# OPS C++ User's Manual

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#### 1 Introduction

OPS is a high-level framework with associated libraries and preprocessors to generate parallel executables for applications on **multi-block structured grids**. Multi-block structured grids consists of an unstructured collection of structured meshes/grids. This document describes the OPS C++ API, which supports the development of single-block and multi-block structured meshes.

Many of the API and library follows the structure of the OP2 high-level library for unstructured mesh applications [1]. However the structured mesh domain is distinct from the unstructured mesh applications domain due to the implicit connectivity between neighbouring mesh elements (such as vertices, cells) in structured meshes/grids. The key idea is that operations involve looping over a "rectangular" multi-dimensional set of grid points using one or more "stencils" to access data. In multi-block grids, we have several structured blocks. The connectivity between the faces of different blocks can be quite complex, and in particular they may not be oriented in the same way, i.e. an i, j face of one block may correspond to the j, k face of another block. This is awkward and hard to handle simply.

To clarify some of the important issues in designing the API, we note here some needs connected with a 3D application:

- When looping over the interior with loop indices i, j, k, often there are 1D arrays which are referenced using just one of the indices.
- To implement boundary conditions, we often loop over a 2D face, accessing both the 3D dataset and data from a 2D dataset.
- To implement periodic boundary conditions using dummy "halo" points, we sometimes have to copy one plane of boundary data to another. e.g. if the first dimension has size I then we might copy the plane i = I 2 to plane i = 0, and plane i = 1 to plane i = I 1.
- In multigrid, we are working with two grids with one having twice as many points as the other in each direction. To handle this we require a stencil with a non-unit stride.
- In multi-block grids, we have several structured blocks. The connectivity between the faces of different blocks can be quite complex, and in particular they may not be oriented in the same way, i.e. an i, j face of one block may correspond to the j, k face of another block. This is awkward and hard to handle simply.

The latest proposal is to handle all of these different requirements through stencil definitions.

## 2 Key concepts and structure

An OPS application can generally be divided into two key parts: initialisation and parallel execution. During the initialisation phase, one or more blocks (ops\_block) are defined: these only have a dimensionality (i.e. 1D, 2D, etc.), and serve to group datasets together. Datasets are defined on a block, and have a specific size (in each dimension of the block), which may be slightly different across different datasets (e.g. staggered grids), in some directions they may be degenerate (a size of 1), or they can represent data associated with different multigrid levels (where their size if a multiple or a fraction of other datasets). Datasets can be declared with empty (NULL) pointers, then OPS will allocate the appropriate amount of memory, may be passed non-NULL pointers (currently only supported in non-MPI environments), in which case OPS will assume the memory is large enough for the data and the block halo, and there are HDF5 dataset declaration routines

which allow the distributed reading of datasets from HDF5 files. The concept of blocks is necessary to group datasets together, as in a multi-block problem, in a distributed memory environment, OPS needs to be able to determine how to decompose the problem.

The initialisation phase usually also consists of defining the stencils to be used later on (though they can be defined later as well), which describe the data access patterns used in parallel loops. Stencils are always relative to the "current" point; e.g. if at iteration (i,j), we wish to access (i-1,j) and (i,j), then the stencil will have two points:  $\{(-1,0),(0,0)\}$ . To support degenerate datasets (where in one of the dimensions the dataset's size is 1), as well as for multigrid, there are special strided, restriction, and prolongation stencils: they differ from normal stencils in that as one steps through a grid in a parallel loop, the stepping is done with a non-unit stride for these datasets. For example, in a 2D problem, if we have a degenerate dataset called xcoords, size (N,1), then we will need a stencil with stride (1,0) to access it in a regular 2D loop.

Finally, the initialisation phase may declare a number of global constants - these are variables in global scope that can be accessed from within user kernels, without having to pass them in explicitly. These may be scalars or small arrays, generally for values that do not change during execution, though they may be updated during execution with repeated calls to <code>ops\_decl\_const</code>.

The initialisation phase is terminated by a call to ops\_partition.

The bulk of the application consists of parallel loops, implemented using calls to <code>ops\_par\_loop</code>. These constructs work with datasets, passed through the opaque <code>ops\_dat</code> handles declared during the initialisation phase. The iterations of parallel loops are semantically independent, and it is the responsibility of the user to enforce this: the order in which iterations are executed cannot affect the result (within the limits of floating point precision). Parallel loops are defined on a block, with a prescribed iteration range that is always defined from the perspective of the dataset written/modified (the sizes of datasets, particularly in multigrid situations, may be very different). Datasets are passed in using <code>ops\_arg\_dat</code>, and during execution, values at the current grid point will be passed to the user kernel. These values are passed wrapped in a templated <code>ACC<></code> object (templated on the type of the data), whose parentheses operator is overloaded, which the user must use to specify the relative offset to access the grid point's neighbours (which accesses have to match the declared stencil). Datasets written may only be accessed with a one-point, zero-offset stencil (otherwise the parallel semantics may be violated).

Other than datasets, one can pass in read-only scalars or small arrays that are iteration space invariant with ops\_arg\_gbl (typically weights,  $\delta t$ , etc. which may be different in different loops). The current iteration index can also be passed in with ops\_arg\_idx, which will pass a globally consistent index to the user kernel (i.e. also under MPI).

Reductions in loops are done using the ops\_arg\_reduce argument, which takes a reduction handle as an argument. The result of the reduction can then be acquired using a separate call to ops\_reduction\_result. The semantics are the following: a reduction handle after it was declared is in an "uninitialised" state. The first time it is used as an argument to a loop, its type is determined (increment/min/max), and is initialised appropriately  $(0, \infty, -\infty)$ , and subsequent uses of the handle in parallel loops are combined together, up until the point, where the result is acquired using ops\_reduction\_result, which then sets it back to an uninitialised state. This also implies, that different parallel loops, which all use the same reduction handle, but are otherwise independent, are independent and their partial reduction results can be combined together associatively and commutatively.

OPS takes responsibility for all data, its movement and the execution of parallel loops. With different execution hardware and optimisations, this means OPS will re-organise data as well as execution (potentially across different loops), and therefore any data accesses or manipulation may only be done through the OPS API.

### $3 \quad OPS C++ API$

#### 3.1 Initialisation declaration and termination routines

### void ops\_init(int argc, char \*\*argv, int diags\_level)

This routine must be called before all other OPS routines.

argc, argv the usual command line arguments

diags\_level an integer which defines the level of debugging diagnostics and reporting to

be performed

Currently, higher diags\_levels does the following checks

 $diags\_level = 1$ : no diagnostics, default to achieve best runtime performance.

diags\_level > 1: print block decomposition and ops\_par\_loop timing breakdown.

diags\_level > 4: print intra-block halo buffer allocation feedback (for OPS internal development only)

diags\_level > 5 : check if intra-block halo MPI sends depth match MPI receives depth (for OPS internal development only)

### ops\_block ops\_decl\_block(int dims, char \*name)

This routine defines a structured grid block.

dims dimension of the block

name a name used for output diagnostics

#### ops\_block ops\_decl\_block\_hdf5(int dims, char \*name, char \*file)

This routine reads the details of a structured grid block from a named HDF5 file

dims dimension of the block

name a name used for output diagnostics

file hdf5 file to read and obtain the block information from

Although this routine does not read in any extra information about the block from the named HDF5 file than what is already specified in the arguments, it is included here for error checking (e.g. check if blocks defined in an HDF5 file is matching with the declared arguments in an application) and completeness.

ops\_dat ops\_decl\_dat(ops\_block block, int dim, int\* size, int \*base, int \*d\_m, int \*d\_p, T \*data, char \*type, char \*name)

This routine defines a dataset.

block	structured block
dim	dimension of dataset (number of items per grid element)
size	size in each dimension of the block
base	base indices in each dimension of the block
$\mathtt{d}_{-\mathtt{m}}$	padding from the face in the negative direction for each dimension (used for block halo) $$
d_p	padding from the face in the positive direction for each dimension (used for block halo)
data	input data of type T
type	the name of type used for output diagnostics (e.g. "double", "float")

The **size** allows to declare different sized data arrays on a given **block**. d\_m and d\_p are depth of the "block halos" that are used to indicate the offset from the edge of a block (in both the negative and positive directions of each dimension).

a name used for output diagnostics

name

# ops\_dat ops\_decl\_dat\_hdf5(ops\_block block, int dim, char \*type, char \*name, char \*file) This routine defines a dataset to be read in from a named hdf5 file

block	structured block
dim	dimension of dataset (number of items per grid element)
type	the name of type used for output diagnostics (e.g. "double", "float")
name	name of the dat used for output diagnostics
file	hdf5 file to read and obtain the data from

### void ops\_decl\_const(char const \* name, int dim, char const \* type, T \* data )

This routine defines a global constant: a variable in global scope. Global constants need to be declared upfront so that they can be correctly handled for different parallelizations. For e.g CUDA on GPUs. Once defined they remain unchanged throughout the program, unless changed by a call to ops\_update\_const(..)

name	a name used to identify the constant
dim	dimension of dataset (number of items per element)
type	the name of type used for output diagnostics (e.g. "double", "float")
data	pointer to input data of type T

## void ops\_update\_const(char const \* name, int dim, char const \* type, T \* data)

This routine updates/changes the value of a constant

name a name used to identify the constant

dim dimension of dataset (number of items per element)

type the name of type used for output diagnostics (e.g. "double", "float")

data pointer to new values for constant of type T

# ops\_halo ops\_decl\_halo(ops\_dat from, ops\_dat to, int \*iter\_size, int\* from\_base, int \*to\_base, int \*from\_dir, int \*to\_dir)

This routine defines a halo relationship between two datasets defined on two different blocks.

from origin dataset

to destination dataset

iter\_size defines an iteration size (number of indices to iterate over in each direction)

from\_base indices of starting point in "from" dataset to\_base indices of starting point in "to" dataset

from\_dir direction of incrementing for "from" for each dimension of iter\_size
to\_dir direction of incrementing for "to" for each dimension of iter\_size

A from\_dir [1,2] and a to\_dir [2,1] means that x in the first block goes to y in the second block, and y in first block goes to x in second block. A negative sign indicates that the axis is flipped. (Simple example: a transfer from (1:2,0:99,0:99) to (-1:0,0:99,0:99) would use iter\_size = [2,100,100], from\_base = [1,0,0], to\_base = [-1,0,0], from\_dir = [0,1,2], to\_dir = [0,1,2]. In more complex case this allows for transfers between blocks with different orientations.)

#### ops\_halo ops\_decl\_halo\_hdf5(ops\_dat from, ops\_dat to, char\* file)

This routine reads in a halo relationship between two datasets defined on two different blocks from a named HDF5 file

from origin dataset

to destination dataset

file hdf5 file to read and obtain the data from

#### ops\_halo\_group ops\_decl\_halo\_group(int nhalos, ops\_halo \*halos)

This routine defines a collection of halos. Semantically, when an exchange is triggered for all halos in a group, there is no order defined in which they are carried out.

nhalos number of halos in halos

halos array of halos

### ops\_reduction ops\_decl\_reduction\_handle(int size, char \*type, char \*name)

This routine defines a reduction handle to be used in a parallel loop

size size of data in bytes

type the name of type used for output diagnostics (e.g. "double", "float")

name of the dat used for output diagnostics

#### void ops\_reduction\_result(ops\_reduction handle, T \*result)

This routine returns the reduced value held by a reduction handle

handle the ops\_reduction handle

result a pointer to write the results to, memory size has to match the declared

#### ops\_partition(char \*method)

Triggers a multi-block partitioning across a distributed memory set of processes. (links to a dummy function for single node parallelizations). This routine should only be called after all the ops\_halo ops\_decl\_block and ops\_halo ops\_decl\_dat statements have been declared

method string describing the partitioning method. Currently this string is not used

internally, but is simply a place-holder to indicate different partitioning

methods in the future.

#### void ops\_exit()

This routine must be called last to cleanly terminate the OPS computation.

#### 3.2 Diagnostics and output routines

#### void ops\_diagnostic\_output()

This routine prints out various useful bits of diagnostic info about sets, mappings and datasets. Usually used right after an ops\_partition() call to print out the details of the decomposition

#### void ops\_printf(const char \* format, ...)

This routine simply prints a variable number of arguments; it is created is in place of the standard C printf function which would print the same on each MPI process

#### void ops\_timers(double \*cpu, double \*et)

gettimeofday() based timer to start/end timing blocks of code

cpu variable to hold the CPU time at the time of invocation
et variable to hold the elapsed time at the time of invocation

#### void ops\_fetch\_block\_hdf5\_file(ops\_block block, char \*file)

Write the details of an ops\_block to a named HDF5 file. Can be used over MPI (puts the data in an ops\_dat into an HDF5 file using MPI I/O)

block ops\_block to be written
file hdf5 file to write to

#### void ops\_fetch\_stencil\_hdf5\_file(ops\_stencil stencil, char \*file)

Write the details of an ops\_block to a named HDF5 file. Can be used over MPI (puts the data in an ops\_dat into an HDF5 file using MPI I/O)

stencil ops\_stencil to be written file hdf5 file to write to

#### void ops\_fetch\_dat\_hdf5\_file(ops\_dat dat, const char \*file)

Write the details of an ops\_block to a named HDF5 file. Can be used over MPI (puts the data in an ops\_dat into an HDF5 file using MPI I/O)

dat ops\_dat to be written file hdf5 file to write to

#### void ops\_print\_dat\_to\_txtfile(ops\_dat dat, chat \*file)

Write the details of an ops\_block to a named text file. When used under an MPI parallelization each MPI process will write its own data set separately to the text file. As such it does not use MPI I/O. The data can be viewed using a simple text editor

dat ops\_dat to to be written file text file to write to

#### void ops\_timing\_output(FILE \*os)

Print OPS performance performance details to output stream

os output stream, use stdout to print to standard out

#### void ops\_NaNcheck(ops\_dat dat)

Check if any of the values held in the dat is a NaN. If a NaN is found, prints an error message and exits.

dat ops\_dat to to be checked

## 3.3 Halo exchange

## $void \ ops\_halo\_transfer(ops\_halo\_group \ group)$

This routine exchanges all halos in a halo group and will block execution of subsequent computations that depend on the exchanged data.

group the halo group

## 3.4 Parallel loop syntax

A parallel loop with N arguments has the following syntax:

```
void ops_par_loop( void (*kernel)(...),
```

char \*name, ops\_blck block, int dims, int \*range, ops\_arg arg1, ops\_arg arg2, ..., ops\_arg argN)

kernel user's kernel function with N arguments

name name of kernel function, used for output diagnostics

block the ops\_block over which this loop executes

dims dimension of loop iteration

range iteration range array

args arguments

The **ops\_arg** arguments in **ops\_par\_loop** are provided by one of the following routines, one for global constants and reductions, and the other for OPS datasets.

#### ops\_arg\_ops\_arg\_gbl(T \*data, int dim, char \*type, ops\_access acc)

Passes a scalar or small array that is invariant of the iteration space (not to be confused with ops\_decl\_const, which facilitates global scope variables).

data data array

dim array dimension

type string representing the type of data held in data

acc access type

#### ops\_arg\_ops\_arg\_reduce(ops\_reduction handle, int dim, char \*type, ops\_access acc)

Passes a pointer to a variable that needs to be incremented (or swapped for min/max reduction) by the user kernel.

handle an ops\_reduction handle

dim array dimension (according to type)

type string representing the type of data held in data

acc access type

#### ops\_arg\_ops\_arg\_dat(ops\_dat dat, ops\_stencil stencil, char \*type, ops\_access acc)

Passes a pointer wrapped in ac ACC<sub>ii</sub> object to the value(s) at the current grid point to the user kernel. The ACC object's parentheses operator has to be used for dereferencing the pointer.

dat dataset

stencil stencil for accessing data

type string representing the type of data held in dataset

acc access type

## ops\_arg\_idx()

Give you an array of integers (in the user kernel) that have the index of the current grid point, i.e. idx[0] is the index in x, idx[1] is the index in y, etc. This is a globally consistent index, so even if the block is distributed across different MPI partitions, it gives you the same indexes. Generally used to generate initial geometry.

#### 3.5 Stencils

The final ingredient is the stencil specification, for which we have two versions: simple and strided.

#### ops\_stencil ops\_decl\_stencil(int dims, int points, int \*stencil, char \*name)

dims dimension of loop iteration

points number of points in the stencil

stencil stencil for accessing data

name string representing the name of the stencil

## ops\_stencil ops\_decl\_strided\_stencil(int dims, int points, int \*stencil, int \*stride, char \*name)

dims dimension of loop iteration

points number of points in the stencil

stencilstencil for accessing datastridestride for accessing data

name string representing the name of the stencil

#### ops\_stencil ops\_decl\_stencil\_hdf5(int dims, int points, char \*name, char\* file)

dims dimension of loop iteration

points number of points in the stencil

name string representing the name of the stencil

file hdf5 file to write to

In the strided case, the semantics for the index of data to be accessed, for stencil point p, in dimension m are defined as:

stride[m]\*loop\_index[m] + stencil[p\*dims+m],

where loop\_index[m] is the iteration index (within the user-defined iteration space) in the different dimensions.

If, for one or more dimensions, both stride[m] and stencil[p\*dims+m] are zero, then one of the following must be true;

- the dataset being referenced has size 1 for these dimensions
- these dimensions are to be omitted and so the dataset has dimension equal to the number of remaining dimensions.

See OPS/apps/c/CloverLeaf/build\_field.cpp and OPS/apps/c/CloverLeaf/generate.cpp for an example ops\_decl\_strided\_stencil declaration and its use in a loop, respectively.

These two stencil definitions probably take care of all of the cases in the Introduction except for multiblock applications with interfaces with different orientations – this will need a third, even more general, stencil specification. The strided stencil will handle both multigrid (with a stride of 2 for example) and the boundary condition and reduced dimension applications (with a stride of 0 for the relevant dimensions).

#### 3.6 Checkpointing

OPS supports the automatic checkpointing of applications. Using the API below, the user specifies the file name for the checkpoint and an average time interval between checkpoints, OPS will then automatically save all necessary information periodically that is required to fast-forward to the last checkpoint if a crash occurred. Currently, when re-launching after a crash, the same number of MPI processes have to be used. To enable checkpointing mode, the OPS\_CHECKPOINT runtime argument has to be used.

#### bool ops\_checkpointing\_init(const char \*filename, double interval, int options)

Initialises the checkpointing system, has to be called after ops\_partition. Returns true if the application launches in restore mode, false otherwise.

filename name of the file for checkpointing. In MPI, this will automatically be post-

fixed with the rank ID.

interval average time (seconds) between checkpoints

options a combinations of flags, listed in ops\_checkpointing.h:

OPS\_CHECKPOINT\_INITPHASE - indicates that there are a number of parallel loops at the very beginning of the simulations which should be excluded from any checkpoint; mainly because they initialise datasets that do not change during the main body of the execution. During restore mode these loops are executed as usual. An example would be the computation of the mesh geometry, which can be excluded from the checkpoint if it is re-computed when recovering and restoring a checkpoint. The API call void ops\_checkpointing\_initphase\_done() indicates the end of this initial phase.

OPS\_CHECKPOINT\_MANUAL\_DATLIST - Indicates that the user manually controls the location of the checkpoint, and explicitly specifies the list of ops\_dats to be saved.

OPS\_CHECKPOINT\_FASTFW - Indicates that the user manually controls the location of the checkpoint, and it also enables fast-forwarding, by skipping the execution of the application (even though none of the parallel loops

would actually execute, there may be significant work outside of those) up to the checkpoint.

OPS\_CHECKPOINT\_MANUAL - Indicates that when the corresponding API function is called, the checkpoint should be created. Assumes the presence of the above two options as well.

#### void ops\_checkpointing\_manual\_datlist(int ndats, ops\_dat \*datlist)

A use can call this routine at a point in the code to mark the location of a checkpoint. At this point, the list of datasets specified will be saved. The validity of what is saved is not checked by the checkpointing algorithm assuming that the user knows what data sets to be saved for full recovery. This routine should be called frequently (compared to check-pointing frequency) and it will trigger the creation of the checkpoint the first time it is called after the timeout occurs.

ndats number of datasets to be saved

datlist arrays of ops\_dat handles to be saved

#### bool ops\_checkpointing\_fastfw(int nbytes, char \*payload)

A use can call this routine at a point in the code to mark the location of a checkpoint. At this point, the specified payload (e.g. iteration count, simulation time, etc.) along with the necessary datasets, as determined by the checkpointing algorithm will be saved. This routine should be called frequently (compared to checkpointing frequency), will trigger the creation of the checkpoint the first time it is called after the timeout occurs. In restore mode, will restore all datasets the first time it is called, and returns true indicating that the saved payload is returned in payload. Does not save reduction data.

nbytes size of the payload in bytes

payload pointer to memory into which the payload is packed

# bool ops\_checkpointing\_manual\_datlist\_fastfw(int ndats, op\_dat \*datlist, int nbytes, char \*payload)

Combines the manual datlist and fastfw calls.

ndats number of datasets to be saved

datlist arrays of ops\_dat handles to be saved

nbytes size of the payload in bytes

payload pointer to memory into which the payload is packed

# bool ops\_checkpointing\_manual\_datlist\_fastfw\_trigger(int ndats, opa\_dat \*datlist, int nbytes, char \*payload)

With this routine it is possible to manually trigger checkpointing, instead of relying on the timeout process. as such it combines the manual datlist and fastfw calls, and triggers the creation of a checkpoint when called.

ndats number of datasets to be saved

datlist arrays of ops\_dat handles to be saved

nbytes size of the payload in bytes

payload pointer to memory into which the payload is packed

The suggested use of these **manual** functions is of course when the optimal location for checkpointing is known - one of the ways to determine that is to use the built-in algorithm. More details of this will be reported in a tech-report on checkpointing, to be published later.

#### 3.7 Access to OPS data

This section describes APIS that give the user access to internal data structures in OPS and return data to user-space. These should be used cautiously and sparsely, as they can affect performance significantly

#### int ops\_dat\_get\_local\_npartitions(ops\_dat dat)

This routine returns the number of chunks of the given dataset held by the current process.

dat the dataset

#### int ops\_dat\_get\_global\_npartitions(ops\_dat dat)

This routine returns the number of chunks of the given dataset held by all processes.

dat the dataset

#### void ops\_dat\_get\_extents(ops\_dat dat, int part, int \*disp, int \*sizes)

This routine returns the MPI displacement and size of a given chunk of the given dataset on the current process.

dat the dataset

dat

part the chunk index (has to be 0)

disp an array populated with the displacement of the chunk within the "global"

distributed array

sizes an array populated with the spatial extents

# char\* ops\_dat\_get\_raw\_metadata(ops\_dat dat, int part, int \*disp, int \*size, int \*stride, int \*d\_m, int \*d\_p)

This routine returns array shape metadata corresponding to the ops\_dat. Any of the arguments that are not of interest, may be NULL.

part the chunk index (has to be 0)

disp an array populated with the displacement of the chunk within the "global" distributed array

size an array populated with the spatial extents

stride an array populated strides in spatial dimensions needed for column-major

indexing

the dataset

d.m an array populated with padding on the left in each dimension. Note that

these are negative values

d\_p an array populated with padding on the right in each dimension

# char\* ops\_dat\_get\_raw\_pointer(ops\_dat dat, int part, ops\_stencil stencil, ops\_memspace \*memspace)

This routine returns a pointer to the internally stored data, with MPI halo regions automatically updated as required by the supplied stencil. The strides required to index into the dataset are also given.

dat the dataset

the chunk index (has to be 0)

stencil a stencil used to determine required MPI halo exchange depths

memspace when set to OPS\_HOST or OPS\_DEVICE, returns a pointer to data in that

memory space, otherwise must be set to 0, and returns whether data is in

the host or on the device

#### void ops\_dat\_release\_raw\_data(ops\_dat dat, int part, ops\_access acc)

Indicates to OPS that a dataset previously accessed with ops\_dat\_get\_raw\_pointer is released by the user, and also tells OPS how it was accessed

dat the dataset

part the chunk index (has to be 0)

acc the kind of access that was used by the user (OPS\_READ if it was read only,

OPS\_WRITE if it was overwritten, OPS\_RW if it was read and written)

#### void ops\_dat\_fetch\_data(ops\_dat dat, int part, int \*data)

This routine copies the data held by OPS to the user-specified memory location, which needs to be at least as large as indicated by the sizes parameter of ops\_dat\_get\_extents.

dat the dataset

part the chunk index (has to be 0)

data pointer to memory which should be filled by OPS

#### void ops\_dat\_set\_data(ops\_dat dat, int part, int \*data)

This routine copies the data given by the user to the internal data structure used by OPS. User data needs to be laid out in column-major order and strided as indicated by the sizes parameter of ops\_dat\_get\_extents.

dat the dataset

part the chunk index (has to be 0)

data pointer to memory which should be copied to OPS

## 4 Tiling for Cache-blocking

OPS has a code generation (ops\_gen\_mpi\_lazy) and build target for tiling. Once compiled, to enable, use the OPS\_TILING runtime parameter - this will look at the L3 cache size of your CPU and guess the correct tile size. If you want to alter the amount of cache to be used for the guess, use the OPS\_CACHE\_SIZE=XX runtime parameter, where the value is in Megabytes. When MPI is combined with OpenMP tiling can be extended to the MPI halos. Set OPS\_TILING\_MAXDEPTH to increase the the halo depths so that halos for multiple ops\_par\_loops can be exchanged with a single MPI message (see [2] for more details)

To test, compile CloverLeaf under apps/c/CloverLeaf, modify clover.in to use a 6144<sup>2</sup> mesh, then run as follows:

```
For OpenMP with tiling:
export OMP_NUM_THREADS=xx;
numactl -physnodebind=0 ./cloverleaf_tiled OPS_TILING

For MPI+OpenMP with tiling:
export OMP_NUM_THREADS=xx;
mpirun -np xx ./cloverleaf_mpi_tiled OPS_TILING OPS_TILING_MAXDEPTH=6

To manually specify the tile sizes (in MB), use the T1, T2, and T3 environment variables:
export T1=600; export T2=200;
export OMP_NUM_THREADS=xx;
numactl -physnodebind=0 ./cloverleaf_tiled OPS_TILING
```

## 5 CUDA and OpenCL Runtime Arguments

The CUDA (and OpenCL) thread block sizes can be controlled by setting the OPS\_BLOCK\_SIZE\_X, OPS\_BLOCK\_SIZE\_Y and OPS\_BLOCK\_SIZE\_Z runtime arguments. For example:

```
./cloverleaf_cuda OPS_BLOCK_SIZE_X=64 OPS_BLOCK_SIZE_Y=4
```

OPS\_CL\_DEVICE=XX runtime flag sets the OpenCL device to execute the code on. Usually OPS\_CL\_DEVICE=0 selects the CPU and OPS\_CL\_DEVICE=1 selects GPUs.

## 6 Executing with GPUDirect

GPU direct support for MPI+CUDA, to enable (on the OPS side) add **-gpudirect** when running the executable. You may also have to use certain environmental flags when using different MPI distributions. For an example of the required flags and environmental settings on the Cambridge Wilkes2 GPU cluster see:

https://docs.hpc.cam.ac.uk/hpc/user-guide/performance-tips.html

### 7 OPS User Kernels

In OPS, the elemental operation carried out per mesh/grid point is specified as an outlined function called a *user kernel*. An example taken from the Cloverleaf application is given in Figure 1.

This user kernel is then used in an ops\_par\_loop (Figure 2). The key aspect to note in the user kernel in Figure 1 is the use of the ACC; objects and their parentheses operator. These specify the stencil in accessing the elements of the respective data arrays.

## References

- [1] OP2 for Many-Core Platforms, 2013. http://www.oerc.ox.ac.uk/projects/op2
- [2] Istvan Z. Reguly, G.R. Mudalige, Mike B. Giles. Loop Tiling in Large-Scale Stencil Codes at Run-time with OPS. (2017) IEEE Transactions on Parallel and Distributed Systems. http://dx.doi.org/10.1109/TPDS.2017.2778161

```
iid accelerate_kernel( const ACC<double> &density0, const ACC<double> &volume,
               ACC<double> &stepbymass, const ACC<double> &xvel0, ACC<double> &xvel1,
2
3
               const ACC<double> &xarea, const ACC<double> &pressure,
               const ACC<double> &yvel0, ACC<double> &yvel1,
               const ACC<double> &yarea, const ACC<double> &viscosity) {
7double nodal_mass;
9//\{0,0,-1,0,0,-1,-1,-1\};
10 \mod 2 \mod 2 = ( \operatorname{density0}(-1,-1) * \operatorname{volume}(-1,-1) 
+ density0(0,-1) * volume(0,-1)
+ density0(0,0) * volume(0,0)
^{13} + density0(-1,0) * volume(-1,0)) * 0.25;
15stepbymass(0,0) = 0.5*dt/ nodal_mass;
17/(\{0,0,-1,0,0,-1,-1,-1\};
18//\{0,0,0,-1\};
20xvel1(0,0) = xvel0(0,0) - stepbymass(0,0) *
           (xarea(0,0) * (pressure(0,0) - pressure(-1,0)) +
             xarea(0,-1) * (pressure(0,-1) - pressure(-1,-1));
24//{0,0, -1,0, 0,-1, -1,-1};
25//{0,0, -1,0};
27yvel1(0,0) = yvel0(0,0) - stepbymass(0,0) *
           (yarea(0,0) * (pressure(0,0) - pressure(0,-1)) +
             yarea(-1,0) * (pressure(-1,0) - pressure(-1,-1));
29
31/(\{0,0,-1,0,0,-1,-1,-1\};
32//\{0,0,0,-1\};
34xvel1(0,0) = xvel1(0,0) - stepbymass(0,0) *
           (xarea(0,0) * (viscosity(0,0) - viscosity(-1,0)) +
             xarea(0,-1) * (viscosity(0,-1) - viscosity(-1,-1));
36
38//\{0,0,-1,0,0,-1,-1,-1\};
39//\{0,0,-1,0\};
41yvel1(0,0) = yvel1(0,0) - stepbymass(0,0) *
           ( yarea(0,0) * ( viscosity(0,0) - viscosity(0,-1) ) +
42
             yarea(-1,0) * (viscosity(-1,0) - viscosity(-1,-1));
44
46
```

Figure 1: example user kernel

```
int rangexy_inner_plus1[] = {x_min,x_max+1,y_min,y_max+1};
2
3 ops_par_loop(accelerate_kernel, "accelerate_kernel", clover_grid, 2, rangexy_inner_plus1,
    ops_arg_dat(density0, 1, S2D_00_M10_0M1_M1M1, "double", OPS_READ),
    ops_arg_dat(volume, 1, S2D_00_M10_0M1_M1M1, "double", OPS_READ),
    ops_arg_dat(work_array1, 1, S2D_00, "double", OPS_WRITE),
    ops_arg_dat(xvel0, 1, S2D_00, "double", OPS_READ),
    ops_arg_dat(xvel1, 1, S2D_00, "double", OPS_INC),
    ops_arg_dat(xarea, 1, S2D_00_0M1, "double", OPS_READ),
    ops_arg_dat(pressure, 1, S2D_00_M10_0M1_M1M1, "double", OPS_READ),
10
    ops_arg_dat(yvel0, 1, S2D_00, "double", OPS_READ),
11
    ops_arg_dat(yvel1, 1, S2D_00, "double", OPS_INC),
12
    ops_arg_dat(yarea, 1, S2D_00_M10, "double", OPS_READ),
    ops_arg_dat(viscosity, 1, S2D_00_M10_0M1_M1M1, "double", OPS_READ));
```

Figure 2: example ops\_par\_loop