Grid support in COMPAS

Functionality that enables users to specify a grid of initial values for both Single Star Evolution (SSE) and Binary Star Evolution (BSE) has been added to the COMPAS code.

For SSE, users can supply a text file that contains initial mass values and, optionally, metallicity values, and COMPAS will evolve individual stars with those initial values (one star per record).

For BSE, users can supply a text file that contains initial mass and metallicity values for the binary constituent stars, as well as the initial separation or orbital period, and eccentricity, of the binary (one binary star per record of initial values).

Changes to COMPAS to support grids are:

- A new Program Option, "grid", of type string. Program option "grid" allows the user to specify the name of the file containing the grid values. The file format is specific to the type of evolution: SSE or BSE (see below for details).

- Changes to the BinaryStar and BaseBinaryStar class constructors to allow specification of initial values.

- Changes to main() to read and parse the grid file, and to call the relevant constructors with the specified initial values.

- Changes to constants.h to add new errors to the error catalogue.

Grid File Format

Grid files are comma-separated text files, with column headers denoting the meaning of the data in the column (with an exception for SSE Grid files – see below for details).

Grid files may contain comments. Comments are denoted by the hash/pound character ('#'). The hash character and any text following it on the line in which the hash character appears is ignored. The hash character can appear anywhere on a line - if it is the first character then the entire line is a comment and ignored, or it can follow valid characters on a line, in which case the characters before the hash are processed, but the hash character and any text following it is ignored. Blank lines are ignored.

Notwithstanding the exception for SSE Grid files mentioned above, the first non-comment, non-blank line in a Grid file must be the header record. The header record is a comma-separated list of strings that denote the meaning of the data in each of the columns in the file.

Data records follow the header record. Data records, with an exception for SSE data files described below, are comma-separated lists of non-negative floating-point numbers. Any data field that contains a negative number, or characters that do not convert to floating-point numbers, is considered an error and will cause processing of the Grid file to be abandoned – an error message will be displayed.

Data records are expected to contain the same number of columns as the header record. If a data record contains more columns than the header record, data beyond the number of columns in the header record is ignored. If a data record contains fewer columns than the header record, missing data values (by position) are set equal to 0.0 – a warning message will be displayed.

BSE Grid File

Header Record

The BSE Grid file header record must be a comma-separated list of strings taken from the following list (case is not significant):

Header String	Column meaning
Mass_1	mass value ($M_\odot$) to be assigned to the primary star
Mass_2	mass value ($M_\odot$) to be assigned to the secondary star
Metallicity_1	metallicity value to be assigned to the primary star
Metallicity_2	metallicity value to be assigned to the secondary star
Separation	separation of the stars (AU) – the semi-major axis value to be assigned to the binary
Eccentricity	eccentricity value to be assigned to the binary
Period	orbital period (days) value to be assigned to the binary

All header strings are required in the header record, with the exception of Separation and Period: one of Separation and Period *must* be present, but both *may* be present.

The order of the columns in the BSE Grid file is not significant.

Data Record

See the general description of data records above. As for the header record, only one of Separation and Period is required to be present, but both may be present. The period may be used to calculate the separation of the binary. If the separation is present it is used as the value for the semi-major axis of the binary, regardless of whether the period is present (Separation has precedence over Period). If the period is present, but separation is not, the separation is calculated form the masses of the stars and the period given.

SSE Grid File

Header Record

The SSE Grid file header record must be a comma-separated list of strings taken from the following list (case is not significant):

Header String	Column meaning
Mass	mass value ($M_\odot$) to be assigned to the star
Metallicity	metallicity value to be assigned to the star

The SSE Grid file is only required to list Mass values for each star, with Metallicity values being optional. If the Metallicity column is omitted, the metallicity value assigned to the star is the user-specified value for metallicity via the program options (OPTIONS→Metallicity()).

If the Metallicity column is ommited from the SSE Grid file, the header is optional: if there is only one column of data in the SSE Grid file it is assumed to be the Mass column, and no header is required (though may be present). If the Metallicity column header is present, the the Mass column header is required.

The order of the columns in the SSE Grid file is not significant.

Data Record

See the general description of data records above. As for the header record, only Mass is required to be present, but Metallicity may also be present. If the Metallicity is omitted, the metallicity value assigned to the star is the user-specified value for metallicity via the program options (OPTIONS→Metallicity()).