to identify possible solutions.

3.1 Score-P and the Score-P ecosystem

The Score-P measurement infrastructure [22] is an open source, highly scalable and easy-to-use tool suite for profiling, event tracing, and online analysis of HPC applications. It is a community project to replace the measurement systems of several performance analysis tools and to provide common data formats to improve interoperability between different analysis tools build on top Score-P. Figure 2 shows a schematic overview of the Score-P ecosystem. Most common HPC programming paradigms are supported by Score-P: MPI (via the PMPI interface), OpenMP (via OPARI2 or the OpenMP tools interface (OMPT) [13]) as well as GPU programming with CUDA, OpenACC or OpenCL. Score-P offers 3 ways to measure application events: (i) Compiler instrumentation, where compiler interfaces are used to insert calls to the measurement system at each function enter and exit, (ii) a user instrumentation API, that enables the application developer to mark specific regions, e.g. kernels, functions or even loops, and (iii) a sampling interface which records the state of the program at specific intervals. All this data is handled in the Score-P measurement core where it can be enriched with hardware counter information from PAPI [35], perf or rusage. Further, Score-P provides a counter plugin interface that enables the user to define its own metric sources. The Score-P measurement infrastructure supports two modes of operation, it can generate event traces in the OFT2 format [12] and profiles in the CUBE4 format [30].

Score-P Python bindings

Traditionally the main programming languages for HPC application development have been C, C++ and Fortran. However, with the advent of high performance Python libraries in the wake of the rise of AI and deep learning, pure Python HPC applications are now a feasible possibility, as pySDC shows. Python has two built-in Performance Analysis Tools, called profile and cProfile. Though they allow profiling Python code, they do not support as detailed application analyses as Score-P does. Therefore, the Score-P Python bindings exist [17], which allow to profile and trace Python applications using Score-P.

The bindings use the Python built-in infrastructure that generates events for each enter and exit of a function. It is the same infrastructure that is used by the profile tool. As the bindings utilise Score-P itself, the different paradigms listed above can be combined and analysed even if they are used from within a Python application. Especially the MPI support of Score-P is
of interest, as **pySDC** uses **mpi4py** for parallelization in time. Moreover, as not each function might be of interest for the analysis of an application, it is possible to manually enable and disable the instrumentation or to instrument regions manually. These techniques can be used to control the detail of recorded information and therefore, to control the instrumentation overhead.

### 3.2 Cube

Cube is the performance report explorer for Score-P as well as for Scalasca (see below). The CUBE data model is a three-dimensional performance space consisting of the dimensions (i) performance metric, (ii) call-path, and (iii) system location. Each dimension is represented in the GUI as a tree and shown in three coupled tree browsers, i.e., upon selection of one tree item the other trees are updated. Non-leaf nodes of each tree can be collapsed or expanded to achieve the desired level of granularity. Figure 3 shows an overview of the Cube GUI. The metrics that are recorded by default contain the time per call, the number of calls to each function and the bytes transferred in MPI calls. Additional metrics depend on the measurement configuration. The CubeGUI is highly customizable and extendable. It provides a plugin interface to add new analysis capabilities [20] and an integrated domain-specific language called CubePL to manipulate CUBE metrics [31].

### 3.3 Scalasca

Scalasca [16] is an automatic analyzer of OTF2 traces generated by Score-P. The idea of Scalasca, as outlined in Figure 4, is to perform an automatic search for patterns indicating inefficient behavior. The whole low-level trace data is considered and only a high-level result in the form of a CUBE report is generated. This report has the same structure as a Score-P profile report, but contains additional metrics for the patterns that Scalasca detected. Scalasca performs three major tasks: (i) an identification of wait states, like the Late Receiver pattern shown in Figure 5 and their respective root-causes [39], (ii) a classification of the behavior and a quantification of its significance and (iii) a scalable identification of the critical path of the execution [2]. As Scalasca is primarily targeted at large-scale applications, the analyzer is a parallel program itself, typically running on the same resources as the original application. This enables a unique scalability to the largest machines available [15].

### 3.4 Vampir

Complementary to the automatic trace analysis with Scalasca - and often more intuitive to the user - is a manual analysis with Vampir. Vampir [21] is a pow-
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Fig. 5: Example of the Late Receiver pattern as detected by Scalasca. Process 0 posts the Send before process 1 posts theRecv. The red arrow indicates waiting time and thus a performance inefficiency.

Fig. 6: Vampir overview showing several of the displays provided by Vampir.

Fig. 6: Vampir overview showing several of the displays provided by Vampir. In contrast to traditional profile viewers, which only visualise the call hierarchy and function runtimes, Vampir allows the investigation of the whole application flow. Figure 6 gives an overview of some of the different views are supported by Vampir. The main view is the Master Timeline which shows the program activity over time on all processes. Further, there is the Process Timeline to display the application call stack of a process over time and a Communication Matrix to analyze the communication between processes. Any metrics collected by Score-P, from PAPI or counter plugins, can be analyzed across processes and time with either a timeline or as a heatmap in the Performance Radar. Recently added was the functionality to visualise I/O-events like reads and writes from and to the hard drive [26]. It is possible to zoom into any level of detail, which automatically updated all views and shows the information from the selected part of the trace. Besides opening an OTF2 file directly, Vampir can connect to VampirServer, which uses multiple MPI processes on the remote system to load the traces. This approach improves scalability and removes the necessity to copy the trace file. VampirServer allows the visualisation of traces from large-scale application runs with multiple thousand processes. The size of such traces is typically in the order of several Gigabyte.

3.5 JUBE

Managing complex workflows of HPC applications can be a complex and error-prone task and often results in significant amounts of manual work. Application parameters may change at several steps in these workflows. In addition, reproducibility of program results is very important but hard to handle when parametrisations change multiple times during the development process. Usually application-specific script based solutions are used to accomplish these tasks.

In contrast, the JUBE benchmarking environment provides a lightweight, command line based, configurable framework to specify, run and monitor the parameter handling and the general workflow execution. This allows a faster integration process and easier adoption of necessary workflow mechanics [24].

Parameters are the central JUBE elements and can be used to configure the application, to replace parts of the source code or to be used within other parameters. Also the workflow execution itself is managed through the parameter setup by automatically looping through all available parameter combinations in combination with a dependency driven step structure. For reproducibility, JUBE also takes care of the directory management to provide a sandbox space for each execution. Finally, JUBE allows to extract relevant patterns from the application output to create a single result overview to combine the input parametrization and the the extracted output results.

To port an application workflow into the JUBE framework, its basic compilation (if requested) and execution command steps have to be listed within a JUBE configuration file. To allow the sandbox directory handling, all necessary external files (source codes, input data and configuration files) have to be listed as well. On top the user can add the specific parametrization by introducing named key/value pairs. These pairs can either provide a fixed one to one key/value mapping or, in case of a parameter study, multiple values can be mapped to the same key. In such a case JUBE starts to spawn a decision tree, by using every available value combination for a separate program step execution. Figure 7 shows a simple graph example where three different program steps (pre-processing, compile and execution) are executed in a specific order and three different parameters (const.p1 and p2) are defined. Once the parameters are defined, they can be used to substitute parts of the
original source files or to directly define certain options within the individual program configuration list.

To take care of the typical HPC environment, JUBE also helps with the job submission part by providing a set of job scheduler specific script templates. This is especially helpful for scaling tests by easily varying the amount of compute devices using one parameter within the JUBE configuration file.

4 Results and Lessons Learned

In the following we consider the two-dimensional Allen-Cahn (or reaction-diffusion) equation

\[ u_t = \Delta u - \frac{2}{\epsilon^2} u(1 - u)(1 - 2u) \]  \hspace{1cm} (5)

with periodic boundary conditions and scaling parameter \( \epsilon > 0 \). The domain in space \([-L/2, L/2]^2\), \(L \in \mathbb{N}\), consists of \( L^2 \) patches of size \( 1 \times 1 \) and in each patch we start with a circle

\[ u_{i,j}(x) = \frac{1}{2} \left( 1 + \tanh \left( \frac{R_{i,j} - |x|}{\sqrt{2} \epsilon} \right) \right), \]

of initial radius \( R_{i,j} > 0 \) which is chosen randomly between 0.5\( \epsilon \) and 3\( \epsilon \) for each patch. For \( L = 1 \) this is precisely the well-known shrinking circle, where the dynamics is known and which can be used to verify the simulation [38]. By increasing the parameter \( L \), the simulation domain can be increased without changing the evolution of the simulation fundamentally. Figure 8 shows the evolution of the system with \( L = 4 \) from the initial condition in 8a to the 24th time-step in 8b.

We split the right-hand side of (5) and treat the linear diffusion part implicitly using the LU trick [37] and the nonlinear reaction part explicitly using the explicit Euler preconditioner. This has been shown to be the fastest SDC variant in [33] and allows us to use the mpi4py-fft library [8] for solving the implicit system, for applying the Laplacian and for transferring data between coarse and fine levels in space.

For the test shown here we use \( L = 4 \), \( N = 576 \) and \( \epsilon = 0.04 \), so that initially about 6 points resolve the interfaces, which have a width of about \( 7 \epsilon \). We furthermore use \( M = 3 \) Gauss-Radau nodes and \( \Delta t = 0.001 < \epsilon^2 \) for the collocation problem and stop the simulation after 24 time-steps at \( T = 0.024 \). The iterations are stopped when a residual tolerance of \( 10^{-8} \) is reached. For coarsening, only 96 points in space were used on the coarse level and, following [4], 3 sweeps are done on the fine level and 1 on the coarse one. All tests were run on the JURECA cluster at JSC [19] using Python 3.6.8 with the Intel compiler and (unless otherwise stated) Intel MPI. The code can be found in the projects/Performance folder of pySDC [34].

4.1 Scalability test with JUBE

In Figure 9 the scalability of the code in space and time is shown. While spatial parallelization stagnates at about 24 cores, adding temporal parallelism with PFASST allows to use 12 times more processors for an additional speedup of about 4. Note that using even more cores in time increases the runtime again due to a much higher number of iterations. Also, using more than 48 cores in space is not possible due to the size of the problem. We do not consider larger-scale problems and parallelization here, since a detailed performance analysis in this case is currently work in progress together with the EU Centre of Excellence “Performance Optimisation and Productivity” (POP CoE, see [6] for details).

The runs were set up and executed using JUBE and all relevant configuration files can be found in the project folder. We split the runs in two groups, one for space-parallel (blue/circles in Figure 9), one for space- and time-parallel runs (red/diamonds). Using the analyze function, a table of results (core counts, timings, iteration counts, etc.) has been generated automatically after each group finished. Using a simple Python script, these tables were read in again and processed into Figure 9. With JUBE, this workflow can be completely automated using only a few configuration files and a post-processing script.
4.2 Performance analysis with Score-P, Scalasca and Vampir

Performance analysis of a parallel application is not an easy task in general and with non-traditional HPC applications in particular. Python applications are still very rare in the HPC landscape and performance analysis tools (and performance analysts for that matter) are not fully prepared for that scenario. In this section we present the challenges we faced and the solutions we found to show what tools can do. We also would like to encourage other application developers not to resign on the first obstacles encountered when using these tools, but seek assistance from the developers and their system administrators in order to get reasonable and satisfactory results.

4.2.1 First measurement attempts

The first obstacle we encountered was that the Score-P Python bindings did not build for the tool-chain of Intel compilers and IntelMPI due to an issue with Intel compiler installation. We thus switched to GNU compilers and ParaStationMPI\(^3\). Using that we were able to obtain a first analysis result. However, this result was basically unusable as it showed all the tiny Python functions that could not be mapped to the actual program execution. To mitigate this we used filtering to reduce the unwanted Python routines and Score-P’s manual instrumentation which allows us to mark the interesting parts of the application.

Another issue we saw was incomplete recording of MPI point-to-point communication. The measurement showed the MPI send operations, but no receive operations. After digging into the source code of mpi4py we discovered that mpi4py uses matched probes and receives (MPI_Mprobe and MPI_Mrecv), which ensures thread safety. However, Score-P does not have support

\(^3\) [https://www.par-tec.com/products/parastation-mpi.html](https://www.par-tec.com/products/parastation-mpi.html)
Fig. 11: Cube Advisor showing the POP metrics for pySDC with ParaStationMPI.

| Metric                      | Value | Status  |
|-----------------------------|-------|---------|
| Parallel Efficiency         | 79%   | Good    |
| Load Balance                | 89%   | Very good |
| Communication Efficiency    | 89%   | Very good |
| Serialisation Efficiency    | 98%   | Very good |
| Transfer Efficiency         | 90%   | Very good |

for Mprobe/Mrecv in the released version, so we had to switch to a development version of Score-P, where the support was added for this project. Full support for matched communication is expected in an upcoming release of Score-P.

Using this setup we were able to get a first usable measurement. A Vampir screenshot of the entire application execution is shown in Figure 10. Even when enlarged properly, this can be a very discouraging view, as very little can be seen at a first glance (beside that around one third of the runtime is initialization). However, it is worth digging deeper with the tools at hand. Profiling showed that the algorithm outlined in Figure 1b worked as expected. We spend the vast majority of the computation time (70 %) in the fine sweep, and only about 3 % in the coarse sweep.

A high-level overview of the parallel performance can be gained with the Advisor mode of Cube [20]. This prints the efficiency metrics developed in the POP project for the entire execution or an arbitrary phase of the application. Figure 11 shows a screenshot of the Advisor result for the computational part of pySDC, i.e. omitting initialization and finalization.

### 4.2.2 Surprising findings

A “Parallel Efficiency”, which is composed of the product of “Load Balance” and “Communication Efficiency”, of 79 % is quite good, but worse than what we expected for this small test case. We know from the algorithm that there will be slight load imbalances, so a Load Balance of 89 % is understood. The “Transfer Efficiency” of 90 % means we lose 10% of the time due to inefficient communication. This was not expected so we assumed either an issue with the implementation of the algorithm or the system environment. A Scalasca analysis shows that the inefficiency originates from a “Late Receiver pattern” (see Figure 5) in the fine sweep phase and a “Late Broadcast” after each time step. A closer look with Vampir at just a single iteration, as shown in Figure 12, finally reveals the issue.

The implementation of pySDC uses non-blocking MPI communication in order to overlap computation and communication. However, Figure 12 clearly shows that this does not work as expected.

In the time of the analysis of the ParaStationMPI runs there was an update of the JURECA software environment which finally enabled the support of the Score-P Python wrappers for the Intel compilers and IntelMPI. So naturally we performed the same analysis again for this constellation, the one we originally intended to analyse. Surprisingly, the results looked much better now. The Cube Advisor analysis now showed nearly perfect Transfer Efficiency and subsequently a much improved Parallel Efficiency, see Figure 13.

Vampir further confirms a very good overlap of computation and communication, the way the implementation intended it to be.

### 4.2.3 Eye for the detail

Thus, the natural question to ask is where these differences between the exactly same code running on two different tool-chains come from. Further investigation showed that the installation of ParaStationMPI provided on JURECA does not provide an MPI progress thread, i.e. MPI communication cannot be performed asynchronously and thus overlapping computation and communication is not possible. IntelMPI on the other hand always uses a progress thread if not explicitly disabled via an environment variable. With a newly installed test version of ParaStationMPI, where an MPI progress thread has been enabled, the overlap of computation and communication is possible there, too. We see an on-par performance of pySDC using the new ParaStationMPI and IntelMPI.

Even though the overlap problem does not seem to be that much of an issue for this small test case, where just 10 % efficiency could be gained, we want to emphasize that these little issues can become severe ones when scaling up. Figure 15 shows the average time per call of the fine sweep. In the Intel case with overlap we see that the fine sweep time is very balanced across the processes (Figure 15b). In the ParaStationMPI case we see that the fine sweep time increases with the process number (Figure 15a). This problem will likely become

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4 https://pop-coe.eu/node/69
Fig. 12: Vampir visualization: user-defined regions, only a single iteration (ParaStation MPI, 4 processes in time, 1 in space).

Fig. 13: Cube Advisor showing the POP metrics for pySDC with IntelMPI.

worse when the problem size is increased, thus limiting the maximum number of processes that can be utilized.

5 Conclusion and Outlook

In this paper we performed and analyzed parallel runs of the PFASST implementation pySDC using the performance tools Score-P, CUBE and Vampir as well as the benchmarking environment JUBE. While the implementation complexity of a time-parallel method may vary, with standard Parareal being on the one side of the spectrum and methods like PFASST on the other, it is crucial to check and analyze the actual performance of the code. This is particularly true for most time-parallel methods with their theoretically grounded low parallel efficiency, since here problems in the communication can easily be mistaken for method-related shortcomings.

As we have shown, the performance analysis tools in the Score-P ecosystem can not only be used to identify tuning potential but also allow to easily check for bugs and unexpected behavior, without the need to do “print”-debugging. While methods like Parareal may straightforward to implement, PFASST is not, in particular due to many edge cases which the code needs to take care of. For example, in the standard PFASST implementation the residual is checked locally for each time-step individually, so that a process working on a later time-step could, erroneously, decide to stop although the iterations on previous time-steps still runs. Vice versa, when previous time-steps did converge, the processes dealing with later ones should not expect to receive new data. Depending on the implementation, those cases could lead to deadlocks (the “good” case) or to unexpected results (the ”bad” case), e.g. when one-sided communication is used, or other unwanted behavior. Many of these issues can be checked by looking at the gathered data after an instrumented run. How many messages were send, how many were received? Is there a wait for each non-blocking communication? Is the communication actually non-blocking or blocking, when it should be? Is the waiting time of the processes as expected? Are the number of solves/evaluations/iterations reasonable? These are potential questions which can be answered just by looking at the data generated by Score-P with Cube and Vampir. This does not, however, replace a careful design of the code, testing, benchmarking, verification and, sometimes, rethinking.
We saw for pySDC that already the choice of the MPI implementation can influence the performance quite severely, let alone the unexpected deviation from the intended workflow of the method. Performance tools as the ones presented here help to verify (or falsify) that the implementation of an algorithm actually does what the developers think it does. They can be used to identify problems in the communication, in the structure of the code and also in the computational parts, e.g. by revealing that due to a bug or an inefficient approach certain regions take much longer than necessary. While there is a lot of documentation on these tools available, it is extremely helpful and quite “accelerating” to get in touch with the core developers, either directly or by attending one of the tutorials e.g. provided by the VI-HPS through the Tuning Workshop series\(^5\). This way, many of the pitfalls and sources of frustration can be avoided and the full potential of these tools becomes visible.

In order to set up experiments using parallel codes in a structured way, be it for performance analysis, parameter studies or scaling tests, tools like JUBE can be used to ease the management of submission, monitoring and post-processing of the jobs. Again, time-parallel method make great candidates for such a tool due to their typically large number of parameters. Besides parameters for the model, the methods in space and time, the iteration and so on, the application of time-parallel methods in combination with spatial parallelism adds another level of complexity, which becomes manageable.

\(^5\) https://www.vi-hps.org/training/tws/tuning-workshop-series.html
with tools like JUBE. For this work, we have used JUBE only for setting up scaling tests with spatial and temporal parallelism to show its ease of use.

The scaling tests as well as the performance analysis made for this work are rather small compared to what joined space and time parallelism can do. The difference when using space-parallel solvers can be quite substantial for the analysis ranging from larger datasets for the analysis and visualization to more complex communication patterns. In addition, the issues experienced can differ, as we already see for the test case at hand. In Figure 16, we now use 2 processes in space and 4 in time. There is still unnecessary waiting time, but its impact is much smaller. This is because progress of MPI calls do not depend on the communicator and for each application of the spatial FFT solver, many MPI calls are made so that progress does happen even in the time-communicator. A more thorough and in-depth analysis of large-scale runs is currently under way together with the EU Centre of Excellence ”Performance Optimisation and Productivity” (POP CoE) and we will report on the outcome of this in a future publication. For this reason, we did not touch e.g. the question of optimal distributions of core in space and time both on the machine and for the method, although this is another highly relevant topic where performance tools can provide valuable and unmatched insights.

Acknowledgements

Parts of this work has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreements No 676553 and 824080. RS thankfully acknowledges the financial support by the German Federal Ministry of Education and Research through the ParaPhase project within the framework “IKT 2020 - Forschung für Innovationen” (project number 01HI15005A).

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