TA3-WP2 ACTIVE MEMBERS

- Lattice QCD
  - Bielefeld*: Olaf Kaczmarek
  - Regensburg*: Daniel Knüttel, Tilo Wettig
- Astro
  - Garching: Salvatore Cielo, Stephan Hachinger
  - Jülich*: Annika Hagemeier, Susanne Pfalzner, Frank Wagner

* Locations with PUNCH funding

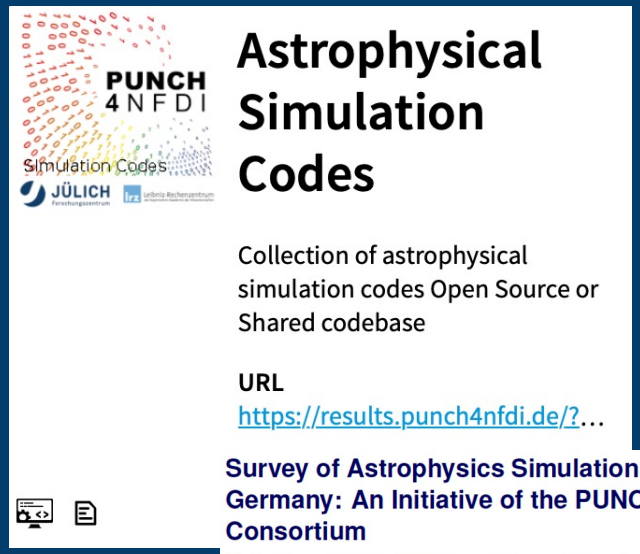
TA3-WP2 DELIVERABLES

- D-TA3-WP2-1 (30 Sep 2026; FZJ, UB, UR): Optimization of performance-critical routines entering data analysis and simulation software on GPU systems, heterogeneous compute clusters, and upcoming processor generations.
- D-TA3-WP2-2 (30 Sep 2026; FZJ, UB, UR): Provision of data-/compute-heavy algorithms with a focus on algorithmic and technical aspects of scientific reproducibility (resilience, uncertainties).

- Will both deliverables be fulfilled? I think so!

ASTRO ACHIEVEMENTS

List of astro codes



Community survey

Survey of Astrophysics Simulation Codes in Germany: An Initiative of the PUNCH4NFDI Consortium

Annika Hagemeier[1]*, Frank W. Wagner[1], Susanne Pfalzner[1], and Ramin Marx[2]

Abstract

PUNCH4NFDI is the consortium of particle and astroparticle physics, astrophysics, and hadronic and nuclear physics in the NFDI (national research data infrastructure), Germany. It aims at developing concepts and tools for efficient management of digital research products in fundamental physics and promotes the idea of FAIR data – which is to make scientific data sets findable, accessible, interoperable, and reusable. Here we concentrate on the aims and measures of PUNCH4NFDI in the context of astrophysics simulations. As a first step towards better understanding the software usage of the astrophysics simulation community in Germany, PUNCH4NFDI developed a 14-question survey. We distributed the survey through various channels (mailing list, conference flyer, personal communication) in 2022. In total, 130 computational astrophysicists responded to our survey. We found that predominantly codes able to simulate gravitational *N*-body problems and magnetohydrodynamics are used by the German astrophysics community. Computer programs typically associated with research in solar physics and numerical relativity turned out to be applied to a lesser degree. The degree to which the FAIR principles are already applied varies greatly. In many cases a basic software version is open access, however, the newest work is often based on modified and unreleased versions. The degree of practising the FAIR principles is often a question of available manpower. Some codes are developed and used by single local research groups, others by large research consortia spread around the globe. While smaller research groups are in principle willing to publish and openly share their simulation data, they often simply lack the manpower to do so. We also found that most astrophysicists in Germany view re-using other researchers' data sets as highly desirable.

Keywords
Astrophysics — Simulations — Survey

[1] *Jülich Supercomputing Centre, Forschungszentrum Jülich, Jülich, Germany*
[2] *Heidelberg-Königstuhl State Observatory, Heidelberg University, Heidelberg, Germany*
***Corresponding author**: a.hagemeier@fz-juelich.de

Paper on the Jülich LOFAR Data Archive

Full length article

Learning from the present for the future: The Jülich LOFAR Long-term Archive

C. Manzano, A. Miskolczi, H. Stiele, V. Vybornov, T. Fieseler, S. Pfalzner

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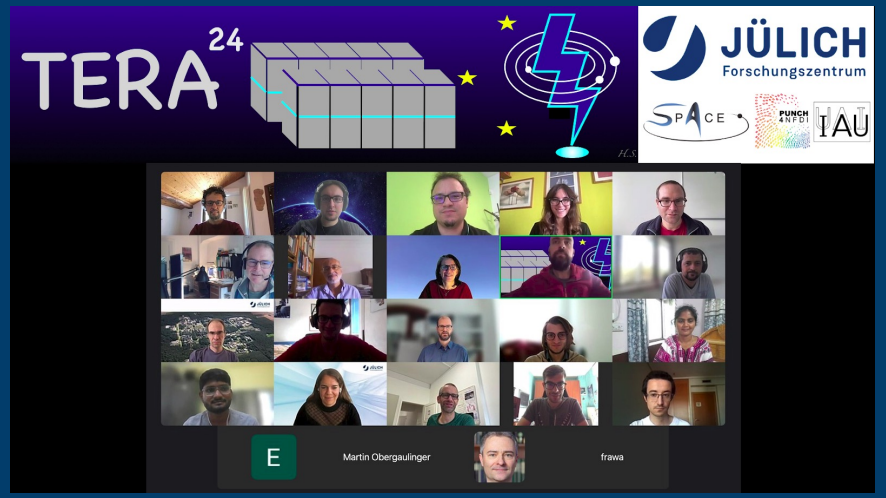
Abstract

The Forschungszentrum Jülich has been hosting the German part of the LOFAR archive since 2013. It is Germany's most extensive radio astronomy archive, currently storing nearly 22 petabytes (PB) of data. Future radio telescopes are expected to require a dramatic increase in long-term data storage. Here, we take stock of the current data management of the Jülich LOFAR Data Archive, describe the ingestion, the storage system, the export to the long-term archive, and the request chain. We analysed the data availability over the last 10 years and searched for the underlying data access pattern and the energy consumption of the process. We determine hardware-related limiting factors, such as network bandwidth and cache pool availability and performance, and software aspects, e.g. workflow adjustment and parameter tuning, as the main data storage bottlenecks. By contrast, the challenge in providing the data from the archive for the users lies in retrieving the data from the tape archive and staging them. Building on this analysis, we suggest how to avoid/mitigate these problems in the future and define the requirements for future even more extensive long-term data archives.



TERA workshop; recorded tutorials available

RECENT ASTRO HIGHLIGHTS

DESTINY as a PUNCH service

DESTINY

DESTINY (Database for the Effects of STellar encounters on dIsks and plaNetary sYstems) is an open-access data portal that provides resources for…

URL https://destiny.fz-juelich.de/

Access Open

Tags Planetary system dynamics, Astrophysics, Astronomy, Database

Data releases via DESTINY / Jülich DATA

Simulation data on the effects of a stellar encounter on the protoplanetary disk of the early Solar System

Version 1.1

Wagner, Frank W.; Pfalzner, Susanne, 2025, "Simulation data on the effects of a stellar encounter on the protoplanetary disk of the early Solar System", https://doi.org/10.26165/JUELICH-DATA/9Z9K47, Jülich DATA, V1

Cite Dataset ▾ Learn about Data Citation Standards.

Simulation data on the long-term evolution of the Solar System following a stellar flyby

Version 1.1

Wagner, Frank W.; Pfalzner, Susanne, 2025, "Simulation data on the long-term evolution of the Solar System following a stellar flyby", https://doi.org/10.26165/JUELICH-DATA/LGBORQ, Jülich DATA, V1

Cite Dataset ▾ Learn about Data Citation Standards.

LATTICE QCD ACHIEVEMENTS

List of lattice QCD codes

ILDG

List of Lattice QCD Codes

Lattice Quantum ChromoDynamics Codes Open Source or Shared codebase

URL
https://results.punch4nfdi.de/?…

Tags Quantum Chromo Dynamics, International Lattice Data Grid

Lattice QCD ensembles published on Zenodo

ldg/rqcd/qcdML/ens_001

Knüttel, Daniel (Producer)[1, 2]; Knüttel, Daniel (Contact person)[1, 2]

A quenched QCD ensemble for machine learning projects.

```
markovChain:
  markovChainURI: "ldg/rqcd/qcdML/ens_001"
  management:
    collaboration: "rqcd"
    projectName: "qcdML"
    archiveHistory:
      - add:
        participant:
          orcid: "0009-0001-9453-4227"
          name: "Daniel Knüttel"
          institution: "Regensburg University"
        date: "2023-06-10T12:00:00+01:00"
```

mc://ldg/rqcd/qcdML/ens_004_selected

Knüttel, Daniel[1]

Selected configurations from a quenched lattice QCD ensemble for machine learning purposes.

```
markovChain:
  markovChainURI: "ldg/rqcd/qcdML/ens_004_selected"
  management:
    collaboration: "rqcd"
    projectName: "qcdML"
    archiveHistory:
      - add:
        participant:
          orcid: "0009-0001-9453-4227"
          name: "Daniel Knüttel"
          institution: "Regensburg University"
        date: "2024-01-14T12:00:00+01:00"
```

AnalysisToolbox Public

A set of Python tools for statistically analyzing data. This includes aspects of lattice QCD applications related to QCD phenomenology.

Python 22 MIT 7 12 0 Updated 4 days ago

SIMULATeQCD Public

SIMULATeQCD is a multi-GPU Lattice QCD framework that makes it easy for physicists to implement lattice QCD formulas while still providing competitive performance.

C++ 36 MIT 15 37 5 Updated last week

Development of numerical libraries and analysis tools

RECENT LATTICE QCD HIGHLIGHTS

QCD_ML library released

The PUNCH4NFDI consortium in the German NFDI

Published May 21, 2025 | Version v0.5.0

Software Open

daknuett/qcd_ml: v0.5.0

Daniel Knuettel[1] ; Simon Pfahler ; Rielco ; Raphael Lehner

Show affiliations

Version 0.5.0. Includes

- Several bugfixes
- added `LGE_CB`
- added `C_Convolution`
- added `topological_charge_density_plaquette`
- made `qcd_ml.compat.gpt` mpi-safe

191 VIEWS

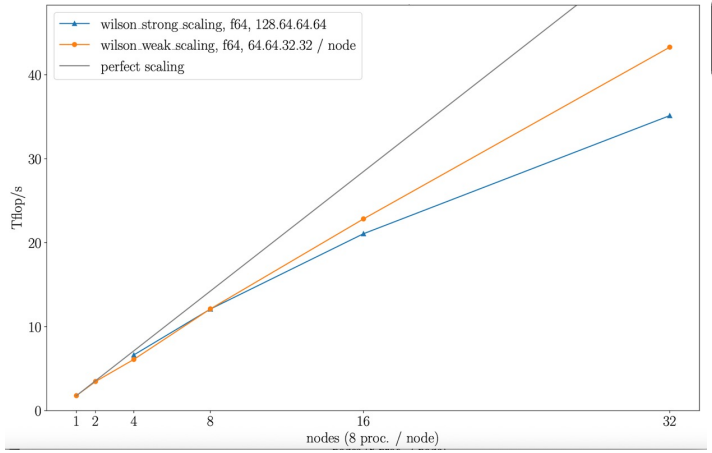
67 DOWNLOADS

Workflow development for lattice QCD

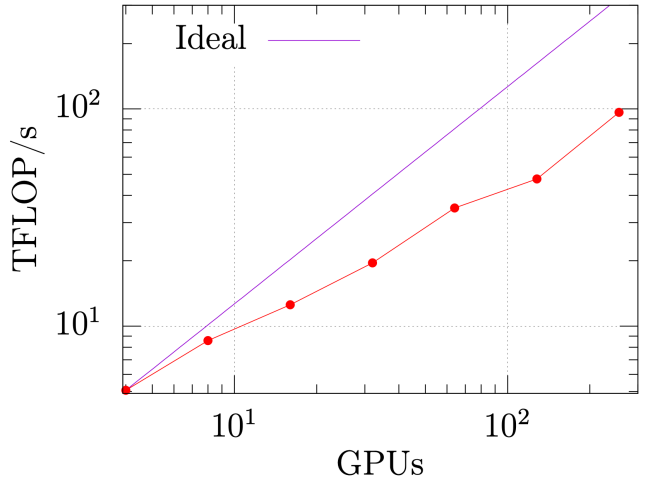
BENCHMARKING ACTIVITIES

Lattice QCD benchmarks
Codes: Bridge++, Grid, SIMULATeQCD

Grid

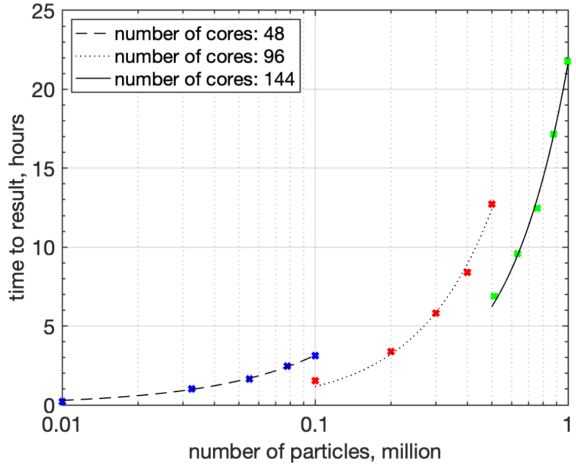


SIMULATeQCD

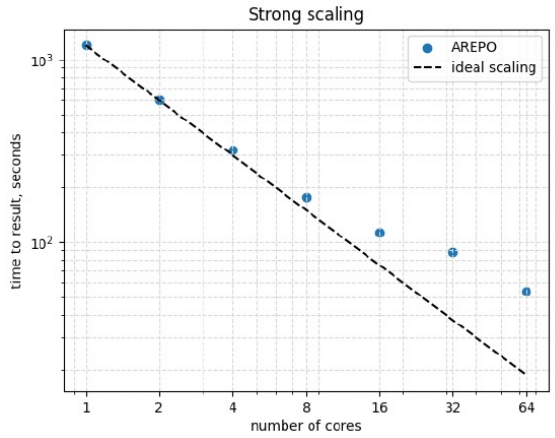


Astro benchmarks
Codes: Arepo, Gadget, Rebound

Rebound

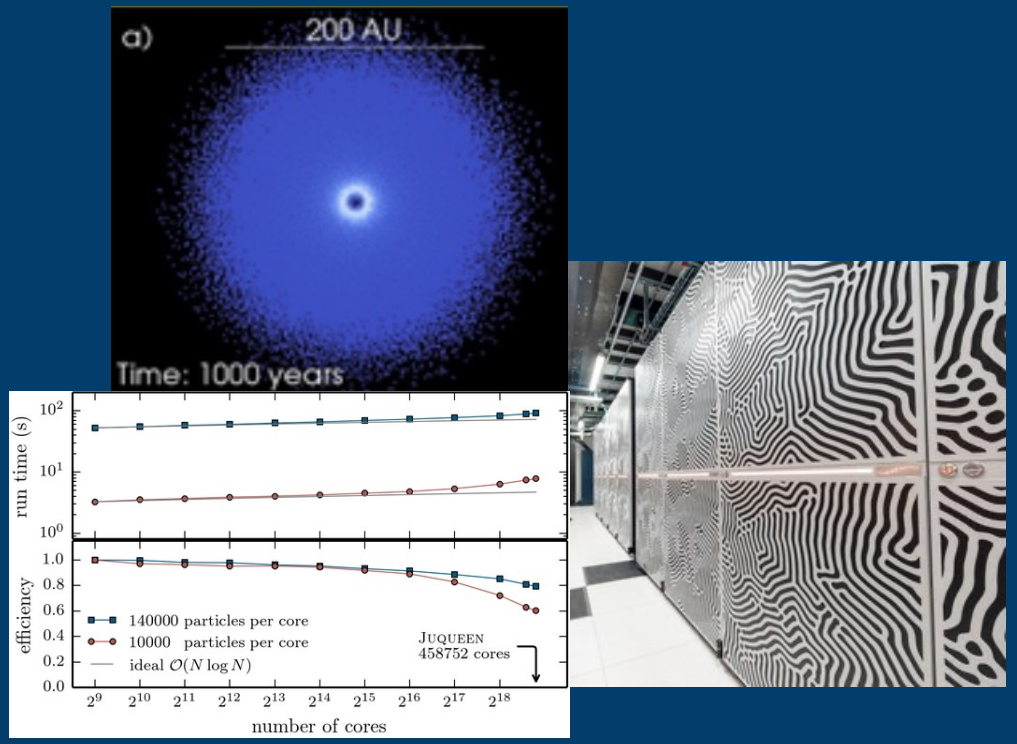


Arepo

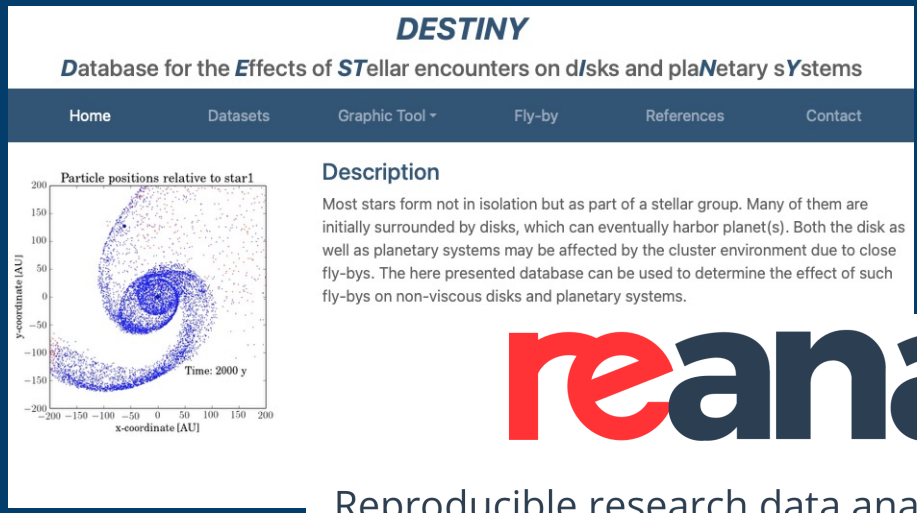


REMINDER OF FUNDING PERIOD / ONGOING ACTIVITIES

- Optimise and benchmark PEPC on JUPITER (D-TA3-WP2-1)



- Integrate REANA with DESTINY to leverage PUNCH resources (D-TA3-WP2-2)

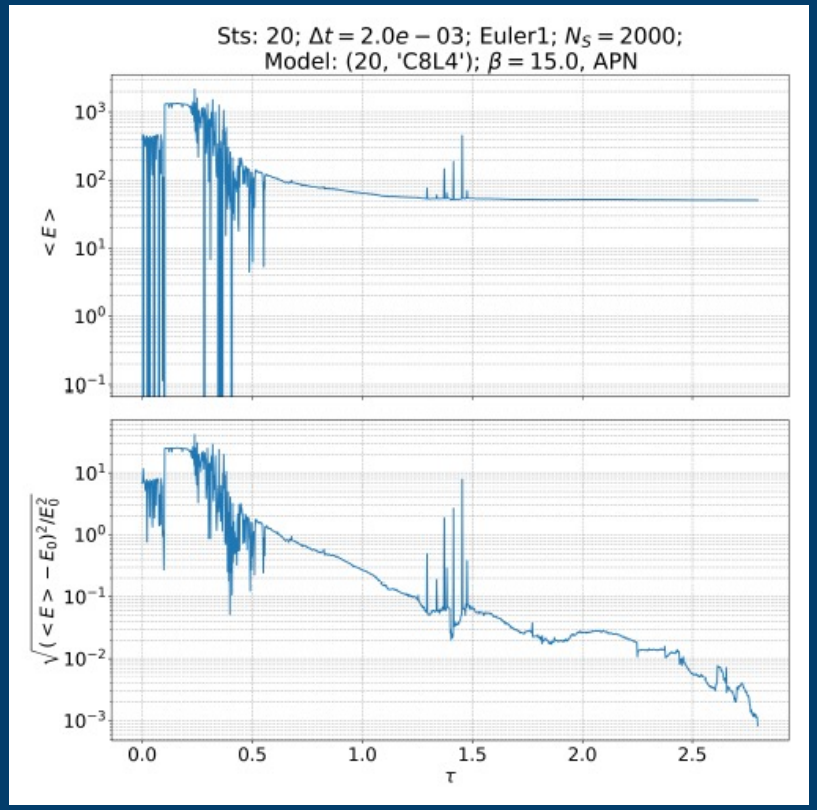


reana

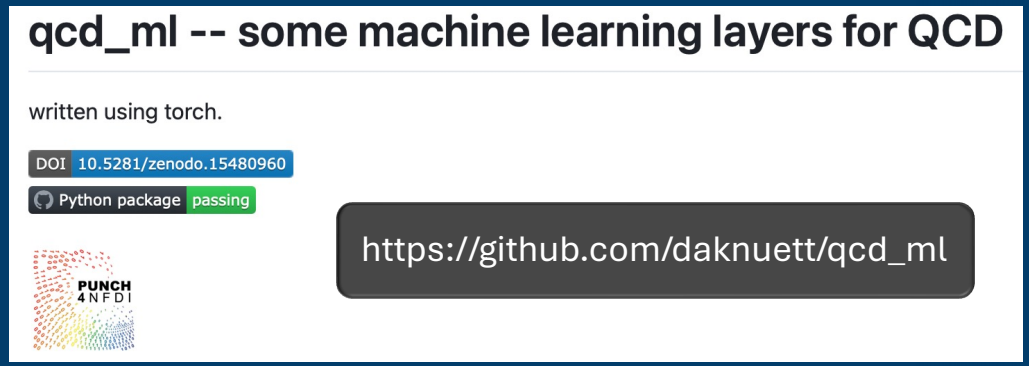
Reproducible research data analysis platform

REMINDER OF FUNDING PERIOD / ONGOING ACTIVITIES

- Novel NQS algorithms for lattice field theory (D-TA3-WP2-2)



- QCD_ML library maintenance (D-TA3-WP2-2)



FURTHER ACTIVITIES

- Participate in the RDM Challenge

- Present PUNCH4NFDI and advertise its services at Astroinformatics 2026

PUNCH_ASTRO COMPUTE PROJECTS

- HPC helpdesk and benchmarking service

https://intra.punch4nfdi.de/?md=/docs/TA3/WP2/compute-projects.md

Project ID	Description	Institution
PA	Code Benchmarking	LRZ, JSC
S1	Quokka Code	Leiden Observatory
GSP24	Guest Student Program	JSC
PA-BP1	PUNCH TA3-WP3	Hamburg Observatory
PA-S1	PUNCH TA3-WP3	JSC
PA-T1	PUNCH TA5-WP4	HTW Berlin
TERA24	TERA Tutorials	Grenoble Alpes University, University of Turin, JSC
GSP25	Guest Student Program	JSC
PA-W1	Stellar Flybys	JSC

PUNCH_ASTRO compute projects

22 April 2024

You wish to test your simulation code on a supercomputer?

Read more

JÜLICH Forschungszentrum

PUNCH_ASTRO COMPUTE PROJECTS

- HPC helpdesk and benchmarking service

https://intra.punch4nfdi.de/?md=/docs/TA3/WP2/compute-projects.md

Project ID	Description	Institution
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TERA24	TERA Tutorials	Grenoble Alpes University, University of Turin, JSC
GSP25	Guest Student Program	JSC
PA-W1	Stellar Flybys	JSC

PA-W1

The Astrophysical Journal Letters, 992:L32 (11pp), 2025 October 20 https://doi.org/10.3847/2041-8213/ae0e74

Trans-Neptunian Object Colors as Evidence for a Past Close Stellar Flyby to the Solar System

Susanne Pfalzner, Frank W. Wagner, and Paul Gibbon
Jülich Supercomputing Center, Forschungszentrum Jülich, 52428 Jülich, Germany
Received 2025 May 13; revised 2025 July 7; accepted 2025 July 8; published 2025 October 17

Abstract

Thousands of small bodies, known as trans-Neptunian objects (TNOs), orbit the Sun beyond Neptune. TNOs are remnants of the planets' formation from a disk of gas and dust, so it is puzzling that they move mostly on eccentric orbits inclined to the planetary plane and show a complex red-to-gray color distribution. A close stellar flyby can account for the TNOs' dynamics, but it is unclear if this can also explain the correlation between their colors and orbital characteristics. Assuming an initial red-to-gray color gradient in the disk, our numerical study finds that the spiral arms induced by the stellar flyby simultaneously lead to the observed TNOs' color patterns and orbital dynamics. The combined explanation of these TNO properties strengthens the evidence for a close flyby of another star to the young solar system. Our study predicts that (1) small TNOs beyond 60 au will mostly be gray, and (2) retrograde TNOs will lack the color most common to high-inclination TNOs. The anticipated TNO discoveries by the Vera Rubin telescope will be able to test these predictions. A confirmed flyby would allow us to reveal the chemical composition of the solar system's primordial disk.

Unified Astronomy Thesaurus concepts: Trans-Neptunian objects (1705)

Materials only available in the online version of record: animation

JÜLICH Forschungszentrum

PUNCH_ASTRO COMPUTE PROJECTS

PA-T1

Software to the data: running container interactively in computing centres

Marcel Trattner

Hochschule für Technik und Wirtschaft (HTW) Berlin

July 24, 2024

Data can be analyzed conveniently, i.e. especially interactively, with Jupyter notebooks, which are consequently popular in many scientific communities. However, this method of working reaches its limits with large volumes of data: for reasons of sustainability, copying large volumes of data to each user is not feasible. Instead, a user copies his analysis pipeline to the data centre that holds the data ("software for the data"). Analysis tools usually require additional software components (such as libraries) that, in general, are not installed on the computers of a data centre. This can be remedied by containers in which the user packs the required components alongside the analysis tools and transfers containers to the data centre.

In elementary particle physics, huge amounts of data are analyzed without user interaction, but with the help of so-called batch jobs. This article demonstrates how container can be used "interactively" at the Jülich Supercomputing Centre, which offers an interface for Jupyter Lab with the added option to start the Jupyter server instance from a custom container. It would be desirable if such a solution could also be implemented in more and more data centres.

GSP24

N-Body Code Optimisation for Stellar Flyby Simulations

A Path to Faster and More Accurate Results

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Heidelberg, Germany
peenalgupta123@gmail.com
&
Frank Wagner
Forschungszentrum Jülich
Jülich, Germany
f.wagner@fz-juelich.de

Abstract *We present an extension of the astrophysical N-body code REBOUND, which enables parallel simulation of stellar flybys. By leveraging the mpi4py package, we harnessed the power of multi-core processors to significantly accelerate simulations. Our approach exploits the non-interacting nature of test particles, allowing us to efficiently distribute the particle cloud across processor cores. Benchmark results demonstrated excellent scalability with both particle number and process count for two popular integration methods, WHfast and IAS15. Furthermore, we developed a post-processing routine using pandas, which converts output data into a human-readable CSV format, enhancing data analysis capabilities. Although this feature introduced a noticeable performance overhead, it substantially improves data accessibility and usability, paving the way for faster and more accurate results in stellar flyby simulations.*

PA

Cuda IPC issue #1036

Open · pgrete opened this issue on Mar 27 · 1 comment

pgrete commented on Mar 27 — Collaborator

I was made aware of a Cuda IPC related issue when running a simple AthenaPK test case in parallel.
Given that the test case mostly exercises Parthenon base features, I'm opening an issue here to raise awareness.

The test setup works on a single rank and on two ranks but fails on 4 ranks on mesh refinement (so sometime not on the first one but on a subsequent one).
Also disabling ipc via

```
export UCX_TLS=rc_x,self,sm,gdr_copy,cuda_copy
```

i.e., removing `cuda_ipc` from that list also fixes the issue.

Might be worth trying to reproduce with the Parthenon advection-example and on other software stacks.
Realistically I'll first be able to have a closer look in about two weeks so if anyone else has ideas in between go for it! I was not able to reproduce on Frontier so might be a CUDA issue, ping **@forrestglines**

Steps to reproduce (using NVHPC/Cuda/OpenMPI 23.1/11.7.64/4.1.4 and 23.7/12.2.91/4.15 on A100s on JUWELS Booster) is compile current AthenaPK `main` and run the advection pgen

PA

nodes	cores	time, sec
1	1	1193.903603
1	2	600.906955
1	4	317.404362
1	8	177.222937
1	16	113.457836
1	32	88.067369
1	64	53.395713