PSyclone Documentation

Release 1.6.0

Rupert Ford, Joerg Henrichs, Iva Kavcic and Andrew Porter

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CONTENTS

PSyclone, the PSy code generator, is being developed for use in finite element, finite volume and finite difference codes. PSyclone development started with the aim to support the emerging API in the GungHo project for a finite element dynamical core.

The GungHo project was initiated in 2011 to address challenges of weather and climate prediction on the next generation of supercomputers. The project ran for 5 years as a collaboration between the Met Office, NERC (via NERC funded academics) and STFC. It laid a foundation for redesign of the heart of the Met Office's Unified Model, known as the dynamical core, from the choices of numerical methods and model grids to the implementation of parallel algorithms that will scale to millions of cores.

The software infrastructure based on the GungHo project recommendations is now being developed in the LFRic project and is expected to be operational in 2022. Its development is led by the requirements to support multiple meshes and element types, thus allowing for future model development.

GungHo also proposed a novel separation of concerns for the software implementation of the dynamical core. This approach distinguishes between three layers: the Algorithm layer, the Kernel layer and the Parallelisation System (PSy) layer. Together this separation is termed PSyKAl.

The Algorithm layer specifies the algorithm that the scientist would like to run (in terms of calls to kernel routines and built-in operations) and logically operates on full fields.

The Kernel layer provides the implementation of the code kernels as subroutines. These subroutines operate on local fields (a set of elements, a vertical column, or a set of vertical columns, depending on the kernel).

The PSy layer sits in-between the algorithm and kernel layers and its primary role is to provide node-based parallel performance for the target architecture. The PSy layer can be optimised for a particular hardware architecture, such as multi-core, many-core, GPGPUs, or some combination thereof with no change to the algorithm or kernel layer code. This approach therefore offers the potential for portable performance.

Rather than writing the PSy layer manually, the PSyclone code generation system can help a user to optimise the code for a particular architecture (by providing optimisations such as blocking, loop merging, inlining etc), or alternatively, generate the PSy layer automatically.

PSyclone is also being extended to support an API being developed in the GOcean project for two finite difference ocean model benchmarks, one of which is based on the NEMO ocean model.

CHAPTER

ONE

GETTING GOING

Download

PSyclone is available on the Python Package Index (pypi.org) and is hosted on github:

`https://github.com/stfc/PSyclone`

The latest release is 1.6.0 and the latest stable version is on the master branch.

PSyclone can be installed using pip:

```
> pip install psyclone
```

or downloaded from github - either see 1.6.0 in the `releases` tab on the PSyclone page or download and extract the latest release of PSyclone directly, e.g.

```
> wget https://github.com/stfc/PSyclone/archive/1.6.0.tar.gz
> gunzip 1.6.0.tar.gz
> tar xf 1.6.0.tar
> rm 1.6.0.tar
> ls
PSyclone-1.6.0
```

Alternatively the PSyclone repository can be cloned:

```
> git clone https://github.com/stfc/PSyclone.git
```

By default you will have access to the master branch if you clone. To change to the latest release then subsequently do the following

```
> git checkout tags/1.6.0
```

Hereon the location where you download or clone PSyclone (including the PSyclone directory itself) will be referred to as <PSYCLONEHOME>

Dependencies

PSyclone is written in Python so needs Python to be installed on the target machine. PSyclone has been tested under Python 2.6.5, 2.7.3 and 3.6.

Warning: As of version 1.6, PSyclone requires version 0.0.7 or greater of fparser.

PSyclone immediately relies on four external Python packages; `six`, `configparser`, `fparser` and `pyparsing`. In order to run the test suite `py.test` is required. The easiest way to satisfy the Python dependencies is to use the Python Package Index (pypi.org) and `pip`. See https://packaging.python.org/installing/ for more information.

If everything is working correctly then using pip to install PSyclone:

```
> pip install psyclone
```

will automatically install the Python dependencies (`fparser` and `pyparsing`).

In addition to the mandatory dependencies just described, PSyclone also has optional dependencies on both `graphviz` and `termcolor`. PSyclone can use graphviz to produce a visualisation of a schedule's dependency graph. If this is desired then the Python package `graphviz` (for the Python bindings) as well as the graphviz package itself must be installed. If the `graphviz` package is not available then the associated PSyclone routines will return silently and no visualisations will be produced. The Python package `termcolor` is used for pretty-printing a schedule in terminals that support coloured text. If the package is not available then the schedule is simply printed in plain text without colour highlighting.

System-specific set-up

System-specific set-up instructions are available for Ubuntu 14.04.2 and OpenSUSE 42.2.

fparser

The fparser package (https://github.com/stfc/fparser) is a Fortran parser originally developed as a part of the f2py project.

The minimum version of fparser required by PSyclone is currently 0.0.7 but we strongly recommend you install the latest version to reduce the chance of encountering problems when parsing existing algorithm or kernel code. (Note that for older versions of PSyclone up to and including 1.5.1 you must use version 0.0.6 of fparser.)

fparser is available from the Python Package Index and thus may be installed using `pip` (https://packaging.python.org/installing/#requirements-for-installing-packages):

```
> pip install fparser
```

If you do not have sufficient permissions to perform a system-wide install then you can instruct pip to do a user-local install:

```
> pip install --user fparser
```

Should you wish to remove fparser then simply do:

```
> pip uninstall fparser
```

If you have already installed fparser and want to upgrade to the latest version simply do:

```
> pip install fparser --upgrade
```

pyparsing

PSyclone requires pyparsing, a library designed to allow parsers to be be built in Python. PSyclone uses pyparsing to parse fortran regular expressions as fparser does not fully parse these, (see http://pyparsing.wikispaces.com for more information).

PSyclone has been tested with pyparsing versions 1.5.2, 2.0.1 and 2.2.0.

You can test whether pyparsing is already installed on your machine by typing `import pyparsing` from the python command line. If pyparsing is installed, this command will complete succesfully. If pyparsing is installed you can check its version by typing `pyparsing.__version__` after succesfully importing it.

If pyparsing is not installed on your system then it may be installed from the Python Package Index using `pip`:

```
> pip install pyparsing
```

Should you wish to, uninstalling is simply performed by doing:

```
> pip uninstall pyparsing
```

If you do not have sufficient privileges for a system-wide install then you can instruct pip to do a user-local install:

```
> pip install --user pyparsing
```

Alternatively, you could follow the instructions here http://pyparsing.wikispaces.com/Download+and+Installation.

graphviz

The data dependencies of a PSy-layer schedule (see Section *Schedule*) determine the validity of changes to a schedule. PSyclone supports the visualisation of these dependencies as a graph using graphviz. This visualisation is not needed to use PSyclone.

If the Python bindings to graphviz are not installed on your system then it may be installed from the Python Package Index using `pip`:

```
> sudo pip install graphviz
```

Should you wish to, uninstalling is simply performed by doing:

```
> sudo pip uninstall graphviz
```

If you do not have sufficient privileges for a system-wide install then you can instruct pip to do a user-local install:

```
> pip install --user graphviz
```

If graphviz itself is not installed on your system and your system supports the `apt` package manager then see below, otherwise please refer to the download and install instructions which are available here http://www.graphviz.org/Download..php.

If your system supports the `apt` package manager then it can be installed and removed in the following way:

```
> sudo apt install graphviz
> sudo apt remove graphviz
```

termcolor

By default, the `view()` method of a `schedule` object (representing the schedule of a PSy-layer routine) prints a plain-text representation to standard-out. However, if the `termcolor` package is available then PSyclone uses this to add colour highlighting to the output text.

Installation (and uninstallation) of this package can be done via `pip` in exactly the same way as for graphviz, as described above.

py.test

The PSyclone test suite uses py.test. This is not needed to use PSyclone but is useful to check whether PSyclone is working correctly on your system. You can test whether it is already installed by simply typing `py.test` at a shell prompt. If it is present you will get output that begins with

```
======================== test session starts ==================
```

If you do not have it then py.test can again be installed using `pip` or from here http://pytest.org/latest/ (or specifically here http://pytest.org/latest/getting-started.html).

Environment

In order to use PSyclone (including running the test suite and building documentation) you will need to install it. The simplest way to do this is to use pip with the supplied `setup.py` file:

```
> cd <PSYCLONEHOME>
> pip install .
```

By default pip will attempt a system-wide install. If you wish to do a user-local install instead then supply the `--user` flag:

```
> pip install --user .
```

This installs the PSyclone modules in ~/.local/lib/pythonX.Y/site-packages (where X.Y is the version of Python that you are using) and the 'psyclone' script in ~/.local/bin. Depending on your linux distribution, you may need to add the latter location to your $PATH.

If for some reason you'd rather not use pip then you can run the setup manually:

```
> python setup.py install
```

or, if you don't have root access:

```
> python setup.py install --user
```

or,

```
> python setup.py install --prefix /my/install/path
```

If using the latter method then it will be necessary to take further action to ensure PSyclone can find the configuration file installed as a part of this process - see below.

Configuration

Various aspects of PSyclone are configured through a configuration file, `psyclone.cfg`. The default version of this file is installed to `<python-base-prefix>/shared/psyclone/` during the installation process. If a system-wide installation is being performed then this will be something like `/usr/share/psyclone/`. If a user-local installation is performed (`--user` flag to `pip install`) then the location will be something like `~/.local/share/psyclone/`.

Warning: if PSyclone is installed to a non-standard location (e.g. by specifying the `--prefix=/some/path` option to `pip install`) then PSyclone will not be able to find the configuration file at execution time. There are two solutions to this: 1. copy the configuration file to a location where PSyclone will find it (see *Configuration*) or 2. set the `PSYCLONE_CONFIG` environment variable to the full-path to the configuration file, e.g.:

```
> export PSYCLONE_CONFIG=/some/path/PSyclone/config/psyclone.cfg
```

Warning: when installing in 'editable' mode (`-e` flag to pip), pip does *not* install the configuration file. You will have to take one of the two actions described above.

See *Configuration* for details of the settings contained within the config file.

Test

Once you have the necessary dependencies installed and your environment configured, you can check that things are working by using the PSyclone test suite. These tests are not required and can be skipped if preferred:

```
> cd <PSYCLONEHOME>/src/psyclone/tests
> py.test
```

If everything is working as expected then you should see output similar to:

```
============================= test session starts ==============================
platform linux2 -- Python 2.6.5 -- py-1.4.29 -- pytest-2.7.2
rootdir: /home/rupert/proj/GungHoSVN/PSyclone_r3373_scripts/src/tests, inifile:
collected 175 items

alggen_test.py .......xxxxxxxxxxx.
dynamo0p1_transformations_test.py .
dynamo0p3_test.py ....................................x
generator_test.py ...................
ghproto_transformations_test.py x
gocean0p1_transformations_test.py .......
gocean1p0_test.py ....
gocean1p0_transformations_test.py ......................x........
parser_test.py ..........
psyGen_test.py ..............................

=================== 160 passed, 15 xfailed in 13.59 seconds ====================
```

Most of the tests use Fortran source files in the `<PSYCLONEHOME>/src/psyclone/tests` directory and many of them can be compiled during the testing process. To enable compilation testing run:

```
> py.test --compile --f90="<compiler_name>" --f90flags="<compiler_flags_list>"
```

`"<compiler_name>"` and `"<compiler_flags_list>"` are optional arguments. The default value for `"<compiler_name>"` is `"gfortran"` and there are no defaults for the `"<compiler_flags_list>"`. Please note that the onus is on the user to provide correct values for these options.

Run

You are now ready to try running PSyclone on the examples. One way of doing this is to use the `psyclone` driver script. Assuming it is on your PATH:

```
> psyclone
usage: psyclone [-h] [-oalg OALG] [-opsy OPSY] [-api API] [-s SCRIPT]
                [-d DIRECTORY] [-l] [-dm] [-nodm]
                filename
psyclone: error: too few arguments
```

As indicated above, the psyclone script takes the name of the Fortran source file containing the algorithm specification (in terms of calls to invoke()). It parses this, finds the necessary kernel source files and produces two Fortran files. The first contains the PSy, middle layer and the second a re-write of the algorithm code to use that layer. These files are named according to the user-supplied arguments (options -oalg and -opsy). If those arguments are not supplied then the script writes the generated/re-written Fortran to the terminal.

Examples are provided in the examples directory. There are 3 subdirectories (dynamo, gocean and gunghoproto) corresponding to different API's that are supported by PSyclone. In this case we are going to use one of the dynamo examples

```
> cd <PSYCLONEHOME>/examples/dynamo/eg1
> psyclone -api dynamo0.1 \
> -oalg dynamo_alg.f90 -opsy dynamo_psy.f90 dynamo.F90
```

You should see two new files created called dynamo_alg.f90 (containing the re-written algorithm layer) and dynamo_psy.f90 (containing the generated PSy- or middle-layer). Since this is a dynamo example the Fortran source code has dependencies on the dynamo system and therefore cannot be compiled stand-alone.

You can also use the runme.py example to see the interactive API in action. This script contains:

```
from psyclone.parse import parse
from psyclone.psyGen import PSyFactory

# This example uses version 0.1 of the Dynamo API
api="dynamo0.1"

# Parse the file containing the algorithm specification and
# return the Abstract Syntax Tree and invokeInfo objects
ast,invokeInfo=parse("dynamo.F90",api=api)

# Create the PSy-layer object using the invokeInfo
psy=PSyFactory(api).create(invokeInfo)
# Generate the Fortran code for the PSy layer
print psy.gen

# List the invokes that the PSy layer has
print psy.invokes.names

# Examine the 'schedule' (e.g. loop structure) that each
# invoke has
schedule=psy.invokes.get('invoke_0_v3_kernel_type').schedule
schedule.view()

schedule=psy.invokes.get('invoke_1_v3_solver_kernel_type').schedule
schedule.view()
```

It can be run non-interactively as follows:

```
> cd <PSYCLONEHOME>/example/dynamo/eg1
> python runme.py
```

However, to understand this example in more depth it is instructive to cut-and-paste from the runme.py file into your own, interactive python session:

```
> cd <PSYCLONEHOME>/example/dynamo/eg1
> python
```

In addition to the runme.py script, there is also runme_openmp.py which illustrates how one applies an OpenMP transform to a loop schedule within the PSy layer. The initial part of this script is the same as that of runme.py (above) and is therefore omitted here:

```
# List the various invokes that the PSy layer contains
print(psy.invokes.names)

# Get the loop schedule associated with one of these
# invokes
schedule = psy.invokes.get('invoke_v3_kernel_type').schedule
schedule.view()

# Get the list of possible loop transformations
from psyclone.psyGen import TransInfo
t = TransInfo()
print(t.list)

# Create an OpenMPLoop-transformation object
ol = t.get_trans_name('OMPLoopTrans')

# Apply it to the loop schedule of the selected invoke
new_schedule, memento = ol.apply(schedule.children[0])
new_schedule.view()

# Replace the original loop schedule of the selected invoke
# with the new, transformed schedule
psy.invokes.get('invoke_v3_kernel_type')._schedule = new_schedule
# Generate the Fortran code for the new PSy layer
print(psy.gen)
```

CHAPTER

TWO

GENERATOR SCRIPT

The simplest way to run PSyclone is to use the generator.py script. This script is located in the <PSYCLONE-HOME>/src directory. The script takes an algorithm file as input and outputs modified algorithm code and generated PSy code. This section walks through its functionality. The *API* section gives a more concise overview.

Running

The generator.py script is designed to be run from the command line. It is typically invoked as an argument to the python interpreter:

```
> python <PSYCLONEHOME>/src/generator.py <args>
```

The optional -h argument gives a description of the options provided by the script:

```
> python <PSYCLONEHOME>/src/generator.py -h

usage: generator.py [-h] [-oalg OALG] [-opsy OPSY] [-api API] [-s SCRIPT]
                    [-d DIRECTORY] [-l] [-dm] [-nodm]
                    filename

Run the PSyclone code generator on a particular file

positional arguments:
  filename              algorithm-layer source code

optional arguments:
  -h, --help            show this help message and exit
  -oalg OALG            filename of transformed algorithm code
  -opsy OPSY            filename of generated PSy code
  -api API              choose a particular api from ['gunghoproto',
                        'dynamo0.1', 'dynamo0.3', 'gocean0.1', 'gocean1.0'],
                        default dynamo0.3
  -s SCRIPT, --script SCRIPT
                        filename of a PSyclone optimisation script
  -d DIRECTORY, --directory DIRECTORY
                        path to root of directory structure containing kernel
                        source code
  -l, --limit           limit the fortran line length to 132 characters
  -dm, --dist_mem       generate distributed memory code
  -nodm, --no_dist_mem  do not generate distributed memory code
```

Basic Use

The simplest way to use generator.py is to provide it with an algorithm file.

```
> python <PSYCLONEHOME>/src/generator.py alg.f90
```

If the algorithm file is invalid for some reason, the script should return with an appropriate error. For example, if we use the Python generator code itself as an algorithm file we get the following:

```
> cd <PSYCLONEHOME>/src
> python ./generator.py generator.py
'Parse Error: Error, program, module or subroutine not found in ast'
```

Warning: In the current version of PSyclone an unhelpful error ending with the following may occur

```
AttributeError: 'Line' object has no attribute 'tofortran'
```

This is due to the parser failing to parse the algorithm code and is very likely to be due to the algorithm code containing a syntax error.

If the algorithm file is valid then the modified algorithm code and the generated PSy code will be output to the terminal screen.

Choosing the API

In the previous section we relied on PSyclone using the default API. The default API, along with the supported API's can be seen by running the generator.py script with the -h option.

If you use a particular API frequently and it is not the default then you can change the default by creating a copy of the default `psyclone.cfg` file and editing it. See *Configuration* for more details.

If your code uses an API that is different to the default then you can specify this as an argument to the generator.py script.

```
> python <PSYCLONEHOME>/src/generator.py -api dynamo0.1 alg.f90
```

File output

By default the modified algorithm code and the generated PSy code are output to the terminal. These can be output to a file by using the -oalg <file> and -opsy <file> options respectively. For example, the following will output the generated psy code to the file 'psy.f90' but the algorithm code will be output to the terminal:

```
> python <PSYCLONEHOME>/src/generator.py -opsy psy.f90 alg.f90
```

Algorithm files with no invokes

If the generator script is provided with a file that contains no `invoke` calls then the script outputs a warning to `stdout` and copies the input file to `stdout`, or to the specified algorithm file (if the -oalg <file> option is used). No PSy code will be output. If a file is specified using the -opsy <file> option this file will not be created.

```
> python <PSYCLONEHOME>/src/generator.py -opsy psy.f90 -oalg alg_new.f90 empty_alg.f90
Warning: 'Algorithm Error: Algorithm file contains no invoke() calls: refusing to
generate empty PSy code'
```

Kernel directory

When an algorithm file is parsed, the parser looks for the associated kernel files. The way this is done requires that any kernel routine specified in an invoke must have an explicit use statement. For example, the following code gives an error:

```
> cat no_use.f90
program no_use
  call invoke(testkern_type(a,b,c,d))
end program no_use
> python <PSYCLONEHOME>/src/generator.py no_use.f90
"Parse Error: kernel call 'testkern_type' must be named in a use statement"
```

If the name of the kernel is provided in a use statement then the parser will look for a file with the same name as the module in the use statement. In the example below, the parser will look for a file called “testkern.f90” or “testkern.F90”:

```
> cat use.f90
program use
  use testkern, only : testkern_type
  call invoke(testkern_type(a,b,c,d))
end program use
```

Therefore, for PSyclone to find Kernel files, the module name of a kernel file must be the same as its filename. By default the parser looks for the kernel file in the same directory as the algorithm file. If this file is not found then an error is reported.

```
> python <PSYCLONEHOME>/src/generator.py use.f90
Kernel file 'testkern.[fF]90' not found in <location>
```

The -d option can be used to tell the generator.py script where to look for Kernel files. The -d option tells the generator.py script that the required Kernel code is somewhere within the specified directory hierarchy. The script will recurse from the specified directory path to look for the required file. There must be only one instance of the specified file within the specified directory:

```
> cd <PSYCLONEHOME>/src
> python ./generator.py -d . use.f90
More than one match for kernel file 'testkern.[fF]90' found!
> python ./generator.py -d tests/test_files/dynamo0p3 -api dynamo0.3 use.f90
[code output]
```

Note: The -d option is limited to a single directory. Therefore a current limitation in PSyclone is that all required Kernel files required by an algorithm file must exist within a directory hierarchy where their file names are unique.

Transformation script

By default the generator.py script will generate 'vanilla' PSy layer code. The -s option allows a python script to be specified which can transform the PSy layer. This option is discussed in more detail in the *Script* section.

Fortran line length

By default the generator.py script will generate fortran code with no consideration of fortran line length limits. As the line length limit for free-format fortran is 132 characters, the code that is output may be non-conformant.

Line length is not an issue for many compilers as they allow compiler flags to be set which allow lines longer than the fortran standard. However this is not the case for all compilers.

When the -l option is specified in the generator.py script, the output will be line wrapped so that the output line lengths are always within the 132 character limit.

The -l option also checks the parsed algorithm and kernel files for conformance and raises an error if they do not conform.

Line wrapping is not performed by default. There are two reasons for this. This first reason is that most compilers are able to cope with long lines. The second reason is that the line wrapping implementation could fail in certain pathological cases. The implementation and limitations of line wrapping are discussed in the *Limitations* section.

Distributed memory

By default the generator.py script will generate distributed memory (DM) code (i.e. parallelised using MPI). As with the choice of API, this default may be configured by editing `psyclone.cfg` - see *Configuration*. Alternatively, whether or not to generate DM code can be specified as an argument to the generator.py script using the `-dm`/`--dist_mem` or `-nodm`/`--no_dist_mem` flags, respectively.

For details of PSyclone's support for generating DM code see *Distributed Memory*.

CHAPTER

THREE

KERNEL LAYER

In the PSyKAl separation of concerns, Kernel code (code which is created to run within the Kernel layer), works over a subset of a field (such as a column). The reason for doing this is that it gives the PSy layer the responsibility of calling the Kernel over the spatial domain which is where parallelism is typically exploited in finite element and finite difference codes. The PSy layer is therefore able to call the kernel layer in a flexible way (blocked and/or in parallel for example). Kernel code in the kernel layer is not allowed to include any parallelisation calls or directives and works on raw fortran arrays (to allow the compiler to optimise the code).

Since a Kernel is called over the spatial domain (by the PSy layer) it must take at least one field or operator as an argument.

API

Kernels in the kernel layer are implemented as subroutines within fortran modules. One or more kernel modules are allowed, each of which can contain one or more kernel subroutines. In the example below there is one module `integrate_one_module` which contains one kernel subroutine `integrate_one_code`. The kernel subroutines contain the code that operates over a subset of the field (such as a column).

Metadata describing the kernel subroutines is required by the PSyclone system to generate appropriate PSy layer code. The metadata is written by the kernel developer and is kept with the kernel code in the same module using a sub-type of the `kernel_type` type. In the example below the `integrate_one_kernel` type specifies the appropriate metadata information describing the kernel code for the `gunghoproto` api.

```
module integrate_one_module
  use kernel_mod
  implicit none

  private
  public integrate_one_kernel
  public integrate_one_code

  type, extends(kernel_type) :: integrate_one_kernel
    type(arg) :: meta_args(2) = (/&
         arg(READ, (CG(1)*CG(1))**3, FE), &
         arg(SUM, R, FE)/)
    integer :: ITERATES_OVER = CELLS
    contains
    procedure, nopass :: code => integrate_one_code
  end type integrate_one_kernel

contains

  subroutine integrate_one_code(layers, p1dofm, X, R)
```

```
    integer, intent(in) :: layers
    integer, intent(in) :: p1dofm(6)
    real(dp), intent(in) :: X(3,*)
    real(dp), intent(inout) :: R
  end subroutine integrate_one_code

end module integrate_one_module
```

Metadata

Kernel metadata is not required if the PSy layer is going to be written manually, its sole purpose is to let PSyclone know how to generate the PSy layer. The content of Kernel metadata differs depending on the particular API and this information can be found in the API-specific sections of this document.

In all API's the kernel metadata is implemented as an extension of the *kernel_type* type. The reason for using a type to specify metadata is that it allows the metadata to be kept with the code and for it to be compilable. In addition, currently all API's will contain information about the arguments in an array called `meta_args`, a specification of what the kernel code iterates over in a variable called `iterates_over` and a reference to the kernel code as a type bound procedure.

```
type, extends(kernel_type) :: integrate_one_kernel
  ...
  type(...) :: meta_args(...) = (/ ... /)
  ...
  integer :: ITERATES_OVER = ...
  ...
  contains
  ...
  procedure ...
  ...
end type integrate_one_kernel
```

CHAPTER

FOUR

ALGORITHM LAYER

In the PSyKAl separation of concerns, the Algorithm layer specifies the algorithm that the scientist would like to run (in terms of calls to kernel routines and Built-in operations) and logically operates on full fields. Algorithm code in the algorithm layer is not allowed to include any parallelisation calls or directives and passes datatypes specified by the particular API.

API

The Algorithm layer is forbidden from calling the Kernel layer directly. In PSyclone, if the programmer would like to call a Kernel routine or a Built-in operation from the algorithm layer they must use the `invoke` call (which is common to all API's). The `invoke` call is not necessary (and indeed will not work) if the PSy layer is written manually.

To make an `invoke` call, the algorithm layer developer adds one or more `call invoke()` statements to their code and within the content of the `invoke` call they add a reference to the required Kernel/Built-in and the data to pass to it. For example,

```
...
call invoke(integrate_one_kernel(arg1,arg2))
...
```

For more information on the concept of Built-in operations see the *Built-ins* Section. Details of which operations are supported for a specific API are given in the documentation of that API.

The algorithm layer can consist of an arbitrary number of files containing fortran code, any of which may contain as many `invoke()` calls as is required. PSyclone is applied to an individual algorithm layer file and must therefore be run multiple times if multiple files containing `invoke()` calls exist in the algorithm layer.

The algorithm developer is also able to reference more than one Kernel/Built-in within an invoke. In fact this feature is encouraged for performance reasons. **As a general guideline the developer should aim to use as few invokes as possible with as many Kernel references within them as is possible**. The reason for this is that it allows for greater freedom for optimisation in the PSy layer as PSy layer optimisations are limited to the contents of individual invoke calls - PSyclone currently does not attempt to optimise the PSy layer over multiple invoke calls.

As well as generating the PSy layer code, PSyclone modifies the Algorithm layer code, replacing `invoke` calls with calls to the generated PSy layer so that the algorithm code is compilable and linkable to the PSy layer and adding in the appropriate `use` statement. For example, the above `integrate_one_kernel` invoke is translated into something like the following:

```
...
use psy, only : invoke_0_integrate_one_kernel
...
call invoke_0_integrate_one_kernel(arg1,arg2)
...
```

You may have noticed from other examples in this guide that an algorithm specification in an invoke call references the metadata `type` in an invoke call, not the `code` directly; this is by design.

For example, in the invoke call below, `integrate_one_kernel` is used.

```
...
call invoke(integrate_one_kernel(arg1,arg2))
...
```

`integrate_one_kernel` is the name of the metadata type in the module, not the name of the subroutine in the Kernel ...

```
module integrate_one_module
  ...
  type, extends(kernel_type) :: integrate_one_kernel
    ...
  end type
  ...
contains
  ...
  subroutine integrate_one_code(...)
  ...
  end subroutine integrate_one_code
  ...
end module integrate_one_module
```

Named Invokes

PSyclone permits the user to optionally specify a label for an invoke call like so:

```
...
call invoke(integrate_one_kernel(arg1,arg2), &
            name="compute something")
...
```

The `name` argument to the invoke call is optional. If supplied it must be a string literal. The content of this string (with any spaces replaced by '_' characters) is used in naming the corresponding PSy-layer routine generated by PSyclone. So, for the above example, the generated PSy-layer subroutine will be named "invoke_compute_something." Each invoke label must currently be unique within an Algorithm source file. Note that, in keeping with the Fortran language, labels are not case sensitive and, after having any spaces replaced by underscores, must be valid Fortran names (e.g. `name="compute(1)"` is invalid). In the future it is intended that the labelling of invokes will help to support invoke-specific optimisations to be applied as well as enabling more readable profiling output. It may also be used to instruct PSyclone to just generate a single subroutine to implement all invokes that share the same label.

Limitations

In order to re-write the Algorithm layer, as just described, PSyclone must obviously be able to parse the invoke calls. Since the Fortran expression parser used by PSyclone is relatively simple, this means there are limitations on what Fortran may be used when specifying kernel arguments in an invoke call. Since these limitations can have a direct impact on the natural science code, the PSyclone developers endeavour to keep them to a minimum.

The current list of known limitations/restrictions on the form of kernel arguments within an invoke is:

- No arithmetic expressions (e.g. `kernel_type(a+b)` or `kernel_type(-a)`)

- No named (optional) arguments (e.g. `kernel_type(fn(my_arg=a))`)

If you encounter any other limitations (or have a burning desire to use one of the above forms) then please contact the PSyclone developers.

CHAPTER

FIVE

PSY LAYER

In the PSyKAl separation of concerns, the PSy layer is responsible for linking together the Algorithm and Kernel layers and for providing the implementation of any Built-in operations used. Its functional responsibilities are to

1. map the arguments supplied by an Algorithm `invoke` call to the arguments required by a Built-in or Kernel call (as these will not have a one-to-one correspondance).
2. call any Kernel routines such that they cover the required iteration space and
3. perform any Built-in operations (either by including the necessary code directly in the PSy layer or by e.g. calling a maths library) and
4. include any required distributed memory operations such as halo swaps and reductions.

Its other role is to allow the optimisation expert to optimise any required distributed memory operations, include and optimise any shared memory parallelism and optimise for single node (e.g. cache and vectorisation) performance.

Code Generation

The PSy layer can be written manually but this is error prone and potentially complex to optimise. The PSyclone code generation system generates the PSy layer so there is no need to write the code manually.

To generate correct PSy layer code, PSyclone needs to understand the arguments and datatypes passed by the algorithm layer and the arguments and datatypes expected by the Kernel layer; it needs to know the name of the Kernel subroutine(s); it needs to know the iteration space that the Kernel(s) is/are written to iterate over; it also needs to know the ordering of Kernels and Built-ins as specified in the algorithm layer. Finally, it needs to know where to place any distributed memory operations.

PSyclone determines the above information by being told the API in question (by the user), by reading the appropriate Kernel and Built-in metadata and by reading the order of Kernels and Built-ins in an invoke call (as specified in the algorithm layer).

PSyclone has an API-specific parsing stage which reads the algorithm layer and all associated Kernel metadata. This information is passed to a PSy-generation stage which creates a high level view of the PSy layer. From this high level view the PSy-generation stage can generate the required PSy code.

For example, the following Python code shows a code being parsed, a PSy-generation object being created using the output from the parser and the PSy layer code being generated by the PSy-generation object.

```python
from parse import parse
from psyGen import PSyFactory

# This example uses version 0.1 of the Dynamo API
api = "dynamo0.1"
```

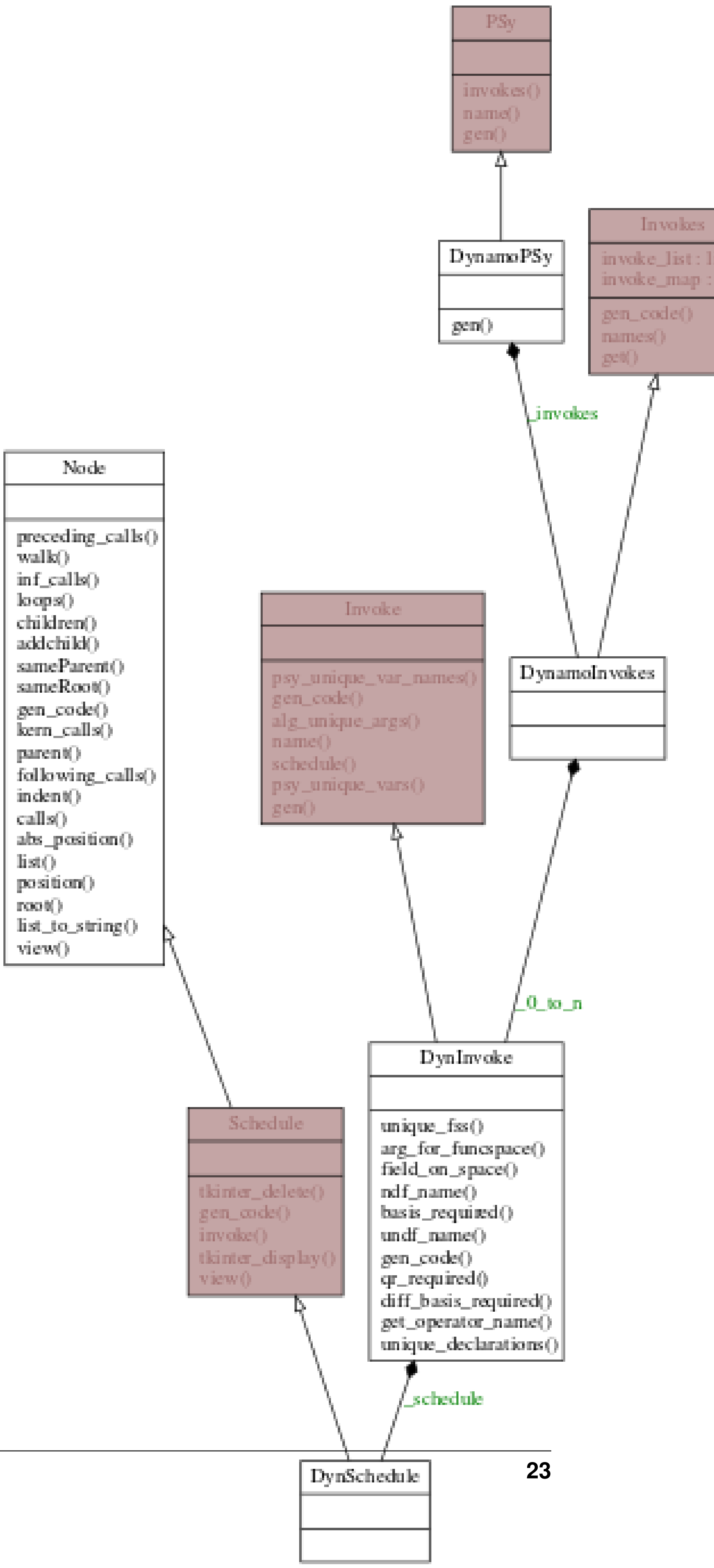
```
# Parse the file containing the algorithm specification and
# return the Abstract Syntax Tree and invokeInfo objects
ast, invokeInfo = parse("dynamo.F90", api=api)

# Create the PSy-layer object using the invokeInfo
psy = PSyFactory(api).create(invokeInfo)
# Generate the Fortran code for the PSy layer
print psy.gen
```

Structure

PSyclone provides a hierarchy of base classes which specific API's can subclass to support their particular API. All API's implemented so far, follow this hierarchy.

At the top level is the **PSy** class. The PSy class has an **Invokes** class. The **Invokes** class can contain one or more **Invoke** classes (one for each invoke in the algorithm layer). Each **Invoke** class has a **Schedule** class.

The class diagram for the above base classes is shown below using the dynamo0.3 API as an illustration. This class diagram was generated from the source code with pyreverse and edited with inkscape.


PSy
invokes()
name()
gen()
DynamoPSy
gen()
Invokes
invoke_list : l
invoke_map :
gen_code()
names()
get()
_invokes
Node
preceding_calls()
walk()
inf_calls()
loops()
children()
addchild()
sameParent()
sameRoot()
gen_code()
kern_calls()
parent()
following_calls()
indent()
calls()
abs_position()
list()
position()
root()
list_to_string()
view()
Invoke
psy_unique_var_names()
gen_code()
alg_unique_args()
name()
schedule()
psy_unique_vars()
gen()
DynamoInvokes
_0_to_n
DynInvoke
unique_fss()
arg_for_funcspace()
field_on_space()
ndf_name()
basis_required()
undf_name()
gen_code()
qr_required()
diff_basis_required()
get_operator_name()
unique_declarations()
Schedule
tkinter_delete()
gen_code()
invoke()
tkinter_display()
view()
_schedule
DynSchedule

API

class `psyclone.psyGen.`**`PSy`**(*invoke_info*)

Base class to help manage and generate PSy code for a single algorithm file. Takes the invocation information output from the function `parse.parse()` as its input and stores this in a way suitable for optimisation and code generation.

Parameters **`invoke_info`** (*`FileInfo`*) – An object containing the required invocation information for code optimisation and generation. Produced by the function `parse.parse()`.

For example:

```
>>> import psyclone
>>> from psyclone.parse import parse
>>> ast, info = parse("argspec.F90")
>>> from psyclone.psyGen import PSyFactory
>>> api = "..."
>>> psy = PSyFactory(api).create(info)
>>> print(psy.gen)
```

`inline`(*module*)

inline all kernel subroutines into the module that are marked for inlining. Avoid inlining the same kernel more than once.

class `psyclone.psyGen.`**`Invokes`**(*alg_calls*, *Invoke*)

Manage the invoke calls

class `psyclone.psyGen.`**`Invoke`**(*alg_invocation*, *idx*, *schedule_class*, *reserved_names=None*)

Manage an individual invoke call

`first_access`(*arg_name*)

Returns the first argument with the specified name passed to a kernel in our schedule

`unique_declarations`(*datatype*, *access=None*)

Returns a list of all required declarations for the specified datatype. If access is supplied (e.g. "gh_write") then only declarations with that access are returned.

`unique_declns_by_intent`(*datatype*)

Returns a dictionary listing all required declarations for each type of intent ('inout', 'out' and 'in').

Parameters **`datatype`** (*`string`*) – the type of the kernel argument for the particular API for which the intent is required

Returns dictionary containing 'intent' keys holding the kernel argument intent and declarations of all kernel arguments for each type of intent

Return type dict

Raises **`GenerationError`** – if the kernel argument is not a valid datatype for the particular API.

class `psyclone.psyGen.`**`Schedule`**(*KernFactory*, *BuiltInFactory*, *alg_calls=[]*)

Stores schedule information for an invocation call. Schedules can be optimised using transformations.

```
>>> from parse import parse
>>> ast, info = parse("algorithm.f90")
>>> from psyGen import PSyFactory
>>> api = "..."
>>> psy = PSyFactory(api).create(info)
>>> invokes = psy.invokes
>>> invokes.names
>>> invoke = invokes.get("name")
>>> schedule = invoke.schedule
>>> schedule.view()
```

coloured_text
Returns the name of this node with appropriate control codes to generate coloured output in a terminal that supports it.

Returns Text containing the name of this node, possibly coloured

Return type string

dag_name
Return the name to use in a dag for this node

view (*indent=0*)
Print a text representation of this node to stdout and then call the view() method of any children.

Parameters **indent** (*integer*) – Depth of indent for output text

Schedule

A PSy **Schedule** object consists of a tree of objects (called Nodes in PSyclone) which can be used to describe the required schedule for a PSy layer subroutine. This subroutine is called by the Algorithm layer and itself calls one or more Kernels and/or implements any required Built-in operations. The Node objects can currently be a **Loop**, a **Kernel**, a **Built-in** (see the *Built-ins* section), a **Directive** (of various types), a **HaloExchange**, or a **GlobalSum** (the latter two are only used if distributed memory is supported and is switched on; see the *Distributed Memory* section). The order of the tree (depth first) indicates the order of the associated Fortran code.

PSyclone will initially create a "vanilla" (functionally correct but not optimised) schedule. This "vanilla" schedule can be modified by changing the objects within it. For example, the order that two Kernel calls appear in the generated code can be changed by changing their order in the tree. The ability to modify this high level view of a schedule allows the PSy layer to be optimised for a particular architecture (by applying optimisations such as blocking, loop merging, inlining, OpenMP parallelisation etc.). The tree could be manipulated directly, however, to simplify optimisation, a set of transformations are supplied. These transformations are discussed in the next section.

Schedule visualisation

PSyclone supports visualising a schedule in two ways. Firstly the *view()* method outputs textual information about the contents of a schedule. If we were to look at the dynamo eg6 example we would see the following output:

```
>>> schedule.view()
Schedule[invoke='invoke_0' dm=True]
    Directive[OMP parallel do]
        Loop[type='dofs',field_space='any_space_1',it_space='dofs']
            Call setval_X_code(p,z)
            Call X_innerproduct_Y_code(rs_old,res,z)
    GlobalSum[scalar='rs_old']
```

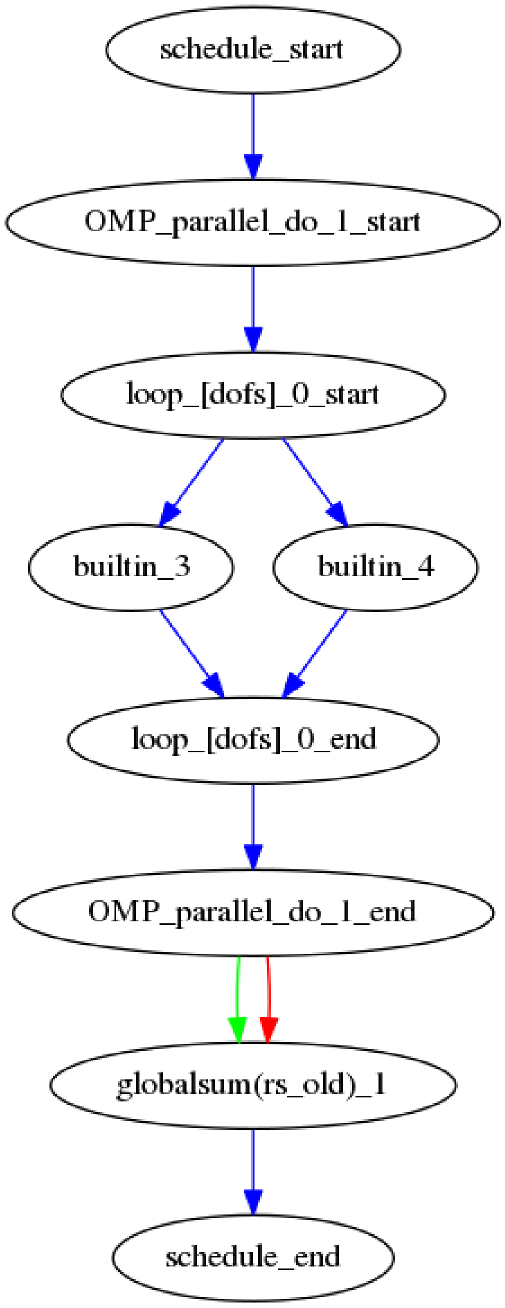
The above output tells us that the invoke name for the schedule we are looking at is *invoke_0* and that the distributed_memory option has been switched on. Within the schedule is an OpenMP parallel directive containing a loop which itself contains two builtin calls. As the latter of the two builtin calls requires a reduction and distributed memory is switched on, PSyclone has added a GlobalSum call for the appropriate scalar.

Secondly, the *dag()* method (standing for directed acyclic graph), outputs the schedule and its data dependencies. By default a file in dot format is output with the name `dag` and a file in svg format is output with the name `dag.svg`. The file name can be changed using the `file_name` optional argument and the output file format can be changed using the `file_format` optional argument. The file_format value is simply passed on to graphviz so the graphviz documentation should be consulted for valid formats if svg is not required.

```
>>> schedule.dag(file_name="lovely", file_format="png")
```

Note: The dag method can be called from any node and will output the dag for that node and all of its children.

If we were to look at the dynamo eg6 example we would see the following image:



In the image, all nodes (Psyclone's generic name for objects in the schedule) with children are split into a start vertex and an end vertex (for example the Schedule node has both *schedule_start* and *schedule_end* vertices). Blue arrows indicate that there is a parent to child relationship (from a start node) or a child to parent relationship (to an end node). Green arrows indicate that a Node depends on another Node later in the schedule (which we call a forward dependence). Therefore the OMP parallel loop must complete before the globalsum is performed. Red arrows indicate that a Node depends on another Node that is earlier in the schedule (which we call a backward dependence). However the direction of the red arrows are reversed to improve the flow of the dag layout. In this example the forward and backward dependence is the same, however this is not always the case. The two built-ins do not depend on each other, so they have no associated green or red arrows.

The dependence graph output gives an indication of whether nodes can be moved in the schedule. In this case it is valid to run the builtin's in either order. The underlying dependence analysis used to create this graph is used to determine whether a transformation of a schedule is valid from the perspective of data dependencies.

CHAPTER

SIX

TRANSFORMATIONS

As discussed in the previous section, transformations can be applied to a schedule to modify it. Typically transformations will be used to optimise the PSy layer for a particular architecture, however transformations could be added for other reasons, such as to aid debugging or for performance monitoring.

Finding

Transformations can be imported directly, but the user needs to know what transformations are available. A helper class **TransInfo** is provided to show the available transformations

class `psyclone.psyGen.`**`TransInfo`**(*module=None*, *base_class=None*)

This class provides information about, and access, to the available transformations in this implementation of PSyclone. New transformations will be picked up automatically as long as they subclass the abstract Transformation class.

For example:

```
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> print(t.list)
There is 1 transformation available:
  1: SwapTrans, A test transformation
>>> # accessing a transformation by index
>>> trans = t.get_trans_num(1)
>>> # accessing a transformation by name
>>> trans = t.get_trans_name("SwapTrans")
```

`get_trans_name`(*name*)

return the transformation with this name (use list() first to see available transformations)

`get_trans_num`(*number*)

return the transformation with this number (use list() first to see available transformations)

`list`

return a string with a human readable list of the available transformations

`num_trans`

return the number of transformations available

Available

Most transformations are generic as the schedule structure is independent of the API, however it often makes sense to specialise these for a particular API by adding API-specific errors checks. Some transformations are API-specific (or specific to a set of API's e.g. dynamo). Currently these different types of transformation are indicated by their names.

The generic transformations currently available are listed in alphabetical order below (a number of these have specialisations which can be found in the API-specific sections).

Note: PSyclone currently only supports OpenACC transformations for the GOcean 1.0 API. Attempts to apply these transformations to (members of) Schedules from other APIs will be rejected.

---

class `psyclone.transformations.`**`ACCDataTrans`**

Adds an OpenACC "enter data" directive to a Schedule. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> dtrans = t.get_trans_name('ACCDataTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> # Add an enter-data directive
>>> newschedule, _ = dtrans.apply(schedule)
>>> newschedule.view()
```

`apply`(*sched*)

Adds an OpenACC "enter data" directive to the invoke associated with the supplied Schedule. Any fields accessed by OpenACC kernels within this schedule will be added to this data region in order to ensure they remain on the target device.

Parameters **`sched`** (sub-class of *`psyclone.psyGen.Schedule`*.) – Schedule to which to add an "enter data" directive.

Returns Tuple of the modified schedule and a record of the transformation.

Return type (*`psyclone.psyGen.Schedule`*, `psyclone.undoredo.Memento`)

Raises

- **`NotImplementedError`** – for any API other than GOcean 1.0.
- ***`TransformationError`*** – if passed something that is not a (subclass of) *`psyclone.psyGen.Schedule`*.

`name`

Returns the name of this transformation.

Return type str

class `psyclone.transformations.`**`ACCLoopTrans`**

Adds an OpenACC loop directive to a loop. This directive must be within the scope of some OpenACC Parallel region (at code-generation time).

For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ltrans = t.get_trans_name('ACCLoopTrans')
>>> rtrans = t.get_trans_name('ACCParallelTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>> new_schedule = schedule
>>>
# Apply the OpenACC Loop transformation to *every* loop
# in the schedule
>>> for child in schedule.children:
>>>     newschedule, memento = ltrans.apply(child, reprod=True)
>>>     schedule = newschedule
>>>
# Enclose all of these loops within a single OpenACC
# PARALLEL region
>>> rtrans.omp_schedule("dynamic,1")
>>> newschedule, memento = rtrans.apply(schedule.children)
>>>
```

`apply`(*node*, *collapse=None*, *independent=True*)

Apply the ACCLoop transformation to the specified node in a Schedule. This node must be a Loop since this transformation corresponds to inserting a directive immediately before a loop, e.g.:

```
!$ACC LOOP
do ...
   ...
end do
```

At code-generation time (when `psyclone.psyGen.ACCLoopDirective.gen_code()` is called), this node must be within (i.e. a child of) a PARALLEL region.

Parameters

- **`node`** (`psyclone.psyGen.Loop.`) – the supplied node to which we will apply the Loop transformation.
- **`collapse`** (*`int`*) – number of loops to collapse into single iteration space or None.
- **`independent`** (*`bool`*) – whether to add the "independent" clause to the directive (not strictly necessary within PARALLEL regions).

Returns (*`psyclone.psyGen.Schedule`*, `psyclone.undoredo.Memento`)

name
Returns the name of this transformation as a string.

---

class `psyclone.transformations.`**`ACCParallelTrans`**
Create an OpenACC parallel region by inserting directives. This parallel region *must* come after an enter-data directive (see *ACCDataTrans*). For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ptrans = t.get_trans_name('ACCParallelTrans')
>>> dtrans = t.get_trans_name('ACCDataTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> # Enclose everything within a single OpenACC PARALLEL region
>>> newschedule, _ = ptrans.apply(schedule.children)
>>> # Add an enter-data directive
>>> newschedule, _ = dtrans.apply(newschedule)
>>> newschedule.view()
```

apply (*nodes*)
Apply this transformation to a subset of the nodes within a schedule - i.e. enclose the specified Loops in the schedule within a single parallel region.

Parameters **nodes** ((list of) `psyclone.psyGen.Node`.) – a single Node or a list of Nodes.

Raises ***TransformationError*** – if the nodes argument is not of the correct type.

name

Returns The name of this transformation as a string.

Return type str

---

class `psyclone.transformations.`**`ColourTrans`**
Apply a colouring transformation to a loop (in order to permit a subsequent parallelisation over colours). For example:

```
>>> invoke = ...
>>> schedule = invoke.schedule
>>>
>>> ctrans = ColourTrans()
>>>
>>> # Colour all of the loops
>>> for child in schedule.children:
>>>     cschedule, _ = ctrans.apply(child)
>>>
>>> csched.view()
```

apply (*node*)

Converts the Loop represented by `node` into a nested loop where the outer loop is over colours and the inner loop is over cells of that colour. :param node: The loop to transform. :type node: `psyclone.psyGen.Loop` :returns: Tuple of modified schedule and record of transformation :rtype: (`psyclone.psyGen.Schedule, :py:class:`psyclone.undoredo.Memento`)

name

Returns the name of this transformation as a string.

---

class `psyclone.transformations.`**`KernelModuleInlineTrans`**

Switches on, or switches off, the inlining of a Kernel subroutine into the PSy layer module. For example:

```
>>> invoke = ...
>>> schedule = invoke.schedule
>>>
>>> inline_trans = KernelModuleInlineTrans()
>>>
>>> ischedule, _ = inline_trans.apply(schedule.children[0].children[0])
>>> ischedule.view()
```

Warning: For this transformation to work correctly, the Kernel subroutine must only use data that is passed in by argument, declared locally or included via use association within the subroutine. Two examples where in-lining will not work correctly are:

1. A variable is declared within the module that `contains` the Kernel subroutine and is then accessed within that Kernel;
2. A variable is included via use association at the module level and accessed within the Kernel subroutine.

There are currently no checks that these rules are being followed when in-lining so the onus is on the user to ensure correctness.

apply (*node*, *inline=True*)

Checks that the node is of the correct type (a Kernel) then marks the Kernel to be inlined, or not, depending on the value of the inline argument. If the inline argument is not passed the Kernel is marked to be inlined.

name

Returns the name of this transformation as a string.

---

class `psyclone.transformations.`**`LoopFuseTrans`**

Provides a loop-fuse transformation. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> ast,invokeInfo=parse("dynamo.F90")
>>> psy=PSyFactory("dynamo0.1").create(invokeInfo)
>>> schedule=psy.invokes.get('invoke_v3_kernel_type').schedule
>>> schedule.view()
>>>
>>> from psyclone.transformations import LoopFuseTrans
>>> trans=LoopFuseTrans()
>>> new_schedule,memento=trans.apply(schedule.children[0],
                                     schedule.children[1])
>>> new_schedule.view()
```

apply (*node1*, *node2*)
Fuse the loops represented by `node1` and `node2`.

name
Returns the name of this transformation as a string.

---

class psyclone.transformations.**MoveTrans**
Provides a transformation to move a node in the tree. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> ast,invokeInfo=parse("dynamo.F90")
>>> psy=PSyFactory("dynamo0.3").create(invokeInfo)
>>> schedule=psy.invokes.get('invoke_v3_kernel_type').schedule
>>> schedule.view()
>>>
>>> from psyclone.transformations import MoveTrans
>>> trans=MoveTrans()
>>> new_schedule, memento = trans.apply(schedule.children[0],
                                        schedule.children[2],
                                        position="after")
>>> new_schedule.view()
```

Nodes may only be moved to a new location with the same parent and must not break any dependencies otherwise an exception is raised.

apply (*node*, *location*, *position='before'*)
Move the node represented by `node` before location `location` (which is also a node) by default and after if the optional *position* argument is set to 'after'. An exception is raised if the move is invalid.

name
Returns the name of this transformation as a string.

---

class psyclone.transformations.**ProfileRegionTrans**
Create a profile region around a list of statements. For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> p_trans = t.get_trans_name('ProfileRegionTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> # Enclose all children within a single profile region
>>> newschedule, _ = p_trans.apply(schedule.children)
>>> newschedule.view()
```

apply (*nodes*)
Apply this transformation to a subset of the nodes within a schedule - i.e. enclose the specified Nodes in the schedule within a single profiler region.

Parameters **nodes** (`psyclone.psygen.Node` or list of `psyclone.psygen.Node`.) – Can be a single node or a list of nodes.

name
Returns the name of this transformation as a string

---

class `psyclone.transformations.`**`OMPLoopTrans`**(*omp_schedule='static'*)
Adds an orphaned OpenMP directive to a loop. i.e. the directive must be inside the scope of some other OMP Parallel REGION. This condition is tested at code-generation time. The optional 'reprod' argument in the apply method decides whether standard OpenMP reduction support is to be used (which is not reproducible) or whether a manual reproducible reproduction is to be used.

Parameters **omp_schedule** (*str*) – The OpenMP schedule to use.

For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>> print psy.invokes.names
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ltrans = t.get_trans_name('OMPLoopTrans')
>>> rtrans = t.get_trans_name('OMPParallelTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>> new_schedule = schedule
>>>
# Apply the OpenMP Loop transformation to *every* loop
# in the schedule
>>> for child in schedule.children:
>>>     newschedule, memento = ltrans.apply(child, reprod=True)
>>>     schedule = newschedule
>>>
# Enclose all of these loops within a single OpenMP
# PARALLEL region
>>> rtrans.omp_schedule("dynamic,1")
>>> newschedule, memento = rtrans.apply(schedule.children)
>>>
>>>
```

apply(*node*, *reprod=None*)
Apply the OMPLoopTrans transformation to the specified node in a Schedule. This node must be a Loop since this transformation corresponds to wrapping the generated code with directives like so:

```
!$OMP DO
do ...
   ...
end do
!$OMP END DO
```

At code-generation time (when `OMPLoopDirective.gen_code()` is called), this node must be within (i.e. a child of) an OpenMP PARALLEL region.

The optional reprod argument will cause a reproducible reduction to be generated if it is set to True, otherwise the default value (as read from the psyclone.cfg file) will be used. Note, reproducible in this case means obtaining the same results with the same number of OpenMP threads, not for different numbers of OpenMP threads.

Parameters

- **node** (`psyclone.psyGen.Node`) – the supplied node to which we will apply the OMPLoopTrans transformation
- **reprod** (*`Boolean or None`*) – optional argument to determine whether to generate reproducible OpenMP reductions (True) or not (False). The default value is None which will cause PSyclone to look up a default value

Returns (*`psyclone.psyGen.Schedule`*, `psyclone.undoredo.Memento`)

name
Returns the name of this transformation as a string.

omp_schedule
Returns the OpenMP schedule that will be specified by this transformation. The default schedule is 'static'.

---

class `psyclone.transformations.`**`OMPParallelLoopTrans`**(*omp_schedule='static'*)
Adds an OpenMP PARALLEL DO directive to a loop.

For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> ast, invokeInfo = parse("dynamo.F90")
>>> psy = PSyFactory("dynamo0.1").create(invokeInfo)
>>> schedule = psy.invokes.get('invoke_v3_kernel_type').schedule
>>> schedule.view()
>>>
>>> from psyclone.transformations import OMPParallelLoopTrans
>>> trans = OMPParallelLoopTrans()
>>> new_schedule, memento = trans.apply(schedule.children[0])
>>> new_schedule.view()
```

apply(*node*)
Apply an OMPParallelLoop Transformation to the supplied node (which must be a Loop). In the generated code this corresponds to wrapping the Loop with directives:

```
!$OMP PARALLEL DO ...
do ...
  ...
end do
!$OMP END PARALLEL DO
```

Parameters **node** (`psyclone.f2pygen.DoGen`) – the node (loop) to which to apply the transformation.

Returns Two-tuple of transformed schedule and a record of the transformation.

Return type (`psyclone.psyGen.Schedule, :py:class:`psyclone.undoredo.Memento`)

name
Returns the name of this transformation as a string.

class `psyclone.transformations.`**`OMPParallelTrans`**

Create an OpenMP PARALLEL region by inserting directives. For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ltrans = t.get_trans_name('GOceanOMPLoopTrans')
>>> rtrans = t.get_trans_name('OMPParallelTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>> new_schedule = schedule
>>>
>>> # Apply the OpenMP Loop transformation to *every* loop
>>> # in the schedule
>>> for child in schedule.children:
>>>     newschedule, memento = ltrans.apply(child)
>>>     schedule = newschedule
>>>
>>> # Enclose all of these loops within a single OpenMP
>>> # PARALLEL region
>>> newschedule, _ = rtrans.apply(schedule.children)
>>> newschedule.view()
```

`name`

Returns The name of this transformation as a string.

Return type str

Note: PSyclone does not support (distributed-memory) halo swaps or global sums within OpenMP parallel regions. Attempting to create a parallel region for a set of nodes that includes halo swaps or global sums will produce an error. In such cases it may be possible to re-order the nodes in the Schedule such that the halo swaps or global sums are performed outside the parallel region. The *MoveTrans* transformation may be used for this.

Applying

Transformations can be applied either interactively or through a script.

Interactive

To apply a transformation interactively we first parse and analyse the code. This allows us to generate a "vanilla" PSy layer. For example ...

```
from parse import parse
from psyGen import PSyFactory

# This example uses version 0.1 of the Dynamo API
api = "dynamo0.1"

# Parse the file containing the algorithm specification and
# return the Abstract Syntax Tree and invokeInfo objects
ast, invokeInfo = parse("dynamo.F90", api=api)

# Create the PSy-layer object using the invokeInfo
psy = PSyFactory(api).create(invokeInfo)

# Optionally generate the vanilla PSy layer fortran
print psy.gen
```

We then extract the particular schedule we are interested in. For example ...

```
# List the various invokes that the PSy layer contains
print psy.invokes.names

# Get the required invoke
invoke = psy.invokes.get('invoke_0_v3_kernel_type')

# Get the schedule associated with the required invoke
schedule = invoke.schedule
schedule.view()
```

Now we have the schedule we can create and apply a transformation to it to create a new schedule and then replace the original schedule with the new one. For example ...

```
# Get the list of possible loop transformations
from psyGen import TransInfo
t = TransInfo()
print t.list

# Create an OpenMPLoop-transformation
ol = t.get_trans_name('OMPParallelLoopTrans')

# Apply it to the loop schedule of the selected invoke
new_schedule,memento = ol.apply(schedule.children[0])
new_schedule.view()

# Replace the original loop schedule of the selected invoke
# with the new, transformed schedule
invoke.schedule=new_schedule

# Generate the Fortran code for the new PSy layer
print psy.gen
```

More examples of use of the interactive application of transformations can be found in the runme*.py files within the examples/dynamo/eg1 and examples/dynamo/eg2 directories. Some simple examples of the use of transformations are also given in the previous section.

Script

PSyclone provides a Python script (**generator.py**) that can be used from the command line to generate PSy layer code and to modify algorithm layer code appropriately. By default this script will generate "vanilla" (unoptimised) PSy layer code. For example:

```
> python generator.py algspec.f90
> python generator.py -oalg alg.f90 -opsy psy.f90 -api dynamo0.3 algspec.f90
```

The generator.py script has an optional **-s** flag which allows the user to specify a script file to modify the PSy layer as required. Script files may be specified without a path. For example:

```
> python generator.py -s opt.py algspec.f90
```

In this case the Python search path **PYTHONPATH** will be used to try to find the script file.

Alternatively, script files may be specified with a path. In this case the file is expected to be found in the specified location. For example ...

```
> python generator.py -s ./opt.py algspec.f90
> python generator.py -s ../scripts/opt.py algspec.f90
> python generator.py -s /home/me/PSyclone/scripts/opt.py algspec.f90
```

PSyclone also provides the same functionality via a function (which is what the **generator.py** script calls internally)

`psyclone.generator.`**`generate`**(*filename*, *api=''*, *kernel_path=''*, *script_name=None*, *line_length=False*, *distributed_memory=None*)

Takes a GungHo algorithm specification as input and outputs the associated generated algorithm and psy codes suitable for compiling with the specified kernel(s) and GungHo infrastructure. Uses the `parse.parse()` function to parse the algorithm specification, the `psyGen.PSy` class to generate the PSy code and the `algGen.Alg` class to generate the modified algorithm code.

Parameters

- **`filename`** (*str*) – The file containing the algorithm specification.
- **`kernel_path`** (*str*) – The directory from which to recursively search for the files containing the kernel source (if different from the location of the algorithm specification)
- **`script_name`** (*str*) – A script file that can apply optimisations to the PSy layer (can be a path to a file or a filename that relies on the PYTHONPATH to find the module).
- **`line_length`** (*bool*) – A logical flag specifying whether we care about line lengths being longer than 132 characters. If so, the input (algorithm and kernel) code is checked to make sure that it conforms. The default is False.
- **`distributed_memory`** (*bool*) – A logical flag specifying whether to generate distributed memory code. The default is set in the config.py file.

Returns The algorithm code and the psy code.

Return type ast

Raises **`IOError`** – if the filename or search path do not exist

For example:

```
>>> from generator import generate
>>> alg, psy = generate("algspec.f90")
>>> alg, psy = generate("algspec.f90", kernel_path="src/kernels")
>>> alg, psy = generate("algspec.f90", script_name="optimise.py")
>>> alg, psy = generate("algspec.f90", line_length=True)
>>> alg, psy = generate("algspec.f90", distributed_memory=False)
```

A valid script file must contain a **trans** function which accepts a **PSy** object as an argument and returns a **PSy** object, i.e.:

```
def trans(psy)
    ...
    return psy
```

It is up to the script what it does with the PSy object. The example below does the same thing as the example in the *Interactive* section.

```
def trans(psy):
    from transformations import OMPParallelLoopTrans
    invoke = psy.invokes.get('invoke_0_v3_kernel_type')
    schedule = invoke.schedule
    ol = OMPParallelLoopTrans()
    new_schedule, _ = ol.apply(schedule.children[0])
    invoke.schedule = new_schedule
    return psy
```

Of course the script may apply as many transformations as is required for a particular schedule and may apply transformations to all the schedules (i.e. invokes) contained within the PSy layer.

An example of the use of transformations scripts can be found in the examples/dynamo/eg3 directory. Please read the examples/dynamo/README file first as it explains how to run the example.

OpenMP

OpenMP is added to a code by using transformations. The three transformations currently supported allow the addition of an **OpenMP Parallel** directive, an **OpenMP Do** directive and an **OpenMP Parallel Do** directive, respectively, to a code.

The generic versions of these three transformations (i.e. ones that theoretically work for all API's) were given in the *Available* section. The API-specific versions of these transformations are described in the API-specific sections of this document.

Reductions

PSyclone supports parallel scalar reductions. If a scalar reduction is specified in the Kernel metadata (see the API-specific sections for details) then PSyclone ensures the appropriate reduction is performed.

In the case of distributed memory, PSyclone will add **GlobalSum's** at the appropriate locations. As can be inferred by the name, only "summation" reductions are currently supported for distributed memory.

In the case of an OpenMP parallel loop the standard reduction support will be used by default. For example

```
!$omp parallel do, reduction(+:x)
!loop
!$omp end parallel do
```

OpenMP reductions do not guarantee to give bit reproducible results for different runs of the same problem even if the same problem is run using the same resources. The reason for this is that the order in which data is reduced is not mandated.

Therefore, an additional **reprod** option has been added to the **OpenMP Do** transformation. If the reprod option is set to “True” then the OpenMP reduction support is replaced with local per-thread reductions which are reduced serially after the loop has finished. This implementation guarantees to give bit-wise reproducible results for different runs of the same problem using the same resources, but will not bit-wise compare if the code is rerun with different numbers of OpenMP threads.

Restrictions

If two reductions are used within an OpenMP region and the same variable is used for both reductions then PSyclone will raise an exception. In this case the solution is to use a different variable for each reduction.

PSyclone does not support (distributed-memory) halo swaps or global sums within OpenMP parallel regions. Attempting to create a parallel region for a set of nodes that includes halo swaps or global sums will produce an error. In such cases it may be possible to re-order the nodes in the Schedule using the *MoveTrans* transformation.

CHAPTER

SEVEN

DISTRIBUTED MEMORY

PSyclone supports the generation of code for distributed memory machines. When this option is switched on, PSyclone takes on responsibility for both performance and correctness, as described below.

Correctness

PSyclone is responsible for adding appropriate distributed memory communication calls to the PSy layer to ensure that the distributed memory code runs correctly. For example, a stencil operation will require halo exchanges between the different processes.

The burden of correctly placing distributed memory communication calls has traditionally been born by the user. However, PSyclone is able to determine the placing of these within the PSy-layer, thereby freeing the user from this responsibility. Thus, the Algorithm and Kernel code remain the same, irrespective of whether the target architecture does or does not require a distributed memory solution.

Performance

PSyclone adds **HaloExchange** and **GlobalSum** objects to the generated PSy **Schedule** (see the *Schedule* Section) at the required locations. The halo-exchange and global-sum objects are exposed here for the purposes of optimisation. For example the halo-exchange and/or global-sum objects may be moved in the schedule (via appropriate transformations) to enable overlap of computation with communication.

Note: When these optimisations are implemented, add a reference to the *Transformations* Section.

A halo exchange is required with distributed memory when a processor requires data from its halo and the halo information is out of date. One example is where a field is written to and then read using a stencil access. Halo exchanges have performance implications so should only be used where necessary.

A global sum is required with distributed memory when a scalar is written to. Global sums can have performance implications so should only be used where necessary. Global sums currently only occur in certain Built-in kernels. The description of Built-ins indicates when this is the case.

Implementation

Within the contents of an `invoke()` call, PSyclone is able to statically determine which communication calls are required and where they should be placed. However, PSyclone has no information on what happens outside `invoke()` calls and thus is unable to statically determine whether communication is required between these calls. The solution we use is to add run-time flags in the PSy layer to keep track of whether data has been written to and read from. These flags are then used to determine whether communication calls are required upon entry to an `invoke()`.

Control

Support for distributed memory can be switched on or off with the default being on. The default can be changed permanently by modifying the `DISTRIBUTED_MEMORY` variable in the `psyclone.cfg` configuration file to `false` (see *Configuration*).

Distributed memory can be switched on or off from the `generator` script using the `-dm`/`--dist_mem` or `-nodm`/`--no_dist_mem` flags, respectively.

For interactive access, the distributed memory option can be changed interactively from the `PSyFactory` class by setting the optional `distributed_memory` flag; for example:

```
psy = PSyFactory(api=api, distributed_memory=False)
```

Similarly the distributed memory option can be changed interactively from the `generate` function by setting the optional `distributed_memory` flag, e.g.:

```
psy, alg = generate("file.f90", distributed_memory=False).
```

Status

Distributed memory support is currently limited to the `dynamo0.3` API. The remaining API's ignore the distributed memory flag and continue to produce code without any distributed memory functionality, irrespective of its value.

CHAPTER

EIGHT

BUILT-INS

Built-ins (named by analogy with the native functionality provided by Python) are operations which can be specified within an invoke call in the algorithm layer but do not require an associated kernel to be implemented as they are provided directly by the infrastructure.

One use of Built-ins is for commonly used operations. In this case Built-ins simplify the use of the system as users do not need to write kernel routines. Built-ins also offer a potential performance advantage as they provide a specification of what is required without an implementation. Therefore the PSy layer is free to implement these operations in whatever way it chooses.

Note: In general, PSyclone will need to know the types of the arguments being passed to any Built-ins. The parser obtains this information from an API-specific file that contains the meta-data for all Built-in operations supported for that API.

Example

In the following example, the invoke call includes a call to a Built-in (`setval_c`) and a user-supplied kernel (`matrix_vector_kernel_mm_type`). The Built-in sets all values in the field `Ax` to `0.0`. Notice that, unlike the kernel call, no use association is required for the Built-in since it is provided as part of the environment (*c.f.* Fortran intrinsics such as `sin()`).

```
subroutine jacobi_solver_algorithm(lhs, rhs, mm, mesh, n_iter)
  use matrix_vector_mm_mod, only: matrix_vector_kernel_mm_type
  integer,               intent(in)    :: n_iter
  type(field_type),      intent(inout) :: lhs, rhs
  type(operator_type),   intent(inout) :: mm
  type(mesh_type),       intent(in)    :: mesh
  type(field_type)                     :: Ax, lumped_weight, res

  real(kind=r_def), parameter :: MU = 0.9_r_def
  ...

  do iter = 1,n_iter
    call invoke( setval_c(Ax, 0.0) )
    call invoke( matrix_vector_kernel_mm_type(Ax,lhs,mm) )
    ...
  end do

end subroutine jacobi_solver_algorithm
```

Below is an example of a kernel that is consistent with the `matrix_vector_kernel_mm_type kernel` specified in the example above.

```
module matrix_vector_mm_mod
  type, public, extends(kernel_type) :: matrix_vector_kernel_mm_type
    private
    type(arg_type) :: meta_args(3) = (/                                  &
         arg_type(GH_FIELD,    GH_INC,  ANY_SPACE_1),                    &
         arg_type(GH_FIELD,    GH_READ, ANY_SPACE_1),                    &
         arg_type(GH_OPERATOR, GH_READ, ANY_SPACE_1, ANY_SPACE_1)        &
         /)
    integer :: iterates_over = CELLS
  contains
    procedure, nopass ::matrix_vector_mm_code
  end type
contains
  subroutine matrix_vector_mm_code(cell,        &
                                   nlayers,     &
                                   lhs, x,      &
                                   ncell_3d,    &
                                   mass_matrix, &
                                   ndf,undf,map)
  end subroutine matrix_vector_mm_code
end module matrix_vector_mm_mod
```

We now translate the algorithm layer code and generate the psy layer code. The algorithm code is assumed to be in a file call *solver_mod.x90*. In this case we use the top level python interface. See the *API* section for different ways to translate/generate code.

```
>>> from generator import generate
>>> alg, psy = generate("solver_mod.x90")
>>> print alg
>>> print psy
```

The resultant generated algorithm code is given below.

Ignoring the difference in case (which is due to the output format of the code parser) the differences between the original algorithm code and the translated algorithm code are:

- the generic calls to `invoke` have been replaced by specific `CALL invoke_xx`. The calls within the invoke are removed, as are duplicate arguments and any literals leaving the three fields being passed in.
- a use statement is added for the each of the new `CALL invoke_xx` which will call the generated PSy layer code.

The existance of a call to a Built-in has made no difference at this point:

```
SUBROUTINE jacobi_solver_algorithm(lhs, rhs, mm, mesh, n_iter)
  USE solver_mod_psy, ONLY: invoke_5_matrix_vector_kernel_mm_type
  USE solver_mod_psy, ONLY: invoke_4
  INTEGER, intent(in) :: n_iter
  TYPE(field_type), intent(inout) :: lhs, rhs
  TYPE(operator_type), intent(inout) :: mm
  TYPE(mesh_type), intent(in) :: mesh
  TYPE(field_type) ax, lumped_weight, res

  REAL(KIND=r_def), parameter :: mu = 0.9_r_def

  INTEGER iter
  INTEGER rhs_fs
  TYPE(function_space_type) fs
  ...
  DO iter = 1,n_iter
    CALL invoke_4(ax)
    CALL invoke_5_matrix_vector_kernel_mm_type(ax, lhs, mm)
    ...
  END DO
END SUBROUTINE jacobi_solver_algorithm
```

A vanilla (not optimised) version of the generated PSy layer is given below. As expected the kernel code is called from the PSy layer. However, in the case of the *setval_c* Built-in, the code for this has been written directly into the PSy layer (the loop setting *ax_proxy%data(df) = 0.0*). This example illustrates that Built-ins may be implemented in whatever way the generator sees fit with no change to the algorithm and kernel layers.

```
MODULE solver_mod_psy
  ...
  SUBROUTINE invoke_4(ax)
    USE mesh_mod, ONLY: mesh_type
    TYPE(field_type), intent(inout) :: ax
    INTEGER df
    INTEGER undf_any_space_1
    TYPE(field_proxy_type) ax_proxy
    !
    ! Initialise field proxies
    !
    ax_proxy = ax%get_proxy()
    !
    ! Initialise sizes and allocate any basis arrays for any_space_1
    !
    undf_any_space_1 = ax_proxy%vspace%get_undf()
    !
    ...
    ! Call our kernels
    !
    DO df=1,undf_any_space_1
      ax_proxy%data(df) = 0.0
    END DO
    !
    ...
    !
  END SUBROUTINE invoke_4
  SUBROUTINE invoke_5_matrix_vector_kernel_mm_type(ax, lhs, mm)
    USE matrix_vector_mm_mod, ONLY: matrix_vector_mm_code
    ...
    TYPE(field_type), intent(inout) :: ax, lhs
    TYPE(operator_type), intent(inout) :: mm
    ...
    !
    ! Initialise field proxies
    !
    ax_proxy = ax%get_proxy()
    lhs_proxy = lhs%get_proxy()
    mm_proxy = mm%get_proxy()
    !
    ! Initialise number of layers
    !
    nlayers = ax_proxy%vspace%get_nlayers()
    !
    ! Initialise sizes and allocate any basis arrays for any_space_1
    !
    ndf_any_space_1 = ax_proxy%vspace%get_ndf()
    undf_any_space_1 = ax_proxy%vspace%get_undf()
    !
    ...
    DO cell=1,mesh%get_last_halo_cell(1)
      !
      map_any_space_1 => ax_proxy%vspace%get_cell_dofmap(cell)
      !
      CALL matrix_vector_mm_code(cell, nlayers, ax_proxy%data,            &
                                 lhs_proxy%data, mm_proxy%ncell_3d,       &
                                 mm_proxy%local_stencil, ndf_any_space_1, &
                                 undf_any_space_1, map_any_space_1)
      ...
      !
    END DO
    !
    ...
    !
  END SUBROUTINE invoke_5_matrix_vector_kernel_mm_type
  ...
END MODULE solver_mod_psy
```

This example is distributed with PSyclone and can be found in `<PSYCLONEHOME>/examples/dynamo/eg4`.

Supported Built-in operations

The list of supported Built-ins is API-specific and therefore is described under the documentation of each API.

Adding new additional Built-in operations

1. Identify the PSyclone source file for the API to be extended. *e.g.* for dynamo0.3 it is `src/dynamo0p3_builtins.py`.
2. Edit this source file to create the class for this new call. It must inherit from the API-specific parent class for Built-in operations (`DynBuiltInKern` for dynamo0.3).
3. Implement `__str__` and `gen_code()` methods for this new class.
4. Add the name of the new Built-in operation and its corresponding class to the `BUILTIN_MAP` dictionary in that source file.
5. Add meta-data describing this call to the appropriate file specified in the `BUILTIN_DEFINITIONS_FILE` in that source file. For dynamo0.3 this is `dynamo0p3_builtins_mod.f90`.
6. Add relevant tests to the PSyclone test file for the API to be extended. *e.g.* for dynamo0.3 it is `src/tests/dynamo0p3_builtins_test.py`. The tests rely on `single_invoke` Fortran examples in the relevant `src/tests/test_files/` subfolder.
7. Add an appropriate Fortran `single_invoke` example for the new Built-in in the relevant `src/tests/test_files/` subfolder. *e.g.* for dynamo0.3 it is `src/tests/test_files/dynamo0p3/`. Names of examples follow the template `<category.number>.<subcategory.number>_<single_invoke_name>.f90`. *e.g.* for dynamo0.3 `<category.number>` is 15.

8. Document the new Built-in in the documentation of the relevant API (*e.g.* `doc/dynamo0p3.rst`).

If the API being extended does not currently support any Built-ins then the `BUILTIN_MAP` and `BUILTIN_DEFINITIONS_FILE` module variables must be added to the source file for the API. A Fortran module file must be created in the PSyclone src directory (with the name specified in `BUILTIN_DEFINITIONS_FILE`) containing meta-data describing the Built-in operations. Finally, `parse.get_builtin_defs()` must be extended to import `BUILTIN_MAP` and `BUILTIN_DEFINITIONS_FILE` for this API.

CHAPTER

NINE

DYNAMO0.3 API

This section describes the Dynamo0.3 application programming interface (API). This API explains what a user needs to write in order to make use of the Dynamo0.3 API in PSyclone.

As with all PSyclone API's the Dynamo0.3 API specifies how a user needs to write the algorithm layer and the kernel layer to allow PSyclone to generate the PSy layer. These algorithm and kernel API's are discussed separately in the following sections.

The Dynamo0.3 API supports the Met Office's finite element (hereafter FEM) based GungHo dynamical core (see *Introduction*). The Met Office Collaboration Wiki (login required) provides more detailed information about the dynamical core's formulation and data model.

Algorithm

The general requirements for the structure of an Algorithm are explained in the *Algorithm layer* section. This section explains the Dynamo0.3-specific specialisations and extensions.

Example

An example Dynamo0.3 API invoke call is given below with various different types of objects supported by the API. These different objects and their use are discussed in the following sections.

```
real(kind=r_def)                  :: scalar1
integer(kind=i_def)               :: stencil_extent
type(field_type)                  :: field1, field2, field3
type(field_type)                  :: field5(3), field6(3)
type(quadrature_type)             :: qr
type(operator_type)               :: operator1
type(columnwise_operator_type) :: cma_op1
...
call invoke( kernel1(field1, field2, operator1, qr),           &
             builtin1(scalar1, field2, field3),               &
             kernel2(field1, stencil_extent, field3, scalar1), &
             assembly_kernel(cma_op1, operator1),             &
             name="some_calculation"                          &
           )
call invoke( prolong_kernel_type(field1, field4),             &
             restrict_kernel_type(field5, field6)
           )
```

Please see the *Algorithm layer* section for a description of the `name` argument.

Objects in the Dynamo0.3 API can be categorised by their functionality as data types and information that specifies supported operations on a particular data type. The above example introduces four of five data types supported by the Dynamo0.3 API: field, scalar, operator and column-wise operator (field vector is the fifth). `qr` represents a quadrature object which provides information required by a kernel to operate on fields (see section *Quadrature* for more details).

Field

Dynamo0.3 API fields, identified with `GH_FIELD` metadata, represent FEM discretisations of various dynamical core prognostic and diagnostic variables. In FEM, variables are discretised by placing them into a function space (see *Supported Function Spaces*) from which they inherit a polynomial expansion via the basis functions of that space. Field values at points within a cell are evaluated as the sum of a set of basis functions multiplied by coefficients which are the data points. Points of evaluation are determined by a quadrature object (*Quadrature*) and are independent of the function space the field is on. Placement of field data points, also called degrees of freedom ("dof"), is determined by the function space the field is on.

Field Vector

Depending on the function space a field lives on, the field data at a point can be a scalar or a vector (see *Supported Function Spaces* for the list of scalar and vector function spaces). There is an additional option which specifies whether the data itself is vector valued and it usually refers to bundles of scalar valued fields. Field vectors are represented as `GH_FIELD*N` where `N` is the size of the vector. The 3D coordinate field, for example, has `(x, y, z)` scalar values at the nodes and therefore has a vector size of 3.

Scalar

In Dynamo 0.3 API a scalar is a single value variable that can be either real or integer. Real scalars are identified with `GH_REAL` and integer scalars are identified with `GH_INTEGER` metadata.

Operator

Represents a matrix constructed on a per-cell basis using Local Matrix Assembly (LMA) and is identified with `GH_OPERATOR` metadata.

Column-Wise Operator

The Dynamo 0.3 API has support for the construction and use of column-wise/Column Matrix Assembly (CMA) operators whose metadata identifier is `GH_COLUMNWISE_OPERATOR`. As the name suggests, these are operators constructed for a whole column of the mesh. These are themselves constructed from the Local Matrix Assembly (LMA) operators of each cell in the column. The rules governing Kernels that have CMA operators as arguments are given in the *Kernel* section below.

There are three recognised Kernel types involving CMA operations; construction, application (including inverse application) and matrix-matrix. The following example sketches-out what the use of such kernels might look like in the Algorithm layer:

```
use field_mod, only: field_type
use operator_mod, only : operator_type, columnwise_operator_type
type(field_type) :: field1, field2, field3
type(operator_type) :: lma_op1, lma_op2
type(columnwise_operator_type) :: cma_op1, cma_op2, cma_op3
real(kind=r_def) :: alpha
```

```
...
call invoke(                                                &
        assembly_kernel(cma_op1, lma_op1, lma_op2),         &
        assembly_kernel2(cma_op2, lma_op1, lma_op2, field3),    &
        apply_kernel(field1, field2, cma_op1),              &
        matrix_matrix_kernel(cma_op3, cma_op1, alpha, cma_op2), &
        apply_kernel(field3, field1, cma_op3),              &
        name="cma_example")
```

The above invoke uses two LMA operators to construct the CMA operator `cma_op1`. A second CMA operator, `cma_op2`, is assembled from the same two LMA operators but also uses a field. The first of these CMA operators is then applied to `field2` and the result stored in `field1` (assuming that the meta-data for `apply_kernel` specifies that it is the first field argument that is written to). The two CMA operators are then combined to produce a third, `cma_op3`. This is then applied to `field1` and the result stored in `field3`.

Note that PSyclone identifies the type of kernels performing Column-Wise operations based on their arguments as described in meta-data (see *Rules for Kernels that work with CMA Operators* below). The names of the kernels in the above example are purely illustrative and are not used by PSyclone when determining kernel type.

A full example of CMA operator construction is available in `examples/dynamo/eg7`.

Quadrature

Kernels conforming to the Dynamo 0.3 API may require quadrature information (specified using e.g. `gh_shape = gh_quadrature_XYoZ` in the kernel meta-data - see Section *gh_shape*). This information must be passed to the kernel from the Algorithm layer in the form of a *quadrature_type* object. This must be the last argument passed to the kernel, e.g.:

```
type( quadrature_type )   :: qr
...
qr = quadrature_type(element_order+2, GAUSSIAN)
call invoke(pressure_gradient_kernel_type(rhs_tmp(igh_u), rho, theta, qr),   &
            kinetic_energy_gradient_kernel_type(rhs_tmp(igh_u), u, chi, qr), &
            geopotential_gradient_kernel_type(rhs_tmp(igh_u), geopotential, qr))
```

This quadrature object specifies the set of points at which the basis/differential-basis functions required by the kernel are to be evaluated.

Stencils

Kernel metadata may specify that a Kernel performs a stencil operation on a field. Any such metadata must provide a stencil type. See the *meta_args* section for more details. The supported stencil types are `X1D`, `Y1D`, `XORY1D` or `CROSS`.

If a stencil operation is specified by the Kernel metadata the algorithm layer must provide the `extent` of the stencil (the maximum distance from the central cell that the stencil extends). The Dynamo0.3 API expects this information to be added as an additional `integer` argument immediately after the relevant field when specifying the Kernel via an `invoke`.

For example:

```
integer :: extent = 2
call invoke(kernel(field1, field2, extent))
```

where `field2` has kernel metadata specifying that it has a stencil access.

`extent` may also be passed as a literal. For example:

```
call invoke(kernel(field1, field2, 2))
```

where, again, `field2` has kernel metadata specifying that it has a stencil access.

Note: The stencil extent specified in the Algorithm layer is not the same as the stencil size passed in to the Kernel. The latter contains the number of cells in the stencil which is dependent on both the stencil type and extent.

If the Kernel metadata specifies that the stencil is of type `XORY1D` (which means `X1D` or `Y1D`) then the algorithm layer must specify whether the stencil is `X1D` or `Y1D` for that particular kernel call. The Dynamo0.3 API expects this information to be added as an additional argument immediately after the relevant stencil extent argument. The argument should be an `integer` with valid values being `x_direction` or `y_direction`, both being supplied by the `LFRic` infrastructure via the `flux_direction_mod` fortran module

For example:

```
use flux_direction_mod, only : x_direction
integer :: direction = x_direction
integer :: extent = 2
! ...
call invoke(kernel(field1, field2, extent, direction))
```

`direction` may also be passed as a literal. For example:

```
use flux_direction_mod, only : x_direction
integer :: extent = 2
! ...
call invoke(kernel(field1, field2, extent, x_direction))
```

If certain fields use the same value of extent and/or direction then the same variable, or literal value can be provided.

For example:

```
call invoke(kernel1(field1, field2, extent,  field3, extent, direction), &
            kernel2(field1, field2, extent2, field4, extent, direction))
```

In the above example `field2` and `field3` in `kernel1` and `field4` in `kernel2` will have the same `extent` value but `field2` in `kernel2` may have a different value. Similarly, `field3` in `kernel1` and `field4` in `kernel2` will have the same `direction` value.

An example of the use of stencils is available in `examples/dynamo/eg5`.

There is currently no attempt to perform type checking in PSyclone so any errors in the type and/or position of arguments will not be picked up until compile time. However, PSyclone does check for the correct number of algorithm arguments. If the wrong number of arguments is provided then an exception is raised.

For example, running test 19.2 from the Dynamo0.3 API test suite gives:

```
cd <PSYCLONEHOME>/src/psyclone/tests
python ../generator.py test_files/dynamo0p3/19.2_single_stencil_broken.f90
"Generation Error: error: expected '5' arguments in the algorithm layer but found '4'.
Expected '4' standard arguments, '1' stencil arguments and '0' qr_arguments'"
```

Inter-grid

From the Algorithm layer, an Invoke for inter-grid kernels (those that map fields between grids of different resolution) looks much like an Invoke containing general-purpose kernels. The only restrictions to be aware of are that inter-grid kernels accept only field or field-vectors as arguments and that an Invoke may not mix inter-grid kernels with any other kernel type. (Hence the second, separate Invoke in the example Algorithm code given at the beginning of this Section.)

PSy-layer

The general details of the PSy-layer are explained in the *PSy layer* section. This section describes any dynamo0p3 specific issues.

Module name

The PSy-layer code is contained within a Fortran module. The name of the module is determined from the algorithm-layer name with "_psy" appended. The algorithm-layer name is the algorithm's module name if it is a module, its subroutine name if it is a subroutine that is not within a module, or the program name if it is a program.

So, for example, if the algorithm code is contained within a module called "fred" then the PSy-layer module name will be "fred_psy".

Kernel

The general requirements for the structure of a Kernel are explained in the *Kernel layer* section. In the Dynamo API there are four different Kernel types; general purpose, CMA, inter-grid and *Built-ins*. In the case of built-ins, PSyclone generates the source of the kernels. This section explains the rules for the other three, user-supplied kernel types and then goes on to describe their metadata and subroutine arguments.

Rules for all User-Supplied Kernels

In the following, 'operator' refers to both LMA and CMA operator types.

1. A Kernel must have at least one argument that is a field, field vector, or operator. This rule reflects the fact that a Kernel iterates over a space and therefore must have some representation over that space.
2. The continuity of the iteration space of the Kernel is determined from the function space of the modified argument (see *Supported Function Spaces*). If more than one argument is modified then the iteration space is taken to be the largest required by any of those arguments. e.g. if a Kernel writes to two fields, the first on W3 (discontinuous) and the second on W1 (continuous), then the iteration space of that Kernel will be determined by the field on the continuous space.
3. If the function space of the modified argument(s) cannot be determined then they are assumed to be continuous. This is the case if any of the modified arguments are declared as `ANY_SPACE` and their actual space cannot be determined statically. This assumption is always safe but leads to additional computation if the quantities being updated are actually on discontinuous function spaces.
4. Operators do not have halo operations operating on them as they are either cell- (LMA) or column-based (CMA) and therefore act like discontinuous fields.
5. Any Kernel that writes to an operator will have its iteration space expanded such that valid values for the operator are computed in the level-1 halo.

6. Any Kernel that reads from an operator must not access halos beyond level 1. In this case PSyclone will check that the Kernel does not require values beyond the level-1 halo. If it does then PSyclone will abort.

Rules specific to General-Purpose Kernels without CMA Operators

1. General-purpose kernels accept arguments of any of the following types: field, field vector, LMA operator, scalar integer, scalar real.
2. A Kernel is permitted to write to more than one quantity (field or operator) and these quantities may be on the same or different function spaces.
3. A Kernel may not write to a scalar argument. (Only *Built-ins* are permitted to do this.) Any scalar aguments must therefore be declared in the meta-data as `GH_READ` - see below.

Rules for Kernels that work with CMA Operators

The Dynamo 0.3 API has support for kernels that assemble, apply (or inverse-apply) column-wise/Column Matrix Assembly (CMA) operators. Such operators may also be used by matrix-matrix kernels. There are thus three types of CMA-related kernels. Since, by definition, CMA operators only act on data within a column, they have no horizontal dependencies. Therefore, kernels that write to them may be parallelised without colouring.

All three CMA-related kernel types must obey the following rules:

1. Since a CMA operator only acts within a single column of data, stencil operations are not permitted.
2. No vector quantities (e.g. "GH_FIELD*3" - see below) are permitted as arguments.

There are then additional rules specific to each of the three CMA kernel types. These are described below.

Assembly

CMA operators are themselves constructed from Local-Matrix-Assembly (LMA) operators. Therefore, any kernel which assembles a CMA operator must obey the following rules:

1. Have one or more LMA operators as read-only arguments.
2. Have exactly one CMA operator argument which must have write access.
3. Other types of argument (e.g. scalars or fields) are permitted but must be read-only.

Application and Inverse Application

Column-wise operators can only be applied to fields. CMA-Application kernels must therefore:

1. Have a single CMA operator as a read-only argument.
2. Have exactly two field arguments, one read-only and one that is written to.
3. The function spaces of the read and written fields must match the from and to spaces, respectively, of the supplied CMA operator.

Matrix-Matrix

A kernel that has just column-wise operators as arguments and zero or more read-only scalars is identified as performing a matrix-matrix operation. In this case:

1. Arguments must be CMA operators and, optionally, one or more scalars.

2. Exactly one of the CMA arguments must be written to while all other arguments must be read-only.

Rules for Inter-Grid Kernels

1. An inter-grid kernel is identified by the presence of a field or field-vector argument with the optional *mesh_arg* meta-data element (see *Inter-Grid Metadata*).
2. An invoke that contains one or more inter-grid kernels must not contain any other kernel types. (This restriction is an implementation decision and could be lifted in future if there is a need.)
3. An inter-grid kernel is only permitted to have field or field-vector arguments.
4. All inter-grid kernel arguments must have the *mesh_arg* meta-data entry.
5. An inter-grid kernel (and meta-data) must have at least one field on each of the fine and coarse meshes. Specifying all fields as coarse or fine is forbidden.
6. Fields on different meshes must always live on different function spaces.
7. All fields on a given mesh must be on the same function space.

A consequence of Rules 5-7 is that an inter-grid kernel will only involve two function spaces.

Metadata

The code below outlines the elements of the Dynamo0.3 API kernel metadata, 1) 'meta_args', 2) 'meta_funcs', 3) 'gh_shape', 4) 'iterates_over' and 5) 'procedure'.

```
type, public, extends(kernel_type) :: my_kernel_type
  type(arg_type) :: meta_args(...) = (/ ... /)
  type(func_type) :: meta_funcs(...) = (/ ... /)
  integer :: gh_shape = gh_quadrature_XYoZ
  integer :: iterates_over = cells
contains
  procedure :: my_kernel_code
end type
```

These five metadata elements are discussed in order in the following sections.

meta_args

The `meta_args` array specifies information about data that the kernel code expects to be passed to it via its argument list. There is one entry in the `meta_args` array for each **scalar**, **field**, or **operator** passed into the Kernel and the order that these occur in the `meta_args` array must be the same as they are expected in the kernel code argument list. The entry must be of `arg_type` which itself contains metadata about the associated argument. The size of the meta_args array must correspond to the number of **scalars**, **fields** and **operators** passed into the Kernel.

Note: it makes no sense for a Kernel to have only **scalar** arguments (because the PSy layer will call a Kernel for each point in the spatial domain) and PSyclone will reject such Kernels.

For example, if there are a total of 2 **scalar / field / operator** entities being passed to the Kernel then the meta_args array will be of size 2 and there will be two `arg_type` entries:

```
type(arg_type) :: meta_args(2) = (/                                     &
     arg_type( ... ),                                                   &
     arg_type( ... )                                                    &
     /)
```

Argument-metadata (metadata contained within the brackets of an `arg_type` entry), describes either a **scalar**, a **field** or an **operator** (either LMA or CMA).

The first argument-metadata entry describes whether the data that is being passed is for a real scalar (`GH_REAL`), an integer scalar (`GH_INTEGER`), a field (`GH_FIELD`) or an operator (either `GH_OPERATOR` for LMA or `GH_COLUMNWISE_OPERATOR` for CMA). This information is mandatory.

Additionally, argument-metadata can be used to describe a vector of fields (see the *Field Vector* section for more details).

As an example, the following `meta_args` metadata describes 4 entries, the first is a real scalar, the next two are fields and the fourth is an operator. The third entry is a field vector of size 3.

```
type(arg_type) :: meta_args(4) = (/                                     &
     arg_type(GH_REAL, ...),                                            &
     arg_type(GH_FIELD, ... ),                                          &
     arg_type(GH_FIELD*3, ... ),                                        &
     arg_type(GH_OPERATOR, ...)                                         &
     /)
```

The second entry to argument-metadata (information contained within the brackets of an `arg_type`) describes how the Kernel makes use of the data being passed into it (the way it is accessed within a Kernel). This information is mandatory. There are currently 5 possible values of this metadata `GH_WRITE`, `GH_READ`, `GH_INC`, `GH_READWRITE` and `GH_SUM`. However, not all combinations of metadata entries are valid and PSyclone will raise an exception if an invalid combination is specified. Valid combinations are specified later in this section (see *Valid Access Modes*).

- `GH_WRITE` indicates the data is modified in the Kernel before (optionally) being read.
- `GH_READ` indicates that the data is read and is unmodified.
- `GH_INC` indicates that different iterations of a Kernel make contributions to shared values. For example, values at cell faces may receive contributions from cells on either side of the face. This means that such a Kernel needs appropriate synchronisation (or colouring) to run in parallel.
- `GH_READWRITE` indicates that different iterations of a Kernel update quantitites which do not share dofs, such as operators and fields over discontinuous function spaces. If a Kernel modifies only discontinuous fields and/or operators there is no need for synchronisation or colouring when running such Kernels in parallel. However, modifying another field with a `GH_INC` access in a Kernel means that synchronisation or colouring is required for parallel runs.
- `GH_SUM` is an example of a reduction and is the only reduction currently supported in PSyclone. This metadata indicates that values are summed over calls to Kernel code.

For example:

```
type(arg_type) :: meta_args(4) = (/                                     &
     arg_type(GH_REAL,   GH_SUM),                                       &
     arg_type(GH_FIELD, GH_INC, ... ),                                  &
     arg_type(GH_FIELD*3, GH_WRITE, ... ),                              &
     arg_type(GH_OPERATOR, GH_READ, ...)                                &
     /)
```

Note: In the Dynamo 0.3 API only *Built-ins* are permitted to write to scalar arguments (and hence perform reductions). Furthermore, this permission is currently restricted to real scalars (`GH_REAL`) as the LFRic infrastructure does not yet support integer reductions.

For a scalar the argument metadata contains only these two entries. However, fields and operators require further entries specifying function-space information. The meaning of these further entries differs depending on whether a field or an operator is being described.

In the case of an operator, the 3rd and 4th arguments describe the `to` and `from` function spaces respectively. In the case of a field the 3rd argument specifies the function space that the field lives on. More details about the supported function spaces are in subsection *Supported Function Spaces*.

For example, the meta-data for a kernel that applies a Column-wise operator to a field might look like:

```
type(arg_type) :: meta_args(3) = (/                          &
     arg_type(GH_FIELD, GH_INC, W1),                         &
     arg_type(GH_FIELD, GH_READ, W2H),                       &
     arg_type(GH_COLUMNWISE_OPERATOR, GH_READ, W1, W2H) &
     /)
```

In some cases a Kernel may be written so that it works for fields and/or operators from any type of w2 space i.e. one of `w2`, `w2h` or `w2v`. In this case the metadata should be specified as being `any_w2`.

Warning: in the current implementation it is assumed that all fields and/or operators specifying `any_w2` within a kernel will use the **same** function space. It is up to the user to ensure this is the case as otherwise invalid code would be generated.

It may be that a Kernel is written such that a field and/or operators may be on/map-between any function space(s). In this case the metadata should be specified as being one of `any_space_1`, `any_space_2`, ..., `any_space_9`. The reason for having different names is that a Kernel might be written to allow 2 or more arguments to be able to support any function space but for a particular call the function spaces may have to be the same as each other.

In the example below, the first field entry supports any function space but it must be the same as the operator's `to` function space. Similarly, the second field entry supports any function space but it must be the same as the operator's `from` function space. Note, the metadata does not forbid `ANY_SPACE_1` and `ANY_SPACE_2` from being the same.

```
type(arg_type) :: meta_args(3) = (/                                &
     arg_type(GH_FIELD, GH_INC, ANY_SPACE_1),                      &
     arg_type(GH_FIELD*3, GH_WRITE, ANY_SPACE_2),                  &
     arg_type(GH_OPERATOR, GH_READ, ANY_SPACE_1, ANY_SPACE_2) &
     /)
```

Note also that the scope of this naming of any-space function spaces is restricted to the argument list of individual kernels. i.e. if an Invoke contains say, two kernel calls that each support arguments on any function space, e.g. `ANY_SPACE_1`, there is no requirement that these two function spaces be the same. Put another way, if an Invoke contained two calls of a kernel with arguments described by the above meta-data then the first field argument passed to each kernel call need not be on the same space.

Note: A `GH_FIELD` argument that specifies `GH_WRITE` or `GH_READWRITE` as its access pattern must be a discontinuous function in the horizontal (see *Valid Access Modes* below). That means it must belong to `w3`, `wtheta` or `w2v` function spaces (see *Supported Function Spaces*). A `GH_FIELD` that specifies `GH_INC` as its access pattern may be continuous in the vertical (and discontinuous in the horizontal), continuous in the horizontal (and discontinuous in the vertical), or continuous in both. In each case the code is the same. However, if a field is discontinuous in the horizontal then it will not need colouring and, if is described as being on any space, there is currently no way to determine this from the metadata (unless we can statically determine the space of the field being passed in). At the moment this type of Kernel is always treated as if it is continuous in the horizontal, even if it is not.

Valid Access Modes

As mentioned earlier, not all combinations of metadata are valid. Valid combinations are summarised here. All types of data (`GH_INTEGER`, `GH_REAL`, `GH_FIELD`, `GH_OPERATOR` and `GH_COLUMNWISE_OPERATOR`) may be read within a Kernel and this is specified in metadata using `GH_READ`. At least one kernel argument must be listed as being modified. When data is *modified* in a Kernel then the permitted access modes depend on the type of data it is and the function space it is on. Valid values are given in the table below.

Argument Type	Function space	Access type
GH_INTEGER	*n/a*	*GH_SUM (Built-ins only)*
GH_REAL	n/a	GH_SUM (Built-ins only)
GH_FIELD	Discontinuous	GH_WRITE, GH_READWRITE
GH_FIELD	Continuous	GH_INC
GH_OPERATOR	Any for both 'to' and 'from'	GH_WRITE, GH_READWRITE
GH_COLUMNWISE_OPERATOR	Any for both 'to' and 'from'	GH_WRITE, GH_READWRITE

Note: As mentioned above, note that only Built-ins may modify scalar arguments. *Since the LFRic infrastructure does not currently support integer reductions, integer scalar arguments are restricted to having read-only access.*

There is no restriction on the number and function-spaces of other quantities that a general-purpose kernel can modify other than that it must modify at least one. The rules for kernels involving CMA operators, however, are stricter and only one argument may be modified (the CMA operator itself for assembly, a field for CMA-application and a CMA operator for matrix-matrix kernels). If a kernel writes to quantities on different function spaces then PSyclone generates loop bounds appropriate to the largest iteration space. This means that if a single kernel updates one quantity on a continuous function space and one on a discontinuous space then the resulting loop will include cells in the level 1 halo since they are required for a quantity on a continuous space. As a consequence, any quantities on a discontinuous space will then be computed redundantly in the level 1 halo. Currently PSyclone makes no attempt to take advantage of this (by e.g. setting the appropriate level-1 halo to 'clean').

PSyclone ensures that both CMA and LMA operators are computed (redundantly) out to the level-1 halo cells. This permits their use in kernels which modify quantities on continuous function spaces and also in subsequent redundant computation of other quantities on discontinuous function spaces. In conjunction with this, PSyclone also checks (when generating the PSy layer) that any kernels which read operator values do not do so beyond the level-1 halo. If any such accesses are found then PSyclone aborts.

Supported Function Spaces

As mentioned in the *Field* and *Field Vector* sections, the function space of an argument specifies how it maps onto the underlying topology and, additionally, whether the data at a point is a vector.

Function spaces can share dofs between cells in the horizontal, vertical or both directions. Depending on the function space and FEM order, the shared dofs can lie on one or more cell entities (faces, edges and vertices) in each direction. This property is referred to as the **continuity** of a function space (horizontal, vertical or full). Alternatively, if there are no shared dofs a function space is described as **discontinuous** (fully or in a particular direction).

The mixed FEM formulation is built on a foundation set of four function spaces described below.

- `w0` is the space of scalar functions with full continuity. The shared dofs lie on cell vertices in the lowest order FEM and on all three entities in higher order FEM.

- `w1` is the space of vector functions with full continuity in the tangential direction only. In the lowest order FEM the shared dofs lie on cell edges for each component, whereas in higher order they also lie on cell faces.
- `w2` is the space of vector functions with full continuity in the normal direction only. The shared dofs lie on cell faces for each component.
- `w3` is the space of scalar functions with full discontinuity. All dofs lie within the cell volume and are not shared across the cell boundaries.

Additional function spaces required for representation of scalar or component-wise vector variables are:

- `wtheta` is the space of scalar functions based on the vertical part of `w2`, discontinuous in the horizontal and continuous in the vertical;
- `w2v` is the space of vector functions based on the vertical part of `w2`, discontinuous in the horizontal and continuous in the vertical;
- `w2h` is the space of vector functions based on the horizontal part of `w2`, continuous in the horizontal and discontinuous in the vertical.

Since the Dynamo0.3 API operates on columns of data, function spaces are categorised as continuous or discontinuous with regard to their horizontal continuity.

- **Continuous** function spaces are `w0`, `w1`, `w2` and `w2h`;
- **Discontinuous** function spaces are `w3`, `wtheta` and `w2v`.

Two additonal function space metadata descriptors as mentioned in sections above are:

- `ANY_W2` for any type of `w2` function spaces;
- `ANY_SPACE` for when the function space of the modified argument(s) cannot be determined and/or for when a Kernel has been written so that it works with fields on any of the available spaces.

As mentioned previously, both `ANY_W2` and `ANY_SPACE` function space types are treated as continuous.

Horizontally discontinuous function spaces and fields over them will not need colouring so PSyclone does not perform it. If such attempt is made, PSyclone will raise a `Generation Error` in the **Dynamo0p3ColourTrans** transformation (see *Transformations* for more details on transformations). An example of fields iterating over a discontinuous function space `wtheta` is given in `examples/dynamo/eg9`, with the `GH_READWRITE` access descriptor denoting an update to the relevant fields. This example also demonstrates how to only colour loops over continuous function spaces when transformations are applied.

Optional Field Metadata

A field entry in the meta_args array may have an optional fourth element. This element describes either a stencil access or, for inter-grid kernels, which mesh the field is on. Since an inter-grid kernel is not permitted to have stencil accesses, these two options are mutually exclusive. The meta-data for each case is described in the following sections.

Stencil Metadata

Stencil metadata specifies that the corresponding field argument is accessed as a stencil operation within the Kernel. Stencil metadata only makes sense if the associated field is read within a Kernel i.e. it only makes sense to specify stencil metadata if the first entry is `GH_FIELD` and the second entry is `GH_READ`.

Stencil metadata is written in the following format:

```
STENCIL(type)
```

where `type` may be one of `X1D`, `Y1D`, `XORY1D` or `CROSS`. As the stencil `extent` (the maximum distance from the central cell that the stencil extends) is not provided in the metadata, it is expected to be provided by the algorithm writer as part of the `invoke` call (see Section *Stencils*). As there is currently no way to specify a fixed extent value for stencils in the Kernel metadata, Kernels must therefore be written to support different values of extent (i.e. stencils with a variable number of cells).

The `XORY1D` stencil type indicates that the Kernel can accept either `X1D` or `Y1D` stencils. In this case it is up to the algorithm developer to specify which of these it is from the algorithm layer as part of the `invoke` call (see Section *Stencils*).

For example, the following stencil (with `extent=2`):

```
| 4 | 2 | 1 | 3 | 5 |
```

would be declared as

```
STENCIL(X1D)
```

and the following stencil (with `extent=2`)

```
|   |   | 9 |   |   |
|   |   | 5 |   |   |
| 6 | 2 | 1 | 3 | 7 |
|   |   | 4 |   |   |
|   |   | 8 |   |   |
```

would be declared as

```
STENCIL(CROSS)
```

Below is an example of stencil information within the full kernel metadata.

```
type(arg_type) :: meta_args(3) = (/                                 &
     arg_type(GH_FIELD, GH_INC, W1),                                &
     arg_type(GH_FIELD, GH_READ, W2H, STENCIL(CROSS)),              &
     arg_type(GH_OPERATOR, GH_READ, W1, W2H)                        &
     /)
```

There is a full example of this distributed with PSyclone. It may be found in `examples/dynamo/eg5`.

Inter-Grid Metadata

The alternative form of the optional fourth metadata argument for a field specifies which mesh the associated field is on. This is required for inter-grid kernels which perform prolongation or restriction operations on fields (or field vectors) existing on grids of different resolutions.

Mesh metadata is written in the following format:

```
mesh_arg=type
```

where `type` may be one of `GH_COARSE` or `GH_FINE`. Any kernel having a field argument with this meta-data is assumed to be an inter-grid kernel and, as such, all of its other arguments (which must also be fields) must have it specified too. An example of the metadata for such a kernel is given below:

```
type(arg_type) :: meta_args(2) = (/                               &
    arg_type(GH_FIELD, GH_INC,  ANY_SPACE_1, mesh_arg=GH_COARSE), &
    arg_type(GH_FIELD, GH_READ, ANY_SPACE_2, mesh_arg=GH_FINE  )  &
    /)
```

Note that an inter-grid kernel must have at least one field (or field- vector) argument on each mesh type. Fields that are on different meshes cannot be on the same function space while those on the same mesh must also be on the same function space.

Column-wise Operators (CMA)

In this section we provide example metadata for each of the three recognised kernel types involving CMA operators.

Column-wise operators are constructed from cell-wise (local) operators. Therefore, in order to **assemble** a CMA operator, a kernel must have at least one read-only LMA operator, e.g.:

```
type(arg_type) :: meta_args(2) = (/                                       &
     arg_type(GH_OPERATOR,            GH_READ,  ANY_SPACE_1, ANY_SPACE_2),&
     arg_type(GH_COLUMNWISE_OPERATOR, GH_WRITE, ANY_SPACE_1, ANY_SPACE_2) &
     /)
```

CMA operators (and their inverse) are **applied** to fields. Therefore any kernel of this type must have one read-only CMA operator, one read-only field and a field that is updated, e.g.:

```
type(arg_type) :: meta_args(3) = (/                                      &
     arg_type(GH_FIELD,    GH_INC,  ANY_SPACE_1),                        &
     arg_type(GH_FIELD,    GH_READ, ANY_SPACE_2),                        &
     arg_type(GH_COLUMNWISE_OPERATOR, GH_READ, ANY_SPACE_1, ANY_SPACE_2) &
     /)
```

Matrix-matrix kernels compute the product/linear combination of CMA operators. They must therefore have one such operator that is updated while the rest are read-only. They may also have read-only scalar arguments, e.g.:

```
type(arg_type) :: meta_args(3) = (/                                        &
     arg_type(GH_COLUMNWISE_OPERATOR, GH_WRITE, ANY_SPACE_1, ANY_SPACE_2), &
     arg_type(GH_COLUMNWISE_OPERATOR, GH_READ, ANY_SPACE_1, ANY_SPACE_2),  &
     arg_type(GH_COLUMNWISE_OPERATOR, GH_READ, ANY_SPACE_1, ANY_SPACE_2),  &
     arg_type(GH_REAL, GH_READ) /)
```

Note: The order with which arguments are specified in meta-data for CMA kernels does not affect the process of identifying the type of kernel (whether it is assembly, matrix-matrix etc.)

meta_funcs

The (optional) second component of kernel meta-data specifies whether any quadrature or evaluator data is required for a given function space. (If no quadrature or evaluator data is required then this meta-data should be omitted.) Consider the following kernel meta-data:

```
type, extends(kernel_type) :: testkern_operator_type
  type(arg_type), dimension(3) :: meta_args =   &
      (/ arg_type(gh_operator,gh_write,w0,w0),  &
         arg_type(gh_field*3,gh_read,w1),       &
         arg_type(gh_integer,gh_read)           &
      /)
  type(func_type) :: meta_funcs(2) =            &
```

```
      (/ func_type(w0, gh_basis, gh_diff_basis) &
         func_type(w1, gh_basis)                &
      /)
  integer, parameter :: gh_shape = gh_quadrature_XYoZ
  integer, parameter :: iterates_over = cells
contains
  procedure() :: code => testkern_operator_code
end type testkern_operator_type
```

The `arg_type` component of this meta-data describes a kernel that takes three arguments (an operator, a field and an integer scalar). Following the `meta_args` array we now have a `meta_funcs` array. This allows the user to specify that the kernel requires basis functions (`gh_basis`) and/or the differential of the basis functions (`gh_diff_basis`) on one or more of the function spaces associated with the arguments listed in `meta_args`. In this case we require both for the W0 function space but only basis functions for W1.

gh_shape

If a kernel requires basis or differential-basis functions then the meta-data must also specify the set of points on which these functions are required. This information is provided by the `gh_shape` component of the meta-data. Currently PSyclone supports two shapes; `gh_quadrature_XYoZ` for Gaussian quadrature points and `gh_evaluator` for evaluation at nodal points. For the latter, the values of the basis/differential-basis functions are computed at the nodes defined by the function space of the quantity that the associated kernel is updating. All necessary data is extracted in the PSy layer and passed to the kernel(s) as required - nothing is required from the Algorithm layer. If a kernel requires quadrature on the other hand, the Algorithm writer must supply a `quadrature_type` object as the last argument to the kernel (see Section *Quadrature*).

Note that it is an error for kernel meta-data to specify a value for `gh_shape` if no basis or differential-basis functions are required.

iterates over

The fourth type of metadata provided is `ITERATES_OVER`. This specifies that the Kernel has been written with the assumption that it is iterating over the specified entity. For user-supplied kernels this currently only has one valid value which is `CELLS`.

Procedure

The fifth and final type of metadata is `procedure` metadata. This specifies the name of the Kernel subroutine that this metadata describes.

For example:

```
procedure :: my_kernel_subroutine
```

Subroutine

Rules for General-Purpose Kernels

The arguments to general-purpose kernels (those that do not involve either CMA operators or prolongation/restriction operations) follow a set of rules which have been specified for the Dynamo0.3 API. These rules are encoded in the `generate()` method within the `ArgOrdering` abstract class in the `dynamo0p3.py` file. The rules, along with PSyclone's naming conventions, are:

1. If an LMA operator is passed then include the `cells` argument. `cells` is an integer and has intent `in`.
2. Include `nlayers`, the number of layers in a column. `nlayers` is an integer and has intent `in`.
3. For each scalar/field/vector_field/operator in the order specified by the meta_args metadata:
   (a) if the current entry is a scalar quantity then include the Fortran variable in the argument list. The intent is determined from the metadata (see *meta_args* for an explanation).
   (b) if the current entry is a field then include the field array. The field array name is currently specified as being `"field_"<argument_position>"_"<field_function_space>`. A field array is a real array of type `r_def` and dimensioned as the unique degrees of freedom for the space that the field is on. This value is passed in separately. Again, the intent is determined from the metadata (see *meta_args*).
      i. If the field entry has a stencil access then add an integer stencil-size argument with intent `in`. This will supply the number of cells in the stencil.
      ii. If the field entry stencil access is of type `XORY1D` then add an integer direction argument with intent `in`.
   (c) if the current entry is a field vector then for each dimension of the vector, include a field array. The field array name is specified as being using `"field_"<argument_position>"_"<field_function_space>"_v"<vector_position>`. A field array in a field vector is declared in the same way as a field array (described in the previous step).
   (d) if the current entry is an operator then first include a dimension size. This is an integer. The name of this size is `<operator_name>"_ncell_3d"`. Next include the operator. This is a real array of type `r_def` and is 3 dimensional. The first two dimensions are the local degrees of freedom for the `to` and `from` function spaces respectively. The third dimension is the dimension size mentioned before. The name of the operator is `"op_"<argument_position>`. Again the intent is determined from the metadata (see *meta_args*).
4. For each function space in the order they appear in the metadata arguments (the `to` function space of an operator is considered to be before the `from` function space of the same operator as it appears first in lexicographic order)
   (a) Include the number of local degrees of freedom (i.e. number per-cell) for the function space. This is an integer and has intent `in`. The name of this argument is `"ndf_"<field_function_space>`.
   (b) If there is a field on this space
      i. Include the unique number of degrees of freedom for the function space. This is an integer and has intent `in`. The name of this argument is `"undf_"<field_function_space>`.
      ii. Include the dofmap for this function space. This is an integer array with intent `in`. It has one dimension sized by the local degrees of freedom for the function space.
   (c) For each operation on the function space (`basis`, `diff_basis`, `orientation`) in the order specified in the metadata
      i. If it is a basis or differential basis function, include the associated argument. This is a real array of kind `r_def` with intent `in`. The rank and extents of this array depend upon the `gh_shape`:
         A. If `gh_shape` is `gh_evaluator` then basis and diff basis are `real` arrays of rank 3 with extent (`dimension`, `number_of_dofs`, `np_xyz`)
         B. If `gh_shape` is `gh_quadrature_xyoz` then basis and diff basis are `real` arrays of rank 4 with extent (`dimension`, `number_of_dofs`, `np_xy`, `np_z`)

         where `dimension` is 1 or 3 and depends upon the function space and whether or not it is a basis or a differential basis function. For the former it is (w0=1, w1=3, w2=3, w3=1, wtheta=1, w2h=3, w2v=3, any_w2=3). For the latter it is (w0=3, w1=3, w2=1, w3=3, wtheta=3, w2h=1, w2v=1, any_w2=3). `number_of_dofs` is the number of degrees of freedom (dofs) associated with the function space and `np_*` are the number of points to be evaluated: i) `*_xyz` in all directions (3D); ii) `*_xy` in the horizontal plane (2D); iii) `*_x, *_y` in the horizontal (1D); and iv) `*_z` in the vertical (1D). The name of the argument is `"basis_"<field_function_space>` or `"diff_basis_"<field_function_space>`, as appropriate.

   ii. If it is an orientation array, include the associated argument. The argument is an integer array with intent `in`. There is one dimension of size the local degrees of freedom for the function space. The name of the array is `"orientation_"<field_function_space>`.

5. If Quadrature or an Evaluator is required (this is the case if any of the function spaces require basis or differential basis functions)

   (a) include integer scalar arguments with intent `in` that specify the extent of the basis/diff-basis arrays:

      i. If `gh_shape` is `gh_evaluator` then pass `n_xyz`

      ii. if `gh_shape` is `gh_quadrature_XYoZ` then pass `n_xy` and `n_z`

   (b) if Quadrature is required (`gh_shape` is of type `gh_quadrature_*`) then include weights which are real arrays of kind `r_def`:

      i. If `gh_quadrature_XYoZ` pass in `w_XZ(n_xy)` and `w_Z(n_z)`

Rules for CMA Kernels

Kernels involving CMA operators are restricted to just three types; assembly, application/inverse-application and matrix-matrix. We give the rules for each of these in the sections below.

Assembly

An assembly kernel requires the column-banded dofmap for both the to- and from-function spaces of the CMA operator being assembled as well as the number of dofs for each of the dofmaps. The full set of rules is:

1. Include the `cell` argument. `cell` is an integer and has intent `in`.
2. Include `nlayers`, the number of layers in a column. `nlayers` is an integer and has intent `in`.
3. Include the number of cells in the 2D mesh, `ncell_2d`, which is an integer with intent `in`.
4. Include the total number of cells, `ncell_3d`, which is an integer with intent `in`.
5. For each argument in the `meta_args` meta-data array:

   (a) If it is a LMA operator, include a real, 3-dimensional array of type `r_def`. The first two dimensions are the local degrees of freedom for the `to` and `from` spaces, respectively. The third dimension is `ncell_3d`.

   (b) If it is a CMA operator, include a real, 3-dimensional array of type `r_def`. The first dimension is is `"bandwidth_"<operator_name>`, the second is `"nrow_"<operator_name>`, and the third is `ncell_2d`.

      i. Include the number of rows in the banded matrix. This is an integer with intent `in` and is named as `"nrow_"<operator_name>`.

      ii. If the from-space of the operator is *not* the same as the to-space then include the number of columns in the banded matrix. This is an integer with intent `in` and is named as `"ncol_"<operator_name>`.

      iii. Include the bandwidth of the banded matrix. This is an integer with intent `in` and is named as `"bandwidth_"<operator_name>`.

      iv. Include banded-matrix parameter `alpha`. This is an integer with intent `in` and is named as `"alpha_"<operator_name>`.

v. Include banded-matrix parameter `beta`. This is an integer with intent `in` and is named as `"beta_"<operator_name>`.

vi. Include banded-matrix parameter `gamma_m`. This is an integer with intent `in` and is named as `"gamma_m_"<operator_name>`.

vii. Include banded-matrix parameter `gamma_p`. This is an integer with intent `in` and is named as `"gamma_p_"<operator_name>`.

(c) If it is a field or scalar argument then include arguments following the same rules as for general-purpose kernels.

6. For each unique function space in the order they appear in the metadata arguments (the `to` function space of an operator is considered to be before the `from` function space of the same operator as it appears first in lexicographic order):

   (a) Include the number of degrees of freedom per cell for the space. This is an integer with intent `in`. The name of this argument is `"ndf_"<arg_function_space>`.

   (b) If there is a field on this space then:

      i. Include the unique number of degrees of freedom for the function space. This is an integer and has intent `in`. The name of this argument is `"undf_"<field_function_space>`.

      ii. Include the dofmap for this space. This is an integer array with intent `in`. It has one dimension sized by the local degrees of freedom for the function space.

   (a) If the CMA operator has this space as its to/from space then include the column-banded dofmap, the list of offsets for the to/from-space. This is an integer array of rank 2. The first dimension is `"ndf_"<arg_function_space>``` and the second is `nlayers`.

Application/Inverse-Application

A kernel applying a CMA operator requires the column-indirection dofmap for both the to- and from-function spaces of the CMA operator. Since it does not have any LMA operator arguments it does not require the `ncell_3d` and `nlayers` scalar arguments. (Since a column-wise operator is, by definition, assembled for a whole column, there is no loop over levels when applying it.) The full set of rules is then:

1. Include the `cell` argument. `cell` is an integer and has intent `in`.

2. Include the number of cells in the 2D mesh, `ncell_2d`, which is an integer with intent `in`.

3. For each argument in the `meta_args` meta-data array:

   (a) If it is a field, include the field array. This is a real array of kind `r_def` and is of rank 1. The field array name is currently specified as being `"field_"<argument_position>"_"<field_function_space>`. The extent of the array is the number of unique degrees of freedom for the function space that the field is on. This value is passed in separately. The intent of the argument is determined from the metadata (see *meta_args*).

   (b) If it is a CMA operator, include it and its associated parameters (see Rule 5 of CMA Assembly kernels).

4. For each of the unique function spaces encountered in the meta-data arguments (the `to` function space of an operator is considered to be before the `from` function space of the same operator as it appears first in lexicographic order):

   (a) Include the number of degrees of freedom per cell for the associated function space. This is an integer with intent `in`. The name of this argument is `"ndf_"<field_function_space>`.

   (b) Include the number of unique degrees of freedom for the associated function space. This is an integer with intent `in`. The name of this argument is `"undf_"<field_function_space>`.

   (c) Include the dofmap for this function space. This is a rank-1 integer array with extent equal to the number of degrees of freedom of the space (`"ndf_"<field_function_space>`).

5. Include the indirection map for the to-space of the CMA operator. This is a rank-1 integer array with extent `nrow`.
6. If the from-space of the operator is *not* the same as the to-space then include the indirection map for the from-space of the CMA operator. This is a rank-1 integer array with extent `ncol`.

Matrix-Matrix

Does not require any dofmaps and also does not require the `nlayers` and `ncell_3d` scalar arguments. The full set of rules are then:

1. Include the `cell` argument. `cell` is an integer and has intent `in`.
2. Include the number of cells in the 2D mesh, `ncell_2d`, which is an integer with intent `in`.
3. For each CMA operator or scalar argument specifed in meta-data:
   (a) If it is a CMA operator, include it and its associated parameters (see Rule 5 of CMA Assembly kernels).
   (b) If it is a scalar argument include the corresponding Fortran variable in the argument list with intent `in`.

Rules for Inter-Grid Kernels

As already specified, inter-grid kernels are only permitted to take fields and/or field-vectors as arguments. Fields (and field-vectors) that are on different meshes must be on different function spaces. Fields on the same mesh must also be on the same function space.

Argument ordering follows the general pattern used for 'normal' kernels with field data being followed by dofmap data. The rules for arguments to inter-grid kernels are as follows:

1. Include `nlayers`, the number of layers in a column. `nlayers` is an integer and has intent `in`.
2. Include the `cell_map` for the current cell (column). This is an integer array of rank one and intent `in` which provides the mapping from the coarse to the fine mesh. It has extent *ncell_f_per_c*.
3. Include `ncell_f_per_c`, the number of fine cells per coarse cell. This is an integer and has intent `in`.
4. Include `ncell_f`, the number of cells (columns) in the fine mesh. This is an integer and has intent `in`.
5. For each argument in the `meta_args` meta-data array (which must be a field or field-vector):
   (a) Pass in field data as done for a regular kernel.
6. For each unique function space (of which there will currently be two) in the order in which they are encountered in the `meta_args` meta-data array, include dofmap information:

   If the dofmap is associated with an argument on the fine mesh:

   (a) Include `ndf_fine`, the number of DoFs per cell for the FS of the field on the fine mesh.
   (b) Include `undf_fine`, the number of unique DoFs per cell for the FS of the field on the fine mesh.
   (c) Include `dofmap_fine`, the *whole* dofmap for the fine mesh. This is an integer array of rank two with intent `in`. The extent of the first dimension is `ndf_fine` and that of the second is `ncell_f`.

   else, the dofmap is associated with an argument on the coarse mesh:

   (a) Include `undf_coarse`, the number of unique DoFs for the coarse field. This is an integer with intent `in`.

(b) Include `dofmap_coarse`, the dofmap for the current cell (column) in the coarse mesh. This is an integer array of rank one and has intent `in`.

Built-ins

The basic concept of a PSyclone Built-in is described in the *Built-ins* section. In the Dynamo 0.3 API, calls to Built-ins generally follow a convention that the field/scalar written to comes first in the argument list. Dynamo 0.3 Built-ins must conform to the following four rules:

1. Built-in kernels must have one and only one modified (i.e. written to) argument.
2. There must be at least one field in the argument list. This is so that we know the number of dofs to iterate over.
3. Kernel arguments must be either fields or scalars.
4. All field arguments to a given Built-in must be on the same function space. This is because all current Built-ins iterate over dofs and therefore all fields should have the same number. It also means that we can determine the number of dofs uniquely when a scalar is written to.

The Built-ins supported for the Dynamo 0.3 API are listed in the related subsections, grouped by the mathematical operation they perform. For clarity, the calculation performed by each Built-in is described using Fortran array syntax; this does not necessarily reflect the actual implementation of the Built-in (*e.g.* it could be implemented by PSyclone generating a call to an optimised maths library).

Naming scheme

The supported Built-ins in the Dynamo 0.3 API are named according to the scheme presented below. Any new Built-in needs to comply with these rules.

1. Ordering of arguments in Built-ins calls follows *LHS (result) <- RHS (operation on arguments)* direction, except where a Built-in returns the *LHS* result to one of the *RHS* arguments. In that case ordering of arguments remains as in the *RHS* expression, with the returning *RHS* argument written as close to the *LHS* as it can be without affecting the mathematical expression.
2. Field names begin with upper case in short form (e.g. **X**, **Y**, **Z**) and any case in long form (e.g. **Field1**, **field**).
3. Scalar names begin with lower case: e.g. **a**, **b**, are **scalar1**, **scalar2**. Special names for scalars are: **constant** (or **c**), **innprod** (inner/scalar product of two fields) and **sumfld** (sum of a field).
4. Arguments in Built-ins variable declarations and constructs (PSyclone Fortran and Python definitions):
   (a) Are always written in long form and lower case (e.g. **field1**, **field2**, **scalar1**, **scalar2**);
   (b) *LHS* result arguments are always listed first;
   (c) *RHS* arguments are listed in order of appearance in the mathematical expression, except when one of them is the *LHS* result.
5. Built-ins names in Fortran consist of:
   (a) *RHS* arguments in short form (e.g. **X**, **Y**, **a**, **b**) only;
   (b) Descriptive name of mathematical operation on *RHS* arguments in the form `<operationname>_<RHSarg>` for one *RHS* argument or `<RHSargs>_<operationname>_<RHSargs>` for more;
   (c) Prefix `"inc_"` where the result is returned to one of the *RHS* arguments (i.e. `"inc_"<RHSargs>_<operationname>_<RHSargs>`).
6. Built-ins names in Python definitions are similar to their Fortran counterparts, with a few differences:

(a) Operators and *RHS* arguments are all in upper case (e.g. **X**, **Y**, **A**, **B**, **Plus**, **Minus**);

(b) There are no underscores;

(c) Common prefix is `"Dyn"`, common suffix is `"Kern"`.

Addition

Built-ins which add (scaled) fields are denoted with the keyword **plus**.

X_plus_Y

X_plus_Y (*field3*, *field1*, *field2*)

Sums two fields (Z = X + Y):

```
field3(:) = field1(:) + field2(:)
```

where:

- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*
- type(field_type), intent(in) :: *field2*

inc_X_plus_Y

inc_X_plus_Y (*field1*, *field2*)

Adds the second field to the first and returns it (X = X + Y):

```
field1(:) = field1(:) + field2(:)
```

where:

- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

aX_plus_Y

aX_plus_Y (*field3*, *scalar*, *field1*, *field2*)

Performs Z = aX + Y:

```
field3(:) = scalar*field1(:) + field2(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*, *field2*

inc_aX_plus_Y

inc_aX_plus_Y (*scalar*, *field1*, *field2*)

Performs X = aX + Y (increments the first field):

```
field1(:) = scalar*field1(:) + field2(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

inc_X_plus_bY

inc_X_plus_bY (*field1*, *scalar*, *field2*)

Performs X = X + bY (increments the first field):

```
field1(:) = field1(:) + scalar*field2(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

aX_plus_bY

aX_plus_bY (*field3*, *scalar1*, *field1*, *scalar2*, *field2*)

Performs Z = aX + bY:

```
field3(:) = scalar1*field1(:) + scalar2*field2(:)
```

where:

- real(r_def), intent(in) :: *scalar1*, *scalar2*
- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*, *field2*

inc_aX_plus_bY

inc_aX_plus_bY (*scalar1*, *field1*, *scalar2*, *field2*)

Performs X = aX + bY (increments the first field):

```
field1(:) = scalar1*field1(:) + scalar2*field2(:)
```

where:

- real(r_def), intent(in) :: *scalar1*, *scalar2*

- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

Subtraction

Built-ins which subtract (scaled) fields are denoted with the keyword **minus**.

X_minus_Y

X_minus_Y (*field3*, *field1*, *field2*)

Subtracts the second field from the first and stores the result in the third (Z = X - Y):

```
field3(:) = field1(:) - field2(:)
```

where:

- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*
- type(field_type), intent(in) :: *field2*

inc_X_minus_Y

inc_X_minus_Y (*field1*, *field2*)

Subtracts the second field from the first and returns it (X = X - Y):

```
field1(:) = field1(:) - field2(:)
```

where:

- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

aX_minus_Y

aX_minus_Y (*field3*, *scalar*, *field1*, *field2*)

Performs Z = aX - Y:

```
field3(:) = scalar*field1(:) - field2(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*, *field2*

X_minus_bY

X_minus_bY (*field3*, *field1*, *scalar*, *field2*)

Performs Z = X - bY:

```
field3(:) = field1(:) - scalar*field2(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*, *field2*

inc_X_minus_bY

inc_X_minus_bY (*field1*, *scalar*, *field2*)

Performs X = X - bY (increments the first field):

```
field1(:) = field1(:) - scalar*field2(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

Multiplication

Built-ins which multiply (scaled) fields are denoted with the keyword **times**.

X_times_Y

X_times_Y (*field3*, *field1*, *field2*)

Multiplies two fields together and returns the result in a third field (Z = X*Y):

```
field3(:) = field1(:)*field2(:)
```

where:

- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*, *field2*

inc_X_times_Y

inc_X_times_Y (*field1*, *field2*)

Multiplies the first field by the second and returns it (X = X*Y):

```
field1(:) = field1(:)*field2(:)
```

where:

- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

inc_aX_times_Y

inc_aX_times_Y (*scalar*, *field1*, *field2*)

Performs X = a*X*Y (increments the first field):

```
field1(:) = scalar*field1(:)*field2(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

Scaling

Built-ins which scale fields are technically cases of multiplying a field by a scalar and are hence also denoted with the keyword **times**.

a_times_X

a_times_X (*field2*, *scalar*, *field1*)

Multiplies a field by a scalar and stores the result in a second field (Y = a*X):

```
field2(:) = scalar*field1(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(out) :: *field2*
- type(field_type), intent(in) :: *field1*

inc_a_times_X

inc_a_times_X (*scalar*, *field*)

Multiplies a field by a scalar value and returns the field (X = a*X):

```
field(:) = scalar*field(:)
```

where:

- real(r_def), intent(in) :: *scalar*
- type(field_type), intent(inout) :: *field*

Division

Built-ins which divide (scaled) fields are denoted with the keyword **divideby**.

X_divideby_Y

X_divideby_Y (*field3*, *field1*, *field2*)

Divides the first field by the second and returns the result in the third (Z = X/Y):

```
field3(:) = field1(:)/field2(:)
```

where:

- type(field_type), intent(out) :: *field3*
- type(field_type), intent(in) :: *field1*, *field2*

inc_X_divideby_Y

inc_X_divideby_Y (*field1*, *field2*)

Divides the first field by the second and returns it (X = X/Y):

```
field1(:) = field1(:)/field2(:)
```

where:

- type(field_type), intent(inout) :: *field1*
- type(field_type), intent(in) :: *field2*

Setting to value

Built-ins which set field elements to some value and hence are denoted with the keyword **setval**.

setval_c

setval_c (*field*, *constant*)

Sets all elements of the field *field* to the value *constant* (X = c):

```
field(:) = constant
```

where:

- type(field_type), intent(out) :: *field*
- real(r_def), intent(in) :: *constant*

Note: The field may be on any function space.

setval_X

setval_X (*field2*, *field1*)

Sets a field *field2* equal to field *field1* (Y = X):

```
field2(:) = field1(:)
```

where:

- type(field_type), intent(out) :: *field2*
- type(field_type), intent(in) :: *field1*

Raising to power

Built-ins which raise field elements to an exponent are denoted with the keyword **powreal** for real exponent or **powint** for integer exponent.

inc_X_powreal_a

inc_X_powreal_a (*field*, *rscalar*)

Raises a field to a real scalar value and returns the field (X = X**a):

```
field(:) = field(:)**rscalar
```

where:

- type(field_type), intent(inout) :: *field*
- real(r_def), intent(in) :: *rscalar*

inc_X_powint_n

inc_X_powint_n (*field*, *iscalar*)

Raises a field to an integer scalar value and returns the field (X = X**n):

```
field(:) = field(:)**iscalar
```

where:

- type(field_type), intent(inout) :: *field*
- integer(i_def), intent(in) :: *iscalar*

Inner product

Built-ins which calculate the inner product of two fields or of a field with itself are denoted with the keyword **inner-product**.

X_innerproduct_Y

X_innerproduct_Y (*innprod*, *field1*, *field2*)

Computes the inner product of the fields *field1* and *field2*, *i.e.*:

```
innprod = SUM(field1(:)*field2(:))
```

where:

- real(r_def), intent(out) :: *innprod*
- type(field_type), intent(in) :: *field1*, *field2*

Note: When used with distributed memory this Built-in will trigger the addition of a global sum which may affect the performance and/or scalability of the code.

X_innerproduct_X

X_innerproduct_X (*innprod*, *field*)

Computes the inner product of the field *field1* by itself, *i.e.*:

```
innprod = SUM(field(:)*field(:))
```

where:

- real(r_def), intent(out) :: *innprod*
- type(field_type), intent(in) :: *field*

Note: When used with distributed memory this Built-in will trigger the addition of a global sum which may affect the performance and/or scalability of the code.

Sum of elements

Built-in which sums the elements of a field is denoted with the keyword *sum*.

sum_X

sum_X (*sumfld*, *field*)

Sums all of the elements of the field *field* and returns the result in the scalar variable *sumfld*:

```
sumfld = SUM(field(:))
```

where:

- real(r_def), intent(out) :: sumfld
- type(field_type), intent(in) :: field

Note: When used with distributed memory this Built-in will trigger the addition of a global sum which may affect the performance and/or scalability of the code.

Boundary Conditions

In the Dynamo0.3 API, boundary conditions for a field or LMA operator can be enforced by the algorithm developer by calling the Kernels `enforce_bc_type` or `enforce_operator_bc_type`, respectively. These kernels take a field or operator as input and apply boundary conditions. For example:

```
call invoke( kernel_type(field1, field2),      &
             enforce_bc_type(field1),          &
             kernel_with_op_type(field1, op1), &
             enforce_operator_bc_type(op1)     &
           )
```

The particular boundary conditions that are applied are not known by PSyclone, PSyclone simply recognises these kernels by their names and passes pre-specified dofmap and boundary_value arrays into the kernel implementations, the contents of which are set by the LFRic infrastructure.

Up to and including version 1.4.0 of PSyclone, boundary conditions were applied automatically after a call to `matrix_vector_type` if the field arguments were on a vector function space (one of `w1`, `w2`, `w2h` or `w2v`). With the subsequent introduction of the ability to apply boundary conditions to operators this functionality is no longer required and has been removed.

Example `eg4` in the `examples/dynamo` directory includes a call to `enforce_bc_kernel_type` so can be used to see the boundary condition code that is added by PSyclone. See the `README` in the `examples/dynamo` directory for instructions on how to run this example.

An example of applying boundary conditions to an operator is the kernel `enforce_operator_bc_kernel_mod.F90` in the `<PSYCLONEHOME>/src/psyclone/tests/test_files/dynamo0p3` directory. Since operators are discontinuous quantities, updating their values can be safely performed in parallel (see Section *Kernel*). The `GH_READWRITE` access is used for updating discontinuous operators (see subsection *Valid Access Modes* for more details).

Conventions

There is a convention in the Dynamo0.3 API kernel code that if the name of the operation being performed is `<name>` then a kernel file is `<name>_mod.[fF90]`, the name of the module inside the kernel file is `<name>_mod`, the name of the kernel metadata in the module is `<name>_type` and the name of the kernel subroutine in the module is `<name>_code`. PSyclone does not need this convention to be followed apart from the stub generator (see the *Stub Generation* Section) where the name of the metadata to be parsed is determined from the module name.

The contents of the metadata is also usually declared private but this does not affect PSyclone.

Finally, the `procedure` metadata (located within the kernel metadata) usually has `nopass` specified but again this is ignored by PSyclone.

Configuration

Annexed DoFs

When a kernel iterates over dofs (rather than cells) for a continuous field using distributed memory (see the *Distributed Memory* Section), then PSyclone need only ensure that dofs owned by a processor are computed. However, for continuous fields, shared dofs at the boundary between processors must be replicated (as different cells share the same dof). Only one processor can own a dof, therefore processors will have continuous fields which contain dofs that the processor does not own. These unowned dofs are called *annexed* in the dynamo0.3 api and are a separate, but related, concept to field halos.

When a kernel that iterates over cells needs to read a continuous field then the annexed dofs must be up-to-date on all processors. If they are not then a halo exchange must be added. Currently PSyclone defaults, for kernels which iterate over dofs, to iterating over only owned dofs. This behaviour can be changed by setting *COMPUTE_ANNEXED_DOFS* to `true` in the *dynamo0.3* section of the configuration file (see the *Configuration* section). PSyclone will then generate code to iterate over both owned and annexed dofs, thereby reducing the number of halo exchanges required (at the expense of redundantly computing annexed dofs). For more details please refer to the *Dynamo0.3* developers section.

Transformations

This section describes the dynamo-api-specific transformations. In all cases, excepting **Dynamo0p3RedundantComputationTrans**, these transformations are specialisations of generic transformations described in the *Transformations* section. The difference between these transformations and the generic ones is that these perform dynamo-api-specific checks to make sure the transformations are valid. In practice these transformations perform the required checks then call the generic ones internally.

The use of the dynamo-api-specific transformations is exactly the same as the equivalent generic ones in all cases excepting **DynamoLoopFuseTrans**. In this case an additional optional argument **same_space** has been added to the **apply** method. The reason for this is to allow loop fusion when one or more of the iteration-spaces is determined by a function space that is unknown by PSyclone at compile time. This is the case when the **ANY_SPACE** function space is specified in the Kernel metadata. By default PSyclone will not allow loop fusion if it does not know the spaces are the same. The **same_space** option allows the user to specify that the spaces are the same. This option should therefore be used with caution. Note, if PSyclone knows the spaces are different this option has no effect and the transformation will always raise an exception.

The **Dynamo0p3RedundantComputationTrans** transformation is only valid for the "Dynamo0p3" API. This is because this API is currently the only one that supports distributed memory. An example of redundant computation can be found in `examples/dynamo/eg8`.

The Dynamo-specific transformations currently available are given below. If the name of a transformation includes "Dynamo0p3" it means that the transformation is only valid for this particular API. If the name of the transformation includes "Dynamo" then it should work with all versions of the Dynamo API.

class `psyclone.transformations.`**`DynamoLoopFuseTrans`**

Performs error checking before calling the `apply()` method of the `base class` in order to fuse two Dynamo loops.

`apply`(*node1*, *node2*, *same_space=False*)

Fuse the two Dynamo loops represented by `node1` and `node2`. The optional same_space flag asserts that an unknown iteration space (i.e. any_space) matches the other iteration space. This is set at the users own risk.

`name`

Returns the name of this transformation as a string.

class `psyclone.transformations.`**`DynamoOMPParallelLoopTrans`**(*omp_schedule='static'*)
Dynamo-specific OpenMP loop transformation. Adds Dynamo specific validity checks. Actual transformation is done by the `base class`.

`apply`(*node*)
Perform Dynamo specific loop validity checks then call the `apply()` method of the `base class`.

`name`
Returns the name of this transformation as a string.

class `psyclone.transformations.`**`Dynamo0p3OMPLoopTrans`**(*omp_schedule='static'*)
Dynamo 0.3 specific orphan OpenMP loop transformation. Adds Dynamo-specific validity checks. Actual transformation is done by `base class`.

`apply`(*node*, *reprod=None*)
Perform Dynamo 0.3 specific loop validity checks then call `OMPLoopTrans.apply()`.

`name`
Returns the name of this transformation as a string.

class `psyclone.transformations.`**`Dynamo0p3ColourTrans`**
Split a Dynamo 0.3 loop over cells into colours so that it can be parallelised. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> import transformations
>>> import os
>>> import pytest
>>>
>>> TEST_API = "dynamo0.3"
>>> _,info=parse(os.path.join(os.path.dirname(os.path.abspath(__file__)),
>>>              "tests", "test_files", "dynamo0p3",
>>>              "4.6_multikernel_invokes.f90"),
>>>              api=TEST_API)
>>> psy = PSyFactory(TEST_API).create(info)
>>> invoke = psy.invokes.get('invoke_0')
>>> schedule = invoke.schedule
>>>
>>> ctrans = Dynamo0p3ColourTrans()
>>> otrans = DynamoOMPParallelLoopTrans()
>>>
>>> # Colour all of the loops
>>> for child in schedule.children:
>>>     cschedule, _ = ctrans.apply(child)
>>>
>>> # Then apply OpenMP to each of the colour loops
>>> schedule = cschedule
>>> for child in schedule.children:
>>>     newsched, _ = otrans.apply(child.children[0])
>>>
>>> newsched.view()
```

Colouring in the Dynamo 0.3 API is subject to the following rules:

- Only kernels with an iteration space of CELLS and which modify a continuous field require colouring. Any other type of loop will cause this transformation to raise an exception.
- A kernel may have at most one field with 'INC' access
- A separate colour map will be required for each field that is coloured (if an invoke contains >1 kernel call)

apply(*node*)
Performs Dynamo0.3-specific error checking and then uses the parent class to convert the Loop represented by `node` into a nested loop where the outer loop is over colours and the inner loop is over cells of that colour.

name
Returns the name of this transformation as a string.

class `psyclone.transformations.`**Dynamo0p3RedundantComputationTrans**
This transformation allows the user to modify a loop's bounds so that redundant computation will be performed. Redundant computation can result in halo exchanges being modified, new halo exchanges being added or existing halo exchanges being removed.

- This transformation should be performed before any parallelisation transformations (e.g. for OpenMP) to the loop in question and will raise an exception if this is not the case.
- This transformation can not be applied to a loop containing a reduction and will again raise an exception if this is the case.
- This transformation can only be used to add redundant computation to a loop, not to remove it.
- This transformation allows a loop that is already performing redundant computation to be modified, but only if the depth is increased.

apply(*loop*, *depth=None*)
Apply the redundant computation tranformation to the loop `loop`. This transformation can be applied to loops iterating over 'cells or 'dofs'. if `depth` is set to a value then the value will be the depth of the field's halo over which redundant computation will be performed. If `depth` is not set to a value then redundant computation will be performed to the full depth of the field's halo.

Parameters

- **loop** (`psyclone.psyGen.DynLoop`) – the loop that we are transforming
- **depth** (*`int or None`*) – the depth of the stencil. Defaults to None if a depth is not provided.

name
Returns the name of this transformation as a string.

CHAPTER

TEN

GOCEAN1.0 API

Introduction

The GOcean 1.0 application programming interface (API) was originally designed to support ocean models that use the finite-difference scheme for two-dimensional domains. However, the approach is not specific to ocean models and can potentially be applied to any finite-difference code.

As with all PSyclone API's, the GOcean 1.0 API specifies how a user must write the Algorithm Layer and the Kernel Layer to allow PSyclone to generate the PSy Layer. These Algorithm and Kernel API's are discussed separately in the sections below. Before these we describe the functionality provided by the GOcean Library.

The GOcean Library

The use of PSyclone and the GOcean 1.0 API implies the use of a standard set of data types and associated infrastructure. This is provided by version 1.0 of the GOcean Library (GOLib v.1.0). Currently this library is distributed separately from PSyclone and is available from http://puma.nerc.ac.uk/trac/GOcean.

Grid

The GOLib contains a `grid_mod` module which defines a `grid_type` and associated constructor:

```
use grid_mod
...
!> The grid on which our fields are defined
type(grid_type), target :: model_grid
...
! Create the model grid
model_grid = grid_type(ARAKAWA_C,                                &
                       (/BC_EXTERNAL,BC_EXTERNAL,BC_NONE/), &
                       OFFSET_NE)
```

Note: The grid object itself must be declared with the `target` attribute. This is because each field object will contain a pointer to it.

The `grid_type` constructor takes three arguments:

1. The type of grid (only ARAKAWA_C is currently supported)
2. The boundary conditions on the domain for the *x*, *y* and *z* dimensions (see below). The value for the *z* dimension is currently ignored.

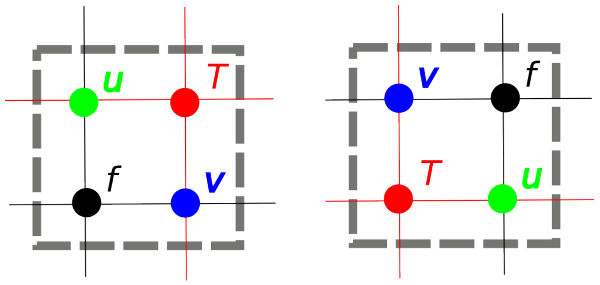
3. The 'index offset' - the convention used for indexing into offset fields.

Three types of boundary condition are currently supported:

Name	Description
BC_NONE	No boundary conditions are applied.
BC_EXTERNAL	Some external forcing is applied. This must be implemented by a kernel. The domain must be defined with a T-point mask (see *The grid_init Routine*).
BC_PERIODIC	Periodic boundary conditions are applied.

The infrastructure requires this information in order to determine the extent of the model grid.

The index offset is required because a model (kernel) developer has choice in how they actually implement the staggering of variables on a grid. This comes down to a choice of which grid points in the vicinity of a given T point have the same array (i, j) indices. In the diagram below, the image on the left corresponds to choosing those points to the South and West of a T point to have the same (i, j) index. That on the right corresponds to choosing those points to the North and East of the T point (this is the offset scheme used in the NEMO ocean model):



The GOcean 1.0 API supports these two different offset schemes, which we term `OFFSET_SW` and `OFFSET_NE`.

Note that the constructor does not specify the extent of the model grid. This is because this information is normally obtained by reading a file (a namelist file, a netcdf file etc.) which is specific to an application. Once this information has been obtained, a second routine, `grid_init`, is provided with which to 'load' a grid object with state. This is discussed below.

The `grid_init` Routine

Once an application has determined the details of the model configuration, it must use this information to populate the grid object. This is done via a call to the `grid_init` subroutine:

```
subroutine grid_init(grid, m, n, dxarg, dyarg, tmask)
  !> The grid object to configure
  type(grid_type), intent(inout) :: grid
  !> Dimensions of the model grid
  integer,          intent(in)    :: m, n
  !> The (constant) grid spacing in x and y (m)
  real(wp),         intent(in)    :: dxarg, dyarg
  !> Optional T-point mask specifying whether each grid point is
  !! wet (1), dry (0) or external (-1).
  integer, dimension(m,n), intent(in), optional :: tmask
```

If no T-mask is supplied then this routine configures the grid appropriately for an all-wet domain with periodic boundary conditions in both the x- and y-dimensions. It should also be noted that currently only grids with constant resolution in x and y are supported by this routine.

Fields

Once a model has a grid defined it will require one or more fields. The GOLib contains a `field_mod` module which defines an `r2d_field` type (real, 2-dimensional field) and associated constructor:

```
use field_mod
...
!> Current ('now') sea-surface height at different grid points
type(r2d_field) :: sshn_u_fld, sshn_v_fld, sshn_t_fld
...

! Sea-surface height now (current time step)
sshn_u = r2d_field(model_grid, U_POINTS)
sshn_v = r2d_field(model_grid, V_POINTS)
sshn_t = r2d_field(model_grid, T_POINTS)
```

The constructor takes two arguments:

1. The grid on which the field exists
2. The type of grid point at which the field is defined (`U_POINTS`, `V_POINTS`, `T_POINTS` or `F_POINTS`)

Note that the grid object need not have been fully configured (by a call to `grid_init` for instance) before it is passed into this constructor.

Example

PSyclone is distributed with a full example of the use of the GOcean Library. See `<PSYCLONEHOME>/examples/gocean/shallow_alg.f90`. In what follows we will walk through a slightly cut-down example for a different program.

The following code illustrates the use of the GOLib in constructing an application:

```
program gocean2d
  use grid_mod   ! From GOLib
  use field_mod ! From GOLib
  use model_mod
  use boundary_conditions_mod

  !> The grid on which our fields are defined. Must have the 'target'
  !! attribute because each field object contains a pointer to it.
  type(grid_type), target :: model_grid

  !> Current ('now') velocity component fields
  type(r2d_field) :: un_fld, vn_fld
  !> 'After' velocity component fields
  type(r2d_field) :: ua_fld, va_fld
  ...

  ! time stepping index
  integer :: istp

  ! Create the model grid. We use a NE offset (i.e. the U, V and F
  ! points immediately to the North and East of a T point all have the
  ! same i,j index).  This is the same offset scheme as used by NEMO.
  model_grid = grid_type(ARAKAWA_C,                              &
                         (/BC_EXTERNAL,BC_EXTERNAL,BC_NONE/),  &
                          OFFSET_NE)
  !! read in model parameters and configure the model grid
  CALL model_init(model_grid)

  ! Create fields on this grid

  ! Velocity components now (current time step)
  un_fld = r2d_field(model_grid, U_POINTS)
  vn_fld = r2d_field(model_grid, V_POINTS)

  ! Velocity components 'after' (next time step)
  ua_fld = r2d_field(model_grid, U_POINTS)
  va_fld = r2d_field(model_grid, V_POINTS)

  ...

  !! time stepping
  do istp = nit000, nitend, 1

    call step(istp,                                  &
              ua_fld, va_fld, un_fld, vn_fld,        &
              ...)
  end do
  ...
end program gocean2d
```

The `model_init` routine is application specific since it must determine details of the model configuration being run, *e.g.* by reading a namelist file. An example might look something like:

```
subroutine model_init(grid)
  type(grid_type), intent(inout) :: grid

  !> Problem size, read from namelist
  integer :: jpiglo, jpjglo
  real(wp) :: dx, dy
  integer, dimension(:,:), allocatable :: tmask

  ! Read model configuration from namelist
  call read_namelist(jpiglo, jpjglo, dx, dy, &
                     nit000, nitend, irecord, &
                     jphgr_msh, dep_const, rdt, cbfr, visc)

  ! Set-up the T mask. This defines the model domain.
  allocate(tmask(jpiglo,jpjglo))

  call setup_tpoints_mask(jpiglo, jpjglo, tmask)

  ! Having specified the T points mask, we can set up mesh parameters
  call grid_init(grid, jpiglo, jpjglo, dx, dy, tmask)

  ! Clean-up. T-mask has been copied into the grid object.
  deallocate(tmask)

end subroutine model_init
```

Here, only `grid_type` and the `grid_init` routine come from the GOLib. The remaining code is all application specific.

Once the grid object is fully configured and all fields have been constructed, a simulation will proceed by performing calculations with those fields. In the example program given above, this calculation is performed in the time-stepping loop within the `step` subroutine. The way in which this routine uses Invoke calls is described in the *Invokes* Section.

Algorithm

The Algorithm is the top-level specification of the natural science implemented in the software. Essentially it consists of mesh setup, field declarations, initialisation of fields and (a series of) Kernel calls. Infrastructure to support these tasks is provided in version 1.0 of the GOcean library (see *The GOcean Library*).

Invokes

The Kernels to call are specified through the use of Invokes, e.g.:

```
call invoke( kernel1(field1, field2),                       &
             kernel2(field1, field3)                        &
           )
```

The location and number of these `call invoke(...)` statements within the source code is entirely up to the user. The only requirement is that PSyclone must be run on every source file that contains one or more Invokes. The body of each Invoke specifies the kernels to be called, the order in which they are to be applied and the fields (and scalars) that they work with.

Note that the kernel names specified in an Invoke are the names of the corresponding kernel *types* defined in the kernel meta-data (see the *Kernel* Section). These are not the same as the names of the Fortran subroutines which contain the actual kernel code. The kernel arguments are typically field objects, as described in the *Fields* Section, but they may also be scalar quantities (real or integer).

In the example `gocean2d` program shown earlier, there is only one Invoke call and it is contained within the `step` subroutine:

```
subroutine step(istp,                    &
                ua, va, un, vn,          &
                sshn_t, sshn_u, sshn_v, &
                ssha_t, ssha_u, ssha_v, &
                hu, hv, ht)
  use kind_params_mod  ! From GOLib
  use grid_mod         ! From GOLib
  use field_mod        ! From GOLib
  use model_mod, only: rdt ! The model time-step
  use continuity_mod,  only: continuity
  use momentum_mod,    only: momentum_u, momentum_v
  use boundary_conditions_mod, only: bc_ssh, bc_solid_u
  !> The current time step
  integer,          intent(inout) :: istp
  type(r2d_field), intent(inout) :: un, vn, sshn_t, sshn_u, sshn_v
  type(r2d_field), intent(inout) :: ua, va, ssha_t, ssha_u, ssha_v
  type(r2d_field), intent(inout) :: hu, hv, ht

  call invoke(                                                  &
              continuity(ssha_t, sshn_t, sshn_u, sshn_v,       &
                         hu, hv, un, vn, rdt),                 &
              momentum_u(ua, un, vn, hu, hv, ht,               &
                         ssha_u, sshn_t, sshn_u, sshn_v),      &
              momentum_v(va, un, vn, hu, hv, ht,               &
                         ssha_v, sshn_t, sshn_u, sshn_v),    &
              bc_ssh(istp, ssha_t),                          &
              bc_solid_u(ua),                                &
              ...
             )
end subroutine step
```

Note that in this example the grid was constructed for a model with 'external' boundary conditions. These boundary conditions are applied through several user-supplied kernels, two of which (`bc_ssh` and `bc_solid_u`) are include in the above code fragment.

Kernel

The general requirements for the structure of a Kernel are explained in the *Kernel layer* section. This section explains the meta-data and subroutine arguments that are specific to the GOcean 1.0 API.

Metadata

The meta-data for a GOcean 1.0 API kernel has four components:

1. 'meta_args',
2. 'iterates_over',
3. 'index_offset' and
4. 'procedure':

These are illustrated in the code below:

```
type, extends(kernel_type) :: my_kernel_type
   type(arg), dimension(...) :: meta_args = (/ ... /)
   integer :: iterates_over = ...
   integer :: index_offset = ...
contains
  procedure, nopass :: code => my_kernel_code
end type my_kernel_type
```

These four meta-data elements are discussed in order in the following sections.

meta_args

The `meta_args` array specifies information about data that the kernel code expects to be passed to it via its argument list. There is one entry in the `meta_args` array for each **scalar**, **field**, or **grid-property** passed into the Kernel. Their ordering in the `meta_args` array must be the same as that in the kernel code argument list. The entry must be of type `arg` which itself contains metadata about the associated argument. The size of the meta_args array must correspond to the total number of **scalars**, **fields** and **grid properties** passed into the Kernel.

For example, if there are a total of two **field** entities being passed to the Kernel then the meta_args array will be of size 2 and there will be two entries of type `arg`:

```
type(arg) :: meta_args(2) = (/                              &
     arg( ... ),                                            &
     arg( ... )                                             &
     /)
```

Argument-metadata (metadata contained within the brackets of an `arg` entry), describes either a **scalar**, a **field** or a **grid property**.

The first argument-metadata entry describes how the kernel will access the corresponding argument. As an example, the following `meta_args` metadata describes four entries, the first one is written to by the kernel while the remaining three are only read.

```
type(arg) :: meta_args(4) = (/                         &
     arg(WRITE, ... ),                                 &
     arg(READ, ... ),                                  &
     arg(READ, ... ),                                  &
     arg(READ, ...)                                    &
     /)
```

The second entry to argument-metadata (information contained within the brackets of an `arg` type) describes the type of data represented by the argument. This type falls into three categories; field data, scalar data and grid properties. For field data the meta-data entry consists of the type of grid-point that field values are defined on. Since the GOcean API supports fields on an Arakawa C grid, the possible grid-point types are `CU`, `CV`, `CF` and `CT`. GOcean Kernels can also take scalar quantities as arguments. Since these do not live on grid-points they are specified as either `R_SCALAR` or `I_SCALAR` depending on whether the corresponding Fortran variable is a real or integer quantity. Finally, grid-property entries are used to specify any properties of the grid required by the kernel (*e.g.* the area of cells at U points or whether T points are wet or dry).

For example:

```
type(arg) :: meta_args(4) = (/                         &
     arg(WRITE, CT, ... ),                             &
     arg(READ,  CU, ... ),                             &
     arg(READ,  R_SCALAR, ... ),                       &
     arg(READ,  GRID_AREA_U)                           &
     /)
```

Here, the first argument is a field on T points, the second is a field on U points, the fourth is a real scalar and the fifth is a property of the grid (cell area at U points).

The full list of supported grid properties in the GOcean 1.0 API is:

Name	Description	Type
grid_area_t	Cell area at T point	Real array, rank=2
grid_area_u	Cell area at U point	Real array, rank=2
grid_area_v	Cell area at V point	Real array, rank=2
grid_mask_t	T-point mask (1=wet, 0=dry)	Integer array, rank=2
grid_dx_t	Grid spacing in x at T points	Real array, rank=2
grid_dx_u	Grid spacing in x at U points	Real array, rank=2
grid_dx_v	Grid spacing in x at V points	Real array, rank=2
grid_dy_t	Grid spacing in y at T points	Real array, rank=2
grid_dy_u	Grid spacing in y at U points	Real array, rank=2
grid_dy_v	Grid spacing in y at V points	Real array, rank=2
grid_lat_u	Latitude of U points (gphiu)	Real array, rank=2
grid_lat_v	Latitude of V points (gphiv)	Real array, rank=2
grid_dx_const	Grid spacing in x if constant	Real, scalar
grid_dy_const	Grid spacing in y if constant	Real, scalar

These are stored in a dictionary named `GRID_PROPERTY_DICT` at the top of the `gocean1p0.py` file. All of the rank-two arrays have the first rank as longitude (*x*) and the second as latitude (*y*).

Scalars and fields contain a third argument-metadata entry which describes whether the kernel accesses the corresponding argument with a stencil. The value `POINTWISE` indicates that there is no stencil access. Metadata for a scalar field is limited to this value. Grid-property arguments have no third metadata argument. If there are no stencil accesses then the full argument meta-data for our previous example will be:

```
type(arg) :: meta_args(4) = (/                          &
     arg(WRITE, CT,       POINTWISE),                   &
     arg(READ,  CU,       POINTWISE),                   &
     arg(READ,  R_SCALAR, POINTWISE),                   &
     arg(READ,  GRID_AREA_U)                            &
     /)
```

If a kernel accesses a field using a stencil then the third argument metadata entry should take the form `stencil(...)`. Note, a stencil access is only allowed for a field that is `READ` by a kernel.

In the GOcean API, fields are implemented as two-dimensional arrays. In Fortran, a standard 5-point stencil would look something like the following:

```
a(i,j) + a(i+1,j) + a(i-1,j) + a(i,j+1) + a(i,j-1)
```

If we view the above accesses as co-ordinates relative to the `a(i,j)` access we get `(0,0), (1,0), (-1,0), (0,1), (0,-1)`. If we then view these accesses in graphical form with `i` being in the horizontal direction and `j` in the vertical and with a `1` indicating a (depth-1) access and a `0` indicating there is no access we get the following:

```
010
111
010
```

In the GOcean API a stencil access is captured as a triplet of integers (one row at a time from top to bottom) using the above view i.e.

```
stencil(010,111,010)
```

So far we have only considered depth-1 stencils. In our notation the depth of access is captured by the integer value (`0` for no access, `1` for depth 1, `2` for depth 2 etc). For example:

```
a(i,j) + a(i,j+1) + a(i,j+2)
```

would be captured as:

```
stencil(020,010,000)
```

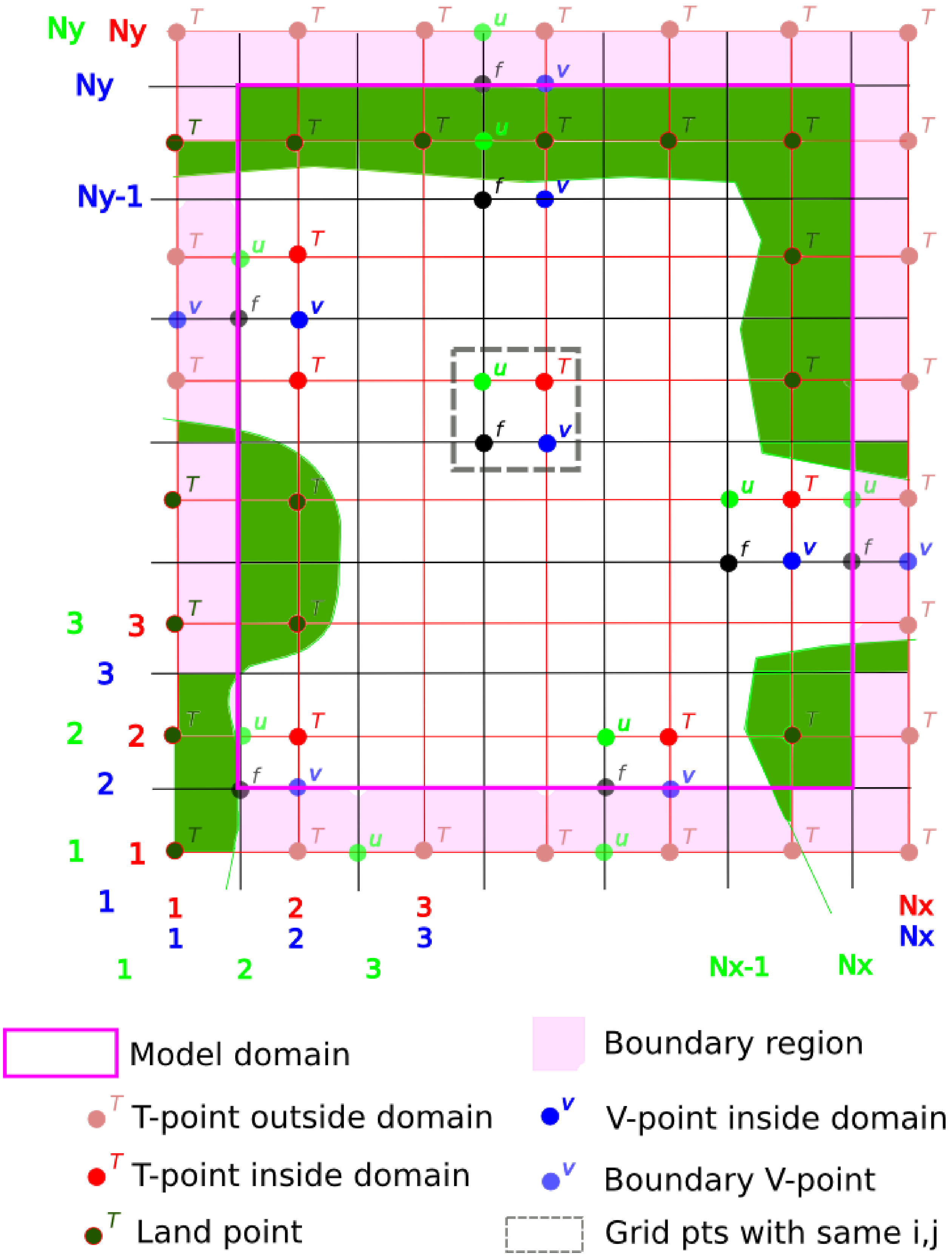
All forms of stencil can be **summarised** using this triplet notation up to a depth of `9` apart from the central `a(i,j)` value which can either be `0` (not accessed) or `1` (accessed). Note, the central value is not currently used by PSyclone. The notation is a **summary** in two ways

1. it only captures the depth of the stencil in a particular direction, not the actual accesses. Therefore, there is no way to distinguish between the stencil `a(i+2,j)` and the stencil `a(i+1,j) + a(i+2,j)`.
2. when there are offsets for both `i` and `j` e.g. `a(i+1,j+1)` it only captures whether there is an access in that direction at a particular depth, not the details of the access. For example, there is no way to distinguish between `a(i+2,j+2)` and `a(i+2,j+2) + a(i+1,j+2) + a(i+2,j+1)`.

Whilst the description is a summary, it is accurate enough for PSyclone as this information is primarily used to determine which grid partitions must communicate with which for the purposes of placing halo exchange calls. In this case, it is the depth and direction information that is most important.

Iterates Over

The second element of kernel meta-data is `ITERATES_OVER`. This specifies that the Kernel has been written with the assumption that it is iterating over grid points of the specified type. The supported values are: `INTERNAL_PTS`, `EXTERNAL_PTS` and `ALL_PTS`. These may be understood by considering the following diagram of an example model configuration:



INTERNAL_PTS are then those points that are within the Model domain (fuscia box), EXTERNAL_PTS are those outside the domain and ALL_PTS encompasses all grid points in the model. The chosen value is specified in the kernel-meta data like so:

```
integer :: iterates_over = INTERNAL_PTS
```

Index Offset

The third element of kernel meta-data, INDEX_OFFSET, specifies the index-offset that the kernel uses. This is the same quantity as supplied to the grid constructor (see the *Grid* Section for a description).

The GOcean 1.0 API supports two different offset schemes; OFFSET_NE, OFFSET_SW. The scheme used by a kernel is specified in the meta-data as, e.g.:

```
integer :: index_offset = OFFSET_NE
```

Currently all kernels used in an application must use the same offset scheme which must also be the same as passed to the grid constructor.

Procedure

The fourth and final type of meta-data is procedure meta-data. This specifies the name of the Kernel Fortran subroutine that this meta-data describes.

For example:

```
procedure :: my_kernel_code
```

Subroutine

Rules

Kernel arguments follow a set of rules which have been specified for the GOcean 1.0 API. These rules are encoded in the gen_code() method of the GOKern class in the gocean1p0.py file. The rules, along with PSyclone's naming conventions, are:

1. Every kernel has the indices of the current grid point as the first two arguments, i and j. These are integers and have intent in.
2. For each field/scalar/grid property in the order specified by the meta_args metadata:
   (a) For a field; the field array itself. A field array is a real array of kind wp and rank two. The first rank is longitude (x) and the second latitude (y).
   (b) For a scalar; the variable itself. A real scalar is of kind wp.
   (c) For a grid property; the array or variable (see the earlier table) containing the specified property.

Note: Grid properties are not passed from the Algorithm Layer. PSyclone generates the necessary lookups in the PSy Layer and includes the resulting references in the arguments passed to the kernel.

As an example, consider the bc_solid_u kernel that is used in the gocean2d program shown earlier. The meta-data for this kernel is:

```
 type, extends(kernel_type) :: bc_solid_u
   type(arg), dimension(2) :: meta_args =  &
        (/ arg(WRITE, CU, POINTWISE),      &
           arg(READ,      GRID_MASK_T)     &
         /)

   !> This is a boundary-conditions kernel and therefore
   !! acts on all points of the domain rather than just
   !! those that are internal
   integer :: ITERATES_OVER = ALL_PTS

   integer :: index_offset = OFFSET_NE

contains
  procedure, nopass :: code => bc_solid_u_code
end type bc_solid_u
```

The interface to the subroutine containing the implementation of this kernel is:

```
subroutine bc_solid_u_code(ji, jj, ua, tmask)
  integer,                 intent(in)    :: ji, jj
  integer,  dimension(:,:), intent(in)    :: tmask
  real(wp), dimension(:,:), intent(inout) :: ua
```

As described above, the first two arguments to this subroutine specify the grid-point at which the computation is to be performed. The third argument is the field that this kernel updates and the fourth argument is the T-point mask. The latter is a property of the grid and is provided to the kernel call from the PSy Layer.

Comparing this interface definition with the use of the kernel in the Invoke call:

```
call invoke ( ...,            &
              bc_solid_u(ua), &
              ... )
```

we see that in the Algorithm Layer the user need only provide the field(s) (and possibly scalars) that a kernel operates on. The index of the grid point and any grid properties are provided in the (generated) PSy Layer where the kernel subroutine proper is called.

Built-ins

The GOcean 1.0 API does not support any built-in operations.

Conventions

There is a convention in the GOcean 1.0 API kernel code that if the name of the operation being performed is `<name>` then a kernel file is `<name>_mod.[fF90]`, the name of the module inside the kernel file is `<name>_mod`, the name of the kernel metadata in the module is `<name>_type` and the name of the kernel subroutine in the module is `<name>_code`. PSyclone does not require this convention to be followed in the GOcean 1.0 API.

The contents of the metadata is also usually declared private but this does not affect PSyclone.

Finally, the `procedure` metadata (located within the kernel metadata) usually has `nopass` specified but again this is ignored by PSyclone.

Transformations

In this section we describe the transformations that are specific to the GOcean 1.0 API. For an overview of transformations in general see *Transformations*.

class `psyclone.transformations.`**`GOceanLoopFuseTrans`**

Performs error checking (that the loops are over the same grid-point type) before calling the `LoopFuseTrans.apply()` method of the `base class` in order to fuse two GOcean loops.

`apply`(*node1*, *node2*)

Fuse the two GOcean loops represented by `node1` and `node2`.

Parameters

- **`node1`** (`psyclone.gocean1p0.GOLoop`) – A node representing a GOLoop.
- **`node2`** (`psyclone.gocean1p0.GOLoop`) – A node representing a GOLoop.

Raises ***`TransformationError`*** – if the supplied node2 can not be fused, e.g. not all nodes are loops, don't have the same parent, are not next to each other or have different iteration spaces.

`name`

Returns the name of this transformation as a string.

---

class `psyclone.transformations.`**`GOceanOMPParallelLoopTrans`**(*omp_schedule='static'*)

GOcean specific OpenMP Do loop transformation. Adds GOcean specific validity checks (that supplied Loop is an inner or outer loop). Actual transformation is done by `base class`.

Parameters **`omp_schedule`** – The omp schedule to be created. Must be one of 'runtime', 'static', 'dynamic', 'guided' or 'auto'.

`apply`(*node*)

Perform GOcean-specific loop validity checks then call `OMPParallelLoopTrans.apply()`.

Parameters **`node`** (`psyclone.psyGen.Loop`) – A Loop node from an AST.

Raises ***`TransformationError`*** – if the supplied node is not an inner or outer loop.

`name`

Returns the name of this transformation as a string.

---

class `psyclone.transformations.`**`GOceanOMPLoopTrans`**(*omp_schedule='static'*)

GOcean-specific orphan OpenMP loop transformation. Adds GOcean specific validity checks (that the node is either an inner or outer Loop). Actual transformation is done by `base class`.

Parameters **`omp_schedule`** – The omp schedule to be created. Must be one of 'runtime', 'static', 'dynamic', 'guided' or 'auto'.

`apply`(*node*)

Perform GOcean specific loop validity checks then call `OMPLoopTrans.apply()`.

Parameters **`node`** (`psyclone.psyGen.Loop.`) – The loop to parallelise using OMP Do.

`name`

Returns the name of this transformation as a string.

---

class psyclone.transformations.**GOConstLoopBoundsTrans**

Switch on (or off) the use of constant loop bounds within a GOSchedule. In the absence of constant loop bounds, PSyclone will generate loops where the bounds are obtained by de-referencing a field object, e.g.:

```
DO j = my_field%grid%internal%ystart, my_field%grid%internal%ystop
```

Some compilers are able to produce more efficient code if they are provided with information on the relative trip-counts of the loops within an Invoke. With constant loop bounds switched on, PSyclone generates code like:

```
ny = my_field%grid%simulation_domain%ystop
...
DO j = 1, ny-1
```

In practice, the application of the constant loop bounds looks something like, e.g.:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> import os
>>> TEST_API = "gocean1.0"
>>> _, info = parse(os.path.join("tests", "test_files", "gocean1p0",
>>>                              "single_invoke.f90"),
>>>                 api=TEST_API)
>>> psy = PSyFactory(TEST_API).create(info)
>>> invoke = psy.invokes.get('invoke_0_compute_cu')
>>> schedule = invoke.schedule
>>>
>>> from psyclone.transformations import GOConstLoopBoundsTrans
>>> clbtrans = GOConstLoopBoundsTrans()
>>>
>>> newsched, _ = clbtrans.apply(schedule)
>>> # or, to turn off const. looop bounds:
>>> # newsched, _ = clbtrans.apply(schedule, const_bounds=False)
>>>
>>> newsched.view()
```

apply (*node*, *const_bounds=True*)

Switches constant loop bounds on or off for all loops in the schedule node. Default is 'on'.

Parameters

- **node** (psyclone.gocean1p0.GOSchedule) – The schedule of which all loops will get the constant loop bounds switched on or off.
- **const_bounds** (*bool*) – If the constant loop should be used (True) or not (False). Default is True.

name

Return the name of the Transformation as a string.

---

class psyclone.transformations.**GOLoopSwapTrans**

Provides a loop-swap transformation, e.g.:

```
DO j=1, m
   DO i=1, n
```

becomes:

```
DO i=1, n
   DO j=1, m
```

This transform is used as follows:

```
>>> from parse import parse
>>> from psyGen import PSyFactory
>>> ast,invokeInfo=parse("shallow_alg.f90")
>>> psy=PSyFactory("gocean1.0").create(invokeInfo)
>>> schedule=psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> from transformations import GOLoopSwapTrans
>>> swap=GOLoopSwapTrans()
>>> new_schedule,memento=swap.apply(schedule.children[0])
>>> new_schedule.view()
```

apply(*outer*)

The argument `outer` must be a loop which has exactly one inner loop. This transform then swaps the outer and inner loop.

Parameters **outer** (`psyclone.psyGen.Loop`) – The node representing the outer loop.

Returns A tuple consistent of the new schedule, and a Memento.

Raises ***TransformationError*** – if the supplied node does not allow a loop swap to be done.

name

Returns the name of this transformation as a string.

CHAPTER ELEVEN

STUB GENERATION

Quick Start

1. Use an existing Kernel file or create a Kernel file containing a Kernel module with the required metadata and an empty Kernel subroutine with no arguments.
2. Run the following command

```
> genkernelstub <PATH>/my_file.f90
```

Introduction

PSyclone provides a kernel stub generator for the Dynamo0.3 API. The kernel stub generator takes a kernel file as input and outputs the kernel subroutine arguments and declarations. The word "stub" is used to indicate that it is only the subroutine arguments and their declarations that are generated; the subroutine has no content.

The primary reason the stub generator is useful is that it generates the correct Kernel subroutine arguments and declarations for the Dynamo0.3 API as specified by the Kernel metadata. As the number of arguments to Kernel subroutines can become large and the arguments have to follow a particular order, it can become burdensome, and potentially error prone, for the user to have to work out the appropriate argument list if written by hand.

The stub generator can be used when creating a new Kernel. A Kernel can first be written to specify the required metadata and then the generator can be used to create the appropriate (empty) Kernel subroutine. The user can then fill in the content of the subroutine.

The stub generator can also be used to check whether the arguments for an existing Kernel are correct i.e. whether the Kernel subroutine and Kernel metadata are consistent. One example would be where a Kernel is updated resulting in a change to the metadata and subroutine arguments.

The Dynamo0.3 API requires Kernels to conform to a set of rules which determine the required arguments and types for a particular Kernel. These rules are required as the generated PSy layer needs to know exactly how to call a Kernel. These rules are outlined in Section *Rules*.

Therefore PSyclone has been coded with the Dynamo0.3 API rules which are then applied when reading the Kernel metadata to produce the require Kernel call and its arguments in the generated PSy layer. These same rules are used by the Kernel stub generator to produce Kernel subroutine stubs, thereby guaranteeing that Kernel calls from the PSy layer and the associated Kernel subroutines are consistent.

Use

Before using the stub generator, PSyclone must be installed. If you have not already done so, please follow the instructions for setting up PSyclone in Section *Getting Going*.

PSyclone will be installed in a particular location on your machine, which will be referred to as the `<PSYCLONEINSTALL>` directory. The stub generator script `genkernelstub` comes with the PSyclone installation. A quick check `> which genkernelstub` should return the location of the `<PSYCLONEINSTALL>/bin` directory.

The easiest way to use the stub generator is to run the supplied `genkernelstub` script.

```
> genkernelstub
usage: genkernelstub [-h] [-o OUTFILE] [-api API] [-l] filename
genkernelstub: error: too few arguments
```

You can get information about the `genkernelstub` arguments using `-h` or `--help`:

```
>  genkernelstub -h
usage: genkernelstub [-h] [-o OUTFILE] [-api API] [-l] filename

Create Kernel stub code from Kernel metadata

positional arguments:
  filename              Kernel metadata

optional arguments:
  -h, --help            show this help message and exit
  -o OUTFILE, --outfile OUTFILE
                        filename of output
  -api API              choose a particular api from ['dynamo0.3'], default
                        dynamo0.3
  -l, --limit           limit the fortran line length to 132 characters
```

As is indicated when using the `-h` option, the `-api` option only accepts `dynamo0.3` at the moment and is redundant as this option is also the default. However the number of supported API's is expected to expand in the future.

The `-o`, or `--outfile` option allows the user to specify that the output should be written to a particular file. If `-o` is not specified then the python `print` statement is used. Typically the print statement results in the output being printed to the terminal.

The `-l`, or `--limit` option utilises the PSyclone support for wrapping of lines within the 132 character limit (please see the *Line Length* chapter for more details).

Kernels

Any Dynamo0.3 kernel can be used as input to the stub generator. Example Kernels can be found in the `examples/dynamo` repository or, for more simple cases, in the `tests/test_files/dynamo0p3` directory. These directories are located in the `<PSYCLONEHOME>/src/psyclone` directory where `<PSYCLONEHOME>` refers to the location where you download or clone PSyclone (*Getting Going*).

In the `tests/test_files/dynamo0p3` directory the majority of examples start with `testkern`. The exceptions are: `simple.f90`, `ru_kernel_mod.f90` and `matrix_vector_mod.F90`. The following test kernels can be used to generate kernel stub code (running stub generation from the `<PSYCLONEHOME>/src/psyclone` directory):

```
tests/test_files/dynamo0p3/testkern_chi_2.F90
tests/test_files/dynamo0p3/testkern_chi.F90
tests/test_files/dynamo0p3/testkern_operator_mod.f90
tests/test_files/dynamo0p3/testkern_operator_nofield_mod.f90
tests/test_files/dynamo0p3/testkern_orientation.F90
tests/test_files/dynamo0p3/testkern_operator_orient_mod.f90
tests/test_files/dynamo0p3/ru_kernel_mod.f90
tests/test_files/dynamo0p3/simple.f90
```

Example

A simple single field example of a kernel that can be used as input for the stub generator is found in `tests/test_files/dynamo0p3/simple.f90` and is shown below:

```
module simple_mod
type, extends(kernel_type) :: simple_type
    type(arg_type), dimension(1) :: meta_args =  &
        (/ arg_type(gh_field,gh_write,w1) /)
    integer, parameter :: iterates_over = cells
  contains
    procedure() :: code => simple_code
end type simple_type
contains
subroutine simple_code()
end subroutine
end module simple_mod
```

Note: The module name `simple_mod` and the type name `simple_type` share the same root `simple` and have the extensions `_mod` and `_type` respectively. This is a convention in Dynamo0.3 and is required by the kernel stub generator as it needs to determine the name of the type containing the metadata and infers this by reading the module name. If this rule is not followed the kernel stub generator will return with an error message (see Section *Errors*).

Note: Whilst strictly the kernel stub generator only requires the Kernel metadata to generate the appropriate stub code, the parser that the generator relies on currently requires a dummy kernel subroutine to exist.

If we run the kernel stub generator on the `simple.f90` example:

```
> genkernelstub tests/test_files/dynamo0p3/simple.f90
```

we get the following kernel stub output:

```
MODULE simple_mod
  IMPLICIT NONE
  CONTAINS
  SUBROUTINE simple_code(nlayers, field_1_w1, ndf_w1, undf_w1, map_w1)
    USE constants_mod, ONLY: r_def
    IMPLICIT NONE
    INTEGER, intent(in) :: nlayers
    INTEGER, intent(in) :: ndf_w1
    INTEGER, intent(in) :: undf_w1
    REAL(KIND=r_def), intent(out), dimension(undf_w1) :: field_1_w1
    INTEGER, intent(in), dimension(ndf_w1) :: map_w1
  END SUBROUTINE simple_code
END MODULE simple_mod
```

The subroutine content can then be copied into the required module, used as the basis for a new module, or checked with an existing subroutine for correctness.

Note: The output does not currently conform to Met Office coding standards so must be modified accordingly.

Note: The code will not compile without a) providing the `constants_mod`, `argument_mod` and `kernel_mod` modules in the compiler include path and b) adding in code that writes to any arguments declared as intent `out` or `inout`. For a quick check, the `USE` declaration and `KIND` declarations can be removed and the `field_1_w1` array can be initialised with some value in the subroutine. At this point the Kernel should compile successfully.

Note: Whilst there is only one field declared in the metadata there are 5 arguments to the Kernel. The first argument `nlayers` specifies the number of layers in a column for a field. The second argument is the array associated with the field. The field array is dimensioned as the number of unique degrees of freedom (undf) which is also passed into the kernel (the fourth argument). The naming convention is to call each field a `field`, followed by its position in the (algorithm) argument list (which is reflected in the metadata ordering). The third argument is the number of degrees of freedom for the particular column and is used to dimension the final argument which is the degrees of freedom map (dofmap) which indicates the location of the required values in the field array. The naming convention for the `dofmap`, `undf` and `ndf` is to append the name with the space that it is associated with.

We now take a look at a more complicated example. The metadata in this example is the same as an actual Dynamo kernel, however the subroutine content and various comments have been removed. The metadata specifies that there are four fields passed by the algorithm layer, the fourth of which is a vector field of size three. All three of the spaces require a basis function and the w0 and w2 function spaces additionally require a differential basis function. The content of the Kernel is given below.

```
module ru_kernel_mod
type, public, extends(kernel_type) :: ru_kernel_type
  private
  type(arg_type) :: meta_args(6) = (/                                    &
       arg_type(GH_FIELD,   GH_INC,  W2),                                &
       arg_type(GH_FIELD,   GH_READ, W3),                                &
       arg_type(GH_INTEGER, GH_READ),                                    &
       arg_type(GH_REAL,    GH_READ),                                    &
       arg_type(GH_FIELD,   GH_READ, W0),                                &
       arg_type(GH_FIELD*3, GH_READ, W0)                                 &
       /)
  type(func_type) :: meta_funcs(3) = (/                                  &
       func_type(W2, GH_BASIS, GH_DIFF_BASIS),                           &
       func_type(W3, GH_BASIS),                                          &
       func_type(W0, GH_BASIS, GH_DIFF_BASIS)                            &
       /)
  integer :: iterates_over = CELLS
  integer :: gh_shape = gh_quadrature_XYoZ
contains
  procedure, nopass ::ru_code
end type
```

```
contains
subroutine ru_code()
end subroutine ru_code
end module ru_kernel_mod
```

If we run the kernel stub generator on this example:

```
> genkernelstub tests/test_files/dynamo0p3/ru_kernel_mod.f90
```

we obtain the following output:

```
MODULE ru_mod
  IMPLICIT NONE
  CONTAINS
  SUBROUTINE ru_code(nlayers, field_1_w2, field_2_w3, iscalar_3, rscalar_4, field_5_
↪w0, field_6_w0_v1, field_6_w0_v2, field_6_w0_v3, ndf_w2, undf_w2, map_w2, basis_w2,␣
↪diff_basis_w2, ndf_w3, undf_w3, map_w3, basis_w3, ndf_w0, undf_w0, map_w0, basis_w0,
↪ diff_basis_w0, np_xy, np_z, weights_xy, weights_z)
    USE constants_mod, ONLY: r_def
    IMPLICIT NONE
    INTEGER, intent(in) :: nlayers
    INTEGER, intent(in) :: ndf_w2
    INTEGER, intent(in) :: undf_w2
    INTEGER, intent(in) :: ndf_w3
    INTEGER, intent(in) :: undf_w3
    INTEGER, intent(in) :: ndf_w0
    INTEGER, intent(in) :: undf_w0
    REAL(KIND=r_def), intent(inout), dimension(undf_w2) :: field_1_w2
    REAL(KIND=r_def), intent(in), dimension(undf_w3) :: field_2_w3
    INTEGER, intent(in) :: iscalar_3
    REAL(KIND=r_def), intent(in) :: rscalar_4
    REAL(KIND=r_def), intent(in), dimension(undf_w0) :: field_5_w0
    REAL(KIND=r_def), intent(in), dimension(undf_w0) :: field_6_w0_v1
    REAL(KIND=r_def), intent(in), dimension(undf_w0) :: field_6_w0_v2
    REAL(KIND=r_def), intent(in), dimension(undf_w0) :: field_6_w0_v3
    INTEGER, intent(in), dimension(ndf_w2) :: map_w2
    REAL(KIND=r_def), intent(in), dimension(3,ndf_w2,np_xy,np_z) :: basis_w2
    REAL(KIND=r_def), intent(in), dimension(1,ndf_w2,np_xy,np_z) :: diff_basis_w2
    INTEGER, intent(in), dimension(ndf_w3) :: map_w3
    REAL(KIND=r_def), intent(in), dimension(1,ndf_w3,np_xy,np_z) :: basis_w3
    INTEGER, intent(in), dimension(ndf_w0) :: map_w0
    REAL(KIND=r_def), intent(in), dimension(1,ndf_w0,np_xy,np_z) :: basis_w0
    REAL(KIND=r_def), intent(in), dimension(3,ndf_w0,np_xy,np_z) :: diff_basis_w0
    INTEGER, intent(in) :: np_xy, np_z
    REAL(KIND=r_def), intent(in), dimension(np_xy) :: weights_xy
    REAL(KIND=r_def), intent(in), dimension(np_z) :: weights_z
  END SUBROUTINE ru_code
END MODULE ru_mod
```

The above example demonstrates that the argument list can get quite complex. Rather than going through an explanation of each argument you are referred to Section *Rules* for more details on the rules for argument types and argument ordering. Regarding naming conventions for arguments you can see that the arrays associated with the fields are labelled as 1-6 depending on their position in the metadata. For a vector field, each vector results in a different array. These are distinguished by appending `_vx` where `x` is the number of the vector.

The introduction of stencil operations on field arguments futher complicates the argument list of a kernel. An example of the use of the stub generator for a kernel that performs stencil operations is provided in `examples/dynamo/eg5`.

```
> genkernelstub ../../examples/dynamo/eg5/conservative_flux_kernel_mod.F90
```

Errors

The stub generator has been written to provide useful errors if mistakes are found. If you run the generator and it does not produce a useful error - and in particular if it produces a stack trace - please contact the PSyclone developers.

The following tests do not produce stub kernel code either because they are invalid or because they contain functionality that is not supported in the stub generator.

```
tests/test_files/dynamo0p3/matrix_vector_mod.F90
tests/test_files/dynamo0p3/testkern_any_space_1_mod.f90
tests/test_files/dynamo0p3/testkern_any_space_4_mod.f90
tests/test_files/dynamo0p3/testkern_invalid_fortran.F90
tests/test_files/dynamo0p3/testkern_short_name.F90
tests/test_files/dynamo0p3/testkern_no_datatype.F90
tests/test_files/dynamo0p3/testkern.F90
tests/test_files/dynamo0p3/testkern_qr.F90
```

`testkern_invalid_fortran.F90`, `testkern_no_datatype.F90`, `testkern_short_name.F90`, `testkern.F90` and `matrix_vector_mod.F90` are designed to be invalid for PSyclone testing purposes and should produce appropriate errors. For example:

```
> genkernelstub tests/test_files/dynamo0p3/testkern_invalid_fortran.F90
Error: 'Parse Error: Code appears to be invalid Fortran'
```

`any_space` is not currently supported in the stub generator so `testkern_any_space_1_mod.f90` and `testkern_any_space_4_mod.f90` should fail with appropriate warnings because of that. For example:

```
> genkernelstub tests/test_files/dynamo0p3/testkern_any_space_1_mod.f90
Error: "Generation Error: Unsupported space for basis function, expecting
one of ['w3', 'wtheta', 'w2v', 'w0', 'w1', 'w2', 'w2h', 'any_w2'] but
found 'any_space_1'"
```

As noted above, if the Dynamo0.3 naming convention for module and type names is not followed, the stub generator will return with an error message. For example:

```
> genkernelstub tests/test_files/dynamo0p3/testkern.F90
Error: "Parse Error: Error, module name 'testkern' does not have
'_mod' as an extension. This convention is assumed."
```

CHAPTER

TWELVE

LINE LENGTH

By default PSyclone will generate fortran code with no consideration of fortran line length limits. As the line length limit for free-form fortran is 132 characters, the code that is output may be non-conformant.

Line length is not an issue for many compilers as they allow compiler flags to be set which allow lines longer than the fortran standard. However this is not the case for all compilers.

PSyclone therefore supports the wrapping of lines within the 132 character limit. The next two sections discuss how this is done when scripting and when working interactively respectively.

Script

The generate.py script provides the -l option to wrap lines. Please see the *Fortran line length* section for more details.

Interactive

When using PSyclone interactively the line length of the input algorithm and Kernel files can be checked by setting the `parse.parse()` function's "line_length" argument to "True".

```
>>> from parse import parse
>>> ast, info = parse("argspec.F90", line_length=True)
```

Similarly the "line_length" argument can be set to "True" if calling the `generator.generate()` function. This function simply passes this argument on to the `parse.parse()` function.

```
>>> from generator import generate
>>> alg, psy = generate("argspec.F90", line_length=True)
```

Line wrapping is performed as a post processing step, i.e. after the code has been generated. This is done by an instance of the `line_length.FortLineLength` class. For example:

```
>>> from generator import generate
>>> from line_length import FortLineLength
>>> psy, alg = generate("algspec.f90", line_length=True)
>>> line_length = FortLineLength()
>>> psy_str = line_length.process(str(psy))
>>> print psy_str
>>> alg_str = line_length.process(str(alg))
>>> print alg_str
```

Limitations

The `line_length.FortLineLength` class is only partially aware of fortran syntax. This awareness is required so that appropriate continuation characters can be used (for example `&` at the end of a line and `!$omp&` at the start of a line for OpenMP directives, `&` at the end of a line for statements and `&` at the end of a line and `&` at the beginning of a line for strings).

Whilst statements only require an `&` at the end of the line when line wrapping with free-form fortran they may optionally also have an `&` at the beginning of the subsequent line. In contrast, when splitting a string over multiple lines an `&` is required at both locations. Therefore an instance of the `line_length.FortLineLength` class will always add `&` at the beginning of a continuation line for a statement, in case the line is split within a string.

One known situation that could cause an instance of the `line_length.FortLineLength` class to fail is when an inline comment is used at the end of a line to make it longer than the 132 character limit. Whilst PSyclone does not generate such code for the PSy-layer, this might occur in Algorithm-layer code, even if the Algorithm-layer code conforms to the 132 line length limit. The reason for this is that PSyclone's internal parser concatenates lines together, thus a long line correctly split with continuation characters in the Algorithm-layer becomes a line that needs to be split by an instance of the `line_length.FortLineLength` class.

CHAPTER THIRTEEN

API

generator.py

-h

-oalg <filename>

-opsy <filename>

-api <api>

-s <script>

-d <directory>

-l

Command line version of the generator. -h prints out the command line options. If -oalg or -opsy are not provided then the generated code is printed to stdout, otherwise they are output to the specified file name. -api specifies the particular api to use. -s allows a script to be called which can modify (typically optimise) the PSy layer. -d specifies a directory to recursively search to find the associated kernel files. -l limits the maximum line length of the fortran output to 132 characters. -l uses a relatively simple algorithm which in pathological cases may produce incorrect output, so it is recommended to only use this option if necessary. generator.py Uses the `generator.generate()` function to generate the code. Please see the run documentation for more details.

For example:

```
> python generator.py algspec.f90
> python generator.py -oalg alg.f90 -opsy psy.f90 -api dynamo0.3 algspec.f90
> python generator.py -d ../kernel -s opt.py algspec.f90
> python generator.py -s ../scripts/opt.py -l algspec.f90
```

This module provides the PSyclone 'main' routine which is intended to be driven from the bin/psyclone executable script. 'main' takes an algorithm file as input and produces modified algorithm code and generated PSy code. A function, 'generate', is also provided which has the same functionality as 'main' but can be called from within another Python program.

`psyclone.generator.`**`generate`**(*filename*, *api=''*, *kernel_path=''*, *script_name=None*, *line_length=False*, *distributed_memory=None*)

Takes a GungHo algorithm specification as input and outputs the associated generated algorithm and psy codes suitable for compiling with the specified kernel(s) and GungHo infrastructure. Uses the `parse.parse()` function to parse the algorithm specification, the `psyGen.PSy` class to generate the PSy code and the `algGen.Alg` class to generate the modified algorithm code.

Parameters

- **`filename`** (*`str`*) – The file containing the algorithm specification.

- **kernel_path** (*str*) – The directory from which to recursively search for the files containing the kernel source (if different from the location of the algorithm specification)
- **script_name** (*str*) – A script file that can apply optimisations to the PSy layer (can be a path to a file or a filename that relies on the PYTHONPATH to find the module).
- **line_length** (*bool*) – A logical flag specifying whether we care about line lengths being longer than 132 characters. If so, the input (algorithm and kernel) code is checked to make sure that it conforms. The default is False.
- **distributed_memory** (*bool*) – A logical flag specifying whether to generate distributed memory code. The default is set in the config.py file.

Returns The algorithm code and the psy code.

Return type ast

Raises `IOError` – if the filename or search path do not exist

For example:

```
>>> from generator import generate
>>> alg, psy = generate("algspec.f90")
>>> alg, psy = generate("algspec.f90", kernel_path="src/kernels")
>>> alg, psy = generate("algspec.f90", script_name="optimise.py")
>>> alg, psy = generate("algspec.f90", line_length=True)
>>> alg, psy = generate("algspec.f90", distributed_memory=False)
```

The parse module

Module implementing classes populated by parsing either kernel meta-data or invoke()'s in the Algorithm layer

psyclone.parse.**parse**(*alg_filename*, *api=''*, *invoke_name='invoke'*, *inf_name='inf'*, *kernel_path=''*, *line_length=False*, *distributed_memory=None*)

Takes a GungHo algorithm specification as input and outputs an AST of this specification and an object containing information about the invocation calls in the algorithm specification and any associated kernel implementations.

Parameters

- **alg_filename** (*str*) – The file containing the algorithm specification.
- **invoke_name** (*str*) – The expected name of the invocation calls in the algorithm specification
- **inf_name** (*str*) – The expected module name of any required infrastructure routines.
- **kernel_path** (*str*) – The path to search for kernel source files (if different from the location of the algorithm source).
- **line_length** (*bool*) – A logical flag specifying whether we care about line lengths being longer than 132 characters. If so, the input (algorithm and kernel) code is checked to make sure that it conforms and an error raised if not. The default is False.

Return type ast,invoke_info

Raises

- `IOError` – if the filename or search path does not exist
- `ParseError` – if there is an error in the parsing

- **RuntimeError** – if there is an error in the parsing

For example:

```
>>> from parse import parse
>>> ast,info=parse("argspec.F90")
```

The transformations module

This module provides the various transformations that can be applied to the schedule associated with an invoke(). There are both general and API-specific transformation classes in this module where the latter typically apply API-specific checks before calling the base class for the actual transformation.

class `psyclone.transformations.`**`ACCDataTrans`**

Adds an OpenACC "enter data" directive to a Schedule. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> dtrans = t.get_trans_name('ACCDataTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> # Add an enter-data directive
>>> newschedule, _ = dtrans.apply(schedule)
>>> newschedule.view()
```

`apply`(*sched*)

Adds an OpenACC "enter data" directive to the invoke associated with the supplied Schedule. Any fields accessed by OpenACC kernels within this schedule will be added to this data region in order to ensure they remain on the target device.

Parameters **sched** (sub-class of *`psyclone.psyGen.Schedule`*.) – Schedule to which to add an "enter data" directive.

Returns Tuple of the modified schedule and a record of the transformation.

Return type (*`psyclone.psyGen.Schedule`*, `psyclone.undoredo.Memento`)

Raises

- **NotImplementedError** – for any API other than GOcean 1.0.
- ***TransformationError*** – if passed something that is not a (subclass of) *`psyclone.psyGen.Schedule`*.

`name`

Returns the name of this transformation.

Return type str

class `psyclone.transformations.`**`ACCLoopTrans`**

Adds an OpenACC loop directive to a loop. This directive must be within the scope of some OpenACC Parallel region (at code-generation time).

For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ltrans = t.get_trans_name('ACCLoopTrans')
>>> rtrans = t.get_trans_name('ACCParallelTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>> new_schedule = schedule
>>>
# Apply the OpenACC Loop transformation to *every* loop
# in the schedule
>>> for child in schedule.children:
>>>     newschedule, memento = ltrans.apply(child, reprod=True)
>>>     schedule = newschedule
>>>
# Enclose all of these loops within a single OpenACC
# PARALLEL region
>>> rtrans.omp_schedule("dynamic,1")
>>> newschedule, memento = rtrans.apply(schedule.children)
>>>
```

`apply`(*node*, *collapse=None*, *independent=True*)

Apply the ACCLoop transformation to the specified node in a Schedule. This node must be a Loop since this transformation corresponds to inserting a directive immediately before a loop, e.g.:

```
!$ACC LOOP
do ...
   ...
end do
```

At code-generation time (when `psyclone.psyGen.ACCLoopDirective.gen_code()` is called), this node must be within (i.e. a child of) a PARALLEL region.

Parameters

- **`node`** (`psyclone.psyGen.Loop.`) – the supplied node to which we will apply the Loop transformation.
- **`collapse`** (*`int`*) – number of loops to collapse into single iteration space or None.
- **`independent`** (*`bool`*) – whether to add the "independent" clause to the directive (not strictly necessary within PARALLEL regions).

Returns (*`psyclone.psyGen.Schedule`*, `psyclone.undoredo.Memento`)

`name`

Returns the name of this transformation as a string.

class psyclone.transformations.**ACCParallelTrans**

Create an OpenACC parallel region by inserting directives. This parallel region *must* come after an enter-data directive (see *ACCDataTrans*). For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ptrans = t.get_trans_name('ACCParallelTrans')
>>> dtrans = t.get_trans_name('ACCDataTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> # Enclose everything within a single OpenACC PARALLEL region
>>> newschedule, _ = ptrans.apply(schedule.children)
>>> # Add an enter-data directive
>>> newschedule, _ = dtrans.apply(newschedule)
>>> newschedule.view()
```

name

Returns The name of this transformation as a string.

Return type str

class psyclone.transformations.**ColourTrans**

Apply a colouring transformation to a loop (in order to permit a subsequent parallelisation over colours). For example:

```
>>> invoke = ...
>>> schedule = invoke.schedule
>>>
>>> ctrans = ColourTrans()
>>>
>>> # Colour all of the loops
>>> for child in schedule.children:
>>>     cschedule, _ = ctrans.apply(child)
>>>
>>> csched.view()
```

apply(*node*)

Converts the Loop represented by `node` into a nested loop where the outer loop is over colours and the inner loop is over cells of that colour. :param node: The loop to transform. :type node: `psyclone.psyGen.Loop` :returns: Tuple of modified schedule and record of transformation :rtype: (`psyclone.psyGen.Schedule, :py:class:`psyclone.undoredo.Memento`)

name

Returns the name of this transformation as a string.

class psyclone.transformations.**Dynamo0p3ColourTrans**

Split a Dynamo 0.3 loop over cells into colours so that it can be parallelised. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> import transformations
>>> import os
>>> import pytest
>>>
>>> TEST_API = "dynamo0.3"
>>> _,info=parse(os.path.join(os.path.dirname(os.path.abspath(__file__)),
>>>              "tests", "test_files", "dynamo0p3",
>>>              "4.6_multikernel_invokes.f90"),
>>>              api=TEST_API)
>>> psy = PSyFactory(TEST_API).create(info)
>>> invoke = psy.invokes.get('invoke_0')
>>> schedule = invoke.schedule
>>>
>>> ctrans = Dynamo0p3ColourTrans()
>>> otrans = DynamoOMPParallelLoopTrans()
>>>
>>> # Colour all of the loops
>>> for child in schedule.children:
>>>     cschedule, _ = ctrans.apply(child)
>>>
>>> # Then apply OpenMP to each of the colour loops
>>> schedule = cschedule
>>> for child in schedule.children:
>>>     newsched, _ = otrans.apply(child.children[0])
>>>
>>> newsched.view()
```

Colouring in the Dynamo 0.3 API is subject to the following rules:

- Only kernels with an iteration space of CELLS and which modify a continuous field require colouring. Any other type of loop will cause this transformation to raise an exception.
- A kernel may have at most one field with 'INC' access
- A separate colour map will be required for each field that is coloured (if an invoke contains >1 kernel call)

apply(*node*)
Performs Dynamo0.3-specific error checking and then uses the parent class to convert the Loop represented by `node` into a nested loop where the outer loop is over colours and the inner loop is over cells of that colour.

name
Returns the name of this transformation as a string.

class psyclone.transformations.**Dynamo0p3OMPLoopTrans**(*omp_schedule='static'*)
Dynamo 0.3 specific orphan OpenMP loop transformation. Adds Dynamo-specific validity checks. Actual transformation is done by *base class*.

apply(*node*, *reprod=None*)
Perform Dynamo 0.3 specific loop validity checks then call *OMPLoopTrans.apply()*.

name
Returns the name of this transformation as a string.

class psyclone.transformations.**Dynamo0p3RedundantComputationTrans**
This transformation allows the user to modify a loop's bounds so that redundant computation will be performed. Redundant computation can result in halo exchanges being modified, new halo exchanges being added or existing halo exchanges being removed.

- This transformation should be performed before any parallelisation transformations (e.g. for OpenMP) to the loop in question and will raise an exception if this is not the case.
- This transformation can not be applied to a loop containing a reduction and will again raise an exception if this is the case.
- This transformation can only be used to add redundant computation to a loop, not to remove it.
- This transformation allows a loop that is already performing redundant computation to be modified, but only if the depth is increased.

apply(*loop*, *depth=None*)
Apply the redundant computation tranformation to the loop `loop`. This transformation can be applied to loops iterating over 'cells or 'dofs'. if `depth` is set to a value then the value will be the depth of the field's halo over which redundant computation will be performed. If `depth` is not set to a value then redundant computation will be performed to the full depth of the field's halo.

Parameters

- **loop** (`psyclone.psyGen.DynLoop`) – the loop that we are transforming
- **depth** (*int or None*) – the depth of the stencil. Defaults to None if a depth is not provided.

name
Returns the name of this transformation as a string.

class `psyclone.transformations.`**DynamoLoopFuseTrans**
Performs error checking before calling the `apply()` method of the `base class` in order to fuse two Dynamo loops.

apply(*node1*, *node2*, *same_space=False*)
Fuse the two Dynamo loops represented by `node1` and `node2`. The optional same_space flag asserts that an unknown iteration space (i.e. any_space) matches the other iteration space. This is set at the users own risk.

name
Returns the name of this transformation as a string.

class `psyclone.transformations.`**DynamoOMPParallelLoopTrans**(*omp_schedule='static'*)
Dynamo-specific OpenMP loop transformation. Adds Dynamo specific validity checks. Actual transformation is done by the `base class`.

apply(*node*)
Perform Dynamo specific loop validity checks then call the `apply()` method of the `base class`.

name
Returns the name of this transformation as a string.

class `psyclone.transformations.`**GOConstLoopBoundsTrans**
Switch on (or off) the use of constant loop bounds within a GOSchedule. In the absence of constant loop bounds, PSyclone will generate loops where the bounds are obtained by de-referencing a field object, e.g.:

```
DO j = my_field%grid%internal%ystart, my_field%grid%internal%ystop
```

Some compilers are able to produce more efficient code if they are provided with information on the relative trip-counts of the loops within an Invoke. With constant loop bounds switched on, PSyclone generates code like:

```
ny = my_field%grid%simulation_domain%ystop
...
DO j = 1, ny-1
```

In practice, the application of the constant loop bounds looks something like, e.g.:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> import os
>>> TEST_API = "gocean1.0"
>>> _, info = parse(os.path.join("tests", "test_files", "gocean1p0",
>>>                              "single_invoke.f90"),
>>>                 api=TEST_API)
>>> psy = PSyFactory(TEST_API).create(info)
>>> invoke = psy.invokes.get('invoke_0_compute_cu')
>>> schedule = invoke.schedule
>>>
>>> from psyclone.transformations import GOConstLoopBoundsTrans
>>> clbtrans = GOConstLoopBoundsTrans()
>>>
>>> newsched, _ = clbtrans.apply(schedule)
>>> # or, to turn off const. looop bounds:
>>> # newsched, _ = clbtrans.apply(schedule, const_bounds=False)
>>>
>>> newsched.view()
```

apply (*node*, *const_bounds=True*)
Switches constant loop bounds on or off for all loops in the schedule `node`. Default is 'on'.

Parameters

- **node** (`psyclone.gocean1p0.GOSchedule`) – The schedule of which all loops will get the constant loop bounds switched on or off.
- **const_bounds** (*bool*) – If the constant loop should be used (True) or not (False). Default is True.

name
Return the name of the Transformation as a string.

class `psyclone.transformations.`**`GOLoopSwapTrans`**
Provides a loop-swap transformation, e.g.:

```
DO j=1, m
   DO i=1, n
```

becomes:

```
DO i=1, n
   DO j=1, m
```

This transform is used as follows:

```
>>> from parse import parse
>>> from psyGen import PSyFactory
>>> ast,invokeInfo=parse("shallow_alg.f90")
>>> psy=PSyFactory("gocean1.0").create(invokeInfo)
>>> schedule=psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> from transformations import GOLoopSwapTrans
>>> swap=GOLoopSwapTrans()
>>> new_schedule,memento=swap.apply(schedule.children[0])
>>> new_schedule.view()
```

apply (*outer*)

The argument `outer` must be a loop which has exactly one inner loop. This transform then swaps the outer and inner loop.

Parameters **outer** (`psyclone.psyGen.Loop`) – The node representing the outer loop.

Returns A tuple consistent of the new schedule, and a Memento.

Raises ***TransformationError*** – if the supplied node does not allow a loop swap to be done.

name

Returns the name of this transformation as a string.

class `psyclone.transformations.`**GOceanLoopFuseTrans**

Performs error checking (that the loops are over the same grid-point type) before calling the *`LoopFuseTrans.apply()`* method of the *`base class`* in order to fuse two GOcean loops.

apply (*node1*, *node2*)

Fuse the two GOcean loops represented by `node1` and `node2`.

Parameters

- **node1** (`psyclone.gocean1p0.GOLoop`) – A node representing a GOLoop.
- **node2** (`psyclone.gocean1p0.GOLoop`) – A node representing a GOLoop.

Raises ***TransformationError*** – if the supplied node2 can not be fused, e.g. not all nodes are loops, don't have the same parent, are not next to each other or have different iteration spaces.

name

Returns the name of this transformation as a string.

class `psyclone.transformations.`**GOceanOMPLoopTrans** (*omp_schedule='static'*)

GOcean-specific orphan OpenMP loop transformation. Adds GOcean specific validity checks (that the node is either an inner or outer Loop). Actual transformation is done by *`base class`*.

Parameters **omp_schedule** – The omp schedule to be created. Must be one of 'runtime', 'static', 'dynamic', 'guided' or 'auto'.

apply (*node*)

Perform GOcean specific loop validity checks then call *`OMPLoopTrans.apply()`*.

Parameters **node** (`psyclone.psyGen.Loop.`) – The loop to parallelise using OMP Do.

name

Returns the name of this transformation as a string.

class `psyclone.transformations.`**GOceanOMPParallelLoopTrans** (*omp_schedule='static'*)

GOcean specific OpenMP Do loop transformation. Adds GOcean specific validity checks (that supplied Loop is an inner or outer loop). Actual transformation is done by *`base class`*.

Parameters **omp_schedule** – The omp schedule to be created. Must be one of 'runtime', 'static', 'dynamic', 'guided' or 'auto'.

apply (*node*)

Perform GOcean-specific loop validity checks then call *`OMPParallelLoopTrans.apply()`*.

Parameters **node** (`psyclone.psyGen.Loop`) – A Loop node from an AST.

Raises ***TransformationError*** – if the supplied node is not an inner or outer loop.

name

Returns the name of this transformation as a string.

class `psyclone.transformations.`**`KernelModuleInlineTrans`**

Switches on, or switches off, the inlining of a Kernel subroutine into the PSy layer module. For example:

```
>>> invoke = ...
>>> schedule = invoke.schedule
>>>
>>> inline_trans = KernelModuleInlineTrans()
>>>
>>> ischedule, _ = inline_trans.apply(schedule.children[0].children[0])
>>> ischedule.view()
```

Warning: For this transformation to work correctly, the Kernel subroutine must only use data that is passed in by argument, declared locally or included via use association within the subroutine. Two examples where in-lining will not work correctly are:

1. A variable is declared within the module that `contains` the Kernel subroutine and is then accessed within that Kernel;
2. A variable is included via use association at the module level and accessed within the Kernel subroutine.

There are currently no checks that these rules are being followed when in-lining so the onus is on the user to ensure correctness.

`apply`(*node*, *inline=True*)

Checks that the node is of the correct type (a Kernel) then marks the Kernel to be inlined, or not, depending on the value of the inline argument. If the inline argument is not passed the Kernel is marked to be inlined.

`name`

Returns the name of this transformation as a string.

class `psyclone.transformations.`**`LoopFuseTrans`**

Provides a loop-fuse transformation. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> ast,invokeInfo=parse("dynamo.F90")
>>> psy=PSyFactory("dynamo0.1").create(invokeInfo)
>>> schedule=psy.invokes.get('invoke_v3_kernel_type').schedule
>>> schedule.view()
>>>
>>> from psyclone.transformations import LoopFuseTrans
>>> trans=LoopFuseTrans()
>>> new_schedule,memento=trans.apply(schedule.children[0],
                                      schedule.children[1])
>>> new_schedule.view()
```

`apply`(*node1*, *node2*)

Fuse the loops represented by `node1` and `node2`.

`name`

Returns the name of this transformation as a string.

class `psyclone.transformations.`**`MoveTrans`**

Provides a transformation to move a node in the tree. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> ast,invokeInfo=parse("dynamo.F90")
>>> psy=PSyFactory("dynamo0.3").create(invokeInfo)
>>> schedule=psy.invokes.get('invoke_v3_kernel_type').schedule
>>> schedule.view()
>>>
>>> from psyclone.transformations import MoveTrans
>>> trans=MoveTrans()
>>> new_schedule, memento = trans.apply(schedule.children[0],
                                        schedule.children[2],
                                        position="after")
>>> new_schedule.view()
```

Nodes may only be moved to a new location with the same parent and must not break any dependencies otherwise an exception is raised.

apply (*node*, *location*, *position='before'*)
Move the node represented by `node` before location `location` (which is also a node) by default and after if the optional *position* argument is set to 'after'. An exception is raised if the move is invalid.

name
Returns the name of this transformation as a string.

class psyclone.transformations.**OMPLoopTrans** (*omp_schedule='static'*)
Adds an orphaned OpenMP directive to a loop. i.e. the directive must be inside the scope of some other OMP Parallel REGION. This condition is tested at code-generation time. The optional 'reprod' argument in the apply method decides whether standard OpenMP reduction support is to be used (which is not reproducible) or whether a manual reproducible reproduction is to be used.

Parameters **omp_schedule** (*str*) – The OpenMP schedule to use.

For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>> print psy.invokes.names
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ltrans = t.get_trans_name('OMPLoopTrans')
>>> rtrans = t.get_trans_name('OMPParallelTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>> new_schedule = schedule
>>>
# Apply the OpenMP Loop transformation to *every* loop
# in the schedule
>>> for child in schedule.children:
>>>     newschedule, memento = ltrans.apply(child, reprod=True)
>>>     schedule = newschedule
>>>
# Enclose all of these loops within a single OpenMP
# PARALLEL region
>>> rtrans.omp_schedule("dynamic,1")
>>> newschedule, memento = rtrans.apply(schedule.children)
```

```
>>>
>>>
```

apply (*node*, *reprod=None*)

Apply the OMPLoopTrans transformation to the specified node in a Schedule. This node must be a Loop since this transformation corresponds to wrapping the generated code with directives like so:

```
!$OMP DO
do ...
   ...
end do
!$OMP END DO
```

At code-generation time (when `OMPLoopDirective.gen_code()` is called), this node must be within (i.e. a child of) an OpenMP PARALLEL region.

The optional reprod argument will cause a reproducible reduction to be generated if it is set to True, otherwise the default value (as read from the psyclone.cfg file) will be used. Note, reproducible in this case means obtaining the same results with the same number of OpenMP threads, not for different numbers of OpenMP threads.

Parameters

- **node** (`psyclone.psyGen.Node`) – the supplied node to which we will apply the OMPLoopTrans transformation
- **reprod** (*Boolean or None*) – optional argument to determine whether to generate reproducible OpenMP reductions (True) or not (False). The default value is None which will cause PSyclone to look up a default value

Returns (*psyclone.psyGen.Schedule*, `psyclone.undoredo.Memento`)

name

Returns the name of this transformation as a string.

omp_schedule

Returns the OpenMP schedule that will be specified by this transformation. The default schedule is 'static'.

class psyclone.transformations.**OMPParallelLoopTrans** (*omp_schedule='static'*)

Adds an OpenMP PARALLEL DO directive to a loop.

For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> ast, invokeInfo = parse("dynamo.F90")
>>> psy = PSyFactory("dynamo0.1").create(invokeInfo)
>>> schedule = psy.invokes.get('invoke_v3_kernel_type').schedule
>>> schedule.view()
>>>
>>> from psyclone.transformations import OMPParallelLoopTrans
>>> trans = OMPParallelLoopTrans()
>>> new_schedule, memento = trans.apply(schedule.children[0])
>>> new_schedule.view()
```

apply (*node*)

Apply an OMPParallelLoop Transformation to the supplied node (which must be a Loop). In the generated code this corresponds to wrapping the Loop with directives:

```
!$OMP PARALLEL DO ...
do ...
  ...
end do
!$OMP END PARALLEL DO
```

Parameters **node** (psyclone.f2pygen.DoGen) – the node (loop) to which to apply the transformation.

Returns Two-tuple of transformed schedule and a record of the transformation.

Return type (psyclone.psyGen.Schedule, :py:class:`psyclone.undoredo.Memento)

name
Returns the name of this transformation as a string.

class psyclone.transformations.**OMPParallelTrans**
Create an OpenMP PARALLEL region by inserting directives. For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> ltrans = t.get_trans_name('GOceanOMPLoopTrans')
>>> rtrans = t.get_trans_name('OMPParallelTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>> new_schedule = schedule
>>>
>>> # Apply the OpenMP Loop transformation to *every* loop
>>> # in the schedule
>>> for child in schedule.children:
>>>     newschedule, memento = ltrans.apply(child)
>>>     schedule = newschedule
>>>
>>> # Enclose all of these loops within a single OpenMP
>>> # PARALLEL region
>>> newschedule, _ = rtrans.apply(schedule.children)
>>> newschedule.view()
```

name

Returns The name of this transformation as a string.

Return type str

class psyclone.transformations.**ParallelLoopTrans**
Adds an orphaned directive to a loop indicating that it should be parallelised. i.e. the directive must be inside the scope of some other Parallel REGION. This condition is tested at code-generation time.

apply (*node*, *collapse=None*)
Apply the Loop transformation to the specified node in a Schedule. This node must be a Loop since this

transformation corresponds to wrapping the generated code with directives, e.g. for OpenMP:

```
!$OMP DO
do ...
   ...
end do
!$OMP END DO
```

At code-generation time (when gen_code()' is called), this node must be within (i.e. a child of) a PARALLEL region.

Parameters

- **node** (`psyclone.psyGen.Node.`) – the supplied node to which we will apply the Loop transformation.
- **collapse** (*int*) – number of loops to collapse into single iteration space or None.

Returns (*psyclone.psyGen.Schedule*, `psyclone.undoredo.Memento`)

name

Returns the name of this transformation as a string.

Return type str

class `psyclone.transformations.`**ParallelRegionTrans**

Base class for transformations that create a parallel region.

apply (*nodes*)

Apply this transformation to a subset of the nodes within a schedule - i.e. enclose the specified Loops in the schedule within a single parallel region.

Parameters **nodes** ((list of) `psyclone.psyGen.Node.`) – a single Node or a list of Nodes.

Raises ***TransformationError*** – if the nodes argument is not of the correct type.

name

Returns the name of this transformation as a string.

class `psyclone.transformations.`**ProfileRegionTrans**

Create a profile region around a list of statements. For example:

```
>>> from psyclone.parse import parse, ParseError
>>> from psyclone.psyGen import PSyFactory, GenerationError
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> p_trans = t.get_trans_name('ProfileRegionTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> # Enclose all children within a single profile region
>>> newschedule, _ = p_trans.apply(schedule.children)
>>> newschedule.view()
```

apply(*nodes*)
Apply this transformation to a subset of the nodes within a schedule - i.e. enclose the specified Nodes in the schedule within a single profiler region.

Parameters **nodes** (`psyclone.psygen.Node` or list of `psyclone.psygen.Node`.) – Can be a single node or a list of nodes.

name
Returns the name of this transformation as a string

exception `psyclone.transformations.`**TransformationError**(*value*)
Provides a PSyclone-specific error class for errors found during code transformation operations.

`psyclone.transformations.`**check_intergrid**(*node*)
Utility function to check that the supplied node does not have an intergrid kernel as a child.

This is used to ensure that we reject any attempt to apply transformations to loops containing inter-grid kernels. (This restriction will be lifted in Issue #134 and this routine can then be removed.)

# TODO remove this routine once #134 is complete.

Parameters **node** (`psyGen.Node`) – the Node in the Schedule to check

Raises ***TransformationError*** – if the supplied node has an inter-grid kernel as a child

The psyGen module

This module provides generic support for PSyclone's PSy code optimisation and generation. The classes in this method need to be specialised for a particular API and implementation.

class `psyclone.psyGen.`**PSy**(*invoke_info*)
Base class to help manage and generate PSy code for a single algorithm file. Takes the invocation information output from the function `parse.parse()` as its input and stores this in a way suitable for optimisation and code generation.

Parameters **invoke_info** (*FileInfo*) – An object containing the required invocation information for code optimisation and generation. Produced by the function `parse.parse()`.

For example:

```
>>> import psyclone
>>> from psyclone.parse import parse
>>> ast, info = parse("argspec.F90")
>>> from psyclone.psyGen import PSyFactory
>>> api = "..."
>>> psy = PSyFactory(api).create(info)
>>> print(psy.gen)
```

inline(*module*)
inline all kernel subroutines into the module that are marked for inlining. Avoid inlining the same kernel more than once.

The algGen module

This module provides the Alg class and supporting exception-handling to translate the original algorithm file into one that can be compiled and linked with the generated PSy code.

class `psyclone.algGen.`**`Alg`**(*ast*, *psy*)

Generate a modified algorithm code for a single algorithm specification. Takes the ast of the algorithm specification output from the function `parse.parse()` and an instance of the `psyGen.PSy` class as input.

Parameters

- **`ast`** (*`ast`*) – An object containing an ast of the algorithm specification which was produced by the function `parse.parse()`.
- **`psy`** (`PSy`) – An object (`psyGen.PSy`) containing information about the PSy layer.

For example:

```
>>> from parse import parse
>>> ast,info=parse("argspec.F90")
>>> from psyGen import PSy
>>> psy=PSy(info)
>>> from algGen import Alg
>>> alg=Alg(ast,psy)
>>> print(alg.gen)
```

`gen`

Generate modified algorithm code

Return type ast

The line_length module

Provides support for breaking long fortran lines into smaller ones to allow the code to conform to the maximum line length limits (132 for f90 free format is the default)

class `psyclone.line_length.`**`FortLineLength`**(*line_length=132*)

This class take a free format fortran code as a string and line wraps any lines that are larger than the specified line length

`length`

returns the maximum allowed line length

`long_lines`(*fortran_in*)

returns true if at least one of the lines in the input code is longer than the allowed length. Otherwise returns false

`process`(*fortran_in*)

takes fortran code as a string as input and output fortran code as a string with any long lines wrapped appropriately

CHAPTER

FOURTEEN

PROFILING

PSyclone has the ability to define regions that can be profiled with various performance measurement tools. The profiling can be enabled automatically using command line parameters like:

```
psyclone --profile kernels ...
```

Or more fine grained by applying a profiling transformation in a transformation script.

PSyclone can be used with a variety of existing profiling tools. It currently supports dl_timer, and comes with a simple stand-alone timer library. An application needs to be able to find the module files for the profile wrapper, and needs to be linked with the included wrapper library that interfaces between the PSyclone API and the tool-specific API. It is the responsibility of the user to supply the corresponding compiler command line options when building the application that incorporates the PSyclone-generated code.

Profiling API

In order to be used with different profiling tools, PSyclone supports a simple profiling API. For each existing profiling tool a simple interface library needs to be implemented that maps the PSyclone profiling calls to the corresponding call for the profiling tool.

PSyclone utilises 4 profiling calls which are described in the following sub-sections.

ProfileInit()

This method needs to be called once to initialise the profiling tool. At this stage this call is not automatically inserted by PSyclone, so it is the responsibility of the user to add the call to an appropriate location in the application:

```
use profile_mod, only : ProfileInit
...
call ProfileInit()
```

The 'appropriate' location might depend on the profiling library used. For example, it might be necessary to invoke this before or after a call to `MPI_Init()`.

ProfileFinalise()

At the end of the program the function `ProfileFinalise()` must be called. It will make sure that the measurements are printed or written to file correctly, and that the profiling tool is closed correctly. Again at this stage it is necessary to manually insert the call at an appropriate location:

```
use profile_mod, only : ProfileFinalise
...
call ProfileFinalise()
```

And again the appropriate location might depend on the profiling library used (e.g. before or after a call to `MPI_Finalize()`).

ProfileStart()/ProfileEnd()

The `ProfileStart` and `ProfileEnd` functions define the beginning and end of a region to be measured. In general it is up to the user what exactly a region is, arbitrary code can be enclosed, as long as it is guaranteed that each call of `ProfileStart` is matched with exactly one corresponding call to `ProfileEnd`. PSyclone supplies one saved (static) variable of type `ProfileData` to each matching Start/End pair.

This is the code sequence which is created by PSyclone:

```
use profile_mod, only : ProfileData, ProfileStart, ProfileEnd
...
type(ProfileData), save :: profiler_data
...
call ProfileStart("Module", "Region", profiler_data)
...
call ProfileEnd(profiler_data)
```

PSyclone guarantees that different ProfileStart/End pairs have different `ProfileData` variables.

Profiling Command Line Options

PSyclone offers two command line options to automatically instrument code with profiling regions. It can create profile regions around a full invoke (including all kernel calls in this invoke), and/or around each individual kernel.

The option `--profile invokes` will automatically add a call to `ProfileStart` and `ProfileEnd` at the beginning and end of every invoke subroutine created by PSyclone. All kernels called within this invoke subroutine will be included in the profiled region.

The option `--profile kernels` will add a call to `ProfileStart` before any loops created by PSyclone, and a `ProfileEnd` call at the end of the loop. Two caveats:

1. In some APIs (for example dynamo when using distributed memory) additional minor code might get included in a profiled kernel section, for example setDirty() calls (expensive calls like HaloExchange are excluded).
2. If loop transforms are applied using a script, the profiling nodes added to the AST will very likely cause errors in the script or in the generated output. As example consider a case where an OMPLoop transform is applied to a loop. With profiling enabled instead of the expected loop there could be a profile node in the AST (with the loop as child). Since an OMP DO directive can only have loops inside, and it now has a call to `ProfileStart`, the generated code is incorrect and will not compile.

In order to avoid the second issue, automatic profiling using `--profile` is not allowed together with a transformation script. On the other hand, since it is possible to write scripts that are more flexible in handling a modified AST, you can use the command line option `--force-profile`. It takes the same parameters as `--profile`, and will allow you to combine a transformation script together with automatic profiling. Use this option at your own risk!

It is also the responsibility of the user to manually add the calls to `ProfileInit` and `ProfileFinalise` to the code base.

PSyclone will modify the schedule of each invoke to insert the profiling regions. Below we show an example of a schedule created when instrumenting invokes - all children of a Profile-Node will be part of the profiling region, including all loops created by PSyclone and all kernel calls:

```
GOSchedule[invoke='invoke_1',Constant loop bounds=True]
    [Profile]
        Loop[type='outer',field_space='cu',it_space='internal_pts']
            Loop[type='inner',field_space='cu',it_space='internal_pts']
                KernCall compute_unew_code(unew_fld,uold_fld,z_fld,cv_fld,h_fld,tdt,
↪dy) [module_inline=False]
        Loop[type='outer',field_space='cv',it_space='internal_pts']
            Loop[type='inner',field_space='cv',it_space='internal_pts']
                KernCall compute_vnew_code(vnew_fld,vold_fld,z_fld,cu_fld,h_fld,tdt,
↪dy) [module_inline=False]
        Loop[type='outer',field_space='ct',it_space='internal_pts']
            Loop[type='inner',field_space='ct',it_space='internal_pts']
                KernCall compute_pnew_code(pnew_fld,pold_fld,cu_fld,cv_fld,tdt,dx,dy)␣
↪[module_inline=False]
```

And now the same schedule when instrumenting kernels. In this case each loop nest and kernel call will be contained in a separate region:

```
GOSchedule[invoke='invoke_1',Constant loop bounds=True]
    [Profile]
        Loop[type='outer',field_space='cu',it_space='internal_pts']
            Loop[type='inner',field_space='cu',it_space='internal_pts']
                KernCall compute_unew_code(unew_fld,uold_fld,z_fld,cv_fld,h_fld,tdt,
↪dy) [module_inline=False]
    [Profile]
        Loop[type='outer',field_space='cv',it_space='internal_pts']
            Loop[type='inner',field_space='cv',it_space='internal_pts']
                KernCall compute_vnew_code(vnew_fld,vold_fld,z_fld,cu_fld,h_fld,tdt,
↪dy) [module_inline=False]
    [Profile]
        Loop[type='outer',field_space='ct',it_space='internal_pts']
            Loop[type='inner',field_space='ct',it_space='internal_pts']
                KernCall compute_pnew_code(pnew_fld,pold_fld,cu_fld,cv_fld,tdt,dx,dy)␣
↪[module_inline=False]
```

Both options can be specified at the same time:

```
GOSchedule[invoke='invoke_1',Constant loop bounds=True]
    [Profile]
        [Profile]
            Loop[type='outer',field_space='cu',it_space='internal_pts']
                Loop[type='inner',field_space='cu',it_space='internal_pts']
                    KernCall compute_unew_code(unew_fld,uold_fld,z_fld,cv_fld,h_fld,
↪tdt,dy) [module_inline=False]
        [Profile]
            Loop[type='outer',field_space='cv',it_space='internal_pts']
                Loop[type='inner',field_space='cv',it_space='internal_pts']
                    KernCall compute_vnew_code(vnew_fld,vold_fld,z_fld,cu_fld,h_fld,
↪tdt,dy) [module_inline=False]
        [Profile]
            Loop[type='outer',field_space='ct',it_space='internal_pts']
                Loop[type='inner',field_space='ct',it_space='internal_pts']
                    KernCall compute_pnew_code(pnew_fld,pold_fld,cu_fld,cv_fld,tdt,dx,
↪dy) [module_inline=False]
```

Profiling in Scripts - ProfileRegionTransform

The greatest flexibility is achieved by using the profiler transformation explicitly in a transformation script. The script takes either a single AST Node or a list of AST Nodes as argument, and will insert a Profile Node into the AST, with the specified nodes as children. At code creation time the listed children will all be enclosed in one profile region. As an example:

```python
from psyclone.transformations import ProfileRegionTrans

t=TransInfo()
p_trans= ProfileRegionTrans()
schedule=psy.invokes.get('invoke_0').schedule
schedule.view()

# Enclose all children within a single profile region
newschedule, _ = p_trans.apply(schedule.children[1:3])
newschedule.view()
```

Warning: It is the responsibility of the user to make sure that a profile region is only created inside a multi-threaded region if the profiling library used is thread-safe!

Interface to Third Party Profiling Tools

PSyclone comes with wrapper libraries to support usage of dl_timer and a simple non-thread-safe timing library. Support for DrHook and TAU will be added in the future.

Any user can create similar wrapper libraries for other profiling tools by providing a corresponding Fortran module. The four profiling calls described in the section about the *ProfilingAPI* must be implemented, and an opaque, user-defined type `ProfileData` needs to be provided in the module.

Note that the `ProfileEnd` call does not have the module or region name as an argument. If this is required by the profiling library, this data must be stored in the `ProfileData` object so that it is available in the `ProfileEnd` call.

The examples in the lib/profiling directory show various ways in which the opaque data type can be used to interface with existing profiling tools - for example by storing an index used by the profiling tool in `ProfileData`, or by storing pointers to the profiling data to be able to print all results in a ProfileFinalise() subroutine.

CHAPTER

FIFTEEN

SYSTEM-SPECIFIC SET-UP

This chapter is split into two sections: *User set-up* describes the setup for a user of PSyclone. It includes all steps necessary to be able to use PSyclone. And while you could obviously do some development, none of the required tools for testing or documentation creation will be installed.

Developer set-up describes the additional installation of all required tools to run tests and create documentation.

Both sections have detailed instructions for Ubuntu 16.04.2 and OpenSUSE 42.2 - if you are working with a different Linux distribution some adjustments will be necessary.

User set-up

This section provides system-specific information on how to set-up your system to use PSyclone for users. It has been tested with a vanilla installation of Ubuntu 16.04.2 and OpenSUSE 42.2. You need a terminal window for entering the commands into.

Installing dependencies

Most required dependencies are installed from the Python Package Index (https://packaging.python.org/installing/) using the program pip ("PIP Installs Packages"). Besides `pip` it is also recommended to install the graphviz package to be able to visualise dependency graphs. This is optional and the associated routine will silently return if the graphviz bindings are not installed.

Installing dependencies on Ubuntu

On Ubuntu `pip` and `graphviz` are installed using `apt-get`. Remember that graphviz is optional and that you'll need to install the graphviz package in addition to the Python bindings.

```
> sudo apt-get install python-pip graphviz
```

Installing dependencies on OpenSUSE

The vanilla OpenSUSE installation includes `pip` for Python 3. Note that the graphviz package is installed by default.

```
> sudo zypper install python-pip
```

Installing PSyclone

Change your working directory to where you would like to place the code and download the latest stable release of PSyclone.

```
> cd <PSYCLONEHOME>
> wget https://github.com/stfc/PSyclone/archive/1.6.0.tar.gz
> gunzip 1.6.0.tar.gz
> tar xf 1.6.0.tar
> rm 1.6.0.tar
> cd PSyclone-1.6.0
> export PYTHONPATH=`pwd`/src:${PYTHONPATH}
> export PATH=`pwd`/bin:${PATH}
```

This sets up your python path and path appropriately. You may want to set these paths permanently (e.g. by editing your ${HOME}/.bashrc file if you run the BASH shell). You can also use the latest version using git, as described in *Installing PSyclone From Git*.

Common installation

To avoid warnings during the dependency installation, it is recommended to update `pip` to the latest version:

```
> sudo pip install --upgrade pip
```

Next you need to install the `fparser` and `pyparsing` packages:

```
> sudo pip install fparser pyparsing
```

Tip: With `pip` it is possible to install packages either system-wide (which requires root privileges) as above, or for a single user only (in ~/.local). While the latter is only useful for one particular user, it means that PSyclone can be installed using `pip` without needing root privileges. In order to install a package for a user, add the –user command line option to all pip commands. This flag requests that the packages be installed locally for the current user rather than requiring root access:

```
> pip install --user fparser pyparsing
```

You may remove the use of `sudo` and add the `--user` option to all pip commands described in this document.

Uninstalling is simply a matter of doing:

```
> sudo pip uninstall fparser pyparsing
```

PSyclone supports the ability to output a schedule dependency graph using the graphviz package. This is optional and the associated routine will silently return if the graphviz bindings are not installed. If you have the graphviz package installed (see especially section *Installing dependencies on Ubuntu* if you are on Ubuntu), you also need to install the python bindings to the graphviz package:

```
> sudo pip install graphviz
```

If you just want to use PSyclone then you've installed all you need and you are ready to go to the getting-going *Run* section.

Developer set-up

This section adds software that is used to develop and test PSyclone. It includes all packages for testing and creation of documentation in html and pdf. We assume you have already installed the software described in the *User set-up* section.

Installing PSyclone From Git

For development it is recommended to get a copy of PSyclone using git to get access to the latest development version.

Installing git for Ubuntu

You need to install the git package:

```
> sudo apt-get install git
```

Installing git on OpenSUSE

You need to install the git package:

```
>> sudo zypper --no-recommends install git
```

Cloning PSyclone using git

Cloning PSyclone from git and setting up your environment is done as follows:

```
> cd <PSYCLONEHOME>
> git clone https://github.com/stfc/PSyclone.git
> cd PSyclone
> pip install --user -e .
```

Note that the "-e" flag causes the project to be installed in 'editable' mode so that any changes to the PSyclone source take effect immediately.

Warning: On OpenSUSE it is necessary to add *$HOME/.local/bin* to your *$PATH* if you have done a user-local install.

Installing documentation tools

Install Sphinx along with bibtex support for creating PSyclone documentation:

```
> sudo pip install sphinx sphinxcontrib.bibtex
```

You can now build html documentation:

```
> cd doc
> make html
```

The latex package is required to create the pdf documentation for PSyclone. Installing the full dependencies can take up several GB, the instructions for Ubuntu and OpenSUSE only install a minimal subset.

Installing LaTeX on Ubuntu

The following three packages need to be installed to create the pdf documentation. It is recommended to install the packages in one `apt-get` command, since otherwise, depending on your filesystem, unnecessary snapshots might be created that take up additional space. The `--no-install-recommends` option significantly reduces the number of installed packages:

```
> sudo apt-get install --no-install-recommends texlive \
texlive-latex-extra latexmk
```

Installing LaTeX on OpenSUSE

The following command installs the minimum number of packages in order to create the pdf documentation - around 130 packages all in all, requiring approximately 300 MB.

Warning: It is important to install the packages in one `zypper` command, since otherwise, depending on your filesystem, unnecessary snapshots might be created after each package, which can add up to several GB of data.

```
> sudo zypper install --no-recommends texlive-latex texlive-latexmk \
texlive-babel-english texlive-cmap texlive-psnfss texlive-fncychap  \
texlive-fancyhdr texlive-titlesec texlive-tabulary texlive-varwidth \
texlive-framed texlive-fancyvrb texlive-float texlive-wrapfig       \
texlive-parskip texlive-upquote texlive-capt-of texlive-needspace   \
texlive-metafont texlive-makeindex texlive-times texlive-helvetic   \
texlive-courier texlive-dvips
```

Creating pdf documentation

You can now build the pdf documentation using

```
> cd doc
> make latexpdf
```

Installing testing tools

The following modules are recommended to get access to testing and formatting tools:

```
> sudo pip install pytest pep8 pylint==1.6.5 pytest-cov pytest-pep8 \
pytest-pylint pytest-flakes pytest-pep257
```

Warning: It appears that the 1.7 series of `pylint` has a bug (at least up to 1.7.2) and does not work properly with PSyclone - it aborts with a "maximum recursion depth exceeded" error message. It is therefore recommended to use version 1.6.5, as specified in the above `pip` command.

You can now run the PSyclone python tests:

```
> cd PSyclone.git
> py.test
```

In order to see whether the Python code conforms to the pep8 standards, use:

```
> pep8 code.py
```

Warning: From release 1.7.1 `pep8` returns a runtime user warning to install and use `pycodestyle` instead.

Verifying the pylint standards is done with:

```
> pylint code.py
```

OK, you're all set up.

CHAPTER

SIXTEEN

CONFIGURATION

PSyclone reads various run-time configuration options from the `psyclone.cfg` file. As described in *Configuration*, the default `psyclone.cfg` configuration file is installed in `<python-base-prefix>/share/psyclone/` during the installation process. (The original version of this file may be found in the `PSyclone/config` directory of the PSyclone distribution.)

At execution-time, PSyclone searches for the configuration file in a number of locations. The ordering of these locations depends upon whether PSyclone is being run within a Python virtual environment (such as `venv`). If no virtual environment is detected then the locations searched, in order, are:

1. `${PWD}/.psyclone/`
2. `${HOME}/.local/share/psyclone/`
3. `<python-base-dir>/share/psyclone/`

where `<python-base-dir>` is the path stored in Python's `sys.prefix`.

If a virtual environment is detected then it is assumed that the `share` directory will be a part of that environment. In order to maintain isolation of distinct virtual environments this directory is then checked *before* the user's home directory. i.e. the list of locations searched is now:

1. `${PWD}/.psyclone/`
2. `<python-base-dir>/share/psyclone/`
3. `${HOME}/.local/share/psyclone/`

If it is desired to use a configuration file in a non-standard location then the search mechanism may be overriden by specifying the (full path to the) configuration file to use via the `PSYCLONE_CONFIG` environment variable. If the specified configuration file is not found then PSyclone will fall back to searching the previously listed locations.

Options

The configuration file is read by the Python ConfigParser class (https://docs.python.org/3/library/configparser.html) and must be formatted accordingly. It currently consists of a `DEFAULT` section e.g.:

```
[DEFAULT]
SUPPORTEDAPIS = gunghoproto, dynamo0.1, dynamo0.3, gocean0.1, gocean1.0
DEFAULTAPI = dynamo0.3
SUPPORTEDSTUBAPIS = dynamo0.3
DEFAULTSTUBAPI = dynamo0.3
DISTRIBUTED_MEMORY = true
REPRODUCIBLE_REDUCTIONS = false
REPROD_PAD_SIZE = 8
```

and a `dynamo0.3` section, e.g.:

```
[dynamo0.3]
COMPUTE_ANNEXED_DOFS = false
```

The meaning of the various entries is described in the following sub-sections.

Note that ConfigParser supports various forms of boolean entry including "true/false", "yes/no" and "1/0". See https://docs.python.org/3/library/configparser.html#supported-datatypes for more details.

`DEFAULT` Section

This section contains entries that are, in principle, applicable to all APIs supported by PSyclone.

Entry	Description
SUPPORTEDAPIS	A comma-separated list of the names of the various APIs that PSyclone supports.
DEFAULTAPI	The API that PSyclone assumes an Algorithm/Kernl conforms to if no API is specified. Must be one of the SUPPORTEDAPIS.
SUPPORTEDSTUBAPIS	Comma-separated list of the APIs that the kernel-stub generator (see *Stub Generation*) supports.
DEFAULTSTUBAPI	The API that the kernel-stub generator assumes by default.
DISTRIBUTED_MEMORY	Whether or not to generate code for distributed-memory parallelism by default. Note that this is currently only supported for the dynamo0.3 API.
REPRODUCIBLE_REDUCTIONS	Whether or not to generate code for reproducible OpenMP reductions (see *Reductions*) by default.
REPROD_PAD_SIZE	If generating code for reproducible OpenMP reductions, this setting controls the amount of padding used between elements of the array in which each thread accumulates its local reduction. (This prevents false sharing of cache lines by different threads.)

`dynamo0.3` Section

This section contains configuration options that are only applicable when using the Dynamo 0.3 API.

Entry	Description
COMPUTE_ANNEXED_DOFS	Whether or not to perform redundant computation over annexed dofs in order to reduce the number of halo exchanges. See *Dof iterators* in the Developers' guide.

CHAPTER

SEVENTEEN

DEVELOPERS' GUIDE

New APIs

TBD

Existing API's

Dynamo0.3

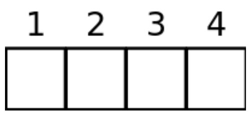
Mesh

The Dynamo0.3 API supports meshes that are unstructured in the horizontal and structured in the vertical. This is often thought of as a horizontal 2D unstructured mesh which is extruded into the vertical. The LFRic infrastructure represents this mesh as a list of 2D cells with a scalar value capturing the number of levels in the vertical "column".

Cells

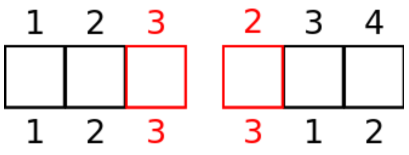
The Dynamo0.3 API currently assumes that all kernels which support iterating over cells work internally on a column of cells. This means that PSyclone need only be concerned with iterating over cell-columns in the horizontal. As a result the LFRic infrastructure presents the mesh information to PSyclone as if the mesh were 2-dimensional. From now on this 2D view will be assumed i.e. a cell will actually be a column of cells. The LFRic infrastructure provides a global 2D cell index from 1 to the number of cells.

For example, a simple quadrilateral element mesh with 4 cells might be indexed in the following way.



When the distributed memory option is switched on in the Dynamo0.3 API (see the *Distributed Memory* Section) the cells in the model are partitioned amongst processors and halo cells are added at the boundaries to a depth determined by the LFRic infrastructure. In this case the LFRic infrastructure maintains the global cell index and adds a unique local cell index from 1 to the number of cells in each partition, including any halo cells.

An example for a depth-1 halo implementation with the earlier mesh split into 2 partitions is given below, with the halo cells being coloured red. An example local indexing scheme is also provided below the cells. Notice the local indexing scheme is set up such that owned cells have lower indices than halo cells.



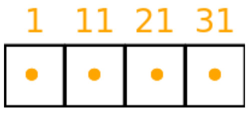
Dofs

In the LFRic infrastructure the degrees-of-freedom (dofs) are indexed from 1 to the total number of dofs. The infrastructure also indexes dofs so that the values in a column are contiguous and their values increase in the vertical. Thus, given the dof indices for the "bottom" cell, the rest of the dof indices can be determined for the column. This set of dof indices for the bottom cell is called a dofmap.

Dofs represent a field's values at various locations in the mesh. Fields can either be continuous or discontinuous. Continuous fields are so named because their values are continuous across cell boundaries. Dofs that represent continuous fields are shared between neighbouring cells. Discontinuous fields have values that are not necessarily related between neighbouring cells (there can be discontinuities across cell boundaries). Dofs that represent discontinuous fields are local to a cell.

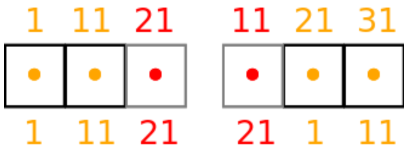
Discontinuous Dofs

A simple example of discontinuous dofs is given below. In this case each cell contains 1 dof and there are 10 cells in a column. We only show the bottom cells and their corresponding dof indices. As explained earlier, the dof indices increase contiguously up the column, so the cell above the cell containing dof index 1 contains dof index 2 and the cell above that contains dof index 3 etc.



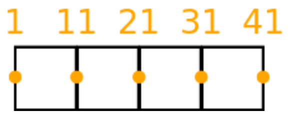
As discussed in the previous section, when the distributed memory option is switched on in the Dynamo0.3 API (see the *Distributed Memory* Section) the cells in the model are partitioned amongst processors and halo cells are added at the boundaries to a depth determined by the LFRic infrastructure. This results in the dofs being replicated in the halo cells, leading to a dof halo. As for cells, the LFRic infrastructure maintains the global dof indexing scheme and adds a local dof indexing scheme from 1 to the number of dofs in each partition, including any halo dofs.

An example for a depth-1 halo implementation with the earlier mesh split into 2 partitions is given below, with the halo cells drawn in grey and halo dofs coloured red. An example local partition indexing scheme is also provided below the dofs. As with cells, notice the local indexing scheme ensures that owned dofs have lower indices than halo dofs.



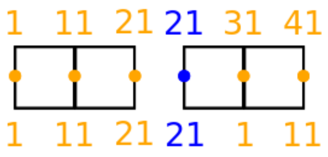
Continuous Dofs

A simple continuous dof example is given below for the same mesh as before. In this case dofs are on cell edges in the horizontal and there are 10 cells in a column. Again we only show the bottom cells and their corresponding dof indices. As explained earlier, the dof indices increase contiguously up the column, so the cell above the cell containing dof index 1 contains dof index 2 and the cell above that contains dof index 3 etc.

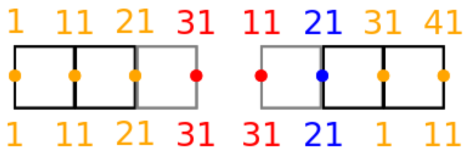


As already explained, when the distributed memory option is switched on in the Dynamo0.3 API (see the *Distributed Memory* Section) the cells in the model are partitioned amongst processors and halo cells are added at the boundaries.

In the example below we ignore the additional halo cells and just look at the partitioning of cells amongst processors (with the same mesh and 2 partitions as shown earlier). It can be seen that the dofs shared between cells which are on different partitions now need to be replicated if fields on continuous dofs are going to be able to be computed locally on each partition. This concept is different to halos as there are no halo cells here, the fact that the cells are partitioned has meant that continuous dofs on the edge of the partition are replicated. The convention used in Dynamo0.3 is that the cell with the lowest global id determines which partition owns a dof and which has the copy. Dofs which are copies are called *annexed*. Annexed dofs are coloured blue in the example:



If we now extend the above example to include the halo cells (coloured grey) then we get:



An example for a depth-1 halo implementation with the earlier mesh split into 2 partitions is given below, with the halo cells drawn in grey and halo dofs coloured red. An example local indexing scheme is also provided below the dofs. Notice the local indexing scheme ensures that owned dofs have lower indices than annexed dofs, which in turn have lower indices than halo dofs.

Cell and Dof Ordering

Cells in a partition are sequentially indexed by the LFRic infrastructure, starting at 1, so that local cells occur first, then level-1 halo cells, then level-2 halo cells etc. A benefit of this layout is that it makes it easy for PSyclone to specify the required iteration space for cells as a single range, allowing a single Fortran do loop (or other language construct as required) to be generated. The LFRic infrastructure provides an API that returns the index of the last owned cell, the index of the last halo cell at a particular depth and the index of the last halo cell, to support PSyclone code generation.

Dofs on a partition are also sequentially indexed by the LFRic infrastructure, starting at 1, so that local dofs occur first, then annexed dofs (if the field is continuous), then level-1 halo dofs, then level-2 halo dofs etc. Again, this layout makes it easy for PSyclone to specify the required iteration space for dofs as a single range. As before, the LFRic infrastructure provides an API that returns the index of the last owned dof, the index of the last annexed dof, the index of the last halo dof at a particular depth and the index of the last halo dof, to support PSyclone code generation.

Loop iterators

In the current implementation of the Dynamo0.3 API it is possible to iterate (loop) either over cells or dofs. At the moment all coded kernels are written to iterate over cells and all builtin kernels are written to iterate over dofs, but that does not have to be the case.

The loop iteration information is specified in the kernel metadata. In the case of builtin's there is kernel metadata but it is part of PSyclone and is specified in *src/psyclone/dynamo0p3_builtins_mod.f90*.

Cell iterators: Continuous

When a kernel is written to iterate over cells and modify a continuous field, PSyclone always computes dofs on owned cells and redundantly computes dofs in the level-1 halo. Users can apply a redundant computation transformation to increase the halo depth for additional redundant computation but it must always at least compute the level-1 halo. The reason for this is to ensure that the shared dofs on cells on the edge of the partition (both owned and annexed) are always correctly computed. Note that the outermost halo dofs are not correctly computed and therefore the outermost halo of the modified field is dirty after redundant computation. Also note that if we do not know whether a modified field is discontinuous or continuous then we must assume it is continuous.

An alternative solution could have been adopted in Dynamo0.3 whereby no redundant computation is performed and partial-sum results are shared between processors in a communication pattern similar to halo exchanges. However, a decision was made to always perform redundant computation.

A downside of performing redundant computation in the level-1 halo is that any fields being read by the kernel must have their level-1 halo clean (up-to-date), which can result in halo exchanges. Note that this is not the case for the modified field, it does not need its halo to be clean, however, at the moment a halo exchange is added in this case. This unecessary halo exchange will be removed in a future release of PSyclone.

Cell iterators: Discontinuous

When a kernel is written to iterate over cells and modify a discontinuous field, PSyclone only needs to compute dofs on owned cells. Users can apply a redundant computation transformation to redundantly compute into the halo but this is not done by default.

Dof iterators

When a kernel that is written to iterate over dofs modifies a field, PSyclone must ensure that all dofs in that field are updated. If the distributed memory flag is set to `false` then PSyclone must iterate over all dofs. PSyclone simply needs to create a loop that iterates from 1 to the total number of dofs. The latter value is provided by the LFRic API.

If the distributed memory flag is set to `true` then PSyclone must ensure that each partition only iterates over owned dofs. Again PSyclone just needs to create a loop that iterates from 1 to the total number of owned dofs on that partition. The latter value is provided by the LFRic API.

When the distributed memory flag is set to `true` an aditional configuration option can be set which makes PSyclone always create loops which iterate over both owned and annexed dofs. Whilst this is not necessary for correctness, it can improve performance by reducing the number of halo exchanges required (at the expense of computing annexed dofs redundantly). The only change for PSyclone is that it calls a different LFRic routine which returns the index of the last annexed dof. This iteration space will necessarily also include all owned dofs due to the ordering of dof indices discussed earlier.

The configuration variable is called *COMPUTE_ANNEXED_DOFS* and is found in the the *dynamo0.3* section of the *psyclone.cfg* configuration file (see *Configuration*). If it is `true` then annexed dofs are always computed in loops that iterate over dofs and if it is `false` then annexed dofs are not computed. The default in PSyclone is `false`.

The computation of annexed dofs could have been added as a transformation optimisation. The reason for using a configuration switch is that it is then guaranteed that annexed dofs are always computed for loops that iterate over dofs which then allows us to always remove certain halo exchanges without needing to add any new ones.

If we first take the situation where annexed dofs are not computed for loops that iterate over dofs i.e. (*COMPUTE_ANNEXED_DOFS* is `false`), then a field's annexed dofs will be dirty (out-of-date) after the loop has completed. If a following kernel needs to read the field's annexed dofs, then PSyclone will need to add a halo exchange to make them clean.

There are 3 cases to consider:

1. the field is read in a loop that iterates over dofs,
2. the field is read in a loop that iterates over owned cells and level-1 halo cells, and
3. the field is read in a loop that iterates over owned cells

In case 1) the annexed dofs will not be read as the loop only iterates over owned dofs so a halo exchange is not required. In case 2) the full level-1 halo will be read (including annexed dofs) so a halo exchange is required. In case 3) the annexed dofs will be read so a halo exchange will be required.

If we now take the case where annexed dofs are computed for loops that iterate over dofs (*COMPUTE_ANNEXED_DOFS* is `true`) then a field's annexed dofs will be clean after the loop has completed. If a following kernel needs to read the field's annexed dofs, then PSyclone will no longer need a halo exchange.

We can now guarantee that annexed dofs will always be clean after a continuous field has been modified by a kernel. This is because loops that iterate over either dofs or cells now compute annexed dofs and there are no other ways for a continuous field to be updated.

We now consider the same three cases. In case 1) the annexed dofs will now be read, but annexed dofs are guaranteed to be clean, so no halo exchange is required. In case 2) the full level-1 halo is read so a halo exchange is still required. Note, as part of this halo exchange we will update annexed dofs that are already clean. In case 3) the annexed dofs will be read but a halo exchange is not required as the annexed dofs are guaranteed to be clean.

Therefore no additional halo exchanges are required when *COMPUTE_ANNEXED_DOFS* is changed from `false` to `true` i.e. case 1) does not require a halo exchange in either situation and case 2) requires a halo exchange in both situations. We also remove halo exchanges for case 3) so the number of halo exchanges may be reduced.

If a switch were not used and it were possible to use a transformation to selectively perform computation over annexed dofs for loops that iterate over dofs, then we would no longer be able to guarantee that annexed dofs would always be clean. In this situation, if the dofs were known to be dirty then PSyclone would need to add a halo exchange and if it were unknown whether the dofs were dirty or not, then a halo exchange would need to be added that uses the run-time flags to determine whether a halo exchange is required. As run-time flags are based on whether the halo is dirty or not (not annexed dofs) then a halo exchange would be performed if the halo were dirty, even if the annexed dofs were clean, potentially resulting in more halo exchanges than are necessary.

Halo Exchange Logic

Halo exchanges are required when the *DISTRIBUTED_MEMORY* flag is set to `true` in order to make sure any accesses to a field's halo or to its annexed dofs receive the correct value.

Operators and Halo Exchanges

Halo Exchanges are only created for fields. This causes an issue for operators. If a loop iterates over halos to a given depth and the loop includes a kernel that reads from an operator then the operator must have valid values in the halos to that depth. In the current implementation of PSyclone all loops which write to, or update an operator are computed redundantly in the halo up to depth-1 (see the *load()* method in the *DynLoop* class). This implementation therefore requires a check that any loop which includes a kernel that reads from an operator is limited to iterating in the halo up to depth-1. PSyclone will raise an exception if an optimisation attempts to increase the iteration space beyond this (see the *gen_code()* method in the *DynKern* class).

To alleviate the above restriction one could add a configurable depth with which to compute operators e.g. operators are always computed up to depth-2, or perhaps up to the maximum halo depth. An alternative would be to halo exchange operators as required in the same way that halo exchanges are used for fields.

First Creation

When first run, PSyclone creates a separate schedule for each of the invokes found in the algorithm layer. A schedule includes all required loops and kernel calls that need to be generated in the PSy layer for the particular invoke call. Once the loops and kernel calls have been created then (if the *DISTRIBUTED_MEMORY* flag is set to `true`) PSyclone adds any required halo exchanges and global sums. This work is all performed in the *DynInvoke* constructor (*__init__*) method.

In PSyclone we apply a lazy halo exchange approach (as opposed to an eager one), adding a halo exchange just before it is required.

It is simple to determine where halo exchanges should be added for the initial schedule. There are three cases:

1. loops that iterate over cells and modify a continuous field will access the level-1 halo. This means that any field that is read within such a loop must have its level-1 halo clean and therefore requires a halo exchange. Note, at the moment PSyclone adds a halo exchange for the modified field (as it is specified as *GH_INC* which requires a read before a write), however this is not required if there is only one field updated in the kernel. This is because we only care about updating owned and annexed dofs, therefore it does not matter what the values of any halo dofs are.
2. continuous fields that are read from within loops that iterate over cells and modify a discontinuous field must have their annexed dofs clean. Currently the only way to make annexed dofs clean is to perform a halo exchange. If the *COMPUTE_ANNEXED_DOFS* configuration variable is set to `true` then no halo exchange is required as annexed dofs will always be clean. If the *COMPUTE_ANNEXED_DOFS* configuration variable is set to `false` then a halo exchange must be added if the previous modification of the field is known to be from within a loop over dofs, or if the previous modification of the field is unknown (i.e. outside the invoke) as the previous modification may have been from within a loop over dofs.
3. fields that have a stencil access will access the halo and need halo exchange calls added.

Halo exchanges are created separately (for fields with halo reads) for each loop by calling the *create_halo_exchanges()* method within the *DynLoop* class.

In the situation where a field's halo is read in more than one kernel in different loops, we do not want to add too many halo exchanges - one will be enough as long as it is placed correctly. To avoid this problem we add halo exchange calls for loops in the order in which they occur in the schedule. A halo exchange will be added before the first loop for a field but the same field in the second loop will find that there is a dependence on the previously inserted halo exchange so no additional halo exchange will be added.

The algorithm for adding the necessary halo exchanges is as follows: For each loop in the schedule, the *create_halo_exchanges()* method iterates over each field that reads from its halo (determined by the *unique_fields_with_halo_reads()* method in the *DynLoop* class).

For each field we then look for its previous dependencies (the previous writer(s) to that field) using PSyclone's dependence analysis. Three cases can occur: 1) there is no dependence, 2) there are multiple dependencies and 3) there is one dependence.

1. If no previous dependence is found then we add a halo exchange call before the loop (using the internal helper method *_add_halo_exchange()*). If the field is a vector field then a halo exchange is added for each component. The internal helper method *_add_halo_exchange* itself uses the internal helper method *_add_halo_exchange_code()*. This method creates an instance of the *DynHaloExchange* class for the field in question and adds it to the schedule before the loop. You might notice that this method then checks that the halo exchange is actually required and removes it again if not. In our current situation the halo exchange will always be needed so this check is not required but in more complex situations after transformations have been applied to the schedule this may not be the case. We discuss this type of situation later.
2. If multiple previous dependencies are found then the field must be a vector field as this is the only case where this can occur. We then choose the closest one and treat it as a single previous dependency (see 3).

3. If a single previous dependency is found and it is a halo exchange then we do nothing, as it is already covered. This will only happen when more than one reader depends on a writer, as discussed earlier. If the dependence is not a halo exchange then we add one.

After completing the above we have all the halo exchanges required for correct execution.

Note that we do not need to worry about halo depth or whether a halo is definitely required, or whether it might be required, as this is determined by the halo exchange itself at code generation time. The reason for deferring this information is that it can change as transformations are added.

Modifying the Schedule

Transformations modify the schedule. At the moment only one of these transformations - the *Dynamo0p3RedundantComputationTrans* class in *transformations.py* - affects halo exchanges. This transformation can mean there is a requirement for new halo exchanges, it can mean existing halo exchanges are no longer required and it can mean that the properties of a halo exchange (e.g. depth) can change.

The redundant computation transformation is applied to a loop in a schedule. When this is done the *update_halo_exchanges()* method for that loop is called - see the *apply()* method in *Dynamo0p3RedundantComputationTrans*.

The first thing that the *update_halo_exchanges()* method does is call the *create_halo_exchanges()* method to add in any new halo exchanges that are required before this loop, due to any fields that now have a read access to their halo when they previously did not. For example, a loop containing a kernel that writes to a certain field might previously have iterated up to the number of owned cells in a partition (*ncells*) but now iterates up to halo depth 1.

However, a field that has its halo read no longer guarantees that a halo exchange is required, as the previous dependence may now compute redundantly to halo depth 2, for example. The solution employed in *create_halo_exchanges()* is to add a halo exchange speculatively and then remove it if it is not required. The halo exchange itself determines whether it is required or not via the *required()* method. The removal code is found at the end of the *_add_halo_exchange_code()* method in the *DynLoop()* class.

The second thing that the *update_halo_exchanges()* method does is check that any halo exchanges after this loop are still required. It finds all relevant halo exchanges, asks them if they are required and if they are not it removes them.

We only need to consider adding halo exchanges before the loop and removing halo exchanges after the loop. This is because redundant computation can only increase the depth of halo to which a loop computes so can not remove existing halo exchanges before a loop (as an increase in depth will only increase the depth of an existing halo exchange before the loop) or add existing halo exchanges after a loop (as an increase in depth will only make it more likely that a halo exchange is no longer required after the loop).

GOcean1.0

TBD

Modules

This section describes the functionality of the various Python modules that make up PSyclone.

f2pygen

f2pygen provides functionality for generating Fortran code from scratch (i.e. when not modifying existing source).

Variable Declarations

Three different classes are provided to support the creation of variable declarations (for intrinsic, character and derived-type variables). An example of their use might be:

```
>>> from psyclone.f2pygen import ModuleGen, SubroutineGen, DeclGen, \
CharDeclGen, TypeDeclGen
>>> module = ModuleGen(name="testmodule")
>>> sub = SubroutineGen(module, name="testsubroutine")
>>> module.add(sub)
>>> sub.add(DeclGen(sub, datatype="integer", entity_decls=["my_int"]))
>>> sub.add(CharDeclGen(sub, length="10", entity_decls=["my_char"]))
>>> sub.add(TypeDeclGen(sub, datatype="field_type", entity_decls=["ufld"]))
>>> gen = str(module.root)
>>> print(gen)
  MODULE testmodule
    IMPLICIT NONE
    CONTAINS
    SUBROUTINE testsubroutine()
      TYPE(field_type) ufld
      CHARACTER(LEN=10) my_char
      INTEGER my_int
    END SUBROUTINE testsubroutine
  END MODULE testmodule
```

The full interface to each of these classes is detailed below:

class `psyclone.f2pygen.`**`DeclGen`**(*parent*, *datatype=''*, *entity_decls=None*, *intent=''*, *pointer=False*, *kind=''*, *dimension=''*, *allocatable=False*, *save=False*, *target=False*, *initial_values=None*)

Generates a Fortran declaration for variables of various intrinsic types (integer, real and logical). For character variables CharDeclGen should be used.

Parameters

- **`parent`** (`psyclone.f2pygen.BaseGen.`) – node to which to add this declaration as a child.
- **`datatype`** (*`str`*) – the (intrinsic) type for this declaration.
- **`entity_decls`** (`list`) – list of variable names to declare.
- **`intent`** (*`str`*) – the INTENT attribute of this declaration.
- **`pointer`** (*`bool`*) – whether or not this is a pointer declaration.
- **`kind`** (*`str`*) – the KIND attribute to use for this declaration.
- **`dimension`** (*`str`*) – the DIMENSION specifier (i.e. the xx in DIMENSION(xx)).
- **`allocatable`** (*`bool`*) – whether this declaration is for an ALLOCATABLE quantity.
- **`save`** (*`bool`*) – whether this declaration has the SAVE attribute.
- **`target`** (*`bool`*) – whether this declaration has the TARGET attribute.
- **`initial_values`** (*`list of str with same no. of elements as entity_decls.`*) – Initial value to give each variable.

Raises **`RuntimeError`** – if datatype is not one of DeclGen.SUPPORTED_TYPES.

class `psyclone.f2pygen.`**`CharDeclGen`**(*parent*, *entity_decls=None*, *intent='‘*, *pointer=False*, *kind='‘*, *dimension='‘*, *allocatable=False*, *save=False*, *target=False*, *length='‘*, *initial_values=None*)

Generates a Fortran declaration for character variables.

Parameters

- **`parent`** (`psyclone.f2pygen.BaseGen`.) – node to which to add this declaration as a child.
- **`entity_decls`** (`list`) – list of variable names to declare.
- **`intent`** (*`str`*) – the INTENT attribute of this declaration.
- **`pointer`** (*`bool`*) – whether or not this is a pointer declaration.
- **`kind`** (*`str`*) – the KIND attribute to use for this declaration.
- **`dimension`** (*`str`*) – the DIMENSION specifier (i.e. the xx in DIMENSION(xx)).
- **`allocatable`** (*`bool`*) – whether this declaration is for an ALLOCATABLE quantity.
- **`save`** (*`bool`*) – whether this declaration has the SAVE attribute.
- **`target`** (*`bool`*) – whether this declaration has the TARGET attribute.
- **`length`** (*`str`*) – expression to use for the (len=xx) selector.
- **`initial_values`** (*`list of str with same no. of elements as entity_decls. Each of these can be either a variable name or a literal, quoted string (e.g. "'hello'")`*) – Initial value to give each variable.

class `psyclone.f2pygen.`**`TypeDeclGen`**(*parent*, *datatype='‘*, *entity_decls=None*, *intent='‘*, *pointer=False*, *dimension='‘*, *allocatable=False*, *save=False*, *target=False*)

Generates a Fortran declaration for variables of a derived type.

Parameters

- **`parent`** (`psyclone.f2pygen.BaseGen`) – node to which to add this declaration as a child
- **`datatype`** (*`str`*) – the type for this declaration
- **`entity_decls`** (`list`) – list of variable names to declare
- **`intent`** (*`str`*) – the INTENT attribute of this declaration
- **`pointer`** (*`bool`*) – whether or not this is a pointer declaration
- **`dimension`** (*`str`*) – the DIMENSION specifier (i.e. the xx in DIMENSION(xx))
- **`allocatable`** (*`bool`*) – whether this declaration is for an ALLOCATABLE quantity
- **`save`** (*`bool`*) – whether this declaration has the SAVE attribute
- **`target`** (*`bool`*) – whether this declaration has the TARGET attribute

Configuration

PSyclone uses the Python `ConfigParser` class (https://docs.python.org/3/library/configparser.html) for reading the configuration file. This is managed by the `psyclone.configuration` module which provides the `ConfigFactory` and `Config` classes. The former's constructor creates a singleton `Config` instance and stores it for return by any future calls to `create`:

class `psyclone.configuration.`**`ConfigFactory`**(*config_file=None*)

Create our singleton Config object. If config_file is specified then we throw-away the old Config and create a new one.

Parameters **`config_file`** (*`str`*) – Specific configuration file to use when creating the Config object.

static **`create`**()

Returns the singleton Config instance

Return type `psyclone.config.Config`

The `Config` class is responsible for finding the configuration file (if no filename is passed to the constructor), parsing it and then storing the various configuration options. It also performs some basic consistency checks on the values it obtains from the configuration file.

Since the default PSyclone API to use is read from the configuration file, it is not possible to have API-specifc sub-classes of `Config` as we don't know which API is in use before we read the file. However, the configuration file can contain API-specific settings. These are placed in separate sections, named for the API to which they apply, e.g.:

```
[dynamo0.3]
COMPUTE_ANNEXED_DOFS = false
```

Having parsed and stored the options from the default section of the configuration file, the `Config` constructor then creates a dictionary using the list of supported APIs to provide the keys. The configuration file is then checked for API-specific sections (again using the API names from the default section) and, if any are found, an API-specifc sub-class is created using the parsed entries from the corresponding section. The resulting object is stored in the dictionary under the appropriate key. The API-specific values may then be accessed as, e.g.:

```
config.api("dynamo0.3").compute_annexed_dofs
```

The API-specific sub-classes exist to provide validation/type-checking and encapsulation for API-specific options. They do not sub-class `Config` directly but store a reference back to the `Config` object to which they belong.

OpenACC Support

PSyclone is able to generate code for execution on a GPU through the use of OpenACC. Support for generating OpenACC code is implemented via *Transformations*. The specification of parallel regions and loops is very similar to that in OpenMP and does not require any special treatment. However, a key feature of GPUs is the fact that they have their own, on-board memory which is separate from that of the host. Managing (i.e. minimising) data movement between host and GPU is then a very important part of obtaining good performance.

Since PSyclone operates at the level of Invokes it has no information about when an application starts and thus no single place in which to initiate data transfers to a GPU. (We assume that the host is responsible for model I/O and therefore for populating fields with initial values.) Fortunately OpenACC provides support for this kind of situation with the `enter data` directive. This may be used to "define scalars, arrays and subarrays to be allocated in the current device memory for the remaining duration of the program" *[ope17]*. The `ACCDataTrans` transformation adds an `enter data` directive to an Invoke:

class `psyclone.transformations.`**`ACCDataTrans`**

Adds an OpenACC "enter data" directive to a Schedule. For example:

```
>>> from psyclone.parse import parse
>>> from psyclone.psyGen import PSyFactory
>>> api = "gocean1.0"
>>> filename = "nemolite2d_alg.f90"
>>> ast, invokeInfo = parse(filename, api=api, invoke_name="invoke")
>>> psy = PSyFactory(api).create(invokeInfo)
>>>
>>> from psyclone.psyGen import TransInfo
>>> t = TransInfo()
>>> dtrans = t.get_trans_name('ACCDataTrans')
>>>
>>> schedule = psy.invokes.get('invoke_0').schedule
>>> schedule.view()
>>>
>>> # Add an enter-data directive
>>> newschedule, _ = dtrans.apply(schedule)
>>> newschedule.view()
```

The resulting generated code will then contain an `enter data` directive protected by an `IF(this is the first time in this Invoke)` block, e.g. (for the GOcean1.0 API):

```
! Ensure all fields are on the device and
! copy them over if not.
IF (first_time) THEN
  !$acc enter data  &
  !$acc& copyin(sshn_t,sshn_t%data,un%grid,un%grid%tmask,...)
  first_time = .false.
  ssha_t%data_on_device = .true.
  ...
```

Note that the `IF` block is not strictly required as the OpenACC run-time identifies when a reference is already on the device and does not copy it it over again. However, when profiling an application, it was seen that there was a small overhead associated with doing the `enter data`, even when the data was already on the device. The `IF` block eliminates this.

Of course, a given field may already be on the device (and have been updated) due to a previous Invoke. In this case, the fact that the OpenACC run-time does not copy over the now out-dated host version of the field is essential for correctness.

BIBLIOGRAPHY

[ope17] *The OpenACC Application Programming Interface, Version 2.6*. 2017.

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