Introduction To GPU Programming

Martin Schwinzerl, Riccardo de Maria HSS Section Meeting, CERN June 3rd, 2020

Goals

- Overview about the GPU computing landscape (Concepts, Hardware)
- ► Introduce the (currently) two most established frameworks
- ▶ Provide Simple Examples to get started
- Outline the typical workflow within a GPU enhanced Program
- ▶ Performance Analysis& Constraints
- **▶ Motivate Design-Decisions & Implementation of SIXTRACKLIB**

Note: This is an interactive Jupyter Notebook - all presented examples are designed to work and allow you to experiment with them. Notbook available from: github.com/martinschwinzerl/sixtracklib-presentations/tree/master/20200603 hss_section_meeting)

- **▶** Low-End Gaming: ≈ 100 EUR
 - Still equal or better FP
 performance than typical CPU in
 SP and DP
 - > DP performance usualy much poorer than SP!

- ► AMD RX 560 TI 4 GByte

 - ⇒ SP Peak Performance 2406

 GFLOP/s
 - DP Peak Performance 163
 GFLOP/s ≈ 1/16 SP
- ▶ NVidia GTX 1050 Ti 4 GByte
 - > 768 Cores
 - ⇒ SP Peak Performance 1981

 GFLOP/s
 - DP Peak Performance 62
 GFLOP/s = 1/32 SP
- ▶ SP ... IEEE754 32Bit single precision floating point numbers
- ▶ DP ... IEEE754 64Bit double precision floating point numbers

- ► Low-End Gaming: ≈ 100 EUR
- **▶** High-End Gaming: ≤ 1000 EUR

 - \triangleright DP performance varies!

- ▶ NVidia GeForce RTX 2080 8GByte
 - ⊳3072 Cores
 - ⊳ SP Peak Performance 8920

GFLOP/s

DP Peak Performance 279

GFLOP/s = 1/32 SP

- ► AMD RX Vega 64 8 GByte
 - > 3840 Cores
 - ⇒ SP Peak Performance 11518

GFLOP/s

DP Peak Performance 720

GFLOP/s = 1/16 SP

- ▶ SP ... IEEE754 32Bit single precision floating point numbers
- ▶ DP ... IEEE754 64Bit double precision floating point numbers

- ► Low-End Gaming: ≈ 100 EUR
- ► High-End Gaming: ≤ 1 kEUR
- **▶** Hybrid HPC: ≈ 3 kEUR 8 kEUR

 - ⊳DP performance ≈ 1/2 SP
- **Server HPC:** ≈ 6 kEUR 8 kEUR
 - Similar performance characteristics as with hybrid HPC, but
 - \triangleright No video outputs, i.e.
 - "Accelerator Card"

- NVidia Titan V 12 GBytes
 - > 3072 Cores
 - > Hybrid card Video outputs available
 - ⊳ SP Peak Performance 12288
 GFLOP/s
 - DP Peak Performance 6144
 GFLOP/s = 1/2 SP
- ► AMD Radeon Instinct MI50 16 GBytes
 - > 3840 Cores
 - ⊳ SP Peak Performance 13400
 GFLOP/s
 - DP Peak Performance 6700 GFLOP/s = 1/2 SP
- ▶ SP ... IEEE754 32Bit single precision floating point numbers
- ▶ DP ... IEEE754 64Bit double precision floating point numbers

- ► Low-End Gaming: ≈ 100 EUR
- ► High-End Gaming: ≤ 1 kEUR
- ► Hybrid HPC: ≈ 3 kEUR 8 kEUR
- ► Server HPC: ≈ 6 kEUR 8 kEUR
- ► AI Server HPC: ≈ 6 kEUR 10 kEUR

- Substancial Integer, SP and Half-Precision Performance or
- ► TOPS ... Trillion operations per second of dedicated neural network computes
- ► Task-specific Hybrid systems with FPGA and/or CPU enhancements
- No classical GPU, no video outputs "Accelerator Card"

</div>

- ▶ SP ... IEEE754 32Bit single precision floating point numbers
- ▶ DP ... IEEE754 64Bit double precision floating point numbers

CPUs versus GPUs

	CPU	GPU	
Cores / Compute Units	2 - 64 (128 HT/SMT)	16 - 80	Compared to CPUs, GPUs have:
Arithmetic Units / Core	2-8	64	 More arithmetic units (in particular SP) Less logic for control flow
Peak Performance SP	24-3200 GFLOP/s	1000-19500 GFLOP/s	 Less registers per arithmetic units Less memory but larger memory bandwidth
Peak Performance DP	12-1600 GFLOP/s	50-9700 GFLOP/s	

- ▶ SP ... IEEE754 32Bit single precision floating point numbers
- ▶ DP ... IEEE754 64Bit double precision floating point numbers
- ► For CPUs: DP performance is roughly 1/2 of SP performance (YMMV)

Introducing Parallelism

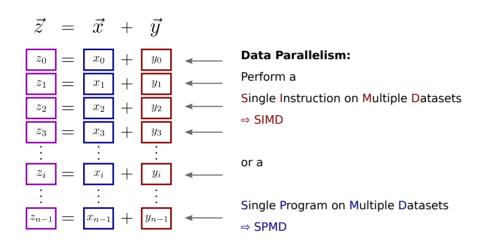
► Task Parallelism: perform multiple tasks on the same dataset

Example: Check if a number is a prime number by checking divisibility in parallel

Introducing Parallelism

 \vec{x} , \vec{y} , $\vec{z} \in \mathbb{R}^n$

▶ **Data Parallelism:** perform the same task on multiple datasets Example: Vector addition



Example: Vector Addtion on the GPU using CuPy

Cf. https://github.com/cupy/cupy and https://cupy.chainer.org/ for reference

```
In [1]: | # If you have a NVidia GPU, one of the simplest ways to offload calculations to
        the GPU is to use CuPv
        import cupy
        import numpy as np
        N = 100000000 # 1.0e7 elements
        x host = np.random.rand( N )
        y host = np.random.rand( N )
        # Create vectors of random numbers. CuPy handles all the required steps behind
        the scenes
        x = cupy.asarray(x host)
        y = cupy.asarray( y host )
        # x and y are cupy entities that "live" on the GPU while
        # x host and y host "live" in regular memory
        # The same applies to the result of the calculation z:
        z = x + y # Vector addition is actually performed on the GPU
```

```
In [2]: # in order to make use of the result outside of the GPU,
# we have to convert z into a regular numpy array
z_host = cupy.asnumpy( z )

# Compare result to calculation on CPU
print( f"calculation on host and device yield same result: {np.allclose( z_host, x_host + y_host, rtol=0.0, atol=1e-16)}" )

del x, y, z, x_host, y_host, z_host
```

calculation on host and device yield same result: True

Overview: Frameworks, Libraries, Toolboxes for GPU Programming

- ▶ High-Level Libraries and Applications
 - CuPy: numpy-like python module for NVIDIA GPUs
 - > Tensorflow: mostly support for NVIDIA GPUs, some opportunities to use other cards via SYCL
 - > Matlab (currently only NVIDIA GPUs are supported)
 - ⊳Julia
 - > Mathematica
 - ▷....
- ► HPC frameworks & libraries
 - > OpenMP: ≥ version 4.5, allows offloading to GPU targets (for AMD, a recent gcc or clang is required)
 - > OpenACC: similar to OpenMP. Traditionally NVIDIA focused but recently got capabilities to offload to AMD
 - ▶ Intel OneAPI
 - > ArrayFire: optimized functions and data-structures to exploit parallelism on both GPUs and CPUs

Overview: Frameworks, Libraries, Toolboxes for GPU Programming

- ► Low-Level Programming Frameworks
 - > ROCm: collection of libraries & tools for AMD GPUs, provides OpenCL backend
 - > HIP: abstract language to write GPU programs (AMD, open-source), allows "automated" translation of CUDA programs into HIP
 - > SyCL: "modernized" abstraction on-top of OpenCL, uses SPIR

 - CUDA C99/C++1x based framework for NVIDIA GPUs (some parts are opensource, drivers etc. are proprietary)
 - ▷ OpenCL: Vendor neutral computing language, allows to target CPUs, GPUs, FPGAs, Signal Processors

► Increasingly Important: Code-Transformation tools and intermediate code representations

▷ PTX: Parallel Thread Execution language, used by NVIDIA for CUDA

▷ SPIR, SPIR-V: Standard Portable Intermediate Representation, cross-platform open standard maintained by the Khronos Group; Central in newer graphic

standards and newer iterations of OpenCL

Comparison: OpenCL versus CUDA

▶ OpenCL

- ▶ Hardware Neutral: GPUs, CPUs,FPGAs, Signal Processors▶ Common, standardized software
- > Common, standardized softward stack (Khronos Group) + vendor specific impl.
- > "Programming to the least common denominator"
- OpenCL 1.2: Still most
 commonly used, C99 kernel
 language, limited set of features
- DopenCL 2.x: some support from AMD and Intel
- DopenCL 3.0: recently specified, modular refactoring of OpenCL 2.x

► CUDA

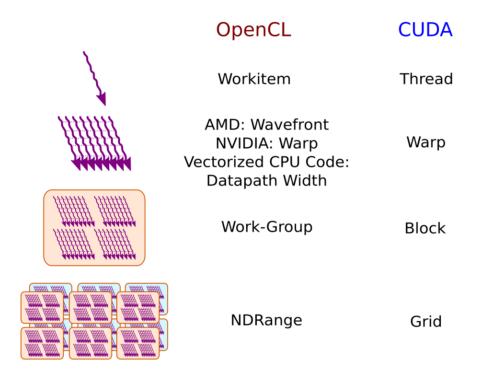
- ⊳ Software implementation only available from NVIDIA, includes libraries, debuggers, profilers, memory checkcers, etc.
- Software and hardware tightly integrated (versioning, "compute capabilites")

- Primarily: Run-time compilation of the kernels
- ► Kernel code has to be available at run time, compile for selected device at runtime
- ► Single-file compilation similar to the default in CUDA available (SyCL)

- ▶ **Primarily**: Single-file compilation. nvcc compiler replaces sysetem compiler for .cu files -> binary compability between system compiler, system libraries, graphic stack, etc. required
- ► Run-time compilation approach simliar to the default with OpenCL is available (NVRTC)

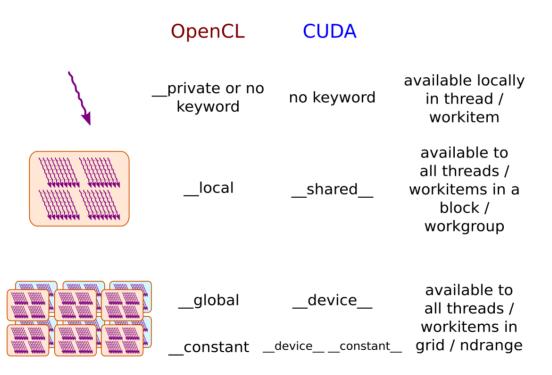
CUDA and OpenCL: Different But Similar - Grid

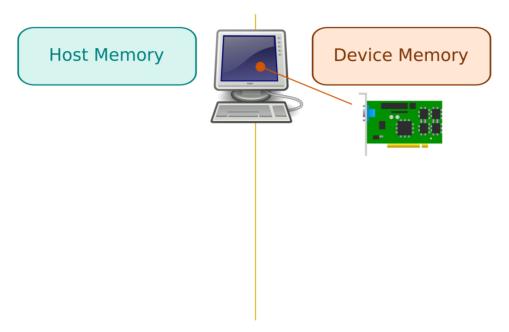
- ▶ Threads are organized in two layers resembling a 3D grid
- ▶ Simpler use-cases only requiring 1D or 2D topologies are mapped on the 3D structure

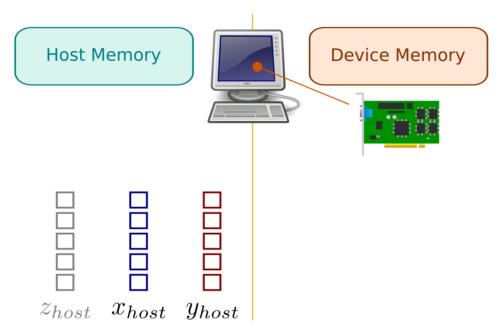


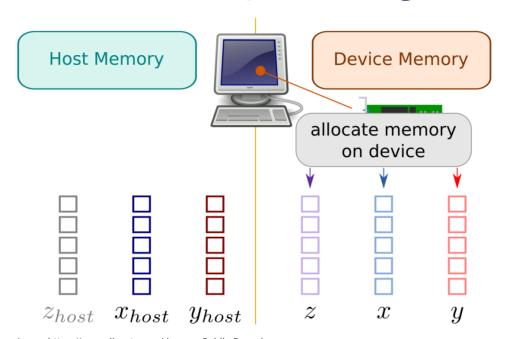
CUDA and OpenCL: Different But Similar - Memory Model

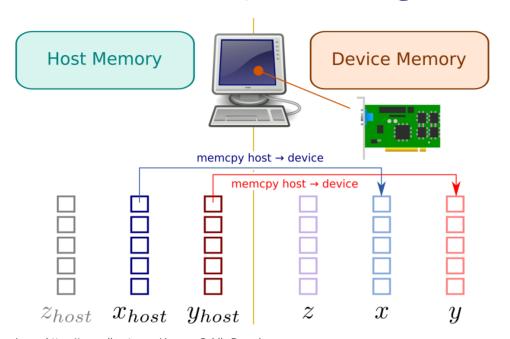
- ► Hierarchical memory model with different "regions"
- ► Visibility allows data exchange across individual threads / work-items but may require synchronization
- ▶ On CUDA, closely linked to Hardware implementation
- ▶ On OpenCL, guarantees about different memory regions are more difficult to give

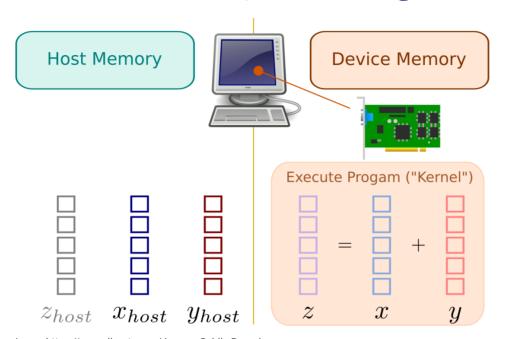


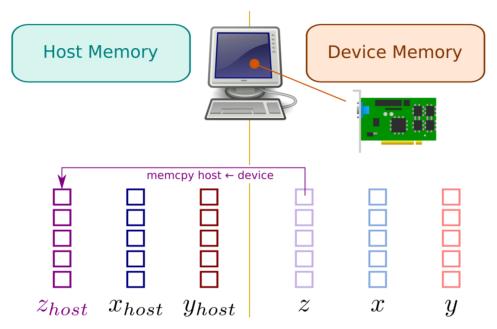


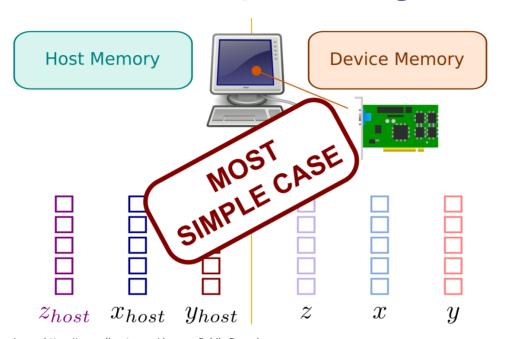












Example: Vector Addtion on the GPU using PyCuda

Cf. https://github.com/inducer/pycuda (https://github.com/inducer/pycuda) for reference

and

```
In [3]:
        # Again, a NVIDIA GPU is required for this example to work!
        import pycuda.autoinit
        import pycuda.driver as cuda
        import numpy as np
        from pycuda.compiler import SourceModule
        # First, we prepare the program that should be applied to our data, i.e. the "K
        ernel"
        vec add program = SourceModule(
        global void sum kernel( double* restrict z,
                                   double const* restrict x,
                                   double const* restrict y, int const N )
            const int threads per block = blockDim.x; /* Assuming 1D grid */
            const int ii = threadIdx.x + blockIdx.x * threads per block; /* Assuming 1D
        grid */
            if(ii < N)
                z[ii] = x[ii] + y[ii];
        # Note: even though we are using CUDA, we are able to specify the kernel at run
        -time ->
        # PyCuda uses the NVRTC implementation!
        vec add kernel = vec add program.get function( "sum kernel" )
```

```
In [4]: # then, we prepare the structures on the host side, allocate the
# required resources on the device side and move things

N = 10000000 # Again, 10^7 elements to the vector

x_host = np.random.randn( N ) # prepare the elements on the host
y_host = np.random.randn( N )

# allocate the structures on the device
x = cuda.mem_alloc( x_host.nbytes )
y = cuda.mem_alloc( y_host.nbytes )
z = cuda.mem_alloc( max( x_host.nbytes, y_host.nbytes ) )

#transfer the memory from the host to the device; htod ... host to device
cuda.memcpy_htod( x, x_host )
cuda.memcpy_htod( y, y_host )
```

```
In [5]:
        # find the grid dimensions:
         threads per block = 128 # This is a pessimistic but educated guess :-)
         num blocks = N // threads per block
         if \overline{N} % threads per block \overline{!} = 0:
             num blocks += 1
         # run the kernel
         N arg = np.int32(N) # pycuda enforces strict type checking
         vec add kernel( z, x, y, np.int32(N), block=(threads per block, 1, 1), grid=(nu
         m blocks,1))
         # copy the result back to the host; dtoh ... device to host
         z host = np.empty like( x host )
         cuda.memcpy dtoh( z host, z )
         # Compare result to calculation on CPU
         print( f"calculation on host and device yield same result: {np.allclose( z hos
         t, x host + y host, rtol=0.0, atol=1e-16)}")
         del x, y, z, x host, y host, z host
```

calculation on host and device yield same result: True

Example: Vector Addtion on the GPU using PyOpenCL

Cf. https://github.com/inducer/pyopencl and https://github.com/inducer/pyopencl and https://https://documen.tician.de/pyopencl for reference

```
In [6]:
        import pyopencl as cl
        import numpy as np
        # setup the OpenCL environment - it's a bit more elaborated as with PyCuda:
        # Shortcut: ctx = cl.create some context() -> create a context with the first a
        vailable device
        platforms = cl.get platforms()
        for p in platforms:
            print( p )
        <pyopencl.Platform 'AMD Accelerated Parallel Processing' at 0x7fc00450a250>
        <pyopencl.Platform 'NVIDIA CUDA' at 0x3d31de0>
        <pyopencl.Platform 'Portable Computing Language' at 0x7fc00dece020>
In [9]:
        platform = platforms[ 0 ] # Let's select the first one
        # get a list of all available devices for a platform
        devices = platform.get devices()
        for d in devices:
            print( d )
```

<pyopencl.Device 'gfx900' on 'AMD Accelerated Parallel Processing' at 0x33ec26
0>

```
In [10]: # Again, let's select the first device
device = devices[ 0 ]

# create a context and a queue
ctx = cl.Context( [device,] )
queue = cl.CommandQueue( ctx )
```

```
In [11]:
         # prepare the program containing the kernel:
         vec add program = cl.Program( ctx,
          kernel void sum kernel( __global double* restrict z,
                                   __global double const* restrict x,
                                   global double const* restrict y, int const N )
             int const ii = (int) get global id(0); /* Assume 1D Grid, 0 .. 0th eleme
         nt of ndrange */
             if(ii < N)
                 z[ii] = x[ii] + y[ii];
         .....
         # Compile the program containing the kernel
         vec add program.build()
         # get kernel function from vec add program
         vec add kernel = vec add program.sum kernel
```

```
In [12]: # then, we prepare the structures on the host side, allocate the
    # required resources on the device side and move things
    N = 10000000 # Again, 10^7 elements to the vector

# create the structures on the host
    x_host = np.random.rand( N )
    y_host = np.random.rand( N )

# allocate the structures on the device
    x = cl.Buffer( ctx, cl.mem_flags.READ_ONLY, x_host.nbytes )
    y = cl.Buffer( ctx, cl.mem_flags.READ_ONLY, y_host.nbytes )
    z = cl.Buffer( ctx, cl.mem_flags.WRITE_ONLY, max( x_host.nbytes, y_host.nbytes )
    )

#transfer the memory from the host to the device
    cl.enqueue_copy( queue, x, x_host )
    cl.enqueue_copy( queue, y, y_host )
```

Out[12]: <pyopencl._cl.NannyEvent at 0x7fc08f85b090>

calculation on host and device yield same result: True

del x, y, z, x host, y host, z host

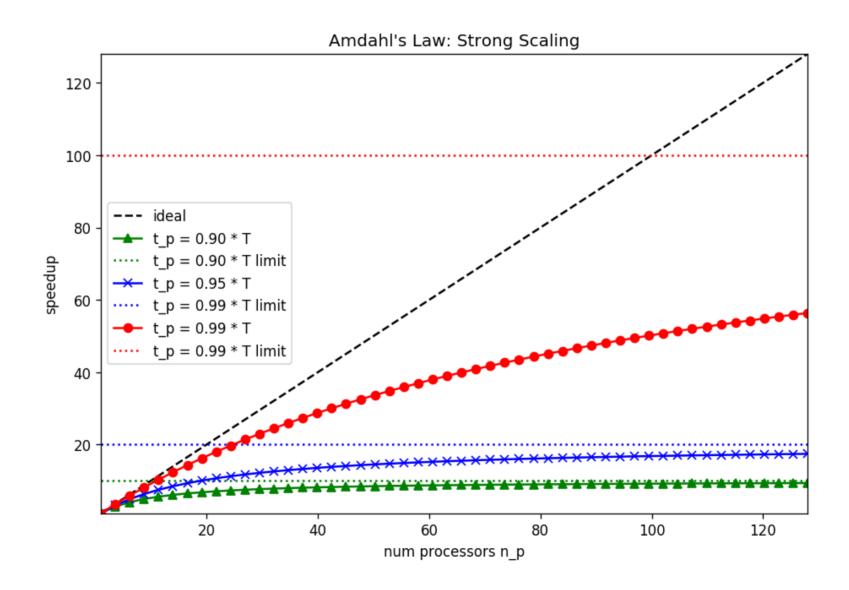
Performance Analysis: Scaling

- ightharpoonup Program with a total run-time T
- \blacktriangleright Assumption: problem size is **constant** (e.g. add vectors of size N, track N particles, etc.)
- Question: how much can we speed up the execution of the problem if we parallelise it, i.e. the speed-up $\eta_s(n_p)$
- $ightharpoonup T = t_p + t_s$
- t_p : fraction of run-time that can be run in "parallel" on n_p "processors"
- t_s : fraction of run-time that is sequential
- ► Amdahls law:

$$\eta_s(n_p) = rac{T}{t_s + rac{t_p}{n_p}}$$

Performance Analysis: Scaling

```
In [16]: from helpers import plot_amdahl_scaling
plot_amdahl_scaling( 1.0, 128.0 )
```



Performance Analysis: Conclusions from Amdahl's Law

- For a given problem with finite t_s , increases in performance are diminishing with rising n_p
- ullet Controlling and limiting t_s is crucial to achieve good parallel performance and speedup
- ullet We assume that $t_s=const.$ for a given problem size. In practice, $t_s=f(n_p)$
- Even with t_s very small, scaling to 10^3 or even 10^4 of parallel processes (as in GPUs) under the assumptions of Amdahl is hard

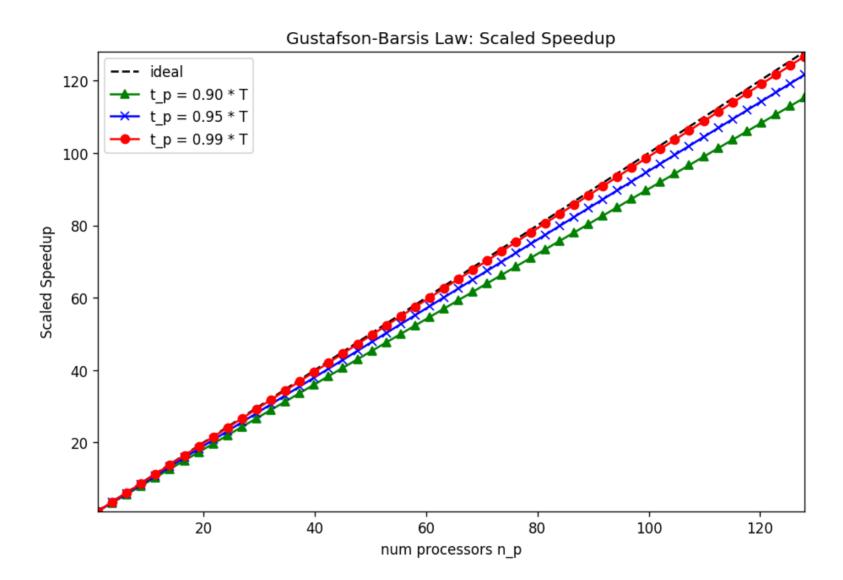
Scaled Speedup, Gustafson-Barsis Law

- Amdahl's Law is a bit pessimistic \leftarrow fixed problem size regardless of n_p
- What if we can **grow** the problem size together with rising number n_p ?
- Scaled Speedup:

$$\eta(n_p) = f_s + n_p \cdot f_p$$

- ullet $f_s=t_s/T$, fraction of the runtime that is serial
- ullet $f_p=t_p/T$, fraction of the runtime that can be run in parallel on n_p processors.
- ullet It holds that $f_s+f_p=1$

In [18]: from helpers import plot_gustafson_scaling
 plot_gustafson_scaling(1.0, 128.0)



Contributions to $oldsymbol{t}_s$ on GPUs

- ► Synchronization overhead between "processes" (threads) → Problems that do not require communication between processes are more suitable to be parallelized (ideal: "Embarrisingly Parallel Problem")
- ▶ Latencies and transfer times for copying memory between host and device
- ▶ latencies in launching kernels
- ► Latencies for accessing resources (different memory regions!)
- During the runtime of the kernel: thread divergence
- ▶ Thread divergence is a consequence of the SPMD model typically implemented on GPUs
- ▶ Remember: Threads/work-items are organized in warps/wavefronts
- ► AMD: 64 work-items / wavefront
- ▶ NVIDIA: 32 threads/workitems / warp
- ► The GPU always executes a multiple of these numbers, even if you only ask to compute 1 work-items / threads
- ▶ All threads execute the **same program** in lock-step
- ightharpoonup Dataparallelism: If the program branches depending on the data, code-paths have to be handled sequentially, thus increasing the t_s !

```
/* Example: Naive implementation of f(c,a,x,y) = c * (a + abs(x) + abs(y)) */
2
 3
     kernel void c times a plus abs x plus v(
         __global double* restrict result,
                                                                 x \ge 0
         double const c, double const a,
 6
         __global double const* restrict y,
         __global double const* restrict x, int const N )
8 🔻
         int const ii = ( int )get_global_id( 0 );
9
10
         /* result[ ii ] = c * ( a + | x[ ii ] | + | y[ ii ] | ) */
11
12
                                                                           active work-items
13
         if(ii < N)
14 ▼
             result[ ii ] = a; 	
15
16
             if(x[ii] >= 0.0)
17
18 ▼
19
                result[ ii ] += x[ ii ];
20
21
             else
22 🔻
23
                result[ ii ] -= x[ ii ];
24
25
26
             if(y[ii] >= 0.0)
27 🔻
28
                result[ ii ] += y[ ii ];
29
30
             else
31 ▼
32
                result[ ii ] -= y[ ii ];
33
34
35
             result[ ii ] *= c;
36
```

```
/* Example: Naive implementation of f(c,a,x,y) = c * (a + abs(x) + abs(y)) */
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     __kernel void c_times_a_plus_abs_x_plus_y(
         __global double* restrict result,
                                                              x \ge 0
         double const c, double const a,
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18 ▼
19
                20
21
             else
22 🔻
                                                                        No Divergence!
23
                result[ ii ] -= x[ ii ];
24
25
26
             if( v[ ii ] >= 0.0 )
27 🔻
28
                result[ ii ] += y[ ii ];
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30
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                                                                         active work-items
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27 🔻
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31 ▼
                                                                         Divergence
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         __global double const* restrict y,
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                                                                 \vee \geq 0
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             if(y[ii] >= 0.0)
26
27 🔻
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29
                                                                           active work-items
30
             else
31 ▼
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33
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                                                                            Divergence
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37
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22 🔻
23
                result[ ii ] -= x[ ii ];
24
25
            if(y[ii] >= 0.0)
26
27 🔻
                                                                       Assumption: already
28
                result[ ii ] += y[ ii ];
29
                                                                       Converged again
30
             else
31 ▼
                result[ ii ] -= y[ ii ];
32
                                                                         active work-items
33
34
35
             36
37
```

Example: Alternative, Branchless Formulation of Kernel

```
/* Example: Naive implementation of f(c,a,x,y) = c * (a + abs(x) + abs(y)) */
2
 3
     __kernel void c_times_a_plus_abs_x_plus_y(
         __global double* restrict result,
         double const c, double const a,
 6
         __global double const* restrict y,
         global double const* restrict x, int const N )
 8 🔻
 9
         int const ii = ( int )get_global_id( 0 );
10
11
        /* result[ ii ] = c * ( a + | x[ ii ] | + | y[ ii ] | ) */
12
13
         if(ii < N)
14 ▼
15
             double temp = a;
16
             temp += x[ii] * (double)((x[ii] > 0.0) - (x[ii] < 0.0));
17
             temp += y[ii] * (double)((y[ii] > 0.0) - (y[ii] < 0.0));
18
             temp *= c;
19
20
            result[ ii ] = temp;
21
22
   }
```

Summary & Conclusions

- ▶ GPUs offer a large number of threads and significant floating-point computing power
- ► There are many options to get started with GPU programming without starting to go fully towards low-level programming
- ▶ The two current main frameworks, OpenCL and CUDA, differ in scope and implementation but are similar enough that a common implementation of Kernels is possible
- ► Controlling and Limiting the sequential run-time component is crucial to achieve good scaling and parallel performance
- ▶ Thread Divergence can be a key contributor to the sequential runtime-portion
- Not covered: optimal grid dimensions and hardware utilization

Thank You For Your Attention!