NVIDIA HPC Software

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October 2022, NERSC GPUs for Science Day

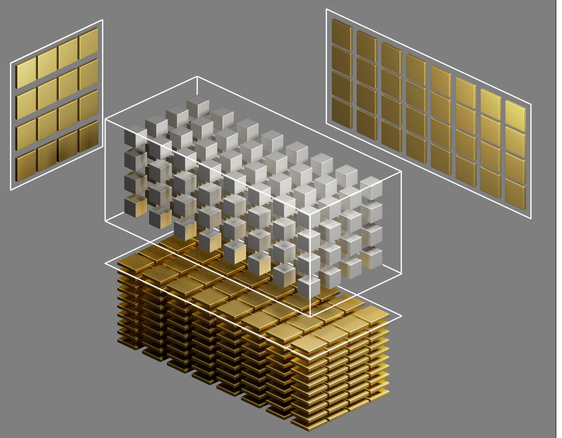
Agenda

- Programming the NVIDIA Platform
- NVIDIA HPC SDK
- Standards-Based Parallel Programming
- Conclusions

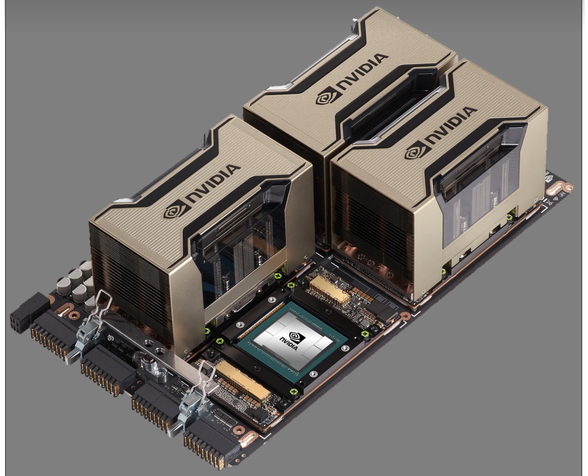
NVIDIA HPC SOFTWARE

Major Initiatives

Seamless Acceleration
Standard Languages, Tensor Cores, GH C2C

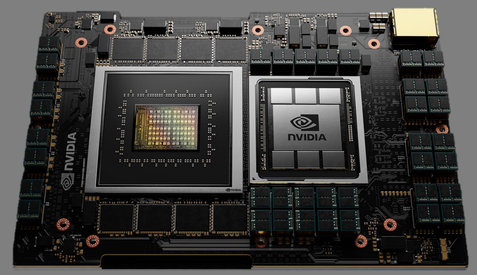


Scaling Up
Multi-GPU and Multi-Node Libraries

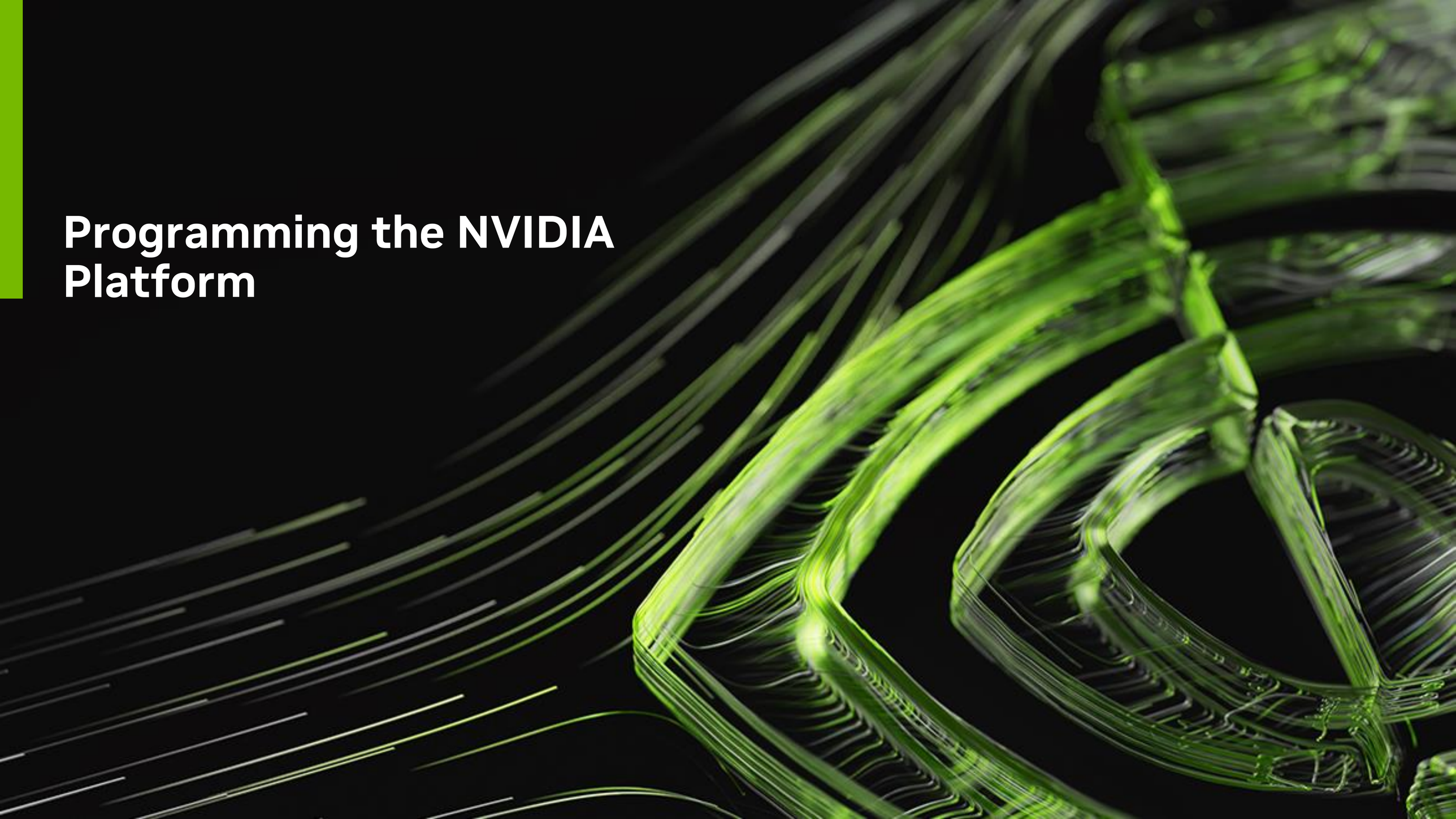


Domain Libraries
Quantum, LQCD, Signal Processing

Arm Software
Compilers, Libraries, Ecosystem



Programming the NVIDIA Platform



Programming the NVIDIA Platform

CPU, GPU, and Network

ACCELERATED STANDARD LANGUAGES

ISO C++, ISO Fortran

```
std::transform(par, x, x+n, y, y,
    [=](float x, float y){ return y + a*x; }
);
```

```
do concurrent (i = 1:n)
   y(i) = y(i) + a*x(i)
enddo
```

```
import cunumeric as np
…
def saxpy(a, x, y):
    y[:] += a*x
```

INCREMENTAL PORTABLE OPTIMIZATION

OpenACC, OpenMP

```
#pragma acc data copy(x,y) {
...
std::transform(par, x, x+n, y, y,
    [=](float x, float y){
        return y + a*x;
});
...
}
```

```
#pragma omp target data map(x,y) {
...
std::transform(par, x, x+n, y, y,
    [=](float x, float y){
        return y + a*x;
});
...
}
```

PLATFORM SPECIALIZATION

CUDA

```
__global__
void saxpy(int n, float a,
           float *x, float *y) {
  int i = blockIdx.x*blockDim.x +
          threadIdx.x;
  if (i < n) y[i] += a*x[i];
}

int main(void) {
  ...
  cudaMemcpy(d_x, x, ...);
  cudaMemcpy(d_y, y, ...);

  saxpy<<<(N+255)/256,256>>>(...);

  cudaMemcpy(y, d_y, ...);
```

ACCELERATION LIBRARIES

Core	Math	Communication	Data Analytics	AI	Quantum

Accelerated Standard Languages

Parallel performance for wherever your code runs

ISO C++

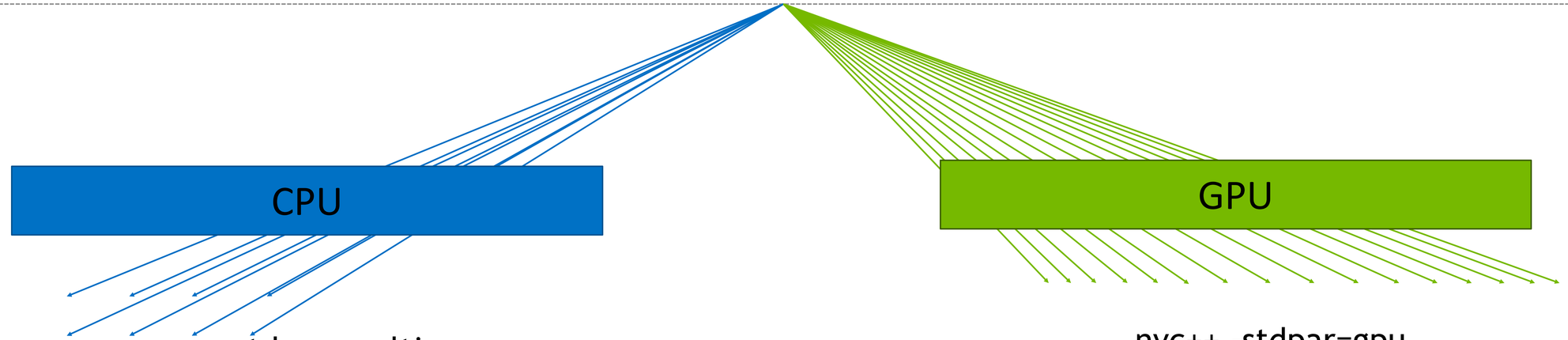
```
std::transform(par, x, x+n, y,
   y,[=](float x, float y){
      return y + a*x;
    }
);
```

ISO Fortran

```
do concurrent (i = 1:n)
   y(i) = y(i) + a*x(i)
enddo
```

Python

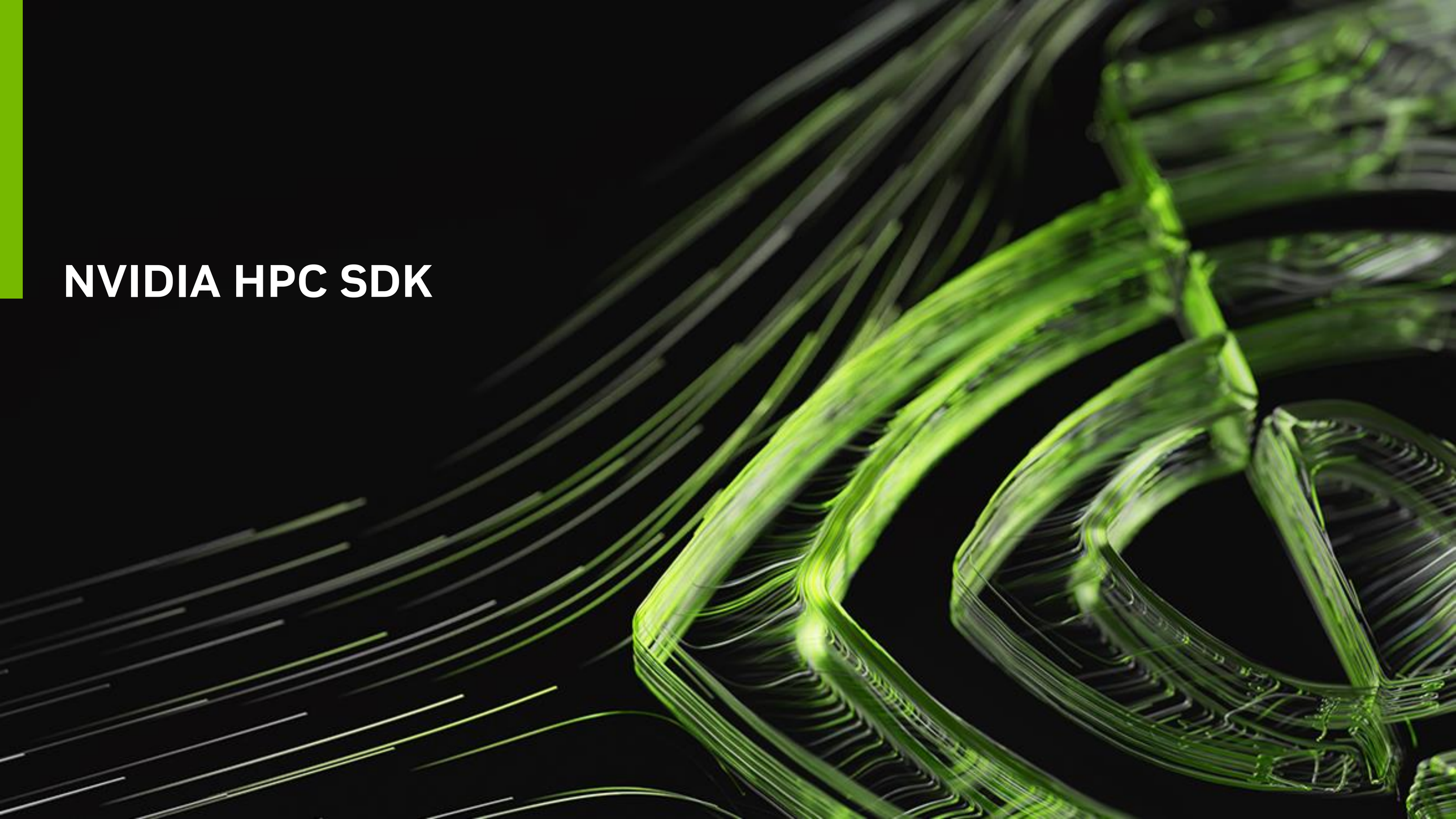
```
import cunumeric as np
…
def saxpy(a, x, y):
    y[:] += a*x
```



nvc++ -stdpar=multicore
nvfortran -stdpar=multicore
legate -cpus 16 saxpy.py

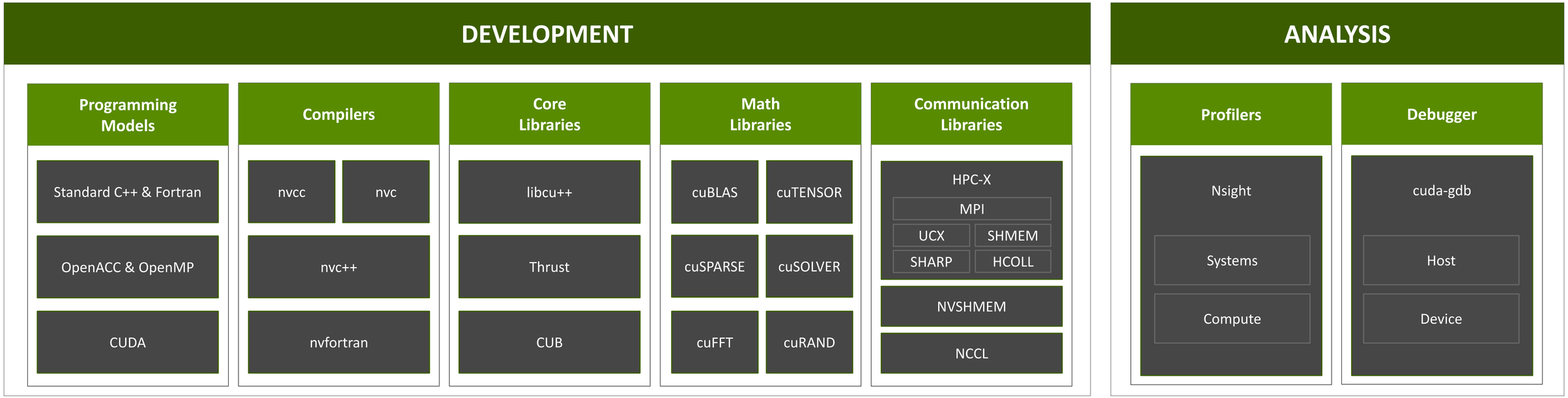
nvc++ -stdpar=gpu
nvfortran -stdpar=gpu
legate -gpus 1 saxpy.py

NVIDIA HPC SDK



NVIDIA HPC SDK

Available at developer.nvidia.com/hpc-sdk, on NGC, via Spack, and in the Cloud



Develop for the NVIDIA Platform: GPU, CPU and Interconnect

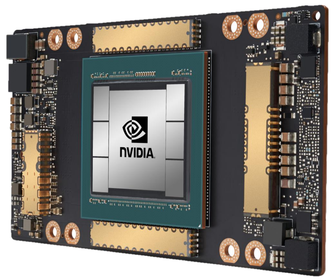
Libraries | Accelerated C++ and Fortran | Directives | CUDA

x86_64 | AArch64 | OpenPOWER

7-8 Releases Per Year | Freely Available

HPC Compilers

NVC | NVC++ | NVFORTRAN



Accelerated
GPU
Automatic

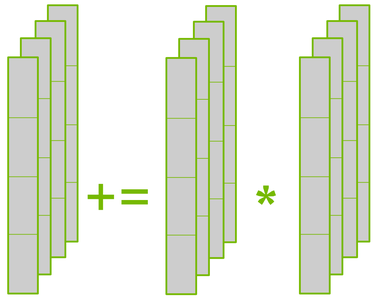
Fortran

NVIDIA CUDA

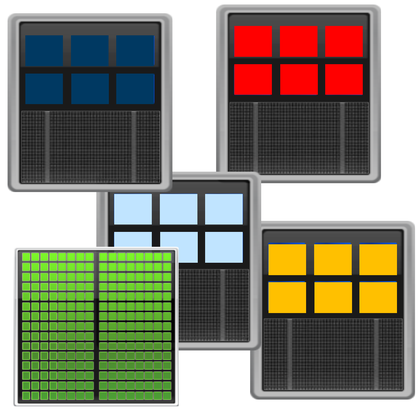
OpenACC
More Science, Less Programming

OpenMP

Programmable
Standard Languages
Directives
CUDA



CPU Optimized
Directives
Vectorization

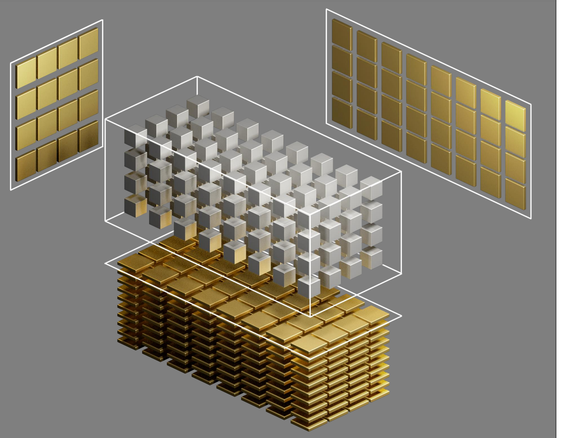


Multi-Platform
x86_64
AArch64
OpenPOWER

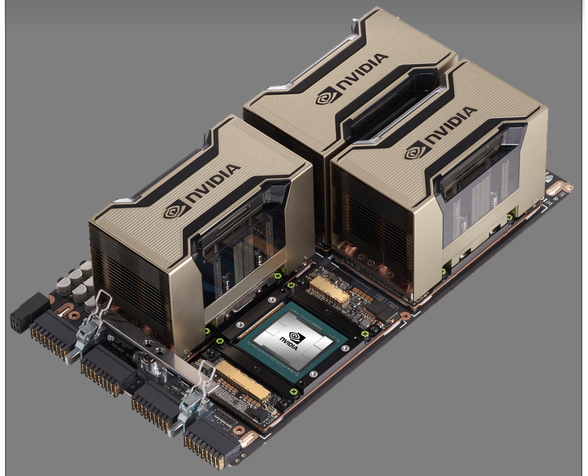
NVIDIA PERFORMANCE LIBRARIES

Core and Math Library Directions

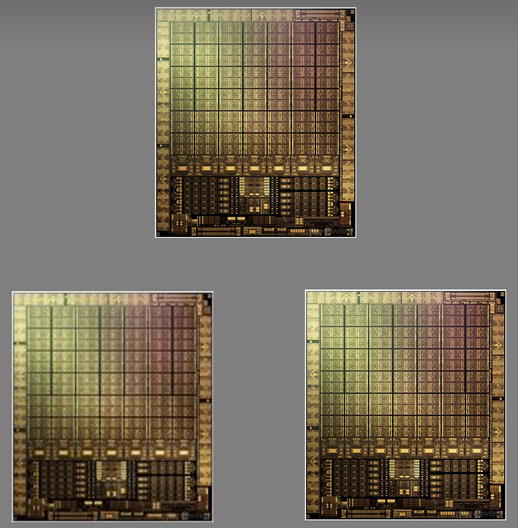
Seamless Acceleration
Tensor Cores, GH C2C



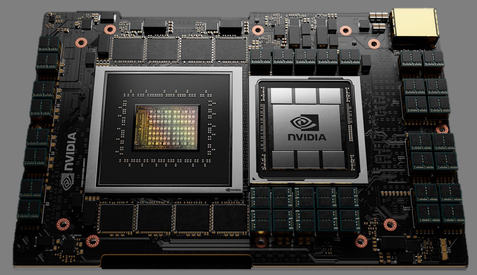
Scaling Up
Multi-GPU and Multi-Node Libraries



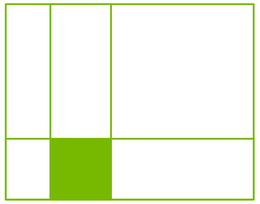
Composability
Device Functions



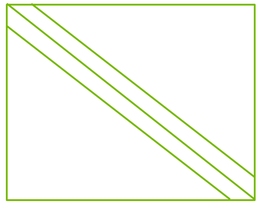
Arm Execution
High Performance CPU Libraries



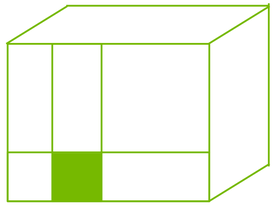
NVIDIA Math Libraries



cuBLAS

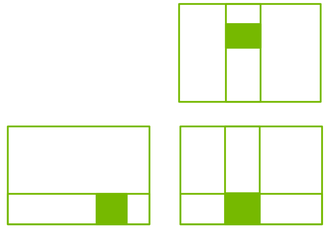


cuSPARSE

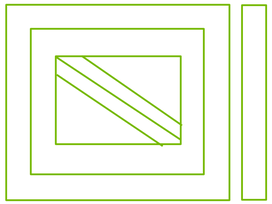


cuTENSOR

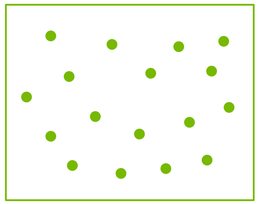
cuSOLVER



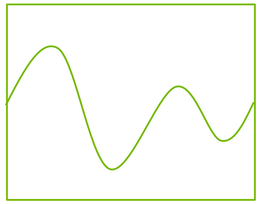
CUTLASS



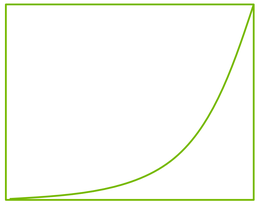
AMGX



cuRAND



cuFFT



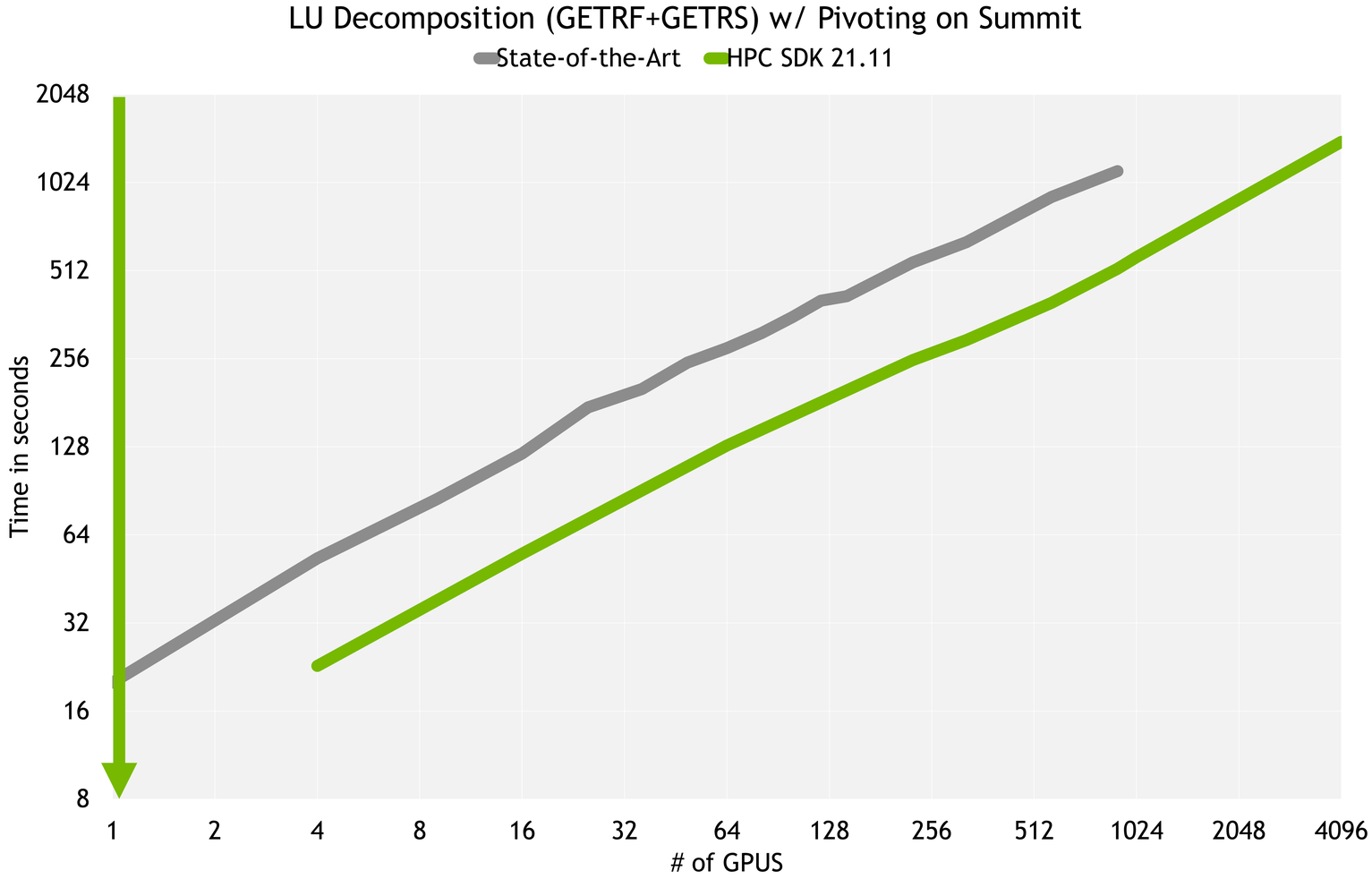
Math API

cuSOLVERMp

Mutli-Node Multi-GPU Solvers

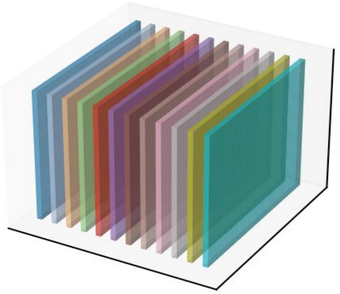
Recent Improvements

- Released in HPC SDK 21.11
- LU Decomposition
- Cholesky



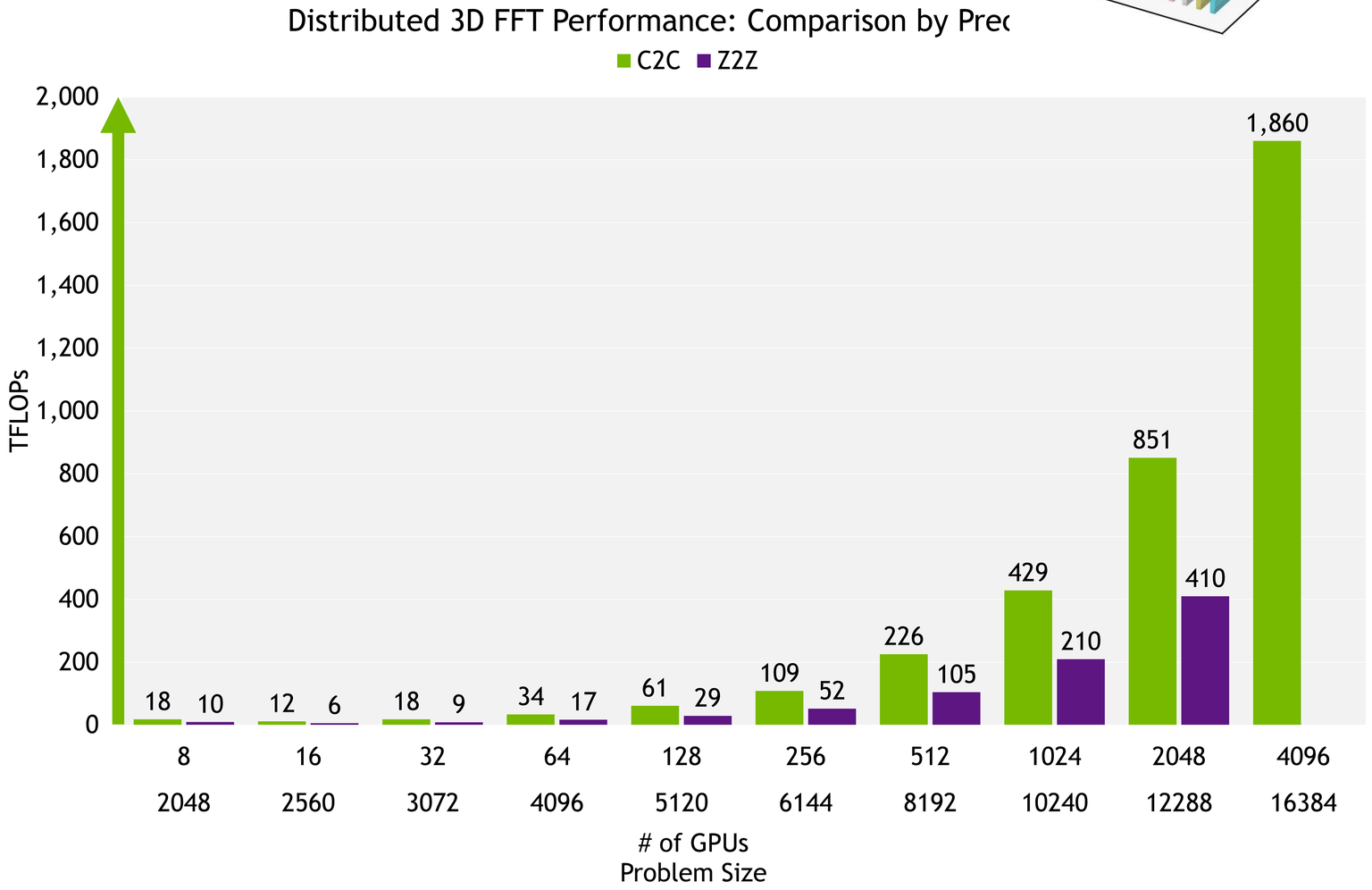
cuFFTMp

Multi-Node Multi-GPU 2D/3D FFTs

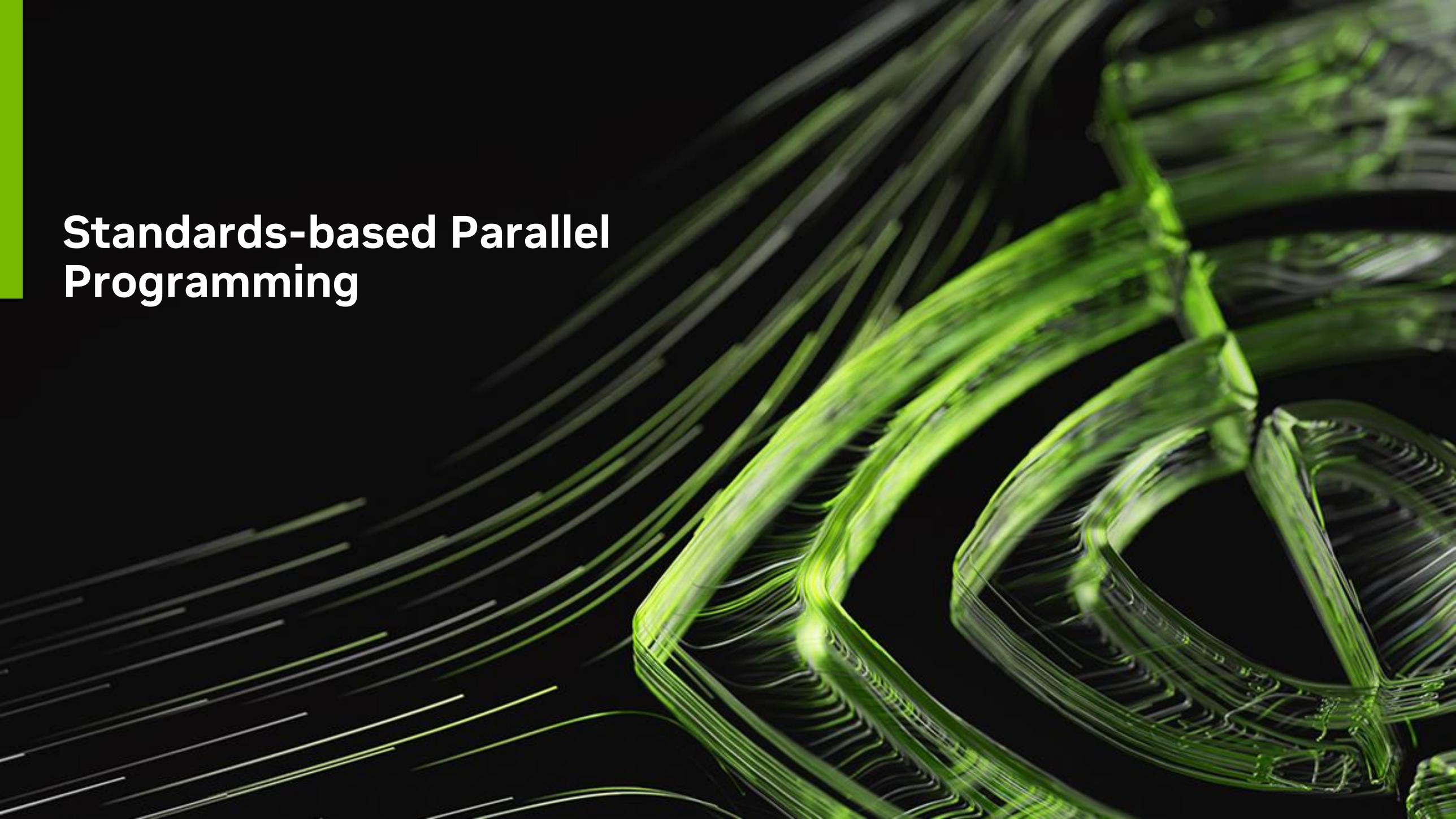


Recent Improvements

- Released in HPC SDK 22.3
- Distributed 2D/3D FFTs
- Slab Decomposition
- Pencil Decomposition (Preview)
- Helper functions: Pencils <-> Slabs



Standards-based Parallel Programming



HPC PROGRAMMING IN ISO C++

ISO is the place for portable concurrency and parallelism

C++17 & C++20

Parallel Algorithms

- In NVC++
- Parallel and vector concurrency

Forward Progress Guarantees

- Extend the C++ execution model for accelerators

Memory Model Clarifications

- Extend the C++ memory model for accelerators

Ranges

- Simplifies iterating over a range of values

Scalable Synchronization Library

- Express thread synchronization that is portable and scalable across CPUs and accelerators
- In libcu++:
  - `std::atomic<T>`
  - `std::barrier`
  - `std::counting_semaphore`
  - `std::atomic<T>::wait/notify_*`
  - `std::atomic_ref<T>`

Preview support coming to NVC++

C++23

`std::mdspan/mdarray`

- HPC-oriented multi-dimensional array abstractions.
- Preview Implementation In Progress!

Range-Based Parallel Algorithms

- Improved multi-dimensional loops

Extended Floating Point Types

- First-class support for formats new and old: `std::float16_t/float64_t`

And Beyond

Executors / Senders-Receivers

- Simplify launching and managing parallel work across CPUs and accelerators
- Preview Implementation In Progress!

Linear Algebra

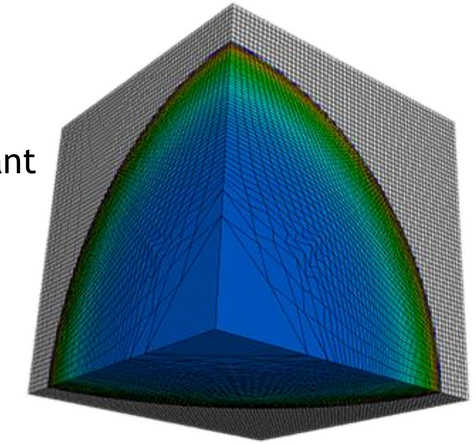
- C++ standard algorithms API to linear algebra
- Maps to vendor optimized BLAS libraries
- Preview Implementation In Progress!

Lulesh with Standard C++

C++ Hydrodynamics Mini-app from LLNL

Rewritten from OpenMP to ISO C++

- More composable, compact, and elegant
- Easier to read and maintain
- ISO Standard
- Portable – nvc++, g++, icpc, MSVC, …



```cpp
static inline
void CalcHydroConstraintForElems(Domain &domain, Index_t length,
    Index_t *regElemlist, Real_t dvovmax, Real_t& dthydro)
{
#if _OPENMP
  const Index_t threads = omp_get_max_threads();
  Index_t hydro_elem_per_thread[threads];
  Real_t dthydro_per_thread[threads];
#else
  Index_t threads = 1;
  Index_t hydro_elem_per_thread[1];
  Real_t dthydro_per_thread[1];
#endif
#pragma omp parallel firstprivate(length, dvovmax)
  {
    Real_t dthydro_tmp = dthydro ;
    Index_t hydro_elem = -1 ;
#if _OPENMP
    Index_t thread_num = omp_get_thread_num();
#else
    Index_t thread_num = 0;
#endif
#pragma omp for
    for (Index_t i = 0 ; i < length ; ++i) {
      Index_t indx = regElemlist[i] ;

      if (domain.vdov(indx) != Real_t(0.)) {
        Real_t dtdvov = dvovmax / (FABS(domain.vdov(indx))+Real_t(1.e-20)) ;

        if ( dthydro_tmp > dtdvov ) {
          dthydro_tmp = dtdvov ;
          hydro_elem = indx ;
        }
      }
    }
    dthydro_per_thread[thread_num] = dthydro_tmp ;
    hydro_elem_per_thread[thread_num] = hydro_elem ;
  }
  for (Index_t i = 1; i < threads; ++i) {
    if(dthydro_per_thread[i] < dthydro_per_thread[0]) {
      dthydro_per_thread[0] = dthydro_per_thread[i];
      hydro_elem_per_thread[0] = hydro_elem_per_thread[i];
    }
  }
  if (hydro_elem_per_thread[0] != -1) {
    dthydro = dthydro_per_thread[0] ;
  }
  return ;
}
```

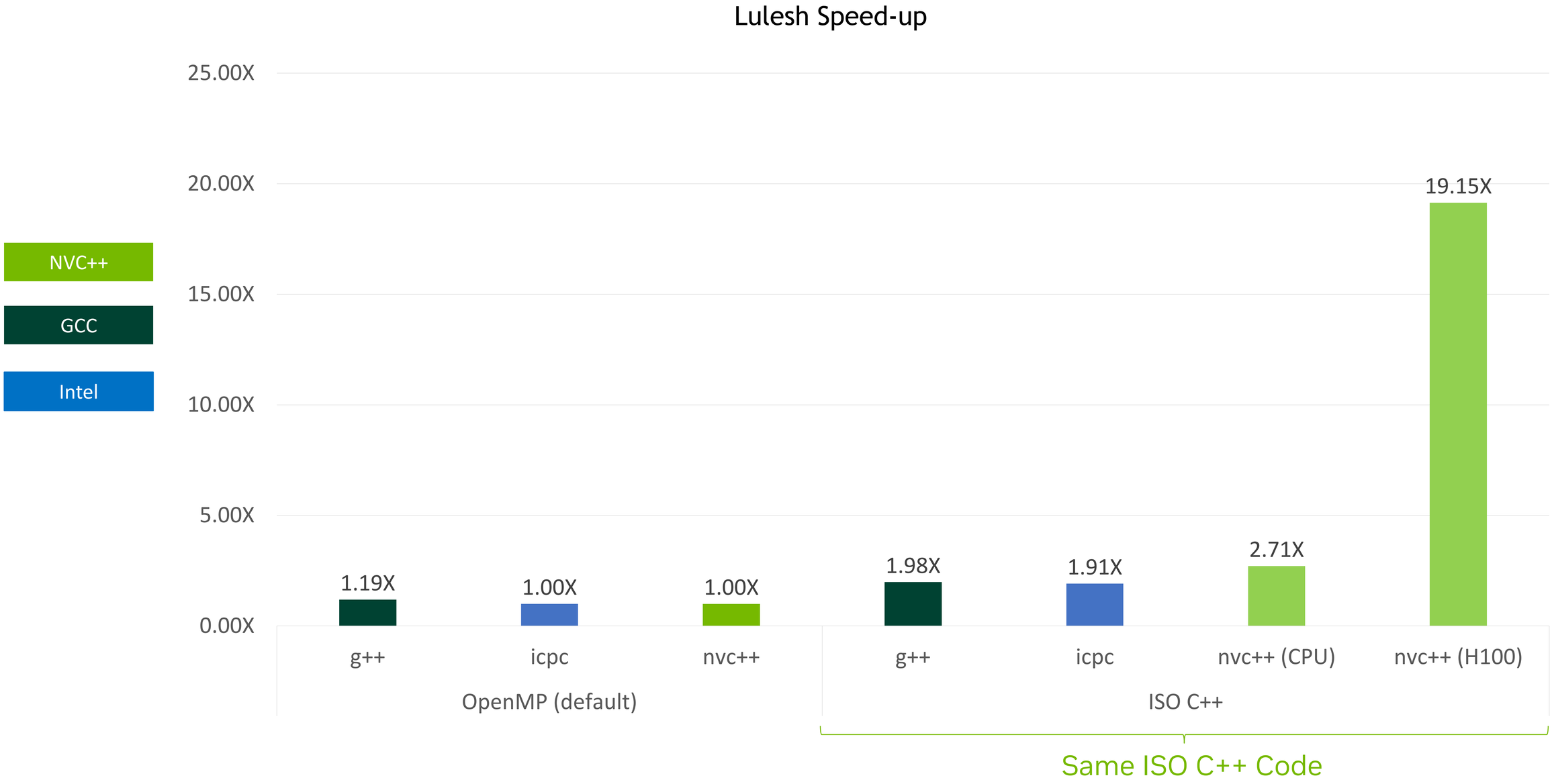
C++ with OpenMP

```cpp
static inline void CalcHydroConstraintForElems(Domain &domain, Index_t length,
                Index_t *regElemlist,
                Real_t dvovmax,
                Real_t &dthydro)
{
  dthydro = std::transform_reduce(
    std::execution::par, counting_iterator(0), counting_iterator(length),
    dthydro, [](Real_t a, Real_t b) { return a < b ? a : b; },
    [=, &domain](Index_t i)
  {
      Index_t indx = regElemlist[i];
      if (domain.vdov(indx) == Real_t(0.0)) {
        return std::numeric_limits<Real_t>::max();
      } else {
        return dvovmax / (std::abs(domain.vdov(indx)) + Real_t(1.e-20));
      }
  });
}
```

Standard C++

codesign.llnl.gov/lulesh

C++ Standard Parallelism

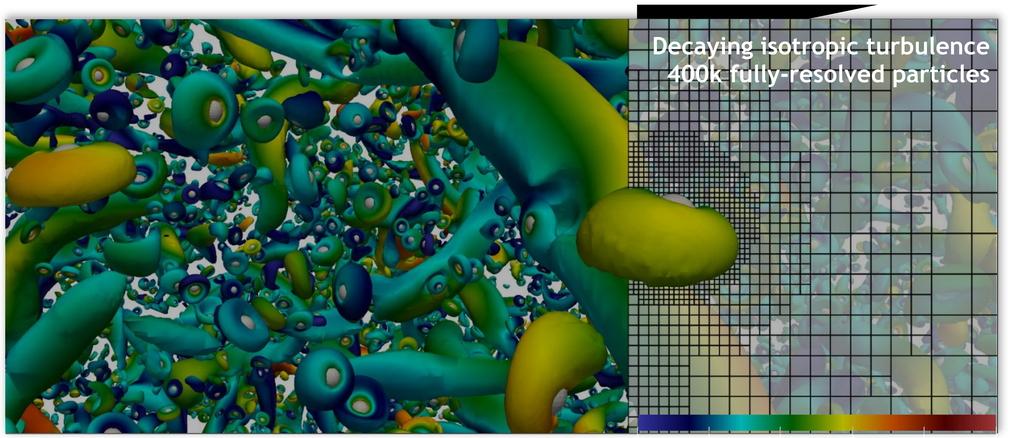


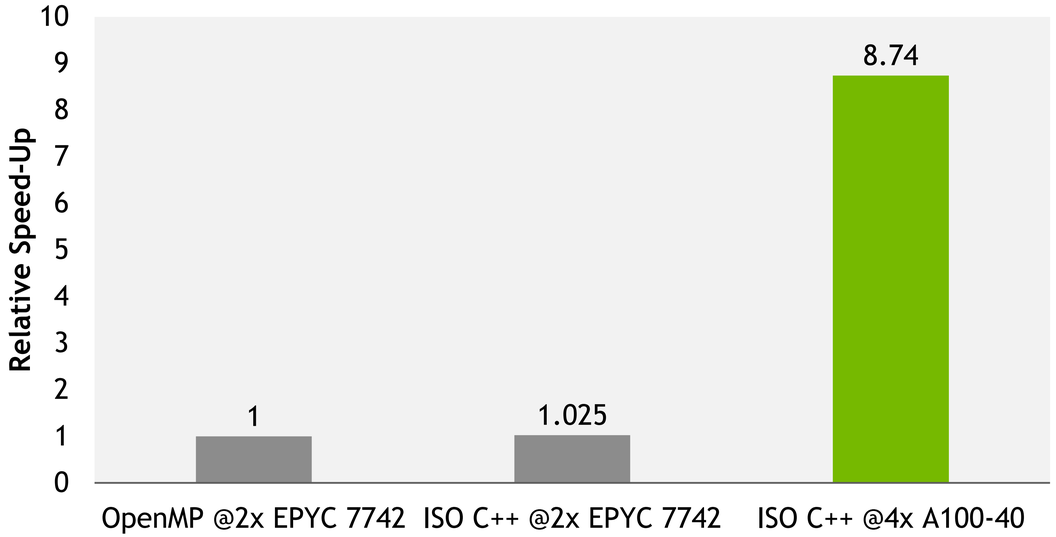
AMD EPYC 7742 CPU, NVIDIA H100 GPU. g++ version 10.3.0, icpc version 2021.5.0, nvc++ version 22.x

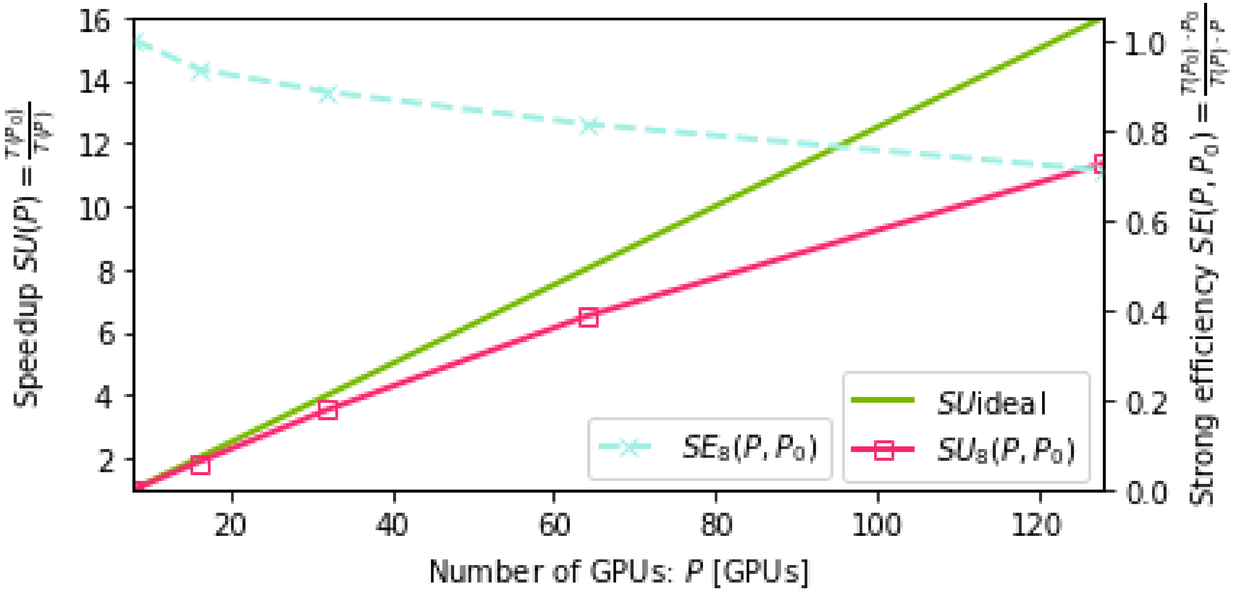
M-AIA

Multi-physics simulation framework developed at the Institute of Aerodynamics, RWTH Aachen University

- Hierarchical grids, complex moving geometries
- Adaptive meshing, load balancing
- Numerical methods: FV, DG, LBM, FEM, Level-Set, ...
- Physics: aeroacoustics, combustion, biomedical, ...
- Developed by ~20 PhDs (Mech. Eng.), ~500k LOC++
- **Programming model:** MPI + **ISO C++ parallelism**







HPC PROGRAMMING IN ISO FORTRAN

ISO is the place for portable concurrency and parallelism

Fortran 2018

Fortran Array Intrinsics

- NVFORTRAN 20.5
- Accelerated matmul, reshape, spread, …

DO CONCURRENT

- NVFORTRAN 20.11
- Auto-offload & multi-core

Co-Arrays

- Not currently available
- Accelerated co-array images

Preview support available now in NVFORTRAN

Fortran 202x

DO CONCURRENT Reductions

- NVFORTRAN 21.11
- `REDUCE` subclause added
- Support for `+`, `*`, `MIN`, `MAX`, `IAND`, `IOR`, `IEOR`.
- Support for `.AND.`, `.OR.`, `.EQV.`, `.NEQV` on `LOGICAL` values

MiniWeather

Standard Language Parallelism in Climate/Weather Applications

MiniWeather

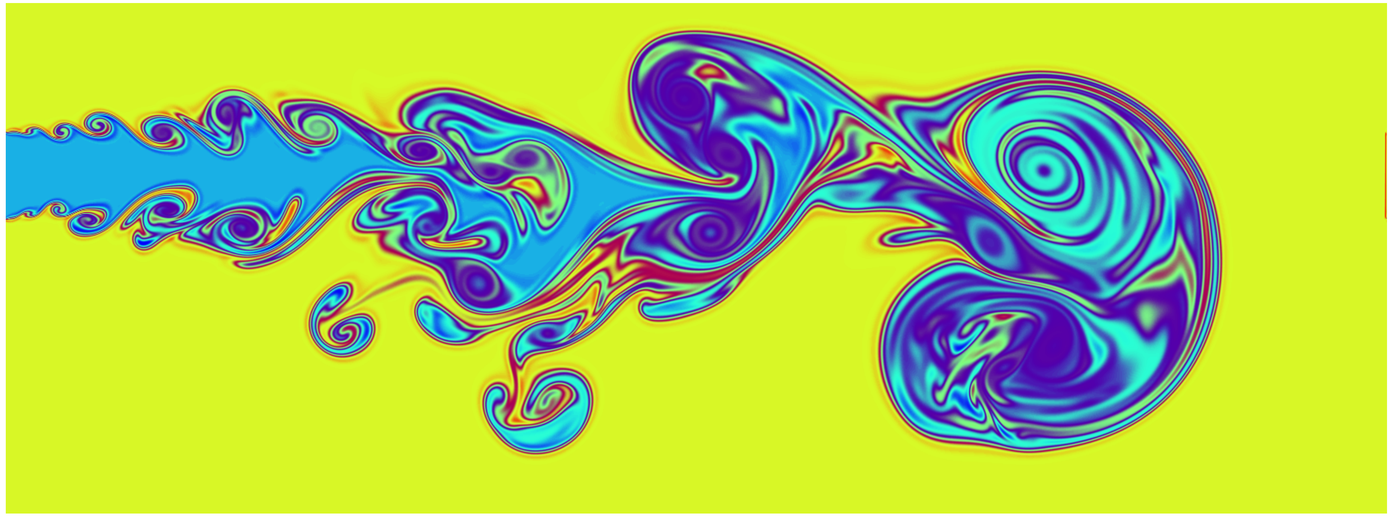
Mini-App written in C++ and Fortran that simulates weather-like fluid flows using Finite Volume and Runge-Kutta methods.

Existing parallelization in MPI, OpenMP, OpenACC, …

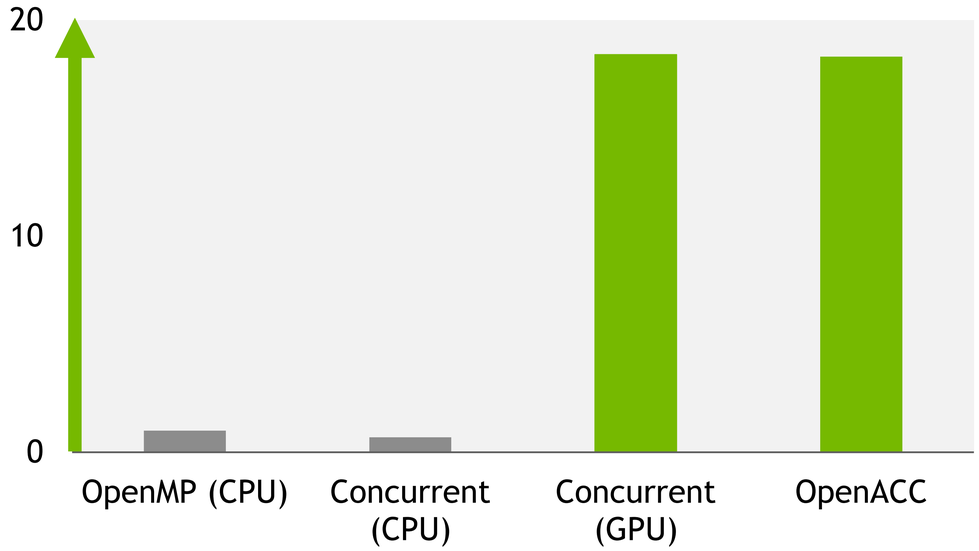
Included in the SPEChpc benchmark suite*

Open-source and commonly-used in training events.

https://github.com/mrnorman/miniWeather/



```
do concurrent (ll=1:NUM_VARS, k=1:nz, i=1:nx)
      local(x,z,x0,z0,xrad,zrad,amp,dist,wpert)

  if (data_spec_int == DATA_SPEC_GRAVITY_WAVES) then
    x = (i_beg-1 + i-0.5_rp) * dx
    z = (k_beg-1 + k-0.5_rp) * dz
        x0 = xlen/8
    z0 = 1000
    xrad = 500
    zrad = 500
    amp = 0.01_rp
    dist = sqrt( ((x-x0)/xrad)**2 + ((z-z0)/zrad)**2 )
         * pi / 2._rp
    if (dist <= pi / 2._rp) then
      wpert = amp * cos(dist)**2
    else
      wpert = 0._rp
    endif
    tend(i,k,ID_WMOM) = tend(i,k,ID_WMOM)
                      + wpert*hy_dens_cell(k)
  endif
  state_out(i,k,ll) = state_init(i,k,ll)
                    + dt * tend(i,k,ll)

enddo
```



Source: HPC SDK 22.1, AMD EPYC 7742, NVIDIA A100. MiniWeather: NX=2000, NZ=1000, SIM_TIME=20 OpenACC version uses -gpu=managed option.

*SPEChpc is a trademark of The Standard Performance Evaluation Corporation

NVIDIA

POT3D: Do Concurrent + Limited OpenACC

POT3D

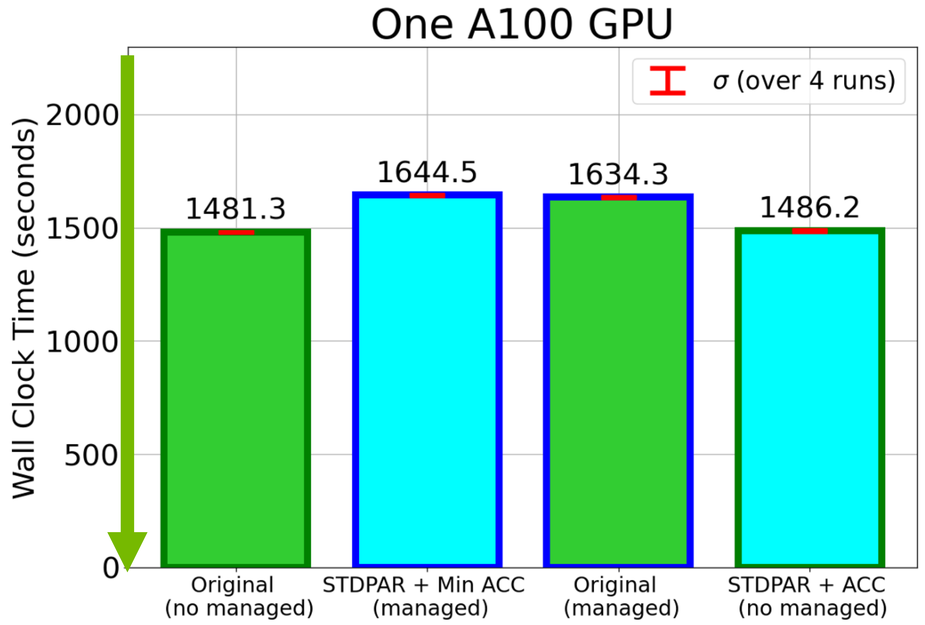
POT3D is a Fortran application for approximating solar coronal magnetic fields.

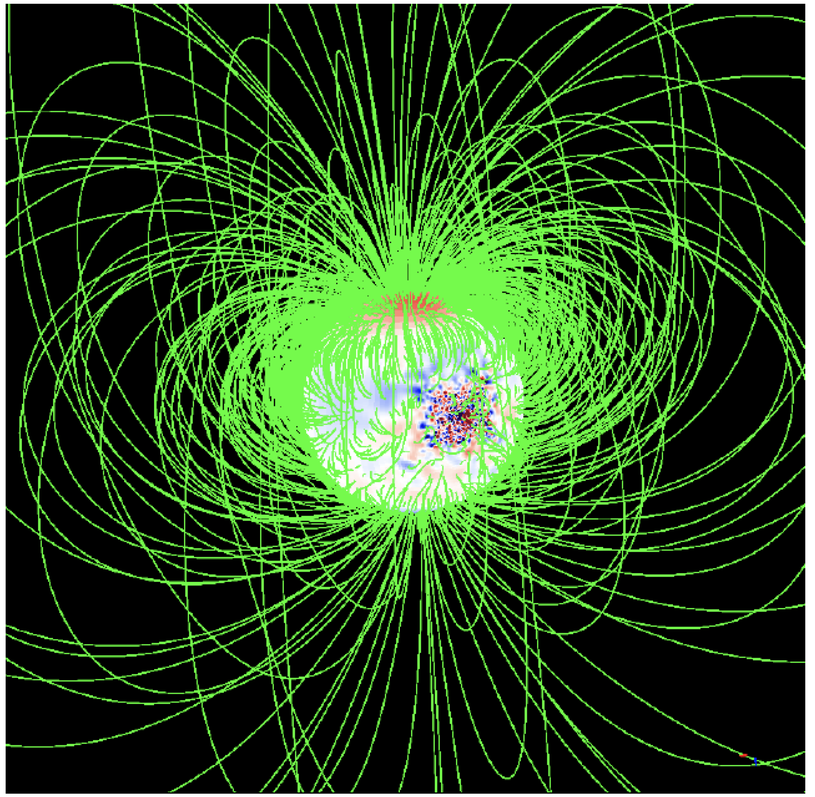
Included in the SPEChpc benchmark suite*

Existing parallelization in MPI & OpenACC

Optimized the DO CONCURRENT version by using OpenACC solely for data motion and atomics

https://github.com/predsci/POT3D





```
!$acc enter data copyin(phi,dr_i)
!$acc enter data create(br)
do concurrent (k=1:np,j=1:nt,i=1:nrm1)
  br(i,j,k)=(phi(i+1,j,k)-phi(i,j,k ))*dr_i(i)
enddo
!$acc exit data delete(phi,dr_i,br)
```

Data courtesy of Predictive Science Inc.

*SPEChpc is a trademark of The Standard Performance Evaluation Corporation

NVIDIA

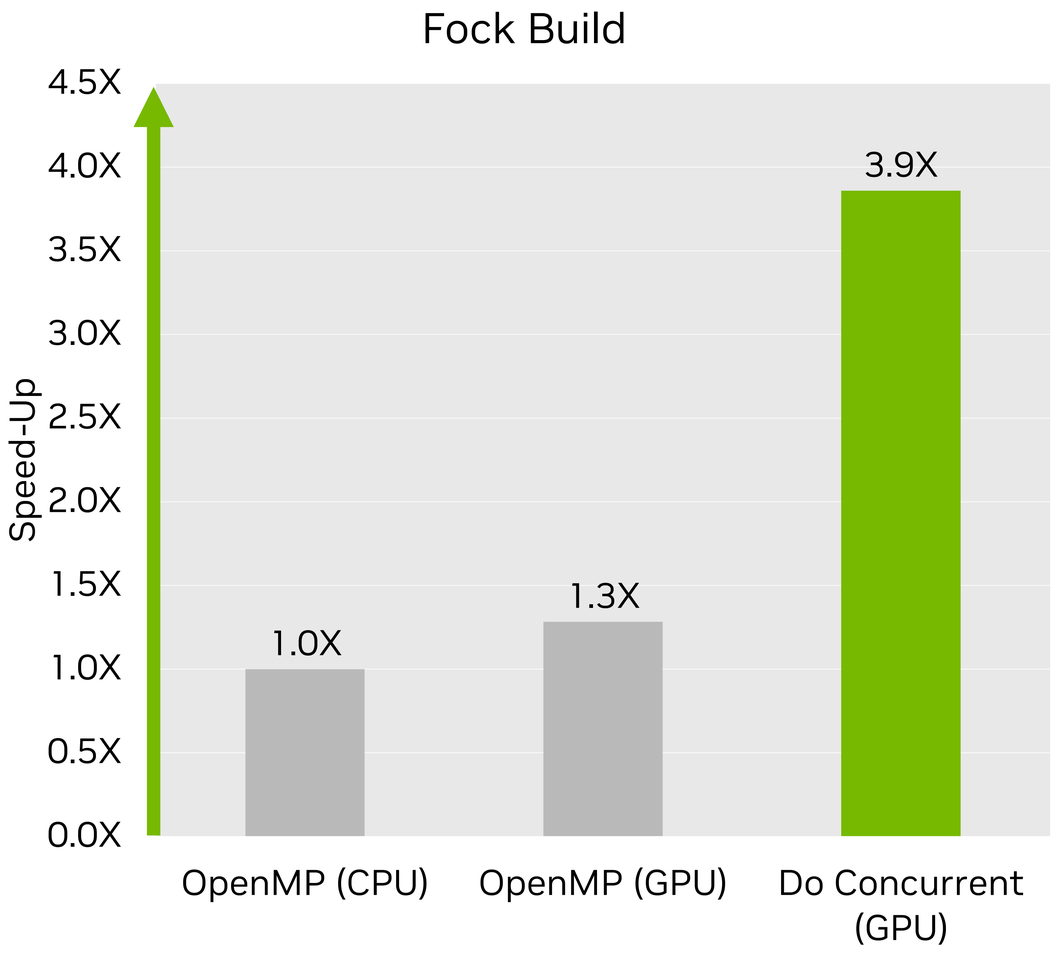
GAMESS

Computational Chemistry with Fortran Do Concurrent

- GAMESS is a popular Quantum Chemistry application.
- More than 40 years of development in Fortran and C
- MPI + OpenMP baseline code
- Hartree-Fock rewritten in Do Concurrent

```
!pre-sorting, screening

!$omp target teams distribute
            parallel do &
!$omp shared() private()
do iquart = 1, ssdd_quarts
!recover shell index
ish=IDX(s_sh)
jsh=IDX(s_sh)
ksh=IDX(d_sh)
lsh=IDX(d_sh)
  !compute ints
  !digest ints
enddo
!$omp end target teams distribute
          parallel do
```

```
!pre-sorting, screening



DO CONCURRENT (iquart=1::ssdd_quarts)&
   SHARED() LOCAL()
!recover shell index
ish=IDX(s_sh)
jsh=IDX(s_sh)
ksh=IDX(d_sh)
lsh=IDX(d_sh)
  !compute ints
  !digest ints
enddo
```



nvfortran 22.7, NVIDIA A100 GPU, AMD “Milan” CPU

* Courtesy of Melisa Alkan, Iowa State University. Not yet published.

ACCELERATED PROGRAMMING IN ISO FORTRAN

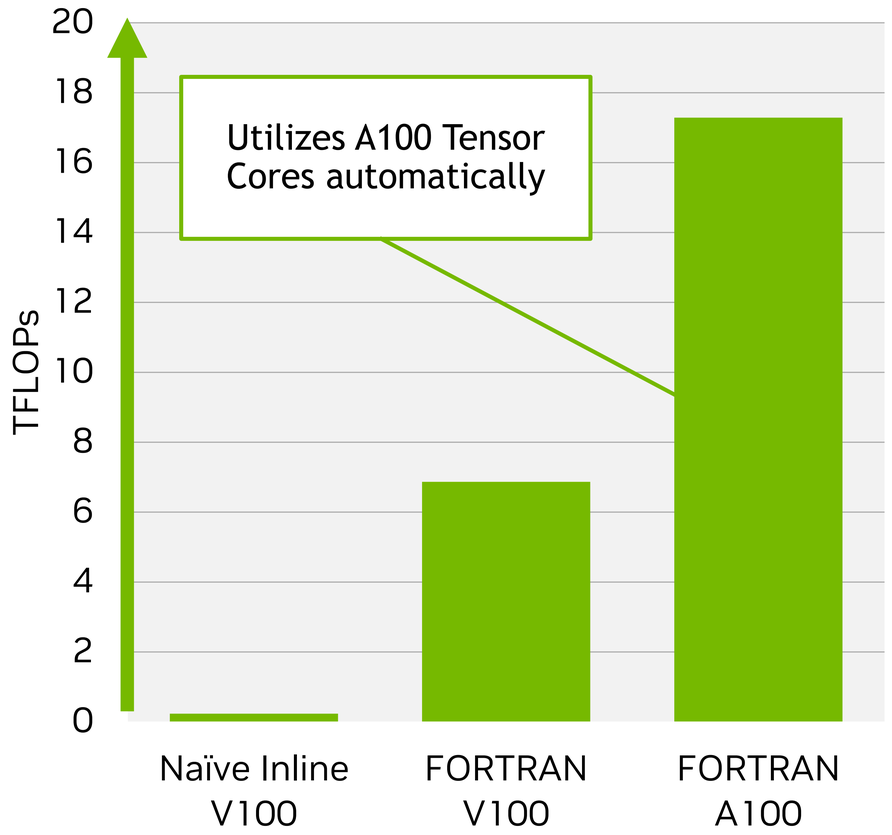
NVFORTRAN Accelerates Fortran Intrinsics with cuTENSOR Backend

```
real(8), dimension(ni,nk) :: a
real(8), dimension(nk,nj) :: b
real(8), dimension(ni,nj) :: c
...
!$acc enter data copyin(a,b,c) create(d)

do nt = 1, ntimes
  !$acc kernels
  do j = 1, nj
    do i = 1, ni
      d(i,j) = c(i,j)
      do k = 1, nk
        d(i,j) = d(i,j) + a(i,k) * b(k,j)
      end do
    end do
  end do
    !$acc end kernels
end do
!$acc exit data copyout(d)
```

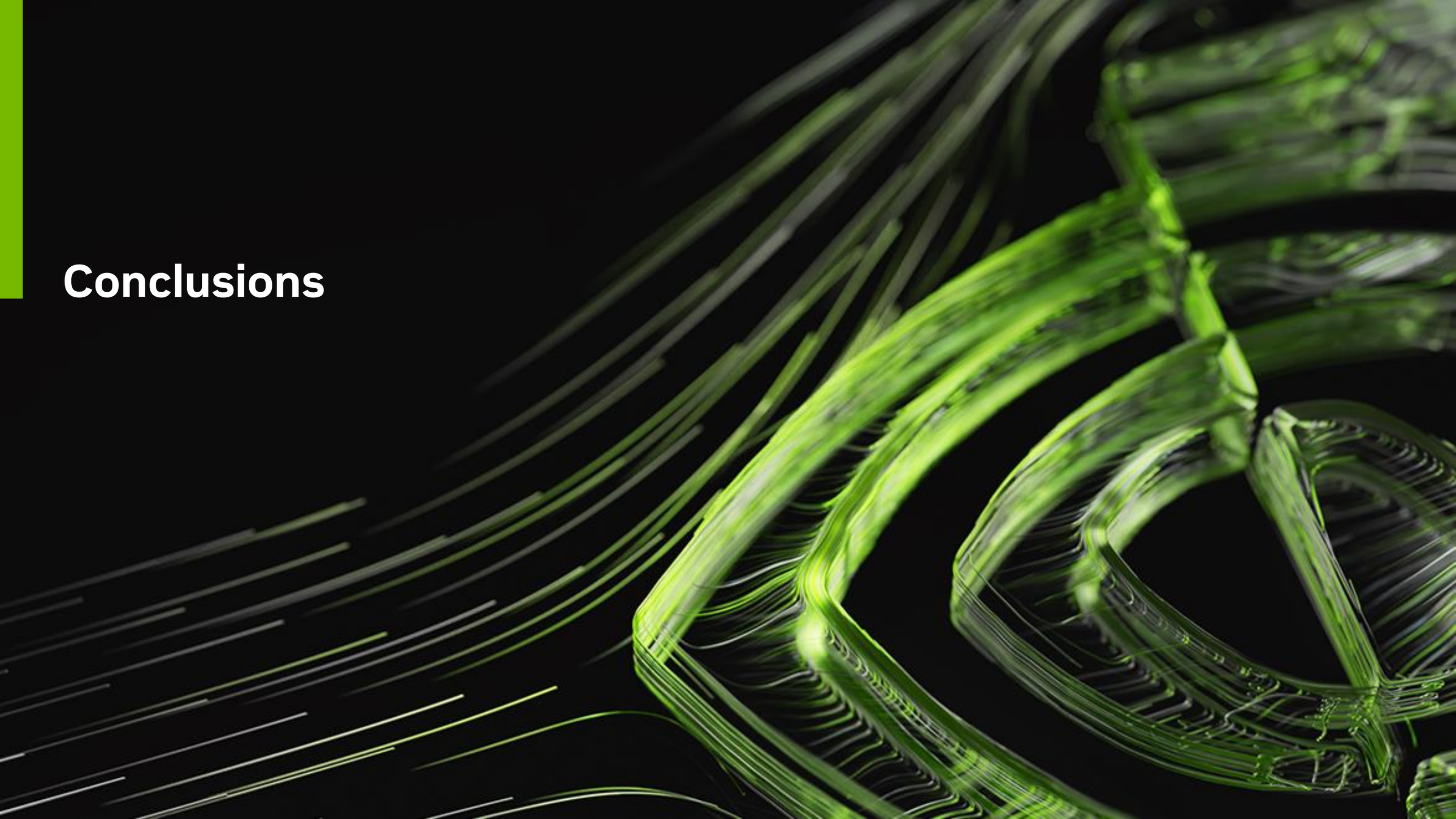
Inline FP64 matrix multiply

```
real(8), dimension(ni,nk) :: a
real(8), dimension(nk,nj) :: b
real(8), dimension(ni,nj) :: c

...

do nt = 1, ntimes
  d = c + matmul(a,b)
end do
```

MATMUL FP64 matrix multiply

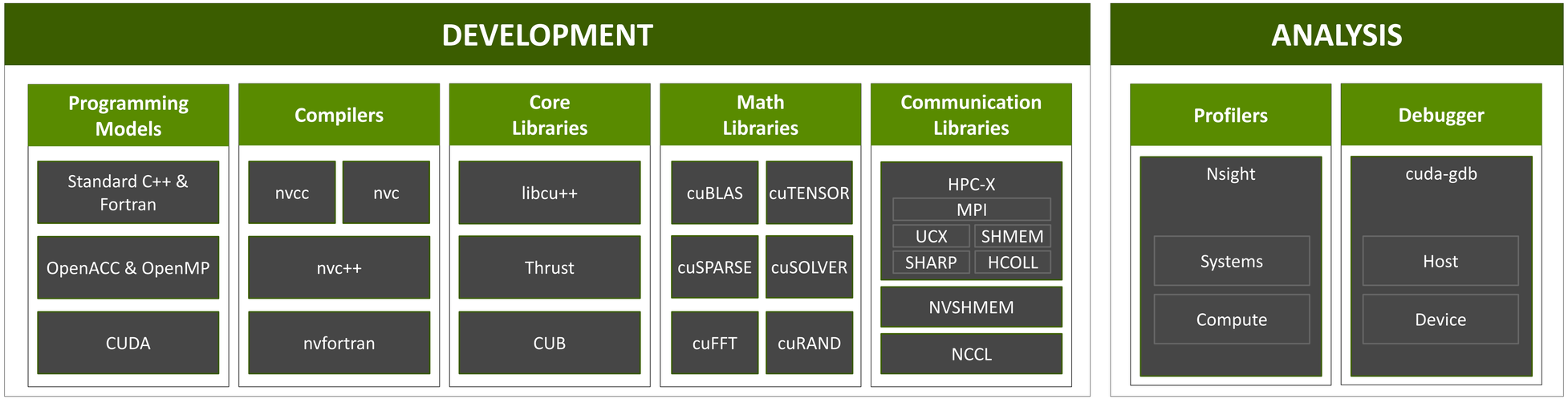


Conclusions



Conclusions

- NVIDIA HPC SDK is a complete and portable toolkit for HPC developers
- NVIDIA supports a wide range of programming models to enable you to choose the right balance of productivity, portability, and performance for your project
- For more information on these topics, see the following on-demand GTC sessions:
  - A Deep Dive into the Latest HPC Software
  - CUDA: New Features and Beyond
  - How CUDA Programming Works
  - Developing HPC Applications with Standard C++, Fortran, and Python

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