reikna Documentation

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Reikna is a library containing various GPU algorithms built on top of PyCUDA and PyOpenCL. The main design goals are:

- separation of computation cores (matrix multiplication, random numbers generation etc) from simple transformations on their input and output values (scaling, typecast etc);
- separation of the preparation and execution stage, maximizing the performance of the execution stage at the expense of the preparation stage (in other words, aiming at large simulations)
- partial abstraction from CUDA/OpenCL

The installation is as simple as

\$ pip install reikna

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CHAPTER 1

Community resources

- Source repository on GitHub;
- Issue tracker, ibid.;
- Discussion forum on Google Groups.

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2.1 Introduction

This section contains a brief illustration of what reikna does. For more details see basic and advanced tutorials.

2.1.1 CLUDA

CLUDA is an abstraction layer on top of PyCUDA/PyOpenCL. Its main purpose is to separate the rest of reikna from the difference in their APIs, but it can be used by itself too for some simple tasks.

Consider the following example, which is very similar to the one from the index page on PyCUDA documentation:

```
import numpy
import reikna.cluda as cluda
N = 256
api = cluda.ocl_api()
thr = api.Thread.create()
program = thr.compile("""
KERNEL void multiply_them(
   GLOBAL_MEM float *dest,
   GLOBAL_MEM float *a,
   GLOBAL_MEM float *b)
 const SIZE_T i = get_local_id(0);
 dest[i] = a[i] * b[i];
""")
multiply_them = program.multiply_them
a = numpy.random.randn(N).astype(numpy.float32)
b = numpy.random.randn(N).astype(numpy.float32)
a_dev = thr.to_device(a)
b_dev = thr.to_device(b)
dest_dev = thr.empty_like(a_dev)
multiply_them(dest_dev, a_dev, b_dev, local_size=N, global_size=N)
print ((dest_dev.get() - a * b == 0).all())
```

If you are familiar with PyCUDA or PyOpenCL, you will easily understand all the steps we have made here. The cluda.ocl_api() call is the only place where OpenCL is mentioned, and if you replace it with cluda.cuda_api() it will be enough to make the code use CUDA. The abstraction is achieved by using generic API module on the Python side, and special macros (KERNEL, GLOBAL_MEM, and others) on the kernel side.

The argument of <code>compile()</code> method can also be a template, which is quite useful for metaprogramming, and also used to compensate for the lack of complex number operations in CUDA and OpenCL. Let us illustrate both scenarios by making the initial example multiply complex arrays. The template engine of choice in <code>reikna</code> is Mako, and you are encouraged to read about it as it is quite useful. For the purpose of this example all we need to know is that <code>\${python_expression()}</code> is a synthax construction which renders the expression result.

```
import numpy
from numpy.linalg import norm
from reikna import cluda
from reikna.cluda import functions, dtypes
N = 256
dtype = numpy.complex64
api = cluda.ocl_api()
thr = api.Thread.create()
program = thr.compile("""
KERNEL void multiply_them(
   GLOBAL_MEM ${ctype} *dest,
   GLOBAL_MEM ${ctype} *a,
   GLOBAL_MEM ${ctype} *b)
  const SIZE_T i = get_local_id(0);
  dest[i] = \$\{mul\}(a[i], b[i]);
""", render_kwds=dict(
   ctype=dtypes.ctype(dtype),
   mul=functions.mul(dtype, dtype)))
multiply_them = program.multiply_them
r1 = numpy.random.randn(N).astype(numpy.float32)
r2 = numpy.random.randn(N).astype(numpy.float32)
a = r1 + 1j * r2
b = r1 - 1j * r2
a_dev = thr.to_device(a)
b_dev = thr.to_device(b)
dest_dev = thr.empty_like(a_dev)
multiply_them(dest_dev, a_dev, b_dev, local_size=N, global_size=N)
print (norm(dest_dev.get() - a \star b) / norm(a \star b) <= 1e-6)
```

Note that CLUDA Thread is created by means of a static method and not using the constructor. The constructor is reserved for more probable scenario, where we want to include some reikna functionality in a larger program, and we want it to use the existing context and stream/queue (see the *Thread* constructor). In this case all further operations with the thread will be performed using the objects provided.

Here we have passed two values to the template: ctype (a string with C type name), and mul which is a Module object containing a single multiplication function. The object is created by a function mul() which takes data types being multiplied and returns a module that was parametrized accordingly. Inside the template the variable mul is essentially the prefix for all the global C objects (functions, structures, macros etc) from the module. If there is only one public object in the module (which is recommended), it is a common practice to give it the name consisting just

of the prefix, so that it could be called easily from the parent code.

For more information on modules, see *Tutorial: modules and snippets*; the complete list of things available in CLUDA can be found in *CLUDA reference*.

2.1.2 Computations

Now it's time for the main part of the functionality. reikna provides GPGPU algorithms in the form of Computation-based cores and Transformation-based plug-ins. Computations contain the algorithm itself; examples are matrix multiplication, reduction, sorting and so on. Transformations are parallel operations on inputs or outputs of computations, used for scaling, typecast and other auxiliary purposes. Transformations are compiled into the main computation kernel and are therefore quite cheap in terms of performance.

As an example, we will consider the matrix multiplication.

```
import numpy
from numpy.linalg import norm
import reikna.cluda as cluda
from reikna.linalg import MatrixMul
api = cluda.ocl_api()
thr = api.Thread.create()
shape1 = (100, 200)
shape2 = (200, 100)
a = numpy.random.randn(*shape1).astype(numpy.float32)
b = numpy.random.randn(*shape2).astype(numpy.float32)
a_dev = thr.to_device(a)
b_dev = thr.to_device(b)
res_dev = thr.array((shape1[0], shape2[1]), dtype=numpy.float32)
dot = MatrixMul(a_dev, b_dev, out_arr=res_dev)
dotc = dot.compile(thr)
dotc(res_dev, a_dev, b_dev)
res_reference = numpy.dot(a, b)
print(norm(res_dev.get() - res_reference) / norm(res_reference) < 1e-6)</pre>
```

Most of the code above should be already familiar, with the exception of the creation of <code>MatrixMul</code> object. The computation constructor takes two array-like objects, representing arrays that will participate in the computation. After that the computation object has to be compiled. The <code>compile()</code> method requires a <code>Thread</code> object, which serves as a source of data about the target API and device, and provides an execution queue.

2.1.3 Transformations

Now imagine that you want to multiply complex matrices, but real and imaginary parts of your data are kept in separate arrays. You could create additional kernels that would join your data into arrays of complex values, but this would require additional storage and additional calls to GPU. Transformation API allows you to connect these transformations to the core computation — matrix multiplication — effectively adding the code into the main computation kernel and changing its signature.

Let us change the previous example and connect transformations to it.

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```
import numpy
from numpy.linalg import norm
import reikna.cluda as cluda
from reikna.core import Type
from reikna.linalg import MatrixMul
from reikna.transformations import combine_complex
api = cluda.ocl_api()
thr = api.Thread.create()
shape1 = (100, 200)
shape2 = (200, 100)
a_re = numpy.random.randn(*shape1).astype(numpy.float32)
a_im = numpy.random.randn(*shape1).astype(numpy.float32)
b_re = numpy.random.randn(*shape2).astype(numpy.float32)
b_im = numpy.random.randn(*shape2).astype(numpy.float32)
arrays = [thr.to_device(x) for x in [a_re, a_im, b_re, b_im]]
a_re_dev, a_im_dev, b_re_dev, b_im_dev = arrays
a_type = Type(numpy.complex64, shape=shape1)
b_type = Type(numpy.complex64, shape=shape2)
res_dev = thr.array((shape1[0], shape2[1]), dtype=numpy.complex64)
dot = MatrixMul(a_type, b_type, out_arr=res_dev)
combine_a = combine_complex(a_type)
combine_b = combine_complex(b_type)
dot.parameter.matrix_a.connect(
   combine_a, combine_a.output, a_re=combine_a.real, a_im=combine_a.imag)
dot.parameter.matrix_b.connect(
   combine_b, combine_b.output, b_re=combine_b.real, b_im=combine_b.imag)
dotc = dot.compile(thr)
dotc(res_dev, a_re_dev, a_im_dev, b_re_dev, b_im_dev)
res_reference = numpy.dot(a_re + 1j * a_im, b_re + 1j * b_im)
print(norm(res_dev.get() - res_reference) / norm(res_reference) < 1e-6)</pre>
```

We have used a pre-created transformation <code>combine_complex()</code> from <code>reikna.transformations</code> for simplicity; developing a custom transformation is also possible and described in <code>Writing a transformation</code>. From the documentation we know that it transforms two inputs into one output; therefore we need to attach it to one of the inputs of <code>dot</code> (identified by its name), and provide names for two new inputs.

Names to attach to are obtained from the documentation for the particular computation; for <code>MatrixMul</code> these are out, a and b.

In the current example we have attached the transformations to both inputs. Note that the computation has a new signature now, and the compiled dot object now works with split complex numbers.

2.2 Tutorial: modules and snippets

Modules and snippets are important primitives in CLUDA which are used in the rest of reikna, although mostly internally. Even if you do not write modules yourself, you will most likely use operations from the functions module, or common transformations from the transformations module, which are essentially snippet and module factories (callables returning Snippet and Module objects). Therefore it helps if you know how they work under the hood.

2.2.1 Snippets

Snippets are Mako template defs (essentially functions returning rendered text) with the associated dictionary of render keywords. Some computations which are parametrized by custom code (for example, <code>PureParallel</code>) require this code to be provided in form of a snippet with a certain call signature. When a snippet is used in a template, the result is quite straightworward: its template function is called, rendering and returning its contents, just as a normal <code>Mako</code> def.

Let us demonstrate it with a simple example. Consider the following snippet:

Now we can compile a template which uses this snippet:

```
program = thr.compile("""

KERNEL void test(int *arr)
{
    const SIZE_T idx = get_global_id(0);
    int a = arr[idx];
    arr[idx] = ${add('x')};
}
""",
render_kwds=dict(add=add))
```

As a result, the code that gets compiled is

```
KERNEL void test(int *arr)
{
    const SIZE_T idx = get_global_id(0);
    int a = arr[idx];
    arr[idx] = x + 1;
}
```

If the snippet is used without parentheses (e.g. \$ {add}), it is equivalent to calling it without arguments (\$ {add()}).

The root code that gets passed to compile() can be viewed as a snippet with an empty signature.

2.2.2 Modules

Modules are quite similar to snippets in a sense that they are also Mako defs with an associated dictionary of render keywords. The difference lies in the way they are processed. Consider a module containing a single function:

Modules contain complete C entities (function, macros, structures) and get rendered in the root level of the source file. In order to avoid name clashes, their def gets a string as a first argument, which it has to use to prefix these entities' names. If the module contains only one entity that is supposed to be used by the parent code, it is a good idea to set its name to prefix only, to simplify its usage.

Let us now create a kernel that uses this module:

```
program = thr.compile("""

KERNEL void test(int *arr)
{
   const SIZE_T idx = get_global_id(0);
   int a = arr[idx];
   arr[idx] = ${add(2)}(x);
}
""",
render_kwds=dict(add=add))
```

Before the compilation render keywords are inspected, and if a module object is encountered, the following things happen:

- 1. This object's render_kwds are inspected recursively and any modules there are rendered in the same way as described here, producing a source file.
- 2. The module itself gets assigned a new prefix and its template function is rendered with this prefix as the first argument, with the positional arguments given following it. The result is attached to the source file.
- 3. The corresponding value in the current render_kwds is replaced by the newly assigned prefix.

With the code above, the rendered module will produce the code

```
WITHIN_KERNEL int _module0_(int x)
{
   return x + 1 + 2;
}
```

and the add keyword in the render_kwds gets its value changed to _module0_. Then the main code is rendered and appended to the previously renderd parts, giving

```
WITHIN_KERNEL int _module0_(int x)
{
    return x + 1;
}

KERNEL void test(int *arr)
{
    const SIZE_T idx = get_global_id(0);
    int a = arr[idx];
    arr[idx] = _module0_(x);
}
```

which is then passed to the compiler. If your module's template def does not take any arguments except for prefix, you can call it in the parent template just as \${add} (without empty parentheses).

Warning: Note that add in this case is not a string, it is an object that has __str__() defined. If you want to concatenate a module prefix with some other string, you have to either call str() explicitly (str(add) + "abc"), or concatenate it inside a template (\${add} abc).

Modules can reference snippets in their render_kwds, which, in turn, can reference other modules. This produces a tree-like structure with the snippet made from the code passed by user at the root. When it is rendered, it is traversed depth-first, modules are extracted from it and arranged in a flat list in the order of appearance. Their positions in render_kwds are replaced by assigned prefixes. This flat list is then rendered, producing a single source file being fed to the compiler.

Note that if the same module object was used without arguments in several other modules or in the kernel itself, it will only be rendered once. Therefore one can create a "root" module with the data structure declaration and then use that structure in other modules without producing type errors on compilation.

2.2.3 Shortcuts

The amount of boilerplate code can be somewhat reduced by using *Snippet.create* and *Module.create* constructors. For the snippet above it would look like:

```
add = Snippet.create(
   lambda varname: "${varname} + ${num}",
   render_kwds=dict(num=1))
```

Note that the lambda here serves only to provide the information about the Mako def's signature. Therefore it should return the template code regardless of the actual arguments passed.

If the argument list is created dynamically, you can use template_def() with a normal constructor:

```
argnames = ['varname']
add = Snippet(
    template_def(argnames, "${varname} + ${num}"),
    render_kwds=dict(num=1))
```

Modules have a similar shortcut constructor. The only difference is that by default the resulting template def has one positional argument called prefix. If you provide your own signature, its first positional argument will receive the prefix value.

```
add = Module.create("""
WITHIN_KERNEL int ${prefix}(int x)
{
    return x + ${num};
}
""",
render_kwds=dict(num=1))
```

Of course, both *Snippet* and *Module* constructors can take already created Mako defs, which is convenient if you keep templates in a separate file.

2.2.4 Module and snippet discovery

Sometimes you may want to pass a module or a snippet inside a template as an attribute of a custom object. In order for CLUDA to be able to discover and process it without modifying your original object, you need to make your object comply to a discovery protocol. The protocol method takes a processing function and is expected to return a

new object of the same class with the processing function applied to all the attributes that may contain a module or a snippet. By default, objects of type tuple, list, and dict are discoverable.

For example:

```
class MyClass:

def __init__(self, coeff, mul_module, div_module):
    self.coeff = coeff
    self.mul = mul_module
    self.div = div_module

def __process_modules__(self, process):
    return MyClass(self.coeff, process(self.mul), process(self.div))
```

2.2.5 Nontrivial example

Modules were introduced to help split big kernels into small reusable pieces which in CUDA or OpenCL program would be put into different source or header files. For example, a random number generator may be assembled from a function generating random integers, a function transforming these integers into random numbers with a certain distribution, and a <code>PureParallel</code> computation calling these functions and saving results to global memory. These two functions can be extracted into separate modules, so that a user could call them from some custom kernel if he does not need to store the intermediate results.

Going further with this example, one notices that functions that produce randoms with sophisticated distributions are often based on simpler distributions. For instance, the commonly used Marsaglia algorithm for generating Gamma-distributed random numbers requires several uniformly and normally distributed randoms. Normally distributed randoms, in turn, require several uniformly distributed randoms — with the range which differs from the one for uniformly distributed randoms used by the initial Gamma distribution. Instead of copy-pasting the function or setting its parameters dynamically (which in more complicated cases may affect the performance), one just specifies the dependencies between modules and lets the underlying system handle things.

The final render tree may look like:

```
Snippet(
   PureParallel,
   render_kwds = {
    base_rng -> Snippet(...)
      gamma -> Snippet(
   }
      Gamma,
      render_kwds = {
      uniform -> Snippet(...)
      normal -> Snippet(
      }
      Normal,
   )
      render_kwds = {
      uniform -> Snippet(...)
      }
      vender_kwds = {
      uniform -> Snippet(...)
      }
}
```

2.3 Tutorial: basics

2.3.1 Usage of computations

All reikna computation classes are derived from the Computation class and therefore share the same API and behavior. A computation object is an opaque typed function-like object containing all the information necessary to

generate GPU kernels that implement some algorithm, along with necessary internal temporary and persistent memory buffers. Before use it needs to be compiled by calling <code>compile()</code> for a given <code>Thread</code> (thus using its associated device and queue). This method returns a <code>ComputationCallable</code> object which takes GPU arrays and scalar parameters and calls its internal kernels.

2.3.2 Computations and transformations

One often needs to perform some simple processing of the input or output values of a computation. This can be scaling, splitting complex values into components, padding, and so on. Some of these operations require additional memory to store intermediate results, and all of them involve additional overhead of calling the kernel, and passing values to and from the device memory. Reikna porvides an API to define such transformations and attach them to "core" computations, effectively compiling the transformation code into the main kernel(s), thus avoiding all these drawbacks.

2.3.3 Transformation tree

Before talking about transformations themselves, we need to take a closer look at the computation signatures. Every *Computation* object has a *signature* attribute containing funcsigs. Signature object. It is the same signature object as can be exctracted from any Python function using funcsigs. signature function (or inspect.signature from the standard library for Python >= 3.3). When the computation object is compiled, the resulting callable will have this exact signature.

The base signature for any computation can be found in its documentation (and, sometimes, can depend on the arguments passed to its constructor — see, for example, <code>PureParallel</code>). The signature can change if a user connects transformations to some parameter via <code>connect()</code>; in this case the <code>signature</code> attribute will change accordingly.

All attached transformations form a tree with roots being the base parameters computation has right after creation, and leaves forming the user-visible signature, which the compiled <code>ComputationCallable</code> will have.

As an example, let us consider a pure parallel computation object with one output, two inputs and a scalar parameter, which performs the calculation out = in1 + in2 + param:

```
future import print_function
import numpy
from reikna import cluda
from reikna.cluda import Snippet
from reikna.core import Transformation, Type, Annotation, Parameter
from reikna.algorithms import PureParallel
import reikna.transformations as transformations
arr_t = Type(numpy.float32, shape=128)
carr_t = Type(numpy.complex64, shape=128)
comp = PureParallel(
   [Parameter('out', Annotation(carr_t, 'o')),
   Parameter('in1', Annotation(carr_t, 'i')),
   Parameter('in2', Annotation(carr_t, 'i')),
   Parameter('param', Annotation(numpy.float32))],
   VSIZE_T idx = \{idxs[0]\};
    ${out.store idx}(
       idx, ${in1.load_idx}(idx) + ${in2.load_idx}(idx) + ${param});
```

2.3. Tutorial: basics

The details of creating the computation itself are not important for this example; they are provided here just for the sake of completeness. The initial transformation tree of comp object looks like:

```
| out | >>
>> | in1 |
>> | in2 |
>> | param |
```

Here the insides of | | are the base computation (the one defined by the developer), and >> denote inputs and outputs provided by the user. The computation signature is:

```
>>> for param in comp.signature.parameters.values():
...    print(param.name + ":" + repr(param.annotation))
out:Annotation(Type(complex64, shape=(128,), strides=(8,)), role='o')
in1:Annotation(Type(complex64, shape=(128,), strides=(8,)), role='i')
in2:Annotation(Type(complex64, shape=(128,), strides=(8,)), role='i')
param:Annotation(float32)
```

Now let us attach the transformation to the output which will split it into two halves: out1 = out / 2, out2 = out / 2:

```
tr = transformations.split_complex(comp.parameter.out)
comp.parameter.out.connect(tr, tr.input, out1=tr.real, out2=tr.imag)
```

We have used the pre-created transformation here for simplicity; writing custom transformations is described in *Writing a transformation*.

In addition, we want in2 to be scaled before being passed to the main computation. To achieve this, we connect the scaling transformation to it:

```
tr = transformations.mul_param(comp.parameter.in2, numpy.float32)
comp.parameter.in2.connect(tr, tr.output, in2_prime=tr.input, param2=tr.param)
```

The transformation tree now looks like:

As can be seen, nothing has changed from the base computation's point of view: it still gets the same inputs and outputs to the same array. But user-supplied parameters (>>) have changed, which can be also seen in the value of the signature:

```
>>> for param in comp.signature.parameters.values():
...    print(param.name + ":" + repr(param.annotation))
out1:Annotation(Type(float32, shape=(128,), strides=(4,)), role='o')
out2:Annotation(Type(float32, shape=(128,), strides=(4,)), role='o')
in1:Annotation(Type(complex64, shape=(128,), strides=(8,)), role='i')
in2_prime:Annotation(Type(complex64, shape=(128,), strides=(8,)), role='i')
param2:Annotation(float32)
param:Annotation(float32)
```

Notice that the order of the final signature is obtained by traversing the transformation tree depth-first, starting from the base parameters. For more details see the note in the documentation for <code>connect()</code>.

The resulting computation returns the value in1 + (in2_prime * param2) + param split in half. In order to run it, we have to compile it first. When prepare_for is called, the data types and shapes of the given arguments

will be propagated to the roots and used to prepare the original computation.

```
api = cluda.ocl_api()
thr = api.Thread.create()

in1_t = comp.parameter.in1
in2p_t = comp.parameter.in2_prime

out1 = thr.empty_like(comp.parameter.out1)
out2 = thr.empty_like(comp.parameter.out2)
in1 = thr.to_device(numpy.ones(in1_t.shape, in1_t.dtype))
in2_prime = thr.to_device(numpy.ones(in2p_t.shape, in2p_t.dtype))

c_comp = comp.compile(thr)
c_comp(out1, out2, in1, in2_prime, 4, 3)
```

2.3.4 Transformation restrictions

There are some limitations of the transformation mechanics:

- 1. Transformations are purely parallel, that is they cannot use local memory. In fact, they are very much like <code>PureParallel</code> computations, except that the indices they use are defined by the main computation, and not set by the GPU driver.
- 2. External endpoints of the output transformations cannot point to existing nodes in the transformation tree. This is the direct consequence of the first limitation it would unavoidably create races between memory writes from different branches. On the other hand, input transformations can be safely connected to existing nodes, including base nodes (although note that inputs are not cached; so even if you load twice from the same index of the same input node, the global memory will be queried twice).

2.4 Tutorial: advanced topics

This tutorial goes into more detail about the internals of computations and transformations, describing how to write them.

2.4.1 Mako basics

Reikna uses Mako extensively as a templating engine for transformations and computations. For the purpose of this tutorial you only need to know several things about the synthax:

- Most of Mako synthax is plain Python, with the set of global variables specified externally by the code doing the template rendering
- \${expr} evaluates Python expression expr, calls str() on the result and puts it into the text
- a pair of <% and %> executes Python code inside, which may introduce some local variables
- a pair of <%def name="func(a, b)"> and </%def> defines a template function, which actually becomes a Python function which can be called as func(a, b) from the other part of the template and returns a rendered string

2.4.2 Writing a transformation

Some common transformations are already available from *transformations* module. But you can create a custom one if you need to. Transformations are based on the class *Transformation*, and are very similar to *PureParallel* instances, with some additional limitations.

Let us consider a (not very useful, but quite involved) example:

```
tr = Transformation(
    [
        Parameter('out1', Annotation(Type(numpy.float32, shape=100), 'o')),
        Parameter('out2', Annotation(Type(numpy.float32, shape=80), 'o')),
        Parameter('in1', Annotation(Type(numpy.float32, shape=100), 'i')),
        Parameter('in2', Annotation(Type(numpy.float32, shape=100), 'i')),
        Parameter('param', Annotation(Type(numpy.float32))),
   ],
    VSIZE\_T idx = ${idxs[0]};
    float i1 = ${in1.load_same};
    float i2 = ${in2.load_idx}(100 - idx) * ${param};
    ${out1.store_same}(i1);
    if (idx < 80)
       ${out2.store_same}(i2);
    m m m
    connectors=['in1', 'out1'])
```

Connectors. A transformation gets activated when the main computation attempts to load some value from some index in global memory, or store one to some index. This index is passed to the transformation attached to the corresponding parameter, and used to invoke loads/stores either without changes (to perform strictly elementwise operations), or, possibly, with some changes (as the example illustrates).

If some parameter is only queried once, and only using <code>load_same</code> or <code>store_same</code>, it is called a *connector*, which means that it can be used to attach the transformation to a computation. Currently connectors cannot be detected automatically, so it is the responsibility of the user to provide a list of them to the constructor. By default all parameters are considered to be connectors.

Shape changing. Parameters in transformations are typed, and it is possible to change data type or shape of a parameter the transformation is attached to. In our example out 2 has length 80, so the current index is checked before the output to make sure there is no out of bounds access.

Parameter objects. The transformation example above has some hardcoded stuff, for example the type of parameters (float), or their shapes (100 and 80). These can be accessed from argument objects out1, in1 etc; they all have the type <code>KernelParameter</code>. In addition, the transformation code gets an <code>Indices</code> object with the name idxs, which allows one to manipulate index names directly.

2.4.3 Writing a computation

A computation must derive *Computation*. As an example, let us create a computation which calculates output = input1 + input2 * param.

Defining a class:

```
import numpy

from reikna.helpers import *
from reikna.core import *
class TestComputation(Computation):
```

Each computation class has to define the constructor, and the plan building callback.

Constructor. Computation constructor takes a list of computation parameters, which the deriving class constructor has to create according to arguments passed to it. You will often need Type objects, which can be extracted from arrays, scalars or other Type objects with the help of from_value() (or they can be passed straight to Annotation) which does the same thing.

```
def __init__(self, arr, coeff):
    assert len(arr.shape) == 1
    Computation.__init__(self, [
        Parameter('output', Annotation(arr, 'o')),
        Parameter('input1', Annotation(arr, 'i')),
        Parameter('input2', Annotation(arr, 'i')),
        Parameter('param', Annotation(coeff))])
```

In addition to that, the constructor can create some internal state which will be used by the plan builder.

Plan builder. The second method is called when the computation is being compiled, and has to fill and return the computation plan — a sequence of kernel calls, plus maybe some temporary or persistent internal allocations its kernels use. In addition, the plan can include calls to nested computations.

The method takes two predefined positional parameters, plus <code>KernelArgument</code> objects corresponding to computation parameters. The plan_factory is a callable that creates a new <code>ComputationPlan</code> object (in some cases you may want to recreate the plan, for example, if the workgroup size you were using turned out to be too big), and <code>device_params</code> is a <code>DeviceParameters</code> object, which is used to optimize the computation for the specific device. The method must return a filled <code>ComputationPlan</code> object.

For our example we only need one action, which is the execution of an elementwise kernel:

```
def _build_plan(self, plan_factory, device_params, output, input1, input2, param):
   plan = plan_factory()
    template = template_from(
        <%def name='testcomp(kernel_declaration, k_output, k_input1, k_input2, k_param)|>
        ${kernel_declaration}
            VIRTUAL_SKIP_THREADS;
            const VSIZE_T idx = virtual_global_id(0);
            ${k_output.ctype} result =
                \{k_{input1.load_idx}\}(idx) +
                ${mul}(${k_input2.load_idx}(idx), ${k_param});
            ${k_output.store_idx}(idx, result);
        </%def>
        """)
    plan.kernel_call(
        template.get_def('testcomp'),
        [output, input1, input2, param],
        global_size=output.shape,
        render_kwds=dict(mul=functions.mul(input2.dtype, param.dtype)))
    return plan
```

Every kernel call is based on the separate Mako template def. The template can be specified as a string using $template_def()$, or loaded as a separate file. Usual pattern in this case is to call the template file same as the file where the computation class is defined (for example, testcomp.mako for testcomp.py), and store it in some variable on module load using $template_for()$ as $template_for()$ as $template_for()$.

The template function should take the same number of positional arguments as the kernel plus one; you can view <%def ... > part as an actual kernel definition, but with the arguments being KernelParameter objects containing parameter metadata. The first argument will contain the string with the kernel declaration.

Also, depending on whether the corresponding argument is an output array, an input array or a scalar parameter, the object can be used as \${obj.store_idx}(index, val), \${obj.load_idx}(index) or \${obj}. This will produce the corresponding request to the global memory or kernel arguments.

If you need additional device functions, they have to be specified between <%def ... > and \${kernel_declaration}. Obviously, these functions can still use dtype and ctype object properties, although store_idx and load_idx will most likely result in compilation error (since they are rendered as macros using main kernel arguments).

Since kernel call parameters (global_size and local_size) are specified on creation, all kernel calls are rendered as CLUDA static kernels (see <code>compile_static())</code> and therefore can use all the corresponding macros and functions (like <code>virtual_global_flat_id()</code> in our kernel). Also, they must have <code>VIRTUAL_SKIP_THREADS</code> at the beginning of the kernel which remainder threads (which can be present, for example, if the workgroup size is not a multiple of the global size).

2.5 API reference

2.5.1 Version queries

This module contains information about the library version.

```
reikna.version.version
```

A tuple with version numbers, major components first.

```
reikna.version.full_version
```

A string fully identifying the current build.

```
reikna.version.git revision
```

A string with Git SHA identifying the revision used to create this build.

```
reikna.version.release
```

A boolean variable, equals True if current version is a release version.

2.5.2 Helpers

This module contains various auxiliary functions which are used throughout the library.

```
reikna.helpers.bounding_power_of_2 (num)
```

Returns the minimal number of the form 2 * *m such that it is greater or equal to n.

```
reikna.helpers.factors(num, limit=None)
```

Returns the list of pairs (factor, num/factor) for all factors of num (including 1 and num), sorted by factor. If limit is set, only pairs with factor <= limit are returned.

```
class reikna.helpers.ignore_integer_overflow
```

Context manager for ignoring integer overflow in numpy operations on scalars (not ignored by default because of a bug in numpy).

```
reikna.helpers.log2(num)
```

Integer-valued logarigthm with base 2. If n is not a power of 2, the result is rounded to the smallest number.

```
reikna.helpers.min_blocks(length, block)
```

Returns minimum number of blocks with length block necessary to cover the array with length length.

```
reikna.helpers.product (seq)
```

Returns the product of elements in the iterable seq.

```
reikna.helpers.template_def(signature, code)
```

Returns a Mako template with the given signature.

Parameters signature – a list of postitional argument names, or a Signature object from funcsigs module.

Code a body of the template.

```
reikna.helpers.template_for (filename)
```

Returns the Mako template object created from the file which has the same name as filename and the extension .mako. Typically used in computation modules as template_for(__filename___).

```
reikna.helpers.template_from(template)
```

Creates a Mako template object from a given string. If template already has render() method, does nothing.

```
reikna.helpers.wrap_in_tuple(seq_or_elem)
```

If seq_or_elem is a sequence, converts it to a tuple, otherwise returns a tuple with a single element seq_or_elem.

2.5.3 CLUDA layer

CLUDA is the foundation of reikna. It provides the unified access to basic features of CUDA and OpenCL, such as memory operations, compilation and so on. It can also be used by itself, if you want to write GPU API-independent programs and happen to only need a small subset of GPU API. The terminology is borrowed from OpenCL, since it is a more general API.

```
class reikna.cluda.Module (template_src, render_kwds=None)
```

Contains a CLUDA module. See Tutorial: modules and snippets for details.

Parameters

- template_src (str or Mako template.) a Mako template with the module code, or a string with the template source.
- render_kwds a dictionary which will be used to render the template. Can contain other modules and snippets.

```
classmethod create (func or str, render kwds=None)
```

Creates a module from the Mako def:

- •if func_or_str is a function, then the def has the same signature as func_or_str (prefix will be passed as the first positional parameter), and the body equal to the string it returns;
- •if func_or_str is a string, then the def has a single positional argument prefix. and the body code.

exception reikna.cluda.OutOfResourcesError

Thrown by compile_static() if the provided local_size is too big, or one cannot be found.

```
class reikna.cluda.Snippet (template_src, render_kwds=None)
```

Contains a CLUDA snippet. See *Tutorial: modules and snippets* for details.

Parameters

• **template_src** (str or Mako template.) – a Mako template with the module code, or a string with the template source.

render_kwds – a dictionary which will be used to render the template. Can contain other
modules and snippets.

```
classmethod create (func_or_str, render_kwds=None)
```

Creates a snippet from the Mako def:

- •if func_or_str is a function, then the def has the same signature as func_or_str, and the body equal to the string it returns;
- •if func or str is a string, then the def has empty signature.

```
reikna.cluda.any_api()
```

Returns one of the API modules supported by the system or raises an Exception if there are not any.

```
reikna.cluda.api_ids()
```

Returns a list of identifiers for all known (not necessarily available for the current system) APIs.

```
reikna.cluda.cuda_api()
```

Returns the PyCUDA-based API module.

```
reikna.cluda.cuda_id()
```

Returns the identifier of the PyCUDA-based API.

```
reikna.cluda.find_devices (api, include_devices=None, exclude_devices=None, include_platforms=None, exclude_platforms=None, include_duplicate_devices=True, include_pure_only=False)
```

Find platforms and devices meeting certain criteria.

Parameters

- api a CLUDA API object.
- include_devices a list of masks for a device name which will be used to pick devices
 to include in the result.
- **exclude_devices** a list of masks for a device name which will be used to pick devices to exclude from the result.
- include_platforms a list of masks for a platform name which will be used to pick platforms to include in the result.
- **exclude_platforms** a list of masks for a platform name which will be used to pick platforms to exclude in the result.
- include_duplicate_devices if False, will only include a single device from the several with the same name available on a platform.
- include_pure_only if True, will include devices with maximum group size equal to 1.

Returns a dictionary with found platform numbers as keys, and lists of device numbers as values.

```
reikna.cluda.get_api(api_id)
```

Returns an API module with the generalized interface reikna.cluda.api for the given identifier.

```
reikna.cluda.ocl_api()
```

Returns the PyOpenCL-based API module.

```
reikna.cluda.ocl id()
```

Returns the identifier of the PyOpenCL-based API.

```
reikna.cluda.supported_api_ids()
```

Returns a list of identifiers of supported APIs.

reikna.cluda.supports_api(api_id)

Returns True if given API is supported.

API module

Modules for all APIs have the same generalized interface. It is referred here (and references from other parts of this documentation) as reikna.cluda.api.

class reikna.cluda.api.Buffer

Low-level untyped memory allocation. Actual class depends on the API: pycuda.driver.DeviceAllocation for CUDA and pyopencl.Buffer for OpenCL.

size

class reikna.cluda.api.Array

A superclass of the corresponding API's native array (pycuda.gpuarray.GPUArray for CUDA and pyopencl.array.Array for OpenCL), with some additional functionality.

shape

dtype

get()

Returns numpy.ndarray with the contents of the array. Synchronizes the parent Thread.

thread

The Thread object for which the array was created.

class reikna.cluda.api.DeviceParameters (device)

An assembly of device parameters necessary for optimizations.

max_work_group_size

Maximum block size for kernels.

max_work_item_sizes

List with maximum local_size for each dimension.

max_num_groups

List with maximum number of workgroups for each dimension.

warp_size

Warp size (nVidia), or wavefront size (AMD), or SIMD width is supposed to be the number of threads that are executed simultaneously on the same computation unit (so you can assume that they are perfectly synchronized).

local mem banks

Number of local (shared in CUDA) memory banks is a number of successive 32-bit words you can access without getting bank conflicts.

local mem size

Size of the local (shared in CUDA) memory per workgroup, in bytes.

min mem coalesce width

Dictionary {word_size:elements}, where elements is the number of elements with size word_size in global memory that allow coalesced access.

supports_dtype (self, dtype)

Checks if given numpy dtype can be used in kernels compiled using this thread.

class reikna.cluda.api.Platform

A vendor-specific implementation of the GPGPU API.

name

Platform name.

vendor

Vendor name.

version

Platform version.

qet devices()

Returns a list of device objects available in the platform.

class reikna.cluda.api.Kernel (thr, program, name, static=False)

An object containing GPU kernel.

max_work_group_size

Maximum size of the work group for the kernel.

```
__call__(*args, **kwds)
```

A shortcut for successive call to <code>prepare()</code> and <code>prepared_call()</code>. In case of the OpenCL backend, returns a <code>pyopencl.Event</code> object.

prepare (global_size, local_size=None, local_mem=0)

Prepare the kernel for execution with given parameters.

Parameters

- global_size an integer or a tuple of integers, specifying total number of work items to run.
- local_size an integer or a tuple of integers, specifying the size of a single work group. Should have the same number of dimensions as global_size. If None is passed, some local_size will be picked internally.
- local_mem (CUDA API only) amount of dynamic local memory (in bytes)

prepared_call(*args)

Execute the kernel. *Array* objects are allowed as arguments. In case of the OpenCL backend, returns a pyopencl. Event object.

class reikna.cluda.api.**Program** (thr, src, static=False, fast_math=False)

An object with compiled GPU code.

source

Contains module source code.

kernel name

Contains Kernel object for the kernel kernel name.

An object containing a GPU kernel with fixed call sizes.

source

Contains the source code of the program.

```
___call___(*args)
```

Execute the kernel. *Array* objects are allowed as arguments. In case of the OpenCL backend, returns a pyopencl. Event object.

class reikna.cluda.api.**Thread**(cqd, async=True, temp_alloc=None)

Wraps an existing context in the CLUDA thread object.

Parameters

- **cqd** a Context, Device or Stream/CommandQueue object to base on. If a context is passed, a new stream/queue will be created internally.
- **async** whether to execute all operations with this thread asynchronously (you would generally want to set it to False only for profiling purposes).

Note: If you are using CUDA API, you must keep in mind the stateful nature of CUDA calls. Briefly, this means that there is the context stack, and the current context on top of it. When the <code>create()</code> is called, the <code>PyCUDA</code> context gets pushed to the stack and made current. When the thread object goes out of scope (and the thread object owns it), the context is popped, and it is the user's responsibility to make sure the popped context is the correct one. In simple single-context programs this only means that one should avoid reference cycles involving the thread object.

Warning: Do not pass one Stream/CommandQueue object to several Thread objects.

api

Module object representing the CLUDA API corresponding to this Thread.

device_params

Instance of DeviceParameters class for this thread's device.

temp alloc

Instance of TemporaryManager which handles allocations of temporary arrays (see temp_array()).

allocate (size)

Creates an untyped memory allocation object of type *Buffer* with size size.

array (shape, dtype, strides=None, allocator=None)

Creates an *Array* on GPU with given shape, dtype and strides. Optionally, an allocator is a callable returning any object castable to int representing the physical address on the device (for instance, *Buffer*).

compile (template_src, render_args=None, render_kwds=None, fast_math=False)

Creates a module object from the given template.

Parameters

- template_src Mako template source to render
- **render_kwds** an iterable with positional arguments to pass to the template.
- render_kwds a dictionary with keyword parameters to pass to the template.
- fast math whether to enable fast mathematical operations during compilation.

Returns a Program object.

Creates a kernel object with fixed call sizes, which allows to overcome some backend limitations. Global and local sizes can have any length, providing that len(global_size) >= len(local_size), and the total number of work items and work groups is less than the corresponding total number available for the device. In order to get IDs and sizes in such kernels, virtual size functions have to be used (see VIRTUAL_SKIP_THREADS and others for details).

Parameters

• **template_src** – Mako template or a template source to render

- name name of the kernel function
- global_size global size to be used, in row-major order.
- local_size local size to be used, in row-major order. If None, some suitable one will be picked.
- local_mem (CUDA API only) amount of dynamically allocated local memory to be used (in bytes).
- render_args a list of parameters to be passed as positional arguments to the template.
- render_kwds a dictionary with additional parameters to be used while rendering the template.
- **fast_math** whether to enable fast mathematical operations during compilation.

Returns a StaticKernel object.

copy_array (arr, dest=None, src_offset=0, dest_offset=0, size=None) Copies array on device.

Parameters

- **dest** the effect is the same as in to_device().
- **src_offset** offset (in items of arr.dtype) in the source array.
- **dest_offset** offset (in items of arr.dtype) in the destination array.
- **size** how many elements of arr.dtype to copy.

classmethod create (interactive=False, device_filters=None, **thread_kwds)

Creates a new Thread object with its own context and queue inside. Intended for cases when you want to base your whole program on CLUDA.

Parameters

- **interactive** ask a user to choose a platform and a device from the ones found. If there is only one platform/device available, they will be chosen automatically.
- **device_filters** keywords to filter devices (see the keywords for find_devices()).
- thread_kwds keywords to pass to Thread constructor.
- **kwds** same as in *Thread*.

empty_like (arr)

Allocates an array on GPU with the same attributes as arr.

from device (arr, dest=None, async=False)

Transfers the contents of arr to a numpy.ndarray object. The effect of dest parameter is the same as in to_device(). If async is True, the transfer is asynchronous (the thread-wide asynchronisity setting does not apply here).

Alternatively, one can use Array.get().

release()

Forcefully free critical resources (rendering the object unusable). In most cases you can rely on the garbage collector taking care of things. Calling this method explicitly may be necessary in case of CUDA API when you want to make sure the context got popped.

synchronize()

Forcefully synchronize this thread with the main program.

```
temp array (shape, dtype, strides=None, dependencies=None)
```

Creates an *Array* on GPU with given shape, dtype and strides. In order to reduce the memory footprint of the program, the temporary array manager will allow these arrays to overlap. Two arrays will not overlap, if one of them was specified in dependencies for the other one. For a list of values dependencies takes, see the reference entry for *TemporaryManager*.

```
to_device (arr, dest=None)
```

Copies an array to the device memory. If dest is specified, it is used as the destination, and the method returns None. Otherwise the destination array is created internally and returned from the method.

```
reikna.cluda.api.get_id()
```

Returns the identifier of this API.

```
reikna.cluda.api.get_platforms()
```

Returns a list of available *Platform* objects. In case of OpenCL returned objects are actually instances of pyopencl.Platform.

Temporary Arrays

Each *Thread* contains a special allocator for arrays with data that does not have to be persistent all the time. In many cases you only want some array to keep its contents between several kernel calls. This can be achieved by manually allocating and deallocating such arrays every time, but it slows the program down, and you have to synchronize the queue because allocation commands are not serialized. Therefore it is advantageous to use *temp_array()* method to get such arrays. It takes a list of dependencies as an optional parameter which gives the allocator a hint about which arrays should not use the same physical allocation.

```
 \begin{array}{ll} \textbf{class} \ \texttt{reikna.cluda.tempalloc.TemporaryManager} \ (\textit{thr}, & \textit{pack\_on\_alloc=False}, \\ & \textit{pack\_on\_free=False}) \end{array}
```

Base class for a manager of temporary allocations.

Parameters

- thr an instance of Thread.
- pack_on_alloc whether to repack allocations when a new allocation is requested.
- pack_on_free whether to repack allocations when an allocation is freed.

array (shape, dtype, strides=None, dependencies=None)

Returns a temporary array.

Parameters

- **shape** shape of the array.
- **dtype** data type of the array.
- **strides** tuple of bytes to step in each dimension when traversing an array.
- **dependencies** can be a *Array* instance (the ones containing persistent allocations will be ignored), an iterable with valid values, or an object with the attribute <u>__tempalloc__</u> which is a valid value (the last two will be processed recursively).

```
pack()
```

Packs the real allocations possibly reducing total memory usage. This process can be slow.

```
 \textbf{class} \ \texttt{reikna.cluda.tempalloc.TrivialManager} \ (*args, **kwds) \\ \textbf{Trivial manager} \ -- \ \text{allocates a separate buffer for each allocation request}.
```

```
class reikna.cluda.tempalloc.ZeroOffsetManager(*args, **kwds)
```

Tries to assign several allocation requests to a single real allocation, if dependencies allow that. All virtual allocations start from the beginning of real allocations.

Function modules

This module contains *Module* factories which are used to compensate for the lack of complex number operations in OpenCL, and the lack of C++ synthax which would allow one to write them.

reikna.cluda.functions.add(*in_dtypes, out_dtype=None)

Returns a *Module* with a function of len(in_dtypes) arguments that adds values of types in_dtypes. If out_dtype is given, it will be set as a return type for this function.

This is necessary since on some platforms the + operator for a complex and a real number works in an unexpected way (returning (a.x + b, a.y + b) instead of (a.x + b, a.y)).

reikna.cluda.functions.cast(out_dtype, in_dtype)

Returns a Module with a function of one argument that casts values of in_dtype to out_dtype.

reikna.cluda.functions.conj(dtype)

Returns a *Module* with a function of one argument that conjugates the value of type dtype (must be a complex data type).

reikna.cluda.functions.div(in_dtype1, in_dtype2, out_dtype=None)

Returns a *Module* with a function of two arguments that divides values of in_dtype1 and in_dtype2. If out dtype is given, it will be set as a return type for this function.

reikna.cluda.functions.exp(dtype)

Returns a *Module* with a function of one argument that exponentiates the value of type dtype (must be a real or complex data type).

reikna.cluda.functions.mul(*in_dtypes, out_dtype=None)

Returns a *Module* with a function of len(in_dtypes) arguments that multiplies values of types in_dtypes. If out_dtype is given, it will be set as a return type for this function.

reikna.cluda.functions.norm(dtype)

Returns a *Module* with a function of one argument that returns the 2-norm of the value of type dtype (product by the complex conjugate if the value is complex, square otherwise).

reikna.cluda.functions.polar(dtype)

Returns a *Module* with a function of two arguments that returns the complex-valued rho \star exp(i \star theta) for values rho, theta of type dtype (must be a real data type).

reikna.cluda.functions.polar unit (dtype)

Returns a *Module* with a function of one argument that returns a complex number (cos(theta), sin(theta)) for a value theta of type dtype (must be a real data type).

reikna.cluda.functions.pow (dtype, exponent_dtype=None, output_dtype=None)

Returns a *Module* with a function of two arguments that raises the first argument of type dtype to the power of the second argument of type exponent_dtype (an integer or real data type). If exponent_dtype or output_dtype are not given, they default to dtype. If dtype is not the same as output_dtype, the input is cast to output_dtype *before* exponentiation. If exponent_dtype is real, but both dtype and output_dtype are integer, a ValueError is raised.

Kernel toolbox

The stuff available for the kernel passed for compilation consists of two parts.

First, there are several objects available at the template rendering stage, namely numpy, reikna.cluda.dtypes (as dtypes), and reikna.helpers (as helpers).

Second, there is a set of macros attached to any kernel depending on the API it is being compiled for:

CUDA

If defined, specifies that the kernel is being compiled for CUDA API.

COMPILE_FAST_MATH

If defined, specifies that the compilation for this kernel was requested with fast_math == True.

LOCAL BARRIER

Synchronizes threads inside a block.

WITHIN KERNEL

Modifier for a device-only function declaration.

KERNEL

Modifier for the kernel function declaration.

GLOBAL MEM

Modifier for the global memory pointer argument.

LOCAL MEM

Modifier for the statically allocated local memory variable.

LOCAL MEM DYNAMIC

Modifier for the dynamically allocated local memory variable.

LOCAL MEM ARG

Modifier for the local memory argument in the device-only functions.

INLINE

Modifier for inline functions.

SIZE T

The type of local/global IDs and sizes. Equal to unsigned int for CUDA, and size_t for OpenCL (which can be 32- or 64-bit unsigned integer, depending on the device).

```
SIZE_T get_local_id (int dim)

SIZE_T get_group_id (int dim)

SIZE_T get_global_id (int dim)

SIZE_T get_local_size (int dim)

SIZE_T get_num_groups (int dim)

SIZE_T get global size (int dim)
```

Local, group and global identifiers and sizes. In case of CUDA mimic the behavior of corresponding OpenCL functions.

VSIZE T

The type of local/global IDs in the virtual grid. It is separate from $SIZE_T$ because the former is intended to be equivalent to what the backend is using, while $VSIZE_T$ is a separate type and can be made larger than $SIZE_T$ in the future if necessary.

ALIGN (int)

Used to specify an explicit alignment (in bytes) for fields in structures, as

```
typedef struct {
    char ALIGN(4) a;
    int b;
} MY_STRUCT;
```

VIRTUAL_SKIP_THREADS

This macro should start any kernel compiled with <code>compile_static()</code>. It skips all the empty threads resulting from fitting call parameters into backend limitations.

```
VSIZE_T virtual_local_id (int dim)

VSIZE_T virtual_group_id (int dim)

VSIZE_T virtual_global_id (int dim)

VSIZE_T virtual_local_size (int dim)

VSIZE_T virtual_num_groups (int dim)

VSIZE_T virtual_global_size (int dim)

VSIZE_T virtual_global_flat_id ()

VSIZE_T virtual_global_flat_size ()
```

Only available in StaticKernel objects obtained from compile_static(). Since its dimensions can differ from actual call dimensions, these functions have to be used.

Datatype tools

This module contains various convenience functions which operate with numpy.dtype objects.

```
reikna.cluda.dtypes.align(dtype)
```

Returns a new struct dtype with the field offsets changed to the ones a compiler would use (without being given any explicit alignment qualifiers). Ignores all existing explicit itemsizes and offsets.

```
reikna.cluda.dtypes.c_constant (val, dtype=None)
```

Returns a C-style numerical constant. If val has a struct dtype, the generated constant will have the form { . . . } and can be used as an initializer for a variable.

```
reikna.cluda.dtypes.c_path(path)
```

Returns a string corresponding to the path to a struct element in C. The path is the sequence of field names/array indices returned from flatten_dtype().

```
reikna.cluda.dtypes.cast (dtype)
```

Returns function that takes one argument and casts it to dtype.

```
reikna.cluda.dtypes.complex_ctr(dtype)
```

Returns name of the constructor for the given dtype.

```
reikna.cluda.dtypes.complex_for(dtype)
```

Returns complex dtype corresponding to given floating point dtype.

```
reikna.cluda.dtypes.ctype(dtype)
```

For a built-in C type, returns a string with the name of the type.

```
reikna.cluda.dtypes.ctype_module(dtype, ignore_alignment=False)
```

For a struct type, returns a <code>Module</code> object with the <code>typedef</code> of a struct corresponding to the given <code>dtype</code> (with its name set to the module prefix); falls back to <code>ctype()</code> otherwise.

The structure definition includes the alignment required to produce field offsets specified in dtype; therefore, dtype must be either a simple type, or have proper offsets and dtypes (the ones that can be reporduced in C using explicit alignment attributes, but without additional padding) and the attribute isalignedstruct == True. An aligned dtype can be produced either by standard means (aligned flag in numpy.dtype constructor and explicit offsets and itemsizes), or created out of an arbitrary dtype with the help of align().

If <code>ignore_alignment</code> is True, all of the above is ignored. The C structures produced will not have any explicit alignment modifiers. As a result, the the field offsets of <code>dtype</code> may differ from the ones chosen by the compiler.

Modules are cached and the function returns a single module instance for equal dtype's. Therefore inside a kernel it will be rendered with the same prefix everywhere it is used. This results in a behavior characteristic for a structural type system, same as for the basic dtype-ctype conversion.

Warning: As of numpy 1.8, the isalignedstruct attribute is not enough to ensure a mapping between a dtype and a C struct with only the fields that are present in the dtype. Therefore, ctype_module will make some additional checks and raise ValueError if it is not the case.

```
reikna.cluda.dtypes.detect_type(val)
     Find out the data type of val.
reikna.cluda.dtvpes.extract field(arr, path)
     Extracts an element from an array of struct dtype. The path is the sequence of field names/array indices
     returned from flatten dtype().
reikna.cluda.dtypes.flatten_dtype(dtype)
     Returns a list of tuples (path, dtype) for each of the basic dtypes in a (possibly nested) dtype. path is
     a list of field names/array indices leading to the corresponding element.
reikna.cluda.dtypes.is_complex(dtype)
     Returns True if dtype is complex.
reikna.cluda.dtypes.is_double(dtype)
     Returns True if dtype is double precision floating point.
reikna.cluda.dtypes.is_integer(dtype)
     Returns True if dtype is an integer.
reikna.cluda.dtypes.is_real(dtype)
     Returns True if dtype is a real.
reikna.cluda.dtypes.min scalar type (val)
     Wrapper for numpy.min_scalar_dtype which takes into account types supported by GPUs.
reikna.cluda.dtypes.normalize_type(dtype)
     Function for wrapping all dtypes coming from the user. numpy uses two different classes to represent dtypes,
     and one of them does not have some important attributes.
reikna.cluda.dtypes.normalize_types(dtypes)
     Same as normalize type (), but operates on a list of dtypes.
reikna.cluda.dtypes.real_for(dtype)
     Returns floating point dtype corresponding to given complex dtype.
reikna.cluda.dtypes.result_type(*dtypes)
     Wrapper for numpy.result_type which takes into account types supported by GPUs.
reikna.cluda.dtypes.zero_ctr(dtype)
     Returns the string with constructed zero value for the given dtype.
```

2.5.4 Core functionality

Classes necessary to create computations and transformations are exposed from the core module.

Computation signatures

```
class reikna.core.Type (dtype, shape=None, strides=None)
Represents an array or, as a degenerate case, scalar type of a computation parameter.
```

shape

A tuple of integers. Scalars are represented by an empty tuple.

dtype

A numpy.dtype instance.

ctype

A string with the name of C type corresponding to dtype, or a module if it is a struct type.

strides

Tuple of bytes to step in each dimension when traversing an array.

```
__call__(val)
```

Casts the given value to this type.

classmethod from_value (val)

Creates a Type object corresponding to the given value.

class reikna.core.Annotation(type_, role=None)

Computation parameter annotation, in the same sense as it is used for functions in the standard library.

Parameters

- type a Type object.
- role any of 'i' (input), 'o' (output), 'io' (input/output), 's' (scalar). Defaults to 's' for scalars and 'io' for arrays.

class reikna.core.Parameter(name, annotation, default=<class 'funcsigs._empty'>)

Computation parameter, in the same sense as it is used for functions in the standard library. In its terms, all computation parameters have kind POSITIONAL_OR_KEYWORD.

Parameters

- **name** parameter name.
- annotation an Annotation object.
- **default** default value for the parameter, can only be specified for scalars.

rename (new_name)

Creates a new Parameter object with the new name and the same annotation and default value.

class reikna.core.Signature (parameters)

Computation signature, in the same sense as it is used for functions in the standard library.

Parameters - a list of Parameter objects.

parameters

An OrderedDict with Parameter objects indexed by their names.

bind_with_defaults (args, kwds, cast=False)

Binds passed positional and keyword arguments to parameters in the signature and returns the resulting BoundArguments object.

Core classes

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class reikna.core.Computation (root_parameters)

A base class for computations, intended to be subclassed.

Parameters root_parameters - a list of Parameter objects.

signature

A Signature object representing current computation signature (taking into account connected transformations).

parameter

A named tuple of ComputationParameter objects corresponding to parameters from the current signature.

_build_plan (plan_factory, device_params, *args)

Derived classes override this method. It is called by <code>compile()</code> and supposed to return a <code>ComputationPlan</code> object.

Parameters

- plan_factory a callable returning a new ComputationPlan object.
- device_params a DeviceParameters object corresponding to the thread the computation is being compiled for.
- args KernelArgument objects, corresponding to parameters specified during the creation of this computation object.

_update_attributes()

Updates signature and parameter attributes. Called by the methods that change the signature.

compile (thread, fast_math=False)

Compiles the computation with the given *Thread* object and returns a *ComputationCallable* object. If fast_math is enabled, the compilation of all kernels is performed using the compiler options for fast and imprecise mathematical functions.

```
connect (_comp_connector, _trf, _tr_connector, **tr_from_comp)
```

Connect a transformation to the computation.

Parameters

- _comp_connector connection target a ComputationParameter object beloning to this computation object, or a string with its name.
- _trf a Transformation object.
- <u>_tr_connector</u> connector on the side of the transformation a **TransformationParameter object beloning to tr, or a string with its name.
- **tr_from_comp** a dictionary with the names of new or old computation parameters as keys, and *TransformationParameter* objects (or their names) as values.

Returns this computation object (modified).

Note: The resulting parameter order is determined by traversing the graph of connections depth-first (starting from the initial computation parameters), with the additional condition: the nodes do not change their order in the same branching level (i.e. in the list of computation or transformation parameters, both of which are ordered).

For example, consider a computation with parameters (a, b, c, d). If you connect a transformation (a', c) \rightarrow a, the resulting computation will have the signature (a', b, c, d) (as opposed to (a', c, b, d) it would have for the pure depth-first traversal).

class reikna.core.**Transformation** (*parameters*, *code*, *render_kwds=None*, *connectors=None*) A class containing a pure parallel transformation of arrays. Some restrictions apply:

•it cannot use local memory;

- •it cannot use global/local id getters (and depends only on externally passed indices);
- •it cannot have 'io' arguments;
- •it has at least one argument that uses <code>load_same</code> or <code>store_same</code>, and does it only once.

Parameters

- parameters a list of Parameter objects.
- **code** a source template for the transformation. Will be wrapped in a template def with positional arguments with the names of objects in parameters.
- render_kwds a dictionary with render keywords that will be passed to the snippet.
- **connectors** a list of parameter names suitable for connection. Defaults to all non-scalar parameters.

Result and attribute classes

```
class reikna.core.Indices (shape)
```

Encapsulates the information about index variables available for the snippet.

```
__getitem__(dim)
```

Returns the name of the index varibale for the dimension dim.

all()

Returns the comma-separated list of all index variable names (useful for passing the guiding indices verbatim in a load or store call).

A result of calling compile () on a computation. Represents a callable opaque GPGPU computation.

thread

A *Thread* object used to compile the computation.

signature

A Signature object.

parameter

A named tuple of *Type* objects corresponding to the callable's parameters.

```
__call__(*args, **kwds)
```

Execute the computation. In case of the OpenCL backend, returns a list of pyopencl. Event objects from nested kernel calls.

```
class reikna.core.computation.ComputationParameter(computation, name, type_)
```

Bases: Type

Represents a typed computation parameter. Can be used as a substitute of an array for functions which are only interested in array metadata.

```
connect (_trf, _tr_connector, **tr_from_comp)
```

Shortcut for *connect* () with this parameter as a first argument.

```
class reikna.core.computation.KernelArgument (name, type_)
```

Bases: Type

Represents an argument suitable to pass to planned kernel or computation call.

```
computation call (computation, *args, **kwds)
```

Adds a nested computation call. The computation value must be a *Computation* object. args and kwds are values to be passed to the computation.

kernel_call (*template_def*, *args*, *global_size*, *local_size=None*, *render_kwds=None*) Adds a kernel call to the plan.

Parameters

- template def Mako template def for the kernel.
- args a list consisting of *KernelArgument* objects, or scalar values wrapped in numpy.ndarray, that are going to be passed to the kernel during execution.
- global_size global size to use for the call, in row-major order.
- local_size local size to use for the call, in row-major order. If None, the local size will be picked automatically.
- render_kwds dictionary with additional values used to render the template.

persistent_array(arr)

Adds a persistent GPU array to the plan, and returns the corresponding KernelArgument.

```
temp_array (shape, dtype, strides=None)
```

Adds a temporary GPU array to the plan, and returns the corresponding *KernelArgument*. Temporary arrays can share physical memory, but in such a way that their contents is guaranteed to persist between the first and the last use in a kernel during the execution of the plan.

```
temp_array_like(arr)
```

Same as temp_array(), taking the array properties from array or array-like object arr.

Represents a typed transformation parameter. Can be used as a substitute of an array for functions which are only interested in array metadata.

```
 \begin{array}{c} \textbf{class} \ \texttt{reikna.core.transformation.KernelParameter} (name, & type\_, & load\_idx=None, \\ & store\_idx=None, & load\_same=None, \\ & store\_same=None, \\ & load\_combined\_idx=None, \\ & store\_combined\_idx=None) \end{array}
```

Providing an interface for accessing kernel arguments in a template. Depending on the parameter type, and whether it is used inside a computation or a transformation template, can have different load/store attributes available.

name

Parameter name

shape

dtype

ctype

strides

Same as in *Type*.

___str___()

Returns the C kernel parameter name corresponding to this parameter. It is the only method available for scalar parameters.

load idx

A module providing a macro with the signature (idx0, idx1, ...), returning the corresponding element of the array.

store idx

A module providing a macro with the signature (idx0, idx1, ..., val), saving val into the specified position.

load combined idx(slices)

A module providing a macro with the signature (cidx0, cidx1, ...), returning the element of the array corresponding to the new slicing of indices (e.g. an array with shape (2, 3, 4, 5, 6) sliced as slices=(2, 2, 1) is indexed as an array with shape (6, 20, 6)).

store combined idx(slices)

A module providing a macro with the signature (cidx0, cidx1, ..., val), saving val into the specified position corresponding to the new slicing of indices.

load_same

A module providing a macro that returns the element of the array corresponding to the indices used by the caller of the transformation.

store same

A module providing a macro with the signature (val) that stores val using the indices used by the caller of the transformation.

2.5.5 Computations

Algorithms

General purpose algorithms.

Pure parallel computations

 $\begin{array}{ll} \textbf{class} \; \texttt{reikna.algorithms.PureParallel} \; (\textit{parameters}, & \textit{code}, & \textit{guiding_array=None}, & \textit{ren-der_kwds=None}) \end{array}$

Bases: Computation

A general class for pure parallel computations (i.e. with no interaction between threads).

Parameters

- parameters a list of Parameter objects.
- **code** a source code for the computation. Can be a *Snippet* object which will be passed *Indices* object for the guiding_array as the first positional argument, and *KernelParameter* objects corresponding to parameters as the rest of positional arguments. If it is a string, such *Snippet* will be created out of it, with the parameter names idxs for the first one and the names of parameters for the remaining ones.
- guiding_array an tuple with the array shape, or the name of one of parameters. By default, the first parameter is chosen.
- render_kwds a dictionary with render keywords for the code.

compiled_signature(*args)

Parameters args – corresponds to the given parameters.

classmethod from_trf (trf, guiding_array=None)

Creates a PureParallel instance from a *Transformation* object. guiding_array can be a string with a name of an array parameter from trf, or the corresponding *TransformationParameter* object.

Transposition (permutation)

```
class reikna.algorithms.Transpose (arr_t, axes=None, block_width_override=None)
    Bases: Computation
```

Changes the order of axes in a multidimensional array. Works analogous to numpy.transpose.

Parameters

- **arr_t** an array-like defining the initial array.
- **axes** tuple with the new axes order. If None, then axes will be reversed.

compiled_signature (output:o, input:i)

Parameters

- output an array with all the attributes of arr_t, with the shape permuted according to axes.
- input an array with all the attributes of arr_t.

Reduction

```
class reikna.algorithms.Predicate(operation, empty)
    A predicate used in Reduce.
```

Parameters

- operation a *Snippet* object with two parameters which will take the names of two arguments to join.
- **empty** a numpy scalar with the empty value of the argument (the one which, being joined by another argument, does not change it).

```
reikna.algorithms.predicate_sum(dtype)
```

Returns a Predicate object which sums its arguments.

```
class reikna.algorithms.Reduce(arr_t, predicate, axes=None)
    Bases: Computation
```

Reduces the array over given axis using given binary operation.

Parameters

- **arr_t** an array-like defining the initial array.
- predicate a Predicate object.
- **axes** a list of non-repeating axes to reduce over. If None, the whole array will be reduced (in which case the shape of the output array is (1,)).

compiled_signature (output:o, input:i)

Parameters

• input – an array with the attributes of arr_t.

• output – an array with the attributes of arr_t, with its shape missing axes from axes.

Linear algebra

Linear algebra algorithms.

Matrix multiplication (dot product)

Bases: Computation

Multiplies two matrices using last two dimensions and batching over remaining dimensions. For batching to work, the products of remaining dimensions should be equal (then the multiplication will be performed piecewise), or one of them should equal 1 (then the multiplication will be batched over the remaining dimensions of the other matrix).

Parameters

- a_arr an array-like defining the first argument.
- **b_arr** an array-like defining the second argument.
- out_arr an array-like defining the output; if not given, both shape and dtype will be derived from a_arr and b_arr.
- block_width_override if provided, it will used as a block size of the multiplication kernel.
- transposed_a if True, the first matrix will be transposed before the multiplication.
- transposed_b if True, the second matrix will be transposed before the multiplication.

compiled_signature (output:o, matrix_a:i, matrix_b:i)

Parameters

- **output** the output of matrix multiplication.
- matrix_a the first argument.
- matrix b the second argument.

Matrix norms

class reikna.linalg.EntrywiseNorm(arr_t, order=2, axes=None)

Bases: Computation

Calculates the entrywise matrix norm (same as numpy.linalg.norm) of an arbitrary order r:

$$||A||_r = \left(\sum_{i,j,\dots} |A_{i,j,\dots}|^r\right)^{1/r}$$

Parameters

- arr_t an array-like defining the initial array.
- **order** the order r (any real number).

axes – a list of non-repeating axes to sum over. If None, the norm of the whole array will
be calculated.

compiled_signature (output:o, input:i)

Parameters

- input an array with the attributes of arr_t.
- output an array with the attributes of arr_t, with its shape missing axes from axes.

Fast Fourier transform and related utilities

Fast Fourier Transform

```
class reikna.fft.FFT(arr_t, axes=None)
    Bases: Computation
```

Performs the Fast Fourier Transform. The interface is similar to numpy.fft.fftn. The inverse transform is normalized so that IFFT (FFT (X)) = X.

Parameters

- arr_t an array-like defining the problem array.
- **axes** a tuple with axes over which to perform the transform. If not given, the transform is performed over all the axes.

Note: Current algorithm works most effectively with array dimensions being power of 2 This mostly applies to the axes over which the transform is performed, beacuse otherwise the computation falls back to the Bluestein's algorithm, which effectively halves the performance.

```
compiled_signature (output:o, input:i, inverse:s)
```

output and input may be the same array.

Parameters

- **output** an array with the attributes of arr t.
- **input** an array with the attributes of arr_t.
- inverse a scalar value castable to integer. If 0, output contains the forward FFT of input, if 1, the inverse one.

FFT frequency shift

```
class reikna.fft.FFTShift (arr_t, axes=None)
    Bases: Computation
```

Shift the zero-frequency component to the center of the spectrum. The interface is similar to numpy.fft.fftshift, and the output is the same for the same array shape and axes.

Parameters

- arr_t an array-like defining the problem array.
- axes a tuple with axes over which to perform the shift. If not given, the shift is performed over all the axes.

compiled signature (output:o, input:i)

output and input may be the same array.

Parameters

- **output** an array with the attributes of arr_t.
- **input** an array with the attributes of arr_t.

Discrete harmonic transform

reikna.dht.get_spatial_grid (modes, order, add_points=0)

Returns the spatial grid required to calculate the order power of a function defined in the harmonic mode space of the size modes. If add_points is 0, the grid has the minimum size required for exact transformation back to the mode space.

reikna.dht.harmonic(mode)

Returns an eigenfunction of order n = mode for the harmonic oscillator:

$$\phi_n = \frac{1}{\sqrt[4]{\pi}\sqrt{2^n n!}} H_n(x) \exp(-x^2/2),$$

where H_n is the n-th order "physicists" Hermite polynomial. The normalization is chosen so that $\int \phi_n^2(x) dx = 1$.

class reikna.dht.DHT (mode_arr, add_points=None, inverse=False, order=1, axes=None)

Bases: Computation

Discrete transform to and from harmonic oscillator modes. With inverse=True transforms a function defined by its expansion C_m , m=0...M-1 in the mode space with mode functions from harmonic(), to the coordinate space (F(x)) on the grid x from $get_spatial_grid()$. With inverse=False guarantees to recover first M modes of $F^k(x)$, where k is the order parameter.

For multiple dimensions the operation is the same, and the mode functions are products of 1D mode functions, i.e. $\phi_{l,m,n}^{3D}(x,y,z) = \phi_l(x)\phi_m(y)\phi_n(z)$.

For the detailed description of the algorithm, see Dion & Cances, PRE 67(4) 046706 (2003)

Parameters

- mode_arr an array-like object defining the shape of mode space. If inverse=False, its shape is used to define the mode space size.
- inverse False for forward (coordinate space -> mode space) transform, True for inverse (mode space -> coordinate space) transform.
- **axes** a tuple with axes over which to perform the transform. If not given, the transform is performed over all the axes.
- **order** if F is a function in mode space, the number of spatial points is chosen so that the transformation DHT [(DHT^{-1} [F]) ^order] could be performed.
- add_points a list of the same length as mode_arr shape, specifying the number of points in x-space to use in addition to minimally required (0 by default).

compiled_signature_forward(modes:o, coords:i)

compiled_signature_inverse (coords:o, modes:i)

Depending on inverse value, either of these two will be created.

Parameters

• modes – an array with the attributes of mode_arr.

• coords — an array with the shape depending on mode_arr, axes, order and add_points, and the dtype of mode_arr.

Counter-based random number generators

This module is based on the paper by Salmon et al., P. Int. C. High. Perform. 16 (2011). and the source code of Random123 library.

A counter-based random-number generator (CBRNG) is a parametrized function $f_k(c)$, where k is the key, c is the counter, and the function f_k defines a bijection in the set of integer numbers. Being applied to successive counters, the function produces a sequence of pseudo-random numbers. The key is an analogue of the seed of stateful RNGs; if the CBRNG is used to generate random numbers in parallel threads, the key is a combination of a seed and a unique thread number.

There are two types of generators available, threefry (uses large number of simple functions), and philox (uses smaller number of more complicated functions). The latter one is generally faster on GPUs; see the paper above for detailed comparisons. These generators can be further specialized to use words=2 or words=4 bitness=32-bit or bitness=64-bit counters. Obviously, the period of the generator equals to the cardinality of the set of possible counters. For example, if the counter consits of 4 64-bit numbers, then the period of the generator is 2^{256} . As for the key size, in case of threefry the key has the same size as the counter, and for philox the key is half its size.

The CBRNG class sets one of the words of the key (except for philox-2x64, where 32 bit of the only word in the key are used), the rest are the same for all threads and are derived from the provided seed. This limits the maximum number of number-generating threads (size). philox-2x32 has a 32-bit key and therefore cannot be used in CBRNG (although it can be used separately with the help of the kernel API).

The CBRNG class itself is stateless, same as other computations in Reikna, so you have to manage the generator state yourself. The state is created by the create_counters() method and contains a size counters. This state is then passed to, and updated by a CBRNG object.

class reikna.cbrng.CBRNG(randoms_arr, generators_dim, sampler, seed=None)
 Bases: Computation

Counter-based pseudo-random number generator class.

Parameters

- randoms_arr an array intended for storing generated random numbers.
- generators_dim the number of dimensions (counting from the end) which will use independent generators. For example, if randoms_arr has the shape (100, 200, 300) and generators_dim is 2, then in every sub-array (j, :, :), j = 0 ... 99, every element will use an independent generator.
- sampler a Sampler object.
- seed None for random seed, or an integer.

 $\textbf{classmethod sampler_name} \ (\textit{randoms_arr}, \textit{generators_dim}, \textit{sampler_kwds=None}, \textit{seed=None})$

A convenience constructor for the sampler sampler_name from <code>samplers</code>. The contents of the dictionary <code>sampler_kwds</code> will be passed to the sampler constructor function (with <code>bijection</code> being created automatically, and <code>dtype</code> taken from <code>randoms_arr</code>).

compiled_signature (counters:io, randoms:o)

Parameters

• counters - the RNG "state". All attributes are equal to the ones of the result of create_counters().

• randoms — generated random numbers. All attributes are equal to the ones of randoms_arr from the constructor.

create_counters()

Create a counter array for use in CBRNG.

Kernel API

class reikna.cbrnq.bijections.Bijection (module, word_dtype, key_dtype, counter_dtype)

Contains a CBRNG bijection module and accompanying metadata. Supports __process_modules__ protocol.

word_dtype

The data type of the integer word used by the generator.

key_words

The number of words used by the key.

counter_words

The number of words used by the counter.

key dtype

The numpy.dtype object representing a bijection key. Contains a single array field v with key_words of word_dtype elements.

counter_dtype

The numpy.dtype object representing a bijection counter. Contains a single array field v with key_words of word_dtype elements.

raw_functions

A dictionary dtype:function_name of available functions function_name in module that produce a random full-range integer dtype from a State, advancing it. Available functions: get_raw_uint32(), get_raw_uint64().

module

The module containing the CBRNG function. It provides the C functions below.

COUNTER_WORDS

Contains the value of counter_words.

KEY WORDS

Contains the value of *key_words*.

Word

Contains the type corresponding to word_dtype.

Key

Describes the bijection key. Alias for the structure generated from key_dtype.

Word v[KEY_WORDS]

Counter

Describes the bijection counter, or its output. Alias for the structure generated from counter_dtype.

Word v[COUNTER_WORDS]

Counter make_counter_from_int (int x)

Creates a counter object from an integer.

Counter bijection (Key key, Counter counter)

The main bijection function.

State

A structure containing the CBRNG state which is used by *samplers*.

State make_state (Key key, Counter counter)

Creates a new state object.

Counter get next unused counter (State state)

Extracts a counter which has not been used in random sampling.

uint32

A type of unsigned 32-bit word, corresponds to numpy.uint32.

uint64

A type of unsigned 64-bit word, corresponds to numpy.uint64.

```
uint32 get_raw_uint32 (State *state)
```

Returns uniformly distributed unsigned 32-bit word and updates the state.

```
uint64 get_raw_uint64 (State *state)
```

Returns uniformly distributed unsigned 64-bit word and updates the state.

reikna.cbrnq.bijections.philox (bitness, counter words, rounds=10)

A CBRNG based on a low number of slow rounds (multiplications).

Parameters

- bitness 32 or 64, corresponds to the size of generated random integers.
- **counter_words** 2 or 4, number of integers generated in one go.
- **rounds** 1 to 12, the more rounds, the better randomness is achieved. Default values are big enough to qualify as PRNG.

Returns a Bijection object.

reikna.cbrng.bijections.threefry(bitness, counter_words, rounds=20)

A CBRNG based on a big number of fast rounds (bit rotations).

Parameters

- bitness 32 or 64, corresponds to the size of generated random integers.
- **counter_words** 2 or 4, number of integers generated in one go.
- rounds 1 to 72, the more rounds, the better randomness is achieved. Default values are big enough to qualify as PRNG.

Returns a Bijection object.

 ${\bf class} \ {\tt reikna.cbrng.samplers.Sampler} \ ({\it bijection, module, dtype, randoms_per_call=1, determinis-per_call=1, determinis-per$

tic=False)

Contains a random distribution sampler module and accompanying metadata. Supports __process_modules__protocol.

deterministic

If True, every sampled random number consumes the same amount of counters.

randoms_per_call

How many random numbers one call to sample creates.

dtype

The data type of one random value produced by the sampler.

module

The module containing the distribution sampling function. It provides the C functions below.

RANDOMS PER CALL

Contains the value of randoms per call.

Value

Contains the type corresponding to dtype.

Result

Describes the sampling result.

value v[RANDOMS PER CALL]

Result sample (State *state)

Performs the sampling, updating the state.

reikna.cbrng.samplers.gamma(bijection, dtype, shape=1, scale=1)

Generates random numbers from the gamma distribution

$$P(x) = x^{k-1} \frac{e^{-x/\theta}}{\theta^k \Gamma(k)},$$

where k is shape, and θ is scale. Supported dtypes: float (32/64). Returns a Sampler object.

reikna.cbrng.samplers.normal_bm(bijection, dtype, mean=0, std=1)

Generates normally distributed random numbers with the mean mean and the standard deviation std using Box-Muller transform. Supported dtypes: float (32/64), complex (64/128). Produces two random numbers per call for real types and one number for complex types. Returns a Sampler object.

Note: In case of a complex dtype, std refers to the standard deviation of the complex numbers (same as numpy.std() returns), not real and imaginary components (which will be normally distributed with the standard deviation std / sqrt(2)). Consequently, while mean is of type dtype, std must be real.

reikna.cbrng.samplers.uniform_float(bijection, dtype, low=0, high=1)

Generates uniformly distributed floating-points numbers in the interval [low, high). Supported dtypes: float (32/64). A fixed number of counters is used in each thread. Returns a Sampler object.

reikna.cbrng.samplers.uniform_integer(bijection, dtype, low, high=None)

Generates uniformly distributed integer numbers in the interval [low, high). If high is None, the interval is [0, low). Supported dtypes: any numpy integers. If the size of the interval is a power of 2, a fixed number of counters is used in each thread. Returns a Sampler object.

reikna.cbrng.samplers.vonmises(bijection, dtype, mu=0, kappa=1)

Generates random numbers from the von Mises distribution

$$P(x) = \frac{\exp(\kappa \cos(x - \mu))}{2\pi I_0(\kappa)},$$

where μ is the mode, κ is the dispersion, and I_0 is the modified Bessel function of the first kind. Supported dtypes: float (32/64). Returns a *Sampler* object.

class reikna.cbrng.tools.KeyGenerator(module, base_key)

Contains a key generator module and accompanying metadata. Supports __process_modules__ protocol.

module

A module with the key generator function:

Key key_from_int (int idx)

Generates and returns a key, suitable for the bijection which was given to the constructor.

classmethod create (bijection, seed=None, reserve_id_space=True)

Creates a generator.

Parameters

- bijection a Bijection object.
- **seed** an integer, or numpy array of 32-bit unsigned integers.
- reserve_id_space if True, the last 32 bit of the key will be reserved for the thread identifier. As a result, the total size of the key should be 64 bit or more. If False, the thread identifier will be just added to the key, which will still result in different keys for different threads, with the danger that different seeds produce the same sequences.

reference (idx)

Reference function that returns the key given the thread identifier. Uses the same algorithm as the module.

2.5.6 Transformations

This module contains a number of pre-created transformations.

```
reikna.transformations.add_const (arr_t, param)
```

Returns an addition transformation with a fixed parameter (1 output, 1 input): output = input + param.

reikna.transformations.add_param(arr_t, param_dtype)

Returns an addition transformation with a dynamic parameter (1 output, 1 input, 1 scalar): output = input + param.

reikna.transformations.broadcast_const(arr_t, val)

Returns a transformation that broadcasts the given constant to the array output (1 output): output = val.

reikna.transformations.broadcast_param(arr_t)

Returns a transformation that broadcasts the free parameter to the array output (1 output, 1 param): output = param.

reikna.transformations.combine_complex(output_arr_t)

Returns a transformation that joins two real inputs into complex output (1 output, 2 inputs): output = real + 1j * imag.

reikna.transformations.copy(arr_t, out_arr_t=None)

Returns an identity transformation (1 output, 1 input): output = input. Output array type out_arr_t may have different strides, but must have the same shape and data type.

reikna.transformations.div const (arr t, param)

Returns a scaling transformation with a fixed parameter (1 output, 1 input): output = input / param.

reikna.transformations.div_param(arr_t, param_dtype)

Returns a scaling transformation with a dynamic parameter (1 output, 1 input, 1 scalar): output = input / param.

reikna.transformations.ignore(arr_t)

Returns a transformation that ignores the output it is attached to.

reikna.transformations.mul_const(arr_t, param)

Returns a scaling transformation with a fixed parameter (1 output, 1 input): output = input * param.

reikna.transformations.mul_param(arr_t, param_dtype)

Returns a scaling transformation with a dynamic parameter (1 output, 1 input, 1 scalar): output = input * param.

reikna.transformations.norm_const(arr_t, order)

Returns a transformation that calculates the order-norm (1 output, 1 input): output = abs(input) ** order.

```
reikna.transformations.norm_param(arr_t)
   Returns a transformation that calculates the order-norm (1 output, 1 input, 1 param): output =
   abs(input) ** order.

reikna.transformations.split_complex(input_arr_t)
   Returns a transformation that splits complex input into two real outputs (2 outputs, 1 input): real =
   Re(input), imag = Im(input).
```

2.6 Release history

2.6.1 0.6.8 (18 Dec 2016)

- ADDED: a von Mises distribution sampler (vonmises ()).
- ADDED: div_const() and div_param() transformations.
- ADDED: Kernel.prepared_call, Kernel.__call__ and StaticKernel.__call__ now return the resulting Event object in case of the OpenCL backend. ComputationCallable.__call__ returns a list of Event objects from the nested kernel calls.
- FIXED: properly handling the case of an unfinished __init__() in Thread (when __del__() tries to access non-existent attributes).
- FIXED: an error when using from_trf() without specifying the guiding array in Py3.
- FIXED: (reported by @mountaindust) Array. copy now actually copies the array contents in CUDA backend.
- FIXED: (reported by @Philonoist) load_idx/store_idx handled expressions in parameters incorrectly (errors during macro expansion).
- FIXED: a minor bug in the information displayed during the interactive Thread creation.
- FIXED: class names in the test suite that produced errors (due to the changed rules for test discovery in py.test).
- FIXED: updated ReturnValuesPlugin in the test suite to conform to py.test interface changes.

2.6.2 0.6.7 (11 Mar 2016)

- ADDED: an example of a transposition-based n-dimensional FFT (demo_fftn_with_transpose.py).
- FIXED: a problem with Beignet OpenCL driver where the INLINE macro was being redefined.
- FIXED: a bug in Reduce where reduction over a struct type with a nested array produced a template rendering error.
- FIXED: now taking the minimum time over several attempts instead of the average in several performance tests (as it is done in the rest of the test suite).
- FIXED: *Transpose* now calculates the required elementary transpositions in the constructor instead of doing it during the compilation.

2.6.3 0.6.6 (11 May 2015)

- FIXED: a bug with the NAN constant not being defined in CUDA on Windows.
- FIXED: (PR by @ringw) copying and arithmetic operations on Reikna arrays now preserve the array type instead of resetting it to PyOpenCL/PyCUDA array.

- FIXED: a bug in virtual size finding algorithm that could cause get_local_id(ndim)/get_global_id(ndim) being called with an argument out of the range supported by the OpenCL standard, causing compilation fails on some platforms.
- FIXED: now omitting some of redundant modulus operations in virtual size functions.
- ADDED: an example of a spectrogram-calculating computation (demo_specgram.py).

2.6.4 0.6.5 (31 Mar 2015)

- CHANGED: the correspondence for numpy.uintp is not registered by default anymore this type is not really useful in CPU-GPU interaction.
- FIXED: (reported by J. Vacher) dtype/ctype correspondences for 64-bit integer types are registered even if the Python interpreter is 32-bit.
- ADDED: ComputationCallable objects expose the attribute thread.
- ADDED: FFTShift computation.
- ADDED: an example of an element-reshuffling transformation.

2.6.5 0.6.4 (29 Sep 2014)

- CHANGED: renamed power_dtype parameter to exponent_dtype (a more correct term) in pow().
- FIXED: (PR by @ringw) exception caused by printing CUDA program object.
- FIXED: pow() (0, 0) now returns 1 as it should.
- ADDED: an example of *FFT* with a custom transformation.
- ADDED: a type check in the FFT constructor.
- ADDED: an explicit output_dtype parameter for pow().
- ADDED: Array objects for each backend expose the attribute thread.

2.6.6 0.6.3 (18 Jun 2014)

- FIXED: (@schreon) a bug preventing the usage of EntrywiseNorm with custom axes.
- FIXED: (PR by @SyamGadde) removed syntax constructions incompatible with Python 2.6.
- FIXED: added Python 3.4 to the list of classifiers.

2.6.7 0.6.2 (20 Feb 2014)

- ADDED: pow() function module in CLUDA.
- ADDED: a function any api() that returns some supported GPGPU API module.
- ADDED: an example of Reduce with a custom data type.
- FIXED: a Py3 compatibility issue in Reduce introduced in 0.6.1.
- FIXED: a bug due to the interaction between the implementation of from_trf() and the logic of processing nested computations.
- FIXED: a bug in FFT leading to undefined behavior on some OpenCL platforms.

2.6.8 0.6.1 (4 Feb 2014)

• FIXED: Reduce can now pick a decreased work group size if the attached transformations are too demanding.

2.6.9 0.6.0 (27 Dec 2013)

- CHANGED: some computations were moved to sub-packages: PureParallel, Transpose and Reduce to reikna.algorithms, MatrixMul and EntrywiseNorm to reikna.linalg.
- CHANGED: scale_const and scale_param were renamed to mul_const() and mul_param(), and the scalar parameter name of the latter was renamed from coeff to param.
- ADDED: two transformations for norm of an arbitrary order: norm_const() and norm_param().
- ADDED: stub transformation ignore().
- ADDED: broadcasting transformations broadcast_const() and broadcast_param().
- ADDED: addition transformations add_const() and add_param().
- ADDED: EntrywiseNorm computation.
- ADDED: support for multi-dimensional sub-arrays in c_constant() and flatten_dtype().
- ADDED: helper functions extract_field() and c_path() to work in conjunction with flatten_dtype().
- ADDED: a function module add().
- FIXED: casting a coefficient in the normal_bm() template to a correct dtype.
- FIXED: cast () avoids casting if the value already has the target dtype (since numpy.cast does not work with struct dtypes, see issue #4148).
- FIXED: a error in transformation module rendering for scalar parameters with struct dtypes.
- FIXED: normalizing dtypes in several functions from dtypes to avoid errors with numpy dtype shortcuts.

2.6.10 0.5.2 (17 Dec 2013)

- ADDED: normal_bm() now supports complex dtypes.
- FIXED: a nested <code>PureParallel</code> can now take several identical argument objects as arguments.
- FIXED: a nested computation can now take a single input/output argument (e.g. a temporary array) as separate input and output arguments.
- FIXED: a critical bug in CBRNG that could lead to the counter array not being updated.
- FIXED: convenience constructors of CBRNG can now properly handle None as samplers_kwds.

2.6.11 0.5.1 (30 Nov 2013)

• FIXED: a possible infinite loop in <code>compile_static()</code> local size finding algorithm.

2.6.12 0.5.0 (25 Nov 2013)

- CHANGED: KernelParameter is not derived from Type anymore (although it still retains the corresponding attributes).
- CHANGED: Predicate now takes a dtype'd value as empty, not a string.
- CHANGED: The logic of processing struct dtypes was reworked, and adjust_alignment was removed. Instead, one should use <code>align()</code> (which does not take a Thread parameter) to get a dtype with the offsets and itemsize equal to those a compiler would set. On the other hand, <code>ctype_module()</code> attempts to set the alignments such that the field offsets are the same as in the given numpy dtype (unless <code>ignore_alignments</code> flag is set).
- ADDED: struct dtypes support in c_constant ().
- ADDED: flatten dtype() helper function.
- ADDED: added transposed_a and transposed_b keyword parameters to MatrixMul.
- ADDED: algorithm cascading to Reduce, leading to 3-4 times increase in performance.
- ADDED: polar_unit () function module in CLUDA.
- ADDED: support for arrays with 0-dimensional shape as computation and transformation arguments.
- FIXED: a bug in Reduce, which lead to incorrect results in cases when the reduction power is exactly equal to the maximum one.
- FIXED: *Transpose* now works correctly for struct dtypes.
- FIXED: bounding_power_of_2 now correctly returns 1 instead of 2 being given 1 as an argument.
- FIXED: compile_static() local size finding algorithm is much less prone to failure now.

2.6.13 0.4.0 (10 Nov 2013)

- CHANGED: supports_dtype() method moved from Thread to DeviceParameters.
- CHANGED: fast_math keyword parameter moved from Thread constructor to compile() and compile_static(). It is also False by default, instead of True. Correspondingly, THREAD_FAST_MATH macro was renamed to COMPILE_FAST_MATH.
- CHANGED: CBRNG modules are using the dtype-to-ctype support. Correspondingly, the C types for keys and counters can be obtained by calling <code>ctype_module()</code> on <code>key_dtype</code> and <code>counter_dtype</code> attributes. The module wrappers still define their types, but their names are using a different naming convention now.
- ADDED: module generator for nested dtypes (ctype_module()) and a function to get natural field offsets for a given API/device (adjust_alignment).
- ADDED: fast_math keyword parameter in <code>compile()</code>. In other words, now fast_math can be set per computation.
- ADDED: ALIGN macro is available in CLUDA kernels.
- ADDED: support for struct types as Computation arguments (for them, the ctypes attributes contain the corresponding module obtained with ctype_module()).
- ADDED: support for non-sequential axes in Reduce.
- FIXED: bug in the interactive Thread creation (reported by James Bergstra).
- FIXED: Py3-incompatibility in the interactive Thread creation.
- FIXED: some code paths in virtual size finding algorithm could result in a type error.

• FIXED: improved the speed of test collection by reusing Thread objects.

2.6.14 0.3.6 (9 Aug 2013)

- ADDED: the first argument to the Transformation or PureParallel snippet is now a reikna.core.Indices object instead of a list.
- ADDED: classmethod PureParallel.from_trf(), which allows one to create a pure parallel computation out of a transformation.
- FIXED: improved Computation.compile() performance for complicated computations by precreating transformation templates.

2.6.15 0.3.5 (6 Aug 2013)

• FIXED: bug with virtual size algorithms returning floating point global and local sizes in Py2.

2.6.16 0.3.4 (3 Aug 2013)

- CHANGED: virtual sizes algorithms were rewritten and are now more maintainable. In addition, virtual sizes
 can now handle any number of dimensions of local and global size, providing the device can support the corresponding total number of work items and groups.
- CHANGED: id- and size- getting kernel functions now have return types corresponding to their equivalents. Virtual size functions have their own independent return type.
- CHANGED: Thread.compile_static() and ComputationPlan.kernel_call() take global and local sizes in the row-major order, to correspond to the matrix indexing in load/store macros.
- FIXED: requirements for PyCUDA extras (a currently non-existent version was specified).
- FIXED: an error in gamma distribution sampler, which lead to slightly wrong shape of the resulting distribution.

2.6.17 0.3.3 (29 Jul 2013)

FIXED: package metadata.

2.6.18 0.3.2 (29 Jul 2013)

- ADDED: same module object, when being called without arguments from other modules/snippets, is rendered
 only once and returns the same prefix each time. This allows one to create structure declarations that can be
 used by functions in several modules.
- ADDED: reworked cbrnq module and exposed kernel interface of bijections and samplers.
- CHANGED: slightly changed the algorithm that determines the order of computation parameters after a transformation is connected to it. Now the ordering inside a list of initial computation parameters or a list of a single transformation parameters is preserved.
- CHANGED: kernel declaration string is now passed explicitly to a kernel template as the first parameter.
- FIXED: typo in FFT performance test.
- FIXED: bug in FFT that could result in changing the contents of the input array to one of the intermediate results.

- FIXED: missing data type normalization in c_constant ().
- FIXED: Py3 incompatibility in cluda.cuda.
- FIXED: updated some obsolete computation docstrings.

2.6.19 0.3.1 (25 Jul 2013)

- FIXED: too strict array type check for nested computations that caused some tests to fail.
- FIXED: default values of scalar parameters are now processed correctly.
- FIXED: Mako threw name-not-found exceptions on some list comprehensions in FFT template.
- FIXED: some earlier-introduced errors in tests.
- INTERNAL: pylint was ran and many stylistic errors fixed.

2.6.20 0.3.0 (23 Jul 2013)

Major core API change:

- Computations have function-like signatures with the standard Signature interface; no more separation of inputs/outputs/scalars.
- Generic transformations were ditched; all the transformations have static types now.
- Transformations can now change array shapes, and load/store from/to external arrays in output/input transformations.
- No flat array access in kernels; all access goes through indices. This opens the road for correct and automatic stride support (not fully implemented yet).
- · Computations and accompanying classes are stateless, and their creation is more straightforward.

Other stuff:

- Bumped Python requirements to >=2.6 or >=3.2, and added a dependency on funcsig.
- ADDED: more tests for cluda.functions.
- ADDED: module/snippet attributes discovery protocol for custom objects.
- ADDED: strides support to array allocation functions in CLUDA.
- ADDED: modules can now take positional arguments on instantiation, same as snippets.
- CHANGED: Elementwise becomes PureParallel (as it is not always elementwise).
- FIXED: incorrect behavior of functions.norm() for non-complex arguments.
- FIXED: undefined variable in functions.exp() template (reported by Thibault North).
- FIXED: inconsistent block/grid shapes in static kernels

2.6.21 0.2.4 (11 May 2013)

- ADDED: ability to introduce new scalar arguments for nested computations (the API is quite ugly at the moment).
- FIXED: handling prefixes properly when connecting transformations to nested computations.
- FIXED: bug in dependency inference algorithm which caused it to ignore allocations in nested computations.

2.6. Release history

2.6.22 0.2.3 (25 Apr 2013)

- ADDED: explicit release() (primarily for certain rare CUDA use cases).
- CHANGED: CLUDA API discovery interface (see the documentation).
- CHANGED: The part of CLUDA API that is supposed to be used by other layers was moved to the __init__.py.
- CHANGED: CLUDA Context was renamed to Thread, to avoid confusion with PyCUDA/PyOpenCL contexts.
- CHANGED: signature of create(); it can filter devices now, and supports interactive mode.
- CHANGED: Module with snippet=True is now Snippet
- FIXED: added transformation.mako and cbrng_ref.py to the distribution package.
- FIXED: incorrect parameter generation in test/cluda/cluda_vsizes/ids.
- FIXED: skipping testcases with incompatible parameters in test/cluda/cluda_vsizes/ids and sizes.
- FIXED: setting the correct length of max num groups in case of CUDA and a device with CC < 2.
- FIXED: typo in cluda.api_discovery.

2.6.23 0.2.2 (20 Apr 2013)

- ADDED: ability to use custom argument names in transformations.
- ADDED: multi-argument mul().
- ADDED: counter-based random number generator CBRNG.
- ADDED: reikna.elementwise.Elementwise now supports argument dependencies.
- ADDED: Module support in CLUDA; see *Tutorial: modules and snippets* for details.
- ADDED: template_def().
- CHANGED: reikna.cluda.kernel.render_template_source is the main renderer now.
- CHANGED: FuncCollector class was removed; functions are now used as common modules.
- CHANGED: all templates created with template_for() are now rendered with from __future__ import division.
- CHANGED: signature of OperationRecorder.add_kernel takes a renderable instead of a full template.
- CHANGED: compile_static() now takes a template instead of a source.
- CHANGED: reikna.elementwise.Elementwise now uses modules.
- FIXED: potential problem with local size finidng in static kernels (first approximation for the maximum workgroup size was not that good)
- FIXED: some OpenCL compilation warnings caused by an incorrect version querying macro.
- FIXED: bug with incorrect processing of scalar global size in static kernels.
- FIXED: bug in variance estimates in CBRNG tests.
- FIXED: error in the temporary variable type in reikna.cluda.functions.polar() and reikna.cluda.functions.exp().

2.6.24 0.2.1 (8 Mar 2013)

- FIXED: function names for kernel polar (), exp() and conj().
- FIXED: added forgotten kernel norm() handler.
- FIXED: bug in Py. Test testcase execution hook which caused every test to run twice.
- FIXED: bug in nested computation processing for computation with more than one kernel.
- FIXED: added dependencies between MatrixMul kernel arguments.
- FIXED: taking into account dependencies between input and output arrays as well as the ones between internal allocations necessary for nested computations.
- ADDED: discrete harmonic transform DHT (calculated using Gauss-Hermite quadrature).

2.6.25 0.2.0 (3 Mar 2013)

- Added FFT computation (slightly optimized PyFFT version + Bluestein's algorithm for non-power-of-2 FFT sizes)
- Added Python 3 compatibility
- · Added Thread-global automatic memory packing
- Added polar(), conj() and exp() functions to kernel toolbox
- · Changed name because of the clash with another Tigger.

2.6.26 0.1.0 (12 Sep 2012)

- · Lots of changes in the API
- · Added elementwise, reduction and transposition computations
- Extended API reference and added topical guides

2.6.27 0.0.1 (22 Jul 2012)

- · Created basic core for computations and transformations
- Added matrix multiplication computation
- · Created basic documentation

2.6. Release history

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