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1 Introduction

Torch is a star formation simulation code with magnetohydrodynamics (FLASH), radiative transfer (Fervent), selfgravity & sinks, star particles, feedback (stellar winds, SNe), stellar evolution tracks (SeBa), and N-body dynamics (AMUSE). Torch features and add-ons are listed in Figure 1, and references for the major components are in Appendix A.

You can find a high-level overview of the code in:

- Wall+ 2019, arXiv:1901.01132
- Wall 2019, Ph.D thesis

Torch comprises (1) interface code that plugs into both FLASH and AMUSE, and (2) a good number of add-on code units for FLASH. To use Torch, you install interface code into both FLASH and AMUSE, compile FLASH alone, and then compile an AMUSE "worker" binary that enables FLASH to be called from AMUSE python scripts.

Flash (AMUSE interface)		ph4 / Multiples / SeBa
MHD (Fryxell+2000)	Atomic cooling (Hill+2012)	N-body (McMillian)
Rad Trans (Bacynzski+2015)	Mol cool (Neufield+1996)	Binary formation (McMillan+)
Winds (Markova+2008,Vink+2000, Kudritzski+2000)	Dust<->Gas (Hollenbach+1989)	Binary dynamics (McMillan+)
SN (Simpson+2016)	Background FUV (Weingartner+2001)	Binary accretion (PZ+1996)
Star formation (Sormani+2017)	Cosmic rays (Galli+2015)	Stellar flux (Lanz+2003)
Ionization fraction solver	Local gas extinction (Banerjee+2006)	SE (PZ+1996)
Ionization heating (Bacynzski+2015)	Radiation momentum	Stellar mass loss rate (other than OB winds) (PZ+1996)
FUV local stellar heating (Weingartner+2001)	EUV on dust (Draine 2011)	

Figure 1. Adapted from Wall+ 2018, MODEST conference proceedings

2 Quick Start

Torch has many moving parts. You'll likely have to adjust the procedure below for your personal setup. In any case, don't despair! Torch has been successfully built and run on a variety of systems.

We assume that you're using (1) the bash shell, and (2) conda for Python package management. But, the setup procedure should work for any shell and Python package manager with some adjustments.

2.1 Prerequisites

- FLASH 4.6.2: http://flash.uchicago.edu/site/flashcode
- AMUSE: https://github.com/amusecode/amuse
- Torch: https://bitbucket.org/torch-sf/torch
- Python 3.X (below setup assumes Conda)
- MPI
- HDF5

• git, wget

To download FLASH, you'll need to register, which takes a few days.

To download AMUSE, do:

```
cd your/code/directory
git clone https://github.com/amusecode/amuse.git
```

To download Torch:

```
cd your/code/directory
git clone https://bitbucket.org/torch-sf/torch.git
```

MPI and HDF5 may be pre-installed if you are using a cluster. If not, you will have to install these packages from source. Be sure to use the same compiler set that you will use for the rest of this Torch build.

Torch is known to work with OpenMPI 2.x, 3.x, and 4.x; HDF5 1.8.x and 1.10.x.

git and wget, if not already provided by your system, can be installed in your custom conda environment (see next section) with conda install git wget.

2.2 Environment setup (Josh thesis Appendix A.1)

Start a new shell session. You may want to check your .bashrc for any old MPI or HDF5 configuration that could conflict with Torch setup – module load commands, environment variable exports, et cetera – and comment them out.

Load MPI and HDF5 into your environment. If you're using shared cluster builds, do something like:

```
module load OpenMPI/x.y.z/blah # for clusters with lmod
module load HDF5/x.y.z/blah
```

Else, if you built MPI or HDF5 from scratch, set your environment manually. You can check what environment variables might be needed by calling module show on existing HDF5 or MPI builds on your cluster. An example for one cluster is below:

```
export MPI_HOME=/path/to/openmpi-x.y.z
export MPI_RUN=/path/to/openmpi-x.y.z/bin/mpirun
export PATH=$MPI_HOME/bin:$PATH
export MANPATH=$MPI_HOME/share/man:$MANPATH
export LD_RUN_PATH=$MPI_HOME/lib:$LD_RUN_PATH
export LD_LIBRARY_PATH=$MPI_HOME/lib:$LD_LIBRARY_PATH
export CPATH=$MPI_HOME/include:$CPATH
export HDF5_HOME=/path/to/hdf5-x.y.z
export HDF5DIR=/path/to/hdf5-x.y.z/lib
export HDF5INCLUDE=/path/to/hdf5-x.y.z/include
export HDF5LIB="hdf5_fortran -lhdf5"
export PATH=${HDF5_HOME}/bin:$PATH
export LD_LIBRARY_PATH=${HDF5_HOME}/lib:$LD_LIBRARY_PATH
export LD_RUN_PATH=${HDF5_HOME}/lib:$LD_RUN_PATH
export LIBRARY_PATH=${HDF5_HOME}/lib:$LIBRARY_PATH
export C_INCLUDE_PATH=${HDF5_HOME}/include:$C_INCLUDE_PATH
export CPLUS_INCLUDE_PATH=${HDF5_HOME}/include:$CPLUS_INCLUDE_PATH
```

Setup a clean, isolated Python environment for AMUSE:

```
mkdir {your/conda_env/directory}
conda create --prefix {your/conda_env/directory}/{env_name} python=3
source activate {your/conda_env/directory}/{env_name} # give absolute path so conda can find your env
```

Install some Python packages required by AMUSE:

conda install ipython matplotlib numpy scipy docutils gsl gmp h5py mpfr nose conda clean --all pip install --no-cache-dir mpi4py

2.3 Install Torch

Declare the following environment variables:

```
export AMUSE_DIR=/path/to/amuse
export FLASH_DIR=/path/to/FLASH4.6.2
export TORCH_DIR=/path/to/torch
```

Then, cd to the torch repo and do:

./install.sh

This will copy interface files from torch to both the AMUSE and FLASH repos.

2.4 Build FLASH (Josh thesis Appendix A.2 + FLASH docs)

Let's cd to the FLASH4.6.2 directory and setup a turbulent sphere collapse problem.

First, create a Makefile.h in FLASH4.6.2/sites/mysitedir. We recommend that you fork an example file from sites/Prototypes. You may have done this already while traversing the FLASH manual's quick start.

If you used the example Makefile.h for the Netherlands supercomputer Cartesius in Josh's thesis, you may need to (1) remove -march=core-avx2 flags throughout, and/or (2) remove -lhdf5_fortran from the LIB_HDF5 variable declaration.

Then, issue the setup command (update "mysitedir"):

```
./setup Cube -auto -3d +amuseUSM +amuseMG +rayPE +HandCnew +amuseSinksAndStars +amuseWind +enerinj \
    +supportPPMupwind +pm4dev -maxblocks=100 +cube16 \
    --site={mysitedir}
```

Compile FLASH. The flash4 binary is not needed for the AMUSE/FLASH bridge, but compiling FLASH alone helps to catch errors and save time in the AMUSE compile step.

<mark>cd</mark> object make -j

2.5 Install AMUSE and Torch as Python packages

Run the following commands:

```
cd $AMUSE_DIR
pip install -e .
cd $TORCH_DIR
pip install -e .
```

The flag -e installs both AMUSE and Torch modules in development mode, so that any changes you make to your AMUSE and Torch directories are immediately visible to your Python installation; Python imports will take the module directly from your git-cloned directories. An alternative to the pip install procedure is to set the PYTHONPATH environment variable manually, like so:

```
export PYTHONPATH=$PYTHONPATH:$AMUSE_DIR/test
export PYTHONPATH=$PYTHONPATH:$AMUSE_DIR/src
export PYTHONPATH=$PYTHONPATH:$TORCH_DIR/src
```

2.6 Configure AMUSE (Josh thesis Appendix A.3 + AMUSE docs)

Now, cd to the AMUSE repository. You can follow the AMUSE docs up to the make step, but take a look at these notes for extra information.

If you used a local conda environment following this guide, you may need to tell **configure** where HDF5, FFTW, GMP, MPFR, and GSL reside.

Here is an example configure call for the Netherlands supercomputer Cartesius (early 2019):

```
./configure \
    --with-fftw=/hpc/eb/RedHatEnterpriseServer7/FFTW/3.3.8-gompi-2018b \
    --with-hdf5=/hpc/sw/hdf5-1.8.12-intel-seq \
    --with-gmp={your/conda_env/directory}/{env_name} \
    --with-mpfr={your/conda_env/directory}/{env_name} \
    --with-gsl-prefix={your/conda_env/directory}/{env_name}
```

Library path errors are rather common at this step. FFTW and NetCDF library errors are OK, but HDF5 library and/or header errors are not OK. The STDOUT from a successful configure build should include something like:

```
checking Using provided HDF5 C wrapper... /path/to/bin/h5pcc
checking for HDF5 type... parallel
checking for HDF5 libraries... yes (version 1.10.5)
checking for hdf5.h... yes
checking for H5Fcreate in -lhdf5... yes
checking for main in -lhdf5_hl... yes
checking for matching HDF5 Fortran wrapper... /path/to/bin/h5pfc
```

See Section 5.3 for more troubleshooting suggestions.

You may need to manually edit the files:

```
config.mk
src/amuse/community/flash/Makefile
```

to select the correct compilers and libraries.

Now, you can make the AMUSE flash_worker, which is basically an AMUSE-hooked replacement for the normal flash4 executable. The standard make takes 10-20 minutes and builds all the codes included in AMUSE. To request only the codes needed for Torch, do:

make framework make flash.code make kepler.code make ph4.code make seba.code make smalln.code

A successful make will create flash_worker in src/amuse/community/flash/.

2.7 Run a Torch simulation (Josh thesis Appendix B)

You are now ready to run a Torch simulation! We will simulate a $3 \times 10^3 M_{\odot}$, 5 pc radius gas sphere in ± 7 pc cubic domain with outflow boundary conditions. In about a free-fall time (≈ 2 Myr), the cloud will collapse under its own gravity, create a sink particle, and begin forming stars.

Choose a directory for your simulation and cd there. Then do:

```
ln -s $TORCH_DIR/cool.dat
ln -s $TORCH_DIR/cube128
cp $TORCH_DIR/torch_user.py torch_user.py
cp $TORCH_DIR/flash.par.turbsph_standard flash.par
mkdir data
```



Figure 2. Density in x-y plane.

The file torch_mainloop.py is the heart of the simulation. It performs the split time-evolution with both FLASH and the n-body integrator ph4, handles stellar evolution, and lots more. torch_user.py is the main source of control for users of Torch, where parameters can be set and initial stellar conditions defined.

The simulation should take 1–10 minutes to reach $t_{\text{max}} = 2 \text{ Myr} = 6.31 \times 10^{13} \text{ s.}$ It will use 7 threads: 2 for FLASH, 1 for n-body integration (ph4), 2 for n-body binary interactions (multiples), 1 for stellar evolution, and 1 for AMUSE itself. At around 1 Myr, a sink particle will form and begin creating stars. One or a few $\geq 7M_{\odot}$ stars may begin blowing a wind, so the time step may drop; you may wish to end the simulation early.

To run the simulation interactively, execute the command:

mpiexec -n 1 python torch_user.py

On a compute cluster with Slurm, copy run.sh from the torch repository to your simulation directory. Edit the SBATCH options as needed. Then do:

sbatch run.sh

If you increase the number of tasks requested, torch_user.py will automatically assign more threads (workers) to FLASH.

Log files will be dumped in your current working directory, and simulation outputs will be written to the data/ directory. If you re-start a simulation, Torch (FLASH) will overwrite existing data, but append to (some) existing logs. You may want to rename or delete your old logs to help keep track of your runs.

2.8 Look at the output

Let's have a quick look at this gestating star cluster. The example plots here were created with the yt package, version 3.4.1. To learn more about yt, visit http://yt-project.org/. To install yt:

conda install yt conda clean --all

We can first look at density-slice plots in the three coordinate planes (x-y, x-z, y-z). At the command line, call:

yt plot data/turbsph_forced_hdf5_plt_cnt_0000

or, if you don't have a "forced" plot output, use the last "plt_cnt" file dumped by the simulation. This will create a new directory **frames**/ with three plots similar to Figure 2.



Figure 3. Star particles. Size is proportional to mass; red particles have dm/dt > 0 (wind-blowing stars), blue particles have dm/dt = 0 (quiescent).

How about the particles? Let's see how they're distributed, and inspect some of their other properties. In a Python session:

```
import numpy as np
import matplotlib.pyplot as plt
import yt
ds = yt.load('data/turbsph_hdf5_plt_cnt_0018')
ad = ds.all_data()
ppx = ad['all', 'particle_posx'].to('pc').value
ppy = ad['all', 'particle_posy'].to('pc').value
ppm = ad['all', 'particle_mass'].to('Msun').value
windy = ad['all', 'particle_dmdt'].value
windy [windy > 0] = 1
plt.scatter(ppx, ppy, s=ppm*6, c=windy, cmap='bwr', alpha=0.5)
plt.gca().set_aspect('equal')
plt.xlim(-2.5, +2.5)
plt.ylim(-2.5, +2.5)
plt.xlabel('x (pc)')
plt.ylabel('y (pc)')
plt.show()
```

In this particular simulation, three stars are massive enough to blow a wind (Figure 3).

2.9 Next steps

To tweak the simulation parameters, you will need to edit flash.par and torch_user.py. These two files specify most of the configuration options for the simulation.

Torch comes packaged with a few simulations in FLASH4.6.2/source/Simulation/SimulationMain/

Cube EnergyInjection StratBox

which provide initial conditions for (1) a turbulent gas sphere initialized from a 128^3 array, (2) a uniform medium for testing a stellar wind or supernova, and (3) a planar gas layer in a periodic domain, driven by random thermal supernova explosions.

It's often useful to reduce the number of Torch features for study or debugging. Below are setup calls showing some reduced feature sets:

Full Torch code with AMUSE/FLASH coupling.

```
./setup Cube -a -3d +amuseUSM +amuseMG +rayPE +HandCnew +amuseSinksAndStars \
        +amuseWind +enerinj +supportPPMupwind +pm4dev -maxblocks=100 +cube16
```

FLASH-only simulation, no AMUSE coupling. Sinks will work, but no stars will form.

```
./setup Cube -a -3d +usm +gravMgrid +rayPE +HandCnew +amuseSinksAndStars \
    +amuseWind +enerinj +supportPPMupwind +pm4dev -maxblocks=100 +cube16
```

FLASH-only simulation, no ray-tracing or sinks/stars. Only self-gravity and heating/cooling.

```
./setup Cube -a -3d +usm +gravMgrid +HandCnew \
    +supportPPMupwind +pm4dev -maxblocks=100 +cube16
```

FLASH-only simulation, only MHD.

./setup Cube -a -3d +usm +supportPPMupwind +pm4dev -maxblocks=100 +cube16

Note that **+rayPE** generally requires **+amuseSinksAndStars**. These setup flags are aliases for various FLASH units; the flags are defined in FLASH4.6.2/bin/setup_shortcuts.txt.

Don't forget that after a fresh setup + compile of FLASH, you will need to recompile the AMUSE worker too.

3 VorAMR: Expanded Options for Initial Conditions

A normal Torch run initializes from a "cubefile" like cube128 or one generated from turb-sphere.py. These initial conditions are currently restricted to spherical clouds with a turbulent velocity distribution and gaussian density profile or something similar. While such ICs make for easy first steps for users to setup a new Torch simulation, ideal ICs would come from systems that evolved self-consistently in galactic environments.

VorAMR was created to allow for output data from other star formation software suites to be used as initial conditions in Torch. Currently, VorAMR has only been shown to be able to convert data from the star formation code AREPO into Torch ICs, but in theory can be easily adapted to convert ANY moving-mesh, AMR, or SPH code into Torch ICs.

3.1 How VorAMR works



Figure 4. VorAMR logic flow.

VorAMR uses output data from other hydro-codes to build a refined grid in FLASH and then populate that grid with field values (density, internal energy, velocity, etc.) via the AMUSE interface. By doing this all within the Torch framework, the resulting grid and initial gas/particle properties allows Torch to immediately launch into a simulation but with external data as its initial conditions.

VorAMR takes advantage of the "refine_on_particle" routines within FLASH to construct a refined grid that as accurately as possible mirrors the local mesh scale of the AREPO data. VorAMR also uses a nearest-neighbor NDInterpolator to fill the FLASH grid cells with the field data of the nearest Voronoi mesh element (and therefore the element which encapsulates the cell center).

3.2 How to use VorAMR

VorAMR is installed alongside Torch but is turned off by default; Torch operates normally with VorAMR turned off. To turn VorAMR on, switches must be flipped in the flash.par file. Note, the file flash.par.turbsph_standard does not have VorAMR switches, flash.par.voramr is meant to be identical but with the VorAMR switches included.

```
# =================
# VorAMR extension
use_voramr = .true. # main control switch
voramr_source = "snapshot_518_9.hdf5" # source data to be converted
voramr_input = "voramr_input.hdf5" # name of file to be read-in by FLASH
refine_on_particle_count = .true. # builds grid based on source data - BE SURE TO TURN OFF FOR NORMAL TORCH
min_particles_per_blk = 4096 # Assumes 16x16x16 blocks
                      = 4096
max_particles_per_blk
pt_maxPerProc
                        = 10000000 # Enough to fit all particles on one proc - CAN BE REDUCED FOR NORMAL
    TORCH
refineonjeanslength = .true.
# Restrict initial refinement by only placing particles within radius
use_localRef = .false.
center_localRef = .false. # Crops FLASH domain centered at localRef_{x,y,z} and centers new domain
# Local refinement center and radius
localRef_x = 3.20621187e+20 # cm
localRef_y = 6.24367575e+20
localRef_z = -1.51873194e+20
localRef_r = 1.543e+20
# Background Potential
sim_withStaticGrav = .true.
            # AREPO 518_9 # Hill et al 2012
sim_aParm1 = 1.31142525e-72 #4.39996789e-9 # [cm/s^2]
                                                           # 1.42E-3 [kpc/Myr^2]
sim_aParm2 = 1.35401904e-52  #5.51293615e-31 # [1/s<sup>2</sup>]
                                                           # 5.49E-4 [1/Myr^2]
sim_aParm3 = -2.36078509e-30 #5.55421965e20 # [cm]
                                                            # 0.18E0 [kpc]
sim_aParm4 = 4.06112841e-11 #1.62715932e-53 # [1/(cm s^2)] #5 .0E-5 [1/kpc Myr^2]
```

Some of these switches are reflected in the torch_user.py file, all flashp['...'] data is extracted directly from flash.par:

```
p = {}
flashp = FlashPar("flash.par")
# <VorAMR>
p['with_voramr'] = flashp['use_voramr']
p['source_file'] = flashp['voramr_source']
p['convert_file'] = True # Runs source_file through src/voramr/hdf5_convert.py
p['use_localRef'] = flashp['use_localRef']
p['local_ref'] = [flashp['localRef_x'], flashp['localRef_y'], flashp['localRef_z'],
flashp['localRef_r']]
p['center_local_ref'] = flashp['center_localRef']
p['input_file'] = flashp['voramr_input']
```

```
p['pickle_kdtree'] = False # saves kdtree built from source_file used in interpolation. Useful if
memory strained.
p['pickle_file_name'] = "kdtree.pickle"
p['numBlocks'] = 15000 # Quirky parameter, just set to any number larger than total num actual blocks
and FLASH will figure it out.
p['cellsPerBlock'] = 16
```

Once VorAMR is turned on, install torch as normal . ./install.sh.

Then, setup FLASH with enough MAXBLOCKS to allow for the expected refined grid to fit on a single processor.

```
./setup Cube -a -3d +amuseUSM +amuseMG +rayPE +HandCnew +amuseSinksAndStars \
    +amuseWind +enerinj +supportPPMupwind +pm4dev -maxblocks=10000 +cube16
```

Change the 'lrefine_max' value in flash.par to be whatever level you wish the grid to reach at its highest refinement regions. To acheive maximum consistency with the structure of the input data, 'lrefine_max' should be set such that the highest refinement FLASH blocks will contain as many input data points as cells (4096 for +cube16 blocks).

If your source data contains star particles that you would like to include in Torch, edit user_initial_conditions() in torch_user.py to read in the particle data, incorporate them into an AMUSE particle set, and initialize them via the hydro class.

It is then recommended to change the following flash.par parameters to force VorAMR to output a checkpoint file as fast as possible. That resulting checkpoint can the be restarted from with VorAMR turned off.

```
tmax = 6.30e8 # two init timesteps
dtinit = 3.15e8
dtmin = 3.15e7
checkpointFileIntervalTime = 3.15e7 # dt_min
plotFileIntervalTime = 3.15e8
particleFileIntervalTime = 3.15e8
```

Finally, run Torch with only 1 processor assigned to flash_worker (if running default worker partitions, this would be 6 total processors: 1 driver, 2 ph4, 1 SeBa, 1 multiples, 1 FLASH). Note, when restarting from a VorAMR checkpoint, any number of processors can be used as long as use_voramr = .false.

In addition to the usual Torch output, VorAMR produces two more files:

- 1. voramr_input.hdf5 the particle data extracted from the source data. This is what FLASH sees and will refine on.
- 2. interp-data.hdf5 the file from which the interpolation kdtree is built. Only AMUSE sees this file, but then passes info from it to FLASH. This file will always contain all data from the source file.

These files are both produced as sometimes we only want FLASH to refine on a portion of the source data, but we want AMUSE to have an accurate kdtree for all data to avoid domain edge effects during interpolation.

4 Caveats and Known Issues

4.1 Torch Issues

Unphysical hot/empty zones are a common problem in finite volume codes, and are readily generated by underresolved supernovae and stellar winds in Torch. To combat such zones, a few tactics include:

- Lower CFL
- Restart with more diffusive hydro solver parameters, temporarily
- Manually smooth out extremely sharp gradients
- Enable or increase artificial shock viscosity.

- Use the time-step limiter for positive-definite cell values (already enabled in the example Torch flash.par files). This is controlled by the FLASH runtime parameter dr_usePosdefComputeDt, among others.
- VorAMR is currently hardcoded to extract data from and refine on data from AREPO file structures. To change to other file structures, edits will need to be made to at least src/voramr/hdf5_convert.py and possibly src/flash/source/Simulation/SimulationMain/Cube/pt_initVoronoiPositions.F90

See http://flash.uchicago.edu/pipermail/flash-users/2019-May/002908.html for a nice explanation by Sasha Tchekhovskoy.

In the FLASH unsplit solver, the logic for the hybrid Riemann solver is slightly altered; see the torch file: src/flash/source/physics/Hydro/HydroMain/unsplit/hy_uhd_dataReconstOneStep.F90

Torch does not support the use of BHTree with AMUSE. Code exists to hook FLASH/BHTree and AMUSE together, but it needs a small update and some testing to work.

Several add-on ParticleInitialization, ParticleMapping, etc. units are provided with Torch. These were created to trace supernova and superbubble ejecta in stratified box simulations run by Ibanez-Mejia et al. (2017). However, these have not been tested with the Torch sink/star framework and probably will not work correctly as is.

The module source/physics/sourceTerms/GridInject is in development and not recommended for use yet.

4.2 VorAMR Issues

VorAMR is capable of building Torch-ready initial conditions from ANY hydrodynamical simulation output. But, VorAMR is limited in how quickly it can complete this process. Luckily, a user will only have to use VorAMR once for a major production run, so the initial cost of time is generally worthwhile.

- VorAMR can only run with ONE oversubscribed processor for the flash_worker due to the use of serial HDF5 open/read calls within FLASH. Data conversion and grid build times can be on the order of days.
- Users are recommended to augment a Torch+VorAMR run to output a checkpoint file after ONE timestep. Then, restart from the checkpoint in a clean Torch build without VorAMR turned on.
- Sometimes VorAMR will run fine, but the resulting grid does not appear to be refined. Check in turbsph.log and see if the number of particles reported matches the dimensions of the array sent so FLASH (reported in slurm file) and what FLASH actually reads (reported in flash_worker.out). If there is a mismatch, then it's likely that some refinement particles are being placed outside of the computational domain. Make sure your domain dimensions correctly reflect the source data.

5 Help!

5.1 General checks

- Are all packages built using the same compiler set?
- Check your environment variables. Is PATH pointing somewhere it shouldn't? Are two different installs/versions of a module visible in PATH?
- Anaconda or Conda may provide its own HDF5. If you are using this HDF5, great, but if you are using a system HDF5 install, not so great. Check your PATH and make sure that the desired system HDF5 comes before the Anaconda/Conda HDF5.
- Check that FLASH, AMUSE, and mpi4py are using the same HDF5 and MPI libraries.
- If you had to swap MPI modules and reinstall mpi4py at any point, pip install needs the --no-cache-dir flag or else mpi4py's compiled object library will not be reinstalled. You can check that mpi4py is linked to the correct MPI library by doing:

ldd {your/conda_env/directory}/{env_name}/lib/python2.7/site-packages/mpi4py/MPI.so

• Here are some commands that may help diagnose library and path problems:

module list
module show some/module/name
which python
which mpiexec
python -c "from mpi4py import MPI; print MPI"
ldd flash4
ldd flash_worker

5.2 FLASH setup/compile problems

- make fails immediately with something like /usr/local/mpich2//bin/mpif90: Command not found. Check that you are using the correct Makefile.h, with MPI_PATH and HDF5_PATH appropriate for your system.
- make is slow.

Try make -j to use multiple processes.

• make succeeds, but flash4 or flash_worker fails at runtime with error like error while loading shared libraries: libhdf5.so.8: cannot open shared object file.

Take a look at http://flash.uchicago.edu/pipermail/flash-users/2013-July/001322.html.

• FLASH runs out of memory.

Reduce MAXBLOCKS or allocate more memory per core. The memory cost can be estimated as:

```
(NUNK_VARS + NFACEVAR + NFLUXVAR) * (NXB + 2*NGUARD) * (NYB + 2*NGUARD) * (NZB + 2*NGUARD) * MAXBLOCKS * (8 bytes)
```

where the variables are defined in FLASH4.6.2/object/Flash.h. For example, with NUNK_VARS=46, NFACEVAR=2, NFLUXVAR=12, NXB=NYB=NZB=16, NGUARD=6, and MAXBLOCKS=100, the memory usage is around 1 GB.

5.3 AMUSE configure/make problems

• How do I troubleshoot X configure error?

A few places to look include: STDOUT from configure, config.log, and the source code of configure itself.

Also, ./configure --help may give an idea of tunable parameters.

• FLASH alone compiles, but the AMUSE flash_worker build fails with library errors.

Try comparing, piece-by-piece, the command-line invocations of mpif90 for FLASH alone versus flash_worker to make sure that -L and -l flags are sensible.

You can manually edit some compiler flags in config.mk, located in the top-level AMUSE directory.

5.4 Runtime and MPI problems

• AMUSE fails spawn processes over > 1 cluster node, but works if all processes are on the same node. MPI may hang, or return errors of form (for Intel MPI).

HYDT_dmx_register_fd ({...}demux.c:101): registering duplicate fd 0
HYDT_bscd_slurm_launch_procs ({...}/slurm_launch.c:258): demux returned error registering fd
...
main (../../ui/mpich/mpiexec.c:1118): process manager error waiting for completion

One known solution: use OpenMPI, and do not overspecify Slurm sbatch or srun options, give only -n. A general solution is not known. This was seen with a relatively old AMUSE version, and may be resolved in newer versions.

For OpenMPI specifically:

• How do I get information about the OpenMPI build on my cluster?

The command ompi_info reports how a given OpenMPI installation was built, e.g., version, compiler, configure flags, etc.

• How do I set MCA parameters?

https://www.open-mpi.org/faq/?category=tuning#setting-mca-params

• How do I fix runtime warnings about infiniband ports?

```
By default, for Open MPI 4.0 and later, infiniband ports on a device
are not used by default. The intent is to use UCX for these devices.
You can override this policy by setting the btl_openib_allow_ib MCA parameter
to true.
...
WARNING: There was an error initializing an OpenFabrics device.
Local host: t035
Local device: mlx5_0
```

Follow the suggestion and set btl_openib_allow_ib=1. The OpenMPI FAQ explains how to set MCA parameters.

5.5 Navigating the source code

• How do I decipher FLASH setup calls and runtime parameters?

Look at bin/setup_shortcuts.txt and object/setup_params. Appendix C lists the file strucutre for Flash when compiled for the turbulent sphere problem.

• A runtime parameter X has little or no documentation in object/setup_params. What do I do?

The file object/setup_params will tell you which unit declared the mysterious parameter. Once you figure out what it does, consider adding some documentation (in the FLASH unit's Config file) and submitting a pull request to the Torch repository!

• How do I quickly track down a FLASH error message?

In the object directory,

grep -I "my error message" *

The flag -I instructs grep to ignore binary files, greatly speeding up the search.

A Torch component references

This list includes most major components, but is not comprehensive.

- FLASH: user's guide, Fryxell+ 2000
- PARAMESH (in vanilla FLASH): archived v4.1 manual
- AMUSE: documentation, book
- Fervent (radiative transfer): Baczynski+ 2015, Baczynski 2015, Ph.D thesis
- Multigrid (self-gravity): Ricker+ 2008
- BHTree (self-gravity): Wünsch+ 2018
- Sink particles: Federrath+ 2010
- Multiples (N-body): AMUSE book (see Sec. 4.5)
- Stratified box setup: Joung & Mac Low 2006, Ibáñez-Mejía+ 2016

B Notes on build process for specific clusters

B.1 Cartesius

CARTESIUS IS NOW DISCONTINUED - We leave the build instructions here as many of the steps are similar to other systems. Also, while SURF has now brought Cartesius offline, its replacement Snellius has a similar module file structure.

Cartesius is the Dutch national supercomputer managed by the cooperative educational and scientific association SURFsara. Many projects have utilized Cartesius and its up-to-date hard/software are well suited for the many projects involving Torch.

To run Torch on Cartesius, you will need to first request an account on the computer. Logging on to Cartesius is straight forward: ssh [username]@doornode.surfsara.nl which will then allow you to select cartesius after asking for your password. At this stage, you will be able to use Cartesius in its full capacity but you will not be able to scp over your FLASH repository until your IP address is whitelisted. This can be accomplished by providing your IP to the Surfsara help center. You will be able to use git to bring over the torch repository to install everything.

Before we install anything however, you must make sure to use the appropriate software packages. Cartesius operates by use of user-chosen modules to be loaded prior to any process you wish to run. Either by editing your .bashrc or creating your own bash script to be run at login, you will need to load the updated module environment, as well as the individual modules required by torch.

```
module load 2019
module load foss/2018b
module load Python/2.7.15-foss-2018b
module load HDF5/1.10.2-foss-2018b
module load h5py/2.8.0-foss-2018b-Python-2.7.15
module load GSL/2.5-iccifort-2018.3.222-GCC-7.3.0-2.30
export MODLOC=/sw/arch/RedHatEnterpriseServer7/EB_production/2019/software
export MPIHOME=$MODLOC/OpenMPI/3.1.1-GCC-7.3.0-2.30
export OMPI_MCA_mpi_warn_on_fork=0
```

At this point, following the installation steps for Torch should result in a fully functioning software suite!

Preparing a run. Make sure to edit the flash.par file you are using such that the output_directory is pointed to your desired directory and make sure your module list script has been executed (an easy check is typing which mpiexec in the command line).

Starting a run. Cartesius uses the **slurm** job managing system and so is fairly straightforward to use. Here I have provided my run.sh script that I deliver to Cartesius with **sbatch run.sh**. The script contains parameters read by the slurm system as well as the command you want executed.

```
#!/bin/sh
#SBATCH --job-name=[informative-job-name]
#SBATCH -n [number of procs]
#SBATCH --time=[day]-[hour]:[min]:[sec]
#SBATCH --mail-user=[your-email@email.com]
#SBATCH --mail-type=[email condition]
mpiexec --mca orte_base_help_aggregate 0 -n 1 python bridge_multiples.py
```

It may take some time before your run makes it through the waitlist. Once it does, there will be some information output in your simulation directory where you ran the script. The most useful file is the one named slurm-#####.out which is where your screen output is redirected to. I check this periodically to see what simulation time my run has achieved, how many stars I've made, if it is hung up on a process, etc.

B.2 Cartesius - Refactor

CARTESIUS IS NOW DISCONTINUED AND THE REFACTOR BRANCH HAS SINCE BEEN MERGED INTO MAIN - The refactored version of Torch (on git branch refactor) uses the latest AMUSE commit on branch master which requires Python 3.X as well as FLASH version 4.6.2. The setup for the refactored version of Torch on Cartesius is largely the same as the master (now called main) branch as described in this document but with a dew caveats.

Firstly, make sure you download and unzip FLASH4.6.2. This can be done from the same FLASH distribution webpage from which FLASH4.5 or earlier versions can be accessed.

Second, make sure to have the AMUSE master branch checked out and is at the most recent commit.

In order to satisfy AMUSE's Python 3.X requirements, we will need to establish a module environment that's a bit different from the one described in Appendix B.1:

```
module load 2019
module load foss/2018b
module load Python/3.6.6-fosscuda-2018b
module load HDF5/1.10.2-foss-2018b
module load h5py/2.10.0-fosscuda-2018b-Python-3.6.6
module load GSL/2.5-iccifort-2018.3.222-GCC-7.3.0-2.30
module load pytest/4.4.0-fosscuda-2018b-Python-3.6.6
export MODLOC=/sw/arch/RedHatEnterpriseServer7/EB_production/2019/software
export MPIHOME=$MODLOC/OpenMPI/3.1.1-GCC-7.3.0-2.30
export OMPI_MCA_mpi_warn_on_fork=0
```

In addition to this slightly altered environment, the Cartesius Python 3.6.6 module does not currently have the matplotlib and docutils libraries installed. This is okay, we can just install them ourselves in our user environment using pip install --user matplotlib docutils after loading the Python/3.6.6-fosscuda-2018b module.

Finally, if running this module environment setup reports any error (such as "XYZ module cannot load due to conflict") try running the same environment setup file again and there should be no issue.

B.3 Snellius

The below modules and setup notes are from Brooke Polak with additions by Sean Lewis. Load the following modules (Summer-Fall 2022):

Load Modules

```
module load 2021
module load Python/3.9.5-GCCcore-10.3.0
module load h5py/3.2.1-foss-2021a
module load GSL/2.7-GCC-10.3.0
#module load Anaconda3/2021.05
#module load HDF5/1.10.7-gompi-2020a
```

```
# Specific Paths
export MODLOC=/sw/arch/Centos8/EB_production/2021/software
export MPIHOME=$MODLOC/OpenMPI/4.1.1-GCC-10.3.0
export MPI_HOME=$MODLOC/OpenMPI/4.1.1-GCC-10.3.0
export MPI_RUN=$MODLOC/OpenMPI/4.1.1-GCC-10.3.0/bin/mpirun
export PATH=$MPI_HOME/bin:$PATH
export MANPATH=$MPI_HOME/share/man:$MANPATH
export LD_RUN_PATH=$MPI_HOME/lib:$LD_RUN_PATH
export LD_LIBRARY_PATH=$MPI_HOME/lib:$LD_LIBRARY_PATH
export CPATH=$MPI_HOME/include:$CPATH
export HDF5_HOME=$MODLOC/HDF5/1.10.7-gompi-2021a
export HDF5DIR=$MODLOC/HDF5/1.10.7-gompi-2021a/lib
export HDF5INCLUDE=$MODLOC/HDF5/1.10.7-gompi-2021a/include
export HDF5LIB="hdf5_fortran -lhdf5"
export PATH=${HDF5_HOME}/bin:$PATH
export LD_LIBRARY_PATH=${HDF5_HOME}/lib:$LD_LIBRARY_PATH
```

```
export LD_RUN_PATH=${HDF5_HOME}/lib:$LD_RUN_PATH
export LIBRARY_PATH=${HDF5_HOME}/lib:$LIBRARY_PATH
export C_INCLUDE_PATH=${HDF5_HOME}/include:$C_INCLUDE_PATH
export CPLUS_INCLUDE_PATH=${HDF5_HOME}/include:$CPLUS_INCLUDE_PATH
export OMPI_MCA_mpi_warn_on_fork=0
export AMUSE_DIR=$HOME/2023feb-vorch/amuse
export FLASH_DIR=$HOME/2023feb-vorch/FLASH4.6.2
export TORCH_DIR=$HOME/2023feb-vorch/torch
export PYTHONPATH=$TORCH_DIR:$PYTHONPATH
export PYTHONPATH=$TORCH_DIR/src:$PYTHONPATH
export PYTHONPATH=$AMUSE_DIR/test:$PYTHONPATH
export PYTHONPATH=$AMUSE_DIR/src:$PYTHONPATH
export CONDA_PATH={path to your conda env.}
# Activate conda environment
conda activate $CONDA_PATH
export PYTHON=$CONDA_PATHbin/python
MCA_Settings='--mca orte_base_help_aggregate 0 '
UCX_Settings='-x UCX_NET_DEVICES=mlx5_0:1'
```

Now follow the usual quickstart procedure. Here are some fixes that might be needed during that process.

- In \$TORCH_DIR/src/flash/source/Particles/ParticlesMain/ray_pe/MultiSourceSimple/HEALPixModule.F90 Lines 209 and 250: iand(int(x),y) i.e. replace the first argument of iand with int(argument)
- In \$FLASH_DIR/bin/setup.py change sys.setcheckinterval() to sys.setswitchinterval()
- In \$FLASH_DIR/sites/snellius.surf.nl/Makefile.h add -fallow-argument-mismatch to FFLAGS_OPT

Then, FLASH can be setup and built.

```
./setup Cube -auto -3d +amuseusm +amusemg +raype +handcnew +amusesinksandstars +amusewinds +enerinj
        +supportppmupwind +pm4dev -maxblocks=100 +cube16 -site={mysitedir}
cd object
make -j
```

And AMUSE can be setup and the individual codes built. Note we need to make some under-the-hood changes to the .mk file after AMUSE is configured.

```
cd amuse
./configure --with-fftw=$MODLOC/FFTW/3.3.9-gompi-2021a
    --with-hdf5=$MODLOC/HDF5/1.10.7-gompi-2021a/bin/h5c++ --with-gmp=$CONDA_PATH --with-mpfr=$CONDA_PATH
    --with-gsl-prefix=/home/bpolak/TORCH/env/amuse_env
#note: some users found that "./configure" was sufficient without any of the --with flags.
#edit in amuse/config.mk:
MPIFC=/sw/arch/Centos8/EB_production/2021/software/OpenMPI/4.1.1-GCC-10.3.0/bin/mpifort
FCFLAGS=-g -O2 -fPIC -fallow-argument-mismatch
pip install -e .
make framework
make flash.code
make kepler.code
make ph4.code
make seba.code
make smalln.code
make petar.code
```

B.4 Mendel

The below modules and setup notes are from Eric Andersson.

All python related software was installed with pip rather than conda (Medndel did not have conda at the time). python venv was used to create a clean python environment for the installation, see details below.

Load the following libraries (note that FFTW is not available on Mendel as of March 21st, 2023) and export all necessary paths.

```
module load Python/python-3.8.5
module load OpenMPI/openmpi-4.0.4
module load HDF5/hdf5-1.10.1
export MPI_HOME=/usr/local/software/OpenMPI/openmpi-4.0.4
export MPI_RUN=/usr/local/software/OpenMPI/openmpi-4.0.4/bin/mpirun
export PATH=$MPI_HOME/bin:$PATH
export MANPATH=$MPI_HOME/share/man:$MANPATH
export LD_RUN_PATH=$MPI_HOME/lib:$LD_RUN_PATH
export LD_LIBRARY_PATH=$MPI_HOME/lib:$LD_LIBRARY_PATH
export CPATH=$MPI_HOME/include:$CPATH
export HDF5_HOME=/usr/local/software/HDF5/hdf5-1.10.1
export HDF5DIR=/usr/local/software/HDF5/hdf5-1.10.1/lib
export HDF5INCLUDE=/usr/local/software/HDF5/hdf5-1.10.1/include
export HDF5LIB="hdf5_fortran -lhdf5"
export PATH=${HDF5_HOME}/bin:$PATH
export LD_LIBRARY_PATH=${HDF5_HOME}/lib:$LD_LIBRARY_PATH
export LD_RUN_PATH=${HDF5_HOME}/lib:$LD_RUN_PATH
export LIBRARY_PATH=${HDF5_HOME}/lib:$LIBRARY_PATH
export C_INCLUDE_PATH=${HDF5_HOME}/include:$C_INCLUDE_PATH
export CPLUS_INCLUDE_PATH=${HDF5_HOME}/include:$CPLUS_INCLUDE_PATH
```

Create a clean python environment and install the following packages. Note that the Quick Guide asks for us to install gmp and mpfr. These are both included in gmpy2.

```
mkdir {directory/for/venv/}
cd {directory/for/venv/}
python3 -m venv {env_name}
source {directory/for/venv/env_name}/bin/activate
pip install ipython matplotlib numpy scipy docutils gsl gmpy2 h5py nose mpi4py
```

Follow the Quick Start Guide to set up AMUSE, FLASH and Torch.

In the FLASH Makefile, update the paths to MPI and HDF5 to point to \$MPI_HOME and \$HDF5_HOME. All other paths are left blank.

Instead of supplying ./configure with arguments when setting up AMUSE, all relevant paths are updated in **\$AMUSE_DIR/config.ml** directly. Note that since FFTW is not on Mendel this is one part where the Mendel set-up deviates from the Quick Start Guide. Ignoring FFTW is fine.

After this point everything is described in the guide.

B.5 Stampede2

This setup guide is credited to Brooke Polak.

After downloading AMUSE, Torch, and FLASH via git, load the following modules in \sim /.profile

```
module load gcc/9.1.0
module load impi/19.0.9
module load python3/3.8.2
module load hdf5/1.10.4
module load gsl/2.6
module load fftw3
```

And, specify your paths in \sim /.bashrc

export	AMUSE_DIR=/home1/05402/bp4928/TORCH/amuse
export	FLASH_DIR=/home1/05402/bp4928/TORCH/FLASH4.6.2
export	TORCH_DIR=/home1/05402/bp4928/TORCH/torch
export	MODLOC=/opt/apps
export	MPIHOME=/opt/intel/compilers_and_libraries_2020.4.304/linux/mpi/intel64
export	MPI_HOME=\$MPI_HOME
export	MPI_RUN=\$MPI_HOME/bin/mpirun
export	PATH=\$MPI_HOME/bin:\$PATH
export	MANPATH=\$MPI_HOME/share/man:\$MANPATH
export	LD_RUN_PATH=\$MPI_HOME/lib:\$LD_RUN_PATH
export	LD_LIBRARY_PATH=\$MPI_HOME/lib:\$LD_LIBRARY_PATH
export	CPATH=\$MPI_HOME/include:\$CPATH
export	HDF5_HOME=\$MODLOC/gcc9_1/hdf5/1.10.4/x86_64
export	HDF5DIR=\$HDF5_HOME/lib
export	HDF5INCLUDE=\$HDF5_HOME/include
export	HDF5LIB="hdf5_fortran -lhdf5"
export	PATH=\${HDF5_HOME}/bin:\$PATH
export	LD_LIBRARY_PATH=\${HDF5_HOME}/lib:\$LD_LIBRARY_PATH
export	LD_LIBRARY_PATH=\${TACC_MKL_LIB}:\$LD_LIBRARY_PATH
export	LD_RUN_PATH=\${HDF5_HOME}/lib:\$LD_RUN_PATH
export	LIBRARY_PATH=\${HDF5_HOME}/lib:\$LIBRARY_PATH
export	LIBRARY_PATH=\${TACC_MKL_LIB}:\$LIBRARY_PATH
export	C_INCLUDE_PATH=\${HDF5_HOME}/include:\$C_INCLUDE_PATH
export	CPLUS_INCLUDE_PATH=\${HDF5_HOME}/include:\$CPLUS_INCLUDE_PATH

Setup your conda environment following these steps:

```
cd /where/you/want/conda/install
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
bash Miniconda3-py39_4.9.2-Linux-x86_64.sh
source ~/.profile
conda deactivate
conda config --set auto_activate_base false
source ~/.profile
mkdir {your/conda_env/directory}
conda create --prefix {your/conda_env/directory}/{env_name} python=3.9
conda activate {your/conda_env/directory}/{env_name} #give absolute path so conda can find your env
conda install ipython matplotlib numpy scipy docutils gsl gmp h5py mpfr nose
conda clean --all
pip install --no-cache-dir mpi4py
```

```
FLASH setup:
```

cd torch ./install.sh FLASH SETUP in \$FLASH_DIR/bin/setup.py change sys.setcheckinterval() to sys.setswitchinterval() in \$FLASH_DIR/sites cp -r sites/cartesius.surfsara.nl sites/stampede2.tacc.utexas.edu in \$FLASH_DIR/sites/stampede2.tacc.utexas.edu/Makefile.h set MPI_PATH = \${MPI_HOME} HDF5_PATH = \${HDF5_HOME} and replace all instances of mpifort with mpif90 in \$FLASH_DIR/sites/Aliases add: stampede2.tacc.utexas.edu login1.stampede2.tacc.utexas.edu stampede2.tacc.utexas.edu login2.stampede2.tacc.utexas.edu stampede2.tacc.utexas.edu login3.stampede2.tacc.utexas.edu

```
./setup Cube -auto -3d +amuseusm +amusemg +raype +handcnew +amusesinksandstars +amusewinds +enerinj
        +supportppmupwind +pm4dev +cube16 -maxblocks=50
cd object
make -j
```

AMUSE setup:

```
cd amuse
./configure --with-fftw=$TACC_FFTW3_INC --with-hdf5=$MODLOC/gcc9_1/hdf5/1.10.4/x86_64/bin/h5c++
    --with-gmp=/home1/05402/bp4928/TORCH/env/torch_env
    --with-mpfr=/home1/05402/bp4928/TORCH/env/torch_env
    --with-gsl-prefix=/home1/05402/bp4928/TORCH/env/torch_env
pip install -e .
make framework
make flash.code
make kepler.code
make ph4.code
make seba.code
make smalln.code
--- petar
in amuse/src/amuse/community/petar/Makefile: if commented out, uncomment the following:
add -I flag before {$INCLUDE}
# arch
CXXFLAGS += -march=core-avx2
CXXFLAGS += -D INTRINSIC_X86
CXXFLAGS += -D USE_SIMD
CXXFLAGS += -D DIV_FIX
make petar.code
```

SLURM submit script:

#!/bin/sh
#SBATCH --job-name=test
#SBATCH -N 1
#SBATCH -N 32
#SBATCH -p skx-dev
#SBATCH --time=0:10:00
export FI_PROVIDER=tcp
ibrun -n 1 /home1/05402/bp4928/TORCH/env/torch_env/bin/python torch_user.py

C Flash file structure

Below is the file structure of the Flash code as defined when using ./setup command for the turbulent sphere example in Section 2.4.

```
+amuseUSM
     +amuseUnsplit
           += Driver/DriverMain/Unsplit/Couple_AMUSE
                 Driver_computeDt.F90
                 Driver_evolveFlash.F90
     +usm
           += physics/Hydro/HydroMain/unsplit/MHD_StaggeredMesh
                 Config
                Makefile
                 amr_runtime_parameters.tpl
                hy_uhd_HLLD.F90
                 hy_uhd_addOhmicHeating.F90
                 hy_uhd_eigenVector.F90
                 hy_uhd_staggeredDivb.F90
                hy_uhd_addBiermannFluxes.F90
                 hy_uhd_addResistiveFluxes.F90
                hy_uhd_getElectricFields.F90
                hy_uhd_unsplit.F90
                 hy_uhd_addHallFluxes.F90
                 hy_uhd_biermannSource.F90
                 hy_uhd_getFluxDeriv.F90
           -= physics/Hydro/HydroMain/split/MHD_8Wave
+amuseMG
     += physics/Gravity/GravityMain/Poisson/Multigrid/Couple_AMUSE
           Config
           Makefile
           Gravity_interface.F90
           Gravity_potentialListOfBlocksPDENonly.F90
           Gravity_getAccelAtPoint.F90
           Gravity_getPotentialAtPoint.F90
           Gravity_potentialListOfBlocks.F90
     -= physics/Gravity/GravityMain/Poisson/BHTree
+ravPE
     += Particles/ParticlesMain/ray_pe/MultiSourceSimple/Active/Sink
           Makefile
           pt_assignRaySink.F90
     += physics/RadTrans/RadTransMain/RayRad/SinksRad
           Config
           Makefile
           RadTrans.F90
           RadTrans_combine2.F90
           RadTrans_computeDt.F90
           calc_ionization.F90
           rt_data.F90
           RadTrans_combine.F90
           RadTrans_combine3.F90
           RadTrans_interface.F90
           get_ionization.F90
           rt_init.F90
+handCnew
     += physics/sourceTerms/Heat/HeatMain/HeatCool/phenHeat/mol_and_dust/solver
           Config
           Makefile
           CoolVars.F90
           Cool_init.F90
```

```
Heat.F90
           HeatCoolInterface.F90
           RadHeat.F90
           heatCool.F90
+amuseSinksAndStars
     += Particles/ParticlesMain/active/Sink/Couple_AMUSE/Couple_AMUSE_Sinks_and_Stars
           Config
           Makefile
           Particles_addNew.F90
           Particles_data.F90
           Particles_sinkCreateAccrete.F90
           Particles_updateGridVarSinksOnly.F90
           Particles_advance.F90
           Particles_init.F90
           Particles_sort.F90
           Particles_computeDt.F90
           Particles_interface.F90
           Particles_updateGridVarMassiveOnly.F90
           pt_gatherGlobal.F90
           sort.F90
           qsort2D.F90
+amuseWinds
     += Particles/ParticlesMain/active/Sink/Couple_AMUSE/wind
           Config
           Makefile
           Particles_computeDt.F90
           Particles_windData.F90
           Particles_advance.F90
           Particles_wind.F90
           pt_windInterface.F90
           inject_direct.F90
           overlap.F90
           normal_rand.F90
+enerInj
     += Particles/ParticlesMain/energyInjection
           Config
           Makefile
           Particles_energyInjection.F90
           pt_enerInjInterface.F90
           overlap.F90
```