Model Coupling between the Weather Research and Forecasting Model and the DPRI Large Eddy Simulator for Urban Flows on GPU-accelerated Multicore Systems

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In this report we present a novel approach to model coupling for shared-memory multicore systems hosting OpenCL-compliant accelerators, which we call The Glasgow Model Coupling Framework (GMCF). We discuss the implementation of a prototype of GMCF and its application to coupling the Weather Research and Forecasting Model and an OpenCL-accelerated version of the Large Eddy Simulator for Urban Flows (LES) developed at DPRI.

The first stage of this work concerned the OpenCL port of the LES. The methodology used for the OpenCL port is a combination of automated analysis and code generation and rule-based manual parallelization. For the evaluation, the non-OpenCL LES code was compiled using gfortran, ifort and pgfortran, in each case with auto-parallelization and auto-vectorization. The OpenCL-accelerated version of the LES achieves a 7× speed-up on a NVIDIA GeForce GTX 480 GPGPU, compared to the fastest possible compilation of the original code running on a 12-core Intel Xeon E5-2640.

In the second stage of this work, we built the Glasgow Model Coupling Framework and successfully used it to couple an OpenMP-parallelized WRF instance with an OpenCL LES instance which runs the LES code on the GPGPU. The system requires only very minimal changes to the original code. The report discusses the rationale, aims, approach and implementation details of this work.
1 Introduction

1.1 The Weather Research and Forecasting Model

The Weather Research and Forecasting Model (WRF) is a mesoscale numerical weather prediction system (NWS) intended both for forecasting and atmospheric research. It is an Open Source project, used by a large fraction of weather and climate scientists worldwide. The WRF code base is written in Fortran-90 and quite complex and extensive (about 1,000,000 lines of code).

1.2 The Large Eddy Simulator for the Study of Urban Boundary-layer Flows

The Large Eddy Simulator for the Study of Urban Boundary-layer Flows (LES) is developed by Hiromasa Nakayama and Haruyasu Nagai at the Japan Atomic Energy Agency and Prof. Tetsuya Takemi at the Disaster Prevention Research Institute of Kyoto University [7,8]. It generates turbulent flows by using mesoscale meteorological simulations, and was designed to explicitly represent the urban surface geometry. Its purpose is to conduct building-resolving large-eddy simulations (LESs) of boundary-layer flows over urban areas under realistic meteorological conditions. WRF is used to compute the wind profile as input for LES, so there is a clear case for coupling both models.

1.3 Model Coupling

“Model coupling” means using data generated by one model as inputs for another model: e.g. climate simulations: atmosphere model, ocean model, land model, ice model. In combination with hardware Acceleration using GPU/manycore/FPGA, model coupling could result in much reduced run times and/or higher accuracy simulations.

Model Coupling is of growing importance because models of e.g. climate need to be as accurate as possible, and therefore include many factors and effects. Creating a single model incorporating all effects is increasingly difficult, and requires very large research teams to cover all specialisms. Combining existing models allows us to model a large variety of very complex systems.

There are a number of existing libraries to support the process of model coupling, e.g. MCT, ESMF, OASIS [6,3,2]. However, each of them requires hand modification of existing model codes, as well as writing of additional code to control the way the coupling is done needs to be written as well. Furthermore, current Model Coupling libraries all use MPI.

1.4 A Novel Approach to Model Coupling for Multicore/GPU Nodes

Creating coupled models using the current approach is very difficult and requires team of experts in various disciplines. As a result model coupling is too hard for most research teams. A better approach will allow more researchers to use model coupling and do better science.

1http://www.wrf-model.org
Furthermore, the current approaches were developed for clusters of single-core machines and are not ideal for multicore/GPU nodes. In particular, the current approach to load balancing requires that every model $i$ gets a fixed number of nodes $m_i$, proportional to its run time, i.e. $m_i = \alpha \Delta t_i$. As a result, data from $m_i$ nodes of model $i$ need to be transferred to $m_j$ nodes of model $j$. This is complex and asymmetrical, esp. for more than two models.

Our proposed approach (Fig. 1) is to limit coupling to processes running on a shared-memory node. The nodes run all processes required for coupling in threads, if a thread is not needed for coupling it goes to sleep and does not consume CPU time. As a result, the cluster communication is more symmetrical, and the load in each node can be balanced more easily.

2 The OpenCL-Accelerated LES

The DPRI Large Eddy Simulator (LES) is a high-resolution simulator which models flow over urban topologies. The main properties of the DPRI LES are:

- Generates turbulent flows by using mesoscale meteorological simulations.
- Explicitly represents the urban surface geometry.
- Used to conduct building-resolving large-eddy simulations (LESs) of boundary-layer flows over urban areas under realistic meteorological conditions.
Figure 2: LES main program (Fortran-77)

- Essentially solves the Poisson equation for the pressure, using Successive Over-Relaxation
- Written in Fortran-77, single-threaded, about a thousand lines of code.

2.1 LES Code Structure – Functional

The LES structure consists of sequential calls to following subroutines for each time step:

velnw: Update velocity for current time step
bondv1: Calculate boundary conditions (initial wind profile, inflow, outflow)
velfg: Calculate the body force
feedbf: Calculation of building effects
les: Calculation of viscosity terms (Smagorinsky model)
adam: Adams-Bashforth time integration
press: Solving of Poisson equation (SOR)
| Subroutine | Block   | Parallelisation                  |
|------------|---------|----------------------------------|
| velnw      |         | data parallel over full domain   |
| bondv1     | init uvw| data parallel over full domain   |
|            | calc uout| reduction over full domain      |
|            | calc uvw| data parallel over boundary planes|
| velfg      |         | data parallel over full domain   |
| feedbf     |         | data parallel over full domain   |
| les        | calc sm | data parallel over full domain   |
|            | bound sm| data parallel over boundary planes|
| adam       | calc visc| data parallel over full domain   |
| pres       | rhsav   | reduction over full domain      |
|            | sor     | reduction over full domain + iteration|
|            | pav     | reduction over full domain      |
|            | adj     | data parallel over full domain   |
|            | boundp  | data parallel over boundary planes|

Table 1: LES Computational structure and parallelization strategy for each block
2.2 LES Code Structure – Computational

2.3 Methodology

In this section we discuss our novel methodology for porting Fortran NWP applications to OpenCL.

The approach used in this work is as follows:

1. Convert the original F77 code to F95, remove common blocks, if required refactor into subroutines. All this is done using our rf4a tool. The resulting F95 code has fully explicit subroutine arguments.

2. For each subroutine that could become a kernel, we created a wrapper in two stages:
   a) We generate a wrapper from the original subroutine using the pragma
      
      ```fortran
      !$ACC KernelWrapper(adam)
      call adam(fgh,fgh_old,im,jm,km)
      !$ACC End KernelWrapper
      ```
      
      This generates a template for a module `module_adam_ocl` which contains a subroutine `adam_ocl`. We manually edit the generated code if required.
      
      • The template file (`module_adam_ocl_TEMPL.f95`) is valid Fortran-95, if compiled and run it will be functionally identical to the original subroutine.
   b) We generate the OpenCL API from the template using the pragma
      
      ```fortran
      !$ACC Kernel(adam_kernel), GlobalRange(im*jm*km), LocalRange(0)
      call adam(fgh,fgh_old,im,jm,km)
      !$ACC End Kernel
      ```
      
      This actually uses even lower-level pragmas underneath, but these are normally not exposed. The code generator requires a Fortran subroutine for `adam_kernel`, which initially is a copy original routine `adam`, but can be edited if the OpenCL kernel arguments would be different.

      This generates `module_adam_ocl.f95` which contains all necessary calls to OpenCL using our `OclWrapper` library.
      
      • If we compile and run the code at this stage it will fail because the actual OpenCL kernel does not yet exist.

3. At this stage we have a wrapper with OpenCL API calls and a “kernel” in Fortran, initially a copy of the original subroutine. We convert this kernel to C using our patched version of `F2C_ACC`. Then we further convert this C code to OpenCL, with some cleaning up. At the moment, this stage is manual, because the conversion script is not yet ready.

   2https://github.com/wimvanderbauwhede/RefactorF4Acc/tree/master/F2C-ACC
Figure 3: LES main program (Fortran-95)
• So at this point we have an actual fully working OpenCL version of the code, albeit a purely sequential one.

4. In this work we manually parallelized the kernels. Ideally, we would like to use some compiler transformation to assist us with this, esp. loop merging.

5. Finally, we merged all kernels into a super-kernel, and also merged the wrappers. In this work we did this manually but the process is straightforward to automate.

2.4 Boundary Conditions Computation

A very effective way to compute boundary conditions in OpenCL is the boundary range approach, where we create a global range consisting of the sum of the products of the domain dimensions for each direction: if the domain is $ip \times jp \times kp$ then the boundary range is $ip \times jp + jp \times kp + ip \times kp$. In this way, the local range can be set to auto. The kernel has an if-statement to calculate the different boundary conditions:

```c
if (gl_id < jp*kp) {
    unsigned int k = gl_id / jp;
    unsigned int j = gl_id % jp;
    // do work
} else if (gl_id < jp*kp + kp*ip) {
    unsigned int k = (gl_id - jp*kp) / ip;
    unsigned int i = (gl_id - jp*kp) % ip;
    // do work
} else if (gl_id < jp*kp + kp*ip + jp*ip) {
    unsigned int j = (gl_id - jp*kp - kp*ip) / ip;
    unsigned int i = (gl_id - jp*kp - kp*ip) % ip;
    // do work
}
```

The global range is padded to a multiple of the product of the suggested number of threads and the number of compute units\(^3\), as this results in much better load balancing:

```c
unsigned int m = nthreads*nunits;
if (range % m) != 0) {
    range += m - (range % m)
}
```

Consequently, the last branch in the if statement in the kernel must also be guarded.

2.5 Some Common Techniques

2.5.1 Using OpenCL Vectors for Locality

The LES uses separate arrays for values in x, y and z directions. We merged those arrays into float4 arrays, to improve locality and alignment. Thus, the arrays f,g,h which are actually the values of the force field f in the x, y and z direction, were merged into fgh.

\(^3\)based on CL_KERNEL_PREFERRED_WORK_GROUP_SIZE_MULTIPLE and CL_DEVICE_MAX_COMPUTE_UNITS
program main

#include "module_and_variable_declarations.inc"

!-----------------------------------------------
!
call set(data0, data1, data20, data21, data22, data23, data24, data25, data26, data27, data30, data31, &
im, jm, km, ifb, t, q, ntheta, ntheta1, nmax, dt, re, vn, alpha, beta)
call grid(dx1, dx2, dy1, dy2, dz1, dz2, dz3, dz4, dy3)

call timedata()

call init(kw, jm, im, u, v, w, p, ifb, cn2s, dxs, cn3s, cn4s, cn5s, cn6s, cn61, nmask1, bmask1, &
call ifdata(ncal, data30, n, time, u, im, jm, km, vn, w, p, usum, vsum, wsum, data31, fold, gold, hold, fghold, &
ifb, delx1, dx1, dy1, dz1, diu1, diu2, diu3, diu4, diu5, diu6, diu7, diu8, diu9, sn, f, g, h, z, dt, dxs, cov1, &
cov2, cov3, dv1, vn, cov4, cov5, cov6, dv1, cov7, cov8, cov9, cov10, dxs, n0, n01, n02, n03, n04, &
n05, n06, n07, n08, bmask1, nmask1, amask1, alpha, beta, fx, fy, fz, amask1, zm)

call initialise_les_kernel( &
p, u, v, w, usum, vsum, wsum, f, g, h, fold, gold, hold, &
diu1, diu2, diu3, diu4, diu5, diu6, diu7, diu8, diu9, &
amask1, bmask1, nmask1, amask1, &
cn1, cn21, cn2s, cn3s, cn4s, &
rhs, sn, dxs, dys, dzs, dx1, dy1, dz1, z2, &
dt, im, jm, km, nmax &
)
!
!------main loop

do n = n0, nmax
!

time = float((n-1)*dt)
!
!-------calculate turbulent flow--------

call run_les_kernel ( &
data0, data2, &
im, jm, km, &
dt, dx1, dy2, dz2, &
n, nmax &
p, u, v, w, f, g, h, fold, gold, hold &
)
!
!--------data output --------------

call timers(n, dt, u, v, w)

call avesflow(n, n0, ifb, cn2s, dxs, cn3s, cn4s, cn5s, cn6s, cn61, nmask1, &
avesu, avesv, avew, avesw, avesuw, avesvw, aveswm, aveswmw, umfx, &
avesus, avesvs, avesuv, avesvw, aveswm, u, v, w, p, sm, nmax, umfx, data18, time, data11)

call anicer(n, n0, nmax, im, jm, km, im, dx1, dx2, dy1, dy2, dz1, z2, data22, data23, u, v, nmask1)
!
if(n == nmax) then
stop
end if
!
end do
!
end program

Figure 4: LES main program with call to OpenCL kernel wrapper
2.5.2 Using Private Scalars Instead of Global Arrays

In several places, the LES computes on global arrays, e.g. the f/g/h arrays. Where possible, we replaced the global access to fgh(i,j,k) by a local scalar fgh_ijk, in effect a form of manual caching.

2.5.3 Pre-computing Neighboring Points

The original computation of f/g/h (in the velfg routine) first computes cov and diu arrays for the full domain, and then accesses them at neighboring points to compute f/g/h:

\[
\begin{align*}
\text{covx1} &= \frac{(dx1(i+1)*cov1(i,j,k)+dx1(i)*cov1(i+1,j,k))}{dx1(i)+dx1(i+1)} \\
\text{covy1} &= \frac{(cov2(i,j,k)+cov2(i,j+1,k))}{2} \\
\text{covz1} &= \frac{(cov3(i,j,k)+cov3(i,j,k+1))}{2} \\
\text{covc} &= \text{covx1}+\text{covy1}+\text{covz1} \\
\text{dfu1}_{ijk} &= 2.0* (-\text{diu}_{ijk}\cdot p(i+1,j,k) + \text{diu}_{ijk}\cdot p(i-1,j,k) + \text{diu}_{ijk}\cdot p(i,j+1,k) + \text{diu}_{ijk}\cdot p(i,j,k+1) - 10) \\
\text{df} &= v*n*\text{dfu1}_{ijk} \\
\text{f}_{ijk} &= (-\text{covc}+\text{df})
\end{align*}
\]

By pre-computing the values for the cov and diu arrays at points i+1/j+1/k+1, the loops can be merged:

\[
\begin{align*}
\text{float covx1} &= \frac{(dx1[i+2]*cov_{ijk}.s0+dx1[i+1]*cov_{ijk\_p1.s0})}{dx1[i+1]+dx1[i+2]} \\
\text{float covy1} &= \frac{(cov_{ijk}.s1+cov_{ijk\_p1.s1})}{2.0F} \\
\text{float covz1} &= \frac{(cov_{ijk}.s2+cov_{ijk\_p1.s2})}{2.0F} \\
\text{float covc} &= \text{covx1}+\text{covy1}+\text{covz1} \\
\text{float dfu1}_{ijk} &= 2.0F* (-\text{diu}_{ijk}\cdot s0+\text{diu}_{ijk\_p1.s0})/(dx1[i+1]+dx1[i+2]) + (-\text{diu}_{ijk}\cdot s1+cov_{ijk\_p1.s1}) \\
\text{float df} &= v*n*dfu1_{ijk} \\
\text{fgh}_{ijk.s0} &= (-\text{covc}+\text{df})
\end{align*}
\]

2.6 SOR Algorithm Implementation

The major bottleneck of the LES is the solver for the Poisson equation, which uses Successive Over-Relaxation. The original algorithm is implemented using the red-black scheme:

\[
\begin{align*}
do \text{nrd} = 0,1 \\
\text{do k = 1,km} \\
\text{do j = 1,jm} \\
\text{do i = 1+mod(k+j+nrd,2),im,2} \\
\text{reltmp} &= \omega*(cn1(i,j,k) *( & \\
& cn2l(i)*p(i+1,j,k) & + & \\
& cn2s(i)*p(i-1,j,k) & + & \\
& cn3l(j)*p(i,j+1,k) & + & \\
& cn3s(j)*p(i,j-1,k) & + & \\
& cn4l(k)*p(i,j,k+1) & + & \\
& cn4s(k)*p(i,j,k-1) & - & \\
\text{reltmp} &= \omega*(cn1(i,j,k) * ( & \\
& cn2l(i)*p(i+1,j,k) & + & \\
& cn2s(i)*p(i-1,j,k) & + & \\
& cn3l(j)*p(i,j+1,k) & + & \\
& cn3s(j)*p(i,j-1,k) & + & \\
& cn4l(k)*p(i,j,k+1) & + & \\
& cn4s(k)*p(i,j,k-1) & - &
\end{align*}
\]
Conceptually, the p array is divided in red and black points so that every red point has black nearest neighbors and vice-versa. The new values for p are computed in two iterations (the nrd-loop in the code example), one for the red, one for the black.

While this is very effective for single-threaded code, and in fact also for parallel code on distributed memory systems, it suffers from poor locality because the accesses to p are strided, and the correction computation requires access to all six neighbors of p. As a result, the threads in each compute unit cannot perform coalesced reads or writes. In[5], Konstantinidis and Cotronis explore a GPU implementation of the SOR method and conclude that their proposed approach of reordering the matrix elements according to their color results in considerable performance improvement. However, their approach is not readily applicable to our problem because one the one hand we have a 3-D array which is much harder to reorder than a 2-D array (i.e. the cost of reordering is higher) and also, we cannot use the reordered array as-is, so we would incur the high reordering cost twice.

Therefore, we developed a new technique which we call “twinred double buffering”: rather than using the read-black scheme for updating p, we use a “double buffer” update scheme for p: for nrd=0, p_1 is updated by values from p_0, and for nrd=1, vice versa. If we would use two arrays for this, locality would still be poor, so instead we use an array of vectors of two floats, which we called a “twinred” array. Using this data structure and the double buffering scheme, and assigning the compute units to the k index and the threads in the compute unit to the i index of the array, we obtain coalesced memory access. The difference in performance is indeed huge: our approach is 6× faster than the parallelized version of the red-black scheme.

2.7 Evaluation

In this section we present a validation study of the OpenCL LES by comparing it to the original Fortran version. We ran the LES on a domain of 150x150x90 points, with 50 iterations for SOR (default setup).

2.7.1 Compilers

The compilers used for the comparison were gfortran 4.8.2 for OpenCL code, as well as pgf77 12.5-0 and ifort 12.0.0 for the reference code. We used the following optimizations for auto-vectorization and auto-parallelization:

- gfortran -Ofast -fl loop-parallelize-all -ftree-parall eize-loops=24
- pgf77 -O3 -fast -Mvect=simd:256

11
|                      | #cores | vector size | Clock speed (GHz) | CPI (~FLOPS) | Memory BW (GB/s) |
|----------------------|--------|-------------|-------------------|--------------|-----------------|
| Intel Xeon E5-2640   | 24     | 8           | 2.5               | 480          | 42.6            |
| Nvidia GeForce GX480 | 15     | 32          | 1.4               | 672          | 177.4           |

Table 2: Hardware Performance Indicators

Figure 5: Comparison of OpenCL LES with original Fortran code

- ifort -O3 -parallel

The run time of the F77 and F95 code is the same with all compilers (to within a few %)

2.7.2 Hardware platforms

The host platform is an Intel Xeon E5-2640 0 @ 2.50GHz, dual-socket 6-core CPU with two-way hyperthreading (i.e. 24 threads), with AVX vector instruction support, 32GB memory, 15MB cache, Intel OpenCL v1.2. The GPU platform is an NVIDIA GeForce GTX 480 @ 1.40 GHz, 15 compute units, 1.5GB memory, 250KB cache, NVIDIA OpenCL 1.1 (CUDA 6.5.12).

Table 2 shows the Hardware Performance Indicators for both systems.

2.7.3 OpenCL LES Results

The results of the comparison of the OpenCL code with the F77 and F95 reference code results are summarized in Figure 5. The OpenCL-LES running on the GPU is 7 times faster than the fastest reference runtime.

We implemented all kernels of the LES in OpenCL, because this allows us to keep all data structures in the GPU memory, rather than copying between the host and the GPU. Figure 6
Figure 6: Proportion of time spent in each routine

shows the breakdown of the run time per subroutine in the original LES code. We see that the press routine, which contains the SOR, takes most of the run time, followed by the velfg and les routines. Figure 2.7.3 shows the corresponding times for the actual OpenCL kernels. It should be noted that 50 SOR iterations is actually on the low side to achieve convergence. So the SOR routine will dominate the run time entirely for more iterations.

2.8 OpenCL LES Evaluation Conclusion

The most important outcome of the effort to convert the LES to OpenCL is the development of an open-source toolchain to facilitate porting of Fortran-77 code to OpenCL. Using this toolchain considerably reduces the porting effort, as illustrated by our work. Furthermore, the porting of the LES specifically has led to the development of a novel parallel implementation of the 3-D Successive Over-relaxation algorithm. The resulting performance is very good: the OpenCL LES running on GPU is seven times faster than the original code running on a multicore CPU.

3 The Glasgow Model Coupling Framework

In this section we introduce the Glasgow Model Coupling Framework. We discuss the the longer-term aims of the framework, and status of the current prototype.
3.1 Longer-term aims

Our longer-term aim is to create a system where there is no need for the end user to write any code at all to achieve model coupling. Instead, we envisage that our system will use a scenario, written in a formal way but in a natural language, to express how the models should be coupled. The scenario will serve as the input to a compilation and code generation system that will create the fully integrated model coupling system.

Designing such a specification language is one of the major research tasks to achieve this goal. We plan to use a system based on Multi-Party Session Types [9] to ensure that the scenario results in a correct system that e.g. is deadlock-free and where data exchanges between incompatible senders and receivers are impossible. The Scribble protocol language [4] uses MPST and therefore constitutes a natural starting point for our investigation.

However, in order to make the scenarios accessible to a large audience, we want to explore the use of natural language based specification, e.g. the Gherkin DSL as used in behavior-driven development [11].

Furthermore, apart from the scenario, there is also a need for a formal specification of each model participating in the scenario. One of the reasons why model coupling is currently very difficult is that it takes a lot of effort and skill to determine where e.g. the wind velocity is generated in a given model, what the time loop is, what the variables and their dimensions are, etc. Our aim is to design a model specification that allows a code analysis tool to work out all necessary information – as opposed to a specification that would provide all this information, as such as specification would be difficult and time consuming to produce.

[4]http://www.scribble.org/
3.2 GMCF Model Coupling Operation

Adopting the classification terminology used by Michalakes\(^5\), GMCF adopts a component-based coupling model with dataflow-style peer-to-peer interaction. There is no centralized control or scheduling. Instead, models communicate using a demand-driven mechanism, i.e., they send request to other models for data or control information. At each simulation time step, each model requests time stamps from the models it is coupled with, and waits until it has received the corresponding time steps. This synchronization step ensures that the timing of data exchanges is correct. After syncing, each model can request and/or send data either before or after computation. When the time loop of a model finishes, the model broadcast a message to all communicating models.

3.3 Approach and Status for Current Prototype

To demonstrate the main concepts of our approach to Model Coupling, we created a prototype with the express aim to couple WRF and the DPRI LES model\(^6\) using a producer/consumer pattern. As we will see, the same prototype is readily useable for symmetrical data exchange as well.

We created a modified version of our Glasgow Parallel Reduction Machine (GPRM) framework\(^7\). GPRM is a framework for task-based parallel computing, and one can consider Model Coupling as a special case of this. We call our new framework the Glasgow Model Coupling Framework (GMCF)\(^8\). The necessary modifications are related two different aspects:

- GPRM is a C++ framework, and most scientific models are written in Fortran. Therefore we developed an automated approach to integrating Fortran code into GPRM.

- GPRM uses run-to-completion semantics, i.e., once a task is started, it runs to completion and only then produces output and checks for new input data. In a long-running, time-step-base application such as a NWP model, this approach is not practical, as it would be a huge effort to lift the the time loop out of the existing model and into GPRM. Therefore we created a new API which allows communication between models from inside the model code, obviously essential for model coupling.

Apart from those major changes, we also changed the code organization and the build system to simplify the creation of a coupled model using GMCF.

3.4 More detail on the GMCF architecture

3.4.1 Run-time architecture

The run-time architecture of GMCF is illustrated in Fig. 3.4.1. On startup, the GMCF runtime system creates a fixed number of threads. Each of these threads contains a main loop which blocks on a FIFO.

\(^5\)http://www2.mmm.ucar.edu/wrf/users/workshops/WS2010/presentations/Tutorials/Coupling%20WRF%20Michalakes.pdf
\(^6\)https://github.com/wimvanderbauwhede/LES
\(^7\)https://github.com/wimvanderbauwhede/GannetCode
\(^8\)https://github.com/wimvanderbauwhede/gmcf
Every model is allocated to a thread and interfaces with the other models through a set of FIFOs. The communication between the models is conceptually based on packets of different types. In other words, GMCF uses a message-passing approach. As a result, it is in principle possible to use GMCF for distributed-memory model coupling as well as shared-memory model coupling. When a packet is read from the main RX fifo it can be either consumed directly by the model or stored in a per-type fifo for later use.

The system is demand-driven: there are request packets and response packets. The information to exchange between the models is either time-related, data-related or control-related.

The low-level GMCF API provides functionality to wait on the main FIFO, to separate packets out into per-type FIFOs, to shift packets from the FIFOs and push packets onto the FIFOs. The higher-level API hides the packet abstraction, instead it expresses synchronization and data transfer.

### 3.4.2 Software architecture

Each of the threads in the GMCF runtime instantiates an object of the Tile class and calls its run() method, which implements the wait loop. The Tile class contains the FIFOs and the Core class, which takes care of the actual model calls (Figure 3.4.2).

Our approach is to transform the Fortran top-level program unit into a subroutine which takes a pointer to the tile as argument (Figure 10). All model subroutines become methods of a singleton Core class which inherits from the base Core class which provides the API calls. This approach allows us to hide any state in the object. The Core class has a run() method which selects the model-specific method based on the thread in which it is called at the start of the run.

Furthermore, the Fortran API consists of a generic part and a per-model part, both implemented as modules. The generic part requires the tile pointer as an argument for each call. The per-model API stores this pointer in its module so that the final API calls require no additional arguments.

![GMCF runtime architecture](image_url)
When the Core.run() method calls the model subroutine, this subroutine can use the GMCF C++ API method calls to interact with the FIFOs and so with the other models in the system.

### 3.4.3 Code generation architecture

The main purpose of GMCF is to make model coupling easier. Therefore, we try to minimize the necessary changes to the original code, and in fact our long-term aim is to entirely automate the process. Currently, the user has to manually insert the actual model coupling API calls.

Apart from that, the build system takes care of the entire integration. This is less obvious than might seem at first: the GMCF runtime and API are written in C++, so it is necessary to generate code to interface with the Fortran model code. The necessary information required from the user is very limited: the full path of the top-level program unit of each model. The build system analyses this program unit and adds the necessary code for GMCF integration, and generates all required interface code.

### 4 Coupling WRF and LES

In this section we present the implementation and preliminary results of coupling WRF and the OpenCL LES using the GMCF.
Figure 10: GMCF Fortran-C++ integration and code generation
WRF is used to compute the wind profile as input for LES. In the original version of the LES, this input is manually extracted from WRF and hardcoded in the Fortran source.

4.1 Implementation Details

In order to achieve coupling, some modifications are required to both WRF and LES. On the one hand, the build system needs to be modified so that the model is compiled into a library rather than an executable. For LES, as we use SCons, this is trivial. WRF uses a complex build infrastructure based on make. The changes are still very small, and some of the changes are actually patches to bugs in the WRF build system. In fact, the modified WRF build system can now build WRF executables using both Fortran and C++ main programs.

The source code of the main program unit needs to be modified to make it a subroutine, this is a very minor change. The other main changes are related to the actual coupling. Our approach is to create a per-model API based on the generic GMCF API. Eventually, this per-model API will be automatically generated. Then the API is used to achieve synchronization and data exchange.

4.1.1 Creating a gmcf subroutine from the main program unit

The changes to main/wrf.F and the LES main.f95 required to be able to use GMCF are shown below; these changes are auto-generated by the build system, the user only needs to provide the name of the original program and of the new top-level subroutine.

```fortran
subroutine program_wrf_gmcf(gmcf_ptr, model_id) ! This replaces 'program wrf'
  use gmcfAPI ! gmcf
  use gmcfAPIwrf ! gmcf
end subroutine program_wrf_gmcf
```
USE module_wrf_top, only : wrf_init, wrf_dfi, wrf_run, wrf_finalize
IMPLICIT NONE

integer(8), intent(In) :: gmcf_ptr  ! gmcf
integer , intent(In) :: model_id  ! gmcf
call gmcfInitWrf(gmcf_ptr, model_id)  ! gmcf
! Set up WRF model.
CALL wrf_init
! Run digital filter initialization if requested.
CALL wrf_dfi
! WRF model time-stepping. Calls integrate().
CALL wrf_run
! WRF model clean-up. This calls MPI_FINALIZE() for DM parallel runs.
CALL wrf_finalize
end subroutine program_wrf_gmcf

And for the LES:

subroutine program_les_gmcf(gmcf_ptr, model_id)
! ... LES-specific use statements ...
use gmcfAPI
use gmcfAPIles
integer(8), intent(In) :: gmcf_ptr
integer , intent(In) :: model_id
! ... LES-specific declarations ...
call gmcfInitLes(gmcf_ptr, model_id)
! ... LES-specific code
end subroutine program_les_gmcf

4.1.2 Time synchronization and data exchange

The actual synchronization and data exchanges also requires very few changes, currently these have to be done manually. In WRF, these are in frame/module_integrate.F:

MODULE module_integrate
CONTAINS
RECURSIVE SUBROUTINE integrate ( grid )
  use gmcfAPI
  use gmcfAPIwrf
! ... WRF-specific code ...
! WRF main time loop
  DO WHILE ( .NOT. domain_clockisstopsubtime(grid) )
    ! Synchronise simulation times between WRF & LES
    call gmcfSyncWrf
! ... Actual model computations ...
    !Prepare the wind profile
    call gmcfCreateWindprofile(grid%u_2,grid%v_2,grid%w_2)
    ! Send the data to the LES when requested
    call gmcfPostWrf
  END DO
call gmcfFinishedWrf
! ... WRF-specific code ... 
END SUBROUTINE integrate 
END MODULE module_integrate

In LES, the time loop is in main.f95:

    do n = n0,nmax
        time = float(n-1)*dt
        ! Synchronise simulation times between WRF & LES
        call gmcfSyncLes
        ! Request and receive the data from WRF
        call gmcfPreLes
        if (can_interpolate == 0) then
            can_interpolate = 1
        else
            ! Interpolate the value for the current LES time step
            call gmcfInterpolateWindprofileLes(u,v,w)
        ! ... Actual model computations
        end if !interpolate guard
    end do 
end do 
call gmcfFinishedLes

Here the code is a little bit more involved because LES only takes data from WRF every simulated minute but simulates with a resolution of half a second. The WRF data are interpolated and the interpolation can only start after two time steps, hence the guard.

The LES required other changes as well, because it used a fixed wind profile rather than taking data from WRF. However, these changes are not specific to model coupling so they are not included.

4.1.3 Per-model API

The changes to the model code are very small because the GMCF operation is abstracted into a per-model API. This API consists of a small number of subroutines:

- The Init call initializes GMCF for the given model.
- The Sync call synchronizes the model with the other models it’s communicating with.
- The Pre and Post calls are taking care of the actual data exchange, Pre is before computation, Post is after computation.
- The Finished call informs all other models that the given model has finished.

These subroutines are currently written manually, the next step is generate the code based on annotations.

- For Init and Sync, what is required is the time step information relative to some reference, typically the model with the largest time step.
• For the Pre and Post calls, we need to know the names, types and sizes of the variables containing the data to be exchanged.

• The Finished call can be generated without extra information.

There are also some API calls that are not as generic as the ones above: the data received from another model must be assigned to a variable in the given model, and often we only want to send a portion of a multidimensional array, so we may want to create intermediate variables. In the case of WRF and LES, we have `gmcfInterpolateWindprofileLes(u,v,w)` and `gmcfCreateWindprofileWrf(u,v,w)` but actually the u,v,w are not quite identical in both models. Currently, these subroutines have to be written by hand. In order to generate the code for these subroutines, we need to describe exactly how a variable from one model maps to a variable of another model. Our approach is to create an intermediate variable for each exchange and define the mapping to that variable for each model.

4.2 Building and Evaluation

Thanks to the extensive code generation and automation, building the GMCF executable is quite simple: first, specify the models to couple using a configuration file. This file is used to build the GMCF framework. Then build each model into a library. Then link the GMCF framework library and the model libraries into the top-level executable. Detailed instructions are available on GitHub.

For the evaluation we tested the correctness of the time step synchronization and the data exchange. And actual evaluation of the performance requires the WRF input files used for creating the simulation that generates the wind profile for the LES, and this has not been done yet.

However, we have successfully built and run a model coupling of WRF using OpenMP on a multicore GPU with the OpenCL LES running on the GPU.

5 Conclusions

The overall conclusions of this two-month pilot project are very encouraging:

• We have demonstrated that our approach to model coupling, aimed at modern heterogeneous manycore nodes, can be used to couple a complex NWP simulator such as WRF, parallelized using OpenMP, with a custom LES simulator running on a GPU using OpenCL.

• The LES is a very high-resolution simulator, therefore GPU acceleration was essential and we have shown that we can achieve a speed-up of seven times using OpenCL on the GPU.

• Furthermore, our model coupling framework is designed to be useable for automatic generation from scenarios and specifications, and this will be the focus of our future work. Already, using GMCF requires only very minor modifications to the original model source code and build system.
• All software developed during this project has been open sourced and is available at
  https://github.com/wimvanderbauwhede

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