Symplectic integrator for near-Keplerian planetary systems

#============================#

README.TXT

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When using orbitN, cite as (ZeebeAJ23 hereafter):

Zeebe, R. E. orbitN: A symplectic integrator for planetary systems dominated by a central mass - Insight into long-term solar system chaos. The Astronomical Journal, 2023.

(0) orbitN

orbitN is a second order symplectic integrator developed with the primary goal of generating accurate and reproducible long-term orbital solutions for near-Keplerian planetary systems with a dominant mass M0. Among other features, orbitN includes M0's quadrupole moment, a lunar contribution, and post-Newtonian corrections (1PN) due to M0 (fast symplectic implementation). To reduce numerical roundoff errors, orbitN features Kahan compensated summation. orbitN version 1.0 focuses on hierarchical systems without close encounters but can be extended to include additional features in future versions. orbitN version 1.0 uses Gaussian units, i.e., length, time, and mass are expressed in units of au, days, and fractions of M0.

(1) Installation

orbitN should run under OSs including Linux and Mac OS. To compile and run orbitN, a C compiler is required. Once a C compiler is available, installing and running orbitN should be fairly simple. Many Linux distributions include, for instance, gcc or provide convenient options to install required packages (see below for Mac OS).

When the C compiler and tools such as 'make' are available, proceed as follows. On github, click on orbitN-x.x.x.tar.gz, then on the symbol "Download raw file". If instead you download the full github main zip package, first extract orbitN-x.x.x.tar.gz from it. Save the compressed file (orbitN-x.x.x.tar.gz) to the directory of your choice, open a terminal, cd to that directory and run (replace x.x.x by actual version number):

```
$ tar -xvf orbitN-x.x.x.tar.gz
$ cd orbitN-x.x.x
$ make
$ ./orbitN
```

Step 3 should produce a number of object files (.o) in the 'src' folder and the executable orbitN in the root folder. Step 4 runs the program.

By default, orbitN output will be written to .dat and .log files in orbitN's root directory, see below for content.

orbitN includes a utility program for post-run conversion of state vectors to Keplerian elements (xv2elm). If the selected conversion involves the masses of individual bodies, the user needs to provide the original mass/coordinate input file of the run. To use xv2elm, edit the input section of xv2elm.c and execute:

```
$ make allelm
$ ./xv2elm
```

(1a) Mac OS

Installing Xcode, for instance, should provide the necessary tools, including a C compiler. The steps to install and run orbitN are then analogous to the Linux steps described above. Xcode may be found on the system install disk or can be downloaded. However, note that the file size for the latest Xcode version may be very large. Alternatively, depending on the Mac OS version, command line tools only may be installed that require less disk space.

(2) Running orbitN

Running orbitN integrations to solve a specific user problem can be accomplished by adjusting orbitN settings, i.e., through user modifications of code and/or input files via different options. (1) By editing the main source code files or (2) by adding custom simulations under ./sim/.. (see below).

For example, the files orbitN.h and orbitN.c include top-level input sections that allow modifying input parameters (C preprocessor macros, see below). Once set, the parameter values take effect after recompilation (use make).

(2a) orbitN Input Sections

The input macros either have values or turn ON/OFF certain options. To turn options off (disable): add a U in front of the macro string. For example,

#define PN

turns Post-Newtonian corrections ON.

#define UPN

double

turns Post-Newtonian corrections OFF.

The input macros of orbitN.h and orbitN.c are included below and should be self-explanatory (for more details, see ZeebeAJ23). Simulations with advanced settings that go beyond the options provided in the input sections will require the user to modify the source code and/or other (non-input) macros.

```
orbitN.h
/*=============== Input Section =============================*/
              /* No. of Bodies incl. central mass
                                                       */
#define JJ 10
/* turn macros off (disable): add U in front of string
#define FASTDRIFT /* merge drift steps
#define PN /* Post-Newton (requires FAST)
#define J2 /* Solar Quadrupole Moment
#define LUNAR /* Lunar: EMB quadrupole (Quinn91)
#define CORR
                /* Symplectic corrector ON/OFF
#define STAGE 6
                /* Symplectic corrector stage: 2, 4, 6
                /* compensated summation (requires FAST) */
#define KAHAN
/* FOR ACCURACY AND STORAGE USE STATE VECTORS X V !
#define ORB_XV /* output state xv. else: orb elements
                                                       */
                                                       */
#define ANG_DEG /* output angle units: deg. else: rad
#define ELM_MJ 1 /* 0/1 use M0 or M0+mj to calc elements */
/* CPU info (log file). disable in case of warnings/errors */
#define CPUINFO
/* set time step (days), t0, tend (days), save interval (steps) */
 /* Y2D = 365.25 (years -> days)
const double in_dt = -2.0;
```

 $in_t0 = 0.e3*Y2D;$

```
double in_tend = -1.e4*Y2D;
const int in_sstep = 73050;
```

/*==============*/

(2b) orbitN Input for Simulations (./sim)

The orbitN package includes several example simulations, see directory ./sim. These can be engaged by running shell scripts in the ./sim/.. subdirectories.

Compiling default- vs. simulation settings is controlled by the macro "SIM", which is set in the Makefile. For example, the command:

\$ make SIM=1

as used in the run/compile scripts under ./sim/.. invokes input parameter values defined in the sim.h and sim.c files in the respective ./sim/.. folder. These parameter values are then used instead of the default parameter values defined in the input sections of orbitN.h and orbitN.c

To run the simulation examples, the user should inspect and, if applicable, modify the scripts in ./sim/.. Note: the simulation ./sim/n-cluster-ensemble may require advanced knowledge of cluster computing, bash, ssh, etc. All scripts need to have executable permission, e.g., to activate and run:

```
$ chmod +x ./run
etc.
$ ./run
```

To activate all scripts, run actvtScripts in ./sim.

Hence the user has at least two options to solve a specific user-defined problem with orbitN. (1) Adjust orbitN settings through modification of input parameter values in the input sections of orbitN.h and orbitN.c. (2) Add custom user simulations, following the examples provided under ./sim.

(2c) orbitN Input File: Masses/Coordinates

orbitN is set to read the input coordinates of the bodies in the simulation from an input file (orbitN-coord.inp). The input includes the body masses (in units of the central mass M0; M0 = index 0) and initial state vectors = position and velocity (in au and au/day) in bodycentric coordinates at time t0. The coordinate input list of bodies starts at index 1.

!!! The input file must maintain the original bit-by-bit format exactly !!!

If the input file is modified (beyond adding/removing bodies and changing masses/state vectors) and after modifying includes, e.g., additional characters and/or spaces, reading of the input file may fail. Note: the backslash character '\' signifies line continuation. Do not add spaces after '\', at end of lines, etc. The text in lines following '#' is ignored.

```
input: state vectors = initial position & velocity (bodycentric)
orbitN-coord.inp
# body 1
m x0 y0 z0 u0 v0 w0
etc.,
  -----
where
SYMBOL m x0 y0 z0 u0 v0 w0
UNIT M0 [... au ...] [... au/d ...]
VARIABLE mass position velocity
(3) orbitN Output
By default, orbitN coordinate output is written to orbitN-j.dat
files (j = body index) in orbitN's root directory with the
following columns.
output option: state vectors = position & velocity (bodycentric)
NOTE: FOR ACCURACY AND STORAGE, STATE VECTORS ARE RECOMMENDED.
output option: Keplerian elements
VARIABLE time [..... see below .....]
where:
a /* semimajor axis */
  /* eccentricity */
i /* inclination
om /* ArgPerihelion */
oom /* LongAscNode */
vpi /* LongPerihelion */
mn /* mean anomaly */
Additional output files are generated as follows:
orbitN-erg.dat
______
SYMBOL t (E-E0)/E0 (Lx-Lx0)/L0 (Ly-Ly0)/L0 (Lz-Lz0)/L0 UNIT day -
VARIABLE time d(Energy) d(Angular Momentum)
```

where d(y) is the fractional change in y.

FILE CONTENT

orbitN.log input values, run log, wallclock time estimates orbitN-final.sve final coordinates for potential restart

The shell script 'cleanup' can be used to clean the orbitN root directory.

!!! CAUTION: all executables, output, object files etc. will be deleted !!! Only source (.c,.h), input, and a few other text files remain.

(4) Checks

The orbitN package includes a check option to test whether orbitN produces accurate output on the user's local machine. For the test, install and compile orbitN out-of-the-box (without any changes). Next, run:

- \$./orbitN
- \$./checkDo

and inspect check.log. The log file should show no differences.

Despite different OS/machines/optimizations, orbitN should produce identical outcome to machine precision. However, *ONLY* when output in STATE VECTORS XV is selected in orbitN.h:

#define ORB_XV

The above has been tested using gcc up to optimization level 3 ('-03'). When output in Keplerian elements is selected, agreement to machine precision can not be guaranteed because of issues with trigonometric functions (see ZeebeAJ23).

(5) Subdirectories

'./check' : check files

'./coords' : example input coordinate files

'./docs' : pdf copy of ZeebeAJ23, README, license, etc.

'./sim' : example simulations

'./src' : C source code files

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\$ soffice --convert-to pdf README.txt