## OP2 C++ User's Manual

## Contents

## 1 Introduction

OP2 is a high-level framework with associated libraries and preprocessors to generate parallel executables for applications on unstructured grids. This document describes the C++ API, but FORTRAN 90 is also supported with a very similar API.

The key concept behind OP2 is that unstructured grids can be described by a number of sets. Depending on the application, these sets might be of nodes, edges, faces, cells of a variety of types, far-field boundary nodes, wall boundary faces, etc. Associated with these are data (e.g. coordinate data at nodes) and mappings to other sets (e.g. edge mapping to the two nodes at each end of the edge). All of the numerically-intensive operations can then be described as a loop over all members of a set, carrying out some operations on data associated directly with the set or with another set through a mapping.

OP2 makes the important restriction that the order in which the function is applied to the members of the set must not affect the final result to within the limits of finite precision floating-point arithmetic. This allows the parallel implementation to choose its own ordering to achieve maximum parallel efficiency. Two other restrictions are that the sets and maps are static (i.e. they do not change) and the operands in the set operations are not referenced through a double level of mapping indirection (i.e. through a mapping to another set which in turn uses another mapping to data in a third set).

OP2 currently enables users to write a single program which can be built into three different executables for different single-node platforms:

- single-threaded on a CPU
- parallelised using CUDA for NVIDIA GPUs
- multi-threaded using OpenMP for multicore CPU systems

A current development branch, also supports AVX vectorisation for x86 CPUs, and OpenCL for both CPUs and GPUS. In addition to this, there is support for distributed-memory MPI parallelisation in combination with any of the above. The user can either use OP2's parallel file I/O capabilities for HDF5 files with a specified structure, or perform their own parallel file I/O using custom MPI code.

## 2 Overview

A computational project can be viewed as involving three steps:

- writing the program
- debugging the program, often using a small testcase
- running the program on increasingly large applications

With OP2 we want to simplify the first two tasks, while providing as much performance as possible for the third.

To achieve the high performance for large applications, a preprocessor is needed to generate the CUDA code for GPUs or OpenMP code for multicore x86 systems. However, to keep the initial development simple, a development single-threaded executable can be created without any special tools; the user's main code is simply linked to a set of library routines, most of which do little more than error-checking to assist the debugging process by checking the correctness of the user's program. Note that this single-threaded version will not execute efficiently. The preprocessor is needed to generate efficient single-threaded and OpenMP code for CPU systems.

Figure ?? shows the build process for a single thread CPU executable. The user's main program (in this case jac.cpp) uses the OP2 header file op\_seq.h and is linked to the appropriate OP2 libraries using g++, perhaps controlled by a Makefile.

Figure ?? shows the build process for the corresponding CUDA executable. The preprocessor parses the user's main program and produces a modified main program and a CUDA file which includes a separate file for each of the kernel functions. These are then compiled and linked to the OP libraries using g++ and the NVIDIA CUDA compiler nvcc, again perhaps controlled by a Makefile.

Figure ?? shows the OpenMP build process which is very similar to the CUDA process except that it uses \*.cpp files produced by the preprocessor instead of \*.cu files.

In looking at the API specification, users may think it is a little verbose in places. e.g. users have to re-supply information about the datatype of the datasets being used in a parallel loop. This is a deliberate choice to simplify the task of the preprocessor, and therefore hopefully reduce the chance for errors. It is also motivated by the thought that "programming is easy; it's debugging which is difficult". i.e. writing code isn't time-consuming, it's correcting it which takes the time. Therefore, it's not unreasonable to ask the programmer to supply redundant information, but be assured that the preprocessor or library will check that all redundant information is self-consistent. If you declare a dataset as being of type OP\_DOUBLE and later say that it is of type OP\_FLOAT this will be flagged up as an error at run-time.

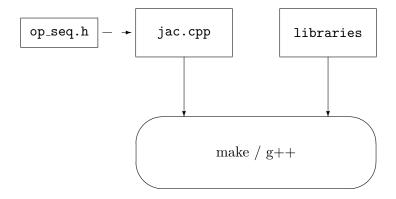


Figure 1: Build process for the development single threaded CPU version

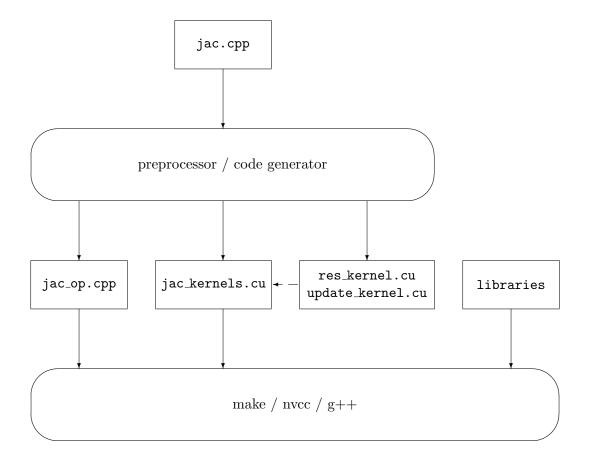


Figure 2: CUDA code build process

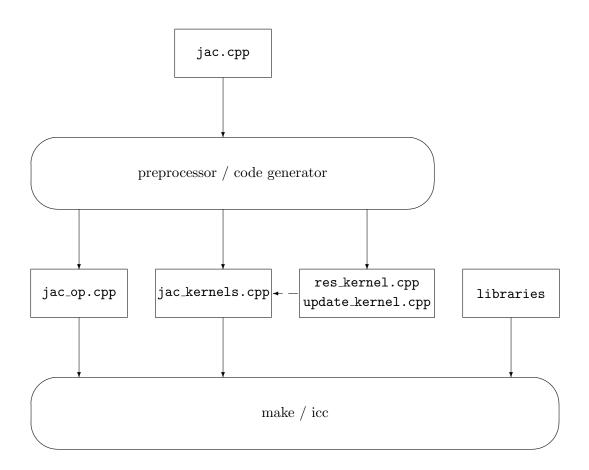


Figure 3: OpenMP code build process

## $3 \quad OP2 C++ API$

#### 3.1 Initialisation and termination routines

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

This routine must be called before all other OP routines. Under MPI back-ends, this routine also calls MPI\_Init() unless its already called previously

argc, argv the usual command line arguments

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

be performed;

0 - none;

1 - error-checking;

2-info on plan construction;

3 – report execution of parallel loops;

4 – report use of old plans;

7 – report positive checks in op\_plan\_check;

### void op\_exit()

This routine must be called last to cleanly terminate the OP computation. Under MPI back-ends, this routine also calls MPI\_Finalize() unless its has been called previously. A runtime error will occur if MPI\_Finalize() is called after op\_exit()

#### op\_set op\_decl\_set(int size, char \*name)

This routine defines a set, and returns a set ID.

size number of elements in the set

name a name used for output diagnostics

## op\_map op\_decl\_map(op\_set from, op\_set to, int dim, int \*imap, char \*name)

This routine defines a mapping from one set to another, and returns a map ID.

from set pointed from

to set pointed to

dim number of mappings per element

imap input mapping table

name a name used for output diagnostics

## void op\_decl\_const(int dim, char \*type, T \*dat, char \*name)

This routine declares constant data with global scope to be used in user's kernel functions. Note: in sequential version, it is the user's responsibility to define the appropriate variable with global scope.

dim dimension of data (i.e. array size)

for maximum efficiency, this should be a literal constant (i.e. a number not

a variable)

type datatype, either intrinsic ("float", "double", "int", "uint", "ll", "ull" or

"bool") or user-defined

dat input data of type T (checked for consistency with type at run-time)

name global name to be used in user's kernel functions;

a scalar variable if dim=1, otherwise an array of size dim

## op\_dat op\_decl\_dat(op\_set set, int dim, char \*type, T \*data, char \*name)

This routine defines a dataset, and returns a dataset ID.

set set

dim dimension of dataset (number of items per set element)

at present this must be a literal constant (i.e. a number not a variable); this restriction will be removed in the future but a literal constant will remain

more efficient

type datatype, either intrinsic or user-defined – expert users can add a qualifier

to control data layout and management within OP2 (see section ??)

data input data of type T (checked for consistency with type at run-time) – for

each element in set, the dim data items muct be contiguous, but OP2 may use a different data layout internally for better performance on certain hard-

ware platforms (see section ??)

name a name used for output diagnostics

## op\_dat op\_decl\_dat\_tmp(op\_set set, int dim, char \*type, char \*name)

This routine defines a temporary dataset, initialises it to zero, and returns a dataset ID.

set set

dim dimension of dataset (number of items per set element)

at present this must be a literal constant (i.e. a number not a variable); this restriction will be removed in the future but a literal constant will remain

more efficient

type datatype, either intrinsic or user-defined – expert users can add a qualifier

to control data layout and management within OP2 (see section ??)

name a name used for output diagnostics

## void op\_free\_dat\_tmp(op\_dat dat)

This routine terminates a temporary dataset.

dat OP dataset ID

## void op\_diagnostic\_output()

This routine prints out various useful bits of diagnostic info about sets, mappings and datasets

## 3.2 Parallel loop syntax

A parallel loop with N arguments has the following syntax:

void op\_par\_loop(void (\*kernel)(...), char \*name, op\_set set, op\_arg arg1, op\_arg arg2, ..., op\_arg argN)

kernel user's kernel function with N arguments

(this is only used for the single-threaded CPU build)

name of kernel function, used for output diagnostics

set OP set ID args arguments

The **op\_arg** arguments in **op\_par\_loop** are provided by one of the following routines, one for global constants and reductions, and the other for OP2 datasets. In the future there will be a third one for sparse matrices to support the needs of finite element calculations.

## op\_arg op\_arg\_gbl(T \*data, int dim, char \*typ, op\_access acc)

data data array

dim array dimension

typ datatype (redundant info, checked at run-time for consistency)

acc access type:

OP\_READ: read-only

OP\_INC: global reduction to compute a sum OP\_MAX: global reduction to compute a maximum OP\_MIN: global reduction to compute a minimum

# op\_arg op\_arg\_dat(op\_dat dat, int idx, op\_map map, int dim, char \*typ, op\_access acc)

dat OP dataset ID

idx index of mapping to be used (ignored if no mapping indirection) – a negative

value indicates that a range of indices is to be used (see section ?? for

additional information)

map OP mapping ID (OP\_ID for identity mapping, i.e. no mapping indirection)

dataset dimension (redundant info, checked at run-time for consistency)

at present this must be a literal constant (i.e. a number not a variable); this restriction will be removed in the future but a literal constant will remain

more efficient

typ dataset datatype (redundant info, checked at run-time for consistency)

acc access type:

OP\_READ: read-only

OP\_WRITE: write-only, but without potential data conflict OP\_RW: read and write, but without potential data conflict OP\_INC: increment, or global reduction to compute a sum

The restriction that OP\_WRITE and OP\_RW access must not have any potential data conflict means that two different elements of the set cannot through a mapping indirection reference the same elements of the dataset.

Furthermore, with OP\_WRITE the user's kernel function must set the value of all DIM components of the dataset. If the user's kernel function does not set all of them, the access should be specified to be OP\_RW since the kernel function needs to read in the old values of the components which are not being modified.

## op\_arg op\_opt\_arg\_dat(op\_dat dat, int idx, op\_map map, int dim, char \*typ, op\_access acc, int flag)

This is the same as op\_arg op\_arg\_dat except for an extra variable flag; the argument is only actually used if flag has a non-zero value. This routine is required for large application codes (such as HYDRA) which has lots of different features turned on and off by logical flags.

Note that if the user's kernel needs to know the value of flag then this must be passed as an additional op\_arg\_gbl argument.

The pointer corresponding to the optional argument in the user kernel must not be dereferenced when the flag is false or not set

## 3.3 Expert user capabilities

#### 3.3.1 SoA data layout

The objective of OP2 is hide all of the complexities involved in achieving high performance on a wide variety of hardware platforms. Unfortunately, there are limits to the extent to which this is possible, and so we have added the capability for expert users to achieve higher performance by providing extra directions to OP2. This is very similar to the use of pragmas in C/C++.

At present we have just one qualifier option, which is to force OP2 to use SoA (struct of arrays) storage internally on GPUs. As illustrated in Figure ?? the user always supplies data in AoS (array of structs) layout, with all of the items associated with one set element stored contiguously. On cache-based CPUs this is almost always the most efficient storage layout because it usually maximises the cache hit ratio and reuse of data. However, when doing vector computing (either on GPUs or in the AVX vector units of CPUs) with no indirect addressing, then the SoA format is more efficient.

OP2 can be directed to use the SoA format by adding the qualifier ':soa' to the datatype, as in 'float:soa'. Note that the data should still be supplied by the user in the standard AoS layout; the transposition to SoA format is handled internally by OP2. Also, this qualifier must be used every time the data is accessed, as well as when it is first defined. If it is not, or if it is accessed indirectly, it will generate a run-time error.

If the data is held in an SoA layout, then there is a non-unit "stride" in accessing the data associated with one set element; this is illustrated in the figure. When executing a parallel loop, this stride is held in a global variable op2\_stride which must be used by the user's kernel, so instead of a data reference data[m] it should be data[m\*op2\_stride]. The sequential implementation defines op2\_stride = 1 so that the user's code works with both SoA and AoS layouts.

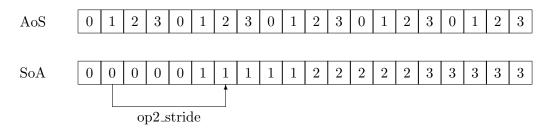


Figure 4: The AoS and SoA layouts for a set with 5 elements, and 4 data items (numbered 0, 1, 2, 3) per element, and the access stride for the SoA storage.

## 3.3.2 Vector maps

When each of the arguments in a parallel loop uses a single mapping index, the corresponding argument in the user's kernel function is a pointer to an array holding the data items for the set element being pointed to. i.e. the kernel declaration may look something like

kernel\_routine(float \*arg1, float \*arg2, float \*arg3, float \*arg4)

If the first 3 arguments correspond to the vertices of a triangle, and the parallel loop is over the set of triangles using a mapping from triangles to vertices, then it may be more natural to combine the first 3 arguments into a single doubly-indexed array as

kernel\_routine(float \*arg1[3], float \*arg4)

This is obtained by a parallel loop argument having a range of mapping indices (instead of just one) which is accomplished by specifying the mapping index to be -range - this means that the set of mapping indices 0 - range-1 is to be used.

## 3.4 MPI message-passing using HDF5 files

HDF5 has become the *de facto* standard format for parallel file I/O, with various other standards like CGNS layered on top. To make it as easy as possible for users to develop distributed-memory OP2 applications, we provide alternatives to some of the OP2 routines in which the data is read by OP2 from an HDF5 file, instead of being supplied by the user:

- op\_decl\_set\_hdf5: similar to op\_decl\_set but with size replaced by char \*file which defines the HDF5 file from which size is read using keyword name
- op\_decl\_map\_hdf5: similar to op\_decl\_map but with imap replaced by char \*file from which the mapping table is read using keyword name
- op\_decl\_dat\_hdf5: similar to op\_decl\_dat but with dat replaced by char \*file from which the data is read using keyword name

In addition, there are the following two routines.

### op\_get\_const\_hdf5(int dim, char \*type, char \*file, char \*name)

This routine reads a constant (or constant array) from an HDF5 file; if required, the user must then call **op\_decl\_const** to declare it to OP2.

dim dimension of data (i.e. array size)

for maximum efficiency, this should be a literal constant (i.e. a number not

a variable)

type datatype, either intrinsic ("float", "double", "int", "uint", "ll", "ull" or

"bool") or user-defined; checked at run-time for consistency with T

file name of the HDF5 file

name global name to be used in user's kernel functions;

a scalar variable if dim=1, otherwise an array of size dim

## 

This routine controls how the various sets are partitioned.

lib\_name A string which declares the partitioning library to be used.

"PTSCOTCH" - PT-Scotch
"PARMETIS" - ParMetis

"INERTIAL" - 3D recursive inertial bisection partitioning in OPlus

"EXTERNAL" - external partitioning read in from hdf5 file

"RANDOM" - select a generic random partitioning (for debugging)

If the OP2 library was not built with the specified third-party library, an error message is displayed at runtime and a trivial block-partitioning is used for the remainder of the application.

prime\_set Specify the geometric coordinates as an op\_dat to be used in when using

"GEOM" or "GEOMKWAY"

Using the above routines, OP2 will take care of everything, reading in all of the sets, mapping and data, partitioning the sets appropriately, renumbering sets as needed, constructing import/export halo lists, etc., and then performing the parallel computation with halo exchange when needed.

Both MPI and single process executables can be generated, depending on the libraries which are linked in.

## 3.5 Other I/O and Miscellaneous Routines

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

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

### void op\_fetch\_data ( op\_dat dat, T\* data)

This routine transfers a copy of the data currently held in an op\_dat from the OP2 back-end to a user allocated memory block.

dat OP dataset ID – The op\_dat whose data is to be fetched from OP2 space to

user space

data pointer to a block of memory of type T – allocated by the user

## void op\_fetch\_data\_hdf5(op\_dat dat, T\* data, int low, int high)

Transfers a copy of the op\_dat's data currently held by OP2 to a user allocated block of memory pointed to by data pointer of type T. The low and high integers gives the range of elements to be fetched. Under MPI (with hdf5) all the processes will hold the same data block(i.e. after an MPI\_Allgather)

dat OP dataset ID – The op dat whose data is to be fetched from OP2 space to

user space

data pointer to a block of memory of type T – allocated by the user

low index of the first element to be fetched high index of the last element to be fetched

## void op\_fetch\_data\_hdf5\_file(op\_dat dat, char const \*file\_name)

Write the data in the op\_dat to an HDF5 file

dat OP dataset ID – The op dat whose data is to be fetched from OP2 space to

user space

file\_name the file name to be written to

#### void op\_print\_dat\_to\_binfile(op\_dat dat, const char \*file\_name)

Write the data in the op\_dat to a binary file

dat OP dataset ID – The op dat whose data is to be fetched from OP2 space to

user space

file\_name the file name to be written to

## void op\_print\_dat\_to\_txtfile(op\_dat dat, const char \*file\_name)

Write the data in the op\_dat to a ASCI text file

dat OP dataset ID – The op dat whose data is to be fetched from OP2 space to

user space

file\_name the file name to be written to

## int op\_is\_root()

A supporting routine that allows to to check for the root process. Intended to be used mainly when the application utilizes HDF5 file I/O and when the user would like to perform some conditional code on the root process. Returns 1 if on MPLROOT else 0

## int op\_get\_size(op\_set set)

Get the global size of an op\_set

set OP set ID

## void op\_dump\_to\_hdf5(char const \* file\_name)

Dump the contents of all the op\_sets, op\_dats and op\_maps to an hdf5 file <u>as held internally by OP2</u>, useful for debugging

file\_name the file name to be written to

## void op\_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 op\_timing\_output()

Print OP2 performance performance details to STD out

## 3.6 MPI message-passing without HDF5 files

Some users will prefer not to use HDF5 files, or at least not to use them in the way prescribed by OP2. To support these users, an application code may do its own file I/O, and then provide the required data to OP2 using the standard routines.

In an MPI application, multiple copies of the same program are executed as separate processes, often on different nodes of a compute cluster. Hence, the OP2 declarations will be invoked on each process. In this case, the behaviour of the OP2 declaration routines is as follows:

- op\_decl\_set: size is the number of elements of the set which will be provided by this MPI process
- op\_decl\_map: imap provides the part of the mapping table which corresponds to its share of the from set
- op\_decl\_dat: dat provides the data which corresponds to its share of set

For example, if an application has 4 processes,  $4\times10^6$  nodes and  $16\times10^6$  edges, then each process might be responsible for providing  $10^6$  nodes and  $4\times10^6$  edges. Process 0 (the one with MPI rank 0) would be responsible for providing the first  $10^6$  nodes, process 1 the next  $10^6$  nodes, and so on, and the same for the edges.

The edge  $\rightarrow$  node mapping tables would still contain the same information as in a single process implementation, but process 0 would provide the first  $4 \times 10^6$  entries, process 1 the next  $4 \times 10^6$  entries, and so on.

This is effectively using a simple contiguous block partitioning of the datasets, but it is very important to note that this will not be used for the parallel computation. OP2 will re-partition the datasets, re-number the mapping tables as needed (as well as constructing import/export lists for halo data exchange) and will move all data/mappings/datasets to the correct MPI process.

## 4 Executing with GPUDirect

GPU direct support for MPI+CUDA, to enable (on the OP2 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 EMERALD GPU cluster see:

www.einfrastructuresouth.ac.uk/cfi/emerald/gpu-programming/

## 5 OP2 Preprocessor/ Code generator

There are three preprocessors for OP2, one developed at Imperial College using ROSE (currently not maintained), a second one developed at Oxford using MATLAB and finally a Python parser/generator also developed at Oxford.

### 5.1 MATLAB preprocessor

The MATLAB preprocessor is run by the command

```
op2('main')
```

where main.cpp is the user's main program. It produces as output

- a modified main program main\_op.cpp which is used for both the CUDA and OpenMP executables;
- for the CUDA executable, a new CUDA file main\_kernels.cu which includes one or more files of the form xxx\_kernel.cu containing the CUDA implementations of the user's kernel functions;
- for the OpenMP executable, a new C++ file main\_kernels.cpp which includes one or more files of the form xxx\_kernel.cpp containing the OpenMP implementations of the user's kernel functions.

If the user's application is split over several files it is run by a command such as

```
op2('main','sub1','sub2','sub3')
```

where sub1.cpp, sub2.cpp, sub3.cpp are the additional input files which will lead to the generation of output files sub1\_op.cpp, sub2\_op.cpp, sub3\_op.cpp in addition to main\_op.cpp, main\_kernels.cu, main\_kernels.cpp and the individual kernel files.

The MATLAB preprocessor was the first prototype source-to-source translator developed in the OP2 project. This has been now superseded by the Python code generator.

#### 5.2 Python code generator

The Python preprocessor is run on the command-line with the command

```
./op2.py main.cpp sub1.cpp sub2.cpp sub3.cpp
```

Assuming that the user's application is split over several files. This will lead to the generation of output files sub1\_op.cpp, sub2\_op.cpp, sub3\_op.cpp in addition to main\_op.cpp, main\_kernels.cu, main\_kernels.cpp and the individual kernel files.

• The modified main program main\_op.cpp is used for the efficient single threaded CPU (also called as generated sequential or Gen\_Seq) OpenMP and CUDA executables;

- For the Gen\_Seq and OpenMP executable, main\_kernels.cpp is a new C++ file which includes one or more files of the form xxx\_kernel.cpp containing the OpenMP implementations of the user's kernel functions.
- For the CUDA executable, main\_kernels.cu is a new CUDA file which includes one or more
  files of the form xxx\_kernel.cu containing the CUDA implementations of the user's kernel
  functions;

## 6 Error-checking

At compile-time, there is a check to ensure that CUDA 3.2 or later is used when compiling the CUDA executable; this is because of compiler bugs in previous versions of CUDA. At run-time, OP2 checks the user-supplied data in various ways:

- checks that a set has a strictly positive number of elements
- checks that a map has legitimate mapping indices, i.e. they map to elements within the range of the target set
- checks that variables have the correct declared type

It would be great to get feedback from users on suggestions for additional error-checking.

## 7 32-bit and 64-bit CUDA

Section 3.1.6 of the CUDA 3.2 Programming Guide says:

The 64-bit version of nvcc compiles device code in 64-bit mode (i.e. pointers are 64-bit). Device code compiled in 64-bit mode is only supported with host code compiled in 64-bit mode.

Similarly, the 32-bit version of nvcc compiles device code in 32-bit mode and device code compiled in 32-bit mode is only supported with host code compiled in 32-bit mode.

The 32-bit version of nvcc can compile device code in 64-bit mode also using the -m64 compiler option.

The 64-bit version of nvcc can compile device code in 32-bit mode also using the -m32 compiler option.

On Windows and Linux systems, there are separate CUDA download files for 32-bit and 64-bit operating systems, so the version of CUDA which is installed matches the operating system. i.e. the 64-bit version is installed on a 64-bit operating system.

Mac OS X can handle both 32-bit and 64-bit executables, and it appears that it is the 32-bit version of nvcc which is installed. Therefore the Makefiles in the OP2 distribution may need the -m64 flag added to NVCCFLAGS to produce 64-bit object code.

The Makefiles in the OP2 distribution assume 64-bit compilation and therefore they link to the 64-bit CUDA runtime libraries in /lib64 within the CUDA toolkit distribution. This will need to be changed to /lib for 32-bit code.