Hydra2.0 Documentation

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Hydra can be obtained from either of the following websites;

- http://coho.astro.uwo.ca/pub/hydra/hydra.html
- http://star-www.maps.susx.ac.uk/\texttt{\~}pat/hydra/hydra.html

1 Documentation

Hydra is an adaptive particle-particle, particle-mesh plus smoothed particle hydro-
dynamics N-body simulation program. It can be used with either periodic or isolated
boundary conditions. A compiler flag allows the gas calculation to be turned off,
converting Hydra to a collisionless mode.

An installation guide comes with the release which provides information about
how to set up and compile Hydra with parameters appropriate for your particular
problem. This documentation describes the Hydra input files in more detail.

In what follows code extracts and variables will be written in \texttt{typewriter font}. Program and subroutine names will appear in \textbf{bold face} and directory names will be bracketed \texttt{<thus>}. 

1.1 Data format

The structure of data files is defined in \texttt{dumpdata.f}:

\begin{verbatim}
real rm(N),r(3,N),v(3,N),dn(N),e(N),h(N)
integer itype(N)
write(8) ibuf,ibuf1,ibuf2
write(8) rm
write(8) r
write(8) v
\end{verbatim}

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write(8) h
write(8) e
write(8) itype
write(8) dn

(i) The first line writes out the values of important parameters and variables as listed in **pinfo.inc**: 

```fortran
common/param/itime, itstop, itdump, itout, time, atime, htime, dtime,
& Est, T, Th, U, Radiation, Esum, Rsum, cpu,
& tstop, tout, icdump, padding, Tlost, Qlost, Ulost
common/start/irun, nobj, ngas, ndark, L, intl, nlmx, perr,
& dtnorm, sft0, sftmin, sftmax, h100, box100, zmet, spc0,
& lcool, rmgas, rmdark, rmnorm, tstart, omega0, xlambda0, h0t0
common/outputtime/tout1
real tout1(25)
dimension ibuf1(100), ibuf2(100), ibuf(200)
equivalence (ibuf1, itime), (ibuf2, irun), (ibuf, tout1)
```

Each of these variables serves the following function:

**itime, itstop, itdump, itout**: step number, stopping step, dumping interval for backups, not used

**time, atime, htime, dtime**: time, expansion factor, hubble parameter, timestep (all in code units)

**Est, T, Th, U**: starting, kinetic, thermal and potential energies in code units

**Radiation, Esum, Rsum, cpu**: radiated energy, energy integral, total radiated energy, cputime counter

**tstop, tout, icdump, padding**: not used, next dump time, position in list of dump times, padding for isolated boundary conditions

**Tlost, Qlost, Ulost**: lost kinetic, thermal and potential energies in grid units (isolated boundary conditions only)

**irun, nobj, ngas, ndark**: run number, total number of particles, number of gas, dark particles

**L, intl, nlmx, perr**: grid size (top level), interlacing switch, max number of refinement levels, maximum 2-body percentage force error

**dtnorm, sft0, sftmin, sftmax**: timestep multiplier, current-day softening (grid units), min, max softening (grid units)

**h100, box100, zmet, sft0**: hubble parameter, boxsize ($h^{-1}Mpc$), metallicity of gas, average particle spacing

**lcool, rmgas, rmdark, rmnorm**: cooling switch, mass of gas, dark matter particle, force normalisation
tstart, omega0, xlambda0, h0t0: start time, omega0, lambda0, H0t0 (last three for expanding box only)
tout1: list of desired output times.

(ii) data arrays

Note that the following arrays are defined for all particles even though some of them are irrelevant for dark matter particles. This is to simplify book-keeping. We recommend setting e, h and dn to zero for dark matter particles.

| Array | used for                        |
|-------|---------------------------------|
| rm    | mass                            |
| r     | positions                       |
| v     | velocities                      |
| e     | thermal energy                  |
| h     | sph smoothing length            |
| dn    | density                         |

Only meaningful for gas

itype particle type (meaning set in itype.inc)

The current settings for itype are:

| itype | used for                                    |
|-------|---------------------------------------------|
| -2    | particle does not exist (useful for merging particles) |
| -1    | star (equivalent to dark matter)           |
| 0     | dark matter                                 |
| 1     | gas                                         |
| 2     | temporary setting for an already completed gas particle |

These can be changed to label particles in different ways but you should check that Hydra handles the resultant types correctly.

1.2 Units

WARNING: the units used internally by Hydra differ from those used in the datafiles. The reason for this is that internally Hydra uses positions in the interval [1,L+1), where L is the number of FFT grid cells across the box. The data is either mapped into this interval exactly or, for isolated boxes and refinements, a padding region is left around the outside of the box. L can be different in different refinements and can vary from run to run - it has no physical meaning but is purely a computational device. The units also differ in isolated and periodic simulations:

(i) isolated simulations (usually compiled with -DISOLATED).

- length: positions run from 0 to 1 in each co-ordinate direction. The length-unit is $\text{box100 } h^{-1} Mpc$.
- mass: currently set to $10^{10} \text{ M}_\odot$. Can be altered.
• time: currently set to $10^{10}$ yr. Can be altered.

• speed: length/time

• density: number of particles per box volume. Converted internally to a number density of ions + electrons using $n_{\text{unit}}$.

• temperature: stored in units of internal energy (ie speed$^2$). Convert to ergs by multiplying by $e_{\text{unit}} = v_{\text{unit}}^2$; convert to temperature by multiplying by $K_{\text{unit}} = e_{\text{unit}}*2.\mu\text{m}/3./K_b$

(ii) cosmological simulations (periodic boxes)

• length: positions run from 0 to 1 in each co-ordinate direction. The length-unit is $a_{\text{time}}*\text{box100}$ $h^{-1}\text{Mpc}$.

• mass: the total mass in the box is normalised to match the desired value of $\Omega_0$. Thus particle masses are all relative.

• time: normalised to unity at the present, ie $t_{\text{unit}}=1$ at the end. $t_0$ is calculated automatically from input cosmological parameters.

• speed: The output velocities are $dx/dt$ where $x$ is the spatial coordinate in the range $[0,1)$. The peculiar velocity is thus $a_{\text{time}} * dx/dt$ and the proper velocity $a_{\text{time}}/dt*x + a_{\text{time}}*dx/dt$.

• density: number of particles per box volume. Converted internally to a number density of ions + electrons using $n_{\text{unit}}$.

• temperature: stored in units of internal energy (ie speed$^2$). Convert to ergs by multiplying by $a_{\text{time}}^2*e_{\text{unit}} = v_{\text{unit}}^2$; convert to temperature by multiplying by $K_{\text{unit}} = a_{\text{time}}^2*e_{\text{unit}}*2.\mu\text{m}/3./K_b$

The units are initialised in the routine $\text{inunit.F}$ to which you should refer if in doubt. They are also written at the head of the log file.

The magnitude of the force-scaling depends upon the system of units which is in use. It is set by the factor $r_{\text{mnorm}}$ defined at the head of $\text{updaterv.F}$.

1.3 Creating initial conditions

The input data arrays which need to be defined for all particle species are $r_{\text{m}}, r, v$ and $i_{\text{type}}$. In addition gas particles need an initial temperature, $e$, and sph smoothing length, $h$. This latter quantity may be estimated as the mean interparticle separation, $dn^{-1/3})$. $dn$ itself is not required.

For dark matter runs the following are the minimum set of input parameters which need to be defined: $i_{\text{time}}, t_{\text{ime}}, i_{\text{run}}, n_{\text{obj}}, h_{100}, \text{box100}, \Omega_0$ (periodic boxes
only), $\lambda_0$ (ditto), $t_{out1}$. In addition for gas runs the cooling flag needs to be set: $l_{cool}=1$ for cooling, 0 otherwise, and for $l_{cool}=1$ then the metallicity, $z_{met}$, should be defined in terms of the Solar value.

An example initial conditions generator for an isolated box is `createtop.f`, included with this distribution. A periodic initial conditions generator is also included, the `cosmic` package.

### 1.4 Running Hydra

Hydra works within and below a runtime directory. An example of the required directory setup was automatically built by unpacking the tar file. The executable (hydrat) will be copied to the run directory `<rundir>` automatically when it is made (the destination directory can be reset by changing RUNDIR in the makefile). When Hydra is executed the runlog (hydrat > runlog) and a summary file (pr????.log where ??? is the run number) are also written out here whilst the data is written to (and read from) a sub-directory `<data>`. The Green’s functions the code uses to do its PM calculation are saved to the sub-directory `<greenfn>`. If you have more than one `<rundir>` then it is usually best to link together the greenfn directories by using `ln -s` .... So the directory tree looks like this:

```
<rundir>  <----- hydra, prun.dat, logfiles
           /  \
           /   \
           /    \
    datafiles --> <data>  <greenfn>  <-- Green’s functions
```

Hydra uses a short file to set its basic run parameters. This file, `<rundir>/prun.dat` has the following format:

- `d3712.0857` startup data file name
- `3724` irun: run number for this run
- `858 10` itstop itdump
- `1.0` dtnorm
- `0.02` sft($h^{-1}$Mpc)
- `1` refinements on/off

The first line contains the name of the datafile you wish to start with. This is built up of d????.nnnn where ??? is a run number and nnnn is the step number. You can reset the run number on the second line. Here we are starting with the 857th step of run 3712, calling this run 3724. The third line contains the step number you wish to stop at and how frequently you require incremental backup files. dtnorm is the timestep normalisation: this should normally be set to unity (see Section 3.8 below). Next comes the Plummer softening in units of $h^{-1}$Mpc (see Section 3.7 below). The
final line contains a switch for turning refinement placing on or off. You can prevent Hydra placing refinements and convert it into a P3M code by setting this parameter to 0.

1.5 Log files

Hydra sends output to the screen and to a summary file. The screen output can be redirected to a log file (e.g. `nohup hydra > run?????.log`) but it is quite large and useful mainly for diagnostic purposes.

The summary file is called `pr?????.log` where `????` is the run number. One line is written to the summary file every step. Its form differs slightly between periodic and isolated runs:

(i) periodic boxes

| step | cputime | time | redshift | $K$ | $U$ | $W$ | error | $(K+U)/a$ | $W/a$ |
|------|---------|------|----------|-----|-----|-----|-------|-----------|-------|
| 857  | 927.48  | 0.5440 | 0.5005   | 5.00E+07 | 2.52E+06 | 7.41E+07 | 0.0065 | 7.89E+07 | 1.11E+08 |
| 858  | 966.93  | 0.5445 | 0.4997   | 5.01E+07 | 2.52E+06 | 7.42E+07 | 0.0065 | 7.88E+07 | 1.11E+08 |

where $K$= Kinetic energy, $U$= Thermal energy, $W$= Potential energy and $a$= atime. The final two columns should be in the ratio 2:3 (approximately - ignoring softening) and should remain constant in time during the linear regime. The error is defined in terms of the ratio of the change in the Layzer-Irvine energy integral, $I$, to the potential energy. $I$ is defined as $I = K + U + W + \int [2(K + U) + W] da/a + \int L dt$ where $L$=radiated power and $t$ = time. See Couchman, Thomas & Pearce (1995) for details.

(ii) isolated boxes

| step | cputime | time | $K$   | $U$   | $W$   | $\text{error}$ | $\text{lost } K$ | $\text{lost } U$ | $\text{lost } W$ |
|------|---------|------|-------|-------|-------|-----------------|-------------------|-------------------|-------------------|
| 0    | 112.58  | 0.0000 | 0.00E+00 | 0.00E+00 | 1.26E+01 | 0.0000         | 0.00E+00         | 0.00E+00         | 0.00E+00         |
| 1    | 112.25  | 0.0438 | 6.12E-03 | 3.20E-10 | 1.26E+01 | 0.0005         | 0.00E+00         | 0.00E+00         | 0.00E+00         |

The error estimate in this case is $[K + U + W - lost(K + U + W) - starting(K + U + W)]/U$.

The screen output begins with some warning messages informing the user if any parameters in the input data file have been altered. It also prints the size, L, of the top-level grid and confirms the presence or absence of refinements. Next follows a list of units (remember to include appropriate atime factors in expanding boxes). Next
comes some diagnostic information:

| Parameter        | Value          |
|------------------|----------------|
| itime, time, atime, htime: | 1295 1.000 1.000 0.667 |
| refinement:      | 0, scaling factor: 1.00 |
| ndark, ngas, ndone, nstar: | 32768 32768 0 0 |
| noveredge, novergrid: | 2578 3697 |
| gravity: av,min,max # neighbours | 110.22 0 1864 |
| sph: av,min,max # neighbours | 23.48 0 161 |
| av,min,max density (ref.) | 7.6971 0.0139 383.5992 |
| av,min,max energy (base) | 50.3896 0.0000 45135.1523 |
| refinement:      | 1, scaling factor: 3.29 |
| ndark, ngas, ndone, nstar: | 2247 906 1241 0 |
| noveredge, novergrid: | 213 94 |
| gravity: av,min,max # neighbours | 41.12 0 391 |
| sph: av,min,max # neighbours | 43.19 28 96 |
| av,min,max density (ref.) | 1.0347 0.0239 7.8099 |
| av,min,max energy (base) | 124.5373 0.0739 433.4357 |

...similarly for other refinements...

timestep = 2.6515502E-04 (2.6515502E-04 7.3740509E-04 9.3750297E-02)

(a) ‘scaling factor’ is the expansion factor of the refinement grid relative to the base level.
(b) ndark, ngas, ndone and nstar give the number of particles of each type within that refinement: ndone refers to those gas particles whose sph forces have already been calculated at the previous level.
(c) The average minimum and maximum number of gravity neighbours refers to the pp force calculation: the average value should be about 100 for efficient distribution of work between PM and PP.
(d) The minimum number of sph neighbours can drop below 32 in low-density regions because we only search for neighbours out to a radius of approximately 2.2 times the grid-spacing: within refinements the minimum number of sph neighbours should be close to 32. The maximum number of sph neighbours can be larger because the smoothing length can never drop below the gravitational softening.
(e) The average, minimum and maximum density of the gas particles is given in refinement units (ie particles per refinement grid cell). The average, minimum and maximum temperature of gas particles is scaled back to the base level units. These units both differ from those in the data files. These entries are omitted from the log if there are no gas particles within that refinement.
(f) The final line gives the timestep and the constraint on the timestep from accelerations, velocities and the hubble expansion (see Section 3.8 below).
1.6  Softening

Hydra uses softening shape function which has compact support:

```fortran
SUBROUTINE S2(r,a,grav,dpot)
    xi=2.*r/a
    if(xi.ge.0. .and. xi.lt.1.)then
        grav=xi*(224.+xi*xi*(-224.+xi*(70.+xi*(48.-xi*21.))))/35./a**2
        dpot=(208.+xi*xi*(-112.+xi*xi*(56.+xi*(-14.
          & +xi*(-8.+xi*3.)))))/70./a
    else if(xi.ge.1. .and. xi.lt.2.)then
        grav=(12./xi**2-224.+xi*(896.+xi*(-840.+xi*(224.+xi*(70.
          & xi*(-48.+xi*7.))))))/35./a**2
        dpot=(12./xi+128.+xi*(224.+xi*(-448.+xi*280.
          & +xi*(-56.+xi*(-14.+xi*(8.-xi))))))/70./a
    else
        grav=1./r**2
        dpot=r*grav
    end if
    RETURN
end
```

It is approximately equivalent to a Plummer softening with extent \( a/2.34 \) (the central value of \( r/force \) is the same in each case). The user supplied value for the softening in prun.dat is assumed to be a Plummer softening and is therefore multiplied by 2.34 before converting to grid units. If the ISOLATED or COMOVING flag is set during compilation then the softening is held fixed. Otherwise it scales with time as \( soft = \min(0.6, sft0/atime) \) where \( sft0 \) is the user-supplied value and the maximum value of 0.6 is a numerical constraint.

When choosing a softening it is important to strike a balance between the competing desires of high spatial resolution and long timesteps. \( dtime \) scales approximately in proportion to \( t_s = \sqrt{(soft^3/Gm)} \) where \( m \) is the mass of the highest-mass objects in the simulation. One should also be aware of the danger of artificial two-body relaxation which will occur in high-density regions on a timescale \( t_2 = \sqrt{45Nt_s} \) where \( N \) is the number of particles within the softening. See Thomas & Couchman (1992) for more detailed discussion.

1.7  Timestepping

Our choice of timestepping algorithm is described in Couchman, Thomas & Pearce (1995). We evaluated several algorithms and settled for a simple PEC scheme which utilises only the current positions (plus velocities and temperatures for gas particles)
to determine the forces. This has the advantage of keeping storage to a minimum and also allowing arbitrary changes in timestep if the force changes abruptly in time (as it can do in the vicinity of shocks). The scheme is equivalent to Leapfrog (but less memory-efficient) if there are no gas forces.

The timestep used by Hydra is not spatially variable but it does vary from one step to the next. The timestep is set by examining the greatest acceleration and velocity present at the current time:

\[
\begin{align*}
  d_{\text{ta}} &= (\text{soft2}/\text{asqmax})^{0.25} \\
  d_{\text{tv}} &= \sqrt{\text{soft2}/\text{vsqmax}} \\
  \text{dtime} &= \min(0.25 \times d_{\text{ta}}, 0.4 \times d_{\text{tv}}) \\
  \text{if} & \ (\text{htime} > 1 \times 10^{-30}) \ \text{then} \\
  & \quad \text{dtime} = \min(\text{dtime}, 0.0625/\text{htime}) \times \text{dtnorm} \\
  \text{else} \\
  & \quad \text{dtime} = \min(\text{dtime}, 1.) \times \text{dtnorm} \\
  \text{end if}
\end{align*}
\]

where \text{soft2} is the softening length squared, \text{asqmax} is the square of the maximum acceleration and \text{vsqmax} is the square of the maximum velocity. For expanding boxes the \text{htime} condition ensures that cooling due to the Hubble expansion is followed accurately: this dominates at early times.

1.8 SPH parameters

The sph smoothing length is chosen so as to encompass approximately 32 neighbours. Some people prefer a higher value but we have found that this makes an imperceptible difference to the results (32 particles gives significant shot-noise scatter in the interpolated density for a Poisson distribution but the actual particle distribution is much more uniform than this). In low-density regions the maximum sph search length (which is limited to approximately 2.2 times the grid-spacing) encloses fewer neighbours; in high-density regions the minimum sph search-length (which is set equal to the S2 softening parameter — see Section 3.7 above) may enclose more particles. If a particle’s sph search length either extends beyond the refinement boundary or is more than 2.2 grid-spacings in size then the sph force for that particle is calculated at the previous refinement level (resulting in a loss of efficiency). The number of particles for which this is done is given in the log.

We use a compact smoothing kernel:

\[
\begin{align*}
  \text{wnorm} &= 1./4./\pi \\
  \text{if} & \ (x \leq 1.0) \ \text{then} \\
  & \quad \text{kernel} = \text{wnorm} \times (4.-6.*x**2+3.*x**3) \\
  \text{else if} & \ (x \leq 2.0) \ \text{then} \\
  & \quad \text{kernel} = \text{wnorm} \times (4.-6.*x**2+3.*x**3) \\
  \text{else} & \end{align*}
\]
where $x=r/h$ is the ratio of the particle separation to the smoothing length, except that the gradient is modified so as to ensure a force which decreases monotonically with radius (see kernel.f and Thomas & Couchman 1992).

The artificial viscosity is based on the bulk divergence of the flow, not on the relative pairwise velocity of particles. Schematically:

$$f_{rc} = \frac{2}{3}e$$
$$\text{if } (\text{divpph} < 0.) f_{rc} = f_{rc} + (b_{visc} \cdot \text{divpph} - a_{visc} \cdot cs) \cdot \text{divpph}$$

where $\text{divpph} = h \cdot \text{div}(v)$, $cs$ is the sound speed and the parameters $a_{visc}$ and $b_{visc}$ are set to 1 and 2, respectively. The actual code, which includes a correction for the hubble expansion, is buried in the heart of shgravsph.F.

### 1.9 Cooling

Cooling can be turned on or off by setting the parameter $lcool$ (0=off, 1=on). The supplied cooling function is a simple series of power-law fits to the optically-thin radiative cooling code of Raymond, Cox & Smith:

$$\text{if } (t < 1e5) \text{ then}$$
$$\quad \Lambda = (1.4e-28 + 1.7e-27 \cdot z_{met}) \cdot t$$
$$\text{else}$$
$$\quad \Lambda = 5.2e-28 \cdot t^{0.5} + 1.4e-18 \cdot t^{-1.0} + 1.7e-18 \cdot t^{-0.8} \cdot z_{met}$$
$$\text{end if}$$

where $t$ is the temperature in Kelvin. This fit contains contributions from both bremsstrahlung and recombination cooling from hydrogen and helium plus a variable contribution from metal lines with an assumed abundance of $z_{met}$ times solar. The fit is good to within about a factor of two above $10^4K$ — below this temperature the cooling function drops precipitously and we take it to be zero. We intend to incorporate a more accurate cooling function in a future release.

Because the cooling time is often shorter than the dynamical time, we do not use it to limit the timestep. Instead we allow the particles to evolve adiabatically, then cool them, assuming a constant density, at the end of the timestep.

### 1.10 Brief description of the code

**MAIN:**

- **startup:** read in parameters and data
inunit: define the units
loop until finished:
updaterv: PEC step
   | accel: acceleration including hubble drag; timestep evaluation
   | force: acceleration evaluation
   | rfin: initialise refinements
   | refforce: see below
   | clist: create particle lists for refinements
   | loop over refinements:
   | | load: load particles into refinement
   | | refforce: see below
   | | unload: unload particles from refinements
   | end loop
| infout: write summary file
| output: write out data and backup files
end loop
end

refforce:

green   : evaluate, or read, green’s function
mesh    : evaluate PM accelerations
list    : sort particles into search cells
refine  : determine the position of subrefinements
shforce : tabulate PP force and potential
shgravsph : apply PP and SPH forces;
               write out diagnostic information

1.11 Cosmological initial conditions

A cosmological initial conditions generator – cosmic comes with the Hydra package. It produces an initial conditions file in Hydra format from a supplied data file, cosmic.dat. There are in act 3 executables in the cosmic package. These are cosmic itself which takes cosmic.dat for input and outputs the Hydra datafile into <data>d????.0000, where ???? is irun from cosmic.dat and r.pert is a perturbation file read by peakfindfft. peakfindfft searches r.pert for peaks of a given size (the default is 8$h^{-1}$Mpc) and outputs the position and $\delta$ of the biggest peak into peak.dat. Finally there is psnum which compares the sums of waves in boxes to the true power spectrum in spheres of radius 8$h^{-1}$Mpc (only useful if boxsize exceeds this) using the parameter file cosmic.dat. cosmic.dat has the following format;
Notes:

- `ndark` must be the cube of a power-of-2
- `omegab=0` for dark matter only, `omegab > 0` gives `ndark` each of dm and gas with correct mass ratio
- if `gamma <= 0` then uses formula in Viana & Liddle (1996)
- `- ipsec = 1 - power law (index ind)`
  - `- ipsec = 2 - cdm`
  - `- ipsec = 3 - hdm`
- `sigma8` is normalised to initial time using formulae in Viana & Liddle (1996)
- `lcool=1` for cooling (0 for no cooling), `zmet` is in solar units

1.12 Utility programs

1.12.1 readheader

The program `readheader` tells you some useful information about your initial conditions (or any dataset). It will automatically be placed into `<rundir>` when made. `readheader` prompts you for the name of a datafile and checks to see if you have set `Nmax` and `Lmax` correctly and also shows the ranges which your data spans if you request further information. This utility is very useful for checking data consistency.

1.12.2 hydra2tipsy

`hydra2tipsy` converts Hydra output files to `tipsy` format. It converts positions to $h^{-1}Mpc$, velocities to km/s, temperatures to Kelvin and densities to overdensities (or atoms per $cm^3$ if an isolated box has been asked for). `hydra2tipsy` is also automatically placed into `<rundir>` by make and prompts for a Hydra datafile. The output file is in the format `tip????..xxxx` where `????` is the run number and `xxxx` is the current step. Tipsy, an N-body visualisation package can be obtained from:

- http://www-hpcc.astro.washington.edu/tools/TIPSY/
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