

Getting Fortran onto GPUs

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Outline

- Where are we now?
 - DO CONCURRENT
 - Data parallel intrinsics
 - Directives
 - CUDA support
- Where do we want to go?
 - Fetching atomics in DO CONCURRENT
 - Asynchrony and task parallelism



Programming the nvidia platform WITH FORTRAN

CPU, GPU, and Network

	ACCELERATED STANDARD MODELS		PLATFORM SPECIALIZATION	
ISO Fortran	OpenACC	OpenMP	CUDA Fortran	
<pre>do concurrent (j=1:order, &</pre>	<pre>!\$acc parallel loop tile(32,32) do j=1,order do i=1,order B(i,j) = A(j,i) enddo enddo</pre>	<pre>!\$omp target teams distribute & parallel do simd & collapse(2) do j=1,order do i=1,order B(i,j) = A(j,i) enddo enddo</pre>	<pre>BIDX = blockIdx%x-1 BIDY = blockIdx%y-1 TIDX = threadIdx%x TIDY = threadIdx%y x = BIDX * TILE + TIDX; y = BIDY * TILE + TIDY; do j = 0,TILE-1,block_rows SM(TIDX,TIDY+j) = A(x,y+j);</pre>	
B = transpose(A)	<pre>!\$acc kernels do j=1,order do i=1,order B(i,j) = A(j,i) enddo enddo !\$acc end kernels</pre>	<pre>!\$omp target teams loop & collapse(2) do j=1,order do i=1,order B(i,j) = A(j,i) enddo enddo</pre>	<pre>end do call syncThreads() x = BIDY * TILE + TIDX; y = BIDX * TILE + TIDY; do j = 0,TILE-1,block_rows B(x,y+j) = SM(TIDY+j,TIDX) end do</pre>	
ACCELERATION LIBRARIES				

CUDA Runtime

CUBLAS

CUTENSOR

CUSOLVER



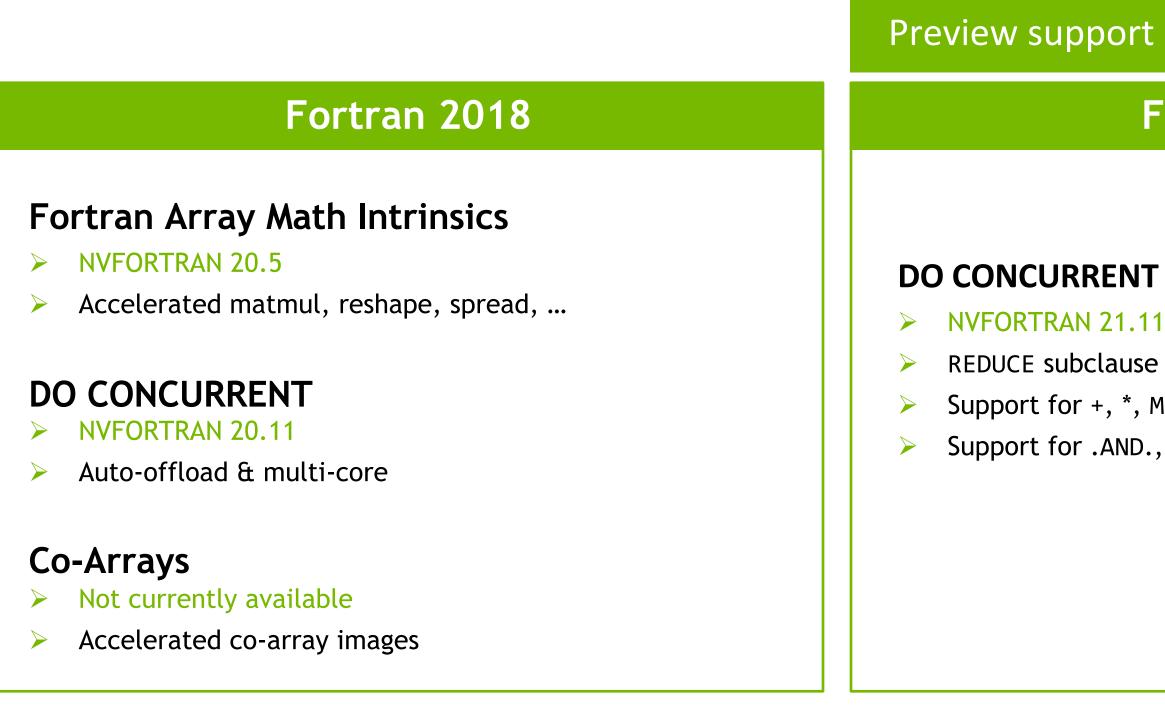
NVSHMEM

•••



HPC PROGRAMMING IN ISO FORTRAN

ISO is the place for portable concurrency and parallelism



Preview support available now in NVFORTRAN

Fortran 202x

DO CONCURRENT Reductions

- **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.

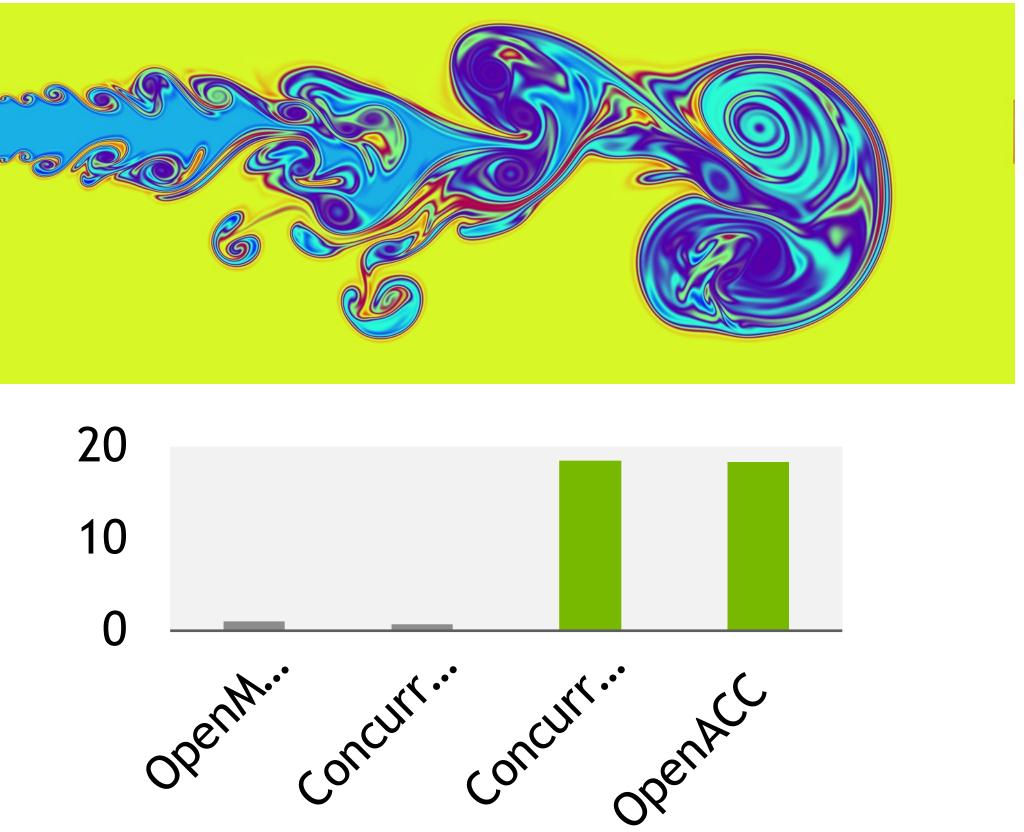
Existing parallelization in MPI, OpenMP, OpenACC, ...

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 \text{ beg-1} + k-0.5 \text{ 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</pre>
      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)
```



Source: HPC SDK 22.1, AMD EPYC 7742, NVIDIA A100. MiniWeather: NX=2000, NZ=1000, SIM_TIME=5. OpenACC version uses -gpu=managed option.

*SPEChpc is a trademark of The Standard Performance Evaluation Corporation

enddo



POT3D: Do Concurrent + Limited OpenACC

POT3D

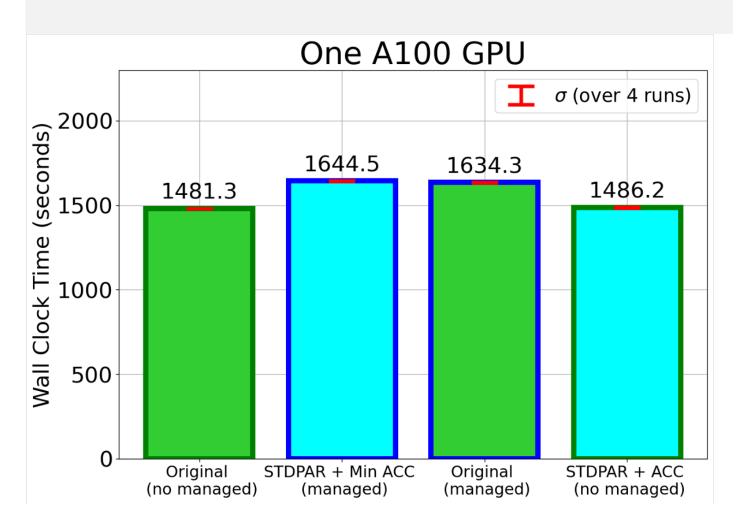
POT3D is a Fortran application for approximating solar coronal magnetic fields.

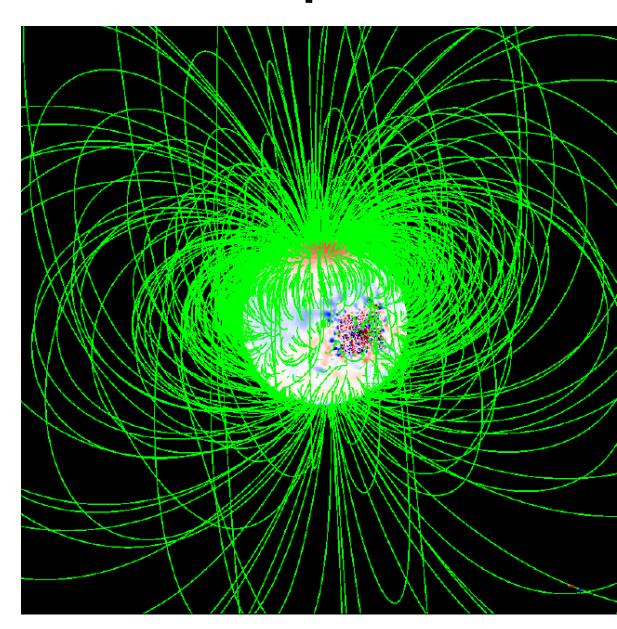
Included in the SPEChpc benchmark suite*

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 Corporation⁶



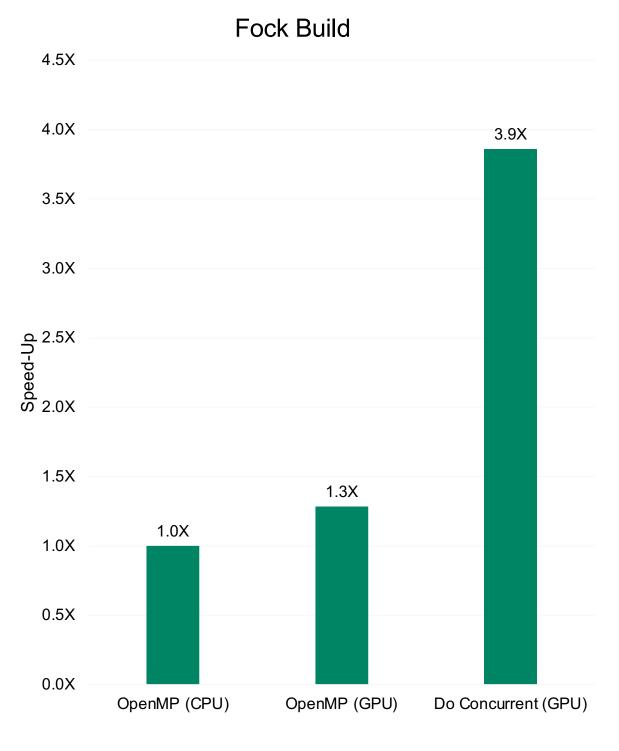
GAMESS

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
                                  !pre-sorting, screening
!$omp target teams distribute &
             parallel do &
!$omp shared() private()
                                  DO CONCURRENT (iquart=1::ssdd quarts) &
do iquart = 1, ssdd quarts
                                     SHARED() LOCAL()
  !recover shell index
                                    !recover shell index
  ish=IDX(s sh)
                                    ish=IDX(s sh)
  jsh=IDX(s sh)
                                    jsh=IDX(s sh)
  ksh=IDX(d sh)
                                    ksh=IDX(d sh)
  lsh=IDX(d sh)
                                    lsh=IDX(d sh)
  !compute ints
                                    !compute ints
  !digest ints
                                    !digest ints
enddo
                                  enddo
```

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



nvfortran 22.7, NVIDIA A100 GPU, AMD "Milan" CPU



ACCELERATED PROGRAMMING IN ISO FORTRAN

NVFORTRAN Accelerates Fortran Intrinsics with cuTENSOR Backend

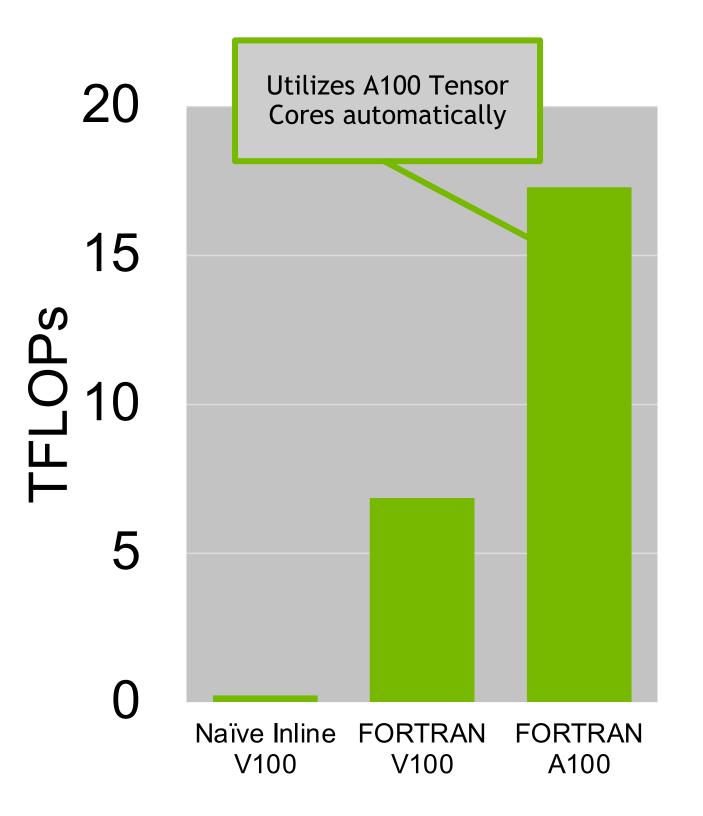
```
real(8), dimension(ni,nk) :: a
real(8), dimension(nk,nj) :: b
real(8), dimension(ni,nj) :: c
. . .
!$acc enter data copyin(a,b,c) create(d)
do nt = 1, ntimes
  !$acc kernels
 do j = 1, nj
   do i = 1, ni
     d(i,j) = c(i,j)
      do k = 1, nk
       d(i,j) = d(i,j) + a(i,k) * b(k,j)
     end do
    end do
  end do
    !$acc end kernels
end do
!$acc exit data copyout(d)
```

```
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
```

Inline FP64 matrix multiply

MATMUL FP64 matrix multiply



HPC PROGRAMMING IN ISO FORTRAN **Examples of Patterns Accelerated in NVFORTRAN**

```
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
```





Identify an important loop nest that can be run in parallel. 1.

do k = 1 , nz+1do i = 1, nx enddo enddo

• • •

enddo enddo

```
!Compute fluxes in the x-direction for each cell
      !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,k-hs-1+s,ll)
        !Fourth-order-accurate interpolation of the state
      !Compute density, u-wind, w-wind, potential
      !temperature, and pressure (r,u,w,t,p respectively)
     r = vals(ID_DENS) + hy_dens_int(k)
     u = vals(ID UMOM) / r
     w = vals(ID_WMOM) / r
     t = ( vals(ID_RHOT) + hy_dens_theta_int(k) ) / r
     p = CO^*(r^*t)^{**}gamma - hy pressure int(k)
```



Identify an important loop nest that can be run in parallel. 1. 2. Replace existing loops with do concurrent loops Note: Multiple loop iteration variables can be used in the same do concurrent loop, if they are all legal to parallelize

enddo enddo

• • •

enddo

```
!Compute fluxes in the x-direction for each cell
do concurrent (k=1:nz, i=1:nx+1)
      !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,k-hs-1+s,ll)
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      !Compute density, u-wind, w-wind, potential
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- Identify an important loop nest that can be run in parallel. 1.
- 2. Replace existing loops with do concurrent loops Note: Multiple loop iteration variables can be used in the same do concurrent loop, if they are all legal to parallelize
- Add local clause for variables that must be privatized for 3. correctness.

enddo enddo

enddo

• • •

```
!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,k-hs-1+s,ll)
```

!Fourth-order-accurate interpolation of the state

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- Recompile with -stdpar and test for correctness. 4.
 - Note 1: Only refactor one loop nest at a time to ensure errors aren't introduced, such as forgetting to localize a variable.
 - Note 2: Performance may get worse at first due to increased memory migration.

- enddo enddo

enddo

• • •

```
!Compute fluxes in the x-direction for each cell
do concurrent (k=1:nz, i=1:nx+1)
                                 &
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```

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- Identify an important loop nest that can be run in parallel. 1.
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- Recompile with -stdpar and test for correctness. 4.
 - Note 1: Only refactor one loop nest at a time to ensure errors aren't introduced, such as forgetting to localize a variable.
 - Note 2: Performance may get worse at first due to increased memory migration.
- Increase the number of concurrent loops to run more work 5. in parallel and reduce memory migration on GPU.

enddo enddo

enddo

. . .

mass = mass + rte enddo

```
!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)
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   !to compute the value at the interface in question
    do ll = 1 , NUM VARS
     do s = 1 , sten size
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```
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w = vals(ID WMOM) / r
t = (vals(ID RHOT) + hy dens theta int(k)) / r
p = CO^*(r^*t)^{**}gamma - hy pressure int(k)
```

```
do concurrent (k=1:nz,i=1:nx) reduce(+:mass,te)
                              *dx*dz ! Accumulate domain mass
        = te + (ke + r*cv*t)*dx*dz
```

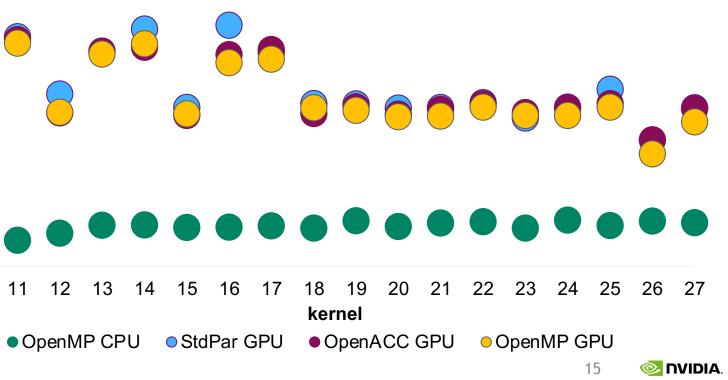


Other Examples

	A100 40GB Cray	Mul - Add -	
 Bristol BabelStream 		Triad - Dot -	_
 Modern Fortran implementation of BabelStream. 	A100 40GB NVHPC	Copy – Mul –	83 85
 Preprint available upon request. 	NVHPC	Add - Triad -	85 85
 <u>https://github.com/jeffhammond/BabelStream/tree/fortran-ports</u> 		Dot -	16 Int
 NWChem TCE CCSD(T) kernels 			DoConcurrent
 6D = 4D x 4D tensor contractions from quantum chemistry with different memory access patterns. 			DoCo
 <u>https://github.com/jeffhammond/nwchem-tce-triples-kernels</u> 			
 Parallel Research Kernels (PRK) 			
 Shows simple patterns implemented in 50+ different programming languages x models, including Fortran StdPar, OpenACC, OpenMP, etc. 		1200	
 <u>https://github.com/ParRes/Kernels/</u> 	S	800	
GPU Gearbox	GF/s	600	
 Based on PRK codes 		400	
 <u>https://www.nvidia.com/en-us/on-demand/session/gtcspring22-s41620/</u> 		200	
		10	11

		0 20	40 60	80 10	0	
	87 86 89	87 86 89	87 86 89	87 86 89		
	89 86 I	89 86 I	89 86 I	89 87 1	1	1
33	89	90	87	87	90	86
35	89	90	86	86	90	86
35	90	88	89	89	88	89
35	90	88	88	88	88	89
91	51	51	92	92	93	93
Doconcurrent -	OpenMPTarget -	OpenMPTargetLoop -	OpenACC -	OpenACCArray -	CUDA -	CUDAKernel -

NWChem TCE CCSD(T) kernels



Fortran Future Features?



Parallelism in Fortran 2018

! fine-grain parallelism	! (
! explicit	np
do concurrent (i=1:n)	n_1
Z(i) = X(i) + Y(i)	
end do	! 2
! implicit	do
MATMUL	
TRANSPOSE	end
RESHAPE	syı

• • •

- coarse-grain parallelism
- = num images()
- local = n / np
- X, Y, Z are coarrays
- i=1,n_local
 - Z(i) = X(i) + Y(i)
- d do
- nc all

Do Concurrent Locality Specifiers and Atomics (2023)

! Scalar reduction - probably implemented with privatization do concurrent (i=1:n) reduce(Z:+) Z = X(i) / Y(i)

end do

! Array reduction - probably implemented with atomics do concurrent (i=1:n) reduce(Z:+) Z(i) = Z(i) + decision(i)end do



What if we need to use the result?

```
! Inserting into an array
offset = 1
do concurrent (i=1:n) shared(X,offset) local(s,stuff)
    stuff = ...
   s = size(stuff)
    !$omp/acc atomic capture
    j = offset
    offset = offset + size
    !$omp/acc end atomic capture
    X(j:j+size) = stuff
end do
```



What if we need to use the result?

! Inserting into an array offset = 1do concurrent (i=1:n) shared(X,offset) local(s,stuff) stuff = ...s = size(stuff) call atomic_fetch_add(offset, size, j) ! coarrays X(j:j+size) = stuffend do

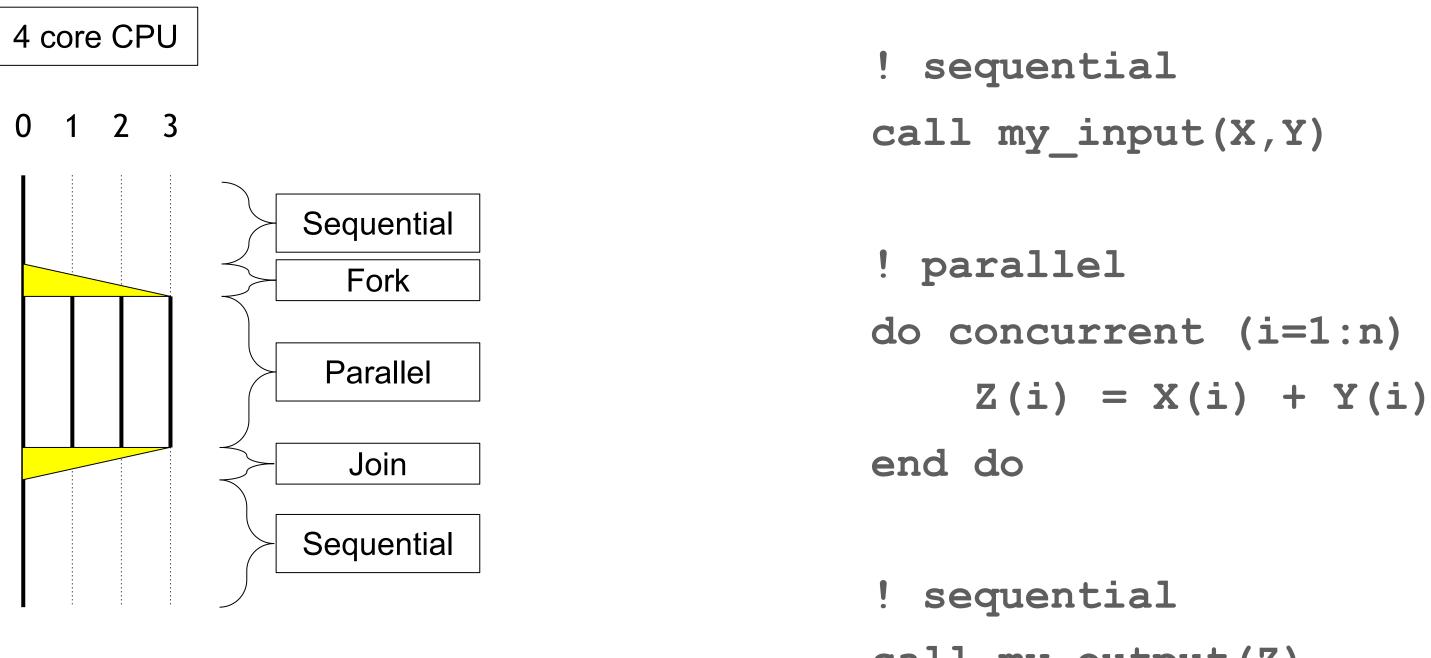


What if we need to use the result?

! Inserting into an array offset = 1do concurrent (i=1:n) shared(X) local(s,stuff) fetched(offset:+) stuff = ...s = size(stuff) j = offset = offset + s ! Syntax to be determined later X(j:j+size) = stuffend do



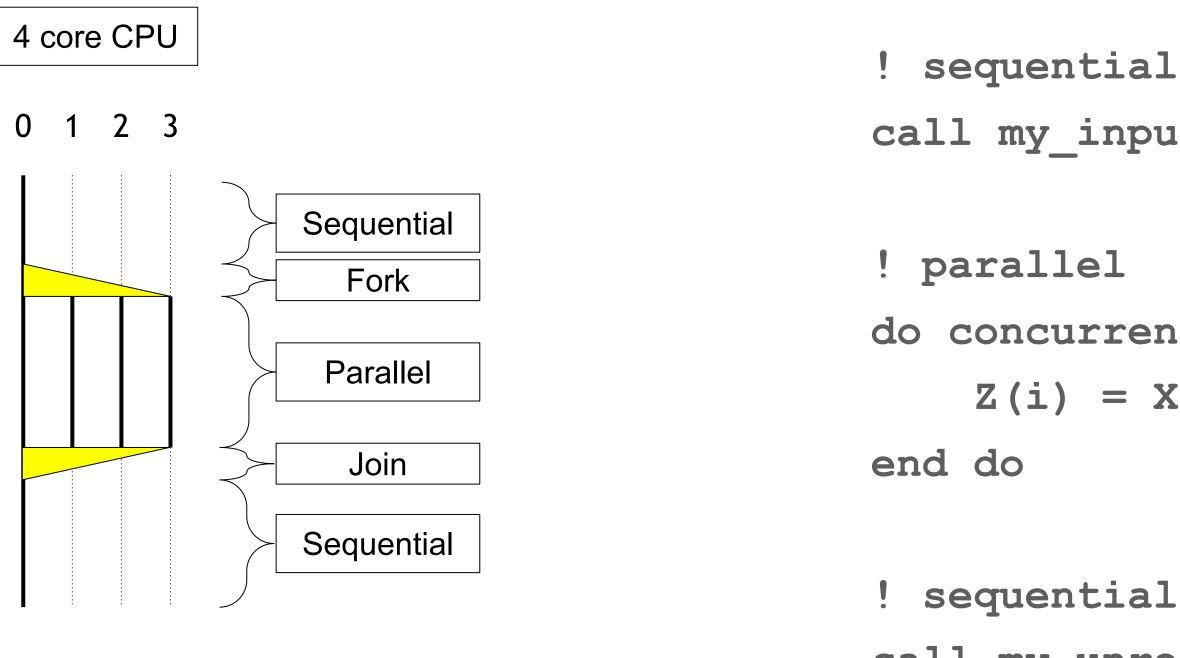
Asynchrony



- call my_input(X,Y)
- do concurrent (i=1:n)

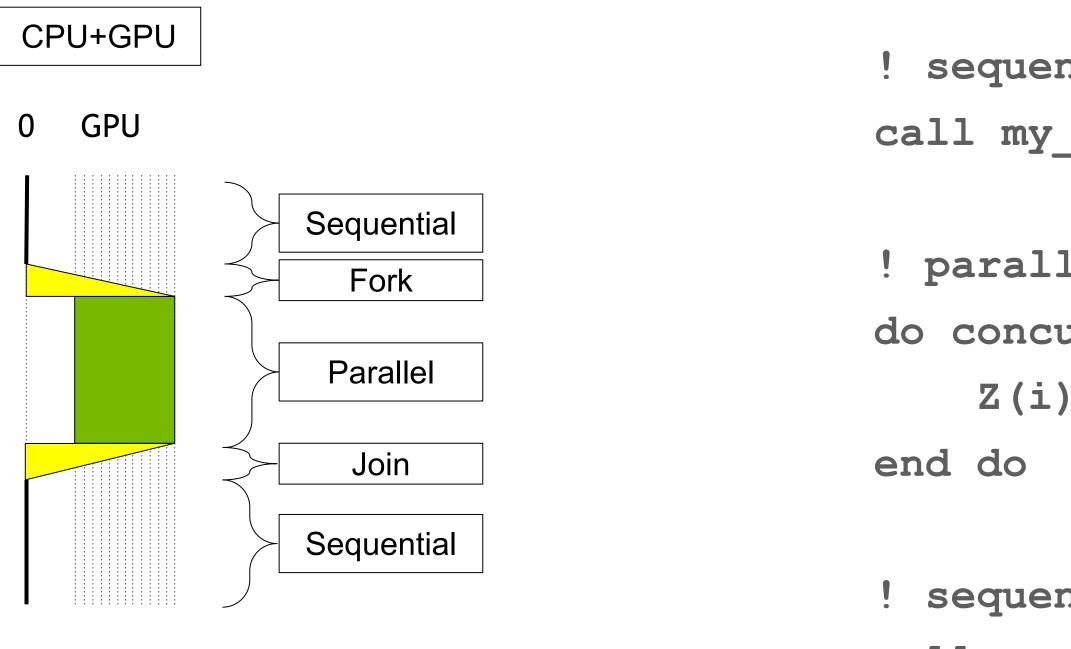
call my output(Z)





- call my_input(X,Y)
- do concurrent (i=1:n)
 - Z(i) = X(i) + Y(i)

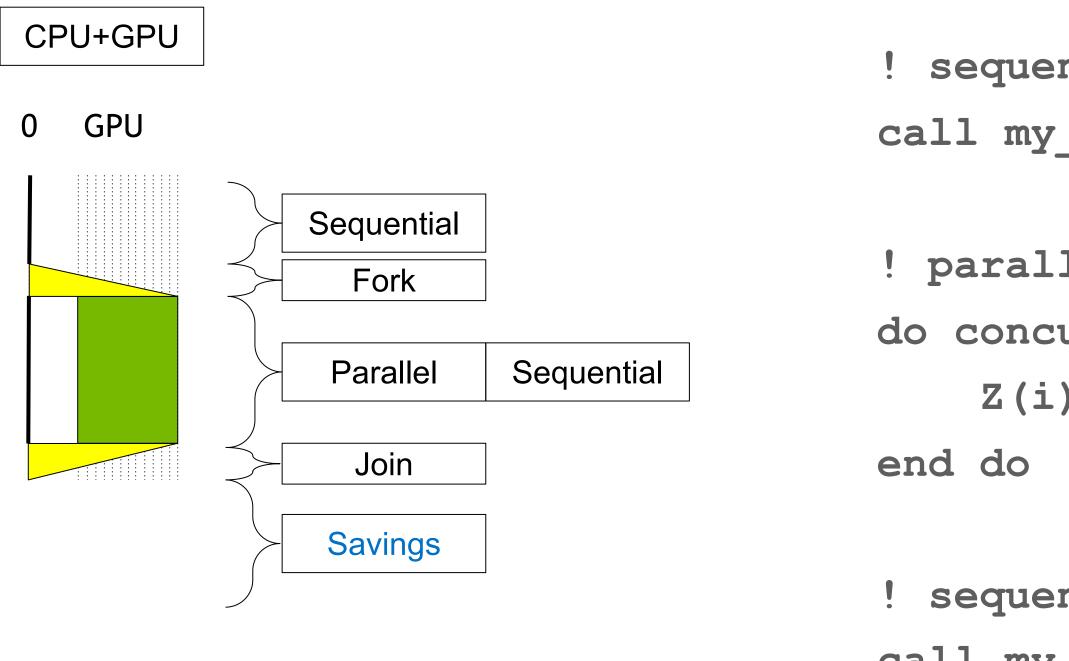
- call my unrelated(A)



- ! sequential on CPU
 call my_input(X,Y)
- ! parallel on GPU
 do concurrent (i=1:n)
 - Z(i) = X(i) + Y(i)

! sequential on CPU call my_unrelated(A)



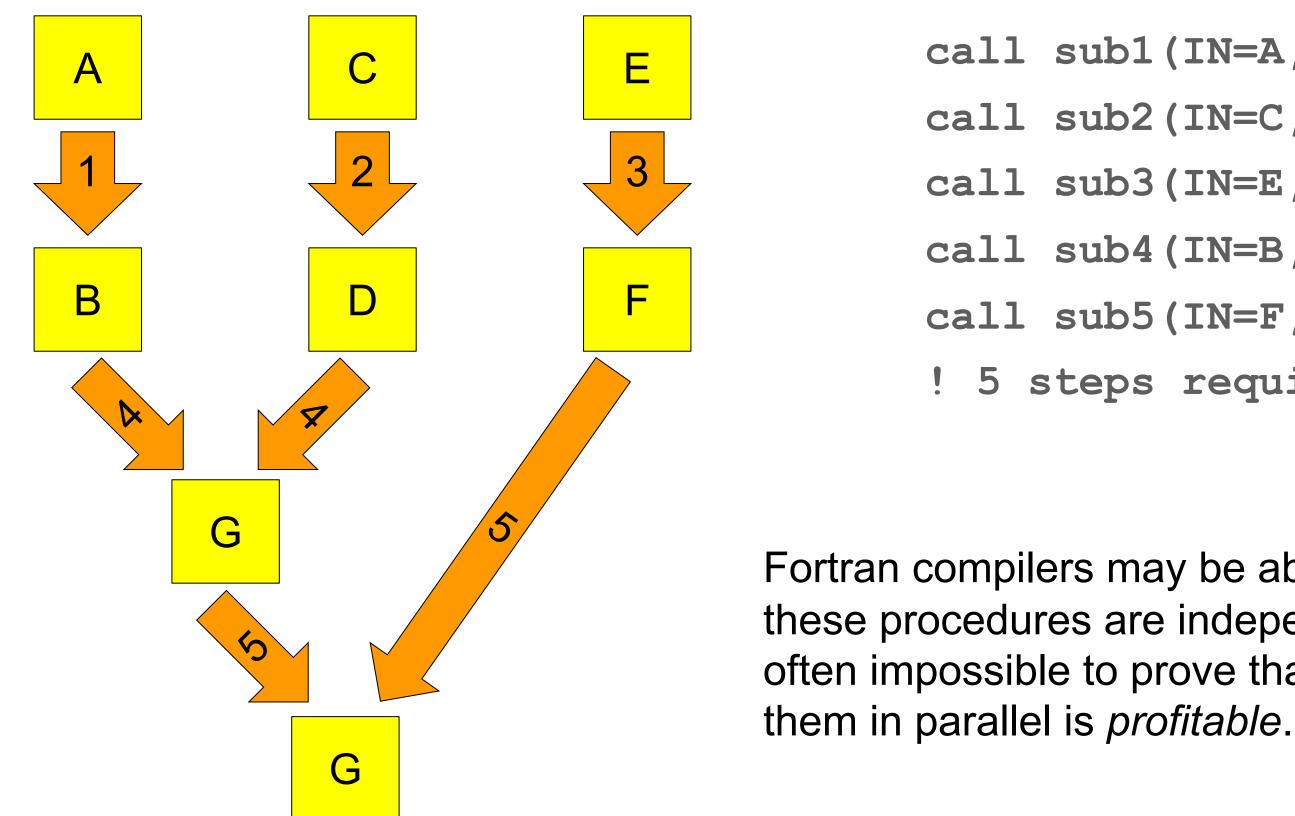


- ! sequential on CPU
 call my_input(X,Y)
- ! parallel on GPU w/ async
- do concurrent (i=1:n)
 - Z(i) = X(i) + Y(i)

! sequential on CPU w/ async call my_unrelated(A)

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Motivation for Asynchrony 2 (synthetic)

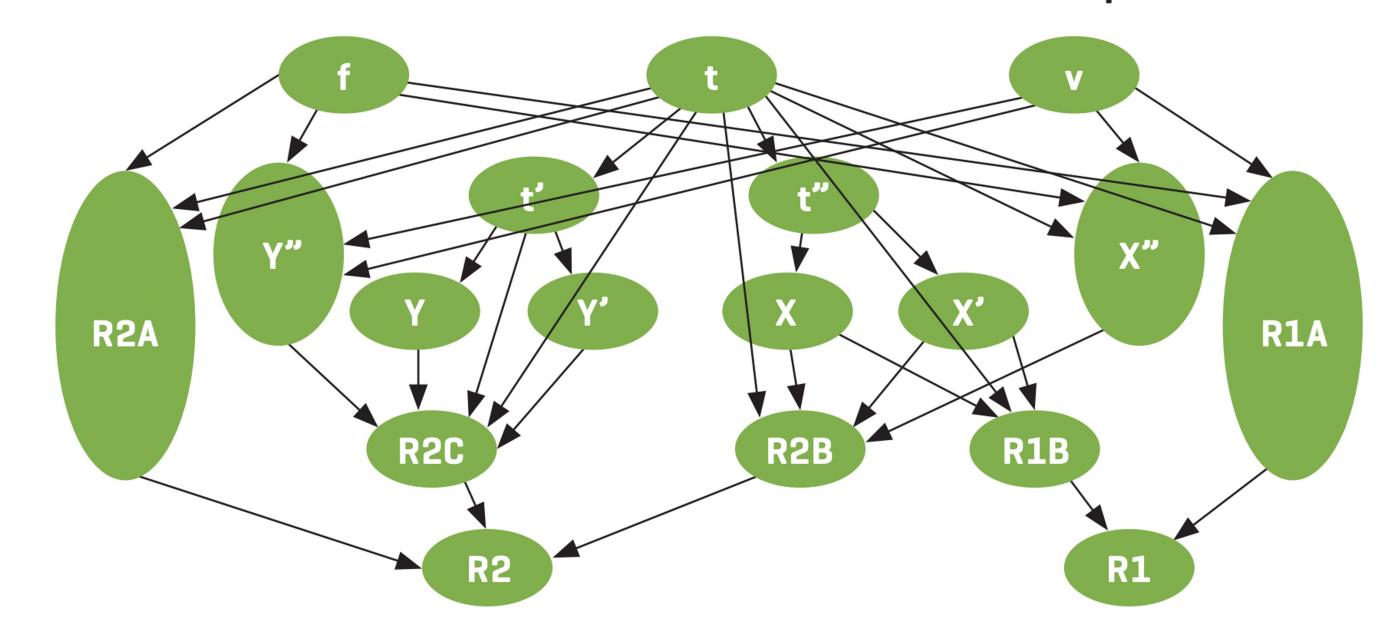


- call sub1(IN=A,OUT=B)
- call sub2(IN=C,OUT=D)
- call sub3(IN=E,OUT=F)
- call sub4(IN=B,IN=D,OUT=G)
- call sub5(IN=F,IN=G,OUT=H)
 - 5 steps require only 3 phases

Fortran compilers may be able to prove these procedures are independent but it is often impossible to prove that executing

Motivation for Asynchrony 2 (realistic)

Figure 3. The directed acyclic graph (DAG) representing data dependencies within one formulation of the CCSD method. The vertex labels are not important.



https://dl.acm.org/doi/10.1145/2425676.2425687 https://pubs.acs.org/doi/abs/10.1021/ct100584w





Prior Art in OpenMP and OpenACC

Both of the popular directive-based models for parallel computing support asynchronous tasks in a range of operations.

OpenACC supports async and wait, with an implicit/default queue (stream) as well as explicit/numbered queues, and the ability to create dependency chains between operations, similar to CUDA streams.

OpenMP supports tasks with dependencies (and without). The syntax for dependencies is finer granularity - based on data references rather than queues - and the implementation may end up using a global queue as a result.

There are merits to both approaches, so the Fortran community will have to think about what form should be standardized.



These are examples of different things. Please don't try to compare them.

Prior Art in OpenMP and OpenACC

do i=1,n	!\$omp par
<pre>!\$acc parallel loop async(i)</pre>	!\$omp mas
do j=1,m	do j=1,n
• • •	do i=1
enddo	!\$omp
enddo	!\$omp
do i=1,n	!\$omp
<pre>!\$acc parallel loop async(i)</pre>	• • •
do j=1,m	!\$omp
• • •	enddo
enddo	enddo
enddo	
!\$acc wait	

- rallel
- ster
- , m
- p task
- mp& depend(in:grid(i-1)) &
- mp& depend(out:grid(j))
- np end task

e.g. https://github.com/ParRes/Kernels/blob/default/FORTRAN/p2p-tasks-openmp.F90



Example

program main				
use numerot				
real :: A(100), B(100), C(100)				
real :: RA, RB, RC				
A = 1; B = 1; C = 1				
RA = yksi(A)				
RB = kaksi(B)				
RC = kolme(C)				
<pre>print*,RA+RB+RC</pre>				
end program main				

https://github.com/jeffhammond/blog/tree/main/CODE

```
module numerot
  contains
    pure real function yksi(X)
      real, intent(in) :: X(100)
      !real, intent(out) :: R
      yksi = norm2(X)
    end function yksi
    pure real function kaksi(X)
      real, intent(in) :: X(100)
     kaksi = 2*norm2(X)
    end function kaksi
    pure real function kolme(X)
      real, intent(in) :: X(100)
      kolme = 3*norm2(X)
    end function kolme
```

end module numerot



A coarray implementation?

<pre>program main use numerot real :: A(100) ! each image has one</pre>	Coarra distrib image
real :: R A = 1	There memo
<pre>if (num_images().ne.3) STOP</pre>	direct
<pre>if (this_image().eq.1) R = yksi(A)</pre>	requir
<pre>if (this_image().eq.2) R = kaksi(A) if (this_image().eq.3) R = kolme(A)</pre>	One of
sync all	task-b balanc
call co_sum(R)	mecha
<pre>if (this_image().eq.1) print*,R end program main</pre>	have t always

rays are designed to support buted memory, hence are based on e-private data.

e is limited opportunity for sharedory optimizations in such codes, as t inter-image copies will be red.

of the common motivations for based models is dynamic loadicing, but coarrays provide no anism for doing this, so users will to write their own, which they ys do poorly.

A do concurrent implementation?

<pre>program main use numerot real :: A(100), B(100), C(100) real :: RA, RB, RC</pre>	This imple independe completel implemen threads fo
integer :: k	
A = 1; B = 1; C = 1 do concurrent (k=1:3) ! reduction, someday	As with co scalable to
if (k.eq.1) RA = yksi(A)	we want a
if (k.eq.2) RB = kaksi(B)	Dath tha
if $(k.eq.3)$ RC = kolme(C)	Both the c
end do print*,RA+RB+RC	and error justification features.
end program main	

ementation only supports lent tasks, and is likely ely useless when the ntation uses SIMD lanes or GPU or DO CONCURRENT (DC).

oarrays, the if (....eq....) is not to more general examples. Do arrays of functions?

coarray and DC are also *tedious r prone*, which is a good ion for adding new language



do i=1,n	The block i
task block async(i)	Droponding
do j=1,m	Prepending is also a ta
• • •	asynchrono
enddo	
end task block	
enddo	
task sync all	Important Is everyt in a task

state?

mechanism is used for scoping.

ig task implies this block scope ask, which can execute ously until synchronized.

questions: thing (e.g. I/O) allowed to be k?

• How do tasks interact with shared



do i=1,n	The block
<pre>task block async(i) type :: private do j=1,m</pre>	Prepending is also a ta
enddo end task block	It is essent private sta by the bloc
enddo	
task sync all	

mechanism is used for scoping.

ng task implies this block scope ask.

itial to be able to have taskate, which is already covered ock feature.



real :: x do i=1, ntask block async(i) shared(x) type :: private do j=1,m• • • enddo end task block enddo task sync all

We also want to be able to describe the intent of data outside of the task, so we could reuse locality specifiers from DO CONCURRENT.

Locality specifiers already match OpenMP syntax, and a related feature in Fortran, so they are likely to be intuitive to Fortran programmers.

Task reductions are supported by OpenMP now, but the concept is tricky.

Atomics would be nice but that's a big bag of worms.

Calling sub
they shoul
reasonable
The right s
but we ca

ibroutines as tasks is useful, but Ild be **pure** in order to have le behavior.

syntax for this is not obvious, an solve that later.



Summary

Fortran has two great ways to write parallel code, but needs a third.

Shared-memory task parallelism is implemented in OpenMP, OpenACC, and in models associated with languages that aren't Fortran.

Task parallelism allows users to solve new types of problems and make better use of existing parallel features, especially DO CONCURRENT (e.g. when executing on GPUs).

Fortran tasks make new things possible and obviate the need for tedious and error prone implementations. They also reduce the need for non-standard extensions like OpenMP and OpenACC.

Please do not let whatever you don't like about my syntax to get in the way \bigcirc





J3/WG5 papers targeting Fortran 2026

https://j3-fortran.org/doc/year/22/22-170.pdf Requirement: fetching atomic operations in DO CONCURRENT https://j3-fortran.org/doc/year/22/22-169.pdf Fortran asynchronous tasks



