Acceleration made easy - Speeding up your science codes with (fairly) little effort

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eResearch NZ 2016

New Zealand eScience Infrastructure

Overview

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2. Accelerating Python with PyOpenCL/PyCUDA
3. Accelerating C, C++, and Fortran with OpenACC
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What accelerators are and when to use them

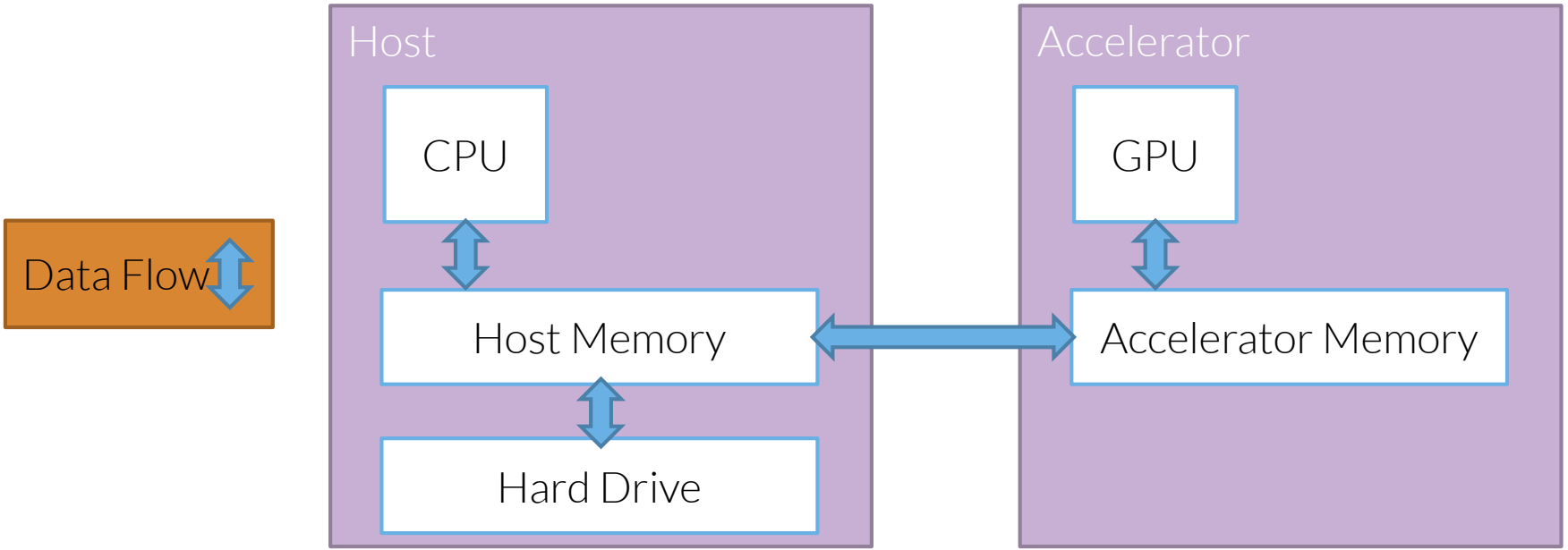
Accelerators

- Accelerators: co-processors that perform some functions faster than CPUs
- Applications include
  - Signal processing, Cryptography, Graphics
  - Scientific computing
- We will focus on scientific computing with GPUs
- Ongoing NeSI project: “Exploring tsunami and flooding code speed-up using GPU processing”

Using accelerators

- CPU – mostly serial computation (each step in a program is executed in order)
- GPU – highly parallel computation (many steps executed at the same time)
- Accelerators only useful for parallel compute-dominated applications (not, e.g., disk I/O)

Typical Accelerator Computing (today!)



Data needs to travel – this takes time and adds complexity

Accelerating Python with PyOpenCL/PyCUDA

PyOpenCL/ PyCUDA

- Python: popular multi-purpose computer language
- PyOpenCL/PyCUDA: extension packages for accelerators
- Full access to OpenCL/CUDA APIs
- We will focus on PyOpenCL Array syntax
- Same code runs on laptop and on HPC (e.g. NeSI Pan cluster, cloud, …)

PyOpenCL/ PyCUDA

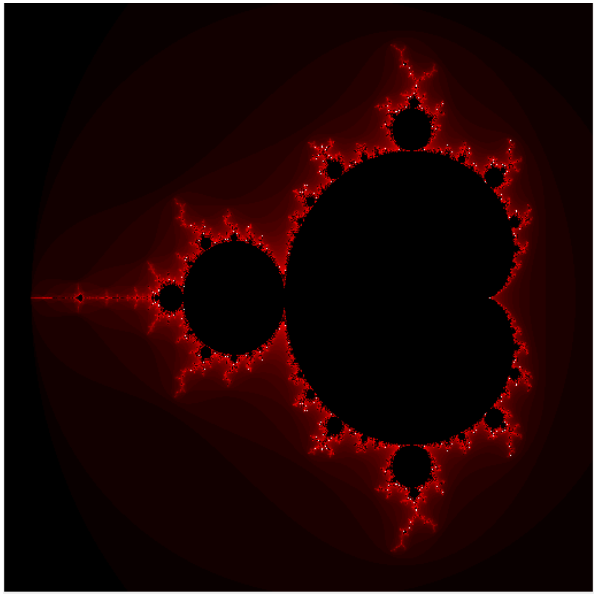
NumPy

```
# Program loads data into “data_np”




# Compute part
x_np = 2 * data_np
result_np = 1.4 * np.exp(-x_np * x_np)




# Rest of program
```

PyOpenCL Arrays

```
# Program loads data into “data_np”
# Program initialises accelerator

# Copy data to accelerator
data_cl = cla.to_device(queue, data_np)

# Compute part – entirely on accelerator!
x_cl = 2 * data_cl
result_cl = 1.4 * clm.exp(-x_cl * x_cl)

# Copy data back to host memory
result_np = result_cl.get()

# Rest of program
```

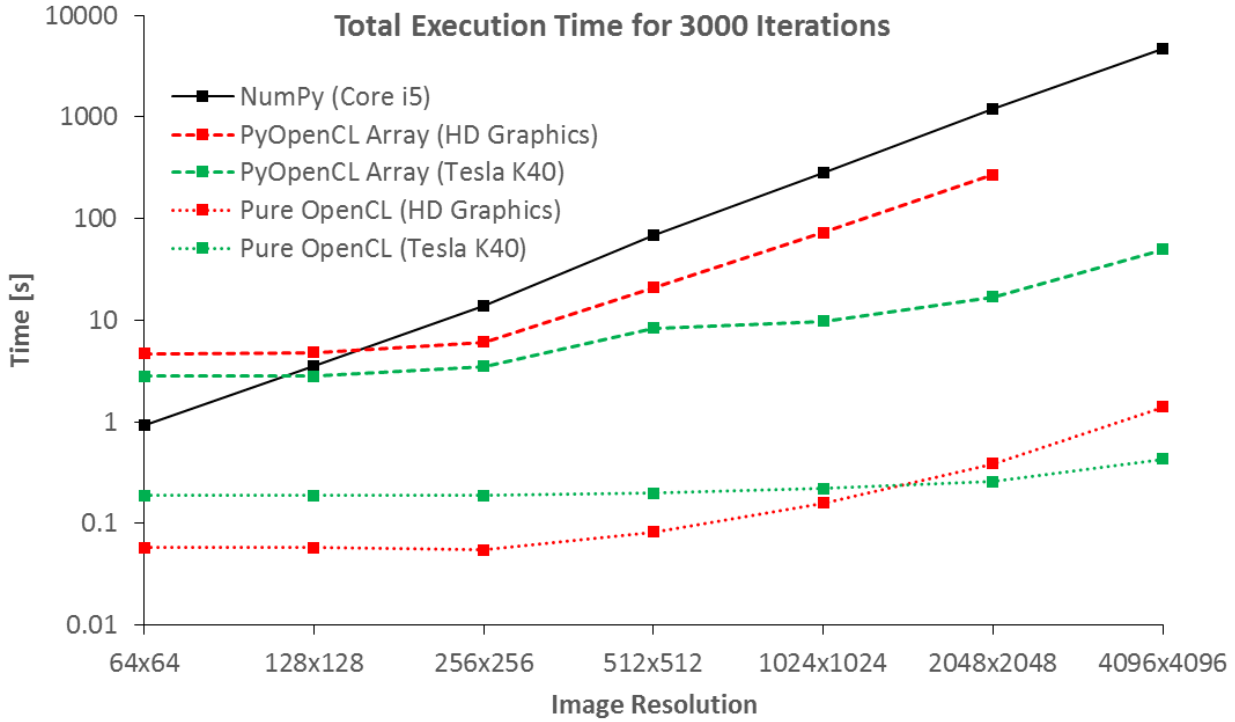
PyOpenCL/ PyCUDA



- Mandelbrot is idealised case - perfect match for GPUs due to inherent parallelism

PyOpenCL/ PyCUDA

Mandelbrot Performance



PyOpenCL/ PyCUDA

- Good speed-up possible with PyOpenCL Arrays, but need large work sizes
- Hand-coded OpenCL is more efficient - just as with NumPy vs. C/Fortran
- NeSI can help with getting you started!

Accelerating C, C++, and Fortran with OpenACC

OpenACC

- Various ways to use accelerators in C, C++ and Fortran: scientific libraries, CUDA, OpenCL, …
- OpenACC: compiler directives for “offloading” loops, main code stays on CPU
- Useful for existing code (NeSI tsunami project)

OpenACC

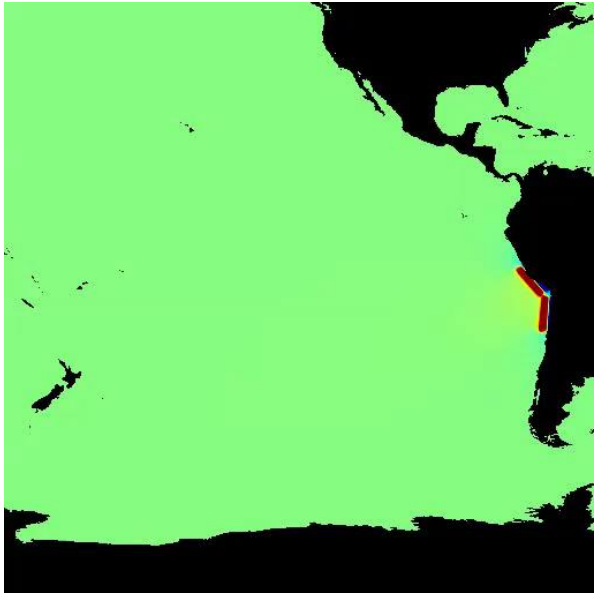
C

```
/* Program loads data into “data” */


/* Compute part */


for (int i = 0; i < n; i++) {
   float x;
   x = 2.0 * data[i];
   result[i] = 1.4 * exp(-x*x);
}

/* Rest of program */
```

C with OpenACC

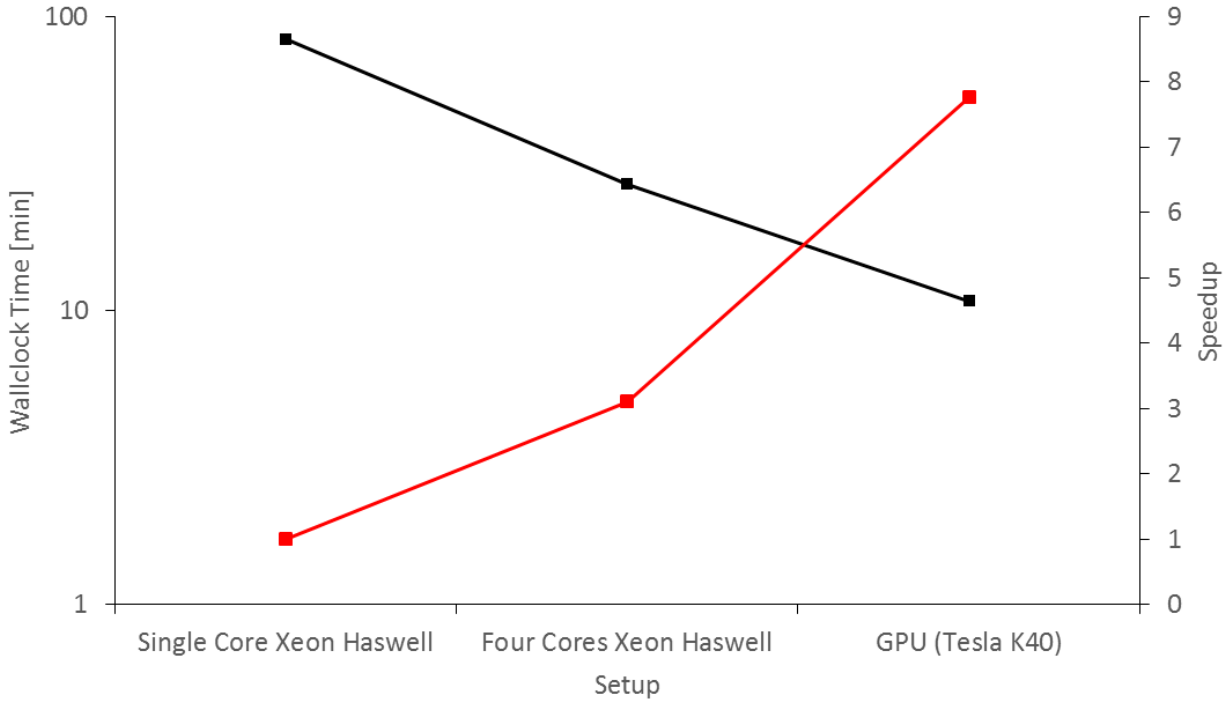
```
/* Program loads data into “data”
    Program initialises accelerator */

/* Offload compute part to accelerator */
#pragma acc kernels \
 copy(data[0:n], result[0:n])
for (int i = 0; i < n; i++) {
   float x;
   x = 2.0 * data[i];
   result[i] = 1.4 * exp(-x*x);
}

/* Rest of program */
```

NeSI Tsunami Project



- Basilisk (www.basilisk.fr)
- Shallow Water simulation of tsunami wave
- Model by Emily Lane, NIWA

Basilisk Performance (preliminary!)



OpenACC

- Good speed-ups, but data locality can be complex
- Hardware knowledge needed for optimisations
- NeSI can help with getting you started!

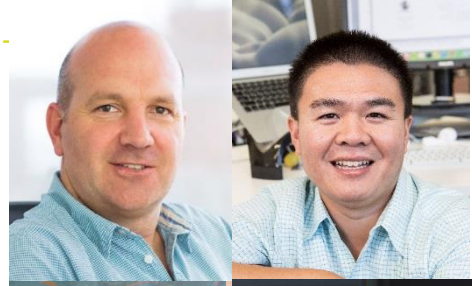
Summary

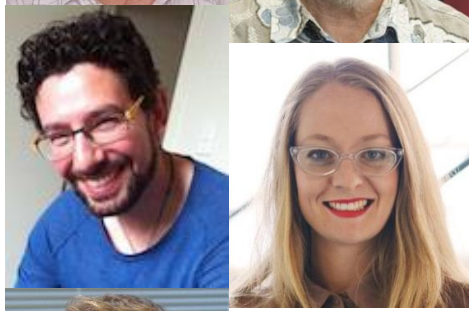
Summary

- PyOpenCL/PyCUDA and OpenACC: easy ways to use accelerators
- Workloads need to be sufficiently large
- Some algorithms may need to be changed
- Talk to us if you would like to try!

NeSI at eResearch NZ 2016

Tuesday 11:15 (Queenstown)	NeSI Update	Nick Jones
Tuesday 11:45 (Remarkables)	Growing NZ's Researcher's Computing Capability	Georgina Rae & John Rugis
Tuesday 14:30 (Queenstown)	An HPC Implementation of the Finite Element Method	John Rugis
Tuesday 16:00 (Queenstown)	The NeSI National Platform Framework	Michael Uddstrom
Tuesday 16:30 (Queenstown)	Early Experiences with Cloud Bursting	Jordi Blasco
Tuesday 16:30 (Remarkables)	NeSI – NZGL Alliance	Dan Sun & Nic Mair
Tuesday 17:00 (Queenstown)	Acceleration Made Easy	Wolfgang Hayek



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Thanks for listening!