December 5, 2014
1:38

Contents

pack. Puts up to six integers (values up to 256) into the **character** variable a.

"utils.f" 0.1 ≡

```
@m ARB 1
@m YES 0
@m NO 1
@m ERR −1

@m BYTES_PER_INTEGER 4
@m LEAST_BYTE 1

@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;

  {
  data b/"␣␣␣␣␣␣␣␣"/;
  a = b;
  a(1 : 1) = char(i);
  a(2 : 2) = char(j);
  a(3 : 3) = char(k);
  a(4 : 4) = char(l);
  a(5 : 5) = char(m);
  a(6 : 6) = char(n);
  return;
  }
```

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

"utils.f" 0.2 ≡

```
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 putint

put integral to file

```
"utils.f" 1 ≡
    subroutine putint(nfile, i, j, k, l, mu, val, pointer, last);
    implicit double precision (a − h, o − z);
    save;
    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/;

    if (last ≡ ERR)
      return;
    iend = NOT_LAST_BLOCK;
    if (pointer ≡ 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 ≡ YES)

      {

      iend = LAST_BLOCK;
      last = ERR;
      write (nfile) pointer, iend, labels, value;

      }

    return;

    }
```

2 getint

Hand out repulsion integrals one at a time

```
"utils.f" 2 ≡
    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 · 10^00D/;

      /* file must be rewound before first use of this function and pointer must be set to 0 */

    if (pointer ≡ maxpointer)     /* pointer must be initialised to 0 */

      {

      if (iend ≡ 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 INDEX

COMMAND LINE: `"fweave utils.web"`.
WEB FILE: `"utils.web"`.
CHANGE FILE: `(none)`.
GLOBAL LANGUAGE: RATFOR.