

Foreword

The Joint Evaluated Fission and Fusion (JEFF) Project is a collaborative effort among the member countries of the OECD Nuclear Energy Agency (NEA) Data Bank to develop a reference nuclear data library. The JEFF library contains sets of evaluated nuclear data, mainly for fission and fusion applications; it contains a number of different data types, including neutron and proton interaction data, radioactive decay data, fission yield data and thermal scattering law data.

The General fission (GEF) model is based on novel theoretical concepts and ideas developed to model low energy nuclear fission. The GEF code calculates designs and associated quantities (e.g. prompt neutron and gamma) for a large range of nuclei and excitation energy. This opens up the possibility of a qualitative step forward to improve further the JEFF fission yields sub-library.

This supplement to JEFF Report 24 provides technical information on the GEF code and subroutines, as well as examples and practical limits.

Acknowledgements

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1 Name of the program

GEF Version 2014/2.1

The official GEF websites are http://www.khs-erzhausen.de and http://www.cenbg.in2p3.fr/GEF.

2 Description of the program

GEF is a computer code for the simulation of the nuclear fission process. The GEF code calculates pre-neutron and post-neutron fission-fragment nuclide yields, angularmomentum distributions, isomeric yields, prompt-neutron yields and prompt-neutron spectra, prompt-gamma spectra, and several other quantities for a wide range of fissioning nuclei from polonium to seaborgium in spontaneous fission and neutron-induced fission. Multi-chance fission (fission after emission of neutrons) is included. For neutroninduced fission, the pre-compound emission of neutrons is considered. Output is provided as tables and as parameters of fission observables on an event by-event basis.

Specific features of the GEF code

- The mass division and the charge polarisation are calculated assuming a statistical population of states in the fission valleys at freeze-out. The freeze-out time considers the influence of fission dynamics and is not the same for the different collective variables.
- The separability principle [1] governs the interplay of macroscopic and microscopic effects. Five fission channels are considered. The strengths of the shells in the fission valleys are identical for all fissioning systems. The mean positions of the heavy fragments in the asymmetric fission channels are essentially constant in atomic number, as suggested by experimental data [2].
- The stiffness of the macroscopic potential with respect to mass asymmetry is deduced from the widths of measured mass distributions [3].
- The excitation-energy-sorting mechanism [4-7] determines the prompt neutron yields and the odd-even effect in fission-fragment yields of even-Z and odd-Z systems.
- Neutron vaporation from the fragments is calculated with a Monte-Carlo statistical code using evel densities from empirical systematics [8] and binding energies with theoretical shall effects with gamma competition included.
- Model incertainties and covariances are determined by a series of calculations with perturbed parameters.

• Multi-chance fission is supported.

• Pre-compound emission is considered for neutron-induced fission.

3 Method of solution

The Monte-Carlo method is used. Uncertainties and co-variances are deduced from perturbed calculations.

4 Computational structure

Gross structure

- User input: Input is provided by dialogue, GUI or by file
- Read tables: Macroscopic masses (Thomas-Fermi masses), Evaluated masses (from 2012 mass table), Shell effects (from P. Möller et al.), Nuclear spectroscopic data (from JEFF3 decay file).
- Begin loop over systems and energies of input file. Synchronize parallel calculations.
- Begin loop of perturbed calculations (optional).
 Sample all model parameters within their uncertainty range.
- - Perform calculations^{*}) with perturbed parameters.
- Establish multi-variant distributions.
 Output of perturbed results, tables and list-mode (optional).
- - End loop of perturbed calculations.
- - Perform calculations^{*}) with nominal parameters.
- - Uncertainties and covariances from multi-variant distributions.
- - Output & nominal results, tables and list-mode (optional).

• End oop over systems and energies of input file.

The calculations are detailed in the next section.

Flow of calculations

- Begin Monte-Carlo event loop (multi-chance fission). Start with target Z, A, entrance channel.
- - Begin Monte Carlo event loop (pre-fission decay).
- - Calculate pre-equilibrium emission (for n-induced reaction)
- Calculate neutron and proton decay widths (compound).
 Calculate fission decay width.
 - - Chose decay at random (fission or particle emission
- - In case of particle emission:
 Determine particle energy at random.
- - In case of fission:
 Build table of fissioning nuclei (2007)
- End Monte-Carlo event loop (pre-fission decay)
 In case of fission or end of particle cascade → next event.
- End Monte-Carlo event loop (molti-chance fission).
- Ordering of multi-chance table (Z_{CN}, A_{CN}, E_{CN}) at fission).
- Begin multi-chance loop. Pick up next Z_{CN} , A_{CN} , E_{CN}^* from multi-chance table.
- - Calculate parameters of distributions for sampling in MC loop.
- - Begin Monte-Carlo loop (sample all distributions).
- - Sample fission channel.
- - Sample A_1 and A_2 (fragments).
 - - Sample Z_1 and Z_2 (fragments).
- - Sample deformation energies of final fragments.
 - - Sample intrinsic excitation energies at scission.
 - - Sample collective excitation energies at scission.
 - - Sum up to E_1^* and E_2^* of fully accelerated fragments.
- - Calculate Q value.
 - -Deduce TKE from energy conservation $(TKE = Q E_1^* E_2^*)$.

- Sample angular momenta of fragments.

- - Prompt-neutron and prompt-gamma emission from fragments.
 - Calculate post-neutron Z'₁, Z'₂, A'₁, A'₂, TKE'.
 Determine relative yields of isomeric states.
- - End Monte-Carlo loop (sample all distributions).
- End multi-chance loop.

5 Subroutines

Function getyield

The function getyield returns the unnormalized yield of a fission chann Input:

- Excitation energy relative to the outer-barrier height.
- Temperature above the barrier (constant-temperature regime).
- Effective temperature below the barrier (for tunneling).

Function masscurv

The function masscurv returns the curvature of the masroscopic potential for massasymmetric distortions according to the systematics of Rusanov et al.

Input:

- -Z of fissioning nucleus
- -A of fissioning nucleus

$Function \ d_e_saddle_scission$

The function d_e_saddle_scission returns the potential-energy gain from fission barrier to scission according to Asghar and Haste.

Input:

 $-Z^2/A^{1/3}$ of fissioning nucleus

Function t_egidy

The function t_egidy returns the temperature parameter of the constant-temperature nuclear-level-density formula of legidy et al.

Input:

– Mass number

– Shell effect

Function trusanov

The function to be the temperature of the Fermi-gas nuclear-level-density formula of Rusanov et al.

Input: – Excitation energy

-Mass number

Function lymass

The function lymass returns the nuclear mass according to the liquid drop model of Myers and Swiatecki.

Input:

- Atomic number Z
- Nuclear mass number A
- Deformation parameter β

Function lypair

The function lypair returns the pairing-fluctuation energy according to the liquid-drop model of Myers and Swiatecki. Input:

- Atomic number Z
- Nuclear mass number A

Function fedefolys

The function fedefolys returns the nuclear deformation energy according to the liquiddrop model of Myers and Swiatecki. Input:

- Atomic number Z
- Nuclear mass number A
- Deformation parameter β

Function ldmass

The function ldmass returns the masroscopic nuclear mass according to the Thomas-Fermi model of Myers and Swiatecki.

Input:

Inpu

- Atomic number $\langle \!\!\! Z \!\!\!\! \rangle$
- Nuclear mass number A
- Deformation parameter

Function ame 2012

The function ame2012 returns the nuclear mass from the 2003 mass evaluation.

Atomic number Z

Nuclear mass number A

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Subroutine

Function u_shell

The function u_shell returns the ground-state shell effect from the Strutinsky-type model calculation of Möller et al.

Input:

- Atomic number Z
- Nuclear mass number A

Function u_shell_exp

The function u_shell_exp returns the ground-state shell effect from the difference of empirical mass and Thomas-Fermi mass without even odd functuations. Input:

– Atomic number Z

- Nuclear mass number A

$Function \ u_shell_e0_exp$

The function u_shell_e0_exp returns the difference of the empirical mass and the Thomas-Fermi mass. It includes shell effect and paring fluctuation. Input:

– Atomic number Z

- Nuclear mass number A

$Function \ u_mass$

The function u_mass returns the Thomas-Fermi macroscopic mass plus the ground-state shell correction of Möller et at Input:

– Atomic number Z

– Nuclear mass number

Function ecoul

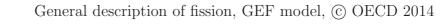
The function equal returns the Coulomb repulsion between two nuclei in the tip-tip configuration.

Input: $-Z_1, A_1, \beta_1, X_2, X_2, \beta_2$, tip distance d

Function beta_light

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The function beta_light returns the mean deformation of the light fragment of the S2 fission channel.



Input:

– Atomic number Z of light fragment

Function beta_heavy

The function beta_light returns the mean deformation of the heavy fragment of the S2 fission channel.

Input:

– Atomic number Z of heavy fragment

Function z_equi

The function z_equi determines the charge polarisation and leturns Z_1 in a configuration of two deformed nuclei $(Z_1, A_1, \beta_1, Z_2, A_2, \beta_2)$ in the tip-configuration with a tip distance d by minimising the total potential energy. Input:

 $-Z_C N, A_1, A_2, \beta_1, beta_2, d$

Subroutine beta_opt_light

The subroutine beta_opt_light determines the optimum deformation β_2 of the light fragment when the deformation β_1 of the heavy fragment is imposed in a tip-tip configuration. Input:

 $-A_1, A_2, Z_1, Z_2, d, \beta_2$

Subroutine beta_equi

The subroutine beta_equi determines the optimum deformation parameters of two deformed nuclei in a tip-tip configuration.

Input: $-A_1, A_2, Z_1, Z_2$, tip distance d

Subroutine eva

The subroutine eva is a simple evaporation code, used for the fragment de-excitation cascade. It considers neutron evaporation and statistical E1 gamma emission. The subroutine eva returns for neutron evaporation the times after scission and the kinetic energies of the neutrons, for gamma emission the energies of the photons, and the composition (Z and A) and the excitation energy of the residual nucleus.

Function u accel

The function u_accel returns the velocity of the fragment 1 at time T_n after scission in units of $\sqrt{(E/MeV)/A}$.

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Subroutin

Input:

 $-A_1, Z_1, A_2, Z_2$, pre-scission TKE

Function p_gamma_low

Random generator of gamma energy for gamma emission below the neutron separation energy.

Input: -Z, A, initial excitation energy E^*

Function p_gamma_high

Random generator of gamma energy for gamma emission neutron separation above the energy.

Input:

-Z, A, initial excitation energy E^*

Function u_ired

The function u_ired returns a reduction factor for the momentum of inertia at the yrast line due to shell effect and pairing correlation Input:

-Z, A

Function u_alev_ld

The function u_alev_ld returns the macroscopic level-density parameter of the Fermi-gas formula according to Ignatyuk Input:

-Z, A

Function u_temp

The function u_temp returns the nuclear temperature parameter from the modified composite level-density formula of Schmidt and Jurado with the influence of shells and pairing correlations (optional). Input:

 $-Z, A, E^*$

Function ggg

gtot returns the probability to emit a gamma of energy E_{γ} in competition The fund ioi with nission.

In

Atomic number Z of emitting nucleus.

- Mass number A of emitting nucleus.
- Excitation energy E^* of the emitting nucleus.
- Energy E_{γ} of the emitted gamma.

Function bftf

The function bftf returns the height of the fission barrier with shell effects and pairing correlations considered (optional).

Input:

-Z, A

Function bftfa

The function bftfa returns the height of the inner fission barrier with shell effects and pairing correlations considered (optional). Input:

-Z, A

Function bftfb

The function bftfb returns the height of the outer fission barrier with shell effects and pairing correlations considered (optional). Input:

-Z, A

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Subroutine

6 Typical running time

A typical calculation with 100 000 events takes about 5 seconds on one processor of an Intel i7 CPU (2.80GHz). Calculations with perturbed parameters and calculations at higher excitation energies, where multi-chance fission occurs, require somewhat more time.

7 Related and auxiliary programs

The main routines are written in $Free BASIC^1$. $Free BASIC^1$ produces compiled binary code that uses the C run-time library. Graphics output is based on the X11 library. A graphical user interface is provided for $WINDOWS^2$, written in $Just Basic^3$, which has a specific run-time library. The $WINDOWS^2$ version of GEF runs also under $WINE^4$ on LINUX.

8 Hardware requirements /

Computing time can be important for calculations with high statistics or for a large number of systems. Parallel computing, e.g. with a multi-core CPU, is supported and can be beneficial.

Memory: minimum ≈ 100 MByte; Disc: minimum ≈ 500 kByte for 1 calculation: eventually more, depending on the option.

9 Programming Language(s) used

Computer language on LINUX: FreeBASIC¹; on $WINDOWS^2$: FreeBASIC¹ and Just-Basic³.

10 Operating system under which the program is executed

a) $WINDOWS XP^2$ or newer

b) Any *LINUX* distribution. Eventually, some additional packages need to be installed, e.g. the X11 developer tools.

¹ Free **R**ASIC is available from http://www.freebasic.net/ with no cost.

 $^{2}WINDOWS$ is either a registered trademark or a trademark of Microsoft Corporation in the United States and/or other countries.

ustBasic is available from http://www.justbasic.com/ with no cost.

⁴ WWNE is a windows compatibility layer for LINUX (http://www.winehq.org/)

11 Other programming or operating information or restrictions

Multi-chance fission is supported, except when a distribution of excitation energies at fission is provided on input. The results on neutron emission prior to fission and promptneutron emission from the fragments are given separately. GEF provides all results event by event in a list-mode file on demand. The sequence of the events in the list-mode output is sorted by energy at fission in the case of multi-chance fission in order to save computing time. Therefore, the event sequence in the list-mode output should be randomly sampled, if the GEF code is to be used as a realistic generator for fission events. An optional enhancement factor may be specified. A value > increases the statistics of the Monte-Carlo calculation and hence reduces the statistical uncertainties of the results. Default value is 10^5 events. With this value, the statistical uncertainties are already smaller than the model uncertainties in most cases. Higher statistics may be used us covariances.

12 Names and adresses of authors

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13 Material available

 $Free BASIC^1$ source files. $Just Basic^3$ executable and run-time-library. Executables for $WINDOWS^2$ and LINUX. Read Me file with technical instructions.

14 Practical hints

Installing and running GEF

Please keep the sub-folder structure of GEF.zip. Sub-folders that are needed by the code are created automatically, if they do not exist. GEF does not overwrite or delete the output files. Kiles in the folders "/out", "/tmp", and "/dmp" that are not needed any more should be deleted.

- "/out" contains the main output as ASCII tables.
- "/tmp" contains more specific or internal information as ASCII tables.
- "/dmp" contains spectra in SATAN analyser format.
- "/gth" contains control files for parallel computing.

(CEP exe) and in the sub-folder GUI - a graphical user interface. GEF is started by

running "GEF.bat" (!) in a command window. All user input must be entered by the CUI window.

If you want to apply any changes, use an IDE (e.g. $FBIDE^5$) for editing any of the source files (*.bas). Compile the main routine GEF.bas under *FreeBASIC*. The other files are automatically included in the compilation process. The GUL is written in $JustBasic^3$.

On *LINUX*: The file GEF.zip provides an executable (GEF) that runs directly in a terminal by entering "./GEF". (Do not forget to set the file properties to "execute as a program".)

The GUI that is provided in the $WINDOWS^2$ version may also be used under LINUX by running the $WINDOWS^2$ version of GEF under $WINE^4$ without any loss of performance.

If you want to make any changes to GEF, prepare an executable, using an IDE (e.g. $GEANY^6$ with the *FreeBASIC*¹ compiler. GEF bas is the main routine. The other files are automatically included in the compilation process. Remark: Installation of additional packages may be required. (See http://www.freebasic.net/ \neq > Documentation - > User Manual - > Using the FreeBASIC Compiler - > Installing FreeBASIC.) E.g. the graphics output requires the installation of the X11 library. If the graphics does not work, you may suppress it by commenting the following line in GEF.bas:

#Include Once "DCLPlotting.bas"

Input

Required input of GEF:

- Z and A of fissioning nucleus or larget.
- Excitation mode and excitation energy.

The user is guided through additional input options by the input dialogue (on LINUX) or by the GUI (on $WINDWS^2$)

Output

Quantities available on output of GEF:

- Contributions of fission chances.
- Relative yields of fission channels.
- Element yield distribution*).

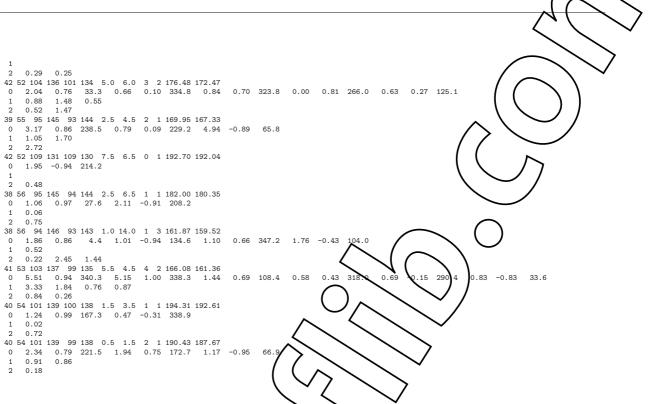
 $^{6}GEANY$ is available from http://fbide.freebasic.net/ with no cost.

- Isotonic-yield distribution (pre- and post-neutron).
- Isobaric-yield distribution*).
- Mass-chain yields (pre- and post-neutron)*).
- Fragment kinetic energies.
- Fragment angular-momentum distributions (for every nuclide).
- Relative independent isomeric yields.
- Prompt-gamma spectrum.
- Prompt-neutron spectrum.
- Neutron-multiplicity distribution.
- Energies and directions of prompt neutrons (pre- and post-scission).
- *) Including uncertainties and covariances. Many more quantities are internally calculated and may be listed.

List-mode output

The optional list-mode output comprises many properties of the fission fragments and the prompt neutrons on an event-by-event basis. A sample is listed below:

- Sample:
 Z1 Z2 Alpre Alpre Alpost Alpost Ilpre I2pre ni ng THEpre Throost Z1: Atomic number of first fragment Z2: Atomic number of second fragment Alpre: Pre-neutron mass number of first fragment Alpost: Post-neutron mass number of second fragment Alpost: Post-neutron mass number of second fragment Ilpre: Spin of first fragment after scission Ilpre: Spin of second fragment after scission I: Prompt neutrons emitted from first tragment TKEpre: Pre-neutron total kinetic energy [NV]
 * TKEpost: Post-neutron total kinetic energy [NV] * In separate lines: Prompt pest-scission meterons (including acceleration phase) * 0 E1, cos(theta1), phi1, E2 cos(theta2), phi2, E3, cos(theta3, phi3,: * Energies [MeV] in lab. fram and angles us. direction of light fragment of all post-scission neutrons * 1 E11, E21, E31,: Energies [MeV] of neutrons emitted from light fragment in frame of light fragment * 2 E1h, E2h, E3h, Energies [NeV] of neutrons emitted from heavy fragment in frame of heavy fragment
* Calculation with normal metal parameters 40 54 98 142 96 140 0 3.0 2 9 172 68 169.51 0 2.85 0.75 182.2 0.80 0.96 240.7 2.80 -0.50 323.4 0.58 0.54 72.3 1 1.30 0.09 2 2.12 1.66 33 61 83 157 82 56 1.6 4.5 1 1 167.69 166.00 0 2.77 0.50 84.3 03 0.69 237.3 1 2.18 2 0.25 39 55 98 142 9 141 4.0 7.0 1 1 177.58 176.00 0 3.19 5.54 157.4 1.90 -0.55 106.7 1 2.27
$\begin{array}{c}2\\42\\52\\0\end{array},137\\105\\-0.96\\55.5\\0.29\\-0.77\\159.2\end{array}$
General description of fission, GEF code, © OECD 2014

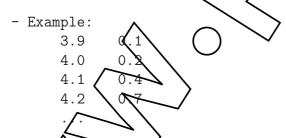


Advanced options

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Uncertainties: Uncertainty analysis from calculations with perturbed parameters is available. These calculations are also used to determine covariances between different observables as given by the model. As an option also the multi-variant distributions of fission-fragment yields can be obtained

Energy distribution: Instead of a single energy, also a distribution of excitation energies above the ground-state a fission may be provided in a file on input. The file name is fixed: Espectrum.in.



Each line gives an energy (in MeV) and a weight. Energy steps of about 100 keV are recommended. The spectrum may be un-normalized. The corresponding option is chosen by the OUI under $WINDOWS^2$ or by the option "ES" under LINUX. Note that GEF calculates only first-chance fission for this option.

the file. This option is chosen if the file. This option is chosen if

Instructions:

1. Create a file with the following information: 0^5 events per First line: Statistical enhancement factor (default = 1 corresponds t ϕ 1 system). A larger factor increases the number of calculated events accord Second line: Energy value or list of energy values. For neutron-induced fission: List of energy values in ascending order. For spontaneous fission: Energy value. (Only one value is allowed.) Following lines: Specification of the fissioning system. $(Z_CN, A_CN, \text{kind of fission})$ - Example for spontaneous fission: 10 0 98, 250, "GS" 98, 252, "GS" . . . - Example for neutron-induced ior 2 8, 0.0253E-6, 0.4, 2 9, 10, 11, 12, 13, 14 1, 92, 234, "EN" 92, 236, "EN" . . . sequence of calculations is performed with the In the case of neutron-induced fission, energies given in the second line of the input file - Example for fission from a shape isomer: Ju**¢**Prop.bas.) (The isomers must be listed in the file l 100 0 IS1' 94. 94

Gle.in": The file "file.in" contains the names of the input files 2. Create the file (one per line). Comments are supported.

xam <u>2SF</u>.in" SF.in"

In this example, only the files U238NF.in and PU240SF.in are treated.

Parallel computing: GEF supports starting several processes in parallel, which calculate the systems given in the input file in parallel in a coordinated way. This enables making efficient use of modern multiprocessor machines. Before starting a new sequence of calculations, the files "/ctl/done.ctl" and "/ctl/thread.ctl" must be deleted.

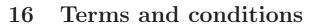
15 Deterministic version of GEF as a subroutine

A deterministic version of the GEF code provides pre-neutron fission-fragment nuclide distributions and excitation energies. It is written as a subroutine that is called with a specific compound nucleus, its excitation energy and its angular momentum on input. Only first-chance fission is calculated. The subroutine is available in FreeBASIC¹ and in FORTRAN. Compilation with the GNU Fortrap 95 compiler was tested.

Computational structure

- Read tables
- Macroscopic masses (Thomas-Fermi masses) Evaluated masses (from 2012 mass table) Shell effects (from P. Möller et al.). Nuclear spectroscopic data (from JEFF3 decay fre).
- Calculate parameters of distributions.
- Calculate distributions.
 Fission-fragment yields (Z and A) for each fission channel.
 Spin distribution per fragment (Z and A) and fission channel.
 Excitation energy per fragment (X and A) and fission channel.
- Fill output arrays of pre-neutron fragment properties. Nuclide yields (Y(Z, A)). Spin distribution (R(J, Z, A)).
 Excitation-energy distribution (P(E*, Z, A)).

In contrast to the Monte-Carlo version, correlations between the fission observables cannot be provided due to the deterministic structure of the computations.



Authors of the GEF code (General description of fission observables) are ©2008, 2010, 2011, 2012, 2013, 2014 Dr. Karl-Heinz Schmidt, Rheinstrasse 4, 64390 Erzhausen, Germany and Dr. Beatriz Jurado, Centre d'Études Nucléaires de Bordeaux-Gradignan, Chemin du Solarium, Le Haut Vigneau, BP 120, 33175 Gradignan, Codex, France.

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fsf

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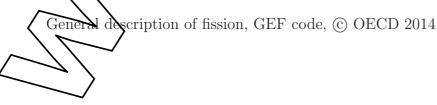
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menu, a prominent item in the list meets this criterion.

1. Source Code.

The "source code" for a work means the preferred form of the work for making modifications to it. "Object code" means any non-source form of a work.

A "Standard Interface" means an interface that either is an official standard defined by a recognized standards body, or, in the case of interfaces specified for a particular programming language, one that is widely used among developers working in that language.

The "System Libraries" of an executable work include anything, other than the work as a whole, that (a) is included in the normal form of packaging a Major Component, but which is not part of that Major Component, and (b) serves only to enable use of the work with that Major Component, or to implement a Standard Interface for which implementation is available to the public in source code А "Major Component", in this context, means a major essential nent (kernel, window system, and so on) of the specific oper rating used (if any) on which the executable work runs, or a comp iler produce the work, or an object code interpreter use o run

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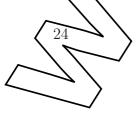
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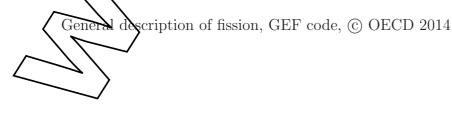
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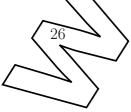
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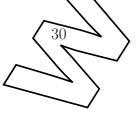
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