GPU Support for Automatic Generation of Finite-Differences Stencil Kernels

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Motivation

 Many physic's problems involve the solution of Partial Difference Equations (PDE)

Poisson's equation:

Wave equation:

$$\nabla^2 u = f(x, y, z)$$

Heat flow equation: $k\frac{\partial}{\partial t}$

$$k\frac{\partial^2 u}{\partial^2 x} = \frac{\partial u}{\partial t}, k > 0$$
$$\nabla^2 u = \frac{1}{v^2}\frac{\partial^2 u}{\partial^2 t}$$

Problem

It is difficult to write computational solutions to these problems and solve them efficiently.

Looking for...

 A solution that will enable field specialists to solve their computational demands without digging into programming technicalities.

Domain Specific Language

- Provides a high-level abstraction for a specific domain
- **2** Divides the matter of problem definition and problem computation
- 3 Enables execution of the same code in different architectures with, ideally, no modifications.
- Examples of DSL for solving PDEs: Devito, Firedrake, FEniCS, and esys-Escript.

Devito



- PDE solver which uses Finite Difference method
- Uses DSL for problem specification in Python
- Automatically generates code in C
- Symbols and loop optimizations: basic, advanced and aggressive

Devito references Luporini et al. 2018[1] and Louboutin et al. 2019[2]

Devito - Example

3D Acoustic Wave Equation with damping

$$m(x,y,z) \frac{d^2u(t,x,y,z)}{dt^2} - \nabla^2 u(t,x,y,z) + \eta \frac{du(t,x,y,z)}{dt} = 0$$

Representation using Devito with Sympy

eqn = model.m * u.dt2 - u.laplace + model.damp * u.dt

Devito - Generated C code

```
1 for (int x = x_m: x \le x_M: x += 1)
    {
 3
      #pragma omp simd aligned(damp,m,u:32)
 4
      for (int v = v_m: v \le v_M: v += 1)
        float r0 = 1.0F*dt*m[x+2][y+2][z+2] +
 7
                    5.0e - 1F * (dt * dt) * damp[x+1][v+1][z+1];
8
9
        u[t1][x+2][y+2][z+2] =
          1.0F*(-dt*m[x+2][y+2][z+2]*u[t2][x+2][y+2][z+2]/r0 +
                 (dt*dt*dt)*u[t0][x + 1][y + 2][z + 2]/r0 +
                  dt*dt*dt)*u[t0][x + 2][y + 1][z + 2]/r0 +
                  dt*dt*dt)*u[t0][x +
                                       21[y +
                                              21[z +
                                                      1 / r0 +
14
                  dt*dt*dt)*u[t0][x + 2][y +
                                              21[z +
                                                      31/r0 +
                  dt*dt*dt)*u[t0][x + 2][y + 3][z +
                                                      21/r0 +
                  dt*dt*dt)*u[t0][x + 3][y + 2][z + 2]/r0) +
          2.0F*dt*m[x+2][y+2][z+2]*u[t0][x+2][y+2][z+2]/r0 +
          5.0e - 1F * (dt * dt) * damp[x+1][y+1][z+1]*u[t2][x+2][y+2][z+2]/r0 - 0
18
          6.0F*dt*dt*dt*u[t0][x + 2][y + 2][z + 2]/r0;
19
21
```

Algorithm 1: A code segment auto generated from Devito using core backend with no optimization. Represents the propagation update for stencil of space order 2.

Stencil - 2nd space order



Figure: 2nd order stencil

 $u_{t+1,x,y,z} =$ $\alpha * u_{t-1,x,y,z} + \beta * u_{t,x,y,z} +$ $\gamma * (u_{t,x+1,y,z} + u_{t,x-1,y,z} +$ $u_{t,x,y+1,z} + u_{t,x,y-1,z} +$ $u_{t,x,y,z+1} + u_{t,x,y,z-1}$)

Stencil - 8th space order



Figure: 8th order stencil

$$u_{t+1,x,y,z} = \alpha * u_{t-1,x,y,z} + \beta * u_{t,x,y,z} + \gamma * (u_{t,x+1,y,z} + u_{t,x-1,y,z} + u_{t,x,y+1,z} + u_{t,x,y-1,z} + u_{t,x,y,z+1} + u_{t,x,y,z-1}) + \delta * (u_{t,x+2,y,z} + u_{t,x-2,y,z} + u_{t,x,y+2,z} + u_{t,x,y-2,z} + u_{t,x,y,z+2} + u_{t,x,y,z-2}) + \epsilon * (u_{t,x+3,y,z} + u_{t,x-3,y,z} + u_{t,x,y+3,z} + u_{t,x,y-3,z} + u_{t,x,y,z+3} + u_{t,x,y,z-3}) + \zeta * (u_{t,x+4,y,z} + u_{t,x-4,y,z} + u_{t,x,y+4,z} + u_{t,x,y-4,z} + u_{t,x,y,z+4} + u_{t,x,y,z-4})$$

Devito works for CPU...



Comparison between x86 CPU and NVIDIA GPUs - (chart from NVDIA presentation)

How can we support GPU...

- So, we now can modify Devito to generate code for GPU architecture
- Which parallel programming platform: CUDA, OpenCL, OpenACC...?

OPS



- Oxford Parallel Structured Software (OPS)
- Framework for the execution of multi-block structured mesh applications
- Uses source-to-source translation
- Generates code for the following platforms
 - CUDA
 - OpenACC
 - OpenCL
 - MPI
 - OpenMP

OPS reference Reguly et al. 2014[3]



To use the GPU's capability to solve PDEs problems

- To use Devito for problem specification and optimizations
- To use OPS framework to generate code targeted for GPU platform
- To integrate Devito and OPS to generate GPU code from a symbolic representation

Diagram displaying Devito and OPS integration



Steps implemented

- 1 Identified parallelizable code
- 2 Translated Devito expressions into OPS expressions
- 3 Generated kernel function
- 4 Partial generation of host code

Step 1 - Devito simple example

```
exemple.py
from devito import Eq, Grid, TimeFunction, Operator
grid_2d = Grid(shape=(4, 4))
v = TimeFunction(name='v', grid=grid_2d, time_order=2, save=10)
equation = Eq(v.forward, v+1)
operator = Operator(equation)
print(operator)
```

Step 2 - Code generated with backend core

```
#define _POSIX_C_SOURCE 200809L
#include "stdlib.h
#include "math.h
#include "sys/time.h'
#include "xmmintrin.h
#include "pmmintrin.h'
struct dataob1 {
      void *restrict data:
      int * npsize:
      int * dsize;
      int * hsize
      int * hofs;
      int * oofs
struct profiler {
    double section0;
int Kernel(struct dataobj *restrict v_vec, const int time_M, const int time_M, struct profiler * timers, const int x_M, const int x_M, const int
v_M. const int v_m) {
    \int_{0}^{1} \int_{0}^{1} \frac{1}{1} 
      /* Flush denormal numbers to zero in hardware */
       _MM_SET_DENORMALS_ZERO_MODE(_MM_DENORMALS_ZERO_ON);
         MM_SET_FLUSH_ZERO_MODE(_MM_FLUSH_ZERO_ON):
      for (int time = time_m; time <= time_M; time += 1){</pre>
             struct timeval start_section0, end_section0;
             gettimeofday(&start_section0, NULL);
             for (int x = x m: x <= x M: x += 1) {
                    #pragma omp simd aligned(v:32)
                   for (int y = y_m; y <= y_M; y += 1) {
    v[time + 1][x + 1][y + 1] = v[time][x + 1][y + 1] + 1;</pre>
             gettimeofday(&end_section0, NULL);
             timers->section0 += (double)(end_section0,tv_sec-start_section0,tv_sec)+(double)(end_section0,tv_usec-start_section0,tv_usec)/1000000;
```

Step 3 - Identify parallelizable region

```
#define _POSIX_C_SOURCE 200809L
#include "stdlib.h"
#include "math.h"
int Kernel(float * v, const int time_M, const int time_m, const int x_M,
            const int x_m, const int y_M, const int y_m)
  for (int time = time_m; time <= time_M; time += 1)</pre>
   for (int x = x_m; x \le x_M; x += 1)
      for (int y = y_m; y \le y_M; y += 1)
        v[time + 1][x + 1][y + 1] = v[time][x + 1][y + 1] + 1;
  return 0;
```

Step 4 - Replacing with OPS API



Step 5 - OPS API - ops_par_loop

```
#define POSIX C SOURCE 200809L
#include "stdlib.h"
#include "math.h"
int Kernel(float * v. const int time M. const int time m. const int x M.
            const int x_m, const int y_M, const int y_m)
  for (int time = time_m: time <= time_M: time += 1)</pre>
   <u>ops_par_loop(0PS_K</u>ernel_0, "0PS_Kernel_0", block, 2, {x_m, x_M, y_m, y_M},
                 ops_arg_dat(v_dat[t0], 1, S2D_VT0_1PT, "float", OPS_READ),
                 ops_arg_dat(v_dat[t1], 1, S2D_VT1_1PT, "float", OPS_WRITE));
  return 0;
```

Step 6 - Device Code



Experiment

3D Acoustic Wave Propagation

- Time step 0.001 s, Total time: 30 s
- Domain size of: $1 \ km \times 1 \ km \times 1 \ km$ with grid points: 32^3 , 64^3 , 128^3 , 256^3 , 512^3
- Ricker source injection with peak frequency 10 Hz
- Space Order: 4, 8, 12, 16 and 24
- Single layer velocity model of 2 km/s
- Absorbing boundary

Compilation and Execution

- Compiler: nvcc 10.1
- Flags: -Xcompiler="-std=c99" -O3
- Median of 5 executions

Architectures Evaluated

	Titan Z	Tesla V100
Memory Bandwidth (GB/s)	336 x2	900
Precision Peak Performance (GFLOPS)	4746	14000
Double Precision Peak Performance (GFLOPS)	1582	7000
Memory (GB)	6 x2	16

Graphical cards specification from vendors

Execution Time

Wave Propagation execution time per grid size in different GPUs



Execution time in different GPUs of an acoustic isotropic 3D wave propagation with 30,000 time steps for 4^{th} space order stencil.

Roofline Model for a Tesla V100 GPU



Roofline Model for a GTX Titan Z



Challenges

Challenges

- To avoid unnecessary memory copies from CPU to GPU
- To keep up with OPS and Devito upgrades

Conclusion

- Created an extension of Devito to enable code generation for the OPS syntax
- Successfully tested the solution with wave propagation algorithm
- Observed that the execution time from approximately 2 hours in GTX Titan Z took 4 minutes in V100
- Achieved up to 63% of the peak performance on V100

Where to find...

Source code

- Devito: https://github.com/opesci/devito
- OPS: https://github.com/OP-DSL/OPS

Website

- https://www.devitoproject.org/index.html
- https://op-dsl.github.io/

Talk to us

Devito slack community: devitocodes.slack.com

References I

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