NVIDIA HPC STANDARD LANGUAGE PARALLELISM

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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

FORTRAN DO CONCURRENT IS STANDARD FORTRAN

Background

Fortran introduced the 'DO CONCURRENT' construct in 2008. We assume the programmer guarantees that there are no dependencies between iterations so that we can run it in parallel on either a GPU or CPU.

```
# This option enables GPU offload
% nvfortran -stdpar source.f90
```

The syntax:

```
DO CONCURRENT (concurrent-header) [locality-spec]
   loop-body
END DO
```

where *locality-spec* is one of the following:

```
local(variable-name-list)
local_init(variable-name-list)
shared(variable-name-list)
default(none)
```

FORTRAN DO CONCURRENT IN MINI-WEATHER

use the local clause, similar to privatizing arrays in OpenACC and OpenMP

```
 !Compute fluxes in the x-direction for each cell
 do concurrent (k=1:nz, i=1:nx+1) local(d3_vals,vals,stencil,ll,s,r,u,t,p,w)
    !Use fourth-order interpolation from four cell averages to compute the
value at the interface in question
    do ll = 1 , NUM_VARS
      do s = 1 , sten_size
        stencil(s) = state(i-hs-1+s,k,ll)
      enddo
      !Fourth-order-accurate interpolation of the state
      vals(ll) = -stencil(1)/12 + 7*stencil(2)/12 + 7*stencil(3)/12 -
stencil(4)/12
      !First-order-accurate interpolation of the third spatial derivative of
the state (for artificial viscosity)
      d3_vals(ll) = -stencil(1) + 3*stencil(2) - 3*stencil(3) + stencil(4)
    enddo

    !Compute density, u-wind, w-wind, potential temperature, and pressure
(r,u,w,t,p respectively)
    r = vals(ID_DENS) + hy_dens_cell(k)
    u = vals(ID_UMOM) / r
    w = vals(ID_WMOM) / r
    t = ( vals(ID_RHOT) + hy_dens_theta_cell(k) ) / r
    p = C0*(r*t)**gamma

    !Compute the flux vector
    flux(i,k,ID_DENS) = r*u     - hv_coef*d3_vals(ID_DENS)
    flux(i,k,ID_UMOM) = r*u*u+p - hv_coef*d3_vals(ID_UMOM)
    flux(i,k,ID_WMOM) = r*u*w   - hv_coef*d3_vals(ID_WMOM)
    flux(i,k,ID_RHOT) = r*u*t   - hv_coef*d3_vals(ID_RHOT)
 enddo
```

```
Minfo Output:

compute_tendencies_x:

    253, Generating NVIDIA GPU code

        253, Loop parallelized across CUDA thread blocks,

                   CUDA threads(32) ! blockidx%x threadidx%x

             Loop parallelized across CUDA thread blocks,

                   CUDA threads(4) blockidx%y threadidx%y

        255, Loop run sequentially

        256, Loop run sequentially

    253, Local memory used for stencil,vals,d3_vals
```

FORTRAN DO CONCURRENT IN MINI-WEATHER

nvfortran supports the reduce clause starting with version 21.11

```
do concurrent (k=1:nz, i=1:nx) reduce(+:mass,te)
   r  =   state(i,k,ID_DENS) + hy_dens_cell(k)              ! Density
   u  =   state(i,k,ID_UMOM) / r                            ! U-wind
   w  =   state(i,k,ID_WMOM) / r                            ! W-wind
   th = ( state(i,k,ID_RHOT) + hy_dens_theta_cell(k) ) / r ! Theta-temp
   p  = C0*(r*th)**gamma      ! Pressure
   t  = th / (p0/p)**(rd/cp)  ! Temperature
   ke = r*(u*u+w*w)           ! Kinetic Energy
   ie = r*cv*t                ! Internal Energy
   mass = mass + r            *dx*dz ! Accumulate domain mass
   te    = te    + (ke + r*cv*t)*dx*dz ! Accumulate domain total energy
enddo

call mpi_allreduce((/mass,te/),glob,2,MPI_REAL8,MPI_SUM,MPI_COMM_WORLD,ierr)
mass = glob(1)
te   = glob(2)
```

```
Minfo Output:

reductions:

    844, Generating NVIDIA GPU code

        844,   ! blockidx%x threadidx%x auto-collapsed

             Loop parallelized across CUDA thread blocks,

                  CUDA threads(128) collapse(2) ! blockidx%x threadidx%x

             Generating reduction(+:te,mass)
```

FORTRAN DO CONCURRENT CURRENT LIMITATIONS

- Do Concurrent requires function and subroutine calls to be pure
- We follow OpenACC and OpenMP defaults for scalars (first-private/local) and arrays (shared)
  - In fact, -stdpar currently enables OpenACC, is built on top of OpenACC.
- Do Concurrent lacks control over GPU scheduling which we have found useful
  - Forcing a “loop seq” inside the region
  - Offloading a serial kernel
  - No control equivalent to OpenACC’s gang, worker, vector
- Interoperability with CUDA is not all there yet
  - We still need to mark some useful device functions as pure (we do support CUDA atomics)
  - No control over the stream which the offloaded region runs on
  - Not interoperable yet with CUDA Fortran device attributed data

FUTURE OF CONCURRENCY AND PARALLELISM IN HPC: STANDARD LANGUAGES

How did we get here?

ON-GOING LONG TERM INVESTMENT

ISO committee participation from industry, academia and government labs.

Fruit born in 2020 was planted over the previous decade.

Focus on enhancing concurrency and parallelism for all.

Open collaboration between partners and competitors.

Past investments in directives enabled rapid progress.

MAJOR FEATURES

Memory Model Enhancements

C++14 Atomics Extensions

C++17 Parallel Algorithms

C++20 Concurrency Library

C++23 Multi-Dim. Array Abstractions

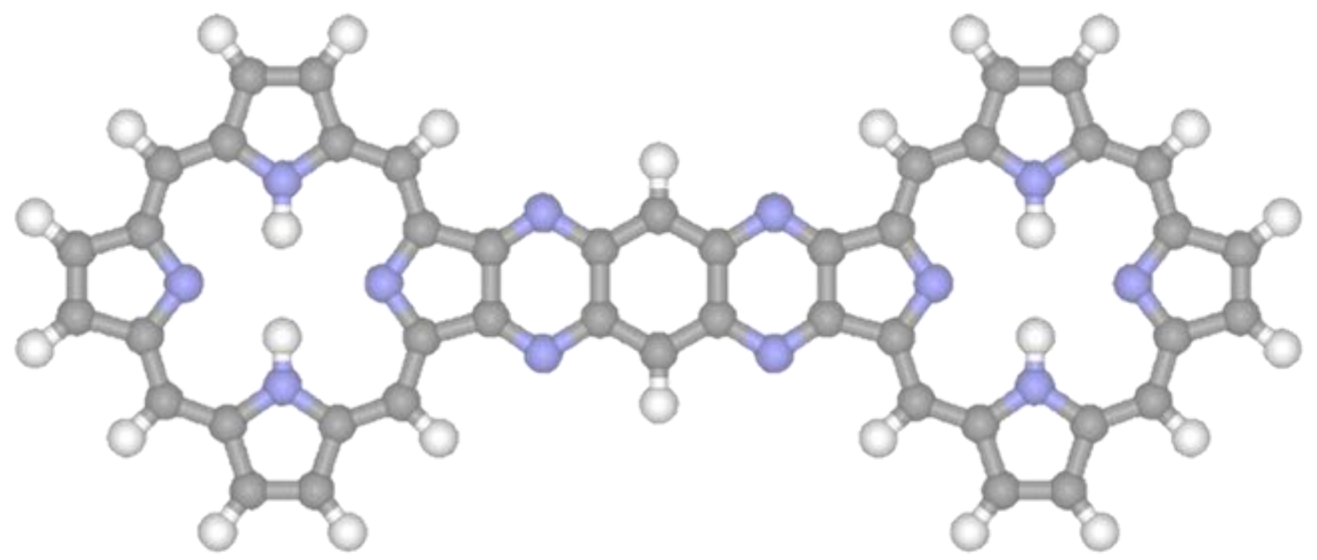
C++2X Executors

C++2X Linear Algebra

C++2X Extended Floating Point Types

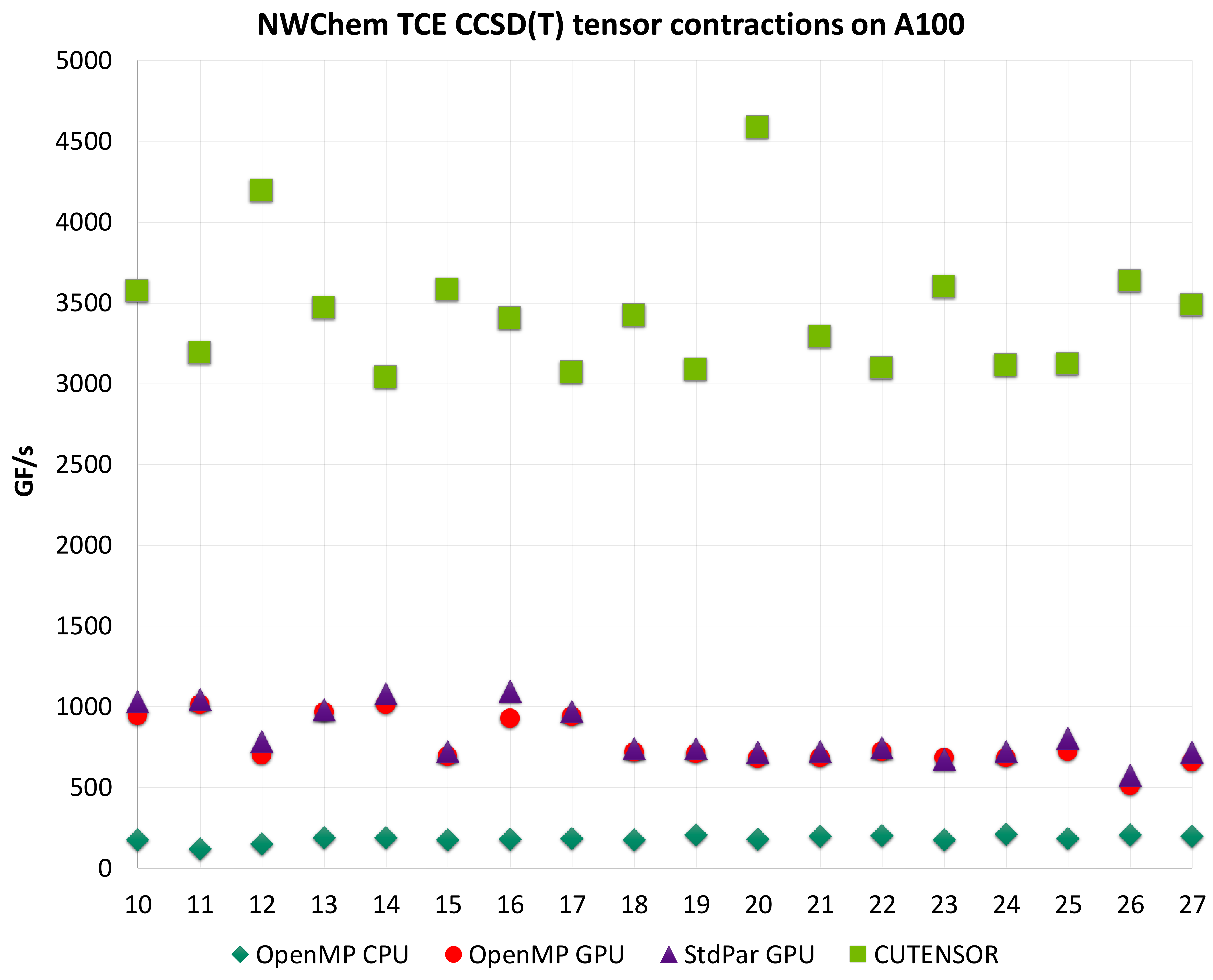
C++2X Range Based Parallel Algorithms

Fortran 2X DO CONCURRENT Reduction



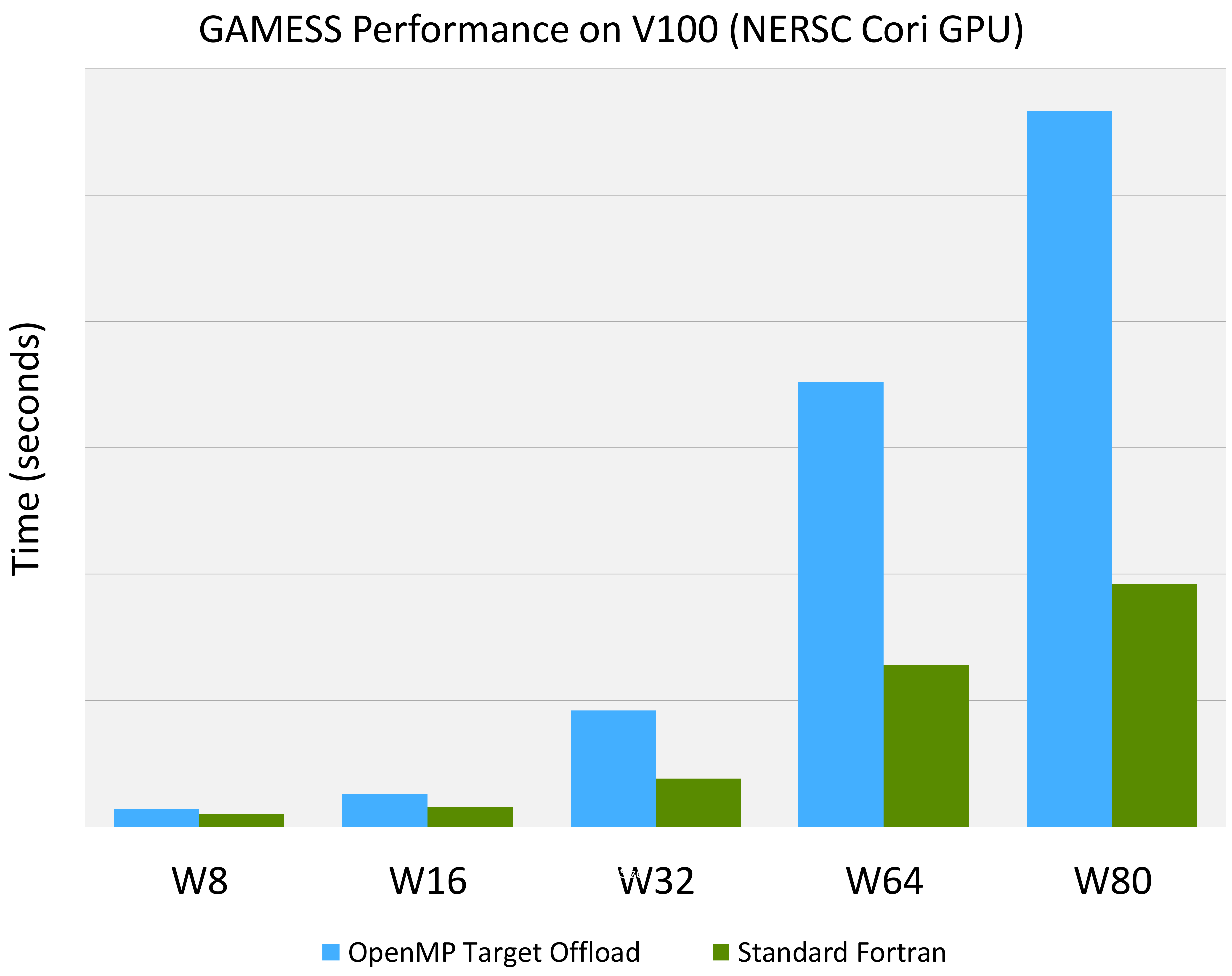
FORTRAN STANDARD PARALLELISM

NWChem and GAMESS with DO CONCURRENT



NWChem TCE CCSD(T) tensor contractions on A100

https://github.com/jeffhammond/nwchem-tce-triples-kernels/



GAMESS Performance on V100 (NERSC Cori GPU)

GAMESS results from Melisa Alkan and Gordon Group, Iowa State

HPC PROGRAMMING IN ISO FORTRAN

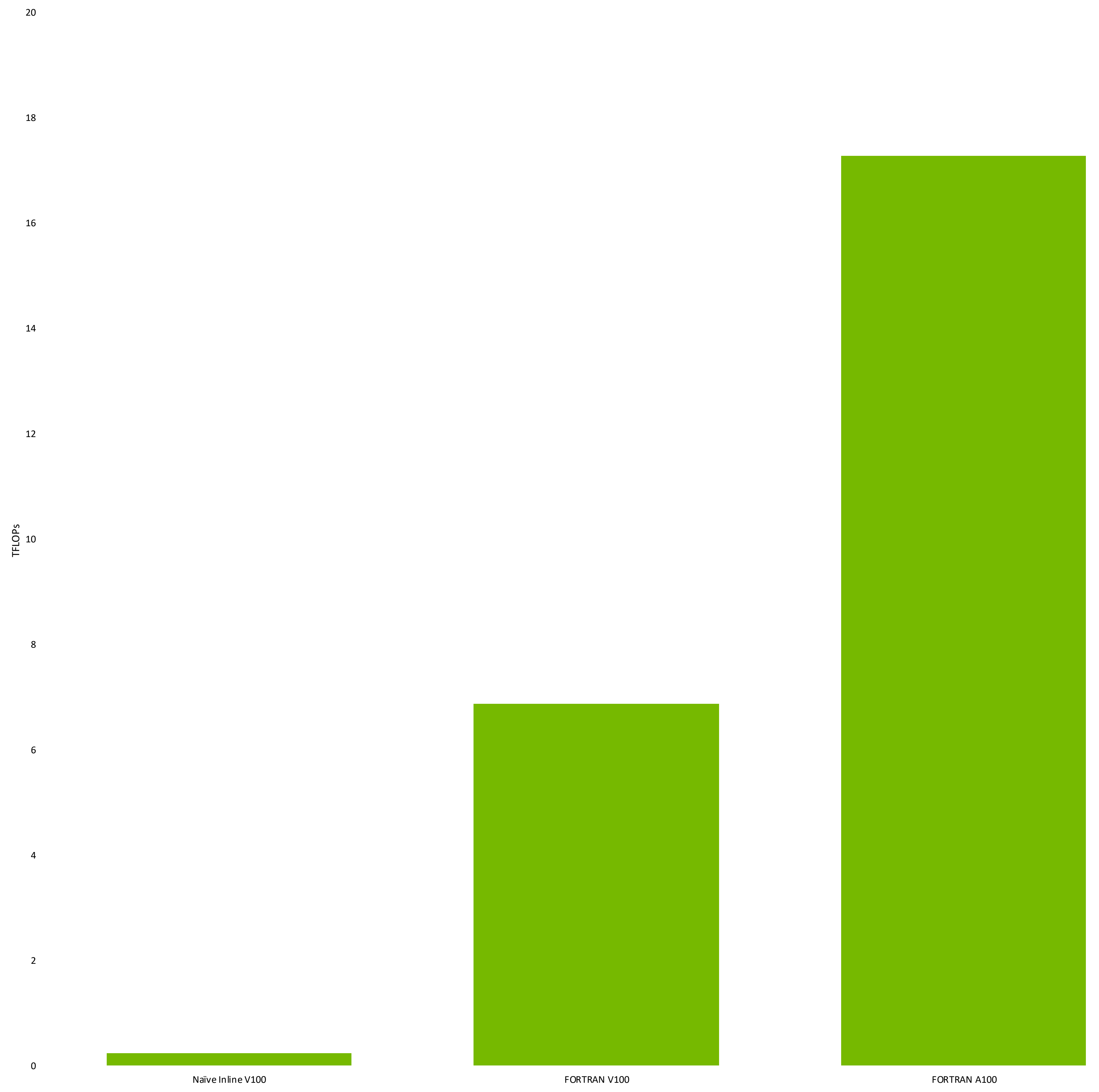
NVFORTRAN Accelerates Fortran Intrinsics with cuTENSOR Backend

```
real(8), allocatable :: a(:,:)
real(8), allocatable :: b(:,:)
real(8), allocatable :: d(:,:)
!@cuf attributes(managed) :: a, b, d
. . .
allocate(a(ni,nk))
allocate(b(nk,nj))
allocate(d(ni,nj))
call random_number(a)
call random_number(b)
d = 0.0d0
do nt = 1, ntimes
  !$cuf kernel do(2) <<<*,*>>>
  do j = 1, nj
    do i = 1, ni
      do k = 1, nk
       d(i,j)= d(i,j) + a(i,k)*b(k,j)
      end do
    end do
  end do
end do
```

Inline FP64 matrix multiply

```
!@cuf use cutensorex
real(8), allocatable :: a(:,:)
real(8), allocatable :: b(:,:)
real(8), allocatable :: d(:,:)
!@cuf attributes(managed) :: a, b, d
. . .
allocate(a(ni,nk))
allocate(b(nk,nj))
allocate(d(ni,nj))
call random_number(a)
call random_number(b)
d = 0.0d0
do nt = 1, ntimes
  d = d + matmul(a,b)
end do
```

MATMUL FP64 matrix multiply



MAPPING FORTRAN INTRINSICS TO CUTENSOR

Examples of Patterns Accelerated with cuTENSOR in HPC SDK since 20.7

```
d = 2.5 * ceil(transpose(a)) + 3.0 * abs(transpose(b))
d = 2.5 * ceil(transpose(a)) + 3.0 * abs(b)
d = reshape(a,shape=[ni,nj,nk])
d = reshape(a,shape=[ni,nk,nj])
d = 2.5 * sqrt(reshape(a,shape=[ni,nk,nj],order=[1,3,2]))
d = alpha * conjg(reshape(a,shape=[ni,nk,nj],order=[1,3,2]))
d = reshape(a,shape=[ni,nk,nj],order=[1,3,2])
d = reshape(a,shape=[nk,ni,nj],order=[2,3,1])
d = reshape(a,shape=[ni*nj,nk])
d = reshape(a,shape=[nk,ni*nj],order=[2,1])
d = reshape(a,shape=[64,2,16,16,64],order=[5,2,3,4,1])
d = abs(reshape(a,shape=[64,2,16,16,64],order=[5,2,3,4,1]))
c = matmul(a,b)
c = matmul(transpose(a),b)
c = matmul(reshape(a,shape=[m,k],order=[2,1]),b)
c = matmul(a,transpose(b))
c = matmul(a,reshape(b,shape=[k,n],order=[2,1]))
```

```
c = matmul(transpose(a),transpose(b))
c = matmul(transpose(a),reshape(b,shape=[k,n],order=[2,1]))
d = spread(a,dim=3,ncopies=nk)
d = spread(a,dim=1,ncopies=ni)
d = spread(a,dim=2,ncopies=nx)
d = alpha * abs(spread(a,dim=2,ncopies=nx))
d = alpha * spread(a,dim=2,ncopies=nx)
d = abs(spread(a,dim=2,ncopies=nx))
d = transpose(a)
d = alpha * transpose(a)
d = alpha * ceil(transpose(a))
d = alpha * conjg(transpose(a))
c = c + matmul(a,b)
c = c - matmul(a,b)
c = c + alpha * matmul(a,b)
d = alpha * matmul(a,b) + c
d = alpha * matmul(a,b) + beta * c
```

https://developer.nvidia.com/blog/bringing-tensor-cores-to-standard-fortran/

NVLAMATH Simplifies Fortran Solver Interfaces

CPU with LAPACK (OpenBLAS)	GPU with cuSOLVER	GPU with NVLAmath
... real*8 , allocatable :: a(:,:) integer, allocatable :: ipiv(:) ... allocate(a(m,n), ipiv(m)) ... call **dgetrf**(m, n, a, lda, ipiv, info) ...	... real*8 , allocatable :: a(:,:) integer, allocatable :: ipiv(:) integer :: istat, lwork type(cusolverDnHandle) :: handle real, allocatable :: work(:) integer :: devinfo(1) ... allocate(a(m,n), ipiv(m)) ... istat = **cusolverDnGetHandle**(handle) istat = **cusolverDnDgetrf_bufferSize**(handle, m, n, a, lda, lwork) allocate(work(lwork)) istat = **cusolverDnDgetrf**(handle, m, n, a, lda, work, ipiv, devinfo(1)) deallocate(work) ...	... real*8 , allocatable :: a(:,:) integer, allocatable :: ipiv(:) ... allocate(a(m,n), ipiv(m)) ... call **dgetrf**(m, n, a, lda, ipiv, info) ...
nvfortran –llapack -lblas	nvfortran –mp=gpu -gpu=managed -cudalib=cusolver	nvfortran –mp=gpu -gpu=managed -cudalib=nvlamath
GFLOPs: ~496	GFLOPs: ~3238	GFLOPs: ~3241

Matrix size: 20k x 20k
CPU: Xeon Gold 6148 w/ multi-threading; GPU: V100

FORTRAN STANDARD LANGUAGE POSSIBLE FUTURE WORK

- Add (non-standard, NVIDIA-specific) capabilities to DO CONCURRENT
- More F90 intrinsic function support in the vein of Matmul, Reshape, Spread, such as Pack and Merge
  - Requires some support for computing the mask argument efficiently
- Add more supported routines to NVLAMATH
  - Some new multi-gpu libraries might be wrapped under SCALAPACK or other interfaces
- Take advantage of new HW and SW Features

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