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# Overview

GElib is a C++/CUDA library implementing various operations related to the representation theory of SO(3) and certain other groups. The primary purpose of GElib is to serve as a backend for building group equivariant neural networks that can take advantage of GPU architectures. The library is built on top of the Cnine tensor library, https://github.com/risi-kondor/cnine.

GElib is under continuous development. Some features described in this document may not be fully implemented yet. GElib is authored by Risi Kondor and Erik H Thiede and released under the Mozilla Public License, version 2.0, https://www.mozilla.org/en-US/MPL/2.0/.

# Installation

GElib is mostly a header library, and does not need to be installed in a specific location on your system. However, if the library is to be used with GPU functionality, certain CUDA object files do have to be separately compiled. This is done by running make all in the cuda directory.

GElib is an extension of the Cnine library, which must be separately pulled from https://github.com/risi-kondor/cnine. Please refer to the Cnine documentation for the description of the basic scalar and tensor classes used in GElib. The only other dependencies of GElib are:

- An appropriate C++11 compiler together with the STL standard template library.
- CUDA and CUBLAS if the library is to be used with GPU functionality.

## Compilation options

Before attempting to compile the CUDA objects or compile your own code against GElib, please copy options\_template.txt to a file named options.txt, and set the following compilation parameters defined within.

Variable	Default value	Description
CC	clang	Name of C++ compiler.
CNINE_ROOT	\$(ROOTDIR)//cnine/	Root directory of the cnine installation.
WITH_CUDA	t	If this variable is defined, the library will link to CUDA. If not
		defined, GPU functionality is disabled.
CUDA_DIR	/usr/local/cuda	Root directory of the CUDA installation on your system.
NVCC	nvcc	Name of CUDA compiler.
NVCCFLAGS	omitted	Various flags to be passed to the NVCC compiler.
WITH_CUBLAS	t	If this variable is defined, the library will link to CUBLAS for
		low level linear algebra functionality on the GPU.

## Usage

To call GElib from your own code C++ code you must do the following:

- #include the relevant header files in your soure files.
- #include the file include/GElib\_base.cpp in your top level source file (the one that contains your main function).
- Define a GElibSession object before calling any Cnine or Cnine objects or functions.
- Link in the appropriate CUDA object files from the cuda directory, as required.

# Reference

<b>E</b> I	This function produces a temporary that is assignable and therefore may be used as an lvalue.

NBU	Bundle dimension. If bundling is off, should be set to $-1$ .
DEVICE	device object specifying the device on which a given variable is initialized or moved to.
	Currently the two possible values are deviceid::CPU and deviceid::GPU0 or 0 and 1.

expr. template	shorthand	description
Conjugate <obj></obj>	conj(x)	The conjugate of x.
Transpose <obj></obj>	transp(x)	The transpose of x.
Hermitian <obj></obj>	herm(x)	The Hermitian conjugate (conjugate transpose) of x.

# SO(3) classes

# S03element

An SO3element object represents a rotation  $R \in SO(3)$ .

## **CONSTRUCTORS**

S03element(double phi, double theta, double psi) The rotation parametrized by Euler angles  $(\phi, \theta, \psi)$ . S03element(fill::uniform) A rotation chosen at random from (uniformly w.r.t. Haar measure on SO(3)).

# S03type

An SO3type object defines the type  $\tau = (\tau_0, \tau_1, \dots, \tau_L)$  of an SO(3)-vector.

Derived from: vector<int>

 $N_1$ 

## **CONSTRUCTORS**

```
S03type(int L) A new type vector \boldsymbol{\tau} = (\tau_0, \tau_1, \dots, \tau_L), where each \tau_\ell is initialized to zero. S03type(initializer_list<int> list) Initialize \boldsymbol{\tau} from list.
```

## MEMBER ACCESS

```
\begin{array}{c} \text{int getL() const} \\ \text{int maxl() const} \\ \text{Return } L. \\ \\ \text{int operator(int 1) const} \\ \text{Return } \tau_{\ell}. \end{array}
```

## **RELATED FUNCTIONS**

```
S03type S03type::CGproduct(S03type& tau1, S03type& tau2) S03type S03type::CGproductroduct(S03type& tau1, S03type& tau2, int maxL) Return the type of \mathbf{v}_1 \otimes \mathbf{v}_2, when \mathbf{v}_1 is of type \tau_1 and \mathbf{v}_2 is of type \tau_2. In the second form of the function, the result is band limited to \ell_{\max}
```

## S03part

An SO3part object stores a single isotypic part  $P = P^{\ell}$  of an SO(3)-vector.

Implemented by: SO3partA (derived from cnine::CtensorA)

## **CONSTRUCTORS**

```
S03part(int 1, int n, [NBU], [FILLTYPE], [DEVICE])
A new S03part object for the \ell'th isotypic consisting of n fragments. FILLTYPE can be cnine::fill::raw (default), cnine::fill::zero or cnine::fill::gaussian.
```

SO3part(int 1, int n, [NBU], std::function<complex<float>(const int i, const int m)> fn) A new SO3part object for the  $\ell$ 'th isotypic consisting of n fragments. The entries of P are computed by the function fn.

## STATIC CONSTRUCTORS

```
S03part S03part::zero(int 1, int n, [NBU], [DEVICE])
S03part S03part::ones(int 1, int n, [NBU], [DEVICE])
S03part S03part::gaussian(int 1, int n, [NBU], [DEVICE])
A new S03part with the given fill pattern.
```

## **VARIANT CONSTRUCTORS**

```
SO3part(const SO3part& P, const device& dev)
Create a copy of P on device dev.
SO3part(const SO3part& P, const cnine::view)
Create a view of P.
```

## MEMBER ACCESS

```
int getl() const
    Return the irrep index \ell.
int getn() const
    Return n, the number of irreducible fragments.
int get_nbu() const
    Return the bundle dimension. If bundling is off, returns -1.
int get_dev() const
    Return the device that this SO3part is stored on.
Cscalar get(int i, int m) const
SO3part& set(int i, int m, const Cscalar& x)
    Return [P_i]_m or set [P_i]_m = x (note that -\ell \le m \le \ell).
complex<float> get_value(int i, int m) const
SO3part& set_value(int i, int m, complex<float> x)
    Return the value of [P_i]_m or set [P_i]_m = x (note that -\ell \le m \le \ell).
operator()(const int i, const int m) 🖘
    Return a temporary for [P_i]_m (note that -\ell \leq m \leq \ell).
fragment(int i) const 🖘
    Return a temporary for the i'th fragment of P.
fragments(int i, int n=1) const [1]
    Return a temporary for the chunk of P consisting of fragments (i, \ldots, i+n-1).
S03part apply(std::function<complex<float>(complex<float> x)> fn)
SO3part apply(std::function<complex<float>(const int i, const int m, complex<float> x)> fn)
    Return the SO3part derived by applying the function fn to each element of P.
ARITHMETIC
c*P
                                                              (complex<float>,SO3part) -> SO3part
c*P
```

```
(cscalar,S03part) -> S03part
P*c
                                                            (SO3part,complex<float>) -> SO3part
P*c
P/c
                                                                    (SO3part,cscalar) -> SO3part
P/c
    Multiply/divide P by the scalar c.
P1+P2
                                                                    (SO3part, SO3part) -> SO3part
P1-P2
                                                                    (SO3part,SO3part) -> SO3part
    Compute P_1 + P_2 resp. P_1 - P_2. The parts must have the same \ell and the same number of fragments.
                                                                    (Ctensor, SO3part) -> SO3part
M*P
    Multiply P by the matrix M.
```

## **IN-PLACE OPERATIONS**

```
+=P2 (S03part,S03part) -> S03part 
-=P2 (S03part,S03part) -> S03part 
Increment/decrement P by P_2.
```

## MEMBER FUNCTIONS

```
SO3part rotate(const SO3element& R) const Rotate P by the rotation R \in SO(3).
```

## **CG-PRODUCTS**

```
CGproduct(P1,P2,1) (SO3part,SO3part,int) -> SO3part Return the \ell'th component of the Clebsch–Gordan product, [P_1 \otimes_{cq} P_2]_{\ell}.
```

## OTHER FUNCTIONS

```
norm2(P) S03part -> Cscalar The squared Frobenius norm \|P\|_{\text{Frob}}^2. inp(P1,P2) (S03part,S03part) -> Cscalar The inner product \langle P_1,P_2\rangle.
```

## 1/0

```
string str(const indent="") const
Print P to string with the optional indentation indent.
```

## S03vec

An SO3vec object stores an SO(3)-covariant vector  $\mathbf{v}$  in "Fourier form", i.e., as a collection of isotypic parts  $(P^0, P^1, \dots, P^L)$ .

## **CONSTRUCTORS**

```
S03vec(const S03part& P0, ..., const S03part& PL) A new SO(3)-vector consisting of parts P^0, P^1, \ldots, P^L. S03vec(const S03type& tau, [NBU], [FILLTYPE], [FORMAT], [DEVICE]) A new S03vec object of type \tau. FILLTYPE may be fill::raw (default), fill::zero or fill::gaussian. FORMAT may be S03vec_format::parts (default), or S03vec_format::compact.
```

## STATIC CONSTRUCTORS

```
S03vec S03vec::zero(const S03type& tau, [NBU], [FORMAT], [DEVICE]) S03vec S03vec::ones(const S03type& tau, [NBU], [FORMAT], [DEVICE]) S03vec S03vec::gaussian(const S03type& tau, [NBU], [FORMAT], [DEVICE]) A new S03vec of type \tau initialized with the given fill pattern.
```

## VARIANT CONSTRUCTORS

```
S03part(const S03vec& v, const device& dev)
   Create a copy of v on device dev.
S03part(const S03vec& v, const S03vec_format& format)
   Create a copy of v with format format.
S03part(const S03vec& v, const cnine::view)
   Create a view of v.
```

## MEMBER ACCESS

#### **ARITHMETIC**

```
(cscalar, S03vec) -> S03vec
                                                                     (complex<float>,S03vec) -> S03vec
C*V
                                                                              (SO3vec,cscalar) -> SO3vec
v*c
                                                                     (SO3vec,complex<float>) -> SO3vec
V*C
                                                                              (SO3vec,cscalar) -> SO3vec
v/c
v/c
                                                                     (SO3vec,complex<float>) -> SO3vec
    Multiply/divide \mathbf{v} by the complex scalar c.
                                                                               (SO3vec,SO3vec) -> SO3vec
11+77
                                                                               (SO3vec, SO3vec) -> SO3vec
u-v
    Compute \mathbf{u} + \mathbf{v} resp \mathbf{u} - \mathbf{v}. The two vectors \mathbf{u} and \mathbf{v} must be of the same type.
                                                                         (CtensorPack,SO3vec) -> SO3vec
    Multiply v by the sequence of matrices stored in the CtensorPack W.
```

## **IN-PLACE OPERATIONS**

```
+=u (S03vec,S03vec) -> S03vec

-=u (S03vec,S03vec) -> S03vec

Increment/decrement v by u.
```

## MEMBER FUNCTIONS

```
S03vec rotate(const S03element& R) const Rotate {\bf v} by the rotation R\in {\rm SO}(3).
```

## OTHER FUNCTIONS

## **CG-PRODUCTS**

 $\begin{array}{ll} \texttt{CGproduct(u,v,[lmax])} & \texttt{(SO3vec,SO3vec,int)} \to \texttt{SO3vec} \\ \texttt{Compute the Clebsch-Gordan product } \mathbf{u} \otimes_{cg} \mathbf{v} \text{ up to } \ell = \ell_{\max}. \end{array}$ 

## I/O

string str(const indent="") const

Print v to string with the optional indentation indent.

## SO3partArray

An SO3partArray [P] is an array of SO3part objects.

Implemented by: SO3partArrayA (derived from cnine::CtensorArrayA)

## **CONSTRUCTORS**

## STATIC CONSTRUCTORS

```
SO3partArray SO3partArray::zero(const Gdims& adims, int 1, int n, [NBU], [DEVICE])
SO3partArray SO3partArray::ones(const Gdims& adims, int 1, int n, [NBU], [DEVICE])
SO3partArray SO3partArray::gaussian(const Gdims& adims, int 1, int n, [NBU], [DEVICE])
Create a new SO3partArray of array dimensions adims using the approriate fill pattern.
```

#### VARIANT CONSTRUCTORS

SO3partArray(const SO3partArray& V, const device& dev) Create a copy of  $\llbracket P \rrbracket$  on device dev.

#### **RESHAPING**

SO3partArray shape(const Gdims& dims) const

Return a copy of the SO3partArray reshaped to dimensions dims.

SO3partArray& reshape(const Gdims& dims)

Change the shape of the array to dims. The total number of cells must be preserved.

SO3partArray as\_shape(const Gdims& dims) const

Return a temporary that reinterprets the shape of the array as dims.

## MEMBER ACCESS

reshape(const Gdims& adims)

Reinterpret [P] as an array of dimensions adims.

```
int getl() const
    Return the irrep index \ell.
int getn() const
    Return \tau_{\ell}, the number of irreducible fragments in this part.
int get_nbu() const
    Return the bundle dimension. If bundling is off, returns -1.
int get_dev() const
    Return the device that this SO3partArray is stored on.
Gdims get_adims()
    Return the array dimensions.
SO3part get_cell(int i1,...,int ik) const
    Return the cell [P](i_1,\ldots,i_k).
CtensorArray& set_cell(int i1,...,int ik, const SO3part& A)
    Set [P](i_1,...,i_k) = A.
SO3part get_cell(Gindex& aix) const
    Return the cell [P](i_1,\ldots,i_k).
CtensorArray& set_cell(Gindex& aix, const SO3part& A)
    Set [P](i_1, ..., i_k) = A.
SO3part cell(const Gindex& aix) 🖘
    Return a temporary SO3part capturing cell aix.
ARRAY OPERATIONS
SO3partArray broaden(int ix, int n) const
    Create a d+1 dimensional array by stacking n copies of [P] along dimension ix.
SO3partArray reduce(int ix) const
    Create a d-1 dimensional array by summing out dimension ix.
SO3part reduce() const
    Reduce [P] by summing all entries into a single SO3part.
```

#### CELL-BY-CELL ARITHMETIC

## **BROADCAST ARITHMETIC**

```
P*=c
                                                         (SO3partArray, Cscalar) -> SO3partArray
P*=c
                                                 (SO3partArray,complex<float>) -> SO3partArray
P/=c
                                                         (SO3partArray, Cscalar) -> SO3partArray
P/=c
                                                 (SO3partArray,complex<float>) -> SO3partArray
    Multiply/divide [P] by the scalar c in-place.
                                                         (Cscalar, SO3partArray) -> SO3partArray
c*P
c*P
                                                 (complex<float>,SO3partArray) -> SO3partArray
                                                         (SO3partArray, Cscalar) -> SO3partArray
P*c
P*c
                                                 (SO3partArray,complex<float>) -> SO3partArray
P/c
                                                         (SO3partArray, Cscalar) -> SO3partArray
                                                 (SO3partArray,complex<float>) -> SO3partArray
P/c
    Multiply/divide [P] by the scalar c.
P1+P2
                                                         (SO3part,SO3partArray) -> SO3partArray
P1+P2
                                                         (SO3partArray,SO3part) -> SO3partArray
                                                         (SO3part,SO3partArray) -> SO3partArray
P1-P2
P1-P2
                                                         (SO3partArray, SO3part) -> SO3partArray
    Compute P_1 + [P_2], [P_1] + P_2, P_1 - [P_2] or [P_1] - P_2.
                                                         (Ctensor, SO3partArray) -> SO3partArray
M*P
    Multiply each cell of \llbracket P \rrbracket by the matrix M.
```

#### SCATTERING ARITHMETIC

## MEMBER FUNCTIONS

SO3partArray rotate(const SO3element& R) const Rotate each cell by  $R \in SO(3)$ .

## OTHER FUNCTIONS

```
norm2(P) S03partArray -> Ctensor The tensor of squared Frobenius norms \|P\|_{\text{Frob}}^2. inp(P1,P2) (S03partArray,S03partArray) -> Ctensor The tensor of inner products \langle P_1, P_2 \rangle.
```

## **CG-PRODUCTS**

```
(SO3partArray,SO3partArray,int) -> SO3partArray
CGproduct(P1,P2,1)
    Compute the \ell'th component of the Clebsch–Gordan product, [P_1 \otimes_{cq} P_2]_{\ell}, cell-by-cell.
                                                     (SO3part,SO3partArray,int) -> SO3partArray
CGproduct(P1,P2,1)
                                                    (SO3partArray,SO3part,int) -> SO3partArray
CGproduct(P1,P2,1)
    Compute the \ell'th component of the Clebsch-Gordan product by broadcasting P_1 resp. P_2.
                                               (SO3partArray,SO3partArray,int) -> SO3partArray
outerprod<CGproduct>(P1,P2,1)
                                               (SO3partArray,SO3partArray,int) -> SO3partArray
matrixprod<CGproduct>(P1,P2,1)
convolution<CGproduct>(P1,P2,1)
                                               (SO3partArray, SO3partArray, int) -> SO3partArray
    Compute the outer product [P_1] and [P_2], matrix-like product, or convolution, where the elementary
    products are Clebsch–Gordan products.
```

## I/O

```
string str(const indent="") const
```

Print P to string with the optional indentation indent.

# S03vecArray

An SO3vecArray  $\llbracket V \rrbracket$  is an array of SO3vec objects.

Derived from: cnine::ArrayPack<SO3partArray>

## **CONSTRUCTORS**

SO3vecArray(const Gdims& adims, const SO3type& tau, [NBU], [FILLTYPE], [DEVICE])

Create an arrray of SO3vec objects. The array dimensions are specified in adims. FILLTYPE can be fill::raw (default), fill::zero or fill::gaussian.

SO3vecArray(const Gdims& adims, const SO3vec& v, [DEVICE]) Create an SO3vecArray in which each cell is a copy of v.

## STATIC CONSTRUCTORS

SO3vecArray SO3vecArray::zero(const Gdims& adims, const SO3type& tau, [NBU], [DEVICE]) SO3vecArray SO3vecArray::ones(const Gdims& adims, const SO3type& tau, [NBU], [DEVICE]) SO3vecArray SO3vecArray::gaussian(const Gdims& adims, const SO3type& tau, [NBU], [DEVICE]) Create a new SO3vecArray on device DEVICE.

## VARIANT CONSTRUCTORS

S03vecArray(const S03vecArray& P, const device& dev) Create a copy of  $[\![V]\!]$  on device dev.

## MEMBER ACCESS

Return L, the highest  $\ell$  index.

int getL() const

```
SO3type get_tau() const
    Return \tau, the type of \mathbf{v}.
int get_nbu() const
    Return the bundle dimension. If bundling is off, returns -1.
int get_dev() const
    Return the device that this SO3vecArray is stored on.
Gdims get_adims()
    Return the array dimensions.
SO3vec get_cell(int i1,...,int ik) const
    Return the cell [V](i_1,\ldots,i_k).
CtensorArray& set_cell(int i1,...,int ik, const SO3vec& A)
    Set [V](i_1,...,i_k) = A.
SO3vec get_cell(Gindex& aix) const
    Return the cell [V](i_1,\ldots,i_k).
CtensorArray& set_cell(Gindex& aix, const SO3vec& A)
    Set [V](i_1, ..., i_k) = A.
SO3vec cell(const Gindex& aix) [1]
    Return a temporary SO3vec capturing cell aix.
SO3partArray get_part(int 1)
SO3vec& set_part(int, 1, const SO3partArray& P)
    Get/set the array of \ell'th isotypic parts.
SO3partArray get(int 1) 🖘
    Return a temporary to the array of \ell'th isotypic parts.
ARRAY OPERATIONS
SO3vecArray broaden(int ix, int n) const
    Create a d+1 dimensional array by stacking n copies of \llbracket V \rrbracket along dimension ix.
SO3vecArray reduce(int ix) const
    Create a d-1 dimensional array by summing out dimension ix.
SO3vec reduce() const
    Reduce \llbracket V \rrbracket by summing all entries into a single S03vec.
reshape(const Gdims& adims)
    Reinterpret \llbracket V \rrbracket as an array of dimensions adims.
```

## **CELL-BY-CELL ARITHMETIC**

## **BROADCASTING ARITHMETIC**

```
(Cscalar,SO3vecArray) -> SO3vecArray
c*V
                                                     (complex<float>,S03vecArray) -> S03vecArray
V*c
                                                             (SO3vecArray, Cscalar) -> SO3vecArray
V*c
                                                     (SO3vecArray,complex<float>) -> SO3vecArray
V/c
                                                             (SO3vecArray, Cscalar) -> SO3vecArray
                                                     (SO3vecArray,complex<float>) -> SO3vecArray
V/c
    Multiply/divide \llbracket V \rrbracket by the scalar c.
V1+V2
                                                              (SO3vec,SO3vecArray) -> SO3vecArray
V1+V2
                                                              (SO3vecArray,SO3vec) -> SO3vecArray
V1-V2
                                                              (SO3vec,SO3vecArray) -> SO3vecArray
V1-V2
                                                              (SO3vecArray, SO3vec) -> SO3vecArray
    Compute P_1 + [P_2], [P_1] + P_2, P_1 - [P_2] or [P_1] - P_2.
                                                        (CtensorPack, SO3vecArray) -> SO3vecArray
W*V
    Multiply each cell of \llbracket V \rrbracket by the CtensorArray W.
```

## SCATTERING ARITHMETIC

```
scatter(C)*V
V*scatter(C)
V/scatter(C)

(Ctensor, SO3vecArray) -> SO3vecArray
(SO3vecArray, Ctensor) -> SO3vecArray
```

Multiply/divide each cell of  $\llbracket V \rrbracket$  by the scalar in the corresponding entry of C.

#### IN-PLACE OPERATIONS

```
+=V2 ($03vecArray,$03vecArray)->$03vecArray -=V2 ($03vecArray,$03vecArray)->$03vecArray ($03vec
```

## MEMBER FUNCTIONS

SO3vecArray rotate(const SO3element& R) const Rotate each cell by  $R \in SO(3)$ .

## OTHER FUNCTIONS

```
norm2(V) S03vecArray -> Ctensor The tensor of squared Frobenius norms \|V\|_{\text{Frob}}^2. inp(V1,V2) (S03vecArray,S03vecArray) -> Ctensor The tensor of inner products \langle V_1, V_2 \rangle.
```

## **CG-PRODUCTS**

```
CGproduct(V1,V2,[lmax])
                                                   (SO3vecArray,SO3vecArray,int) -> SO3vecArray
    Compute the Clebsch–Gordan product, V_1 \otimes_{cq} V_2, up to band limit \ell_{\text{max}} cell-by-cell.
CGproduct(V1,V2,[lmax])
                                                        (SO3vec,SO3vecArray,int) -> SO3vecArray
                                                        (SO3vecArray,SO3vec,int) -> SO3vecArray
CGproduct(V1,V2,[lmax])
    Compute the \ell'th component of the Clebsch-Gordan product by broadcasting V_1 resp. V_2.
Outer<CGproduct>(V1,V2,[lmax])
                                                   (SO3vecArray,SO3vecArray,int) -> SO3vecArray
Mprod<CGproduct>(V1,V2,[lmax])
                                                   (SO3vecArray,SO3vecArray,int) -> SO3vecArray
                                                   (SO3vecArray,SO3vecArray,int) -> SO3vecArray
Convolve<CGproduct>(V1,V2,[lmax])
    Compute the outer product of [V_1] and [V_2], matrix-like product, or convolution, where the elementary
    products are Clebsch–Gordan products.
```

## 1/0

```
string str(const indent="") const Print \llbracket V \rrbracket to string with the optional indentation indent.
```