Program Reference

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Overview of libcint usage

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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 ζ
  - `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 intialized

  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_opimizer. "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);
```

In libcint-3 or above, new integral function signature are provided.

```
int1e_xxx(buf, dims, shls, atm, natm, bas, nbas, env, opt, cache);
int2e_xxx(buf, dims, shls, atm, natm, bas, nbas, env, opt, cache);
```

In the new function signature, the shape of output buffer (in column-major order) can be specified. It's the second argument `dims`. Integrals can be written to the sub-block or the output buffer according to the information of `dims`. Another change is the runtime `cache` for integral intermediates, which comes as the last arguments of the new signature. If `cache` is specified, all integral intermediates will be put in the `cache`. The library will not use extra main memory during computatin. The size of cache can be determined by the function if the first argument is set to `NULL`

```
int cache_size = int1e_xxx(NULL, dims, shls, atm, natm, bas, nbas, env, opt, NULL);
```

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 intialized by

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

The optimizier can be banned by setting the "optimizier" 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 tensor component takes the biggest strides.

- 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`
  $$0.5i\langle\vec{p}\cdot\vec{p}i|U_gj\rangle$$
  - `cint1e_iovlpg_cart`
  $$i\langle i|U_gj\rangle$$
  - `cint1e_inucg_cart`
  $$i\langle i|V_{nuc}|U_gj\rangle$$
  - `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
$$i(iU_g j|kl)$$
- 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
$$0.5\langle i|\vec{p}\cdot pj\rangle$$
  - 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
$$0.5i\langle \vec{p}\cdot \vec{p}i|U_g j\rangle$$
  - cint1e_iovlpg_sph
$$i\langle i|U_g j\rangle$$
  - cint1e_inucg_sph
$$i\langle i|V_{nuc}|U_g j\rangle$$
  - 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
$$i(iU_g j|kl)$$
- 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
$$\langle i|V_{nuc}|U_g j\rangle$$
  - 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
$$0.5\langle\vec{\nabla}i|p\cdot pj\rangle$$
- 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

$$(i U_g j | kl)$$

- cint2e_spgsp1

$$(\vec{\sigma} \cdot \vec{p} i U_g \vec{\sigma} \cdot \vec{p} j | kl)$$

- cint2e_g1spsp2

$$(i U_g j | \vec{\sigma} \cdot \vec{p} k \vec{\sigma} \cdot \vec{p} l)$$

- cint2e_spgsp1spsp2

$$(\vec{\sigma} \cdot \vec{p} i U_g \vec{\sigma} \cdot \vec{p} j | \vec{\sigma} \cdot \vec{p} k \vec{\sigma} \cdot \vec{p} l)$$

- cint2e_ip1

$$(\vec{\nabla} i j | kl)$$

- cint2e_ipspsp1

$$(\vec{\nabla} \vec{\sigma} \cdot \vec{p} i \vec{\sigma} \cdot \vec{p} j | kl)$$

- cint2e_ip1spsp2

$$(\vec{\nabla} i j | \vec{\sigma} \cdot \vec{p} k \vec{\sigma} \cdot \vec{p} l)$$

- 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

$$(i \vec{\sigma} \vec{\sigma} \cdot \vec{p} j | k \vec{\sigma} \vec{\sigma} \cdot \vec{p} l)$$