Project INF in the CRC CIM

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TUD

Spring 2022

Available in the very near future

- GitLab for the CIM
- Compute cluster
- Data server

Now 2023

Available and could be used

- GitLab for the CIM
- Compute cluster
- Data server





Where to find it? https://gitlab.ruhr-uni-bochum.de/sfb1491

How to register? Send an email request to me (grauer@tp1.rub.de)

or to **Andreas Schramm** (Andreas.Schramm@ruhr-uni-bochum.de)

What is it good for? Documentation on how to reproduce a paper (DFG guidelines):

paper, source codes, pre- and post processing scripts

Must be approved by another member of another project!

Each project is different, thus no general applicable procedure.

Let's have a look at examples ...





S SFI

SFB1491 ⊕

Group ID: 2084 [Leave group

Cosmic Interacting Matters - From Source to Signal

Subgroups and projects Shared projects Archived projects

> % C CompSchool2023 Maintainer we discuss later

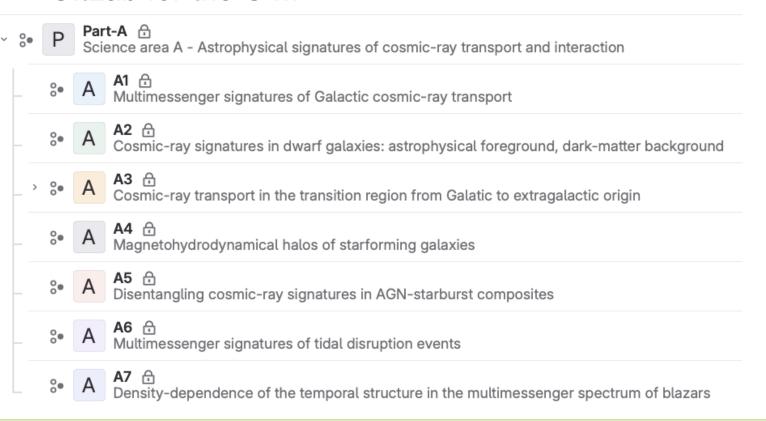
> % P Part-F Science area F - Fundamental properties of matter

> % P Part-A Science area A - Astrophysical signatures of cosmic-ray transport and interaction





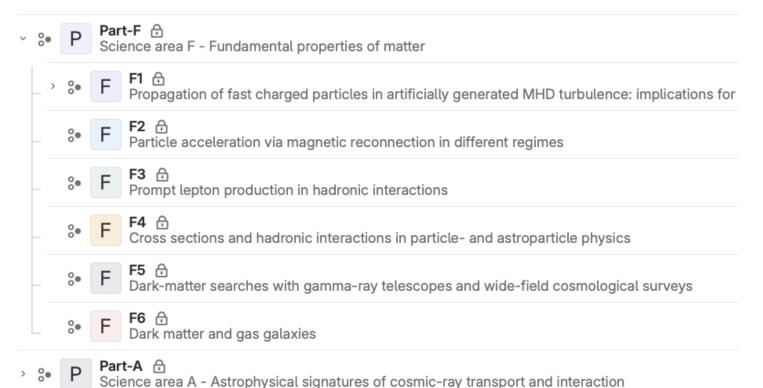








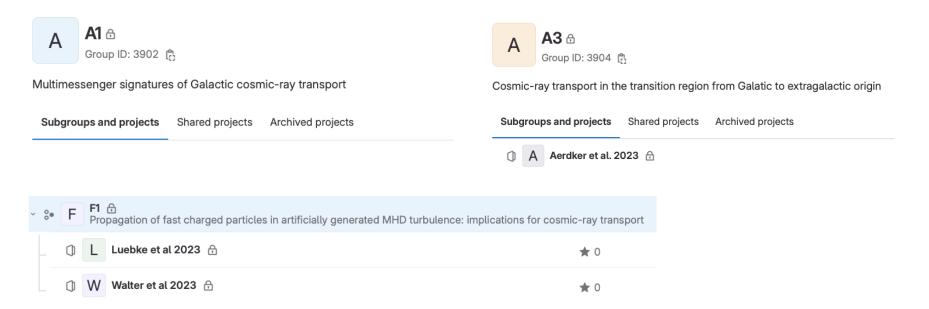












Presently, 4 papers are approved in GitLab. Needs to be improved!







Example



Walter et al 2023 ∆

Project ID: 2542 👸

□ Doc	Upload New File
□ Papers	Upload New File
□ Source	Upload New File
M* README.md	Update README.md







Walter et al 2022

Documentation and Code for the Paper Walter et al. 2022 https://pubs.aip.org/aip/pop/article-abstract/29/7/072302/2844126/A-nonlinear-model-ofdiffusive-particle

Authors: Dominik Walter, Frederic Effenberger, Horst Fichtner, Yuri Litvinenko

This repo contains a documentation for the whole numerical Setup, the purpose and function of the seperated codes and theirs distinct outputs. The details of the codes itself, will be discussed in different files, referenced here.

The main code is a variation of the open access fortran-code VLUGR3, named cartesian_ref_nonlin.f Here all the numerical solutions used in the paper are produced, it calculates the shock acceleration models for linear and nonlinear cases. The code produces an output in the form of a sol.dat file, where it gives the output-times as well as the solution at the points x,y,z,numsol. More details for the setup in this code, are given in "DocumentationMainCode".

The file exaktlnt.f can take the file sol.dat and puts out several files, containing the spectrum at the shock for different points in time in the form of p,solexap^2,r,t,solnump^2. More details in "DocumentationexaktCode"

The file Spatial f takes the solution provided by the main code and derives a integrated spatial distribution, by sorting and integrating the output. More details can be found in "DocumentationSpatials".

The file Contour.f takes the solution provided by the main code and provides the resulting diffusion-coefficient and a file that is suitable for 2D plots.

The files derived by exaktlnt.f or Spatial.f can now easily be plotted by a plotting routine of choice (e.g. gunplot).

In the file 'InstructionsforCompiling' you can find a short example, that shows how to compile and run the codes. Using the gfortran-compiler no additional compiler options were necessary, to compile the code.

A Link to the original VLUGR3 code can be found here: https://dl.acm.org/doi/abs/10.1145/232826.232853

A file diff.txt was edited, that compares the probia f example of the official main code (link above) to our version of the code, hihadlighting the differences.







Another example



Name	Last commit
DSA_JupyterNotebooks	Fix file name in comment.
□ VLUGCODE	Restructuring of directories and typo corrections
□ VLUGDATA	Merge branch 'main' into cleanup
□ VLUGDOCUMENTATION	Update vlugr3 documentation
◆ .gitignore	Typos, additional comments, etc.
™ README.md	Update vlugr3 documentation





1. Installation of CRPropa

Install CRPropa version (2777730f094640d09202e5cac65c50a0467bcd48), which can be found in this separate repository: https://github.com/sophieaerdker/CRPropa3/tree/DSAEnergyDependence. Detailed information on how to install CRPropa can be found on the webpage (crpropa.desy.de) and on the public GitHub repository (github.com/crpropa/crpropa3).

2. Installation of VLUGR3

Install a Fortran compiler version (90+), which is suitable for your system. The used programs are stored in (./VLUGCODE/). A detailed documentation together with explanations on how to run them can be found in (./VLUGDOCUMENTATION). In this way the already produced data (./VLUGDATA) can be verified.

3. Running Simulation and Analysis

Run the jupyter notebooks. The notebooks themself contain further explanations. Jupyter notebooks are independed of each other. To follow the publication we recommend the following order:

- 1. StationarySolution.ipynb
- 2. ParticleSplitting.ipynb
- 3. Constraints_AdvectiveStep.ipynb (+ AdvectiveStep_Steering.py)
- 4. Constraints_DiffusiveStep.ipynb (+ DiffusiveStep_Steering.py)
- 5. BurstLikelnjection.ipynb
- 6. EnergyDependentDiffusion.ipynb
- 7. InjectedSpectra.ipynb (+ InjectedSpectra_Steering.py)
- 8. ObliqueShock.ipynb
- 9. RadialShock.ipvnb (+ RadialShock_Steering.pv)







WE NEED YOUR HELP:

Look at the examples

and ... do it!

If you need help: Kevin Kröninger (Particles)

Angus Wright (Astro)

Rainer Grauer (Simulations)

It is important in applying for the second phase.

Responsibility: PIs





In addition:

Use the gitlab to store info and data for schools, workshops, seminar series ...

Let's have a look at an example ...

С	CompSchool2023 ⊕ Group ID: 5182 Ĉ Leave group
Subgro	pups and projects Shared projects Archived projects
0	G GeneralInfo (#)
0 7	Turbulence ⊕
	ParticleInCell 🕆
	C CosmicRayTransport 🙃
	MultiPhysics ⊕
1	MHD ☆







Compute Cluster

galileo.cim.ruhr-uni-bochum.de

managed by Jürgen Möllenhoff@tp1 some technical data

- 1 x Head-Node (galileo.cim.rub.de, login and cluster management)
- ssh galileo.cim.rub.de
- cluster view via https://galileo.cim.rub.de
- 1 x AMD EPYC 7313P 16-Core Processor 3.0 GHz, 128MB L3 cache, (16 real kernels, 32 with HT)
- 256 GB DDR4-3200MHz ECC-RAM
- user directories located on 2 x 1 TB M.2 SSD as RAID1 → 1 TB can be used (/home)
- more information here: https://www.gigabyte.com/Enterprise/Rack-Server/R272-Z30-rev-A00
- 8 x Compute CPU-Nodes (c1-c8)
- 4 nodes each share one cabinet
- access only via **SLURM** using the head node
- 2 x Intel(R) Xeon(R) Gold 5318Y CPU @ 2.10GHz, max. 3.4 GHz, 36 MB cache, 24 kernels (48 real kernels, 96 with HT)
- 256 GB DDR4-3200MHz ECC-RAM
- user directories and storage connected via NFSv4
- more information here: https://www.gigabyte.com/Enterprise/High-Density-Server/H262-NO0-rev-100







Compute Cluster

galileo.cim.ruhr-uni-bochum.de

- 1 x Compute GPU-Node (c9)
- access only via **SLURM** using the head-node
- 1 x AMD EPYC 7313P 16-Core Processor 3.0 GHz, 128MB L3 Cache, (16 real kernels, 32 with HT)
- 128 GB DDR4-3200MHz ECC-RAM
- 2 x NVIDIA® A100 80GB Tensor-Core-GPU (https://www.nvidia.com/de-de/data-center/a100/)
- space for 8 GPU-cards, 6 cards could be added

needs to be improved

- Benutzerverzeichnisse bzw. Speicherlaufwerk via NFS angebunden
- further information here: https://www.gigabyte.com/Enterprise/GPU-Server/G292-Z20-rev-A00
- 1 x storage (fs)
- access only via NFSv4 (/home/fs/users/)
- 1 x AMD EPYC 7313P 16-Core Processor 3.0 GHz, 128MB L3 cache, (16 real kernels, 32 with HT)
- 128 GB DDR4-3200MHz ECC-RAM
- 11 TB Speicherplatz via ZFS-RAID6, harddiscs RAID with 1 TB SSD-cache
- We could add 7 more discs
- further information here: https://www.gigabyte.com/Enterprise/Rack-Server/R272-Z30-rev-A00

nodes connected 2 x 10 GB Ethernet

needs to be improved

Presently 22 users (apply by writing an email to RG)





Data server

storing observational data (Dettmar)

similar to the John Hopkins turbulence database https://turbulence.pha.jhu.edu/ store data from large scale MHD simulations on JUWELS (Mike Wilbert) to use as turbulent background

HIT, various background fields, different resolutions, decaying and forced ...

Thanks



