

基于DPCT的序列比对软件 迁移与性能评估

2023



intel[®]

Contents

01



背景介绍

02



迁移过程

03



实验结果

04



总结

/01

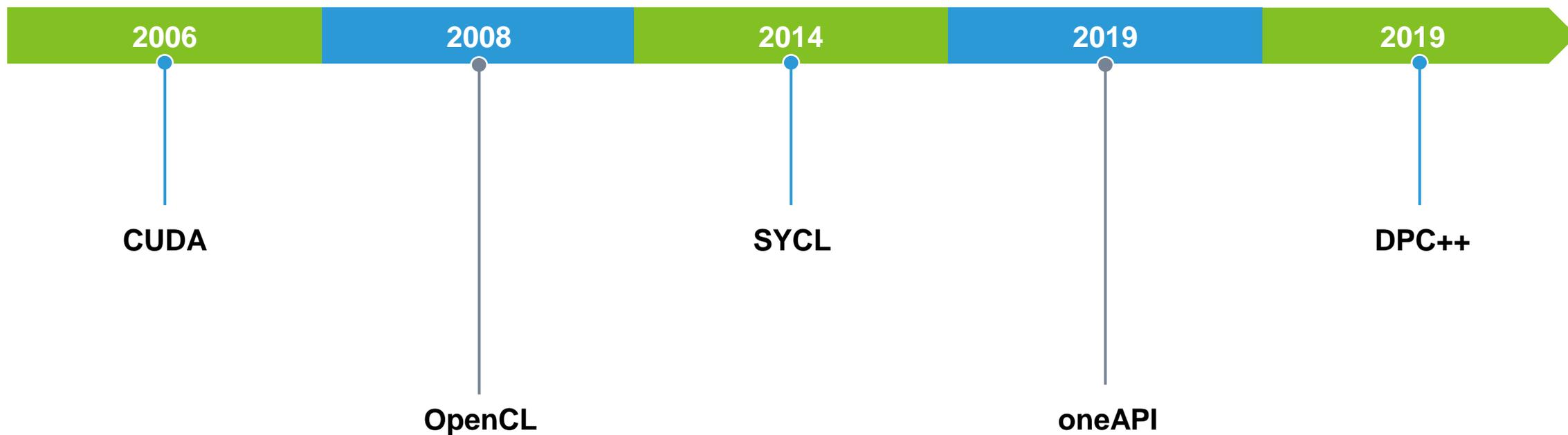
背景介绍



异构计算在HPC领域中的优势



异构编程架构的发展



SYCL的主要实现

ComputeCpp™

ComputeCpp is SYCL v1.2.1 conformant. It is Codeplay Software's implementation of the standard and is available to download today.

[Find Out More](#)

DPC++ and oneAPI

Data Parallel C++ (DPC++) is an evolution of C++ that incorporates SYCL. The SYCL Compiler compiles C++-based SYCL source files with code for both CPU and a wide range of compute accelerators.

[Find Out More](#)

hipSYCL

The goal of the hipSYCL project is to develop a SYCL 1.2.1 implementation that builds upon NVIDIA CUDA/AMD HIP.

[Find Out More](#)

triSYCL

triSYCL is an open-source implementation test-bed to experiment with the specification of the OpenCL SYCL 2.2 C++ layer and to give feedback to the Khronos group.

[Find Out More](#)

DPC++的优势

Diverse accelerators needed to meet today's performance requirements:

48% of developers target heterogeneous systems that use more than one kind of processor or core¹

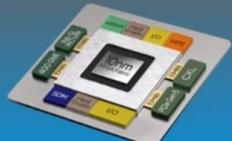
CPU



GPU



FPGA



Other Accelerators



Developer Challenges: Multiple Architectures, Vendors, and Programming Models



Open, Standards-based, Multiarchitecture Programming

跨架构性

可以在不同架构上的GPU, CPU, AI加速器上编写程序并且运行

跨架构性



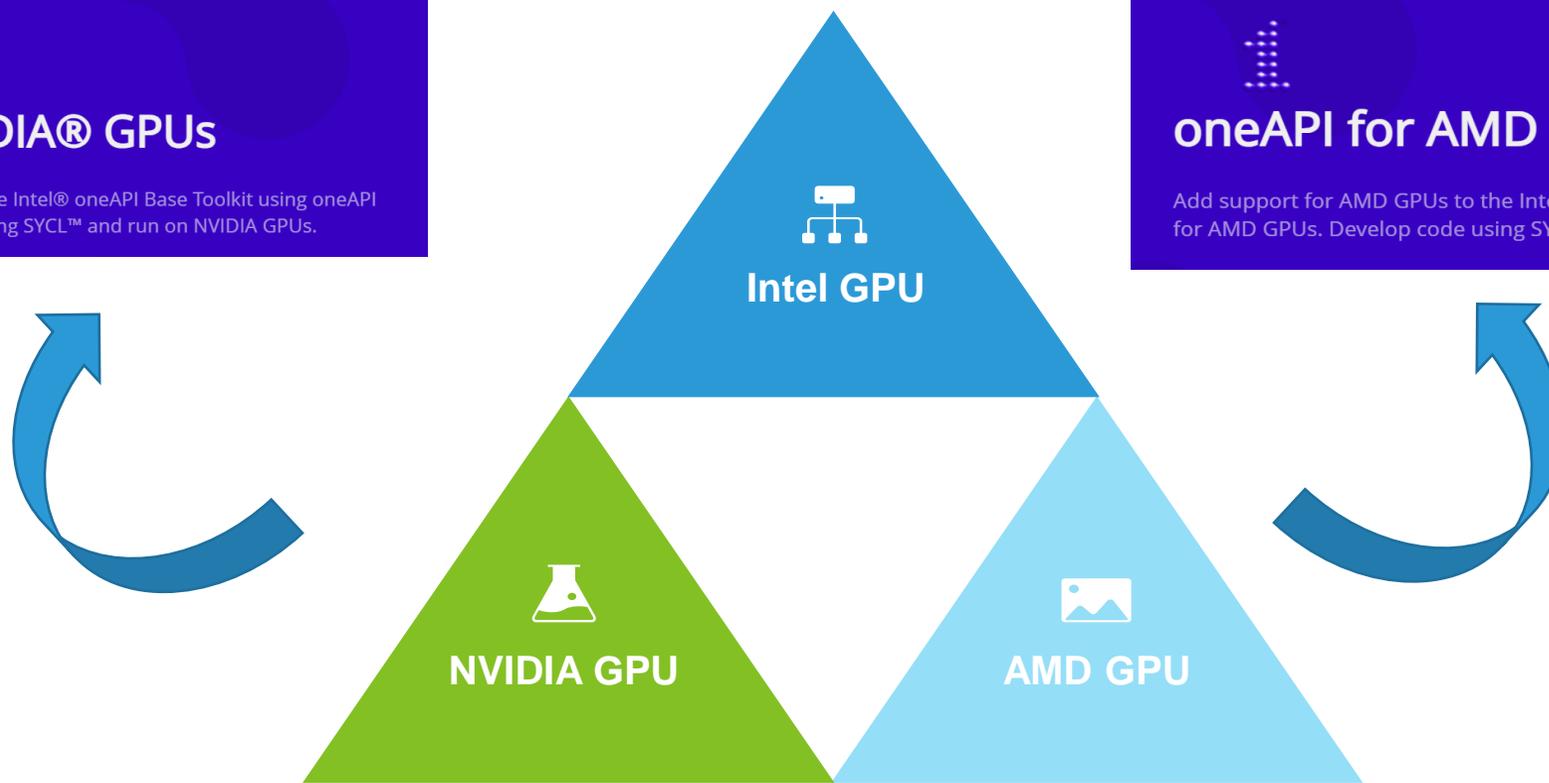
oneAPI for NVIDIA® GPUs

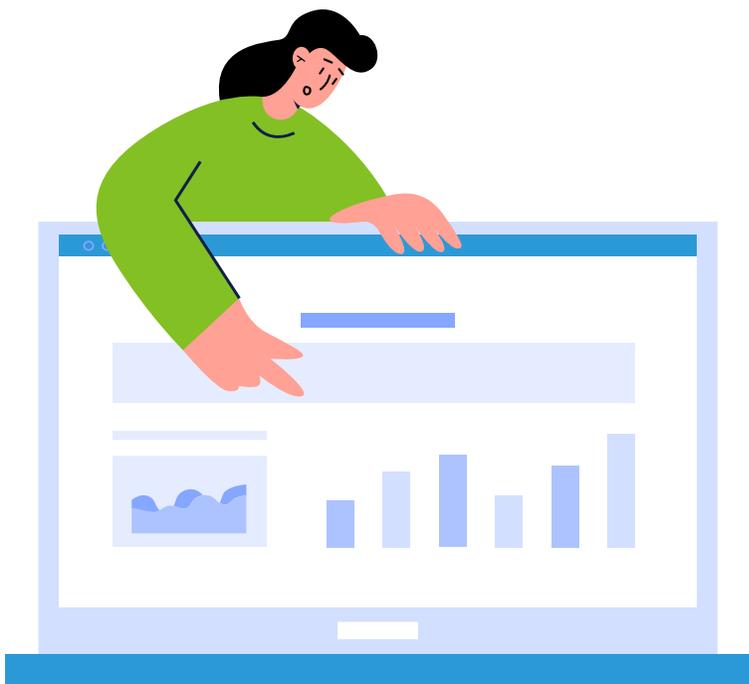
Add support for NVIDIA GPUs to the Intel® oneAPI Base Toolkit using oneAPI for NVIDIA GPUs. Develop code using SYCL™ and run on NVIDIA GPUs.



oneAPI for AMD GPUs (beta)

Add support for AMD GPUs to the Intel® oneAPI Base Toolkit using oneAPI for AMD GPUs. Develop code using SYCL™ and run on AMD GPUs.





灵活性

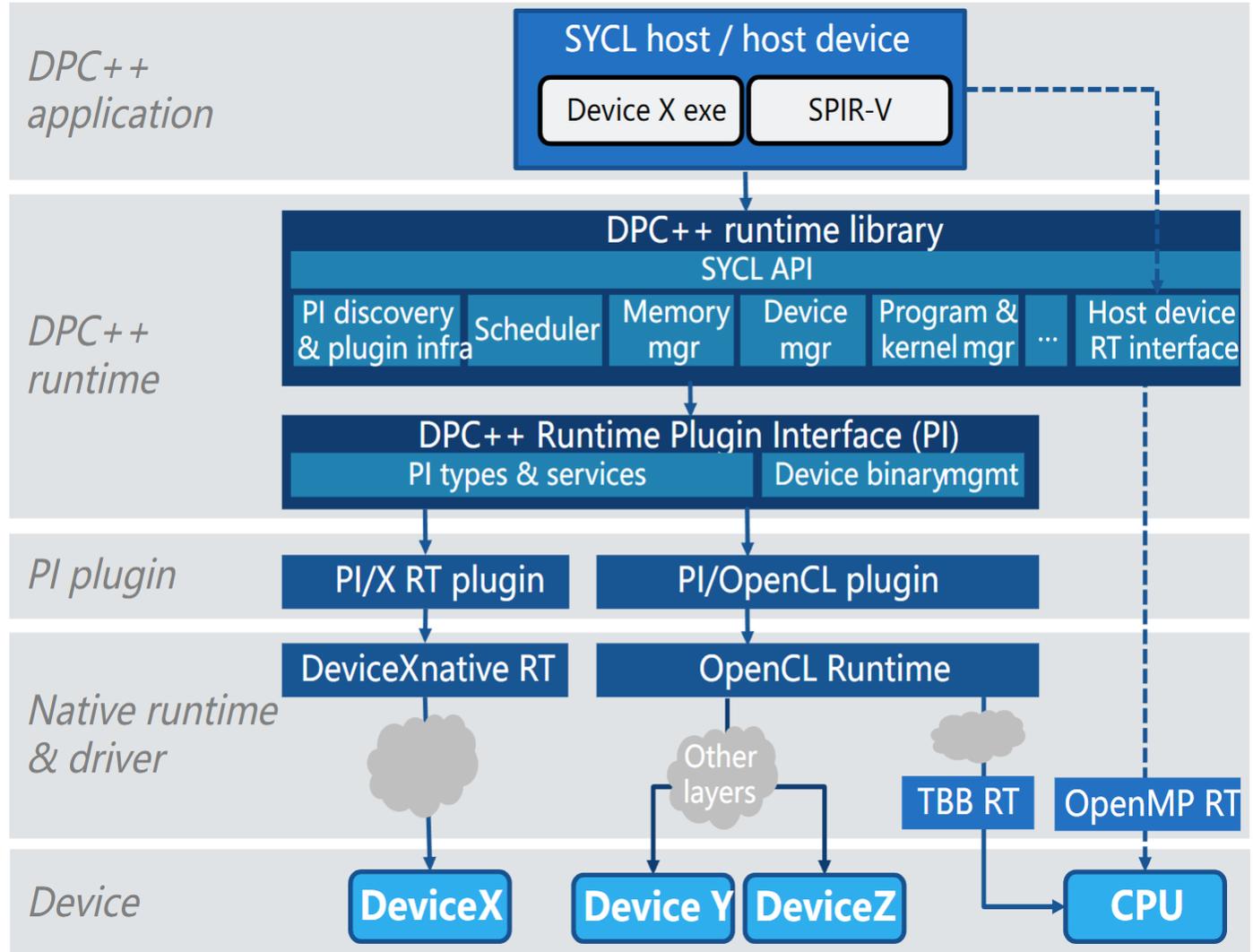
- DPC++ 设计时考虑了可移植性，使得编写的代码可以在不同类型的硬件上运行

易开发性

- DPC++基于SYCL标准实现，SYCL标准是C++的扩展，没有特定的针对某种特定架构，有C++开发经验可以很快上手

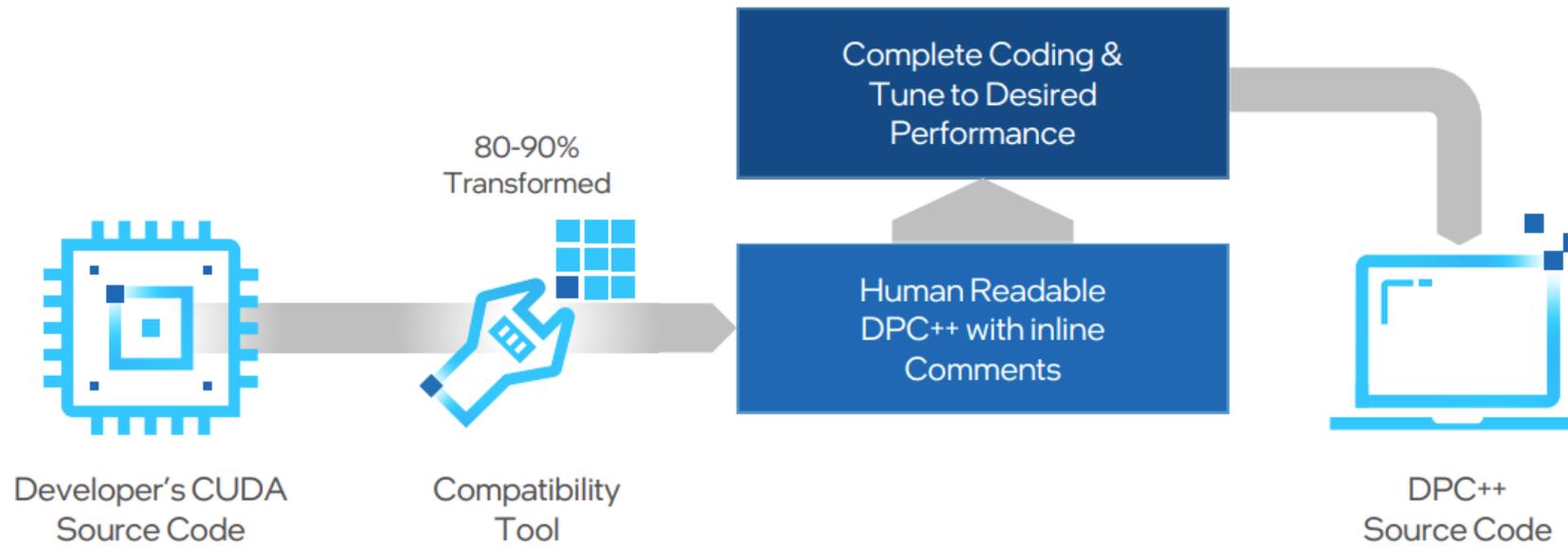
DPC++

Compiler



DPCT

Intel DPC ++ Compatibility Tool Usage Flow



/02

迁移过程



GASAL2

Software | [Open Access](#) | [Published: 25 October 2019](#)

GASAL2: a GPU accelerated sequence alignment library for high-throughput NGS data

[Nauman Ahmed](#) , [Jonathan Lévy](#), [Shanshan Ren](#), [Hamid Mushtaq](#), [Koen Bertels](#) & [Zaid Al-Ars](#)

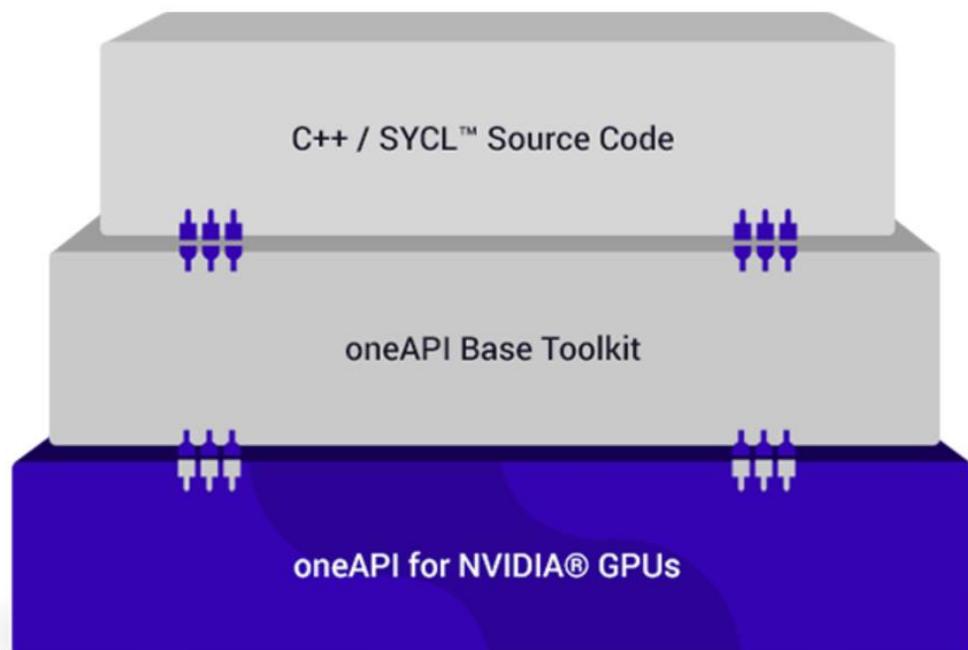
[BMC Bioinformatics](#) **20**, Article number: 520 (2019) | [Cite this article](#)

12k Accesses | **27** Citations | **3** Altmetric | [Metrics](#)

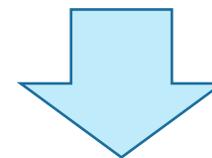
<https://github.com/nahmedraja/GASAL2>

实验环境

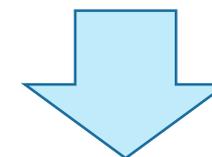
oneAPI for NVIDIA® GPUs



1、下载安装包



2、安装安装包



3、激活环境

实验环境

表 1 NVIDIA 平台信息

Table1 NVIDIA platform information

属性	NVIDIA 平台
GPU	2* NVIDIA Tesla P100
CPU	2* Intel(R) Xeon(R) Gold 5120 CPU @ 2.20GHz
GPU 核心数	56 SMs
CPU 核心数	56
L1/2/3	32K/1024K/19712K
CUDA	11.1
oneAPI-for-nvidia	2023.0.0
oneAPI	2023.0.0
操作系统	Ubuntu 20.04.4 LTS
SP	10.6TFlops
DP	5.3TFlops



表 2 Intel DevCloud 平台信息

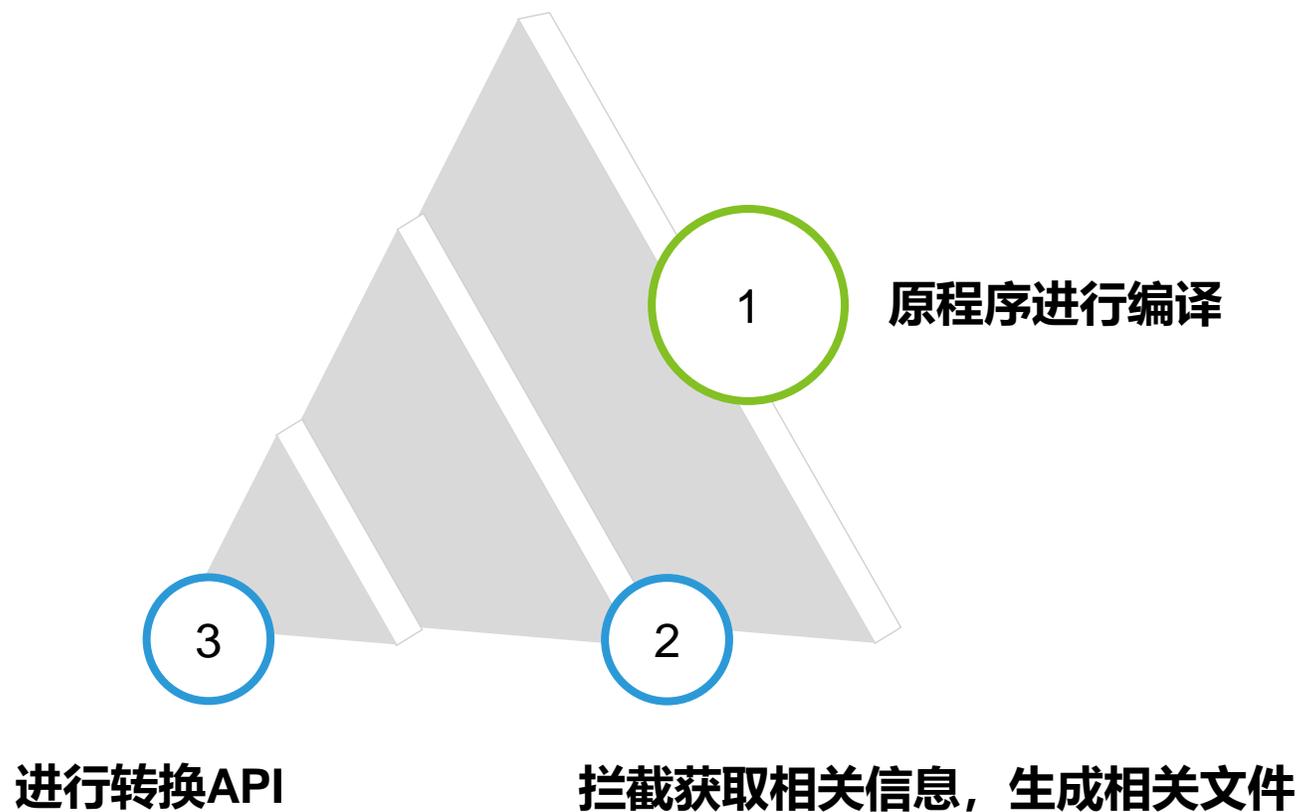
Table2 Intel DevCloud Platform information

属性	Gen9 节点	Gen11 节点
GPU	2*Intel Corporation UHD Graphics P630	2*Intel(R) UHD Graphics [0x9a60]
CPU	Intel(R) Xeon(R) E- 2176G CPU @3.70GHz	11th Gen Intel(R) Core(TM) i9-11900KB @ 3.30GHz
GPU 核 心	24EUs	32EUs
CPU 核 心	6	8
L1/2/3	192KiB/1.5 MiB/12 MiB	256 KiB/10 MiB/24 MiB
oneAPI	2023.0.0	2023.0.0
操作系统	Ubuntu 20.04.6 LTS	Ubuntu 20.04.6 LTS
SP	441.6GFlops	537.6GFlops
DP	220.8GFlops	268.8GFlops

DPCT迁移流程



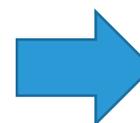
DPCT迁移流程



DPCT迁移流程

一、运行intercept-build脚本，它能自动跟踪编译时相关需要修改的信息

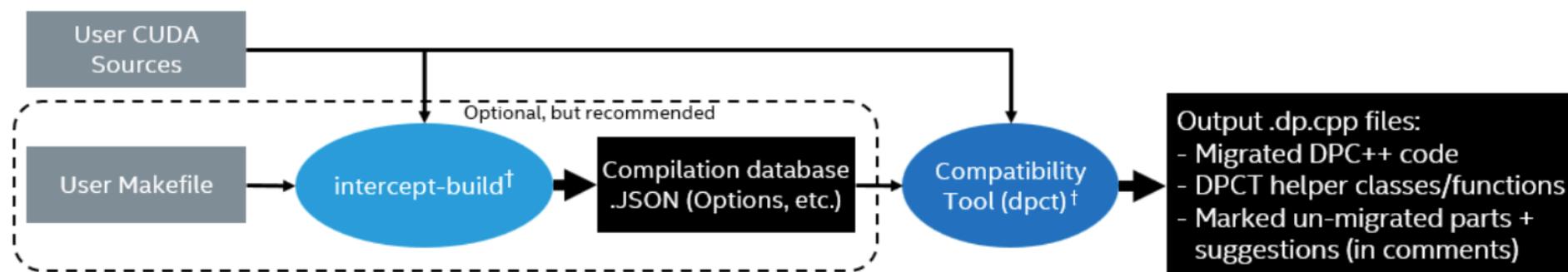
```
intercept-build make
```



```
compile_commands.json
```

二、运行DPCT

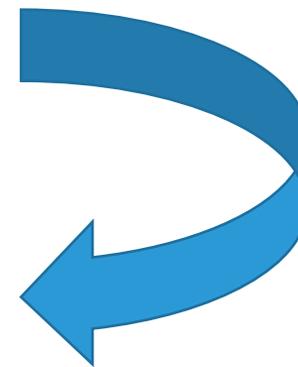
```
dpct -p ./ --in-root=./ --out-root=output *.cu
```



† Certain CUDA language header files may need to be accessible to the Intel® DPC++ Compatibility Tool

迁移过程

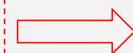
```
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2# intercept-build make GPU_SM_ARCH=sm_60 MAX_QUERY_LEN=300 N_CODE=0x4E N_PENALTY=1
rm -f -r ./obj/ ./lib/ ./include/ *.exe *.cppo *.cuo *.txt *.w
g++ -c -g -O3 -std=c++11 -Wall -DMAX_QUERY_LEN=300 -DN_CODE=0x4E -DN_PENALTY=1 -Werror src/args_parser.cpp -o ./obj/args_parser.cppo
g++ -c -g -O3 -std=c++11 -Wall -DMAX_QUERY_LEN=300 -DN_CODE=0x4E -DN_PENALTY=1 -Werror src/host_batch.cpp -o ./obj/host_batch.cppo
g++ -c -g -O3 -std=c++11 -Wall -DMAX_QUERY_LEN=300 -DN_CODE=0x4E -DN_PENALTY=1 -Werror src/ctors.cpp -o ./obj/ctors.cppo
g++ -c -g -O3 -std=c++11 -Wall -DMAX_QUERY_LEN=300 -DN_CODE=0x4E -DN_PENALTY=1 -Werror src/interfaces.cpp -o ./obj/interfaces.cppo
g++ -c -g -O3 -std=c++11 -Wall -DMAX_QUERY_LEN=300 -DN_CODE=0x4E -DN_PENALTY=1 -Werror src/res.cpp -o ./obj/res.cppo
/usr/local/cuda/bin/nvcc -c -g -O2 -std=c++11 -Xcompiler -Wall,-DMAX_QUERY_LEN=300,-DN_CODE=0x4E,-DN_PENALTY=1 -Xptxas -Werror --gpu-architecture=compute_60 --gpu-code=sm_60
ar -csru ./lib/libgasal.a ./obj/args_parser.cppo ./obj/host_batch.cppo ./obj/ctors.cppo ./obj/interfaces.cppo ./obj/res.cppo ./obj/gasal_align.cuo
ar: 'u' modifier ignored since 'D' is the default (see 'U')
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2# dpct --in-root=. -p compile_commands.json --cuda-include-path=/usr/local/cuda/include --out-root=./dpct_gasal2
Processing: /workspace/source_code/dpct/GASAL2/src/gasal_align.cu
In file included from /workspace/source_code/dpct/GASAL2/src/gasal_align.cu:5:
In file included from /workspace/source_code/dpct/GASAL2/src/gasal_kernels.h:71:
```



■ 操作简单

■ 自动转换

```
__deprecated.cpp
args_parser.cpp
args_parser.h
ctors.cpp
ctors.h
gasal.h
gasal_align.cu
gasal_align.h
gasal_header.h
gasal_kernels.h
host_batch.cpp
host_batch.h
interfaces.cpp
interfaces.h
kernels
├── __ksw_deprecated.h
├── banded.h
├── get_tb.h
├── global.h
├── ksw_kernel_template.h
├── local_kernel_template.h
├── pack_rc_seqs.h
├── semiglobal_kernel_template.h
res.cpp
res.h
```



```
args_parser.h
gasal.h
gasal.h.yaml
gasal_align.dp.cpp
gasal_align.h
gasal_align.h.yaml
gasal_kernels.h
gasal_kernels.h.yaml
host_batch.h
kernels
├── banded.h
├── banded.h.yaml
├── get_tb.h
├── get_tb.h.yaml
├── global.h
├── global.h.yaml
├── ksw_kernel_template.h
├── ksw_kernel_template.h.yaml
├── local_kernel_template.h
├── local_kernel_template.h.yaml
├── pack_rc_seqs.h
├── pack_rc_seqs.h.yaml
├── semiglobal_kernel_template.h
├── semiglobal_kernel_template.h.yaml
res.h
```

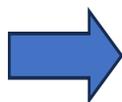
迁移过程

- 在Int2Type这种语法下尖括号匹配转换时会多一个尖括号

```
gasal_semi_global_kernel < Int2Type<a>, Int2Type<s>,  
                          Int2Type<b>, Int2Type<h>,  
                          Int2Type<t>>>>
```

- 有些关于设备状态或者队列信息的API转换需要自己去查阅相关资料去手动实现

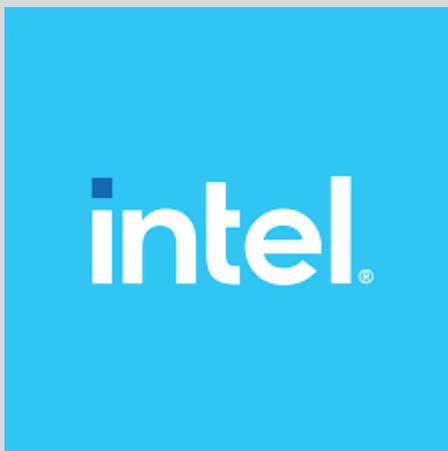
```
1 int gasal_is_aln_async_done(gasal_gpu_storage_t *gpu_storage)  
2 {  
3     cudaError_t err;  
4     if(gpu_storage->is_free == 1) return -2;//if no work is launced in this stream, return -2  
5     err = cudaStreamQuery(gpu_storage->str);//check to see if the stream is finished  
6     if (err != cudaSuccess) {  
7         if (err == cudaErrorNotReady) return -1;  
8         else{  
9             fprintf(stderr, "[GASAL CUDA ERROR:] %s(CUDA error no.=%d). \\  
10                Line no. %d in file %s\n", cudaGetErrorString(err), err, __LINE__, __FILE__);  
11                exit(EXIT_FAILURE);  
12            }  
13        }  
14        gasal_host_batch_reset(gpu_storage);  
15        gpu_storage->is_free = 1;  
16        gpu_storage->current_n_alns = 0;  
17        return 0;  
18    }
```



```
1 int gasal_is_aln_async_done(gasal_gpu_storage_t *gpu_storage) try {  
2     int err;  
3     if(gpu_storage->is_free == 1) return -2;//if no work is launced in this stream, return -2  
4     if(!gpu_storage->str->ext_oneapi_empty())  
5         return -1; // check to see if the stream is finished  
6  
7     gasal_host_batch_reset(gpu_storage);  
8     gpu_storage->is_free = 1;  
9     gpu_storage->current_n_alns = 0;  
10    return 0;  
11 }  
12 catch (sycl::exception const &exc) {  
13     std::cerr << exc.what() << "Exception caught at file:" << __FILE__  
14         << ", line:" << __LINE__ << std::endl;  
15     std::exit(1);  
16 }
```

编译文件

DPC++采用C++17标准,采用跨架构GPU编译运行的时候只需修改编译器就可



Intel平台: `icpx -fsycl -fsycl-targets=spir64_gen`



Nvidia平台: `clang++ -fsycl -fsycl-targets=nvptx64-nvidia-cuda`

`-arch=compute_60;-code=sm_60`



`-Xsycl-target-backend=nvptx64-nvidia-cuda --
cuda-gpu-arch=sm_60`

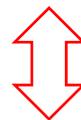
/03

实验结果



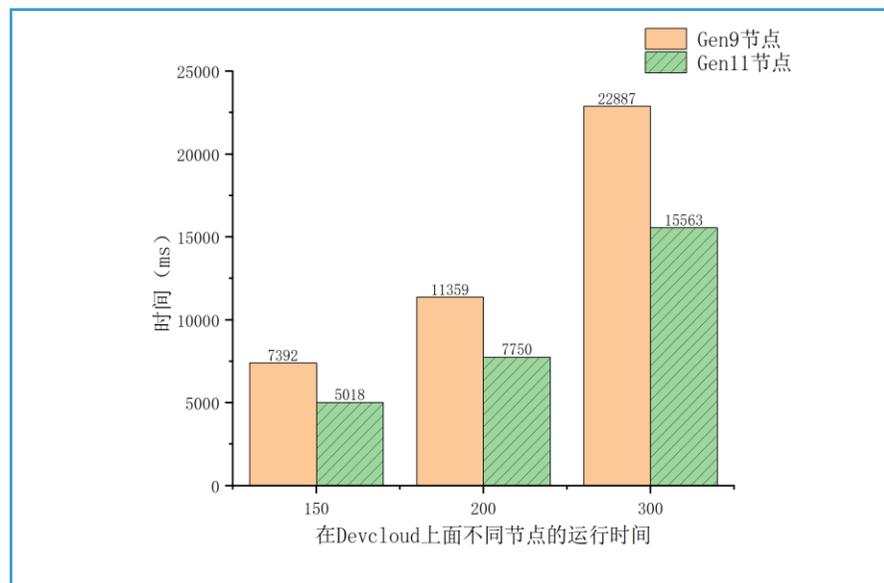
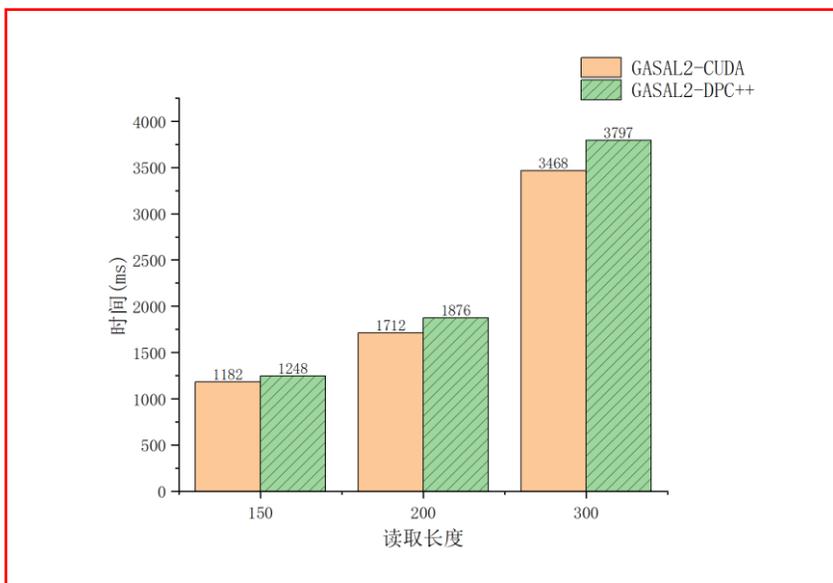
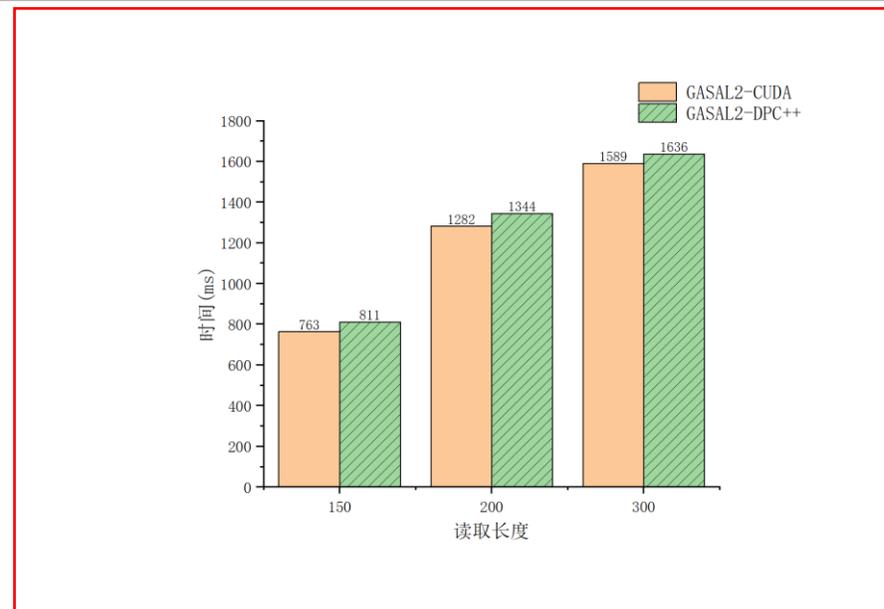
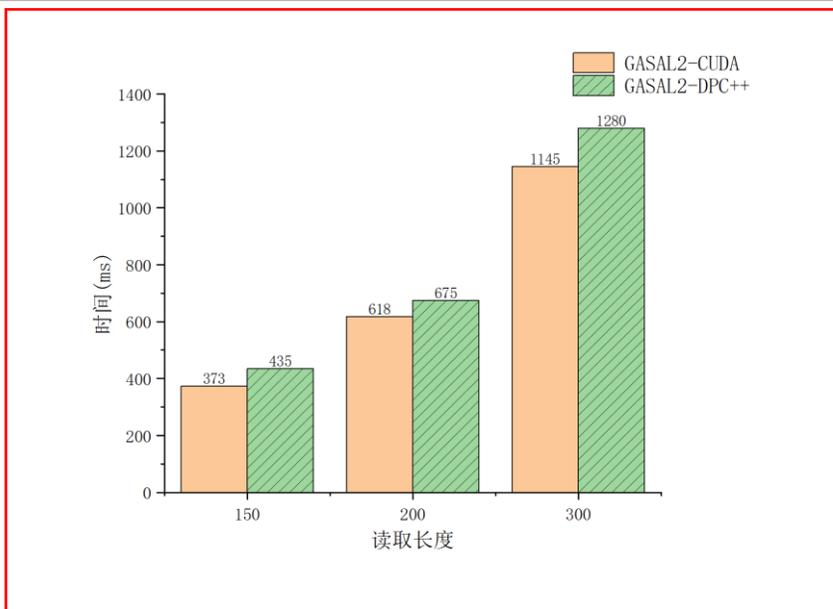
实验结果

```
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# ./test_prog.out -p -y local query_batch_2000000.fasta target_batch_2000000.fasta > local_cuda.out 2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# sha256sum local_cuda.out
b5374189941d93263410c3f6bcbbaa8b316f1f9380566f8d04f1894eeb54e32c8 local_cuda.out
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# ./test_prog.out -p -y semi-global query_batch_2000000.fasta target_batch_2000000.fasta > semi-global_cuda.out
2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# sha256sum semi-global_cuda.out
456cffc3f583ac242b364bf107ded68eb6883894210b2c7932c33b03a5671635 semi-global_cuda.out
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# ./test_prog.out -p -y global query_batch_2000000.fasta target_batch_2000000.fasta > global_cuda.out 2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# sha256sum global_cuda.out
74379c71f29adc5f5d1848f9d45307c9905c5a8f70149fc956f6461f77c75e44 global_cuda.out
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# ./test_prog.out -p -y ksw query_batch_2000000.fasta target_batch_2000000.fasta > ksw_cuda.out 2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/test_prog# sha256sum ksw_cuda.out
dafffdc454dc37bb91f125cda4f747b0b3a08d3ee9dcb23d25de7b3071dd0445 ksw_cuda.out
```

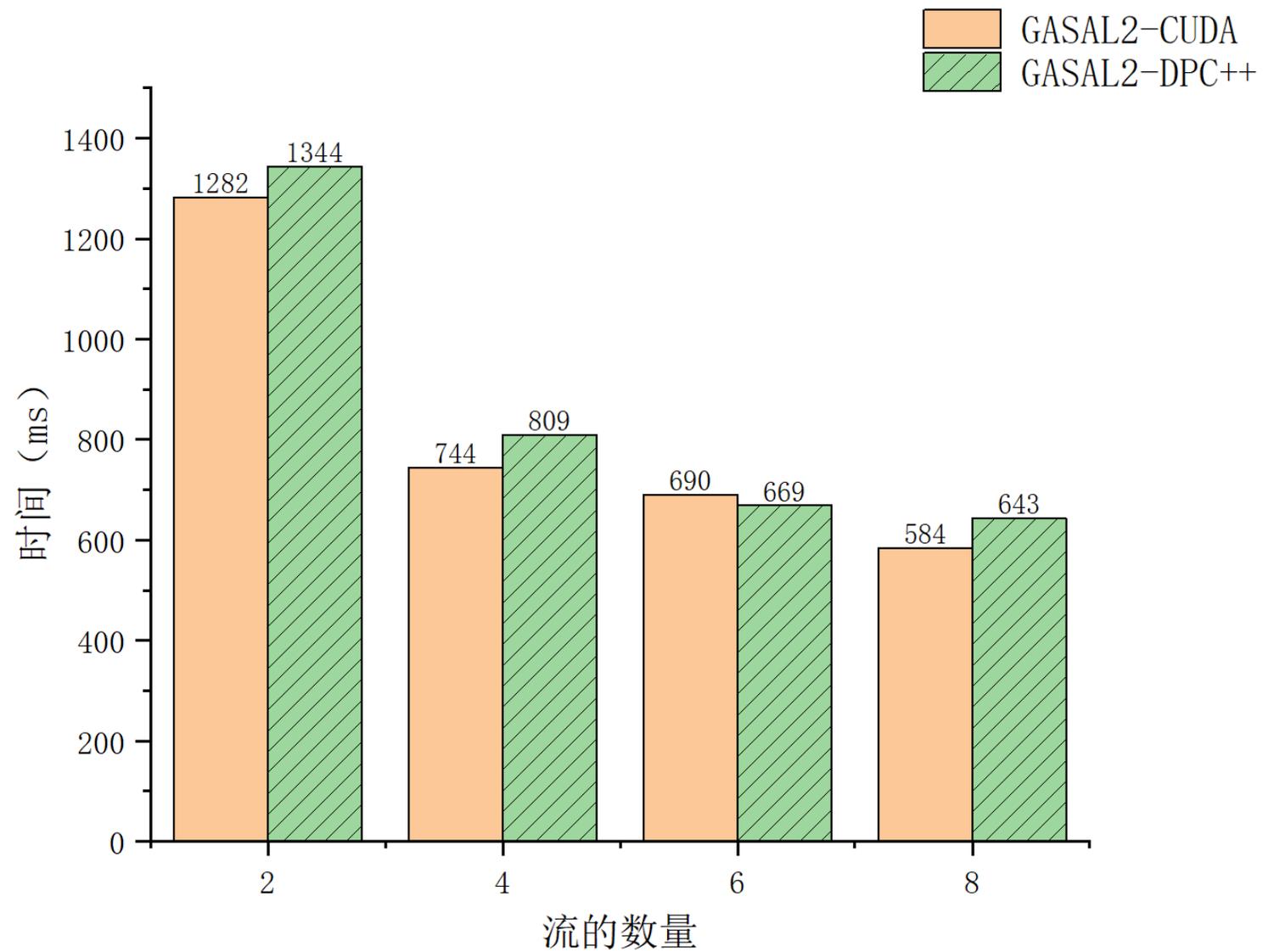


```
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# ./test_prog_dpcpp.out -p -y local query_batch_2000000.fasta target_batch_2000000.fasta > local_dp
cpp.out 2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# sha256sum local_dpcpp.out
b5374189941d93263410c3f6bcbbaa8b316f1f9380566f8d04f1894eeb54e32c8 local_dpcpp.out
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# ./test_prog_dpcpp.out -p -y semi-global query_batch_2000000.fasta target_batch_2000000.fasta > se
mi-global_dpcpp.out 2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# sha256sum semi-global_dpcpp.out
456cffc3f583ac242b364bf107ded68eb6883894210b2c7932c33b03a5671635 semi-global_dpcpp.out
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# ./test_prog_dpcpp.out -p -y global query_batch_2000000.fasta target_batch_2000000.fasta > global_
dpcpp.out 2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# sha256sum global_dpcpp.out
74379c71f29adc5f5d1848f9d45307c9905c5a8f70149fc956f6461f77c75e44 global_dpcpp.out
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# ./test_prog_dpcpp.out -p -y ksw query_batch_2000000.fasta target_batch_2000000.fasta > ksw_dpcpp.
out 2>/dev/null
root@e1389a78eac3:/workspace/source_code/dpct/GASAL2/dpct_output/test_prog# sha256sum ksw_dpcpp.out
dafffdc454dc37bb91f125cda4f747b0b3a08d3ee9dcb23d25de7b3071dd0445 ksw_dpcpp.out
```

性能对比



实验结果



/04

总结



总结



可以快速转化



需要细粒度的优化



强大的跨架构性



需要进行适度修改

The Intel logo is centered on a solid blue background. It features the word "intel" in a white, lowercase, sans-serif font. A small blue square is positioned above the letter "i". To the right of the word "intel" is a registered trademark symbol (®).

intel®