NBODY6++

Manual for the Computer Code

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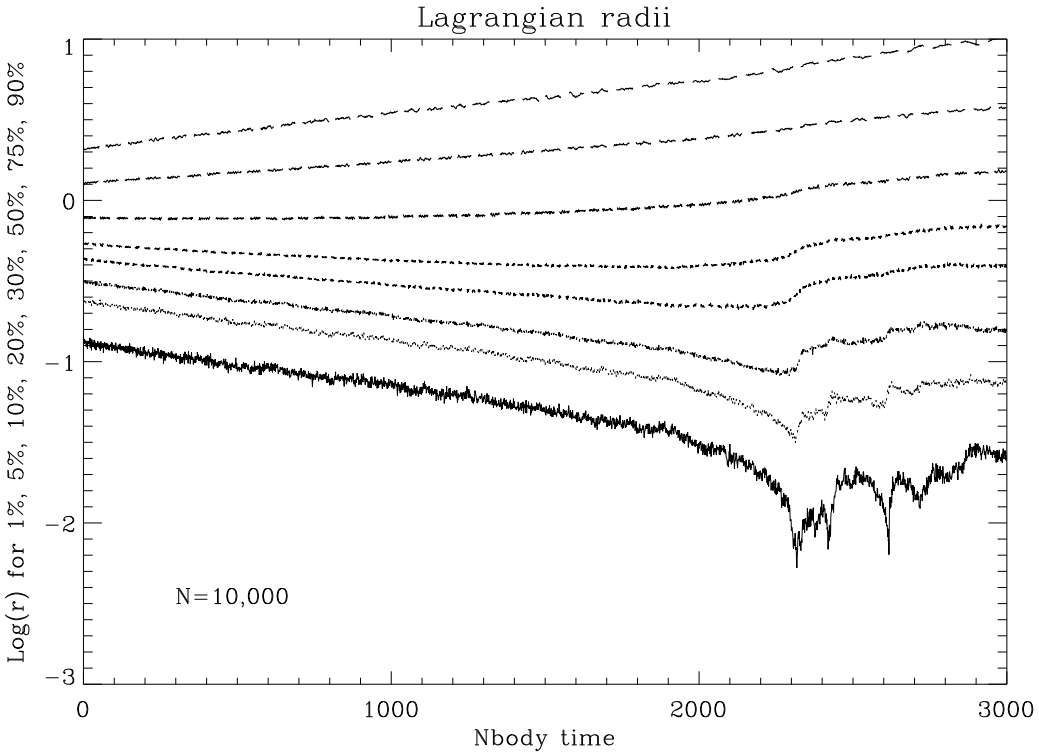

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1 Introduction

Gravity is an ever–present force in the Universe and is involved into the dynamics of all kinds of bodies, from the tiny atom to the clusters of galaxies. At small spatial scales, its influence is covered by other strong forces (e.g. magnetic, pressure, radiation induced), while on the very large scale it becomes the most dominant power. In astrophysics, it governs the dynamical evolution of many self–gravitating systems. Here, we concentrate on such systems that are dominated by mutual gravitation between particles.

The numerical star-by-star simulation of a simple cluster containing some more than hundred thousand members still places heavy demands on the available hard- and software. A balance has to be found between two constraints: On one hand the *realism*, i.e. the input of profound physics, inclusion of all astrophysical effects as well as the maintenance of the accuracy of calculations; and on the other hand, the *efficiency*, i.e. the limitations given by the computational possibilities and suitable codes to be finished in a reasonable time. Many different kinds of approaches have been undertaken to suffice both:

- codes based on the direct force integration [2], [5], [6], see also: `http://www.sverre.com/` ,
- statistical models, which themselves divide into several subgroups (Fokker–Planck approximation by [10]; Monte–Carlo method by [13]; Gas models by [27]),
- usage of high-performance parallel computers [28], [11],
- or the construction of special hardware devoted for these purposes (GRAPE [19], see also: `http://www.astrograpе.org/` and `http://www.cs.rit.edu/~grapecluster/` .

The code NBODY6++ described in this manual is designed for an accurate integration of many bodies (e.g. in a star cluster, planetary system, galactic nucleus) based on the direct integration of the Newtonian equations of motion. It is optimal for collisional systems, where long times of integration and high accuracy or both are required, in order to follow with high precision the secular evolution of the objects.

NBODY6++ is a descendant of the family of NBODY codes initiated by Sverre Aarseth [4], which has been extended to be suitable for parallel computers [28]. The basic features of the code increasing the efficiency may be considered under four separate headings: fourth order prediction–correction method (Hermite scheme), individual and block time–steps, regularization of close encounters and few-body subsystems, and a neighbour scheme (Ahmad–Cohen scheme). We briefly describe these ideas in this booklet, while a detailed description can be found in [3] as well as his book [6].

While NBODY6++ is not that different from NBODY6 to justify a completely new name, the user should, however, be aware that in order to make a parallelization of regular and irregular force computations possible at all, some significant changes in the order of operations became necessary. As a consequence, trajectories of the same initial system, simulated by NBODY6 and NBODY6++ will diverge from each other, due to the inherent exponential instability and deterministic chaos in N-body systems. Still one should always expect that the *global* properties are well behaved in both cases (e.g. energy conservation). While much effort is taken to keep NBODY6 and NBODY6++ as close as possible this is never 100% the case, and the interested should always contact Sverre Aarseth or Rainer Spurzem if in doubt about these matters.

This manual should serve as a practical starter kit for new students working with NBODY6++. It is not meant as a complete reference or scientific paper; for that see the references and in particular the excellent compendium of Aarseth's book on Gravitational N-Body Simulations [6].

Acknowledgements

The authors of this manual would like to express their sincere gratitude to Sverre Aarseth and Seppo Mikkola, for their continuous support and work over the decades. Also, many students and postdocs in Heidelberg and elsewhere have contributed towards development, debugging and improving the software for the benefit of the community. This booklet was written at the Astronomisches Rechen–Institut Heidelberg under the supervision of Rainer Spurzem.

2 Code versions

The development of the NBODY code has begun in the 1960s [1], though there exist some earlier precursors [29], [30]. It has set a quasi-standard for the precise direct integration of gravitating many-body systems. There exist several code groups (NBODY0–7, and a number of special implementations) for different usage, some of which are rather of historical interest.

The current NBODY6++ code is available publicly under Subversion or Github. You can download the beta version by using: `svn co http://silkroad.bao.ac.cn/repos/betanb6`
`git clone https://github.com/lwang-astro/betanb6pp.git`
The stable version will be avaiable under `svn co http://silkroad.bao.ac.cn/repos/releasenb6`
The documents and input samples are included.

The original *N*–body codes can be accessed publicly via Sverre Aarseth's ftp and web sites at `ftp://ftp.ast.cam.ac.uk/pub/sverre/` and `http://www.sverre.com/`.

A brief comparison of the code versions:

ITS: Individual time–steps
ACS: Neighbour scheme (Ahmad–Cohen scheme) with block time–steps
KS: KS–regularization of few-body subsystems
HITS: Hermite scheme integration method combined with hierarchical block time steps
PN: Post-Newtonian terms
AR: Algorithmic regularization

	ITS	ACS	KS	HITS	PN	AR
NBODY1	✓					
NBODY2		✓		✓		
NBODY3	✓		✓			
NBODY4			✓	✓		
NBODY5	✓	✓	✓			
NBODY6		✓	✓	✓		
NBODY7		✓	✓	✓	✓	✓

3 Getting started

After checkout the NBODY6++ by Subversion or Github (Ch. 2), A directory will be created containing all the source files (routines and functions), documents and input samples. By default the directory is called `betanb6` for beta version and `relnb6` for stable version. The current version use "configure" scripts generated by GNU Autoconf `http://www.gnu.org/software/autoconf/` to manage the installation. You can check README file for basic examples of using "configure" to select different features of NBODY6++ for compilation. More details of configure options can be found by using:
`./configure -help`

The simple way to use configure is just type: `./configure` Then the configure script will check your system environments to find avaiable compilers, make decision for several features like CUDA, SIMD and HDF5. In this simple example, if all checking pass successfully, there will be a summary showing the name of excutable file (nbody6++.**), the supported features, installation path and basic parameters for simulation (`NMAX`, `KMAX`, `LMAX`,`MMAX`). Here `NMAX` is the maximum number of particles, `KMAX` is the maximum number of KS pairs, `LMAX` is the maximum neighbor number and `MMAX` is the maximum merger number ($\geq$ 3 bodies stable hierarchical system).

The default installation path is "/user/local". If you want to change it, use:
`./configure -prefix=Installpath` Then the code will be installed in "Installpath".

After successful configure, you just use
make
for compiling the code and
make install
for installation.

The most important options of configure you need to care is shown in Table 3.

Figure 3.0: Options of configure script

Option	Description
–prefix=`path`	Installation path
–disable-gpu	Disable GPU acceleration (In the case you don't have Nvidia GPU with cuda support)
–enable-simd=`avx/sse/no`	Switch the features of SIMD parallel method (AVX / SSE / NONE)
–disable-mpi	Disable MPI parallelization
–disable-openmp	Disable OpenMP support
–with-par=`size`	Choose the simulation parameters (NMAX, KMAX, LMAX, MMAX), see detail by "./configure –help"

The document file is saved in "Installpath/share/doc". The input samples are in directory samples in your code directory.

The code NBODY6++ is written in Fortran 77 and consists of about 300 files. Their functionality was improved as well as new routines included all the way through the decades along with the technological achievements of the hardware. The starting (main) routine is called `nbody6.F`.

Most of the files have the suffix `.f`, `.F`, `.cu` or `.h`. All `.f` files are directly read by a Fortran compiler. The `.F` files will pass preprocessor first, which selects code lines separated by preprocessor options, e.g. between `#ifdef PARALLEL` and `#endif`, for they activate the parallel code on different multiprocessor machines. By this, some portability between different hardware is ensured at least, and a single processor version of the code can easily be compiled as well. The `.h`

are header files and declare the variables and their blocks.

Depending on the user's individual research, the Nbody code opens a wide field of application possibilities. The user has to define his model by a number of input control variables, e.g. number of stars, the size of the cluster, a mass function, profile, and many more. These control variables are gathered in the input files. The detailed explanation of its handling is given in Chapter 4. Alternatively, a data file named `dat.10` can be used, which contains data for an initial configuration (see Ch. 4). If the model criteria are defined, a single processor simulation run is started with the command

homedir`/Nbody/Run> ./nbody6++.** < input > output &`

In this example, the code reads the control variables given in the input file from Unix standard input *stdin*. Then, a star cluster is created according to the user's instructions, and the bodies are moved one by one with respect to their time maturity. Some first results and error checks are directed via the Unix standard output *stdout* to `output` . This file provides snapshots of the state of the system for a brief overview of some key data of the simulation to judge about the quality and performance of the run.

There are several more files created. Most important are `fort.1` and `fort.2`, which contain dumps of the complete common blocks for a restart and checkpoint purposes, and `conf.3_*`, `bdat.9_*`, `bwdat.19_*`, `sev.83_*`, `bev.82_*` that contain the particle data for the user's analysis. The detail descriptions of output files are shown in Ch. 13. In the `conf.3_*`, many details of the run are saved, e.g. positions, velocities, neighbour densities, potential of *each* particle in *any* predefined time interval. The volume of data in all three mentioned files critically depends on the dimensions of vectors in `params.h` . Here, the particle data plus some user-defined dimensions are given a threshold in order to save disk space when outputting to `conf.3` — see Chapter 5.

At the time of this writing, the user has to provide own routines to postprocess the particle data from the simulation, using e.g. additional routines or programs (like IDL, gnuplot etc.), in order to extract the binary data from this file and plot graphics. Work is in progress to provide a better visual interface delivered with the program.

A run will be finished when one of 4 conditions becomes true:

- the specified CPU–time on the computer is exceeded (variable `TCOMP` in the input file), or
- the maximum Nbody–time (see Ch. 4) is reached (variable `TCRIT`), or
- the physical cluster time in Myr is reached (variable `TCRITp`), or
- the number of cluster stars has fallen below a minimum (variable `NCRIT`).

A soft termination of a running simulation can be realized by generating of a file `STOP` in the executing directory:

homedir`/Nbody/Run> touch STOP`

In that case, a checkpoint of the code is done, which is located in the routine `intgr.F` and shown in Figure 3.1. The program writes out the current variables, saves a complete common dump in `fort.1` or `fort.2` and terminates. The run can be restarted and continued from the same point where it was left.

Before a restart, it is recommendable to copy or rename the files, otherwise they may be overwritten. Any file `fort.1` and `fort.2` is restartable. The different names are just for getting common dumps at different time units. For example, if an irregular termination takes place, `fort.2` contains the data at some earlier time point, while `fort.1` always contains the last time data.

To restart a run, a different very short input control data file needs to be used, because most of the control data are already stored in `fort.1` . Only the first line corresponds to the standard input file, but the first input variable, `KSTART`, has to be changed to "2" or higher. In this case, the routine `modify.F` will be entered.

KSTART	Function
1	new run, start from initial values given in `data.F`
2	continuation of a run without changes
3	restart of a run with changes of the following parameters given in the second line of a newly created input file: DTADJ, DELTAT, TADJ, TNEXT, TCRIT, QE, J, K where the options KZ can be changed via KZ(J)=K
4	restart of a run with following parameters changed in the second line: ETAI, ETAR, ETAU, DTMIN, RMIN, NCRIT, NNBOPT, SMAX
5	restart of a run with all parameter changes in the run control index 3 and 4. The changes must succeed the first line.

"0" values in the fields are interpreted as: Do not change the value of this parameter.

The details of input and restart are discussed in Ch. 4.

```
*
*       Include facility for termination of run (create dummy file STOP).
      IF(rank.EQ.0)THEN
      OPEN (99,FILE='STOP',STATUS='OLD',FORM='FORMATTED',IOSTAT=IO)
      IF (IO.EQ.0) THEN
          CLOSE (99)
          IF (NSUM.EQ.0.and.rank.eq.0) WRITE (6,90)
   90     FORMAT  (/,9X,'TERMINATION BY MANUAL INTERVENTION')
          CPU = 0.0
      END IF
      END IF
*
```

Figure 3.1: Soft interruption of a simulation run in `intgr.F`: If the dummy file "STOP" exists, then the run terminates.

4 Input variables

The input control file of NBODY6++ (see below), contains a minimum of 90 parameters which guide one simulation run for its technical and physical properties (it is very similar but not identical to the one used for NBODY6). As for the technical aspect, the file supervises the run e.g. for its duration, intervals of the output, or error check; the physical parameters concern the size of a cluster, initial conditions, or a number of optional features related to the numerical problem to be studied. The handling of this input file appears rather entangled at first sight, for it has grown rather historically and "ready–for–use" than custom–oriented. Thus, the input variables are read by different routines (functions) in the code, and the nature of the parameters are woven with each other in some cases. Also, some parameters require additional input, such that the total number of lines and parameters may vary.

In the following, we explain the main input file and give an example of typical values for a simulation of an isolated globular cluster. Then, we proceed to the thresholds.

`Input with all options:`

nbody6.F	KSTART	TCOMP	TCRITp	isernb	iserreg	iserks				
input.F	N	NFIX	NCRIT	NRAND	NNBOPT	NRUN				
	ETAI	ETAR	RS0	DTADJ	DELTAT	TCRIT	QE	RBAR	ZMBAR	
	KZ(1)	KZ(2)	KZ(3)	KZ(4)	KZ(5)	KZ(6)	KZ(7)	KZ(8)	KZ(9)	KZ(10)
	KZ(11)	KZ(12)	KZ(13)	KZ(14)	KZ(15)	KZ(16)	KZ(17)	KZ(18)	KZ(19)	KZ(20)
	KZ(21)	KZ(22)	KZ(23)	KZ(24)	KZ(25)	KZ(26)	KZ(27)	KZ(28)	KZ(29)	KZ(30)
	KZ(31)	KZ(32)	KZ(33)	KZ(34)	KZ(35)	KZ(36)	KZ(37)	KZ(38)	KZ(39)	KZ(40)
	KZ(41)	KZ(42)	KZ(43)	KZ(44)	KZ(45)	KZ(46)	KZ(47)	KZ(48)	KZ(49)	KZ(50)
	DTMIN	RMIN	ETAU	ECLOSE	GMIN	GMAX	SMAX			
data.F	ALPHA	BODY1	BODYN	NBIN0	NHI0	ZMET	EPOCH0	DTPLOT		
setup.F	AP0	ECC	N2	SCALE						(KZ(5)=2)
	AP0	ECC	SCALE							(KZ(5)=3)
	AP0	ECC	SCALE							(KZ(5)=3)
	SEMI	ECC	M1	M2						(KZ(5)=4)
	ZMH	RCUT							(KZ(5)=6&&KZ(24)<0)	
scale.F	Q	VXROT	VZROT	RTIDE						
xtrnl0.F	GMG	RG0								(KZ(14)=2)
	GMG	DISK	A	B	VCIRC	RCIRC	RG	VG		(KZ(14)=3)
	MP	AP	MPDOT	TDELAY					(KZ(14)=3||KZ(14)=4)	
binpop.F	SEMI	ECC	RATIO	RANGE	NSKIP	IDORM			(KZ(8)=1||KZ(8)>4)	
hipop.F	SEMI	ECC	RATIO	RANGE					(KZ(8)>0&&KZ(18)>1)	
imbhinit.F	MMBH	XBH(1)	XBH(2)	XBH(3)	VBH(1)	VBH(2)	VBH(3)	DTBH		(KZ(24)=1)
cloud0.F	NCL	RB2	VCL	SIGMA	CLM	RCL2				(KZ(13)>0)

`nbody6.F:`

KSTART Run control index
=1: new run (construct new model or read from `dat.10`)
=2: restart/continuation of a run, needs `fort.1`
=3: restart + changes of DTADJ, DELTAT, TADJ, TNEXT, TCRIT, QE, J, KZ(J)
=4: restart + changes of ETAI, ETAR, ETAU, DTMIN, RMIN, NCRIT, NNBOPT, SMAX
=5: restart containing the combination of the control index 3 and 4

TCOMP Maximum wall-clock time in seconds (parallel runs: wall clock)

TCRITP Termination time in Myr

isernb For MPI parallel runs: only irregular block sizes larger than this value are executed in parallel mode (dummy variable for single CPU)

iserreg For MPI parallel runs: only regular block sizes larger than this value are executed in parallel mode (dummy variable for single CPU)

iserks	For MPI parallel runs: only ks block sizes larger than this value are executed in parallel mode (dummy variable for single CPU)

`input.F`:

N	Total number of particles (single + c.m.s. of binaries; singles + 3×c.m.s. of binaries < NMAX−2)
NFIX	Multiplicator for output interval of data on `conf.3` and of data for binary stars (output each DELTAT×NFIX time steps; compare KZ(3) and KZ(6))
NCRIT	Minimum particle number (alternative termination criterion)
NRAND	Random number seed; any positive integer
NNBOPT	Desired optimal neighbour number (< LMAX−5)
NRUN	Run identification index

ETAI	Time–step factor for irregular force polynomial
ETAR	Time–step factor for regular force polynomial
RS0	Initial guess for all radii of neighbour spheres (*N*–body units)
DTADJ	Time interval for parameter adjustment and energy check (*N*–body units)
DELTAT	Time interval for writing output data and diagnostics, multiplied by NFIX (*N*–body units)
TCRIT	Termination time (*N*–body units)
QE	Energy tolerance: – immediate termination if DE/E > 5*QE & KZ(2) $\leq$ 1; – restart if DE/E > 5*QE & KZ(2) > 1 and termination after second restart attempt.
RBAR	Scaling unit in pc for distance (*N*–body units)
ZMBAR	Scaling unit for average particle mass in solar masses (in scale-free simulations RBAR and ZMBAR can be set to zero; depends on KZ(20))

KZ(1)	Save COMMON to file `fort.1` = 1: at end of run or when dummy file STOP is created = 2: every 100*NMAX steps
KZ(2)	Save COMMON to file `fort.2` = 1: save at output time = 2: save at output time and restart simulation if energy error DE/E > 5*QE
KZ(3)	Save basic data to file `conf.3` at output time (unformatted)
KZ(4)	(Suppressed) Binary diagnostics on `bdat.4` (# = threshold levels <10)
KZ(5)	Initial conditions of the particle distribution, needs KZ(22)=0 = 0: uniform & isotropic sphere = 1: Plummer random generation = 2: two Plummer models in orbit (extra input) = 3: massive perturber and planetesimal disk (each pariticle has circular orbit, constant separation along radial direction between each neighbor and random phase) (extra input) = 4: massive initial binary (extra input) = 5: Jaffe model (extra input) $\geq$ 6: Zhao BH cusp model (extra input if KZ(24)<0)
KZ(6)	Output of significant and regularized binaries at main output (`bodies.f`)

= 1: output regularized and significant binaries (|E|>0.1 ECLOSE)
= 2: output regularized binaries only
= 3: output significant binaries at output time and regularized binaries with time interval DELTAT
= 4: output of regularized binaries only at output time

KZ(7) Determine Lagrangian radii and average mass, particle counters, average velocity, velocity dispersion, rotational velocity within Lagrangian radii (`lagr.f`)
= 1: Get actual value of half mass radius RSCALE by using current total mass
$\geq$ 2: Output data at main output and `lagr.7`
$\geq$ 6: Output Lagrangian radii for two mass groups at `lagr.31` and `lagr.32` (`lagr2.f`; based on KZ(5)=1,2; cost is O(N^2))
—- methods:
= 2,4: Lagrangian radii calculated by initial total mass
= 3,$\geq$ 5: Lagrangian radii calculated by current total mass (The single/K.S-binary Lagrangian radii are still calculated by initial single/binary total mass)
= 2,3: All parameters are averaged within the shell between two Lagrangian radii neighbors
$\geq$ 4: All parameters are averaged from center to each Lagrangian radius

KZ(8) Primordial binaries initialization and output (`binpop.f`)
—- Initialization:
= 0: No primordial binaries
= 1,$\geq$ 3: generate primordial binaries based on KZ(41) and KZ(42) (`binpop.F`)
= 2: Input primordial binaries from first 2$\times$NBIN0 lines of `dat.10`
—- Output:
> 0: Save information of primordial binary that change member in `pbin.18`; binary diagnostics at main output (`binout.f`)
$\geq$ 2: Output KS binary in `bdat.9`, soft binary in `bwdat.19` at output time

KZ(9) Binary diagnostics
= 1,3: Output diagnostics for the hardest binary below ECLOSE in `hbin.39` (`adjust.f`)
$\geq$ 2: Output binary evolution stages in `binev.17` (`binev.f`)
$\geq$ 3: Output binary with degenerate stars in `degen.4` (`degen.f`)

KZ(10) K.S. regularization diagnostics at main output
> 0: Output new K.S. information
> 1: Output end K.S. information
$\geq$ 3: Output each integrating step information

KZ(11) (Suppressed)

KZ(12) HR diagnostics of evolving stars with output time interval DTPLOT in `sse.83` (single star) and `bse.82` (K.S. binary)

KZ(13) Interstellar clouds
= 1: constant velocity for new cloud
> 2: Gaussian velocity for new cloud

KZ(14) External tidal force
= 1: standard solar neighbor tidal field
= 2: point-mass galaxy with circular orbit (extra input)
= 3: point-mass + disk + halo + Plummer (extra input)
= 4: Plummer model (extra input)

KZ(15) Triple, quad, chain and merger search

≥ 1: Switch on triple, quad, chain (KZ(30)>0) and merger search (`impact.f`)
≥ 2: Diagnostics at main output at begin and end of triple, quad
≥ 3: Save first five outer orbits every half period of wide quadruple before merger and stable quadruples accepted for merger in `quastab.89`

KZ(16) Auto-adjustment of regularization parameters
≥ 1: Adjust RMIN, DTMIN & ECLOSE every DTADJ time
≥ 3: modify RMIN for GPERT > 0.05 or < 0.002 in chain; output diagnostics at `kscrit.77`

KZ(17) Auto-adjustment of ETAI, ETAR and ETAU by tolerance QE every DTADJ time (`check.f`)
≥ 1: Adjust ETAI, ETAR
≥ 2: Adjust ETAU

KZ(18) Hierarchical systems
$= 1,3$: diagnostics (`hiarch.f`)
≥ 2: Initialize primordial stable triples, number is NHI0 (`hipop.F`)
≥ 4: Data bank of stable triple, quad in `hidat.87` (`hidat.f`)

KZ(19) Stellar evolution mass loss
$= 1,2$: supernova scheme
≥ 3: Eggleton, Tout & Hurley
≥ 5: extra diagnostics (mdot.F)
$= 2,4$: Input stellar parameters from `fort.21` (`instar.f`)
N lines of (MI, KW, M0, EPOCH1, OSPIN)
MI: Current mass
KW: Kstar type
M0: Initial mass
EPOCH1: evolved age of star (Age = TIME[Myr] − EPOCH1)
OSPIN: angular velocity of star

KZ(20) Initial mass functions, need KZ(22)−0 or 9:
$= 0$: self-defined power-law mass function using ALPHAS (`data.F`)
$= 1$: Miller-Scalo-(1979) IMF (`imf.f`)
$= 2,4$: KTG (1993) IMF (`imf2.f`)
$= 3,5$: Eggleton-IMF (`imf2.f`)
$= 6,7$: Kroupa(2001) (`imf2.f`), extended to Brown Dwarf regime (`imfbd.f`)
—- Primordial binary mass
$= 2,6$: random pairing (`imf2.f`)
$= 3,4,5,7$: binary mass ratio corrected by $(m_1/m_2)\prime = (m_1/m_2)^{0.4}$ + constant (Eggleton, `imf2.f`)
$= 8$: binary mass ratio $q = m_1/m_2$ ($m_2 \leq m_1$) use distribtution $0.6q^{-0.4}$ (Kouwenhoven)

KZ(21) Extra diagnostics information at main output every DELTAT interval (`output.F`)
≥ 1: output NRUN, MODEL, TCOMP, TRC, DMIN, AMIN, RMAX, RSMIN, NEFF
≥ 2: Number of escapers NESC at main output will be counted by Jacobi escape criterion (cost is O(N^2), `jacobi.f`)

KZ(22) Initialization of basic particle data mass, position and velocity (`data.F`)
—- Initialization with internal method
$= 0,1$: Initial position, velocity based on KZ(5), initial mass based on KZ(20)
$= 1$: write initial conditions in `dat.10` (`scale.F`)

—- Initialization by reading data from `dat.10`
= 2: input through NBODY-format (7 parameters each line: mass, position(1:3), velocity(1:3))
= 3: input through Tree-format (`data.F`)
= 4: input through Starlab-format
= 6: input through NBODY-format and do scaling
= 7: input through Tree-Format and do scaling
= 8: input through Starlab-format and do Scaling
= 9: input through NBODY-format but ignore mass (first column) and use IMF based on KZ(20), then do scaling

KZ(23) Removal of escapers (`escape.F`)
≥ 1: remove escapers and ghost particles generated by two star coalescence (collision)
$= 2,4$: write escaper diagnostics in `esc 11`
≥ 3: initialization & integration of tidal tail

KZ(24) Initial conditions for subsystems
< 0: ZMH & RCUT (N-body units) Zhao model (Need KZ(5)$\geq$6, `setup.F`)
$= 1$: Add one massive black hole (extra input: mass, position, velocity and output frequency), will output black hole data in `mbh.45` and its neighbor data in `mbhnb.46`

KZ(25) Velocity kicks for white dwarfs (`kick.F`)
$= 1$: Type 10 Helium white dwarf & 11 Carbon-Oxygen white dwarf
$= 2$: All WDs (type 10, 11 and type 12 Oxygen-Neon white dwarf)

KZ(26) Slow-down of two-body motion, increase the regularization integration efficiency
≥ 1: Apply to KS binary
≥ 2: Apply to chain
$= 3$: Rectify to get better energy conservation

KZ(27) Two-body tidal circularization (Mardling & Aarseth, 2001; Portegies Zwart et al. 1997)
(Please suppress in KS parallel version)
$= 1$: sequential
$= 2$: chaos
$= 3$: GR energy loss
$= -1$: Only detect collision and suppress coalescence

KZ(28) Magnetic braking and gravitational radiation for NS or BH binaries (Need KZ(19)=3 and based on KZ(27))
≥ 1: GR coalescence for NS & BH (`brake.f`, `brake3.f`)
≥ 2: Diagnostics at main output (`brake.f`)
$= 3$: Input of ZMH = 1/SQRT(2*N) (Need KZ(5)$\geq$6) (`setup.F`)
$= 4$: Set every star as type 13 Neutron star (Need KZ(27)=3) (`instar.f`)

KZ(29) (Suppressed) Boundary reflection for hot system

KZ(30) Hierarchical system regularization
$= -1$: Use chain only
$= 0$: No triple, quad and chain regularization, only merger
$= 1$: Use triple, quad and chain (`impact.f`)
≥ 2: Diagnostics at begin/end of chain at main output
≥ 3: Diagnostics at each step of chain at main output

KZ(31) Centre of mass correction after energy check (`cmcorr.f`)

KZ(32) Adjustment (increase) of adjust interval DTADJ, output interval DELTAT and energy error criterion QE based on binding eneryg of cluster (`check.f`)

KZ(33) Block-step statistics at main output (diagnostics)
≥ 1: Output irregular block step; and K.S. binary step if KZ(8)>0
≥ 2: Output regular block step

KZ(34) Roche-lobe overflow
$= 1$: Roche & Spin synchronisation on binary with circular orbit (`synch.f`)
$= 2$: Roche & Tidal synchronisation on binary with circular orbit by BSE method (`bsetid.f`)

KZ(35) TIME reset to zero every 100 time units, total time is TTOT = TIME + TOFF (`offset.f`)

KZ(36) (Suppressed) Step reduction for hierarchical systems

KZ(37) Neighbour list additions (`checkl.F`)
≥ 1: Add high-velocity particles into neighbor list
≥ 2: Add small time step particle (like close encounter particles near neighbor radius) into neighbor list

KZ(38) Force polynomial corrections during regular block step calculation
$= 0$: no corrections
$= 1$: all gains & losses included
$= 2$: small regular force change skipped
$= 3$: fast neighbour loss only

KZ(39) Neighbor radius adjustment method
$= 0$: The system has unique density centre and smooth density profile
$= 1, \geq 3$: The system has no unique density centre or smooth density profile
skip velocity modification of RS(I) (`regint.f`, `regcor_gpu.f`)
do not reduce neighbor radius if particle is outside half mass radius
reduce RS(I) by multiply 0.9 instead of estimation of RS(I) based on NNBOPT/NNB when neighbor list overflow happens (`fpoly0.F`, `util_gpu.F`)
$= 2, 3$: Consider sqrt(particle mass / average mass) as the factor to determine the particle's neighbor membership. (`fpoly0.F`, `util_gpu.F`)

KZ(40) (Suppressed)

KZ(41) proto-star evolution of eccentricity and period for primordial binaries initialization (`proto_star_evol`, `binpop.F`)

KZ(42) Initial binary distribution
$= 0$: RANGE>0: uniform distribution in log(semi) between SEMI0 and SEMI0/RANGE
RANGE<0: uniform distribution in semi between SEMI0 and -1*RANGE.
$= 1$: linearly increasing distribution function $f = 0.03438 * logP$
$= 2$: $f = 3.5 logP / [100 + (logP) * *2]$
$= 3$: $f = 2.3(logP - 1) / [45 + (logP - 1) * *2]$; This is a "3rd" iteration when pre-ms evolution is taken into account with KZ(41)=1
$= 4$: $f = 2.5(logP - 1) / [45 + (logP - 1) * *2]$; This is a "34th" iteration when pre-ms evolution is taken into account with KZ(41)=1 and RBAR<1.5
$= 5$: Duquennoy & Mayor 1991, Gaussian distribution with mean $\log P = 4.8$, SDEV in $\log P = 2.3$. Use Num.Recipes routine `gasdev.f` to obtain random deviates given "idum1"

KZ(43) (Unused)

KZ(44) (Unused)

KZ(45)	(Unused)
KZ(46)	HDF5/CSV format output (name,time,x,v,m,f,fdot,kstar,rho,phi,L,radius,Teff,m_{core},$radius_{core}$) $= 1,3$: HDF5 format $= 2,4$: CSV format $= 1,2$: Only output active stars with time interval defined by KZ(47) $= 3,4$: Output full particle list with time interval defined by KZ(47)
KZ(47)	Frequency for KZ(46) output $= 0$: Output data during each irregular block time step $= 1 \sim 63$: Output data with time interval $0.5^{KZ(47)}$
KZ(48)	(Unused)
KZ(49)	Computation of Moments of Inertia (with Chr. Theis) in `fort.60` (`ellan.f`)
KZ(50)	(Unused)

DTMIN	Time–step criterion for regularization search
RMIN	Distance criterion for regularization search
ETAU	Regularized time-step parameter (6.28/ETAU steps/orbit)
ECLOSE	Binding energy per unit mass for hard binary (positive)
GMIN	Relative two-body perturbation for unperturbed motion
GMAX	Secondary termination parameter for soft KS binaries
SMAX	Maximum time-step (factor of 2 commensurate with 1.0)

`data.F:`	
ALPHA	Power-law index for initial mass function, routine `data.F`
BODY1	Maximum particle mass before scaling (based on KZ(20); solar mass unit)
BODYN	Minimum particle mass before scaling
NBIN0	Number of primordial binaries (need KZ(8)>0) – by routine `imf2.F` using a binary IMF (KZ(20)$\geq$2) – by routine `binpop.F` splitting single stars (KZ(8)>0) – by reading subsystems from `dat.10` (KZ(22)$\geq$2)
ZMET	Metal abundance (in range 0.03 - 0.0001)
EPOCH0	Evolutionary epoch (in 10^6 yrs)
DTPLOT	Plotting interval for stellar evolution HRDIAG (N-body units; $\geq$ DELTAT)

`setup.F:`	`if (kz(5)=2)`
APO	Separation of two Plummer models in *N*–body units (SEMI = APO/(1 + ECC). (Notice SEMI will be limited between 2.0 and 50.0)
ECC	Eccentricity of two-body orbit (ECC $\geq$0 and ECC < 0.999)
N2	Membership of second Plummer model (N2 <= N)
SCALE	Scale factor for the second Plummer model, second cluster will be generated by first Plummer model with $X \times SCALE$ and $V \times \sqrt{SCALE}$($\geq$ 0.2 for limiting minimum size)
	`if (kz(5)=3)`
APO	Separation between the perturber and Sun in *N*–body units
ECC	Eccentricity of orbit (=1 for parabolic encounter)
SCALE	Perturber mass scale factor, perturber mass = Center star mass $\times$ SCALE (=1 for Msun)

	`if (kz(5)=4)`
SEMI	Semi-major axis (slightly modified; ignore if ECC > 1)
ECC	Eccentricity (ECC > 1: NAME = 1 & 2 free-floating)
M1	Mass of first member (in units of mean mass)
M2	Mass of second member (rescaled total mass = 1)
	`if (kz(5)≥6) and (kz(24)<0)`
ZMH	Mass of single BH (in N-body units)
RCUT	Radial cutoff in Zhao cusp distribution (MNRAS, 278, 488)

`scale.F:`

Q	Virial ratio (routine `scale.F`; Q=0.5 for equilibrium)
VXROT	XY–velocity scaling factor (> 0 for solid-body rotation)
VZROT	Z–velocity scaling factor (not used if VXROT = 0)
RTIDE	Unscaled tidal radius for KZ(14)=2 and KZ(22)≥2. If not zero, RBAR = RT/RTIDE where RT[pc] is tidal radius calculated from input GMG and RG0

`xtrnl0.F:` `if (kz(14)=2)`

GMG	Point-mass galaxy (solar masses, linearized tidel field in circular orbit)
RG0	Central distance (in kpc)
	`if (kz(14)=3)`
GMG	Point-mass galaxy (solar masses)
DISK	Mass of Miyamoto disk (solar masses)
A	Softening length in Miyamoto potential (in kpc)
B	Vertical softening length (kpc)
VCIRC	Galactic circular velocity (km/sec) at RCIRC (=0: no halo)
RCIRC	Central distance for VCIRC with logarithmic potential (kpc)
RG	Initial position; DISK+VCIRC=0, VG(3)=0: A(1+E)=RG(1), E=RG(2)
VG	Initial cluster velocity vector (km/sec)
	`if (kz(14)=3,4)`
MP	Total mass of Plummer sphere (in scaled units)
AP	Plummer scale factor (N-body units; square saved in AP2)
MPDOT	Decay time for gas expulsion (MP = MP0/(1 + MPDOT*(T-TD))
TDELAY	Delay time for starting gas expulsion (T > TDELAY)

`binpop.F:` `if (kz(8)=1 or kz(8)>2)`

SEMI	Initial semi-major axis limit
ECC	Initial eccentricity < 0: thermal distribution, $f(e) = 2e$ ≥ 0 and ≤ 1: fixed value of eccentricity $= 20$: uniform distribution $= 30$: distribution with $f(e) = 0.1765/(e^2)$ $= 40$: general $f(e) = a * e^b$, $e0 <= e <= 1$ with $a = (1+b)/(1-e0^(1+b))$, current values: $e0 = 0$ and $b = 1$ (thermal distribution)
RATIO	KZ(42)$\leq$ 1: Binary mass ratio $M1/(M1+M2)$ KZ(42)= 1.0: $M1 = M2 = \langle M \rangle$

RANGE	KZ(42)= 0: semi-major axis range for uniform logarithmic distribution; not used for other KZ(42)
NSKIP	Binary frequency of mass spectrum (starting from body #1)
IDORM	Indicator for dormant binaries (> 0: merged components)

`hipop.F:` `if (kz(8)>0 and kz(18)>1)`

SEMI	Max semi-major axis in model units (all equal if RANGE = 0)
ECC	Initial eccentricity (< 0 for thermal distribution)
RATIO	Mass ratio ($= 1.0$: $M1 = M2$; random in $[0.5 \sim 0.9]$)
RANGE	Range in SEMI for uniform logarithmic distribution (> 0)

`imbhinit.F:if (kz(24)=1)`

MMBH	Mass of massive black hole in solar mass unit
XBH(1:3)	3 dimensional position of massive black hole in pc
VBH(1:3)	3 dimensional velocity of massive black hole in km/s
DTBH	Output interval for massive black hole data in `mbh.45` and `mbhnb.46` (N-body unit)

`cloud0.F: if (kz(13)>0)`

NCL	Number of interstellar clouds
RB2	Radius of cloud boundary in pc (square is saved)
VCL	Mean cloud velocity in km/sec
SIGMA	Velocity dispersion (KZ(13)>1: Gaussian)
CLM	Individual cloud masses in solar masses (maximum MCL)
RCL2	Half-mass radii of clouds in pc (square is saved)

A typical input file can look like as follows. It defines a new simulation running for 1,000,000 CPU–minutes with $N = 16,000$ particles distributed from a Plummer profile (KZ(5)=1). The run may alternatively terminate when TCRIT=1000.0 N–body units. or if the final particle number of NCRIT=10 has been reached. The output and adjustment time interval DELTAT/DTADJ are 1.0 N-body unit. The initial mass function follows Kroupa, (2001) with mass ranging from $m_{\max} = 20.0 M_{\odot}$ to $m_{\min} = 0.08 M_{\odot}$ (BODY1 and BODYN). The initial virial ratio is 0.5 (equilibrium). The stellar evolution is switched on (KZ(19)=3) and initial metallicity is 0.001. Multiples and chain regularization are switched on (KZ(15)=2 and KZ(30)=2). It uses solar neighbor tidal field (KZ(14)=1).

```
1 1000000.0 1.E6 40 40 640
16000 1 10 43532 100 1
0.02 0.02 0.1 1.0 1.0 1000.0 2.0E-05 1.0 0.7
0 1 1 0 1 0 4 0 0 2
0 1 0 1 2 1 0 0 3 6
1 0 2 0 0 2 0 0 0 2
1 0 2 1 1 0 1 1 0 0
0 0 0 0 0 0 0 0 0 0
1.0E-06 1E-4 0.2 1.0 1.0E-06 0.01 1.0
2.35 20.0 0.08 0 0 0.001 0 1.0
0.5 0.0 0.0 0.0
```

Input variables for primordial Binaries

Many star clusters contain initial hard binaries with binding energies much larger than the thermal energy (the threshold ECLOSE is a suitable division between hard and soft binaries). There are two ways to initialise primordial binaries:

The first one always starts from some initial mass function (IMF) provided by the routines `imf.f` or `imf2.f`. The option KZ(8)=1 or ≥ 3 invokes the routine `binpop.F`, which reads the last line of the input file containing NBIN and the parameters of their distribution (see above). In this case, binaries are created either by random pairing of single stars obtained from the IMF or by splitting them, depending on the value of KZ(20) (see above).

The second way assumes that particle data, including the binaries, are provided via the input data on file `dat.10` (as e.g. in the Kyoto–II collaborative experiment). In such a case KZ(8)=2 and NBIN0 should be set to the expected number of primordial binaries from the file. The code will first create NBIN0 centers of masses, and then use those for scaling, before regularizing the pairs and the calculation begins.

A typical input file with primordial binaries looks as follows. Here, we use binary random pairing from `imf2.f` and `binpop.F` (KZ(20)=6 and KZ(8)=3, respectively) for 1000 initial binaries. The semi-major axes of binaries use uniform distribution in log(semi) with a range from 41.3 AU to 0.00413 AU. The eccentricity of binaries use thermal distribution. It was created from this input file running for 1000 time units. Stellar evolution was also switched on in this file (KZ(19)=3). In the package of the code, the file `N10k_B1k.input` is included.

```
1 1000000.0 1.E6 40 40 640
10000 1 10 43532 100 1
0.02 0.02 0.17 1.0 1.0 800.0 5.0E-05 1.0 0.7
0 1 1 0 1 0 4 3 0 2
0 1 0 1 2 1 0 0 3 6
1 0 2 0 0 2 0 0 0 2
1 0 2 1 1 0 1 1 0 0
0 0 0 0 0 0 0 0 0 0
5.0E-06 3E-4 0.2 1.0 1.0E-06 0.01 0.5
2.35 100.0 0.08 1000 0 0.001 0 1.0
0.5 0.0 0.0 0.0
2E-4 -1.0 1.0 1E4 5 0
```

Stellar Evolution

Stellar evolution is invoked by KZ(19)=1,2 or KZ(19)≥3, offering two different schemes. The simpler one is KZ(19)=1, while the more complex one, K(19)≥3, is based on the Cambridge stellar evolution package (Hurley, Pols, Tout 2000). The common envelope, roche transfering binaries are also considered. The main effects are changing stellar masses, radii, and luminosities, which give rise to cluster mass loss. The mass is assumed to escape from the cluster immediately and possible collisions depend on stellar radii.

With the additional option KZ(12)>0, information on binaries and single stars is written on two files (unit 82, file `bev.82` and unit 83, file `sev.83`) in regular time intervals determined by TPLOT (See details in Section Output).

Restart

It's very common that in the computer cluster every job has running time limit, or the simulation stop due to some energy conservation problem or the normal stop when the stop criterion is reached. In this case the user may want to continue the simulation from the last time point. Thus the input parameter should changed to restart mode. The first line of input shown above combined together with two extra lines (See the description of KSTART in the parameter table above). A simple example is :

```
2 1000000.0 1.E6 40 40 640
```

Here KSTART=2 means every parameter keeps the same value as before and just restarts from the last saved file `fort.1`. If the user wants to change some parameters of simulation, KSTART=3,5 can be set. For example:

```
3 1000000.0 1.E6 40 40 640
2.0 2.0 0.0 0.0 0.0 0.0 16 0
```

This restart file will change DTADJ and DELTAT to 2.0. The KZ(16) is changed to 0. All other parameters that are set to 0.0 (TADJ, TNEXT, TCRIT, QE) keep same as before.

5 Thresholds for the variables

Before the compilation of the code (Chapter 3), the parameter file (`params.h`) should be consulted to check whether some vector dimensions are in the desired range. Most important are

- the maximum particle number `NMAX`,
- the maximum number of regularised KS pairs `KMAX`, and
- the maximum number of neighbours per particle `LMAX`.

The particles are saved in various lists which serve to distinguish between their funcionality. The table below explains their nomenclature. "KS–pairs" are particles that approach each other in a hyperbolic encounter; they are given a special treatment by the code (see Chapter 11). If NPAIRS is the amount of KS–pairs, then IFIRST = 2*NPAIRS + 1 is the first single particle (not member of a KS pair), and N the last one. NTOT = N + NPAIRS is the total number of particles plus c.m.'s. Therefore NMAX, the dimension of all vectors containing particle data should be at least of size N + KMAX, where N is the number of particles and KMAX the maximum number of expected KS pairs. If one starts with single particles, KMAX = 10 or 20 should usually be enough, but in clusters with a large number of primordial binaries, KMAX must be large.

N:	Total number of particles
NBIN0:	number of primordial binaries (physical bound stars)
NBIN:	???
NPAIRS:	Number of binaries (KS–pairs, see Chapter 11), transient unbound pairs as well as persistent binaries
NTOT:	= N + NPAIRS; Number of single particles plus centres of masses of regularized (KS) pairs
KMAX:	threshold for the amount of allowed KS pairs
NMAX:	= N + KMAX; threshold for the total number of particles and the centre of masses

Hier gibt's noch ein Bildchen!

6 How to read the diagnostics

The diagnostics is the ASCII readable text printed on unit 6 *stdout* ("out1000" in Chapter 3) that gives a brief overview of the global status and progress of the cluster simulation. Different routines write into that file, depending on the options chosen as the input variables. The following lines occur:

```
      N  NFIX  NCRIT  NRAND  NNBOPT  NRUN
   1000     5     10   1006      50     1

    ETAI      ETAR      RS0       DTADJ     DELTAT     TCRITp    TCRIT     QE        RBAR       ZMBAR
    1.0E-02   2.0E-02   3.0E-01   1.0E+01   1.0E+01   1.0E+06   2.0E+01   2.0E-05   1.0E+00   7.0E-01

    OPTIONS
   1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
   1  1  1  0  1  0  4  0  0  2  1  0  0  0  1  1  1  0  0  0  1  0  1  0  0  2  0  0  0  2  0  0  2  0  1  0  1  1  0  1

    OPTIONS BK:
   1  2  3  4  5  6  7  8  9 10
   0  0  0  0  0  0  0  0  0  0

    DTMIN     RMIN      ETAU      ECLOSE    GMIN      GMAX
    1.0E-04   1.0E-02   1.0E-01   1.0E+00   1.0E-06   1.0E-02
****** NOTE: new random number seed initialisation!
****** AND new ran2 from new ed. of Press et al.
```

written by the routine: `input.F`

Usage: Repetition of the input variables

```
STANDARD IMF    ALPHA = 2.35  BODY1 = 20.0  BODYN = 0.10 ZMASS = 3.36752E+02 NBIN0=    0 ZMET = 0.00 EPOCH0 = 0.00
.....................................................................................................
BINARY STAR IMF:   NB =  400  RANGE =  3.27E+01  2.14E-01 ZMB = 3.74E+02  <MB> = 9.36E-01
SINGLE STAR IMF:   NS = 1200  RANGE =  7.76E+00  1.01E-01 ZMS = 5.25E+02  <MS> = 4.38E-01
```

IMF power law index, max. mass, min. mass, total mass, # of primordial bin., metallicity, evolution. epoch [Myrs].
.....
number of objects, mass range, average mass before scaling.

`data.F`, (if KZ(20)=0 & BODY1≠BODYN)

or

`imf2.F`, if KZ(20)≥2

Information about initial mass function (IMF).

```
      SCALING:   SX =  1.00421D+00  E = -2.49E-01  M(1) = 5.94E-02  M(N) = 2.97E-04  <M> = 1.00E-03

      TIME SCALES:   TRH = 2.8E+01  TCR = 2.8E+00  2<R>/<V> = 2.8E+00


 PHYSICAL SCALING:    R* = 1.0000E+00  M* = 7.0000E+02  V* = 1.7348E+00  T* = 5.6466E-01  <M> = 7.0000E-01
                      SU = 4.4335E+07  AU = 2.0627E+05  YRS = 3.5408E+06
```

scale.F, units.f

scaling factor for energy, total energy, max. mass, min. mass, average mass *after scaling*;
Spitzer's half-mass relaxation time, crossing time obtained from total energy and mass, crossing time obtained from virial radius (see 12);
information about physical scaling: values of one N–body unit in length (pc), mass (solar masses), velocity (km/s), time (million years), average mass of particles (solar massses), astronomical units (one N–body unit) and years (one N–body unit).

```
fpoly1 time=  0.1200000035762785
fpoly2 time=  0.2100000062584875
```

start.F

CPU (wall clock in parallel execution) time for initialising the force and its time derivative (`fpoly1, fpoly_mpi.f`) and the second and third time derivative of the force (`fpoly2, fpoly2_mpi.f`). The mpi-versions are called for initialisation in case of parallel runs.

---

lagr.F

```
   TIME  M/MT:    1.00D-02  2.00D-02  5.00D-02  1.00D-01  2.00D-01  3.00D-01  4.00D-01  5.00D-01  7.00D-01  9.00D-01  1.00D+00 <RC
     0.0 RLAGR:   1.52D-01  1.81D-01  1.91D-01  2.83D-01  4.33D-01  5.22D-01  6.17D-01  7.52D-01  1.16D+00  1.96D+00  5.86D+00  2.97D-01
     0.0 AVMASS:  6.26D-04  4.26D-03  6.13D-04  9.45D-04  7.82D-04  1.11D-03  1.09D-03  8.35D-04  9.19D-04  1.25D-03  9.01D-04  1.23D-03
     0.0 NPARTC:        17         9         2        53       130        90        91       122       216       163       107        90
     0.0 SIGR2:   2.19D-01  1.70D-01  7.37D-01  2.44D-01  1.89D-01  2.33D-01  2.16D-01  2.43D-01  1.72D-01  8.36D-02  5.09D-02  2.09D-01
     0.0 SIGT2:   2.01D-01  8.25D-02  4.46D-02  2.12D-01  3.39D-01  2.42D-01  1.71D-01  1.83D-01  1.51D-01  1.03D-01  6.16D-02  1.63D-01
     0.0 VROT:   -8.34D-02  4.41D-01 -6.28D-01  3.14D-02 -1.54D-01 -9.44D-02 -6.45D-02  1.17D-02  5.35D-02  1.98D-02 -3.46D-02  4.46D-01
```

Time, specification of the Lagrangian radii, core radius
Time, Lagrangian radii, core radius (if primordial binaries: separately for singles and binaries, not shown above)
Time, average mass between Lagrangian radii, avmass in the core
Time, number of particles within the shell, in the core
Time, radial velocity dispersion within the shell, in the core
Time, tangential vel. dispersion within the shell, in the core
Time, rotational vel. within the shell, in the core (not shown above)

```
 0 ADJUST:  TIME =    1.00000D+01  T[Myr] =     5.65  Q = 0.52  DE =  -1.403819E-05  E =  -2.500038E-01 EBIN=   0.000000E+00 EMERGE=   0.000000E+00
```

adjust.F

rank, “ADJUST:”, total time in NB units, physical time, virial ratio, relative energy error, total energy, total energy of regularized pairs, energy of mergers

---

```
 RMIN = 1.1E-03  DTMIN = 3.5E-05 RHOM = 3.5E+02 RSCALE = 9.5E-01 RSMIN = 2.2E-01  ECLOSE = 1.05  TC =    3
 PE  N       ttot      treg      tirr      tpredtot  tint      tinit      tks      ttcomm    tadj     tmov      tprednb  tsub     tsub2    xtsub1   xtsub2
  0  1000     41.46000     29.54      7.23      0.63     40.39      0.99      0.07      0.00      0.59      0.00      1.50      0.00      0.00  0.00000D+00  0.00000D+00
```

close encounter distance and minimum time step (for regularization search, updated from input parameters if KZ(16)=1), maximum density, virial radius, minimum neighbour sphere, hard binary threshold energy, total run time in units of initial crossing times

number of processors, number of particles, total processing time, total regular processing, total irregular processing, processing of prediction, time spent in `intgrt.F`, for initialisation, for KS integration, for communication, for adjust and energy check, for overhead of moving data in parallel runs, for neighbour predictions, for MPI communication after irregular (tsub) and regular (tsub2) blocks, number of bytes transferred respectively. From xtsub1/tsub and xtsub2/tsub2 the sustained bandwidth of MPI communication can be read off. Note, that the determination of these quantities involves a certain overhead by many calls of `cputim.F` per block, so for critically large production runs one may want to comment these out (most of them in `intgrt.F`).

adjust.F

```
 0 T =   10.0  N = 1000  <NB> = 20  KS =    0  NM = 0 MM = 0 NS =  1000 NSTEPS =    1610624       273    321696       1016  DE =  -0.140382E-04  E =       -0.250004

NRUN =  1  M# =  1  CPU = 6.91000E-01  TRC =  0.0  DMIN = 6.6E-05 6.6E-05 1.0E+02 1.0E+02  AMIN = 1.0E+02  RMAX = 0.0E+00  RSMIN = 0.22  NEFF =   128

   <R>  RTIDE  RDENS   RC      NC   MC   RHOD   RHOM  CMAX   <Cn>  Ir/R    UN    NP    RCM    VCM         AZ      EB/E   EM/E   TCR     T6
#1 0.95   9.5   0.21  0.08      5  0.073  159.   350.    5.  37.0  0.13     0     0    0.000  0.0000   0.006197  0.000  0.000  2.83     5

      NNPRED    NBCORR  NBFULL  NBVOID  NRCONV    NICONV  NBSMIN  NBDIS  NBDIS2  NCMDER  NBDER  NFAST  NBFAST    NBLOCK     NBPRED
#2     20204    294307       0      98    2664      9227    1576      0       0      33      0      0       0     58132    3045868

    NKSTRY  NKSREG  NKSHYP     NKSPER  NPRECT  NKSREF  NKSMOD  NTTRY  NTRIP  NQUAD  NCHAIN  NMERG  NSTEPT  NSTEPQ  NSTEPC    NBLCKR    NBFLUX
#3   14463      45      33          0       0       0       0      0      0      0       0      0       0       0       0     10333   1903963
```

output.F

time, actual particle number, average neighbour number, number of KS pairs, number of merged KS pairs, number of hierarchical subsystems, number of single stars, step numbers (irregular, irr. c.m., regular, KS), relative energy error since last output, total energy

several more lines uncommented here....

```
STEP I     0    3   63   91  154  220  160  133  109   44   19    4
STEP R     0    4   77  133  249  310  179   45    3
Max Speedup Irr:     4 3.76D+00    8 6.82D+00   16 1.14D+01   32 1.66D+01   64 2.15D+01  128 2.49D+01  256 2.66D+01  512 2.74D+01 1024 2.77D+01
Max Speedup Reg:     4 3.71D+00    8 6.69D+00   16 1.12D+01   32 1.67D+01   64 2.22D+01  128 2.62D+01  256 2.91D+01  512 3.04D+01 1024 3.11D+01
```

levels.f

histogram of distribution of irregular (STEP I), regular (STEP R)
If there are p step distribution (not appearing here, STEP U, in physical time), statistics of parallel work for irr. and reg. steps, figures given are theoretical speedups for infinitely fast communication (limit of large block sizes)

```
        END RUN    TIME[Myr] =   11.29  TOFF/TIME/TTOT=      0.00000000     20.00000000     20.00000000  CPUTOT =    1.6  ERRTOT =-5.15000D-05  DETOT =-1.28197D-05

       0 INTEGRATION INTERVAL =   20.00    NIRR=    3237662 NIRRB=       1245 NREG=     779010 NKS=       4625

         PER TIME UNIT: NIRR= 1.61883D+05 NIRRB= 6.22500D+01 NREG= 3.89505D+04 NKS= 2.31250D+02
 Total CPU=   97.11000289410342
```

adjust.F

This is the regular end of a run giving: the integration time, total cumulative absolute and relative errors, cumulative number of regular, irregular, KS steps, the step numbers per time unit and the total CPU (wall clock for parallel) time in minutes.

To check a regular stop of the run, look at the end of the diagnostics first. If there are failures, the line "`CALCULATION HALTED`" appears and means that the energy conservation could not be guaranteed. A restart with smaller steps (ETAI, ETAR) and larger neighbour number NNBOPT may cure the problem, but not always; persistent problems should be reported to Rainer Spurzem.

The unix command on the output file, e.g.

homedir`> grep ADJUST out1000`

produces an overview of the accuracy (energy error at every DTADJ interval). It may show where problems originated; a restart from the last ADJUST before the error with smaller output intervals is one way to look after it. Watch out, because sometimes errors are not reproducible, because changes in ADJUST intervals change frequencies of prediction and small differences can build up. A quick possibility to see the real evolution of the system is to `grep` for the lines with Lagrangian radii and other quantities (see above), which can directly be plotted, e.g. with gnuplot, because the first column is always the time.

7 Runs on parallel machines

For parallel runs, the file `mpif.h` is very important, and system specialists should be consulted in addition to us what to use. Again, for some standard systems templates are provided (e.g. `mpif.t3e.h` or `mpif.mpich.h`). The routine providing CPU–time measurements, `cputim.F` , and the use of the function `flush.f` may need special attention depending on the hardware.

8 The Hermite integration method

Each particle is completely specified by its mass m, position $\mathbf{r}_0$, and velocity $\mathbf{v}_0$, where the subscript 0 denotes an initial value at a time t_0. The equation of motion for a particle i is given by its momentary acceleration $\mathbf{a}_{0,i}$ due to all other particles and its time derivative $\dot{\mathbf{a}}_{0,i}$ as

$$\mathbf{a}_{0,i} = -\sum_{i\neq j} Gm_j \frac{\mathbf{R}}{R^3}, \tag{1}$$

$$\dot{\mathbf{a}}_{0,i} = -\sum_{i\neq j} Gm_j \left[\frac{\mathbf{V}}{R^3} + \frac{3\mathbf{R}(\mathbf{V}\cdot\mathbf{R})}{R^5}\right], \tag{2}$$

where G is the gravitational constant; $\mathbf{R} = \mathbf{r}_{0,i} - \mathbf{r}_{0,j}$ is the relative coordinate; $R = |\mathbf{r}_{0,i} - \mathbf{r}_{0,j}|$ the modulus; and $\mathbf{V} = \mathbf{v}_{0,i} - \mathbf{v}_{0,j}$ the relative space velocity to the particle j.

The Hermite scheme employed in NBODY6++ follows the trajectory of the particle by firstly "predicting" a new position and new velocity for the next time step t. A Taylor series for $\mathbf{r}_i(t)$ and $\mathbf{v}_i(t)$ is formed:

$$\mathbf{r}_{p,i}(t) = \mathbf{r}_0 + \mathbf{v}_0(t-t_0) + \mathbf{a}_{0,i}\frac{(t-t_0)^2}{2} + \dot{\mathbf{a}}_{0,i}\frac{(t-t_0)^3}{6}, \tag{3}$$

$$\mathbf{v}_{p,i}(t) = \mathbf{v}_0 + \mathbf{a}_{0,i}(t-t_0) + \dot{\mathbf{a}}_{0,i}\frac{(t-t_0)^2}{2}. \tag{4}$$

The predicted values of $\mathbf{r}_p$ and $\mathbf{v}_p$, which result from this simple Taylor series evaluation, using the force and its time derivative at t_0, do not fulfil the requirements for an accurate high–order integrator; they just give a first approximation to $\mathbf{r}_1$ and $\mathbf{v}_1$ at the upcoming time t_1. Even if the time step, $t_1 - t_0$, is chosen impracticably small, a considerable error will quickly occur, let alone the inadequate computational effort. Therefore, an improvement is made by the Hermite interpolation which approximates the higher accelerating terms by another Taylor series:

$$\mathbf{a}_i(t) = \mathbf{a}_{0,i} + \dot{\mathbf{a}}_{0,i}\cdot(t-t_0) + \frac{1}{2}\mathbf{a}^{(2)}_{0,i}\cdot(t-t_0)^2 + \frac{1}{6}\mathbf{a}^{(3)}_{0,i}\cdot(t-t_0)^3, \tag{5}$$

$$\dot{\mathbf{a}}_i(t) = \dot{\mathbf{a}}_{0,i} + \mathbf{a}^{(2)}_{0,i}\cdot(t-t_0) + \frac{1}{2}\mathbf{a}^{(3)}_{0,i}\cdot(t-t_0)^2. \tag{6}$$

Here, the values of $\mathbf{a}_{0,i}$ and $\dot{\mathbf{a}}_{0,i}$ are already known, but a further derivation of equation (2) for the two missing orders on the right hand side turns out to be quite cumbersome. Instead, one determines the additional acceleration terms from the predicted ("provisional") $\mathbf{r}_p$ and $\mathbf{v}_p$; we calculate their acceleration and time derivative according to the equations (1) and (2) anew and call these new terms $\mathbf{a}_{p,i}$ and $\dot{\mathbf{a}}_{p,i}$, respectively. Because these values ought to be generated by the former high–order terms also (which we avoided), we put them into the left–hand sides of (5) and (6). Solving equation (6) for $\mathbf{a}^{(2)}_{0,i}$, then substituting it into (5) and simplifying yields the third derivative:

$$\mathbf{a}^{(3)}_{0,i} = 12\frac{\mathbf{a}_{0,i} - \mathbf{a}_{p,i}}{(t-t_0)^3} + 6\frac{\dot{\mathbf{a}}_{0,i} + \dot{\mathbf{a}}_{p,i}}{(t-t_0)^2}. \tag{7}$$

Similarly, substituting (7) into (5) gives the second derivative:

$$\mathbf{a}^{(2)}_{0,i} = -6\frac{\mathbf{a}_{0,i} - \mathbf{a}_{p,i}}{(t-t_0)^2} - 2\frac{2\dot{\mathbf{a}}_{0,i} + \dot{\mathbf{a}}_{p,i}}{t-t_0}. \tag{8}$$

Note, that the desired high–order accelerations are found just from the combination of the low–order terms for $\mathbf{r}_0$ and $\mathbf{r}_p$. We never derived higher than the first derivative, but achieved the higher orders easily through (1) and (2). This is called the Hermite scheme.

Previously, a four–step Adams–Bashforth–Moulton integrator was used (especially in NBODY5, [2]), however, the new Hermite scheme allows twice as large timesteps for the same accuracy. Also its storage requirements are less [16], [17], [4], [5].

Finally, we extend the Taylor series for $\mathbf{r}_i(t)$ and $\mathbf{v}_i(t)$, eqs. (3) and (4), by two more orders, and find the "corrected" position $\mathbf{r}_{1,i}$ and velocity $\mathbf{v}_{1,i}$ of the particle i at the computation time t_1 as

$$\mathbf{r}_{1,i}(t) = \mathbf{r}_{p,i}(t) + \mathbf{a}^{(2)}_{0,i}\frac{(t-t_0)^4}{24} + \mathbf{a}^{(3)}_{0,i}\frac{(t-t_0)^5}{120}, \tag{9}$$

$$\mathbf{v}_{1,i}(t) = \mathbf{v}_{p,i}(t) + \mathbf{a}^{(2)}_{0,i}\frac{(t-t_0)^3}{6} + \mathbf{a}^{(3)}_{0,i}\frac{(t-t_0)^4}{24}. \tag{10}$$

The integration cycle for other upcoming steps may now be repeated from the beginning, eqs. (1) and (2). The local error in $\mathbf{r}$ and $\mathbf{v}$ within the two time steps $\Delta t = t_1 - t_0$ is expected to be of order $\mathscr{O}(\Delta t^5)$, the global error for a fixed physical integration time scales with $\mathscr{O}(\Delta t^4)$ [15].

9 Individual and block time steps

Stellar systems are characterized by a huge dynamical range in radial and temporal scales. The time scale varies e.g. in a star cluster from orbital periods of binaries of some days up to the relaxation of a few hundred million years, or even billions of years. Even if we put for a moment the very close binaries aside, which are treated differently (by regularization methods), there typically is a large dynamic range in the average local stellar density from its centre to the very outskirts, where it dissolves into the galactic tidal field. In a classical picture, the two closest bodies would determine the time–step of force calculation for the whole rest of the system. However, for bodies in regions where the changes of the force are relatively small, a permanent re–computing of the terms appears time consuming. So, in order to economize the calculation, these objects shall be allowed to move a longer distance before a recomputation becomes necessary. In between there is always the possibility to acquire particle positions and velocities via a Taylor series prediction, as described in Chapter 8. This is the idea of a vital method for assigning different time–steps, $\Delta t = t_1 - t_0$, between the force computations, the so–called "individual time–step scheme" [1], which was later advanced to the hierarchical block steps.

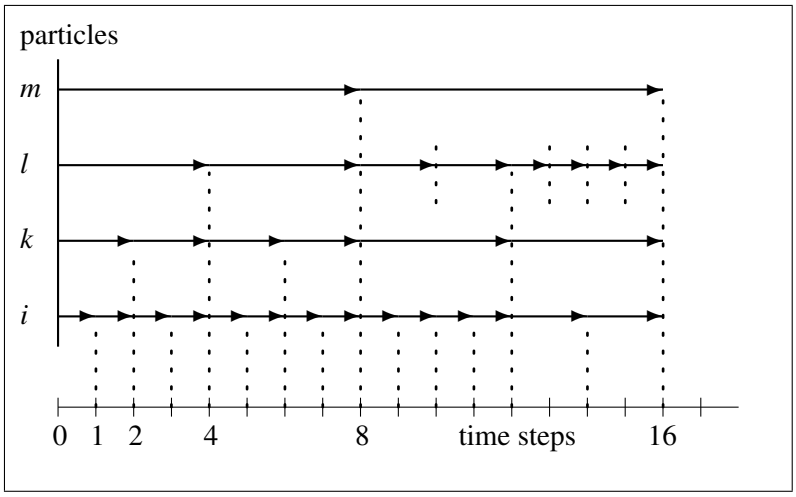


Figure 9.1: Block time steps exemplary for four particles.

Each particle is assigned its own Δt_i which is first illustrated for the case of "block time–steps" in Figure 9.1. The particle named i has the smallest time step at the beginning, so its phase space coordinates are determined at each time step. The time step of k is twice as large as i's, and its coordinates are just extrapolated ("predicted") at the odd time steps, while a full force calculation is due at the dotted times. The step width may be altered or not after the end of the integration cycle for the special particle, as demonstrated for k and l beyond the label "8". The time steps have to stay commensurable with both, each other as well as the total time, such that a hierarchy is guaranteed. This is the block step scheme.

As a first estimate, the rate of change of the acceleration seems to be a reasonable quantity for the choice of the time step: $\Delta t_i \propto \sqrt{\mathbf{a}_i/\dot{\mathbf{a}}_i}$. But it turns out that for special situations in a many-body system, it provides some undesired numerical errors. After some experimentation, the following formula was adopted [2]:

$$\Delta t_i = \sqrt{\eta \frac{|\mathbf{a}_{1,i}||\mathbf{a}^{(2)}_{1,i}| + |\dot{\mathbf{a}}_{1,i}|^2}{|\dot{\mathbf{a}}_{1,i}||\mathbf{a}^{(3)}_{1,i}| + |\mathbf{a}^{(2)}_{1,i}|^2}}, \tag{11}$$

where η is a dimensionless accuracy parameter which controls the error. In most applications it is taken to be $\eta \approx 0.01$ to 0.02, see also next chapter.

For the block–time steps, the synchronization is made by taking the next–lowest integer of Δt_i; the time steps are quantized to powers of 2 [15]. Then, there will be a group (block) of several particles which are due to movement at each time step. If one keeps the exact Δt_i's evaluated from (11) for each particle, the commensurability is destroyed, and we arrive at the so–called "individual time steps"; in this case, there exists one sole particle being due. The latter concept is realized in the earlier codes NBODY1, NBODY3, NBODY5, where a neighbour scheme is renounced. NBODY4, NBODY6, and NBODY6++ use a block step scheme.

Subsystems like star binaries, triples or a similar subgroups (they are termed KS pairs, chains, hierarchies) enter the time–step scheme with their respective centre's of masses only. Their internal motion is treated in a different way by a regularized integration (Chapter 11).

10 The Ahmad–Cohen scheme

The computation of the full force for each particle in the system makes simulations very time–consuming for large memberships. Therefore, it is desirable to construct a method in order to speed up the calculations while retaining the collisional approach. One way to achieve this is to employ a "neighbour scheme", suggested by [9].

The basic idea is to split the force polynomial (5) on a given particle i into two parts, an irregular and a regular component:

$$\mathbf{a}_i = \mathbf{a}_{i,\mathrm{irr}} + \mathbf{a}_{i,\mathrm{reg}}. \tag{12}$$

The irregular acceleration $\mathbf{a}_{i,\mathrm{irr}}$ results from particles in a certain neighbourhood of i (in the code, FI and FIDOT are the irregular force and its time derivative at the last irregular step; internally some routines use FIRR and FD as a local variable). They give rise to a stronger fluctuating gravitational force, so it is determined more frequently than the regular one of the more distant particles that do not change their relative distance to i so quickly (in the code, FR and FRDOT are the regular force and its time derivative at the last regular step; some routines use as a local variable FREG and FDR). We can replace the full summation in eq. (1) by a sum over the N_{nb} nearest particles for $\mathbf{a}_{i,\mathrm{irr}}$ and add a distant contribution from all the others. This contribution is updated using another Taylor series up to the order FRDOT, the time derivative of FR at the last regular force computation[1].

Wether a particle is a neighbour or not is determined by its distance; all members inside a specified sphere ("neighbour sphere" with radius r_{s}) are held in a list, which is modified at the end of each "regular time–step" when a total force summation is carried out. In addition, approaching particles within a surrounding shell satisfying $\mathbf{R}\cdot\mathbf{V} < 0$ are included. This "buffer zone" serves to identify fast approaching particles before they penetrate too far inside the neighbour sphere. The neighbour criterion should be improved according to relative forces rather than distances, in particular, if there are very strong mass differences between particles (black holes!) — such kind of work is under progress.

Figures 10.1 and 10.2 show how the Ahmad–Cohen scheme works for one particle [17]. At the beginning of the force calculation, a list of neighbour objects around the particle i is created first (filled dots). From this neighbour list the irregular component $\mathbf{a}_{i,\mathrm{irr}}$ is calculated, and then the summation is continued to the distant particles obtaining $\mathbf{a}_{i,\mathrm{reg}}$. At the same time we also calculate the first time derivative. From the equations (5) and (6) the position and velocity of the particle i are predicted. At time $t_{1,\mathrm{irr}}$ we apply the "corrector" only for $\mathbf{a}_{i,\mathrm{irr}}$ from the neighbours; the regular component we do not correct, but obtain by extrapolating $\mathbf{a}_{i,\mathrm{reg}}$. At the next step, $t_{2,\mathrm{irr}}$, the same predictor–corrector method proceeds for the neighbour particles, while the correction of the distant acceleration term is still neglected. When t_1 is reached, the total force is calculated on the basis of the full application of the Hermite predictor–corrector method. Also, a new neighbour list is constructed using the positions at time t_1. Thus, we calculate at certain times only the forces from neighbours (irregular time–step, t_{irr}), while at other times we calculate both the forces from neighbours and distant particles (regular time–step, t_{reg}).

For a neighbour list of size $N_{\mathrm{nb}} \ll N$, this procedure can lead to a significant gain in efficiency, provided the respective time scales for $\mathbf{a}_{i,\mathrm{irr}}$ and $\mathbf{a}_{i,\mathrm{reg}}$ are well separated.

[1] Note, that the code also keeps the variables F and FDOT, which contain one half (!) of the *total* force, and one sixth (!) of the *total* time derivative of the force; this just a handy assignment for the frequent predictions of equation 3.

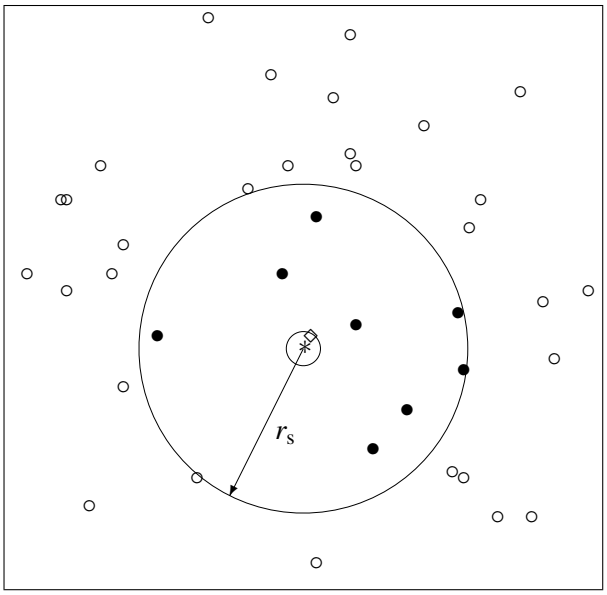


Figure 10.1: Illustration of the neighbour scheme for particle i marked as the asterisk (after [2]).

The actual size of neighbour spheres in NBODY6++ is controlled iteratively by a requirement in order to keep a certain optimal number of neighbours. This variable, NNBOPT, can be adjusted according to performance requirements. Its typical values are between 50 and 200 for a very wide range of total particle numbers N. Outside of the half-mass radius, the requirement of having NNBOPT neighbours is relaxed due to low local densities. Insisting on NNBOPT neigbours could result in undesired large amplitude fluctuations of the neighbour radii.

While [18] claim that the optimal neighbour number should grow as $N^{3/4}$ (which would be unsuitable for the performance on parallel computers), this is still an unsettled question. [2] advocates the coupling of the neighbour radius to the local density contrast, but NBODY6++ does *not* use that, since it makes average neighbour numbers much less predictable, which is bad for the performance and profiling issues on supercomputers, again.

Resuming, the method of the two particle groups is squeezed into the hierarchical time–step scheme making the overall view quite complex. Each particle is moved due to its time–step order *and* the time–steps, because the force calculation is divided: In eq. (11) a further subscript is needed which distinguishes the regular and irregular time step. The accuracy can be tuned by

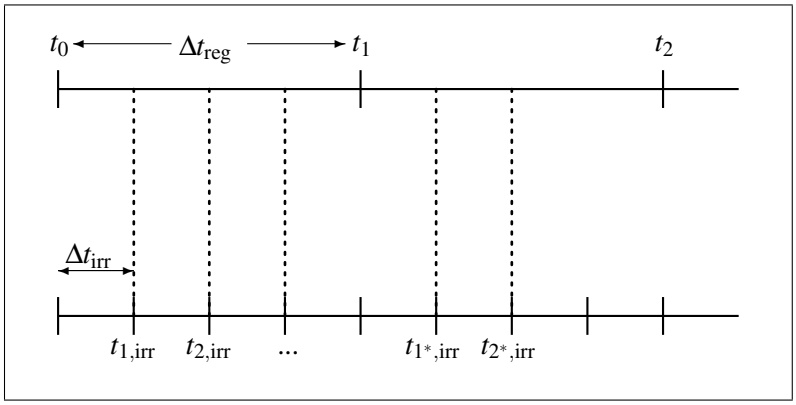


Figure 10.2: Regular and irregular time steps (after [17]).

$\eta_{\rm irr} \approx 0.01$ and $\eta_{\rm reg} \approx 0.02$, again.

Both, the neighbour scheme and the hierarchical time–step scheme have in common that they are centered on one particle i, and they distinguish between nearby and remote stars, and they save computational time. One may ask: What is the intriguing difference between them? — The neighbour scheme is a *spatial* hierarchy, which avoids a frequent force calculation of the remote particles, because their totality provides a smooth potential which does not vary so much with respect to the particle i; that potential is rather superposed by some fluctuating peaks of close–by stars which will be "worked in" by the more often force determination. The time step scheme, in contrast, exhibits the *temporal* behaviour of the intervals for re–calculation of the full force in order to maintain the exactness of the trajectory; time steps chosen too small slow down the advancing calculation losing the computer's efficiency.

11 KS–Regularization

The fourth main feature of the codes since NBODY3 is a special treatment of close binaries. A close encounter is characterised by an impact parameter that is smaller than the parameter for a 90 degree deflection

$$p_{90} = 2G(m_1 + m_2)/v_\infty^2 \tag{13}$$

where G, m_1, m_2, v_∞ are the gravitational constant, the masses of the two particles and their relative velocity at infinity. In the cluster centre, it is very likely that two (or even more) stars come very close together in a hyperbolic encounter. As the relative distance of the two bodies becomes small ($R \to 0$), their timesteps are reduced to prohibitively small values, and truncation errors grow due to the singularity in the gravitational potential, eqs. (1) and (2). In the NBODY code, the parameter RMIN is used to define a close encounter, and it is kept to the value of equation 13 (if KZ(16) > 0 is chosen in the control parameters). The corresponding time step DTMIN can be estimated from

$$dt_{\min} = \kappa \Big[\frac{\eta}{0.03}\Big] \Big(\frac{r_{\min}^3}{\langle m \rangle}\Big)^{1/2} \tag{14}$$

where κ is a free numerical factor, η the general time step factor, and $\langle m \rangle$ the average stellar mass [2]. If two particles are getting closer to each other than RMIN, and their time steps getting smaller than DTMIN, then they are candidates for "regularization".

Regularization is an elegant trick in order to deal with such particles which are as close as the diamond in the Figure 10.1. The idea is to take both stars out of the main integration cycle, replace them by their centre of mass (c.m.) and advance the usual integration with this composite particle instead of resolving the two components. The two members of the regularized pair (henceforth KS pair) will be relocated to the beginning of all vectors containing particle data, while at the end one additional c.m. particle is created (see below). One of the purposes of the code variable NAME(I) is to identify particles after such a reshuffling of data.

To be actually regularized, the two particles have to fulfil two more sufficient criteria: that they are approaching each other, and that their mutual force is dominant. In the equations in routine `search.f`, these sufficient criteria are defined as

$$\mathbf{R} \cdot \mathbf{V} > 0.1 \sqrt{(G(m_1 + m_2)R}$$
$$\gamma := \frac{|\mathbf{a}_{\text{pert}}| \cdot R^2}{G(m_1 + m_2)} < 0.25$$

Here, $\mathbf{a}_{\text{pert}}$ is the vectorial differential force exerted by other perturbing particles onto the two candidates, R, $\mathbf{R}$, $\mathbf{V}$ are scalar and vectorial distance and relative velocity vector between the two candidate, respectively. The factor 0.1 in the upper equation allows nearly circular orbits to be regularized; $\gamma < 0.25$ demands that the relative strength of the perturbing forces to the pairwise force is one quarter of the maximum. These conditions describe quantitatively that a two-body subsystem is dynamically separated from the rest of the system, but not unperturbed.

The internal motion of a KS pair will be determined by switching to a different (regularized) coordinate system. This transformation can be traced back to the square in quaternion space, where — by sacrificing some commutativity rules — it is guaranteed that the real-space motion does not leave the three-dimensional Cartesian space. It involves a set of four regular spatial coordinates and a fictitious time $s(t)$, obtained in its simplest variant by the transformation $dt = Rds$. Any unperturbed two–body orbit in real space is mapped onto a harmonic oscillator in KS–space with double the frequency. Since the harmonic potential is regular, numerical integration with high accuracy can proceed with much better efficiency, and there is no danger of truncation errors for

arbitrarily small separations. The internal time–step of such a KS–regularized pair is independent of the eccentricity and, depending on the parameter ETAU, of the order of some 50–100 steps per orbit. The method of regularization goes back to [14] and makes an accurate calculation of a perturbed two–body motion possible. A modern theoretical approach to this subject can be found in [25]; the Hamiltonian formalism of the underlying transformations is nicely explained in [20].

While regularization can be used for any analytical two–body solution across a mathematical collision, it is practically applied to perturbed pairs only. Once the perturbation γ falls below a critical value (input parameter GMIN $\approx 10^{-6}$), a KS–pair is considered unperturbed, and the analytical solution for the Keplerian orbit is used instead of doing numerical integration. A little bit misleading is that such unperturbed KS–pairs are denoted in the code as "mergers", e.g. in the number or merges (NM) and the energy of the mergers (EMERGE). Merged pairs can be resolved at any time if the perturbation changes. The two–body KS regularization occurs in the code either for short-lived hyperbolic encounters or for persistent binaries.

In the code, the KS–pair appears as a new particle at the postion of the centre of mass. The variable NTOT, that contains the total number of particles N plus the c.m.'s, is increased by 1. When the pair is disrupted, NTOT is decreased again. The maximum number of possible KS–pairs is saved in the variable KMAX, which sets a threshold for the extension of the vector NTOT (see Chapter 5).

Close encounters between single particles and binary stars are also a central feature of cluster dynamics. Such temporary triple systems often reveal irregular motions, ranging from just a perturbed encounter to a very complex interaction, in which disruption of binaries, exchange of components and ejection of one star may occur. Although not analytically solvable, the general three–body problem has received much attention. So, the KS–regularization was expanded to the isolated 3– and 4–body problem, and later on to the perturbed 3–, 4–, and finally to the N–body problem. The routines are called

- `triple.f` (unperturbed 3-body subsystems, [8]),
- `quad.f` (unperturbed 4-body subsystems), and
- `chain.f` with different stages of implementation (slow-down, Stumpff functions, see for consecutive references Mikkola & Aarseth 1990, 1993, 1996, 1998, and [20]).

While occurrences of "triple" and "quad" will be rare in a simulation, the chain regularization is invoked if a KS–pair has a close encounter with another single star or another pair. Especially, if systems start with a large number of primordial binaries, such encounters may lead to stable (or quasi-stable) hierarchical triples, quadruples, and higher multiples. They have to be treated by using special stability criteria. Some of them are actually already implemented, but there is ongoing research and development in the field.

A typical way to treat all such special higher subsystems is to define their c.m. to be a pseudo-particle, i.e. a particle with a known sub-structure (very much like nodes in a TREE code). The members of the pseudo-particles will be deactivated by setting their mass to zero (ghost particles). At present there can only exist one chain at a time in the code, while merged KS binaries, and hierarchical subsystems can be more frequent. Details of these procedures are beyond the scope of this introductory manual.

Every subsystem — KS pair, chain or hierarchical subsystem — is perturbed. Perturbers are typically those objects that get closer to the object than $R_{\rm sep} = R/\gamma_{\rm min}^{1/3}$, where R is the typical size of the subsystem; for perturbers, the components of the subsystem are resolved in their own force computation as well (routines `cmfreg.f`, `cmfirr.f`).

12 Nbody–units

The NBODY–code uses Dimensionless units, so–called "Nbody units". They are obtained when setting the gravitational constant G and the initial total cluster mass M equal to 1, and the initial total energy E to $-1/4$ (see [12], [7]).

Since the total energy E of the system is $E = K + W$ with $K = \frac{1}{2}M\langle v^2\rangle$ being the total kinetic energy and $W = -(3\pi/32)GM^2/R$ the potential energy of the Plummer sphere, we find from the virial theorem that

$$E = \frac{1}{2}W = -\frac{3\pi}{64}\frac{GM^2}{R}. \tag{15}$$

R is a quantity which determines the length scale of a Plummer sphere. Using the specific definitions for G, M, and E above, this scaling radius becomes $R = 3\pi/16$ in dimensionless units. The half mass radius $r_{\rm h}$ can easily be evaluated by the formula (e.g. [26]):

$$M(r) = M\frac{r^3/R^3}{(1+r^2/R^2)^{3/2}} \tag{16}$$

when setting $M(r_{\rm h}) = \frac{1}{2}M$. It yields $r_{\rm h} = (2^{2/3}-1)^{-1/2}R = 1.30R$. The half–mass radius is located at $R = 0.766$, or about 3/4 "Nbody–radii".

The virial radius of a system is defined by $R_{\rm vir} = GM^2/2|W|$, while the r.m.s. velocity is $\langle v^2\rangle^{1/2} = 2K/M$. In virial equilibrium $|W| = 2K$, so it follows for the crossing time

$$t_{\rm cr} := \frac{2R_{\rm vir}}{\langle v^2\rangle^{1/2}} = \frac{GM^{5/2}}{(2|E|)^{3/2}}. \tag{17}$$

The setting of $G = M = 1$ and $E = -0.25$ also determines the unit of time; so it follows that $t_{\rm cr} = 2\sqrt{2}$ in N-body units. By inversion we have

$$\tau_{\rm NB} = \frac{GM^{5/2}}{(4|E|)^{3/2}}, \tag{18}$$

for the unit of time $\tau_{\rm NB}$. The virial radius of Plummer's model is $R_{\rm vir} = 1$ in N-body units.

13 Output

Table 17: Definition of parameters

Global properties	
TIME	time of simulation
RSCALE	Half mass radius
RTIDE	Tidal radius
RC	Core radius
NC	Number of stars inside core radius
MC	Core mass
VC	r.m.s velocity inside core radius
CMAX	Maximum number density / half mass mean value
RDENS(1:3)	Density center position
RHOD	Density weighted average density $\Sigma RHO^2/\Sigma RHO$
RHOM	Maximum mass density / half mass mean value
$\langle M \rangle$	Average mass of star
M1	Mass of most massive star
ZMASS	Total mass of cluster
MODEL	Snapshot counter in output
NRUN	Run identification index
TIDAL4	Twice angular velocity for linearised tidel force
Energy	
DE	relative energy error
DELTA	absolute energy error
BE(1)	Intial total energy
BE(2)	Last adjust total energy
BE(3)	Current total energy
ZKIN	Kinetic energy
POT	Potential energy
ETIDE	Tidal energy
ETOT	Total energy
E	Mechanical energy: ZKIN - POT + ETIDE (E(3))
ESUB	Binding energy of unperturbed triples and quadruples
EMERGE	Binding energy of mergers (E(9))
EBIN	Binding energy of KS binaries
ECOLL	The difference of binding energy of inner binary at the end and begin of hierarchical systems (E(10))
EMDOT	Mechanical energy of mass loss due to stellar evolution (E(12))
ECDOT	Energy of velocity kick due to stellar evolution
ECH	Binding energy of chain
EBINP	Primordial KS binary energy (E(1))
EBINN	Energy of new KS binary formed by dynamics (E(2))
EESCS	Single escaper mechanical energy (E(4))
EESCPB	Binding energy of primordial KS binary escapers (E(5))

EESCPC	Mechanical energy of center mass of primordial KS binary escapers (E(6))
EESCNB	Binding energy of new formed KS binary escapers (E(7))
EESCNC	Mechanical energy of center mass of new KS binary escapers (E(8))
Scaling factors (Astronomical units = *N*–body units × scaling factor)	
RBAR	PC
TSCALE	Myr
TSTAR	Myr
VSTAR	km/s
RAU	AU
ZMBAR	Solar mass
SU	Solar radius
Astronomical units	
R*	Solar radius
L*	Solar luminosity
M*	Solar mass
Status number	
NTOT	Total number of particles (include all binary components, single stars and center of mass)
N	Total number of stars (binary counts as two stars)
NS	Single star number
NPAIRS	Number of KS regularization pairs
NMERGE	Number of mergers (stable triples)
MULT	Number of ≥ 4 bodies merger
NZERO	Initial particle number (2* binaries + singles, initial N)
NB0	Primordial binary number
NUPKS	Unperturbed KS
NPKS	Total perturber number of KS
NTYPE(1:16)	Number of stars with type 1 to 16
For stars	
I	Index of star (position in particle data array)
NAME	Identification of individual star, it's constant and unique value for each star (exclude un-physical particles like center mass and ghosts) during the whole simulation
K*	KSTAR type, see Table
M	Mass of star
X(1:3)	Three dimension position
V(1:3)	Three dimension velocity
DM	Current mass loss due to stellar evolution (*N*–body units)
DMA	Accumulated mass loss due to stellar evolution
STEP	Irregular time step of star
STEPR	Regular time step of star
ZKIN	Kinetic energy
POT	Potential
NB	Neighbor number

RNB	Neighbor radius
RHO	Mass density of individual star calculated by nearest 5 neighbors, (only avaiable for particles inside core radius
Stellar evolution of star	
RS	star radius
L	luminosity
Teff	effective temperature
ROT	angular velocity of star
For binaries	
SEMI	semi-major axis
ECC	eccentricity
PERI	Pericenter distance
R12	distance between two members of binary
RI	distance to density center
VI	velocity of center of mass
P	Orbit period
I1/I2	Index for binary component 1/2 (Not always equal name)
ICM	Index for center mass particle (Not always equal name)
NP	perturber number
H	Binary energy per unit mass
EB	Binary energy: M(I1)*M(I2)/M(ICM)*H
GAMMA	Perturbation on KZ binary
IPAIR	Pair index for binary
STEP(I1)	KS time step of binary
TC	circularization timescale for current pericenter
FLAG-PB	Primordial binary indicator. -1: Primordial bianry; 0: New binary
INEW	Index of new star generated by binary collision or coalescence
For hierarchical systems	
IM	merger index
IMC	Number count of current merger
INPAIR	Index of inner binary
INCM	Inner binary center mass index
NAME(IM)	Merger center mass name
I1/I2	Inner binary two component indexs
I3	Outer particle index
ECC0	Inner binary orbit eccentricity
ECC1	Outer orbit eccentricity
EB0	Inner binary energy
EB1	Outer orbit energy
P0	Inner binary orbit period
P1	Outer orbit period
R12	Inner binary components seperation
RIN3	Separation between inner center mass and outer component
TG	Inner orbit eccentricity growth timescale
ECCMIN	Minimum eccentricity of inner binary orbit

ECCMAX	Maximum eccentricity of inner binary orbit
PERIM	smallest pericenter distance of outer particle orbit
PCR	Stability triple system criterion for PERIM (assess.f), the real stability criterion is more complicated and depend on the ECC1
SEMI0	Inner binary orbit semi-major axis
SEMI1	Outer orbit semi-major axis
INA	Inclination angle in unit degree
FLAG-H	Hierarchical system indicator. -1: merger, triple, chaotic binary, tidal circularization binary...; 0: normal binary
For quadruple systems	
OCM	Outer binary center of mass index
OCPAIR	Index of outer binary
I3/I4	Outer binary two component index
ECC2	Outer binary eccentricity
EB2	Outer binary energy
SEMI2	Outer binary orbit semi-major axis
R34	Outer binary components seperation
DP34	Difference potential correction for the outer binary
For chain	
IC	Chain index
NCH	Number of chain members
ECH	Total energy of perturbed system (N-body interface)
NP	Perturbers of chain
ENERGY	Total energy of chain
RSUM	Sum of all chain distances
RGRAV	Gravitational radius ((sum M(I)*M(J))/ABS(ENERGY))
TCR	Local crossing time ((sum M(I))**2.5/ABS(2*ENERGY)**1.5)
RMAXS	Maximum size of unperturbed configuration
RIJ(i-j)	Distance between member i and j
ICM1	First binary index after termination
ICM2	Second binary index after termination
For kick	
M0	mass before kick
MN	mass after kick
VK	kick velocity after limit check
VI	Initial velocity of kick star in cluster
VF	Final velocity of kicked star in cluster
VK0	Kick velocity generated from Henon's method (Douglas Heggie 22/5/97)
FB	Fallback ratio, VK = VK*(1-FB)
VESC	cluster escape velocity
VDIS	escape velocity from binary system: SQRT(2*M(ICM)/R12)

Table 18: Notice for Table19

File format

Header-*	The Header of file with line number *, the description of it is shown in the right cell
H-Label-*	Content labels are shown at the line number *, data begin from the next line
F-Label	Content labels are shown at the beginning of each line
I-Label	Content labels are shown before each data
N-Label	No labels in file

Frequency (freq.)	
T_{event}	Output when event is triggered
T_0	Output during initialization
ΔT_{out}	Output time interval (input parameter DELTAT)
ΔT_{adj}	Adjust time interval (input parameter DTADJ)
ΔT_{HR}	Stellar evolution output time interval (input parameter DTPLOT)
NFIX	Frequency of output (input parameter)
option	
#[*num*]	KZ option [num]
$\|\|$	logical or
&&	logical and
CHAIN	Use chain: $\#15 > 0 \&\& (\#30 > 0 \| \| \#30 = -1)$
USE_GPU	switch on GPU during compiling code
USE_HDF5	switch on HDF5 during compiling code

Table19 show all output files of *NBODY6++*. The filename will be named as "[name].[unit]". The first column [name] with suffix "*" means this file will output as seperated snaphshots split by TIME[NB] (shown as suffix of file name).

Table 19: Output file information

name	unit	code	option	freq.	content
conf*	3	output.F	$\#3 > 0$	ΔT_{out} × NFIX	Basic data snapshots
Header-1		NTOT, MODEL, NRUN, NK			
Header-2		TIME[NB], NPAIRS, RBAR, ZMBAR, RTIDE, TIDAL4, RDENS(1:3), TIME/TCR, TSCALE, VSTAR, RC, NC, VC, RHOM, CMAX, RSCALE, RSMIN, DMIN1			
N-Label		M, RHO, XNS, X(1:3), V(1:3), POT, NAME (All in NB unit)			
Notice the file is unformatted (binary file). Each item output continually from 1 to NTOT. All items output in one line after two header lines. NK : The number of parameters in Header-2, right now is always 20 TCR : Crossing time RSMIN : Smallest neighbor radius obtained in last output (output.F) time DMIN1 : Smallest two body distance XNS : The fifth nearest neighbor distance, (only avaiable for particles inside core radius					
degen	4	degen.f	$\#9 \geq 3$	T_{event}	Binary with degenerate stars
Header-1		RBAR, $\langle M \rangle$[M*], M1[M*], TSCALE, NB0, NZERO			

H-Label-2	ICASE, TIME[Myr], SEMI[AU], ECC, PERI/RS, P[days], RI[PC], M(I1)[M*], M(I2)[M*], K*(I1),K*(I2),K*(ICM), NAME(I1),NAME(I2)
ICASE: 3: normal binary; 4: CE binary; 5: physical collision binary PERI/RS: Pericenter / maximum stellar radius of two members	

lagr	7	lagr.f	#7 ≥ 3	ΔT_{out}	Lagrangian radii, average mass, average velocity, velocity dispersion output (calculation of Lagrangian radii use initial total mass of cluster)
Header-1		Labels and column number for each output			
H-Label-2		R_{lagr}, $R_{lagr,s}$, $R_{lagr,b}$, $\langle M\rangle$, N_{Shell}, $\langle V_x\rangle$, $\langle V_y\rangle$, $\langle V_z\rangle$, $\langle V\rangle$, $\langle V_r\rangle$, $\langle V_t\rangle$, σ^2, σ_r^2,σ_t^2,$\langle V_{rot.}\rangle$ (All in NB units)			
For each items above, there are 18 columns with different mass fraction(%): 0.1, 0.3, 0.5, 1, 3, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 95, 99, 100 and inside core radius (exclude $R_{lagr,s}$, $R_{lagr,b}$)					
R_{lagr}: Lagrangian radius $R_{lagr,s}$: Single star Lagrangian radius $R_{lagr,b}$: KZ binaries Lagrangian radius $\langle M\rangle$: Average mass of a spherical shell defined by R_{lagr} $\langle V_{x/y/z}\rangle$: Mass weighted average velocity in x/y/z direction $\langle V_t\rangle$: Mass weighted average tangential velocity $\langle V_r\rangle$: Mass weighted average radial velocity σ^2: Mass weighted velocity dispersion square σ_r^2: Mass weighted radius velocity dispersion square σ_t^2: Mass weighted tangential velocity dispersion square $\langle V_{rot.}\rangle$: Mass weighted average rotational velocity projected in x-y plane					

bdat	8	ksin2.f	#8 > 0	T_{event}	New hierarchical (B-S)-S binary information
		ksinit.F	#8 > 0		New binary information
		ksterm.F	#8 > 0		End binary information
I-Label		TIME[NB], NAME(I1) NANE(I2), FLAG-PB, M(I1)[NB], M(I2)[NB], EB[NB], SEMI[NB], R12[NB], GAMMA[NB], RI[NB]			

bdat*	9	bindat.f	#8 ≥ 2	ΔT_{out}	KS binary output
Header-1		NPAIRS, MODEL, NRUN, N, NC, NMERGE, TIME[NB], RSCALE[NB], RTIDE[NB], RC[NB], TIME[Myr], ETIDC[NB], 0			
Header-2		EBINP, EBINN, E, EESCS, EESCPB, EESCPC, EESCNB, EESCNC, EMERGE, ECOLL (All in NB unit)			
Header-3		SBCOLL, BBCOLL, ZKIN, POT, EBIN0, EBIN, ESUB, EMERGE, BE(3), ZMASS, ZMBIN, CHCOLL, ECOLL (All in NB unit)			
H-Label-4		NAME(I1), NAME(I2), M1[M*], M2[M*], E[NB], ECC, P[days], SEMI[AU], RI[PC], VI[km/s], K*(I1), K*(I2), ZN[NB], RP[NB], STEP(I1)[NB], NAME(ICM), ECM[NB], K*(ICM)			
ETIDC[NB]: escape energy due to tidal force SBCOLL: The difference of binding energy of inner binary at the end and begin of unperturbed triples					

BBCOLL: The difference of binding energy of inner binary at the end and begin of unperturbed B-B quadruples
ZMBIN : Total KS binary masses
CHCOLL: The difference of binding energy of inner binary at the end and begin of chain

dat	10	start.F	#22 = 1	T_0	Basic data after initialization
N-label		M[NB], X(1:3)[NB], V(1:3)[NB]			

esc	11	escape.f	#23 = 2, 4	ΔT_{adj}	escaping star output
H-Label-1		TIME[Myr], M[M*], EESC, VI[km/s], K*, NAME			

EESC: dimensionless escape energy

hiarch	12	hiarch.f	#18 = 1, 3	T_{event}	New/End stable hierarchical system (mergers) information
Header-1		RBAR, $\langle M \rangle$[M*], M1[M*], TSCALE, NB0, NZERO			
F-Label		TIME, SEMI0, SMEI1, ECC1, PERI0, PERI0M, P1/P0, M(INCM)/M(I3), PCR/SEMI0, M(INCM)/<M>, MR, INA, NAME(I1), NAME(I2), NAME(I3), K*(INCM), ECC0, ECCMIN, ECCMAX, K*(I1), K*(I2), RSM (All in NB unit)			
F-Label		TIME RI/RC, SEMI0, ECC0, PERI0, P0F/P0I, RC/RSCALE, GAMMA(INCM), NKI, NKF, NPAIRS, NAME(I2) (All in NB unit)			

PERI0: Inner binary pericenter distance
PERI0M: Inner binary minimum pericenter distance
MR: Mass ratio of inner binary components (> 1)
PSM: Maximum stellar radius of two members of inner binary
P0F/P0I: Period of inner binary at the end of merger over at the beginning of merger
NKI: Orbit number the inner binary during the life of merger over the period of inner binary at the beginning of merger
NKF: Orbit number the inner binary during the life of merger over the period of inner binary at the end of merger

coll	13	mix.f	#19 $\geq$ 3	T_{event}	Mixed star (physical collision of binary without evolved stars) information
Header-1		RBAR, $\langle M \rangle$[M*], M1[M*], TSCALE, NB0, NZERO			
H-Label-2		TIME[NB], NAME(I1), NAME(I2), K*(I1), K*(I2), K*(INEW), M(I1)[M*], M(I2)[M*], M(INEW)[M*], DM[M*], RS(I1)[R*], RS(I2)[R*], RI/RC, R12[R*], ECC, P[days]			

shrink	14	shrink.f		T_{event}	Diagnostics for shrink regular time step for incoming high velocity star coming
F-Label		I, RN, FI/FJ, DT, STEPR (All in NB unit)			

RN: Next distance from high velocity star after DT
FI/FJ: force at minimum distance / current force
DT: evaluated time of minimum approach truncated to next time

mix	15	mix.f	#19 $\geq$ 3	T_{event}	Mixed star information for the case NS/BH form
F-Label		K*(I1), K*(I2), K*(INEW), M(I1)[M*], M(I2)[M*], M(INEW)[M*]			

hirect	16	hirect.f	#27 = 2 (hi-grow.f) ‖ #34 > 0 (brake2.f) ‖ #28 > 0 (brake3.f)	T_{event}	Diagnostics for rectification of hierarchical binary due to the internal energy change of system
F-Label		TIME[Nb],NAME,K*,ECC,R12/SEMI,H,DB,DH/H			
H: inner binary energy DM: change of binding energy					
		ksrect.f		T_{event}	Diagnostics for rectification of KS orbit.
F-Label		TIME[NB], IPAIR, R12/SEMI, H, GAMMA, DB, DH/H			
binev	17	binev.f	#9 ≥ 2	T_{event}	Binary evolution stage, output when binary change type
H-Label-1		TIME[Myr], NAME(I1), NAME(I2), K*(I1), K*(I2), K*(ICM), M(I1)[M*], M(I2)[M*], RS(I1)[R*], RS(I2)[R*], RI[PC], ECC, SEMI[R*], P[days], IQCOLL			
IQCOLL: Type of stage, need table in the future					
pbin	18	binout.f	#8 > 0	ΔT_{out}	Diagnostics for the primordial binary which exchanges members
I-Label		TIME[NB], NAME(I1), NAME(I2), Flag-PB, Flag-H, M(I1)[NB], M(I2)[NB], EB[NB], SEMI[NB], ECC, GX, RI[NB], VR[NB]			
GX: maximum perturbation (near apocenter)					
VR: radial velocity					
bwdat*	19	bindat.f	#8 ≥ 2		Wide Non-KS bianry output
Header-1		TIME[NB],TIME[Myr], N			
H-Label-2		NAME(I1), NAME(I2), M1[M*], M2[M*], E[NB], ECC, P[days], SEMI[AU], RI[PC], VI[km/s], K*(I1), K*(I2)			
symb	20	mdot.F	#19 ≥ 3	T_{event}	Symbiotic stars information
F-Label		NAME, K*, TIME[Myr], M[M*], SEMI[R*], DM, DMA??			
JC: Companion star index DMX(JC): Mass loss from stellar wind of companion star DMA: Accreted mass from companion star					
rocdeg	22	roche.f	#34 > 0	T_{event}	Roche overflow binary involving degenerate objects
F-Label		NAME(I1), NAME(I2), K*(I1), K*(I2), M(I1)[M*], M(I2)[M*], TIME[Myr], SEMI[R*], P[days], MD(I1)[M*/Myr], MD(I2)[M*/Myr]			
MD: Mass loss rate					
ibeigen	23	binpop.F	(#8 = 1 ‖ #8 ≥ 3) && #42 = 6	T_0	Initial binary data by using eigen-evolution
F-Label		ITER, I1, M(ICM)[M*], ECCI, ECCC, SEMII, SEMIC, P[days]			
ITER: Iteraction times to generate parameter that satisfy the input criterions					

ECCI: Initial eccentricity from thermal distribution
ECCC: Circularized eccentricity
SEMII: Initial semi-major axis generated by ECC0 and period
SEMIC: Circularized semi-major axis generated by ECCC and period

coal	24	coal.f	#19 ≥ 3	T_{event}	Binary coalescence (Stellar type with cores and circular orbit)
Header-1		RBAR,$\langle M \rangle$,M1,TSCALE,NB0,NZERO			
H-Label-2		TIME[NB], NAME(I1), NAME(I2), K*(I1), K*(I2), K*(INEW), IQCOLL, M(I1)[M*], M(I2)[M*], M(INEW)[M*], DM[M*], RS(I1)[R*], RS(I2)[R*], RI/RC, R12[R*], ECC, P[days], RCOLL[R*], EB[NB], DP[NB], VINF[km/s]			

DP: Potential energy correction to perturbers due to binary exchanged to single star
RCOLL: Binary distance before coalescence
VINF: Velocity at infinity for hyperbolic coalescence

sediag	25	unpert.f	#27 > 0	T_{event}	Diagnostics for the stellar evolution next look-up time of unpert KS
F-Label		IPAIR, K*(I1), K*(I2), K*(ICM), TEVNXT[NB], STEP(I1)[NB] (No more output when NWARN$\geq$ 1000)			

TEVNXT: Next time to check stellar evolution

highv	29	hivel.f		T_{event}	Diagnostics for high-velocity particle added or removed from LISTV
F-Label		(REMOVE) TIME[NB], I, NAME, RI(NB), VI(NB)			
F-Label		(ADD NS, terminated KS/chain) TIME[NB], NHI, I, NAME, K*, VI[NB], RI[NB], STEP[NB]			
F-Label		(ADD fast single) TIME[NB], NHI, NAME, IPHASE, VI[NB], RI[NB], STEP[NB]			
F-Label		(ADD hyperbolic two-body motion) TIME[NB], NHI, NAME(I1), NAME(I2), IPHASE, RIJ[NB]			

NHI: high-velocity particle number
IPHASE: Internal status of code (check nbody6.F for details)

global	30	output.F		ΔT_{out}	Global features of cluster and event counters
H-Label-1		TIME[NB], TIME[Myr], TCR[Myr], DE, BE(3), RSCALE[PC], RTIDE[PC], RDENS[PC], RC[PC], RHOD[PC], RHOM[PC], MC[M*], CMAX, $\langle Cn \rangle$, Ir/R, RCM[NB], VCM[NB], AZ, EB/E, EM/E, VRMS[km/s], N, NS, NPAIRS, NUPKS, NPKS, NMERGE, MULT, $\langle NB \rangle$, NC, NESC, NSTEPI, NSTEPB, NSTEPR, NSTEPU, NSTEPT, NSTEPQ, NSTEPC, NBLOCK, NBLCKR, NNPRED, NIRRF, NBCORR, NBFLUX, NBFULL, NBVOID, NICONV, NLSMIN, NBSMIN, NBDIS, NBDIS2, NCMDER, NFAST, NBFAST, NKSTRY, NKSREG, NKSHYP, NKSPER, NKSMOD, NTTRY, NTRIP, NQUAD, NCHAIN, NMERG, NEWHI			

TCR: Crossing time
RDENS: density center to coordinate center distance
$\langle Cn \rangle$: frequency $1/STEP$ weighted averaged neighbor number
Ir/R: Irregular cost ($\sum NB/STEP$) over regular cost ($N/\sum STEPR$)
RCM: Center mass distance to coordinate center

VCM: Center mass velocity
AZ: Angular momentum in z axis including tidal effect (Chandrasekhar equation 5.530)
VRMS: root mean square velocity of cluster
NESC: Escapers
NSTEPI: Irregular integration steps
NSTEPB: Irregular integration steps of binary center mass particles
NSTEPR: Regular integration steps
NSTEPU: Regularized integration steps
NSTEPT: Triple regularization integration steps (#15 $>$ 0)
NSTEPQ: Quadruple regularization integration steps (#15 $>$ 0)
NSTEPC: Chain regularization steps (# DIFSY calls)
NBLOCK: Number of irregular blocks (block-step version)
NBLCKR: Number of regular blocks (block-step version)
NNPRED: Coordinate & velocity predictions of all particles
NIRRF : Calculated irregular force
NBCORR: Force polynomial corrections
NBFLUX: Number of changes in neighbor lists (NBLOSS+NBGAIN)
NBFULL: Neighbor number overflows with standard criterion
NBVOID: No neighbours inside 1.26 times the basic sphere radius
NICONV: Irregular step reduction (force convergence test)
NLSMIN: Small step neighbours selected from other neighbour lists
NBSMIN: Retained neighbours inside 2*RS (STEP < SMIN)
NBDIS : Second component of recent KS pair added as neighbour (#18)
NBDIS2: Second component of old KS pair added as neighbour (#18 $>$ 1)
NCMDER: C.m. values for force derivatives of KS component
NFAST : Fast particles included in LISTV (#18 $>$ 0)
NBFAST: Fast particles included in neighbour list (#18 $>$ 0)
NKSTRY: Two-body regularization attempts
NKSREG: Total KS regularizations
NKSHYP: Hyperbolic KS regularizations
NKSPER: Unperturbed KS binary orbits
NKSMOD: Slow KS motion restarts (#26 $>$ 0)
NTTRY : Search for triple, quad & chain regularization or mergers
NTRIP : New three-body regularizations (#15 $>$ 0)
NQUAD : New four-body regularizations (#15 $>$ 0)
NCHAIN: New chain regularizations (#15 $>$ 0&&#30 $>$ 0)
NMERG : New mergers of stable triples or quadruples (#15 $>$ 0)
NEWHI : New hierarchical systems (counted by routine HIARCH)

lagr1	31	lagr2.f	#7 $\geq$ 5	ΔT_{out}	Two mass group systems Lagrangian radii (first group)
N-Label		TIME[NB], R_{lagr}[NB] (mass fraction: 0.01, 0.02, 0.05 ,0.1, 0.2, 0.3, 0.4, 0.5, 0.625, 0.75, 0.9) (Here calculation of R_{lagr} use the current total mass)			

lagr2	32	lagr2.f	#7 $\geq$ 5	ΔT_{out}	Two mass group systems Lagrangian radii (second group)
N-Label		see Unit 31			

ns	33	degen.f	#9 $\geq$ 3	T_{event}	Neutron stars (never used)
F-Label		I, NAME, IFIRST, K*, TIME[Myr], VI[km/s]			

bh	34	degen.f	#9 ≥ 3	T_{event}	Black holes (never used)
F-Label		I, NAME, IFIRST, K*, TIME[Myr], VI[km/s]			
event	35	events.f	#19 $>$ 0$\|\|$#27 $>$ 0	ΔT_{out}	Stellar evolution and tidal capture event counter and energy
H-Lable-1		TIME[Myr], NDISS, NTIDE, NSYNC, NCOLL, NCOAL, NDD, NCIRC, NROCHE, NRO, NCE, NHYP, NHYPC, NKICK, EBIN, EMERGE, ECOLL, EMDOT, ECDOT, EKICK, ESESC, EBESC, EMESC, DEGRAV, EBIND, MMAX, NMDOT, NRG, NHE, NRS, NNH, NWD, NSN, NBH, NBS, ZMRG, ZMHE, ZMRS, ZMNH, ZMWD, ZMSN, ZMDOT, NTYPE(1:16)			

NDISS: Tidal dissipations at pericentre (#27 $>$ 0)
NTIDE: Tidal captures from hyperbolic motion (#27 $>$ 0)
NSYNC: Number of synchronous binaries (#27 $>$ 0)
NCOLL: Stellar collisions
NCOAL: Stellar coalescence
NDD: Double WD/NS/BH binaries
NCIRC: Circularized bianries (#27 $>$ 0)
NROCHE: Roche stage triggered times
NRO: Roche binary events
NCE: Common envelope binaries
NHYP: Hyperbolic collision
NHYPC: Hyperbolic common envelope binaries
NKICK: WD/NS/BH kick
NSESC: Escaped single particles (#23 $>$ 0)
NBESC: Escaped binaries (#23 $>$ 0)
NMESC: Escaped mergers (#15 $>$ 0&&#23 $>$ 0)
EKICK: KICK energy of WD/NS/BH

ESESC: Single star escaper energy
EBESC: KS Binary star escaper energy
EMESC: Merger escaper energy
DEGRAV: Change of binary energy compared to initial value
EBIND: Binding energy of cluster (E)
MMAX: Maximum stellar mass
NMDOT: Stellar mass loss event
NRG: New red giants
NHE: New helium stars
NRS: New red supergiants
NNH: New naked Helium stars
NWD: New white dwarfs
NSN: New neutron stars
NBH: New black holes
NBS: New blue stragglers
ZMRG: New red giants mass
ZMHE: New helium stars mass
ZMRS: New red supergiants mass
ZMNH: New naked Helium stars mass

ZMWD: New white dwarfs mass ZMSN: New neutron stars mass					
sediag	38	expel2.f	#19 $\geq$ 3 && Chain	T_{event}	Diagnostics for common envelop type change
N-Label					
		mix.f	#19 $\geq$ 3	T_{event}	Diagnostics for mixed stars
N-Label					
		trflow.f	#19 $\geq$ 3	T_{event}	Diagnostics for iteration convergency check until Roche-lobe overflow
N-Label					
stellar evolution health check					
hbin	39	adjust.F	#9 = 1,3	ΔT_{out}	The hardest binary below ECLOSE
F-Label		TIME[NB], NAME(I1), NAME(I2), K*, NP, ECC, SEMI[NB], P[days], EB[NB], EM[NB]			
data .h5part	40	custom_ output.F	USE_ HDF5 && #46 > 0	#47	HDF5 or CSV output of basic data
		NAME, TIME[NB], X(1:3)[NB], V(1:3)[NB], M[NB], F[NB], FD[NB], K*, RHO[NB], PHI[NB], L[L*], RS[R*], Teff[K], MCORE[M*], RSCORE[R*]			
RHO: Local density PHI: potential MCORE: Stellar core mass RSCORE: Stellar core radius					
nbflow	41	fpoly0.F	USE_GPU	T_0	Diagnostics for neighbor list overflow from GPU regular force initialization
F-Label		NSTEPR, NAME, NB, RNB[NB], RI[NB]			
		util_gpu.F	USE_GPU	T_{event}	Diagnostics for neighbor list overflow from GPU regular force calculation
I-Label		I,NAME, NNPRE, NBNEW, RNB[NB], RI[NB], TIME[NB]			
NBPRE: previous neighbor number					
NBNEW: new neighbor number that cause overflow					
ibcoll	42	binpop.F	#8 = 1,$\geq$ 3	T_0	Diagnostics for the binary physical collision cases when initializing primordial binaries
I-Label		I1, M(I1)[M*], M(I2)[M*], ECC, SEMI[AU], PERI[R*], RS(I1)[R*], RS(I2)[R*]			
sediag	43	mdot.F	#19 $\geq$ 3	T_{event}	Diagnostics of warning when stellar radius expand more than 1.5x
F-Label		I, NAME, TIME[Myr], DT[Myr], K*0, K*N, M0[M*], MN[M*], RS0[R*], RSN[R*]			
K*0: Previous stellar type K*N: New stellar type M0: Initial stellar mass					

MN: Current new stellar mass RS0: Previous stellar radius RSN: New stellar radius					
hinc	44	induce.f	#27 > 0	T_{event}	Information of high inclinations and TC2 $< 10^7$ yrs of hierarchical binary
F-Label		ECC0, ECCMIN, ECCMAX, K*(I1), K*(I2), K*(ICM), SEMI0[NB], PERIM[NB], IN, TG[Myr], TC[Myr], TCM[Myr], TIME[Myr]			
IN: Indicator of inclination: 1 + AIN*360/(2*pi*22.5), where AIN is inclination angle TCM: Circularization timescale for smallest pericenter					
mbh	45	bhplot.f	#24 $= 1$	ΔT_{BH}	Mass black hole information
H-Label-1		STAT, TIME[Myr], IBH, X(1:3)[PC], V(1:3)[km/s], NB, XAVE(1:3)[AU], VAVE(1:3)[km/s], DEN[M*/PC^3], RIJMAX[PC], VSIGMA(1:3)[km^2/s^2]			
Notice the XAVE, VAVE, DEN, VSIGMA is not accurate due to the neighbor criterion STAT: Status showing whether black hole is in binary system or single IBH: Index of massive black hole XAVE: Density center vector of black hole neighbors (relative to black hole velocity) VAVE: Average velocity vector of black hole neighbors (relative to black hole velocity) DEN: Local density of black hole calculated by neighbors within RNB (exclude black hole mass) RIJMAX: Maximum distance from neighbor star to black hole VSIGMA: 3-dimensional velocity dispersion of black hole neighbors (relative to black hole velocity)					
mbhnb	46	bhplot.f	#24 $= 1$	ΔT_{BH}	Mass black hole neighbor information
Header-1		TIME[Myr], NB			
N-Label		NAME, M[M*], XREL(1:3)[AU], RIJ[AU], VREL(1:3)[km/s], K*			
XREL: Position vector relative to black hole RIJ: Distance to black hole VREL: Velocity vector relative to black hole velocity					
itid3	52	xtrnl0.F	#14 $= 3$	T_0	Initialization of circular velocity in the plane for galaxy tidal force
F-Label		VC[km/s], RI[KPC]			
VC: Circular velocity					
hypcep	54	ksint.f	#19 ≥ 3	T_{event}	Close encounter for hyperbolic motion (pericenter $< 5.0\times$ Maximun stellar radius of two stars
F-Label		TIME[NB], NAME(I1), NAME(I2), K*(I1), K*(I2), VINF[km/s], RCAP[R*], RX[R*], PERI[R*]			
VINF: Velocity at infinity for hyperbolic coalescence RCAP: Capture distance of hyperbolic encounters (binary will form) RX: Maximum stellar radius of two stars					
hypcec	55	ksint.f	#19 ≥ 3	T_{event}	Close encounter for hyperbolic motion (physical collision case)

F-Label	TIME[NB], IPAIR, NAME(I1), NAME(I2), K*(I1), K*(I2), K*(ICM), VINF, ECC, H[NB], R12[NB], SEMI[NB], PERI[NB], M(I1)[NB], M(I2)[NB], M(ICM)[M*], RI[RC], VI[km/s], RHOD, RS(I1)[R*], RS(I2)[R*], RCAP[R*], RX/PERI, RCOLL/PERI
RCOLL: If #27 $>$ 2 Relativistic collision criterion, otherelse normal collision criterion RX: Maximum stellar radius of two stars	

*fort	60	ellan.f	#49 $>$ 0	ΔT_{out}	Moments of Inertia ??
N-Label		??			

cirdiag	71	spiral.f	#27 $>$ 0	T_{event}	Diagnostics for skip removal of chaos binary if this is member of single/double (stable quadruple) merger.
F-Label		NCHAOS, NAMEC, NAME(IM), NAME(I3)			
NCHAOS: Number of chaos binaries NAMEC: Name for chaos binaries					

histab	73	impact.f	#15 $>$ 0	T_{event}	Diagnostics for checking Zare exchange stability criterion (exchange of outer particle with inner member of binary), but the slingshot still can happen, thus not triple system stablility criterion.
F-Label		TIME[NB], M(I3)/M(INCM), ECC0, ECC1, SEMI0[NB], PERIM[NB], PCR[NB], TG[Myr], SP, INA[deg], K*			
SP: $>=$ 1, no exchange; $<$ 1, will be exchange					

cirdiag	75	decide.f	#27 = 2	T_{event}	Diagnostics output for large eccentricity ($>$ 0.9) during merger decision (deny stable triple forming if circularization timescale is short).
F-Label		NAME, TIME[NB], ECC0, ECC1, EMIN, EMAX, ECCD[1/Myr], EDT[NB], TG[Myr], TC[Myr], EDAV[1/Myr], PERIM[RSM]			
ECCD: Eccentricity change rate EDAV: Average eccentricity change rate RSM: Maximum stellar radius of two stars EDT: Tidal circularization timescale for current eccentricity					

kscrit	77	chmod.f	#16 $>$ 2 && CHAIN	T_{event}	Diagnostics for increasing or decreasing regularization parameters in chain
F-Label		TIME[NB], KSMAG, GPERT, RMIN, RIJ[NB]			
KSMAG: Indicator of increasing and decreasing times GPERT: Dimensionless perturbation of chain RMIN: Distance criterion for regularization (also is input parameter) RIJ: Distance between chain center mass and perturber					

chstab	81	chstab.f	CHAIN	T_{event}	New hierarchical system with stability condition for bound close pair (RB $>$ semi) (formed from 4th body escape or perturber make it stable).

I-Label		TIMEC, RI[NB], NAME(I3), M(I3)/M(INCM), ECC0, ECCMAX, ECC1, SEMI0[NB], SEMI1[NB], PCR/PERIM, INA[deg]			
		cstab2.f	CHAIN	T_{event}	Hierarchical stability condition (SEMI1 $>0 \Rightarrow$ ECC1 <1).
N-Label		TIMEC[NB], RI[NB], NAME(I3), ECC0, ECC1, ECCMAX, SEMI0[NB], SEMI1[NB], PCR/PERIM, INA[deg]			
		cstab3.f	CHAIN	T_{event}	Continued chain integration if outer orbit unstable or large pert.
N-Label		TIMEC[NB], RI[NB], NAME(I3), ECC0, ECC1, ECCMAX, SEMI0[NB], SEMI1[NB], PCR/PERIM, INA[deg]			
		cstab4.f	CHAIN	T_{event}	Check hierarchical stability condition for bound close pair.
N-Label		TIMEC[NB], RI[NB], NAME(I3), ECC0, ECC1, ECCMAX, SEMI0[NB], SEMI1[NB], PCR/PERIM, INA[deg]			
TIMEC: time when chain formed					
bev*	82	hrplot.F	#12 >0	ΔT_{HR}	KS binary stellar evolution data
Header-1		NPAIRS, TIME[Myr]			
N-Label		TIME[NB], I1, I2, NAME(I1), NAME(I2), K*(I1), K*(I2), K*(ICM), RI[RC], ECC, log10(P[days]), log10(SEMI[R*]), M(I1)[M*], M(I2)[M*], log10(L(I1)[L*]), Log10(L(I2)[L*]), Log10(RS(I1)[R*]), Log10(RS(I2)[R*]), Log10(Teff(I1)[K]), Log10(Teff(I2)[K])			
sev*	83	hrplot.F	#12>0		Single star stellar evolution data
Header-1		NS, TIME[Myr]			
N-Label		TIME[NB], I, NAME, K*, RI[RC], M[M*], log10(L[L*]), log10(RS[R*]), log10(Teff[K])			
merger	84	bindat.f	#8 ≥ 2	ΔT_{out}	Extra mergers information (main merger output is in hidat.87_*)
F-Label		TIME[NB], NAME[I1], NAME[I3], K*[I1], K*[I3], K*[IM], ECC0, ECC1, PERI(I3)/PCR, PERI(INCM)[RSM], P0[days], P1[days], SEMI1[NB]			
roche	85	roche.f	#34 >0	T_{event}	Roche overflow stage data
H-Label		NAME(I1), NAME(I2), K*(I1), K*(I2), TIME[Myr], AGE(I1), AGE(I2), M0(I1), M0(I2), M(I1), M(I2), Z, ECC, P[days], JSPIN(I1), JSPIN(I2), STAT			
AGE: Stellar age JSPIN: Angular momentum of star STAT: Type of binary Z: Metallicity *M0: Stellar mass before mass transfer?					
hidat*	87	hidat.f	#18 >3	ΔT_{out}	Hierarchical data of mergers (stable triples, quadruples)
Header-1		NPAIRS, NRUN, N, NC, NMERGE, MULT, NEWHI, TIME[NB]			
H-Label		NAME(I1), NAME(I2), NAME(I3), K*(I1), K*(I2), K*(I3), M(I1)[M*], M(I2)[M*], M(I3)[M*], RI[NB], ECCMAX, ECC0, ECC1, P0[days], P1[days]			
MULT: Number of deeper mergers (4 bodies ((B-S)-S) or 5 bodies ((B-S)-S)-S)					

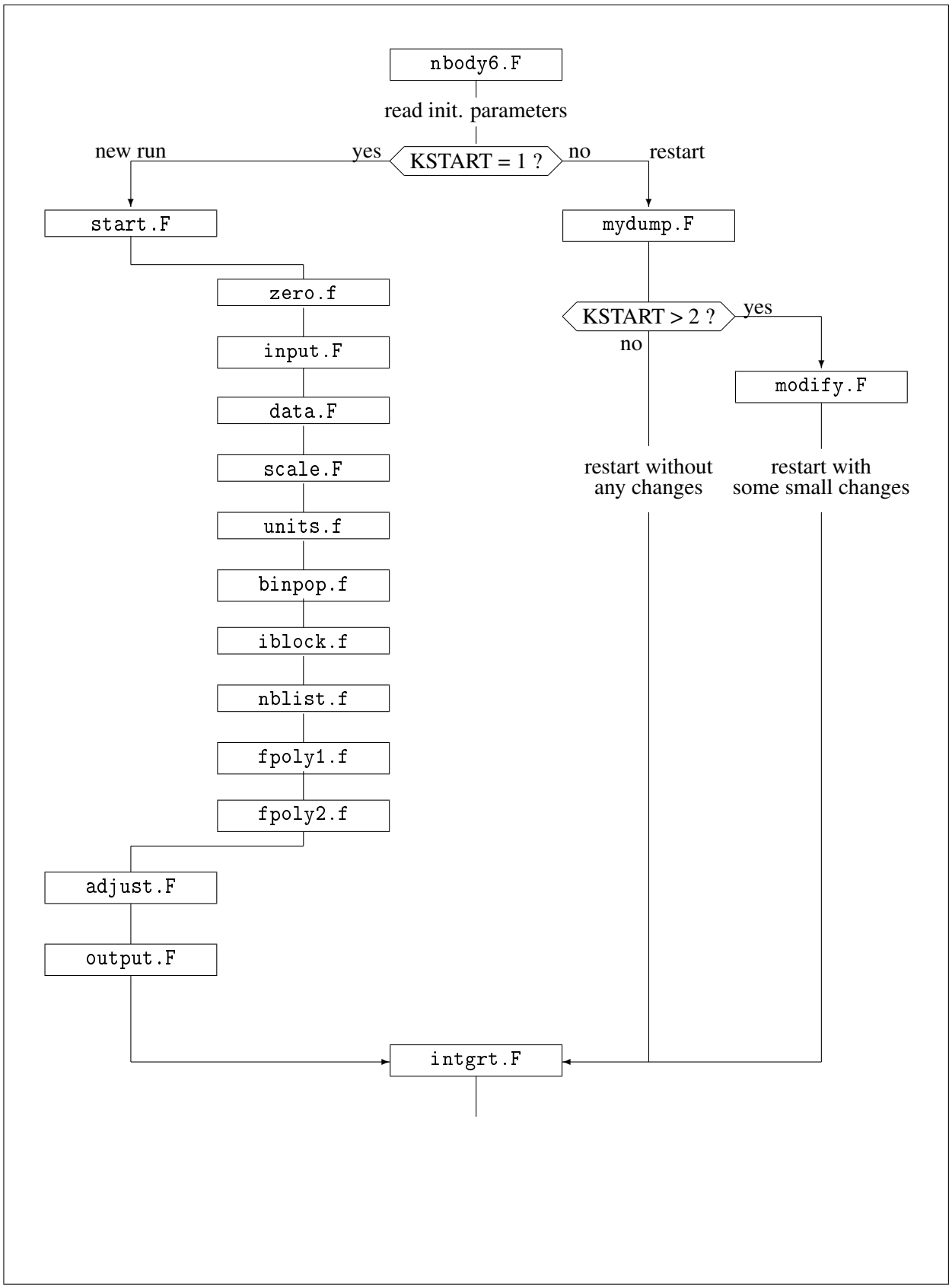
NEWHI: Counter of new hierarchical systems in chain					
quastab	89	impact.f	#15 ≥ 3	T_{event}	Diagnostics for stability criterion of two binaries in quadruple
F-Label		TIME[NB], NAME(I1), NAME(J1), LQ, RI[NB], ECC1, EB[NB], EB2[NB], EB1[NB], P1[days], PERIM[NB], PCR[NB]			
J1: Index of first member in second binary LQ: orbit counter for diagnostics output ECC1: Outer orbit eccentricity in B-B quadruple EB: Quadruple binding energy EB1: First binary binding energy EB2: Second binary binding energy P1: Outer orbit period					
bs	91	mix.f	#19 ≥ 3	T_{event}	Blue straggler information
F-Label		TIME[NB], NAME(I1), NAME(I2), M(INEW), ECC, P[days], P(I1)[days], P(I2)[days]			
wdcirc	95	spiral.f	#27 > 0	T_{event}	Diagnostics for recent WD as the second component of binary system involving tidal circularization
F-Label		TIME[NB], NAME(I2), NAME(I1), K*(I1), ROT(I1)[NB], ROT(I2)[NB], $\langle$motion$\rangle$, SPIN(I2)[NB]			
$\langle$motion$\rangle$: sqrt(M(ICM) / (RSM * SEMI)**3) [NB] *SPIN: spin of star ?					
cirdiag	96	hut.f	#27 > 0	T_{event}	Diagnostics for reducing steps of integration equations for eccentricity and angular velocites of stars (Equation 15.22 in Sverre, 2003 book)
F-Label		NSTEPS, IT, U, UD, DTAU (All in NB unit)			
NSTEPS: Step number for integration IT: Iteration times for reduction U: KS vector U UD: KS vector UDOT DTAU: KS integration time step					

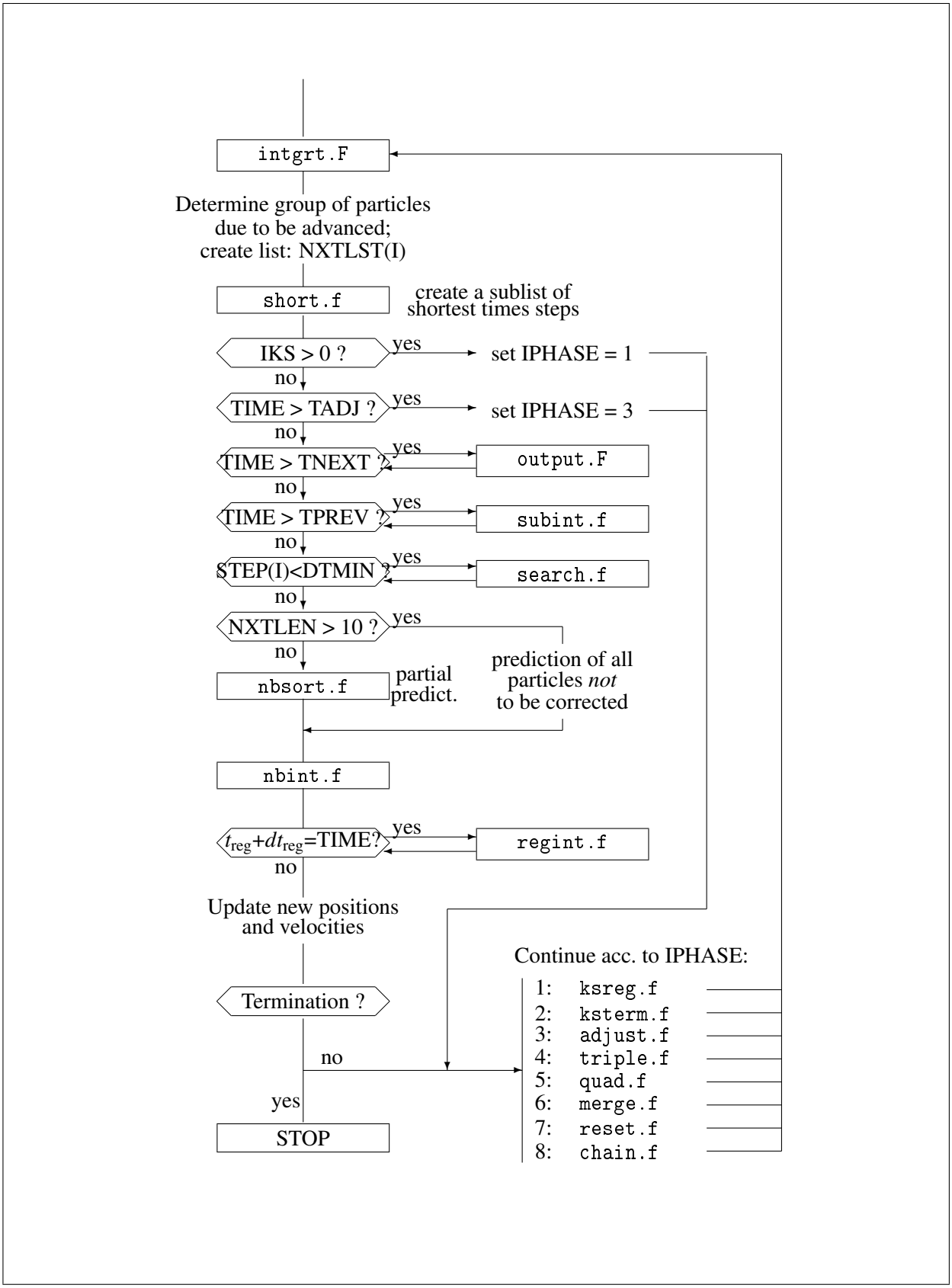
14 Python and IDL scripts

TODO

15 AMUSE

TODO


nbody6.F
read init. parameters
new run
yes
KSTART = 1 ?
no
restart
start.F
mydump.F
zero.f
KSTART > 2 ?
yes
input.F
no
modify.F
data.F
scale.F
restart without
any changes
restart with
some small changes
units.f
binpop.f
iblock.f
nblist.f
fpoly1.f
fpoly2.f
adjust.F
output.F
intgrt.F


intgrt.F
Determine group of particles due to be advanced; create list: NXTLST(I)
short.f
create a sublist of shortest times steps
IKS > 0 ?
yes
set IPHASE = 1
no
TIME > TADJ ?
yes
set IPHASE = 3
no
TIME > TNEXT ?
yes
output.F
no
TIME > TPREV ?
yes
subint.f
no
STEP(I)<DTMIN ?
yes
search.f
no
NXTLEN > 10 ?
yes
no
nbsort.f
partial predict.
prediction of all particles *not* to be corrected
nbint.f
$t_{reg}+dt_{reg}$=TIME?
yes
regint.f
no
Update new positions and velocities
Continue acc. to IPHASE:
Termination ?
1: ksreg.f
2: ksterm.f
3: adjust.f
4: triple.f
5: quad.f
6: merge.f
7: reset.f
8: chain.f
no
yes
STOP

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