The dust post-processing code Paperboats

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1 INTRODUCTION

Paperboats is a parallelized, grid-based post-processing code to compute the evolution of dust material in a moving gas. Based on the output of an MHD code – which provides all required information of the gas phase – the dust transport, dust destruction and potential dust growth is calculated. The code was originally developed to study the destruction of dust grains in a clumpy supernova remnant, however, it was also applied to study the dust destruction of a supernova blastwave in a turbulet ISM or in a turbulent ISM without supernova blastwave.

The code is based on an approach we call "Dusty grid approach", at which the full dust number density distribution is traced in all cells of the domain and at each time-step. This approach is unique in that it allows for the simultaneous simulation of the entire dust distribution rather than just tracking the paths of a finite number of tracer particles as has been done in the past. Moreover, it allows to generate dust maps for different dust grain sizes. The dusty grid approach is somewhat comparable to gas in MHD simulations where one is not interested in individual gas atoms, ions or molecules, but in the number density of them.
The dust transport in Paperboats considers drag by gas-grain collisions, plasma drag, and the acceleration of charged grains in magnetic fields (gyration due to Lorentz force). Dust destruction processes include sputtering (thermal and kinetic sputtering) and grain-grain collisions (fragmentation, vaporisation). Moreover, there are three different dust growth processes included: Coagulation due to grain-grain collisions at low velocities, ion trapping of gas, and the accretion of gas. All processes can be simulated simultaneously or individually by turning some of the processes on or off. It is possible to follow a grain size distribution based on N dust grain sizes, with typical numbers for N used in previous simulations ranging from 2 to 40. The dust processing is calculated separately for each grain size, so that the evolution of dust number densities can be followed for each specific grain size. The initial grain size distributions follow a log-normal or a power-law function, but are easily adaptable to other size distributions. The grain material comprise silicate dust, carbonaceous dust, or a mixture of both materials.
Paperboats can manage 2D or 3D MHD simulations, however, depending on the grid size, the number of snapshots and the number of dust grain sizes, 3D simulations can be very computationally intensive. In this case it is preferable to run slices of 3D simulations: a 2D simulation and the third dimension consists of a single cell.

In order to conduct post-processing simulations with Paperboats, the following is needed:
The 2D or 3D output of an MHD code, namely for the gas density, gas temperature, gas velocity vector, and the magnetic field vector – for all quantities on a regular Cartesian grid. Typical numbers for the number of grid cells are a few 10^5 to 10^6 cells. This information is needed for different snapshots, with between 100 and 4000 snapshots used in previous studies. The time steps do not need to be equally sized. Currently, Paperboats is able to use the output of the MHD codes AstroBEAR, Pencil, Arepo and Amun. It is extendible to each other MHD code, even SPH, if an appropriate interface is used which converts the data onto a Cartesian grid. Supported data formats are hdf5 and Ascii.

Paperboats will then provide the following results:
- Gas maps for each snapshot, for the density, temperature, and magnetic field,
- Density maps for the dust, for each snapshot and for multiple dust grain sizes,
- Grain size distribution (number of grain sizes as a function of grain size, integrated over the full domain), for each snapshot,
- The total dust survival rate as a function of time.

A more detailed description of processes and methods considered in Paperboats can be found in Kirchschlager et al. (2019). The code is constantly being further developed, several adjustments and new implementations are described in the publications listed at the end of this manual. Please also have a look at the following short movies.

Gas maps of the cloud-crushing problem:
χ = 100: https://youtu.be/ufjy58X2xHo
χ = 300: https://youtu.be/6ZmppLkGHFw
SN blastwave expanding in turb. ISM (low density):
Gas maps: https://youtu.be/Mz2cuEVm_eY
Dust maps: https://youtu.be/byw8LQ38i8M
SN blastwave expanding in turb. ISM (moderate density):
Gas maps: https://youtu.be/oGXh6piIqlA
Dust maps: https://youtu.be/w8ZJqZK63KY
Turbulent ISM:
Gas maps: https://youtu.be/HEJ-4CZl-ZQ
Dust maps: https://youtu.be/36nB1aAL-2o

2 OBTAINING AND COMPILING THE SOURCE CODE

The installation is taking place on a Linux system with a f90 or f95 compiler and hdf5 installed. The packages “tar”, “mogrify” and “ffmpeg” are required for a smooth sequence. The graphing utility gnuplot is required at the beginning but can be replaced later with own plot scripts if necessary.

The complete source code for Paperboats is provided in a single gzipped tarfile. After downloading Paperboats, create a working directory (here as an example: “River”) where you would like Paperboats to reside. Remove the date specification of the file (though this is not necessary), copy the gzipped tarfile of Paperboats to this working directory and extract the files from the gzipped tarfile:

mv Paperboats_2023_01_13.tar.gz   Paperboats.tar.gz

cp Paperboats.tar.gz   River/

cd River/

tar -xf Paperboats.tar.gz

rm Paperboats.tar.gz

In order to run post-processing simulations for AstroBEAR, Pencil, Arepo, or Amun, change the flag l_hydrocode in “Paperboats/Process.tab” to 1, 2, 4, or 5, respectively. Please note, that l_hydrocode=3 is reserved for the code Swift. Further procedures for the individual MHD codes can be found in the following subsections.

AstroBEAR

In case AstroBear is the MHD code, “River/” has to be the project folder of the AstroBEAR simulation. This means, “River/” contains in addition to the folder “Paperboats/” all files to run a separate AstroBEAR simulation (esp. “global.data”, “physics.data”, “problem.data”, “scales.data”) and the folder “out/”. “out/” contains all hdf5-files (e.g. “chombo00000.hdf”) and the files “child_boxes.txt” and “totals.dat”. Please note, “child_boxes.txt” is not automatically generated by AstroBEAR but has to be produced using the tool HDFView. “totals.dat” contains the list of timesteps in code units.
In short, the “Paperboats/” folder just needs to be copied into the project folder of AstroBEAR.

Pencil

In case Pencil is the MHD code and the data are provided in Ascii-files (which is not the general case), “River/” has to contain two folders: The "Paperboats/" folder and a folder “Pencil_data/”. In "Pencil_data", the files "meta.pencil" and a folder "Ascii_data/" are needed. Please copy all Ascii-files and also "totals.dat" into the folder "Ascii_data".

If you want to change the names of these folders, you have to change also these names in “Paperboats/src/variable.f90” and “Paperboats/src/init_pencil.f90”. “totals.dat” contains the list of timesteps in code units. In case you change the time intervals, total number of timesteps or code units in the MHD simulation, you have to change this list as well. “meta.pencil” contains a few meta-parameters of the MHD simulation: The code units, the number of grid cells, and the lengths of the 2D or 3D box. In case you change them in the MHD simulation, make sure that you change them in this file as well. An example for “meta.pencil” is available in “Paperboats/misc/”.

Arepo

In case Arepo is the MHD code, the procedure is analog to the case for Pencil. Please replace “Pencil_data/”, “Ascii_data/” and “meta.pencil” by “Arepo_data/”, “data/” and “meta.arepo”, respectively. Please copy all hdf5-files and also “totals.dat” into the folder “data/”. An example for “meta.arepo” is available in “Paperboats/misc/”.

Amun

In case Amun is the MHD code, the procedure is analog to the case for Pencil. Please replace “Pencil_data/”, “Ascii_data/” and “meta.pencil” by “Amun_data/”, “data/” and “meta.amun”, respectively. Please copy all hdf5-files and also “totals.dat” into the folder “data/”. An example for “meta.amun” is available in “Paperboats/misc/”.

3 RUNNING PAPERBOATS

To start Paperboats, please go to the folder “Paperboats/” and type in the bash:

chmod u+x Run.sh

./Run.sh

This starts a series of processes:
Paperboats should compile and start now automatically. Results are written into the folder “Results/” which is automatically generated. Please be aware: If there exists already a folder “Results/”, **all existing files in this folder will be deleted or overwritten.** It is recommended to rename the folder “Results/” after completing a simulation.

After finishing Paperboats, a plotting script will produce plots in the folder “Results”. The plotting script uses gnuplot, so in case gnuplot is not installed on the machine, you should do so or write your own plotting script. For the beginning, the usage of gnuplot is recommended. The plots produced are in pdf format.

After the plotting, a video generator starts to produce videos from the pdf plots. This can take a while, depending on the number and size (MBs) of the pdfs between seconds and hours. Moreover, other packages like mogrify and ffmpeg are required. For the beginning, videos are not needed and the sequence can be simply interrupted.

4 PARAMATERS FOR THE SET-UP AND THE DUST

All changes to the post-processing have to be done in the files “Dust.tab” and “Process.tab” (which are the only two input files) in the “Paperboats” folder before starting “Run.sh”.

In “Process.tab”, dust processes can be selected or switched off, and the number of cores, the MHD code, the boundary conditions and the evolution scenario are specified.

In “Dust.tab”, all dust parameters are specified: Number of grain sizes, number and kind of grain size distributions, distribution parameters, dust materials, grain size limits as well as the gas-to-dust mass ratio.

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