

# Program Reference

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## Overview of libcint usage

### Preparing args

...

### Interface

#### C routine

```
dim = CINTgto_cart(bas_id, bas);
dim = CINTgto_spheric(bas_id, bas);
dim = CINTgto_spinor(bas_id, bas);
f1e(buf, shls, atm, natm, bas, nbas, env);
f2e(buf, shls, atm, natm, bas, nbas, env, opt);
f2e_optimizer(&opt, atm, natm, bas, nbas, env);
CINTdel_optimizer(&opt);
```

- buf: column-major double precision array.

- for 1e integrals of shells (i,j), data are stored as [i1j1 i2j1 ... ]
  - for 2e integrals of shells (i,j|k,l), data are stored as  
[i1j1k1l1 i2j1k1l1 ... i1j2k1l1 ... i1j1k2l1 ... ]
  - complex data are stored as two double elements, first is real, followed by imaginary, e.g. [Re Im Re Im ...]
  - shls: 0-based basis/shell indices.
    - int[2] for 1e integrals
    - int[4] for 2e integrals
  - atm: int[natm\*6], list of atoms. For ith atom, the 6 slots of atm[i] are
    - atm[i\*6+0] nuclear charge of atom i
    - atm[i\*6+1] env offset to save coordinates (env[atm[i\*6+1]], env[atm[i\*6+1]+1], env[atm[i\*6+1]+2]) are (x,y,z)
    - atm[i\*6+2] nuclear model of atom i, = 2 indicates gaussian nuclear model  $\rho(r) = Z(\frac{\zeta}{\pi})^{3/2} \exp(-\zeta r^2)$
    - atm[i\*6+3] env offset to save the nuclear charge distribution parameter  $\zeta$
    - atm[i\*6+4] unused
    - atm[i\*6+5] unused
  - natm: int, number of atoms, natm has no effect **except nuclear attraction** integrals
  - bas: int[nbas\*8], list of basis. For ith basis, the 8 slots of bas[i] are
    - bas[i\*8+0] 0-based index of corresponding atom
    - bas[i\*8+1] angular momentum
    - bas[i\*8+2] number of primitive GTO in basis i
    - bas[i\*8+3] number of contracted GTO in basis i
    - bas[i\*8+4] kappa for spinor GTO.
      - < 0 the basis ~ j = l + 1/2.
      - > 0 the basis ~ j = l - 1/2.
      - = 0 the basis includes both j = l + 1/2 and j = l - 1/2
    - bas[i\*8+5] env offset to save exponents of primitive GTOs. e.g. 10 exponents env[bas[i\*8+5]] ... env[bas[i\*8+5]+9]
    - bas[i\*8+6] env offset to save column-major contraction coefficients. e.g. 10 primitive -> 5 contraction needs a 10 × 5 array
- |                   |  |                    |  |     |  |                    |
|-------------------|--|--------------------|--|-----|--|--------------------|
| env[bas[i*8+6] ]  |  | env[bas[i*8+6]+10] |  |     |  | env[bas[i*8+6]+40] |
| env[bas[i*8+6]+1] |  | env[bas[i*8+6]+11] |  |     |  | env[bas[i*8+6]+41] |
| .                 |  | .                  |  | ... |  | .                  |
| .                 |  | .                  |  |     |  | .                  |
| env[bas[i*8+6]+9] |  | env[bas[i*8+6]+19] |  |     |  | env[bas[i*8+6]+49] |
- ‘bas[i\*8+7]’ unused
  - nbas: int, number of bases, nbas has no effect, can be set to 0
  - env: double[], save the value of coordinates, exponents, contraction coefficients
  - struct CINTOpt \*opt: so called “optimizer”, it needs to be initialized

```
CINTOpt *opt = NULL; intname_optimizer(&opt, atm, natm, bas, nbas,
env);
```

every integral type has its own optimizer with the suffix `_optimizer` in its name, e.g. the optimizer for `cint2e_sph` is `cint2e_sph_optimizer`. “optimizer” is an optional argument for the integrals. It can roughly speed the integration by 10% without affecting the value of integrals. If no optimizer is wanted, set it to `NULL`.

optimizer needs to be released after using.

```
CINTdel_optimizer(&opt);
```

- if the return value equals 0, every element of the integral is 0
- short example

```
#include "cint.h"
...
CINTOpt *opt = NULL;
cint2e_sph_optimizer(&opt, atm, natm, bas, nbas, env);
for (i = 0; i < nbas; i++) {
    shls[0] = i;
    di = CINTcgto_spheric(i, bas);
    ...
    for (l = 0; l < nbas; l++) {
        shls[3] = l;
        dl = CINTcgto_spheric(l, bas);
        buf = malloc(sizeof(double) * di * dj * dk * dl);
        cint2e_cart(buf, shls, atm, natm, bas, nbas, env, opt);
        free(buf);
    }
}
CINTdel_optimizer(&opt);
```

## Fortran routine

```
dim = CINTgto_cart(bas_id, bas)
dim = CINTgto_spheric(bas_id, bas)
dim = CINTgto_spinor(bas_id, bas)
call f1e(buf, shls, atm, natm, bas, nbas, env)
call f2e(buf, shls, atm, natm, bas, nbas, env, opt)
call f2e_optimizer(opt, atm, natm, bas, nbas, env)
call CINTdel_optimizer(opt)
```

- atm and bas are 2D integer array
  - atm(1:6,i) is the (charge, offset\_coord, nuclear\_model, unused, unused, unused) of the ith atom

- bas(1:8,i) is the (atom\_index, angular, num\_primitive\_GTO, num\_contract\_GTO, kappa, offset\_exponent, offset\_coeff, unused) of the ith basis

- parameters are the same to the C function. Note that those offsets atm(2,i) bas(6,i) bas(7,i) are 0-based.

- buf is 2D/4D double precision/double complex array

- opt: an integer(8) to hold the address of so called “optimizer”, it needs to be initialized by

```
integer(8) opt call f2e_optimizer(opt, atm, natm, bas, nbas, env)
```

The optimizer can be banned by setting the “optimizer” to 0\_8

```
call f2e(buf, atm, natm, bas, nbas, env, 0_8)
```

To release optimizer, execute

```
call CINTdel_optimizer(opt);
```

- short example

```
...
integer,external CINTcgto_spheric
integer(8) opt
call cint2e_sph_optimizer(opt, atm, natm, bas, nbas, env)
do i = 1, nbas
  shls(1) = i - 1
  di = CINTcgto_spheric(i-1, bas)
  ...
  do l = 1, nbas
    shls(4) = l - 1
    dl = CINTcgto_spheric(l-1, bas)
    allocate(buf(di,dj,dk,dl))
    call cint2e_sph(buf, shls, atm, natm, bas, nbas, env, opt)
    deallocate(buf)
  end do
end do
call CINTdel_optimizer(opt)
```

## Supported angular momentum

$$l_{max} = 6$$

## Data ordering

- for Cartesian GTO, the output data in buf are sorted as

s shell	p shell	d shell	...
...	...	...	
s	p $x$	d $xx$	
s	p $y$	d $xy$	
...	p $z$	d $xz$	
	p $x$	d $yy$	
	p $y$	d $yz$	
	p $z$	d $zz$	
	...	...	

- for real spheric GTO, the output data in buf are sorted as

s shell	p shell	d shell	f shell	...
...	...	...	...	
s	p $x$	d $xy$	f $y(3x^2 - y^2)$	
s	p $y$	d $yz$	f $xyz$	
...	p $z$	d $z^2$	f $yz^2$	
	p $x$	d $xz$	f $z^3$	
	p $y$	d $x^2 - y^2$	f $xz^2$	
	p $z$	...	f $z(x^2 - y^2)$	
	...		f $x(x^2 - 3y^2)$	
			...	

- for spinor GTO, the output data in buf correspond to

...	kappa=0,p shell	kappa=1,p shell	kappa=0,d shell	...
	...	...	...	
	$p_{1/2}(-1/2)$	$p_{1/2}(-1/2)$	$d_{3/2}(-3/2)$	
	$p_{1/2}(1/2)$	$p_{1/2}(1/2)$	$d_{3/2}(-1/2)$	
	$p_{3/2}(-3/2)$	$p_{1/2}(-1/2)$	$d_{3/2}(1/2)$	
	$p_{3/2}(-1/2)$	$p_{1/2}(1/2)$	$d_{3/2}(3/2)$	
	$p_{3/2}(1/2)$	$p_{1/2}(-1/2)$	$d_{5/2}(-5/2)$	
	$p_{3/2}(3/2)$	$p_{1/2}(1/2)$	$d_{5/2}(-3/2)$	
	$p_{1/2}(-1/2)$	...	$d_{5/2}(-1/2)$	
	$p_{1/2}(1/2)$		$d_{3/2}(-3/2)$	
	$p_{3/2}(-3/2)$		$d_{3/2}(-1/2)$	
	$p_{3/2}(-1/2)$		...	
	...			

## Tensor

Integrals like Gradients have more than one components. The output array is ordered in Fortran-contiguous. The tensors are ordered as

- 3-component tensor
  - X buf(:,0)
  - Y buf(:,1)
  - Z buf(:,2)
- 9-component tensor
  - XX buf(:,0)
  - XY buf(:,1)
  - XZ buf(:,2)
  - YX buf(:,3)
  - YY buf(:,4)
  - YZ buf(:,5)
  - ZX buf(:,6)
  - ZY buf(:,7)
  - ZZ buf(:,8)

## Built-in function list

- Cartesian GTO integrals
  - CINTcgto\_cart(int shell\_id, int bas[]): Number of cartesian functions of the given shell
  - cint1e\_ovlp\_cart
 
$$\langle i|j \rangle$$
  - cint1e\_nuc\_cart
 
$$\langle i|V_{nuc}|j \rangle$$
  - cint1e\_kin\_cart
 
$$.5\langle i|\vec{p} \cdot \vec{p}|j \rangle$$
  - cint1e\_ia01p\_cart
 
$$\langle i|\frac{\vec{r}}{r^3} \times \vec{\nabla}|j \rangle$$
  - cint1e\_irixp\_cart
 
$$\langle i|(\vec{r} - \vec{R}_i) \times \vec{\nabla}|j \rangle$$
  - cint1e\_ircxp\_cart
 
$$\langle i|(\vec{r} - \vec{R}_o) \times \vec{\nabla}|j \rangle$$
  - cint1e\_iking\_cart
 
$$0.5i\langle \vec{p} \cdot \vec{p}|U_g j \rangle$$
  - cint1e\_iovlp\_cart
 
$$i\langle i|U_g j \rangle$$
  - cint1e\_inucg\_cart
 
$$i\langle i|V_{nuc}|U_g j \rangle$$
  - cint1e\_ipovlp\_cart
 
$$\langle \vec{\nabla}_i|j \rangle$$

- cint1e_ipkin_cart	$0.5\langle\vec{\nabla}i \vec{p}\cdot\vec{p}j\rangle$
- cint1e_ipnuc_cart	$\langle\vec{\nabla}i V_{nuc} j\rangle$
- cint1e_iprinv_cart	$\langle\vec{\nabla}i r^{-1} j\rangle$
- cint1e_rinv_cart	$\langle i r^{-1} j\rangle$
- cint2e_cart	$(ij kl)$
- cint2e_ig1_cart	$i(iU_gj kl)$
- cint2e_ip1_cart	$(\vec{\nabla}ij kl)$
• Spheric GTO integrals	
- CINTcgto_spheric(int shell_id, int bas[]):	Number of spheric functions of the given shell
- cint1e_ovlp_sph	$\langle i j\rangle$
- cint1e_nuc_sph	$\langle i V_{nuc} j\rangle$
- cint1e_kin_sph	$0.5\langle i \vec{p}\cdot\vec{p}j\rangle$
- cint1e_ia01p_sph	$\langle i \frac{\vec{r}}{r^3} \times\vec{\nabla}j\rangle$
- cint1e_irixp_sph	$\langle i (\vec{r}_c - \vec{R}_i)\times\vec{\nabla}j\rangle$
- cint1e_ircxp_sph	$\langle i (\vec{r}_c - \vec{R}_o)\times\vec{\nabla}j\rangle$
- cint1e_iking_sph	$0.5i\langle\vec{p}\cdot\vec{p}i U_gj\rangle$
- cint1e_iovlp_sph	$i\langle i U_gj\rangle$
- cint1e_inucg_sph	$i\langle i V_{nuc} U_gj\rangle$
- cint1e_ipovlp_sph	$\langle\vec{\nabla}i j\rangle$

- cint1e_ipkin_sph	$0.5\langle\vec{\nabla}i \vec{p}\cdot pj\rangle$
- cint1e_ipnuc_sph	$\langle\vec{\nabla}i V_{nuc} j\rangle$
- cint1e_iprinv_sph	$\langle\vec{\nabla}i r^{-1} j\rangle$
- cint1e_rinv_sph	$\langle i r^{-1} j\rangle$
- cint2e_sph	$(ij kl)$
- cint2e_ig1_sph	$i(iU_gj kl)$
- cint2e_ip1_sph	$(\vec{\nabla}ij kl)$
• Spinor GTO integrals	
- CINTcgto_spinor(int shell_id, int bas[]):	Number of spinor functions of the given shell
- cint1e_ovlp	$\langle i j\rangle$
- cint1e_nuc	$\langle i V_{nuc} j\rangle$
- cint1e_nucg	$\langle i V_{nuc} U_gj\rangle$
- cint1e_srsr	$\langle\vec{\sigma}\cdot\vec{r}i \vec{\sigma}\cdot\vec{r}j\rangle$
- cint1e_sr	$\langle\vec{\sigma}\cdot\vec{r}i j\rangle$
- cint1e_srsp	$\langle\vec{\sigma}\cdot\vec{r}i \vec{\sigma}\cdot\vec{p}j\rangle$
- cint1e_spsp	$\langle\vec{\sigma}\cdot\vec{p}i \vec{\sigma}\cdot\vec{p}j\rangle$
- cint1e_sp	$\langle\vec{\sigma}\cdot\vec{p}i j\rangle$
- cint1e_spspsp	$\langle\vec{\sigma}\cdot\vec{p}i \vec{\sigma}\cdot\vec{p}\vec{\sigma}\cdot\vec{p}j\rangle$
- cint1e_spnuc	$\langle\vec{\sigma}\cdot\vec{p}i V_{nuc} j\rangle$

– cint1e_spnucsp	$\langle \vec{\sigma} \cdot \vec{p}i   V_{nuc}   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint1e_srnucsr	$\langle \vec{\sigma} \cdot \vec{r}i   V_{nuc}   \vec{\sigma} \cdot \vec{r}j \rangle$
– cint1e_sa10sa01	$0.5 \langle \vec{\sigma} \times \vec{r}_c i   \vec{\sigma} \times \frac{\vec{r}}{r^3}   j \rangle$
– cint1e_ovlpg	$\langle i   U_g j \rangle$
– cint1e_sa10sp	$0.5 \langle \vec{r}_c \times \vec{\sigma} i   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint1e_sa10nucsp	$0.5 \langle \vec{r}_c \times \vec{\sigma} i   V_{nuc}   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint1e_sa01sp	$\langle i   \frac{\vec{r}}{r^3} \times \vec{\sigma}   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint1e_spgsp	$\langle U_g \vec{\sigma} \cdot \vec{p}i   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint1e_spgnucsp	$\langle U_g \vec{\sigma} \cdot \vec{p}i   V_{nuc}   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint1e_spgsa01	$\langle U_g \vec{\sigma} \cdot \vec{p}i   \frac{\vec{r}}{r^3} \times \vec{\sigma}   j \rangle$
– cint1e_ipovlp	$\langle \vec{\nabla} i   j \rangle$
– cint1e_ipkin	$0.5 \langle \vec{\nabla} i   p \cdot p j \rangle$
– cint1e_ipnuc	$\langle \vec{\nabla} i   V_{nuc}   j \rangle$
– cint1e_iprinv	$\langle \vec{\nabla} i   r^{-1}   j \rangle$
– cint1e_ipspnucsp	$\langle \vec{\nabla} \vec{\sigma} \cdot \vec{p}i   V_{nuc}   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint1e_ipsprinvsp	$\langle \vec{\nabla} \vec{\sigma} \cdot \vec{p}i   r^{-1}   \vec{\sigma} \cdot \vec{p}j \rangle$
– cint2e	$(ij kl)$

- cint2e\_spsp1  $(\vec{\sigma} \cdot \vec{p}i\vec{\sigma} \cdot \vec{p}j|kl)$   
 - cint2e\_spsp1spsp2  $(\vec{\sigma} \cdot \vec{p}i\vec{\sigma} \cdot \vec{p}j|\vec{\sigma} \cdot \vec{p}k\vec{\sigma} \cdot \vec{p}l)$   
 - cint2e\_srsr1  $(\vec{\sigma} \cdot \vec{r}i\vec{\sigma} \cdot \vec{r}j|kl)$   
 - cint2e\_srsr1srsr2  $(\vec{\sigma} \cdot \vec{r}i\vec{\sigma} \cdot \vec{r}j|\vec{\sigma} \cdot \vec{r}k\vec{\sigma} \cdot \vec{r}l)$   
 - cint2e\_sa10sp1  $0.5(\vec{r}_c \times \vec{\sigma}i\vec{\sigma} \cdot \vec{p}j|kl)$   
 - cint2e\_sa10sp1spsp2  $0.5(\vec{r}_c \times \vec{\sigma}i\vec{\sigma} \cdot \vec{p}j|\vec{\sigma} \cdot \vec{p}k\vec{\sigma} \cdot \vec{p}l)$   
 - cint2e\_g1  $(iU_{gj}|kl)$   
 - cint2e\_spgsp1  $(\vec{\sigma} \cdot \vec{p}iU_g\vec{\sigma} \cdot \vec{p}j|kl)$   
 - cint2e\_g1spsp2  $(iU_{gj}|\vec{\sigma} \cdot \vec{p}k\vec{\sigma} \cdot \vec{p}l)$   
 - cint2e\_spgsp1spsp2  $(\vec{\sigma} \cdot \vec{p}iU_g\vec{\sigma} \cdot \vec{p}j|\vec{\sigma} \cdot \vec{p}k\vec{\sigma} \cdot \vec{p}l)$   
 - cint2e\_ip1  $(\vec{\nabla}ij|kl)$   
 - cint2e\_ipspsp1  $(\vec{\nabla}\vec{\sigma} \cdot \vec{p}i\vec{\sigma} \cdot \vec{p}j|kl)$   
 - cint2e\_ip1spsp2  $(\vec{\nabla}ij|\vec{\sigma} \cdot \vec{p}k\vec{\sigma} \cdot \vec{p}l)$   
 - cint2e\_ipspsp1spsp2  $(\vec{\nabla}\vec{\sigma} \cdot \vec{p}i\vec{\sigma} \cdot \vec{p}j|\vec{\sigma} \cdot \vec{p}k\vec{\sigma} \cdot \vec{p}l)$   
 - cint2e\_ssp1ssp2  $(i\vec{\sigma}\vec{\sigma} \cdot \vec{p}j|k\vec{\sigma}\vec{\sigma} \cdot \vec{p}l)$