December 5, 2014 1:38

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§0.1 [#1]

pack. Puts up to six integers (values up to 256) into the **character** variable a. "utils.f" $0.1 \equiv$ **@m** ARB 1 $@\mathbf{m} YES 0$ **@m** *NO* 1 $@\mathbf{m} \ \mathsf{ERR} \ -1$ @m BYTES_PER_INTEGER 4 **@m** *LEAST_BYTE* 1 $@\mathbf{m}\ END_OF_FILE\ -1$ $@m\ NO_OF_TYPES\ 20$ @m INT_BLOCK_SIZE 20 @m LAST_BLOCK 1 $@m\ NOT_LAST_BLOCK\ 0$ @m ERROR_OUTPUT_UNIT 6 @m MAX_BASIS_FUNCTIONS 255 **@m** *MAX_PRIMITIVES* 1000 **@m** *MAX_CENTRES* 50 @m MAX_ITERATIONS 60 @m UHF_CALCULATION 10 @m CLOSED_SHELL_CALCULATION 20 subroutine pack(a, i, j, k, l, m, n); **character***8 a, b;integer i, j, k, l, m, n; $\det b/$ """/; a = b: $a(1:1) = \mathbf{char}(i);$ $a(2:2) = \mathbf{char}(j);$ $a(3:3) = \mathbf{char}(k);$ $a(4:4) = \mathbf{char}(l);$ a(5:5) = char(m); $a(6:6) = \mathbf{char}(n);$ return; }

§0.2 [#2] 2

unpack. Extracts the six integers from the **character** variable a.

```
"utils.f" 0.2 \equiv subroutine unpack(a, i, j, k, l, m, n); character*8 a; integer i, j, k, l, m, n; { i = ichar(a(1:1)); j = ichar(a(2:2)); k = ichar(a(3:3)); l = ichar(a(4:4)); m = ichar(a(5:5)); n = ichar(a(6:6)); return; }
```

§1 [#3] putint 3

1 putint

```
put integral to file
"utils.f" 1 \equiv
    subroutine putint(nfile, i, j, k, l, mu, val, pointer, last);
    implicit double precision (a - h, o - z);
    integer nfile, i, j, k, l, mu, pointer, last;
     double precision val;
     double precision value(INT_BLOCK_SIZE);
     character*8 labels(INT_BLOCK_SIZE);
     data maxpointer/INT_BLOCK_SIZE/, id/0/;
    \mathbf{if} \ (\mathit{last} \equiv \mathtt{ERR})
       return;
     iend = NOT\_LAST\_BLOCK;
     if (pointer \equiv maxpointer)
       write(nfile) pointer, iend, labels, value;
       pointer = 0;
       }
     pointer = pointer + 1;
     call pack(labels(pointer), i, j, k, l, mu, id);
     value(pointer) = val;
    if (last \equiv YES)
       {
       iend = LAST\_BLOCK;
       last = ERR;
       write (nfile) pointer, iend, labels, value;
    return;
     }
```

 $\S2$ [#4] getint 4

2 getint

```
Hand out repulsion integrals one at a time
"utils.f" 2 \equiv
    integer function getint(file, i, j, k, l, mu, val, pointer);
    integer file, i, j, k, l, mu, pointer;
    double precision val;
    {
    save;
    integer maxpointer, id, iend;
    double precision zero;
    double precision value(INT_BLOCK_SIZE);
    character*8 labels(INT_BLOCK_SIZE);
    data maxpointer/0/, iend/NOT_LAST_BLOCK/, zero/0.0 \cdot 10^{00} D/;
      /* file must be rewound before first use of this function and pointer must be set to 0 */
    if (pointer \equiv maxpointer) /* pointer must be initialised to 0 */
      {
      if (iend \equiv LAST\_BLOCK)
        val = zero;
        i = 0;
        j = 0;
        k=0;
        l = 0;
        maxpointer = 0;
        iend = NOT_{-}LAST_{-}BLOCK;
        return (END_OF_FILE);
      read(file) maxpointer, iend, labels, value;
      pointer = 0;
      }
    pointer = pointer + 1;
    call unpack(labels(pointer), i, j, k, l, mu, id); /* id is unused */
    val = value(pointer);
    return (OK);
    }
```

§3 [#5] INDEX 5

3 INDEX

 $value: \underline{1}, \underline{2}.$

 $YES: \underline{0.1}, 1.$

zero: $\underline{2}$.

 $\begin{array}{ccc} a \colon & \underline{0.1}, \, \underline{0.2}. \\ ARB \colon & \underline{0.1}. \end{array}$

b: 0.1.

 $BYTES_PER_INTEGER: 0.1.$

char: 0.1.

 $CLOSED_SHELL_CALCULATION: 0.1.$

 $END_OF_FILE: 0.1, 2.$

ERR: 0.1, 1.

 $ERROR_OUTPUT_UNIT: 0.1.$

 $\quad \text{file:} \quad \underline{2}.$

getint: 2.

 $i: \ \underline{0.1}, \ \underline{0.2}, \ \underline{1}, \ \underline{2}.$

ichar: 0.2.

 $id\colon \ \underline{1},\,\underline{2}.$

 $iend: 1, \underline{2}.$

 INT_BLOCK_SIZE : 0.1, 1, 2.

j: 0.1, 0.2, 1, 2.

 $k: \quad \underline{0.1}, \, \underline{0.2}, \, \underline{1}, \, \underline{2}.$

 $l: \ \underline{0.1}, \ \underline{0.2}, \ \underline{1}, \ \underline{2}.$

labels: $\underline{1}, \underline{2}$.

 $last: \underline{1}.$

 $LAST_BLOCK: 0.1, 1, 2.$

 $LEAST_BYTE: 0.1$.

m: 0.1, 0.2.

 $MAX_BASIS_FUNCTIONS: \underline{0.1}.$

 $MAX_CENTRES$: 0.1.

 $MAX_ITERATIONS: 0.1.$

 $MAX_PRIMITIVES: 0.1.$

maxpointer: $\underline{1}, \underline{2}$.

 $mu: \underline{1}, \underline{2}.$

n: 0.1, 0.2.

 $nfile: \underline{1}.$

NO: 0.1.

 $NO_{-}OF_{-}TYPES: \underline{0.1}.$

 $NOT_{-}LAST_{-}BLOCK: \underline{0.1}, 1, 2.$

OK: 2.

pack: 0.1, 1.

pointer: 1, 2.

 $put int \colon \ \underline{1}.$

 $UHF_{-}CALCULATION: 0.1.$

unpack: 0.2, 2.

 $val: \underline{1}, \underline{2}.$

COMMAND LINE: "fweave utils.web".

WEB FILE: "utils.web". CHANGE FILE: (none).

GLOBAL LANGUAGE: RATFOR.