SPH-EXA: Enhancing the Scalability of SPH codes Via an Exascale-Ready SPH Mini-App

Danilo Guerrera¹, Aurélien Cavelan¹, Rubén M. Cabezón², David Imbert³ and Jean-Guillaume Piccinali⁴, Ali Mohammed¹, Lucio Mayer⁵, Darren Reed⁵, and Florina M. Ciorba¹

¹ Department of Mathematics and Computer Science, University of Basel, Switzerland
   {firstname.lastname}@unibas.ch,
² Scientific Computing Center (sciCORE), University of Basel, Switzerland,
   ruben.cabezon@unibas.ch,
³ XXX Software, YYY, ZZZ,
   contact@xxx.com,
⁴ Scientific Computing Support, Swiss National Supercomputing Centre, Lugano,
   Switzerland,
   jgp@cscs.ch,
⁵ Center for Theoretical Astrophysics and Cosmology, Institute for Computational Science, University of Zürich, Switzerland,
   {lmayer,reed}@physik.uzh.ch

Abstract Numerical simulations of fluids in astrophysics and computational fluid dynamics (CFD) are among the most computationally-demanding calculations, in terms of sustained floating-point operations per second, or FLOP/s. It is expected that these numerical simulations will significantly benefit from the future Exascale computing infrastructures, that will perform $10^{18}$ FLOP/s. The performance of the SPH codes is, in general, adversely impacted by several factors, such as multiple time-stepping, long-range interactions, and/or boundary conditions. In this work an extensive study of three SPH implementations SPHYNX [1], ChaNGa [2], and XXX [?] is performed, to gain insights and to expose any limitations and characteristics of the codes. These codes are the starting point of an interdisciplinary co-design project, SPH-EXA, for the development of an Exascale-ready SPH mini-app. We implemented a rotating square patch [4] as a joint test simulation for the three SPH codes and analyzed their performance on a modern HPC system, Piz Daint. The performance profiling and scalability analysis conducted on the three parent codes allowed to expose their performance issues [5], such as load imbalance, both in MPI and OpenMP. Two-level load balancing has been successfully applied to SPHYNX to overcome its load imbalance. The performance analysis shapes and drives the design of the SPH-EXA mini-app towards the use of efficient parallelization methods, fault-tolerance mechanisms, and load balancing approaches.
1 Introduction

 Faster, Higher, Stronger is the Olympic motto proposed by Pierre de Coubertin upon the creation of the Olympic Committee in 1894. One hundred and twenty-five years later, this motto’s fundamental idea represents somehow the computational effort done in high-performance computing and its scientific applications in the last decades, although re-phrased to Bigger, Faster, Longer. Numerical simulations grow more complex and, as a consequence, more computationally demanding, while addressing more detailed and intricated scientific questions. One paradigmatic example of this can be found in Computational Astrophysics. This is a field where our ability to understand complex processes, like those that form the stars or make them explode as Supernovas, is not only limited by our incomplete knowledge of the underlying physics, but also by our capability to harness the current computational power. Bigger simulations are needed to include all relevant processes for the scenario at study. This implies that they should be faster to compensate for the additional computational expense that detailed physics entail. Finally, we are usually interested in longer simulations, that allow a consistent study of a process and its consequences ab initio, but also in terms of resilience, so that the simulations can perform their calculations accurately even when external factors, like silent data corruption, occur.

The SPH-EXA project was born with these ideas in mind: developing a mini-app to perform Smoothed Particle Hydrodynamics (SPH) simulations that are Bigger, Faster, Longer. To that extent, we brought together a group of Computational Scientists, Astrophysicists, and Fluid Dynamics experts to share their respective knowledge and find a common ground where the SPH-EXA mini-app could be built, targeting the upcoming Exascale infrastructures. In this respect, this is a co-design project in terms of interdisciplinarity.

– Contribution details

Interdisciplinary co-design and co-development is the recommended approach for developing a mini-app, to leverage the involvement of the developers of the parent codes in the mini-app design and implementation process [10]. The SPH-EXA project follows such recommendation, as both computer scientists and computational scientists (that developed the three parents codes) are part of the team working on the SPH-EXA mini-app. The development has thus followed a building blocks approach, with the resulting mini-app being shaped while adding new features both on the SPH side (e.g., SPH operands) and the HPC side (e.g., adopting a specific data structure or parallel algorithm). Lighter than production codes, mini-apps are algorithm oriented and allow modifications and experiments [9]. Replacing a data structure or a specific algorithm can be easily done without additional cost. Immediate results and computation time obtained by the mini-app allow anyone to make is own idea about the efficiency of one or an other algorithm.

Mini-apps have been a privileged area for high performance computing [9,10]. single function can be evaluated using different strategies leading to different performances, even if the physical result is still the same. These evaluation strategies
may rely on vectorisation, node level multi-threading, cross-node parallelism. Their efficiency also depends on platforms configuration: presence of accelerators, CPU generation, interconnection network. Therefore, a mini-app is a perfect portable sandbox to optimize a numerical method such as the SPH method.

Mini-apps also help testing new technical features which could not be available in large production codes. For example, the three SPH codes are implemented with different languages, are built with different compilers versions, rely on different dependencies, and targets different operating systems and platforms. Therefore, last SIMD instructions, last C++ standard, or a new library, may not be tested in all production codes without a high development cost to adapt these codes. A freshly designed mini-app does not suffer from maintenance costs and allows estimating potential benefits of new features before implementing them in production context.

Parts of the mini-app can be organized as independent libraries to help integration of new features in production code. This organization avoids implementing two times an interesting feature: one time in the mini-app, one other time in the production code. Interfaces to this library should be generic enough to work with any production code.

The mini-app introduced in this work is still in its early stages and offers limited capabilities for SPH simulations. As it has been designed with the goal to allow interfacing with production code and as a testing ground for new features, it is expected to benefit from the ideas and interest of the SPH community. A request for a new test cases could turn into the development of a missing SPH-related functionality and allow the exploration of alternative solutions on the HPC side.

2 Related Work

Mini-apps or proxy-apps have received great attention in recent years, with several projects being developed or under development. The Mantevo Suite [10], from the high performance computing (HPC) community, and developed at Sandia National Laboratory is one of the first large mini-app set. It includes mini-apps that represent the performance of finite-element codes, molecular dynamics, and contact detection, to name a few.

Another example is CGPOP [16], a mini-app from the oceanographic community, that implements a conjugate gradient solver to represent the bottleneck of the full Parallel Ocean Program application. CGPOP is used for experimenting new programming models and to ensure performance portability.

At Los Alamos National Laboratory, MCMini [17] was developed as a co-design application for Exascale research. MCMini implements Monte Carlo neutron transport in OpenCL and targets accelerators and coprocessor technologies.

The CESAR Proxy-apps [18] represent a collection of mini-apps belonging to three main fields: thermal hydraulics (for fluid codes), neutronics (for neutronics codes), and coupling and data analytics (for data-intensive tasks).
One of the motivation behind the European ESCAPE project [19] is to define and encapsulate the fundamental building blocks (‘Weather & Climate Dwarfs’) that underlie weather and climate services. This serves as a prerequisite for any subsequent co-design, optimization, and adaptation efforts. One of the ESCAPE outcomes is Atlas [20], a library for numerical weather prediction and climate modeling, with the primary goals to exploit the emerging hardware architectures forecasted to be available in the next few decades. Interoperability across the variegated solutions that the hardware landscape offers is a key factor for an efficient software and hardware co-design [21], thus of great importance when targeting Exascale systems.

Similar to these works, the creation of a mini-app directly from existing codes rather than the development of a code that mimics a class of algorithms has been recently discussed [22]. A scheme to follow was proposed therein that must be adapted according to the specific field the parent code originates in. To maximize the impact of a mini-app on the scientific community, it is important to keep the build and run system easy enough, to not discourage potential users. The building should be kept as simple as a Makefile and the preparation of the run to a handful of command line arguments: “if more than this level of complexity seems to be required, it is possible that the resulting MiniApp itself is too complex to be human-parseable, reducing its usefulness.” [22]. The present work introduces the interdisciplinary co-design of an SPH-EXA mini-app with three parent SPH codes originating in the astrophysics academic community and the industrial CFD community. This represents a category not discussed in [22].

Skeleton applications, the name used to refer to reduced versions of applications that produce the same network traffic of the full ones, are of interest to model the performance of networks through simulation. An auto-skeletonization approach has recently been proposed to auto-skeletonize a full application via compiler pragmas: an interesting idea to produce flexible skeletons, that serve as a tool to study balanced Exascale interconnect designs [23]. Such a skeletonization approach may be of interest in annotating a full application to obtain a mini-app that reflects exactly the corresponding production code.

3 Co-Design of the Mini-App

Being optimization critical to achieve the scalability needed to exploit Exascale computers, the long-term goal of SPH-EXA [6] is to provide a parallel, optimized, state-of-the-art implementation of basic SPH operands with classical test cases used by the SPH user community. This can be implemented at different levels: employing state-of-the-art dynamic load balancing algorithms, fault-tolerance techniques, programming languages, tools, and libraries.

In reaching this goal, interdisciplinary co-design and co-development is the recommended approach for developing a mini-app, to leverage the involvement of the developers of the parent codes in the mini-app design and implementation process [10].
Thanks to the co-design and co-development, it is straightforward in the analysis phase to individuate the common and best features of the state-of-the-art parent codes, with a focus on the physics therein, highlighted in Table 1. In the first stage the focus has been on implementing a vanilla SPH solver, representing the basis of the future mini-app. The momentum equation implemented can be found in [1], while the artificial viscosity has been derived from [25]. To calculate the value of the next timestep the Courant condition is applied; the updates of the positions and the energy follow a Press and Adams-Bashforth method, respectively. While not all existing techniques and algorithms need to be implemented, some of them, such as the SPH interpolation kernels, can be later developed as separate interchangeable modules. In that sense, Table 1 shows also the domain science techniques and algorithms that the mini-app features.

Simultaneously to the effort on the SPH solver implementation, HPC related aspects regarding the development of the code have been addressed. The solver has evolved from being sequential, to having intra-node parallel capabilities via OpenMP, to inter-node parallelism via MPI.

The goal is to provide a reference implementation in MPI+X. MPI is the de facto standard for HPC applications, due to the lack of a valid alternative for the inter-node communication. The MPI+OpenMP programming model represents a starting point, since it does not fully exploit the heterogeneous parallelism in the newest architectures. While OpenMP 4.5 [26] offers support for accelerators, in the meanwhile other languages directly targeting accelerators have being proposed and accepted by the community, such as OpenACC (a directive-based programming model targeting a CPU+accelerator system, similar to OpenMP), CUDA (an explicit programming model for GPU accelerators) and OpenCL. In programming models, research has been focusing on the efficient use of intra-node parallelism, able to properly exploit the underlying communication system through a fine grain task-based approach, ranging from libraries (Intel TBB [27]) to language extensions (Intel Cilk Plus [28] or OpenMP), to experimental programming languages with focus on productivity (Chapel [29]). Kokkos [30] offers a programming model, in C++, to write portable applications for complex many-core architectures, aiming for performance portability. HPX [31] is a task-based asynchronous programming model that offers a solution for homogeneous execution of remote and local operations. It is planned to port the mini-app to at least one of the paradigms described, between the ones described previously to explore their efficiency and potential on Exascale ready machines.

Then, Table 2 reveals the computer science-related similarities and differences of the codes, i.e., algorithms, techniques, and other implementation-specific choices. Each code has a different history, has been used for different purposes, and, therefore, uses different approaches in its simulations. For example, all applications use standard checkpoint/restart mechanisms to enable fault-tolerance when executing at scale. Yet, they all use different domain-decomposition methods and scheduling techniques. It is important to note that such features can dramatically affect the scalability of the application, as shown in Section 4.
Table 1: Differences and similarities between SPHYNX, ChaNGa, XXX, and the SPH-EXA mini-app

| SPH Code | Code Version | Kernel Calculation | Volume Gradients | Mass of Elements | Time-Stepping | Neighbour Discovery | Self-Gravity |
|----------|---------------|---------------------|-----------------|-----------------|---------------|---------------------|--------------|
| SPHYNX   | 1.3.1         | Sinc IAD Generalized | Equal or Variable | Global Tree Walk | Multipoles (4-pole) |
| ChaNGa   | 3.3           | Wendland, M4 spline | Kernel derivatives | Standard | Equal or Variable | Individual Tree Walk | Multipoles (16-pole) |
| XXX      | 17.6          | Wendland Kernel derivatives | Standard | Equal or Adaptive Global | Tree Walk | No |
| mini-app | 0.5           | Sinc, Wendland, IAD (in development) | Generalized (in development) | Equal or Variable Global | Tree Walk | Multipoles (16-pole) (in development) |

Table 2: Different and similar computer science-related aspects between SPHYNX, ChaNGa, XXX, and the SPH-EXA mini-app

| SPH Code | Domain Load Checkpoint- Precision Language Parallelization #LOC Code Decomposition Balancing Restart |
|----------|---------------------------------------------|-------------------------------------------------|-----------------------------------|----------------|-------------------|----------------|----------------|
| SPHYNX   | Straightforward None (static) Yes 64-bit Fortran 90, MPI+OpenMP 25,000 |
| ChaNGa   | Space Filling Curve Dynamic Yes 64-bit C++ MPI 37,000 |
| XXX      | Orthogonal Recursive Bisection Local-Inner-Outer Yes 64-bit Fortran 90 MPI |
| mini-app | HTree based None (static) No 64-bit C++ MPI+OpenMP 3,500 |

In its current status, the mini-app provides two different implementations for the SPH kernel, namely Sinc, whose benefits are described in [32] and Wendland, originally presented in [33]. The Sinc functions has been defined as:

\[
W_n^s(v, h, n) = \frac{B_n}{h^d} S_n\left(\frac{\pi}{2} v\right) \text{for } 0 \leq v \leq 2, \tag{1}
\]

where \(S_n(.) = sinc_n(.)\), and where n is the index of the kernel and \(B_n\) a normalization constant. The function \(sinc(\frac{\pi}{2} v) = \frac{\sin(\frac{\pi}{2} v)}{\frac{\pi}{2} v}\), widely used in spectral theory, has been chosen.

The Wendland kernel instead, has been defined as:

\[
W(v, h, n) = \begin{cases} 
\sigma_W (1 - \frac{v}{2})^4 (2v + 1) & \text{for } 0 \leq v \leq 2, \\
0 & \text{for } v > 2,
\end{cases} \tag{2}
\]

where the normalization \(\sigma_W\) is \(21/(16\pi)\).

Additional kernels can be plugged in, upon implementation (in the above cases 6 LOC only), proving how such a mini-app can result useful in allowing easy and quick modification to experiment alternative solutions.

On current HPC systems it is common to have more than one programming environment installed. On Piz Daint (at least) 4 compiler suites (Intel, GNU, PGI and Cray) are available to the users together with communication and scientific libraries tuned by Cray and CSCS. As the programming environment and operating system gets updated regularly, it is considered good practice to continuously test that a code repeatedly builds and runs correctly independently of any given change to the software stack and/or code base. In order to achieve this goal of continuous integration, all involved steps of the project have been designed to run fully automated with Jenkins. As a result, the mini-app has been tested with the following compilers: gcc/6.2.0, gcc/7.3.0, gcc/8.2.0, intel/18.0, intel/19.0, cce/8.6.1, cce/8.7.6, pgi/18.7 and clang/7.0.0. While continuous testing
gives information about the current state of the code, it also allows to quickly pinpoint sources of problems and to apply changes when needed. History on the information about previous failures or success can easily be accessed on the Jenkins dashboard. The regression tests for the mini-app have been generated using the ReFrame framework.

Jenkins is a self-contained, open source automation server which can be used to automate all sorts of tasks related to building, testing, and delivering or deploying software.

ReFrame is a framework for writing regression tests for HPC systems. The goal of this framework is to abstract away the complexity of the interactions with the system, separating the logic of a regression test from the low-level details, which pertain to the system configuration and setup. This allows users to write easily portable regression tests, focusing only on the functionality.

Regression tests in ReFrame are simple Python classes that specify the basic parameters of the test. The framework will load the test and will send it down a well-defined pipeline that will take care of its execution. The stages of this pipeline take care of all the system interaction details, such as programming environment switching, compilation, job submission, job status query, sanity checking and performance assessment.

Writing system regression tests in a high-level modern programming language, like Python, poses a great advantage in organizing and maintaining the tests. Users can create their own test hierarchies, create test factories for generating multiple tests at the same time and also customize them in a simple and expressive way. Of the three SPH codes, two are in Fortran 90 (SPHYNX and XXX) and one in C++ (ChaNGa); note that the future version of XXX in development is in C++. As a compiled static language, both C++ and Fortran allows a close management of memory and higher performance than Python, Matlab, or R [14].

Fortran is a procedural language suffering from severe maintenance issues: global variables, complex divisions, interlinking. Therefore, Fortran code is hard to modify, unit test, and extend [14]. Fortran 2003 goal was to become object-oriented; but in 2017, the 2003 standard was still not completely supported by all compilers [15]. On the contrary, C++ is close to the hardware and also completely supports object-oriented [14]. That is why C++ has been chosen as the mini-app language.

C++ also supports header-only libraries which does not require a software factory. Header files just have to stand near the client "cpp" files. This is an asset to spread more easily the mini-app in the community.

Moreover, header-only libraries can completely benefit from template meta programming to perform operations or detect errors during compile-time instead of runtime. This also leads to higher runtime performance [13]. Template meta programming allows generating custom code based on policy choices. The mini-app introduced in this work is still in its early stages and offers limited capabilities for SPH simulations. As it has been designed with the goal of allowing an easy interface with production codes and as a testing ground for new features,
it is expected to benefit from the ideas and interests of the SPH community. A request for a new test case could turn into the development of a missing SPH-related functionality and allow the exploration of alternative solutions on the HPC side.

4 Status of the Mini-App

The complexity of the scenarios simulated in CFD and Astrophysics usually forbids the possibility to perform simulations with continuously increased resolution and different codes, so that a convergence to zero differences on the results can be found. Often, it is neither possible nor reasonable to obtain sufficient computational resources to perform simulations that are “converged” throughout the computational domain in a mathematical sense. It is much more important to limit the deviations in under-resolved regimes by enforcing fundamental conservation laws. Additionally, the emergence of stochastic processes, like turbulence, renders the pursuit for mathematical convergence impossible, yet still constrained by conservation laws. As a consequence, overall physics properties of the simulated scenarios remain robust, even if slightly different results are obtained when using different codes to “solve” the same set of equations. Therefore, comparing results of different hydrodynamical codes to the same initial conditions has been proved to be highly beneficial to gain understanding in complex scenarios, in the behavior of the codes, and to discover strengths and weaknesses of those. These comparisons are not uncommon in CFD and Astrophysics [7,8,11,12]. The SPH codes comparison presented herein is in this spirit, yet with a focus on performance-related aspects from computer science.

| Test Simulation         | Description                  | Domain Size | Simulation Length | SPH Code              | Test Platform |
|-------------------------|------------------------------|-------------|-------------------|-----------------------|---------------|
| Rotating Square Patch   | Rotation of a free-surface 3D, 10^6 particles 40 time-steps |             | SIHYNX, ChaNGa    | XXX, mini-app         | Piz Daint     |

The common test case chosen to validate the results obtained through the mini-app against the ones of the parent codes is the Rotating Square Patch. This test was first proposed by [4] as a demanding scenario for SPH simulations. The presence of negative pressures stimulates the emergence of unphysical tensile instabilities that destroy the system. Nevertheless, these can be suppressed either using a tensile stability control or increasing the order of the scheme [3]. As a consequence, this is a commonly used test in CFD to verify hydrodynamical codes, and it is employed in this work as a common test for the three codes.

The setup here is similar to that of [4], but in 3D. The original test was devised in 2D, but the SPH codes used in this work normally operate in 3D. To use a test that better represents the regular operability of the target codes, the
A square patch was set to [100 x 100] particles in 2D and this layer was copied 100 times in the direction of the Z-axis. This results in a cube of $10^6$ particles that, when applying periodic boundary conditions in the Z direction, is equivalent to solving the original 2D test 100 times, while conserving the 3D formulation of the codes. The initial conditions are the same for all layers, hence they depend only on the X and Y coordinates. The initial velocity field is given such that the square rotates rigidly:

$$v_x(x, y) = \omega y; \quad v_y(x, y) = -\omega x,$$

where $v_x$ and $v_y$ are the X and Y coordinates of the velocity, and $\omega = 5$ rad/s is the angular velocity. The initial pressure profile consistent with that velocity distribution can be calculated from an incompressible Poisson equation and expressed as a rapidly converging series:

$$P_0 = \rho \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{-32\omega^2}{m\pi^2 \left( \left( \frac{m\pi}{L} \right)^2 + \left( \frac{n\pi}{L} \right)^2 \right)} \times \sin \left( \frac{m\pi x}{L} \right) \sin \left( \frac{n\pi x}{L} \right),$$

where $\rho$ is the density and $L$ is the side length of the square.

### 4.1 Experimental Results

**System overview - Piz Daint** The experiments were performed on the hybrid partition of the Piz Daint supercomputer using PrgEnv-Intel, Cray MPICH 7.7.2 and OpenMP 4.0 (version 201611). At the time of writing, this supercomputer consisted of a multi-core partition of more than 1,600 Cray XC40 nodes with two Intel Xeon E5-2695 v4 (codename Broadwell) processors, which were not used in this study, as well as the hybrid partition of more than 5,000 Cray XC50 nodes. These hybrid nodes are equipped with an Intel E5-2690 v3 CPU (codename Haswell) and a PCIe version of the NVIDIA Tesla P100 GPU (codename Pascal) with 16 GB second generation high bandwidth memory (HBM2). The nodes of both partitions are interconnected in one fabric based on Aries technology in a Dragonfly topology.

**Runtime evaluation** Figure 1 shows the average execution time per timestep (in seconds), out of 40 time-steps, on Piz Daint up to 32 nodes (i.e., 384 cores). The SPH-EXA mini-app is able to complete a timestep circa 6 times faster than the production codes, with different number of nodes. Indeed, the proposed mini-app has been designed from scratch with performance in mind. The straightforward SPH implementation, together with the minimal and modern code style lead to increased performance compared to the legacy codes. However, the SPH-EXA mini-app is currently limited to the bare SPH implementation.

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6. [https://www.cscs.ch/computers/piz-daint/](https://www.cscs.ch/computers/piz-daint/)

7. [http://www.cray.com/sites/default/files/resources/CrayXCNnetwork.pdf](http://www.cray.com/sites/default/files/resources/CrayXCNnetwork.pdf)
Figure 1: Average execution time per timestep (out of 40 timesteps) of ChaNGa (12 OpenMP tasks and 1 MPI rank per node), SPHYNX (12 OpenMP tasks and 1 MPI rank per node), XXX (12 MPI ranks per node) and SPH-EXA mini-app (12 MPI ranks per node), in function of the number of nodes used (1 node = 12 cores) on Piz Daint.

**Strong scaling evaluation** The measure of parallel scalability indicates how efficiently an application is in utilizing an increasing number of processing elements. In the case of strong scaling the problem size is fixed, while the number of processing elements increases. Its goal is to find a “sweet spot”, where the computation completes in a reasonable amount of time, while not wasting too many cycles due to the parallel overhead. The applications exhibit good strong scaling up to 16 compute nodes. The scaling stalls when there are not enough particles/core (typically $10^4$) to keep the compute nodes busy. The measured global efficiency decreases steadily from 4 nodes on (i.e., 48 cores on), the main cause being an increasing load imbalance, caused by high idle times of worker tasks/threads (to be addressed in future work). However, realistic scientific simulations deal with both, more calculations per particle (i.e. detailed physics) and larger numbers of particles, where strong scaling is expected up to thousands of cores. We also stress here that the results with $10^6$ particles should not be generalized. This relatively low count of particles/core was chosen knowing that the codes will rapidly encounter a limit in their strong scaling due to reduced particles count per node with increasing node count, and reckoning the limits (in terms of maximum amount of particles that can be handled) of some of the production codes. This easily exposed scalability limits of the codes and targets of interest for improvement. Additionally, setup and execute experiments with larger amount of particles is much easier when using the mini-app than when
dealing with its parent codes: express and quick testing is one of the “raison d’être” of the mini-app.

The experiments show that the selected parent implementations already suffer from load imbalance. Acknowledging that imbalance will become an even more important problem on exascale (-ready) machines, the SPH-EXA mini-app is being designed to take it into account, already in its early development phases, and addressing it via state-of-the-art, scalable dynamic load balancing mechanisms within a single compute node and across massive numbers of nodes.

![Figure 2: Parallel efficiency of ChaNGa(12 OpenMP tasks and 1 MPI rank per node), SPHYNX (12 OpenMP tasks and 1 MPI rank per node), XXX (12 MPI ranks per node) and SPH-EXA mini-app (12 MPI ranks per node) under strong scaling, in function of the number of nodes used (12 cores per node) on Piz Daint.](image)

**Weak scaling evaluation** Figure 3 shows the efficiency of the SPH-EXA mini-app while weak scaling. While performing weak scaling, the problem size assigned to each processing element is constant and additional elements are used to solve a larger problem. The efficiency of weak scaling can be measured as:

\[ E = \frac{t_s}{t_p}, \]

where \( t_s \) is the time of the reference execution and \( t_p \) is the time of the execution using \( p \) processors. The linear scaling (best case scenario) is achieved if
the runtime stays constant while increasing the workload (proportionally to the number of processing elements).

![Parallel efficiency of the SPH-EXA mini-app (12 MPI ranks per node) under weak scaling, in function of the number of nodes used (12 cores per node) on Piz Daint.](image)

Compared to the previous strong-scaling experiments where the efficiency drops to 0.3 upon reaching 32 nodes, weak scaling results show that the proposed SPH-EXA mini-app can scale up to 512 nodes (6144 cores) before the efficiency reaches 0.3.

5 Conclusion

Based on interdisciplinary co-design, we identified the differences and similarities between SPHYNX, ChaNGa and XXX, both in terms of computer science-related features and physical models implemented therein. This results in a list of selected features, algorithms, and physics modules that are partially incorporated in the SPH-EXA mini-app.

To expose any limitations of the codes that may represent a major performance degradation today or in the future Exascale era, we have compared the codes through a common test cases that serves both as a test, and as a validation and acceptance proof for the mini-app, in the form of reproducible experiment. The result of this work is a deeper understanding of the three parent SPH codes, with a direct feedback to their developers, that already benefit from this work in terms of unveiling parallelization problems and improving overall scalability.
Furthermore, the prototype mini-app has shown promising results at scale, that will be complemented and improved by the features under development.

The SPH-EXA mini-app is expected to enable highly parallelized, scalable, reproducible, portable and fault-tolerant production SPH codes in different scientific domains. Addressing the performance and scalability challenges of SPH codes requires a versatile collaboration with and support from supercomputing centers, such as CSCS, such that our results can be taken into account for the design of the next generation HPC infrastructures.

An extensive analysis of the load imbalance in the mini-app both at process and thread level is planned in the future. Based on the load imbalance analysis, the thread-level load imbalance can be addressed using dynamic loop scheduling techniques implemented in the extended GNU OpenMP runtime library [34] or the extended LLVM OpenMP runtime library [35], whereas DLS4LB [36] can be used to address process-level load imbalance. Two-level dynamic load balancing ensures improved performance via balanced load execution at both levels [37].

In the long-term the goal is to provide a large number of complementary physics modules, thus enabling the mini-app to serve as a production code, that is more diverse and can be used for a broader set of tests than any single of the current parent production codes. Ongoing efforts are the extension to support the integral approach to derivatives and the multipolar expansion. The latter will allow to implement the gravity features thus enabling the mini-app to execute additional simulation scenarios, such as the Evrard collapse and star collision.

Portability is targeted through the porting to HPX, a task-based asynchronous programming model that offers a solution for homogeneous execution of remote and local operations, enabling the exploration of its efficiency and potential on Exascale ready machines.

Faults, errors and failures have become the norm rather than the exception in large-scale systems [38–40]. Providing adequate fault-tolerance mechanisms has become mandatory. While checkpointing, rollback and recovery [41,42] is the de-facto general-purpose recovery technique to tolerate failures during the execution, optimal multilevel checkpointing can leverage the different storage mediums available to greatly enhance performance. Additional mechanisms to handle silent errors, or silent data corruptions will also be considered [43,44].

Reproducibility is at the core of the scientific method, its cornerstone being the ability to independently reproduce and reuse experimental results to prove and build upon them. While the concept of reproducibility has always been part of the science, in certain computational sciences it has long been neglected. A framework has been proposed to support reproducible research [45] and will be analyzed, evaluated, and adopted as in the design of the SPH-EXA mini-app.

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