Program Reference

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Contents

Overview of libcint usage

Preparing args

...

Interface

C routine

```
f(buf, shls, atm, natm, bas, nbas, env);
```

- 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
  - `atm[i*6+3]` unused
  - `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 $\sim$ j = l + 1/2.
    > 0 the basis $\sim$ 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
- env: double[], save the value of coordinates, exponents, contraction coefficients

Fortran routine

```
call f(buf, shls, atm, natm, bas, nbas, env)
```

- 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

Supported angular momentum

- 1e integrals $l_{max} = 6$
- 2e integrals $l_{max} = 4$

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 y	d xy	f $y(3x^2-y^2)$	
s	p z	d yz	f xyz	
...	p x	d z^2	f yz^2	
	p y	d xz	f z^3	
	p z	d x^2-y^2	f xz^2	
	p x	...	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 tensor components. the output data is

- 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)`

function list

- Cartesian GTO integrals
  - `cgto_cart(int ishell, 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`
  $$0.5i\langle\vec{p}\cdot\vec{p}i|U_g j\rangle$$
  - `cint1e_iovlpg_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`

$$i(iU_g j|kl)$$

- `cint2e_ip1_cart`

$$(\vec{\nabla} ij|kl)$$

- Spheric GTO integrals
  - `cgto_spheric(int ishell, 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`

$$i(iU_gj|kl)$$

- `cint2e_ip1_sph`

$$(\vec{\nabla}ij|kl)$$

• Spinor GTO integrals

- `cgto_spinor(int ishell, 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

$$0.5\langle\vec{\nabla}i|p\cdot pj\rangle$$

- 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

$$(iU_gj|kl)$$

– 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

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