PLATYPUS: A code for reaction dynamics of weakly-bound nuclei at near-barrier energies within a classical dynamical model

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A B S T R A C T

A self-contained Fortran-90 program based on a three-dimensional classical dynamical reaction model with stochastic breakup is presented, which is a useful tool for quantifying complete and incomplete fusion, and breakup in reactions induced by weakly-bound two-body projectiles near the Coulomb barrier. The code calculates (i) integrated complete and incomplete fusion cross sections and their angular momentum distribution, (ii) the excitation energy distribution of the primary incomplete-fusion products, (iii) the asymptotic angular distribution of the incomplete-fusion products and the surviving breakup fragments, and (iv) breakup observables, such as angle, kinetic energy and relative energy distributions.

Program summary

Program title: PLATYPUS
Catalogue identifier: AEIG_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEIG_v1_0.html
Program obtainable from: CPC Program Library, Queen’s University, Belfast, N. Ireland
No. of lines in distributed program, including test data, etc.: 332 342
No. of bytes in distributed program, including test data, etc.: 344 124
Distribution format: tar.gz
Programming language: Fortran-90
Computer: Any Unix/Linux workstation or PC with a Fortran-90 compiler
Operating system: Linux or Unix
RAM: 10 MB
Classification: 16.9, 17.7, 17.8, 17.11
Nature of problem: The program calculates a wide range of observables in reactions induced by weakly-bound two-body nuclei near the Coulomb barrier. These include integrated complete and incomplete fusion cross sections and their spin distribution, as well as breakup observables (e.g. the angle, kinetic energy, and relative energy distributions of the fragments).
Solution method: All the observables are calculated using a three-dimensional classical dynamical model combined with the Monte Carlo sampling of probability-density distributions. See Refs. [1,2] for further details.
Restrictions: The program is suited for a weakly-bound two-body projectile colliding with a stable target. The initial orientation of the segment joining the two breakup fragments is considered to be isotropic.
Additional comments: Several source routines from Numerical Recipes, and the Mersenne Twister random number generator package are included to enable independent compilation.
Running time: About 75 minutes for input provided, using a PC with 1.5 GHz processor.
1. Introduction

Nuclear physics research has entered a new era with developments of rare-isotope beam facilities, where investigations are highly focused on understanding astrophysically important reaction rates involving exotic nuclei. These are often weakly-bound with a few-body, cluster structure that can easily be dissociated in their interaction with other nuclei. Understanding the breakup mechanism and its impact on nuclear reaction dynamics is essential. A major consequence of breakup is that a rich scenario of reaction pathways arises, such as events where (i) not all the resulting breakup fragments might be captured by the target, termed incomplete fusion (ICF), (ii) the entire projectile is captured by the target, termed complete fusion (CF), and (iii) none of the breakup fragments are captured, termed no-capture breakup (NCBU), which is expected to be predominant at energies below the fusion barrier. Some of these are presented in Fig. 1. Although it is not illustrated there, the transfer process is also very important [1–5].

The experimental disentanglement of all these reaction processes is very complex. Also their modelling within a unified framework is an outstanding problem. The continuum-discretized coupled-channels (CDCC) model, for instance, can make reliable predictions of the NCBU and TF processes. However, this approach and other existing quantum models have limitations [6], as they cannot calculate integrated incomplete and complete fusion cross sections unambiguously [7,8]. Neither, after the formation of incomplete fusion products, can these follow the evolution of the surviving breakup fragment(s) since incomplete fusion results in depletion of the total few-body wave-function. A quantum model is very desirable, as it can deal with quantum tunnelling that is essential for understanding astrophysical reaction rates involving exotic nuclei. Nevertheless, some difficulties are overcome by the present classical dynamical reaction model.

This paper describes a computer program of the three-dimensional classical dynamical reaction model with stochastic breakup, recently published in Refs. [9,10]. This approach exploits concepts and techniques (e.g., classical trajectory, Monte Carlo sampling) that overlap with some involved in dynamical models of multi-fragmentation and ICF in heavy-ion induced reactions at energies well-above the Coulomb barrier (>10 MeV/nucleon), as in Refs. [11,12]. A crucial input of the present model is a stochastically sampled breakup function suggested in Ref. [13], which can be determined from sub-barrier breakup measurements [4,13]. This function encodes the effects of the Coulomb and nuclear interactions that cause the projectile breakup. Hence, this approach is not a breakup model, rather it is a quantitative dynamical model for relating the sub-barrier NCBU to the above-barrier ICF and CF of weakly-bound nuclei [13]. The model has successfully been applied to interpreting fusion and breakup measurements of weakly-bound nuclei [4,5,14], and isomer ratio measurements [15]. Other applications in γ-ray spectroscopy are discussed in Ref. [10].

Since the code is very user-friendly and useful for researchers involved in fusion and breakup measurements of weakly-bound nuclei at near-barrier energies, it will be beneficial make the program accessible to everyone. In Section 2 the program and the input file are explained. The code is illustrated in Section 3 with the reaction of a pseudo-8Be projectile (assuming a weakly-bound state of two α-particles [9]) with a 208Pb target. Very recent measurements [4] have shown that prompt 8Be breakup occurs dominantly through an excited 8Be nucleus, validating the approximation of a 8Be projectile by 1Be. The good agreement of the classical model calculations for the NCBU process with those of the CDCC quantum mechanical model shows the reliability of the classical dynamical approach (see Ref. [9] for details).

2. Computer program and input file

2.1. Structure of the code

The code has a main program and ten modules. The main program breakup3D directs the input to be read, the problem to be solved, and details of the calculation to be written in output files. The modules are kinds, global data, potentials, mt19937, nrutit, initial conditions, fusion, angular momentum distribution, input values and incomplete fusion products.

The main program breakup3D calls the module input values first, in which the subroutine input file reads the input file described below. For a given partial wave between the projectile and the target (IMPACTMIN up to IMPACTMAX), the subroutines projectile trajectory and trajectory arrays of this module calculate the orbit of the bound projectile and store it for interpolations in the module initial conditions. Thereafter, ISSEEDMAX breakup events with sampled initial conditions are calculated for every partial wave. The initial conditions for the propagation in time of the three bodies are fixed by the subroutine initial values of the module initial conditions, whilst the classical trajectory of the breakup fragments and the target are calculated by the driver-subroutine ODEINT of the module nrutit. During the time propagation, the possible capture of the breakup fragments by the target is determined by the subroutine fusion events in the module fusion. Here, the relative energy and angular momentum between the nuclei, and the initial conditions for the time propagation in the two ICF channels are calculated as well. The spin distribution and cross sections for CF and ICF, and for the breakup process are calculated by the subroutine spin distribution in the module angular momentum distribution. Here, other observables such as the angle, kinetic energy and relative energy distributions of the fragments from NCBU events are also computed. Finally, the asymptotic angular distribution of the ICF products and the surviving breakup fragments is calculated by the subroutine propagating icf product in the module incomplete fusion products. This subroutine also provides the excitation energy distribution of the primary ICF products. Depending on the value of the output control variables (FILE1, FILE2, FILE3, FILE4, FILE5 and FILE6), details of the calculation can be written into output files. The output file TRACKING CALCULATIONS contains information on the evolution of the calculations.

Module kinds. This defines the kind type parameter for real values.

Module global data. This defines global variables used in different modules.

Module potentials. Here the nuclear and Coulomb interactions between the participants of the reaction (projectile fragments and the target) are defined.

Module mt19937. It contains the Mersenne Twister random number generator, written by Makoto Matsumoto and Takuji Nishimura [16].

References:

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Module \textit{nrutil}. In this module several subroutines from Numerical Recipes are included, which are mainly related to integrating the classical equations of motion. \textit{ODEINT} is the integrator driver that calls the subroutine \textit{RKQC} which is a fourth-order Runge–Kutta integrator ensuring accuracy and adjusted stepsizes. The forces are defined in the subroutine \textit{DERIVS}. The module also contains subroutines (\textit{printout1} and \textit{printout2}) for writing into output files the trajectory of the nuclei along with the value of the integrals of motion. The latter is crucial for checking the accuracy of the integration of the classical equations of motion.

Module \textit{initial conditions}. This module defines the initial conditions for the propagation in time of the three bodies, following the breakup of the two-body projectile. This task is performed by the subroutine \textit{initial values}, which is guided by the conservation of energy, linear momentum and angular momentum in the overall centre-of-mass frame of the projectile and target system. This is transformed to the laboratory reference frame (with Galilean kinematical relations) where the equations of motion are solved using a system of spherical coordinates. This module calls the module \textit{mt19937} in the sampling of (i) the initial excitation energy of the projectile, (ii) the initial relative angular momentum between the projectile fragments, (iii) the initial separation between the fragments, (iv) the breakup radius, (v) the initial orientation of the segment joining the two fragments of the projectile, and (vi) the initial direction of the radial velocity along that segment. If the output control variables are activated, the initial conditions will be written into output files.

Module \textit{fusion}. In this module the subroutine \textit{fusion events} analyses the possible capture of any of the breakup fragments by the target. Here, the relative energy and angular momentum between the nuclei during the time propagation are calculated by the subroutines \textit{relative energy} and \textit{relative spin}. The subroutine \textit{icf product} calculates the initial positions and velocities for the time propagation in the two \textit{icf} channels.

Module \textit{angular momentum distribution}. Knowing the statistics of fusion and \textit{ncbu} events after a large number of sampling (1000 per partial wave in the example given below), the subroutine \textit{spin distribution} calculates observables related to \textit{cf} and \textit{icf} processes (spin distribution and cross sections). The angle, kinetic energy and relative energy distributions of the \textit{ncbu} events and the breakup cross section are also computed here. This subroutine extensively calls the subroutine \textit{LOCATE} of the module \textit{nrutil}. All observables are written into output files.

Module \textit{input values}. Here the input file is read by the subroutine \textit{input data}. It also calculates the s-barrier features (radius and height) between (i) the projectile and the target, (ii) the projectile fragments and the target, and (iii) the two fragments of the projectile. The module also contains the subroutines \textit{projectile trajectory} and \textit{trajectory arrays} mentioned above.

Module \textit{incomplete fusion products}. This module includes the subroutines \textit{propagating icf product} and \textit{icf trajectory}. The former carries out the time propagation of the \textit{icf} products and the remaining breakup fragments, whilst the latter analyses this propagation in order to determine their asymptotic angles. The angular distributions, and the excitation energy distribution of the primary \textit{icf} products are constructed like those in the module \textit{angular momentum distribution}. All observables are also written into output files.

### 2.2. Input file

**Fig. 2** shows the input file of the program. At the bottom of the figure, the namelist of the input variables appearing in the code are shown. The lines related to the potentials (lines 12–21) are self-explanatory, whilst some variables in previous lines have already been mentioned in the description of the program. We will here describe lines 1–11 only.

The integer variables of the first line allow the user to write details of the dynamical calculations into output files, when they are equal to one. FILE1 and FILE2 open output files to write the trajectory of the breakup fragments and the initial projectile-target, respectively. The file opened by FILE3 contains details of breakup events, and FILE4 is for plotting the trajectory of the breakup fragments. FILE5 opens a file to write the asymptotic angles and energy of the breakup fragments, and FILE6 provides a file for the asymptotic angles of the \textit{icf} products and the surviving breakup fragments. Line 2 defines the window of orbital angular momentum of the incident projectile (IMPACTMIN, IMPACTMAX) in units of \(\hbar\), and the number of breakup events per partial wave (ISEEDMAX). PARTICULAR IMPACT in line 3 is to select a partial wave, whose associated dynamical calculations are written into the file opened by FILE3. Line 4 refers to the incident energy of the projectile in MeV (E0). Lines 5–6 define the range of initial excitation energy (EXCMIN, EXCMAX) in MeV and relative angular momentum (L12MIN, L12MAX) in units of \(\hbar\) for the breakup fragments. In line 7, \textsc{type} EXC controls the sampling function for excitation
**Fig. 2.** Input file for PLATYPUS code (PLATYPUS.inp).

The above text describes the potential for ICF channel 2: \((\text{AT}+\text{AP}2)\) and \(\text{AP}1\) and the potential for ICF channel 1: \((\text{AT}+\text{AP}1)\) and \(\text{AP}2\).

### Line 19: Fragment1-Fragment2 potential (\(V01, rr01, a01\)) and Coulomb radius (\(rrc01\))

- In the potential, the radius parameters are multiplied by \((\text{AP}1)^{(1/3)}\).

### Line 18: Target-Fragment2 potential (\(V02, rr02, a02\)) and Coulomb radius (\(rrc02\))

- In the potential, the radius parameters are multiplied by \((\text{AP}2)^{(1/3)}\).

### Line 21: Potential for ICF channel 2: \((\text{AT}+\text{AP}1)\) and \(\text{AP}2\) (\(V02ICF, r02ICF, A02ICF\)) and Coulomb radius (\(rcc1CF\)) and Qvalue (\(\text{Qvalue01}\)) for the ICF process

- In the potential, the radius parameters are multiplied by \((\text{AP}2)^{(1/3)}\).

### Fig. 3.

**Fig. 3.** ICF angular momentum distribution (ICF SPIN DISTRIBUTION).

Regarding angular momentum distribution, for \(\text{TYPE EXC}=0\) the weighting is uniform, and for \(\text{TYPE EXC}=1\) it is exponentially decreasing with a coefficient \(\alpha_{\text{exc}}\). Line 8 defines the centroid (\(d012\)) and width (\(\text{sig012}\)) in fm of the Gaussian function that describes the radial probability distribution of projectile ground-state wave function. It is used to sample the initial separation between the breakup fragments. The breakup function [see expression (1) in Refs. [9,10]] is given in line 9 by the parameters alpha and beta, being beta = \(\ln(A)\). Line 10 defines a maximal projectile-target separation for sampling the breakup radius, whilst line 11 allows the user to carry out the time propagation in the ICF channels, when ICF PROPAG=1.
The code also calculates nontrivial component related to the capture of all the projectile suggestions. The work was supported by an ARC Discovery Grant M. Dasgupta and L.R. Gasques for discussions and constructive Acknowledgements.

REFERENCES


3. Test run

Using the input file of Fig. 2, Figs. 3–5 show output files for angular momentum distribution in icf, cf and ncbu processes, respectively. The angular momenta are in the first column, whilst in the second and third columns are partial probabilities and cross sections. The total angular momentum distribution in Fig. 4 shows the orbital angular momentum of the incident projectile. The former has been employed very recently to understand isomer ratios and the UK Science and Technology Facilities Council (STFC) Grant No. ST/F012012/1.

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