**SUBROUTINES AND FUNCTIONS FOR SPECIAL UTILITIES**

**[HELP INDEX]**

[ • WORKS • WORKS WITH SOME RESTRICTIONS • DON’T KNOW ]

* **FUNCTIONS RELATED TO THE GAMMA FUNCTION.**

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| **NAME** | **DESCRIPTION** |
| DGAMMA(XX)  QGAMMA(XX)  DGAMI(A,X)  QGAMI(A,X)  DGAMIC(A,X)  QGAMIC(A,X) | FUNCTION TO CALCULATE THE GAMMA FUNCTION OF XX (IT ADMITS NEGATIVE AND POSITIVE VALUE OF XX). NUMERICAL RECIPES PG. 207 (MODIFIED). |
| DGAMMAP(A,X)  QGAMMAP(A,X)  DGAMMAQ(A,X)  QGAMMAQ(A,X) | FUNCTION TO CALCULATE THE INCOMPLETE GAMMA FUNCTION P(a,x). NUMERICAL RECIPES PG. 211 (MODIFIED). |
| DGSER(A,X)  QGSER(A,X) | FUNCTION TO CALCULATE THE INCOMPLETE GAMMA FUNCTION P(a,x), EVALUATED BY ITS SERIES REPRESENTATION. NUMERICAL RECIPES PG. 212 (MODIFIED). |
| DGCF(A,X)  QGCF(A,X) | FUNCTION TO CALCULATE THE INCOMPLETE GAMMA FUNCTION P(a,x), EVALUATED BY ITS CONTINUED FRACTION REPRESENTATION. NUMERICAL RECIPES PG. 212 (MODIFIED). |

* **FUNCTIONS RELATED TO THE FACTORIAL FUNCTION.**

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| **NAME** | **DESCRIPTION** |
| DFACT(NUM)  QFACT(NUM) | FUNCTION TO CALCULATE FACTORIAL FUNCTION OF NUM. |
| DFACTI(NUM)  QFACTI(NUM) | FUNCTION TO CALCULATE THE FACTORIAL FUNCTION OF AN ODD NUMBER (NUM). |
| NFACT(NUM) | FUNCTION TO CALCULATE THE FACTORIAL FUNCTION OF AN INTEGER NUMBER (NUM). |
| DSFACT(NUM)  QSFACT(NUM) | FUNCTION TO CALCULATE POSITIVE SEMI-FACTORIAL (NUM+1/2)! |

* **FUNCTIONS RELATED TO SPECIAL FUNCTIONS.**

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| **NAME** | **DESCRIPTION** |
| DELTAK(N,M) | FUNCTION TO CALCULATE KRONEKER'S DELTA FUNCTION. |

* **SUBROUTINES AND FUNCTIONS RELATED FOR MATRIX OPERATIONS.**

Funciona, pero sobrescribe la matriz de salida

en la de entrada

Sólo funcionan para matrices simétricas

Antes eran MANTINV

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| **NAME** | **DESCRIPTION** |
| MATOUT(N,M,A,C,F) | SUBROUTINE TO WRITE A NxM MATRIX (N=ROWS,M=COLUMNS). |
| DMATINVSYM(N,SS,SR)  QMATINVSYM(N,SS,SR) | SUBROUTINE TO CALCULATE SS^(-1) (SS=NxN MATRIX). |
| DMATINVR(N,SS,SR)  QMATINVR(N,SS,SR) | SUBROUTINE TO CALCULATE SS^(-1/2) (SS=NxN MATRIX). |
| DTRACE(N,M)  QTRACE(N,M) | FUNCTION TO CALCULATE THE TRACE OF A MATRIX. |
| DJACOBIM(N,A,TT)  QJACOBIM(N,A,TT)  DJACOBI(N,A,T,SORT)  QJACOBI(N,A,T,SORT) | SUBROUTINE TO DIAGONALIZE A SYMMETRIC MATRIX. NUMERICAL RECIPES PG. 460 (MODIFIED). |
| DJACOBI\_JAIME(N,B,X,V,NORD)  QJACOBI\_JAIME(N,B,X,V,NORD) | SUBROUTINE TO DIAGONALIZE A SYMMETRIC MATRIX (JAIME MODIFICATION). |
| DGAUSSJ(a,n,np,b,m,mp)  QGAUSSJ(a,n,np,b,m,mp) | SUBROUTINE TO SOLVE EQUATIONS SYSTEM, GAUSS-JORDAN MATRIX INVERSION AND LINEAR EQUATION SOLUTION, NUMERICAL RECIPES PG. 30 (MODIFIED). |

* **SUBROUTINES AND FUNCTIONS RELATED TO COORDINATES CONVERSION.**

Antes eran

SPHER2CAR

Antes eran

POLAR2CAR

Antes eran

CAR2POLAR

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| **NAME** | **DESCRIPTION** |
| DCAR2SPHER(P,PP)  QCAR2SPHER(P,PP) | SUBROUTINE TO CONVERT CARTESIAN COORDINATES TO POLAR RECEIVES THE DATA X,Y,Z AND RETURNS R, COS(THETA) AND PHI. |
| DSPHER2CAR(PP,P)  QSPHER2CAR(PP,P) | SUBROUTINE TO CONVERT POLAR COORDINATES TO CARTESIAN RECEIVES A VECTOR R, COS(THETA), PHI AND RETURNS OTHER WITH X,Y,Z. |
| DELLIP2CAR(PP,DISTCENTROS,P)  QELLIP2CAR(PP,CENTERSDIST,P) | SUBROUTINE TO CONVERT ELLIPSOIDAL COORDINATES TO CARTESIAN RECEIVES A VECTOR R=LAMBDA, COS(THETA)=MU, PHI=PHI AND RETURNS OTHER WITH X,Y,Z. |

* **SUBROUTINES AND FUNCTIONS TO DETERMINE THE TIME.**

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| **NAME** | **DESCRIPTION** |
| CAL\_TIME(SS,D,H,M,S,T) | SUBROUTINE TO GET THE TIME TAKEN. |

* **SUBROUTINES OF NUMBERS AND DATA CONVERTION (NUMBERS TO STRINGS AND STRINGS TO NUMBERS).**

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| **NAME** | **DESCRIPTION** |
| STRTODBLE(STR)  STRTOQUAD(STR) | SUBROUTINES THAT RETURNS A REAL NUMBER FROM A STRING. |
| REALDTOSTR(NUMBER)  REALQTOSTR(NUMBER) | FUNCTION THAT RECEIVES A REAL NUMBER AND RETURNS A STRING. |
| STRTOINT(STR) | SUBROUTINE THAT RETURNS AN INTEGER FROM A STRING. |
| INTTOSTR(NUMBER) | FUNCTION THAT RECEIVES A POSITIVE INTEGER NUMBER AND RETURNS A STRING. |
| ISNUMBER(STR) | FUNCTION THAT RETURNS TRUE IN CASE THE STRING GIVEN IS NUMERIC. |
| ISPAR(N) | FUNCION THAT INDICATES IF A NUMBER IS ODD OR EVEN. |
| ISINT(NUMI) | FUNCTION THAT RETURNS TRUE IF THE NUMBER IS AN INTEGER AND FALSE OTHERWISE. |

* **SUBROUTINES AND FUNCTIONS FOR TREATING STRINGS.**

En pantalla no reconoce el espacio en blanco definido como splitter

en la subrutina

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| **NAME** | **DESCRIPTION** |
| SPLIT(STRING,SPLITTER,SUBSTRING) | SUBROUTINE TO CONVERT A STRING INTO AN ARRAY OF WORDS DEPENDING ON THE WORD SEPARATOR. |
| CMAYMIN(C,MM) | SUBROUTINE TO CONVERT ALL THE CHARACTER TO CAPITAL CHARACTER IF (MM=1) OR TO SMALL LETTER IF (MM=0). |
| COMPARESTR(C1,C2) | FUNCTION TO COMPARE TWO STRINGS. RETURNS 1 IF THEY ARE EQUALS AND 0 OHTERWISE. IT IS NOT CASE SENSITIVE. |

* **SUBROUTINES TO IMPROVE THE DATA WRITING.**

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| **NAME** | **DESCRIPTION** |
| BLANKLINES(N,NUNIT) | SUBROUTINE FOR ADDING N BLANK LINES. |
| CHARDASH(N,NUNIT,J) | SUBROUTINE TO ADD A LINE WITH N DASHES. |
| SPLITTER(NCHAR,CHAR,NLINES,SFILE) | SUBROUTINE TO SPLIT DATA. |

* **SUBROUTINES FOR TREATMENT OF FILES.**

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| **NAME** | **DESCRIPTION** |
| GET\_UNIT() | FUNCTION THAT RETURNS THE NUMBER OF THE NON-USED FILE. |
| GET\_PATH(STR) | FUNCTION THAT RETURNS THE PATH. |
| GET\_FILENAME(STR) | FUNCTION THAT RETURNS THE COMPLETE NAME OF THE FILE (W/ EXTENSION). |
| GET\_BASENAME(STR) | FUNCTION THAT RETURNS THE COMPLETE NAME OF THE FILE (WO/ EXTENSION). |
| GET\_EXT(STR) | FUNCTION THAT RETURNS THE FILE EXTENSION. |
| REPLACE\_EXT(STR,NEWEXT,IFPATH) | FUNCTION THAT RETURNS THE FILE CHANGING THE EXTENSION (IFPATH=TRUE/FALSE WITH PATH/WITHOUT PATH). |
| REPLACE\_CHAR(STR,CHIN,CHOUT)  REPLACE\_CHAR1(STRIN,CHIN,CHOUT,STROUT) | FUNCTION THAT RETURNS THE FILE CHANGING A CHARACTER (CHIN) FOR OTHER (CHOUT). |
| POSCHAR(STR,CH,DIR) | FUNCTION THAT RETURNS THE POSITION OF THE FIRST/LAST (DIR=FALSE/TRUE) GIVEN CHARACTER (CH) IN THE STRING (STR) DISTINGUISH BETWEEN MAYUS AND MINUS. |

* **SUBROUTINES AND FUNCTIONS FOR INI FILES.**

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| **NAME** | **DESCRIPTION** |
| EXE\_PATH() | FUNCTION TO RETURN THE PATH OF THE \*.EXE SOFTWARE. |
| MAKESECTION(FILEN,SECTION) | SUBROUTINE TO CREATE A NEW SECTION IN THE GIVEN FILE. IF THE SECTION ALREADY EXISTS, THE SECTION IS NOT CREATED. |
| SAVEVALUE(FILEN,SECTION,KEY,VALUE\_K) | SUBROUTINE TO SAVE THE VALUE ASSOCIATED TO THE KEY AND SECTION. IF THE KEY DOES NOT EXIT, IT WILL BE CREATED, IF DOES, IT WILL BE AMENDED. |
| READVALUE\_GEN(FILEN,SECTION,KEY,OPT\_VALUES,NSUB) | FUNCTION TO READ A VALUE ASSOCIATED TO THE GIVEN KEY AND SECTION FROM THE DATA FILE AND CHECK THE COMPLIMENT OF THE ALLOWED OPTIONS. IF THE VALUE IS NOT FOUND, AN EMPTY STRING IS RETURNED. |
| READVALUE(FILEN,SECTION,KEY) | FUNCTION TO READ A VALUE ASSOCIATED TO THE GIVEN KEY AND SECTION FROM THE DATA FILE. IF THE VALUE IS NOT FOUND, AN EMPTY STRING IS RETURNED. |
| READVALUE\_INT(FILEN,SECTION,KEY,MINV,MAXV) | FUNCTION TO READ AN INTEGER NUMBER FROM THE DATA FILE. |
| READVALUE\_REAL(FILEN,SECTION,KEY) | FUNCTION TO READ A REAL NUMBER FROM THE DATA FILE. |

* **SUBROUTINES FOR TREATMENT OF NAMES AND SYMBOLS OF ATOMS.**

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| **NAME** | **DESCRIPTION** |
| CHARGETOSYMBOL(NUM,SB) | SUBROUTINE TO FIND OUT THE SYMBOL OF AN ELEMENT FROM ITS CHARGE (Z) AND VICE VERSA. |
| CHARGETONAMESP(NUM,NB) | SUBROUTINE TO FIND OUT THE NAME OF AN ELEMENT FROM ITS CHARGE (Z) AND VICE VERSA (SPANISH). |
| CHARGETONAMEEN(NUM,NB) | SUBROUTINE TO FIND OUT THE NAME OF AN ELEMENT FROM ITS CHARGE (Z) AND VICE VERSA (ENGLISH). |