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HIGH-LEVEL SUPPORT FOR SIMULATIONS IN ASTRO- AND ELEMENTARY PARTICLE PHYSICS

G. Poghosyan [*]

Steinbuch Centre for Computing, Karlsruhe Institute of Technology, Karlsruhe, Germany

To fully exploit the potential of modern supercomputing systems, when performing particle and astrophysics simulations, the special user support instrument called the Simulation Laboratory "Elementary Particle and Astroparticle Physics" (SimLab E&A Particle) is established at Steinbuch Centre for Computing of the Karlsruhe Institute of Technology. SimLab is providing advanced support to scientific groups in developing the simulation software and porting them into up-to-date supercomputing infrastructures. Some details of how the SimLab is governed and cooperation with developers and users of codes are presented in this work including examples about code THiSMPI for simulation of particle accelerations in supernovae shock fronts and the KB3D code for solving quantum kinematic equations that could be used in simulations of heavy-ion collisions or laser excited semiconductor systems.

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INTRODUCTION

Computational Software during the past decades became a fundamental tool for scientific research in particle and astrophysics. Rarely, solution of modern scientific problems in astro- and elementary particle physics is achieved without development of computer simulation software. But adaptation of even off-the-shelf scientific simulation codes into up-to-date high-performance computing (HPC) infrastructures and/or distributed computing infrastructures like Grid or Cloud Computing often requires not only substantial knowledge of how to use those modern computing systems, but it leads to necessary essential changes in the scientific simulation code as well.

In addition, the necessity of optimal and effective use of limited and expensive computational time on any HPC systems is crucial and seldom can be

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[*] E-mail: gevorg.poghosyan@kit.edu

reached without long-term re-engineering of the scientific simulation codes, resulting in changes of the scientific concepts and architecture, practically leading to fundamentally new software and maybe scientific results. Hence, HPC hard- and software installation need to be complemented by a brainware component, i.e., trained HPC specialists supporting performance optimization of users' codes [1].

Simulation Laboratories recently established in Jülich and Karlsruhe Computing Centres [2] are aiming to provide the necessary brainware and support or even to fully take over the part of research activities of scientific groups related to the mentioned computational, often initially unplanned subjects. In particular, SimLab E&A Particle support scientific groups from particle and astrophysics in mastering S.P.O.R.A.D.I.C. changes in their simulation codes and conduct necessary tests and productive runs for improving scientific codes [3].

We define S.P.O.R.A.D.I.C. changes for scientific simulation software as

Standardization — making codes object-oriented, adapting Input-Output to modern standards,

Parallelization — scientific exploitation of the code to find parallelization strategies,

Optimization — infrastructure-dependent performance-analysis, code profiling,

Release — publicly available deduced parts of transfer code and simulated results to libraries,

Adaptation — porting code to up-to-date HPC, Grid/Cloud,

Data — managing huge amount of data produced by large-exascale simulations,

Intensive — data mining, visualization, statistic,

Computing — monitoring of computing time used, bookkeeping for large scale parameter studies.

1. STEERING AND OPTIMALLY USING THE BRAINWARE RESOURCES OF SimLab

The persons involved in a SimLab have been actively engaged with user groups from their respective communities during many years, through joint research and development activities, cooperations and workshops. To channel these activities and optimally use the limited man and computing resources provided for SimLabs by computing centres, a common governance metrics and workflow for managing SimLab activities is established. These must help to optimally use the brainware in productive long-term simulations, joint research and development activities as well as identify interest of computing centres to generate new explicit labs out of existing ones, when particular scientific community based projects are becoming big or important enough with potential to "consume" future supercomputing power at exascales level, one of the main challenges in Horizon 2020 — research and innovation framework programme of the European Union.

SimLabs could be considered as flexible expert pools where from the "task force" teams could be established, governed and sunset depending on the current needs of a particular research field facing the challenge to solve problems arising when supercomputing facilities must often be optimally utilized and counted in limited amount of CPU Hours available for a particular scientific community. Potentially such teams consist of both experts in supercomputing and in a particular scientific domain, e.g., visiting scientist working for a given period of time in supercomputing centres jointly with computing experts. The formation of teams could often be realized through 3rd party funding that SimLab in joint applications with scientific communities aspire to get.

Workflow to manage the brainware in SimLabs is presented in diagram in Fig. 1. The element "Joint R&D Call" defines the process of receiving and arranging of requests/applications from different scientific communities. Here the selection of corresponding SimLab responsible for the topic of scientific community is especially made. The next stage is "Analyzing Performance and Size of Simulation", where the brainware-manpower allocated in the computing centre is used to exploit potential scalability and estimate the size of the problem, e.g., in

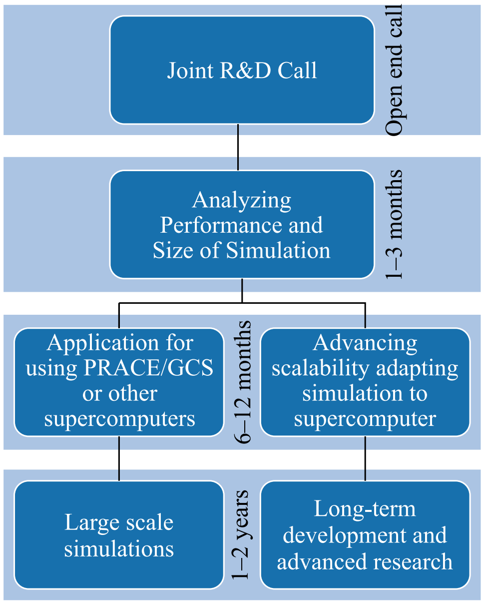

Fig. 1. Workflow for optimally channelling activities of an advanced support

CPU Hours or amount of Floating-point Operations (FloP). Depending on the performance and need of future optimization for scientific problem, the next stage — long-term R&D cooperation — is started to port and perform simulations on HPC systems in Europe like PRACE in national supercomputing centres like GCS. In case the code is not scaling or even not yet parallelized to be used on supercomputers, the development has to be organized in joint projects with scientific groups to be able to use present and especially future supercomputing facilities. The last two steps in workflow are most manpower and time consuming, and so could be organized only based on the procurement of the third-party financial support for joint research activities of SimLab experts and groups of scientists from a particular domain, e.g., particle physics, astrophysics or nuclear physics at SimLab E&A Particle.

Steering and governance of SimLab based on such a workflow allows brainware to act dynamically for many different scientific topics — building the "task force" groups depending on the needs of scientists from a given domain. Also accumulation of knowledge in SimLab, not only in thematic but in computational science as well, allows other scientific communities to profit from it, without necessity to "spend" resources and accumulate the same knowledge within their own scientific domain. The leader of SimLab is often a scientist involved more in the scientific domain to be able to "speak" the language of scientists because the author is very often an important "portion" of the simulation code whith rare documentation and at suboptimal level, from the point of view of computational science.

2. EXAMPLES OF COOPERATIONS IN SIMULATIOIN LABORATORY FOR ELEMENTARY AND ASTROPARTICLES

In cooperation with many groups in KIT and beyond, SimLab E&A Particle is acting in joint research in the fields of Cosmic Rays, Nuclear Physics, Heavy-Ion Collisions and Astrophysics. Brainware of SimLab is not only active as an HPC tuning expert, but in many different forms closing the gap between HPC and topical software. As a representative example of support, we discuss next the works in progress concerning two scientific simulation codes: THiSMPI — Two-and-a-Half-Dimensional Stanford code with Message Passing Interface for simulation of fully electromagnetic and relativistic particle dynamics, and KB3D — code for solution of Kadanoff–Baym equations. These are two representative cases showing different stages of codes — one simply needs to be optimized and go into productive runs on supercomputers, whereas the other needs long-term development to be able at all to run on up-to-date HPC systems.

2.1. "THiSMPI" Simulation of Acceleration of Particles in Supernovae Shock Fronts. THiSMPI is fully relativistic Particle-In-Cell code used for plasma physics computations. The code self-consistently solves the full set of Maxwell's

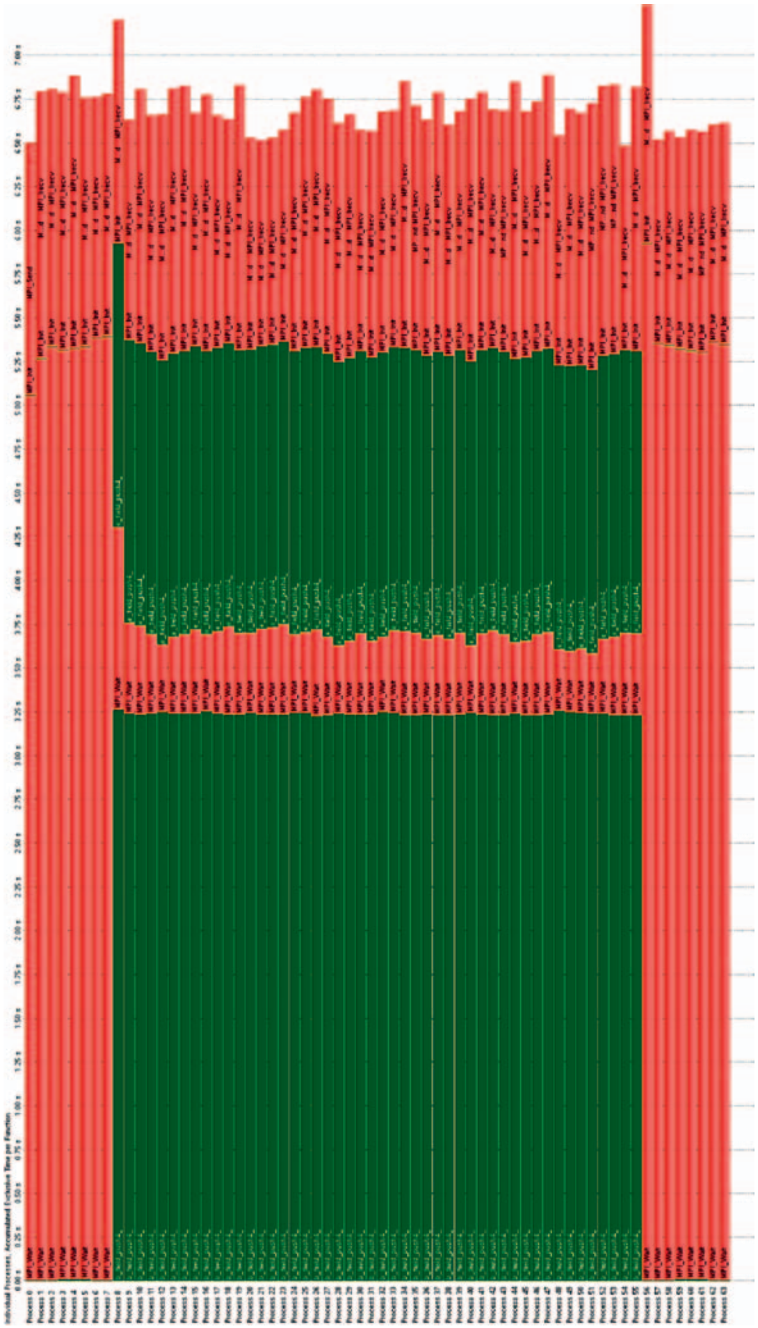

Fig. 2 (color online). Process Summary using VAMPIR for THiSMPI on 64 parallel Cores and 8 × 8 cells equations, along with the relativistic equations of motion for the charged particles [4].

Analyzing the performance of the code by using VAMPIR tool, we were able to identify the necessity of changing the strategies for balancing computation on different cells. As one can see in Fig. 2, initial and final 8 processors are mainly in waiting non-computing state (red color) as of mesh of cells where the simulation of plasma and particles is performed is simply directly distributed to available computational units without a priori estimation of computation need of each cell. Also, data optimal transfer bandwidth has to be developed for automated tracking and storage of bookkeeping information between cells, which promises to be a major advantage for improving the efficiency when simulation at large scales would be done.

2.2. "KB3D" Code for Solution of Kadanoff–Baym Equations. Solving Kadanoff–Baym 3D equations, one can simulate evolution in excited quantum kinematic systems [5]. For instance, simulation of a flash of laser on the semiconductor or heavy-ion collisions (HIC), when spin-polarized protons accelerated up to 100 GeV are colliding with another proton or gold or copper atoms. In KB3D the process of equilibration — thermalization — is modelled using non-equilibrium Green functions. Current version is an old code from 1999 written in Fortran77, where Green functions convolutions were computed using Fast Fourier Transformation functions of Mathkeisan commercial libraries, especially available only on Cray, SGI, NEC supercomputers. Here the use of other standard FFT libraries would be implemented and also a potential speedup when use of GPU for FFT calculations is planned.

CONCLUSIONS

The efficiency of brainware could be increased if this would be allocated into SimLabs, where special S.P.O.R.A.D.I.C. actions could be performed — like providing Key Performance Indicators or Benchmarks for different simulation codes, showing the time efficiency or potential amount of possible productive simulations. As well as performing long-term joint research for particular scientific code, it is crucial to be able to reach in short time highly effective usage of supercomputing facilities especially at large scale that would be available in next decades at supercomputing centres as well as distributed in many dedicated or remote computing units. Accumulated brainware in SimLabs the time scales for performing code optimization could be reduced as of necessary knowledge would be available and do not need to be accumulated again.

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