1 Modifications of the TALYS file 'checkkeyword.f'

TALYS only accepts input data according to a pre-defined set of keywords. In order to be able to pass information about unique file names to TALYS, a new keyword 'geffissionfileid' was added to the list of eligible keywords and the number of keywords was extended by one. On a side note, it does not matter whether the value for the keyword is given in upper or lower case letters, because TALYS has an internal function that converts all input to lower case. This means that the actual file names given to the file that TALYS shall use must be in lower case. Otherwise TALYS can not find the file and an error occurs. The necessary modifications to 'checkkeyword.f' are highlighted in yellow.

```
      subroutine checkkeyword
c
c +-------------------------------------------------------------------
c  Author:  Arjan Koningc  Date : March 7, 2023
c  Task :  Check for errors in keywords
c  Edited: Peter Karlsson; Date: May 7, 2023
c +-------------------------------------------------------------------
c
c ******************** Editing information *********************************
c Added one keyword: geffissionfileid, and increased numkey to 397 (from 396)
c  (new keyword placed in last position in list of keywords)
c ***************************************************************************
c
c ****************** Declarations and common blocks *******************
c
      include "talys.cmb"
      integer numkey
      parameter (numkey=397)
      integer i,j
      character*132 keyword(numkey),word(40),key
c
c Although it is difficult to prevent the user from all possible input
c errors, we can check for the use of wrong keywords and for unphysical
c values for most of the input variables.
c
c ********************** Check for wrong keywords *********************
c
c keyword: keyword
c numkey : number of keywords
c
c TALYS will stop if a keyword is incorrect
c
      data (keyword(i),i=1,numkey) /
     + ' ', 'a', 'aadjust', 'abundance', 'adddiscrete', 'addelastic',
     + 'adepthcor', 'alimit', 'alphald', 'alphaomp', 'anfit', 'angles',
     + 'anglescont', 'anglesrec', 'aradialcor', 'area', 'astro',
     + 'astroe', 'astroex', 'astrogs', 'astrot', 'asys',
     + 'autorot', 'avadjust', 'avadjustf', 'avdadjust', 'avdadjustf',
     + 'avsoadjust', 'avsoadjustf', 'awadjust', 'awadjustf',
     + 'awdadjust',
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+ 'awdadjustf', 'awsoadjust', 'awsoadjustf', 'axtype', 'bdamp',
+ 'bdampadjust', 'best', 'bestbranch', 'bestend', 'bestpath',
+ 'beta2', 'betafiscor', 'betafiscoradjust', 'betald', 'bins',
+ 'block', 'branch',
+ 'breakupmodel', 'cbreak', 'cfermi', 'cglobal',
+ 'channelenergy', 'channels', 'cknock', 'class2', 'class2file',
+ 'class2width', 'cnubar1', 'cnubar2', 'colenhance', 'colldamp',
+ 'components', 'compound',
+ 'core', 'coulomb', 'cpang', 'cstrip', 'ctable',
+ 'ctableadjust', 'ctmglobal', 'd0', 'd1adjust', 'd2adjust',
+ 'd3adjust', 'ddxmode', 'deformfile', 'deltaw', 'densfile',
+ 'deuteronomp',
+ 'disctable', 'dispersion', 'dnfit', 'e0', 'e0adjust', 'e1file',
+ 'eciscalc', 'eciscompound', 'ecisdwba', 'ecissave', 'eback',
+ 'ebeam', 'egr', 'egradjust', 'ejectiles', 'ejoin',
+ 'electronconv', 'element', 'elow', 'elwidth', 'emsdmin',
+ 'endf', 'endfdetail', 'endfecis', 'energy', 'epr',
+ 'epradjust', 'equidistant', 'equispec', 'estop', 'esurf',
+ 'etable', 'etableadjust', 'exmatch', 'exmatchadjust', 'expmass',
+ 'ffevaporation', 'ffmodel',
+ 'ffspin', 'fileangle', 'filechannels', 'fileddxa', 'fileddxe',
+ 'filedensity', 'filediscrete', 'fileelastic', 'filefission',
+ 'filegamdis',
+ 'filepsf', 'filerecoil', 'fileresidual', 'filespectrum',
+ 'filetotal',
+ 'fisbar', 'fisbaradjust', 'fisfeed', 'fishw', 'fishwadjust',
+ 'fismodel', 'fismodelalt', 'fispartdamp', 'fiso', 'fisom',
+ 'fission', 'fit', 'fsadjust',
+ 'ftable', 'ftableadjust', 'fullhf', 'fymodel', 'g', 'gadjust',
+ 'gamgam', 'gamgamadjust', 'gammald', 'gammashell1',
+ 'gammashell2',
+ 'gammax', 'gefran', 'ggr', 'ggradjust', 'giantresonance',
+ 'gn', 'gnadjust', 'gnfit', 'gnorm', 'gp', 'gpadjust',
+ 'gpr', 'gpradjust', 'group', 'gshell', 'hbstate',
+ 'hbtransfile', 'ibeam','incadjust', 'inccalc', 'integral',
+ 'isomer', 'isofit', 'jlmmode', 'jlmomp',
+ 'kph', 'krotconstant',
+ 'kvibmodel', 'labddx', 'ldmodel', 'ldmodelcn', 'ldmodelracap',
+ 'levelfile', 'liso', 'localomp', 'ltarget', 'lurr', 'lv1adjust',
+ 'lvadjust', 'lvsoadjust', 'lw1adjust', 'lwadjust', 'lwsoadjust',
+ 'm1file', 'm2constant', 'm2limit', 'm2shift', 'mass',
+ 'massdir', 'massdis', 'massexcess', 'massmodel', 'massnucleus',
+ 'maxband', 'maxchannel', 'maxenrec', 'maxlevelsbin',
_ 'maxlevelsres',
+ 'maxlevelstar', 'maxn', 'maxnrp', 'maxrot', 'maxz',
+ 'maxzrp', 'micro', 'mpreeqmode', 'msdbins', 'multipreeq',
+ 'nafit', 'nffit', 'ngfit', 'nlevels', 'nlow', 'nnfit',
+ 'nonthermlev', 'ntop', 'nulldev',
+ 'ompenergyfile', 'omponly', 'onestep', 'optmod', 'optmodall',
+ 'optmodfilen', 'optmodfilep', 'outangle', 'outbasic',
```

```
     + 'outbinspectra',
     + 'outcheck','outdecay', 'outdensity', 'outdirect', 'outdiscrete',
     + 'outdwba', 'outecis', 'outexcitation', 'outfission', 'outfy',
     + 'outgamdis', 'outgamma', 'outinverse', 'outkd', 'outlegendre',
     + 'outlevels',
     + 'outmain', 'outomp', 'outpopulation', 'outpreequilibrium',
     + 'outspectra',
     + 'outtransenergy', 'pair', 'pairconstant', 'pairmodel', 'parity',
     + 'partable', 'pfnsmodel', 'pglobal', 'phmodel', 'pnfit',
     + 'popeps', 'popmev', 'preeqcomplex', 'preeqmode', 'preeqspin',
     + 'preeqsurface', 'preequilibrium',
     + 'production', 'projectile', 'pshift', 'pshiftadjust',
     + 'pshiftconstant',
     + 'psfglobal', 'ptable', 'ptableadjust', 'racap', 'radialfile',
     + 'radialmodel', 'radiounit', 'rcadjust', 'rclass2mom',
     + 'reaction',
     + 'recoil', 'recoilaverage', 'relativistic', 'rescuefile',
     + 'reslib',
     + 'resonance', 'rfiseps', 'rgamma', 'rho', 'riplomp', 'riplrisk',
     + 'risomer',
     + 'rnunu', 'rnupi', 'rotational', 'rpevap', 'rpinu', 'rpipi',
     + 'rprime', 'rspincut', 'rspincutff', 'rspincutpreeq',
     + 'rtransmom', 'rvadjust', 'rvadjustf', 'rvdadjust', 'rvdadjustf',
     + 'rvsoadjust', 'rvsoadjustf', 'rwadjust',
     + 'rwadjustf', 'rwdadjust', 'rwdadjustf', 'rwsoadjust',
     + 'rwsoadjustf',
     + 's2adjust', 'sacs', 'segment', 'sfexp', 'sfth',
     + 'sgr', 'sgradjust', 'shellmodel', 'skipcn', 'soswitch',
     + 'soukho',
     + 'spherical', 'spincutmodel', 'spr', 'spradjust', 'statepot',
     + 'strength', 'strengthm1', 'strucpath', 'sysreaction', 't',
     + 'tadjust', 'tcool', 'tirrad', 'tjadjust', 'tmadjust',
     + 'transeps', 'transpower', 'tres', 'twocomponent', 'ufermi',
     + 'upbend', 'upbendc', 'upbende', 'upbendf', 'urr',
     + 'urrnjoy', 'v1adjust', 'v2adjust', 'v3adjust', 'v4adjust',
     + 'vfiscor', 'vfiscoradjust', 'vso1adjust', 'vso2adjust',
     + 'vinfadjust', 'w1adjust',
     + 'w2adjust', 'w3adjust', 'w4adjust', 'wfcfactor', 'widthfluc',
     + 'widthmode', 'wso1adjust', 'wso2adjust', 'wtable',
     + 'wtableadjust', 'xsalphatherm', 'xscaptherm', 'xseps',
     + 'xsptherm', 'yieldfile', 'yieldunit','geffissionfileid'/
c
c A keyword can be de-activated by putting a # in front of it.
c All first words of the input lines are checked against the list
c of keywords.
c
c nlines : number of input lines
c getkeywords: subroutine to retrieve keywords and values from input
c line
c inline : input line
```

```
c word : words on input line
c key : keyword
c
c The keyword is identified.
c
      Loop1: do i=1,nlines
        call getkeywords(inline(i),word)
        key=word(1)
        if (key(1:1).eq.'#') cycle Loop1
        do j=1,numkey
          if (keyword(j).eq.key) cycle Loop1
        enddo
        write(*,'(/" TALYS-error: Wrong keyword: ",a20)') key
        stop
      enddo Loop1
      return
      end
```