Developing NEPTUNE for U.S. Naval Weather Prediction

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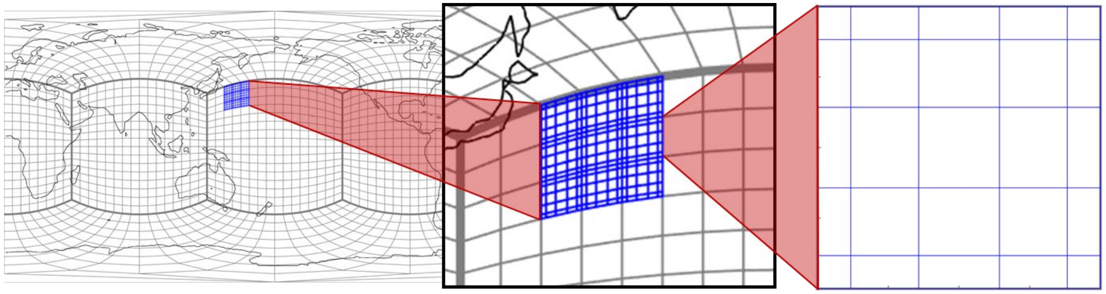
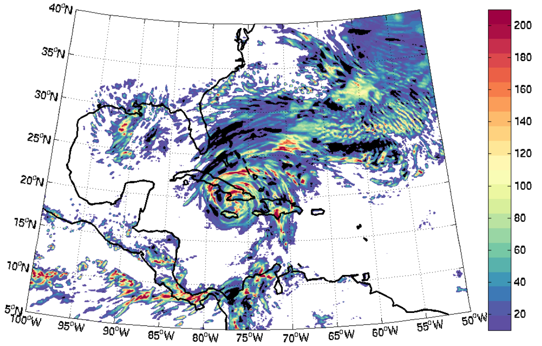
- Vendors: Cavium, Intel, NEC, NVIDIA, Portland Group

NEPTUNE/NUMA

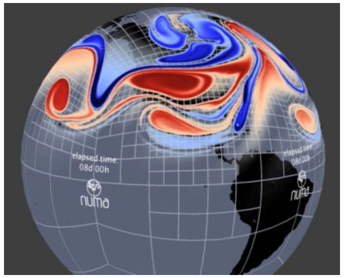
- Navy's Next Generation Prediction System
- Spectral element dynamics on a cubed sphere
  - Based on NUMA (Frank Giraldo, NPS)
  - Higher-order continuous Galerkin
  - Cubed sphere grid





NEPTUNE 72-h forecast (5 km resolution) of accumulated precipitation for Hurr. Sandy

- Computationally dense but highly scalable
  - Constant width-one halo communication
  - Good locality for next generation HPC



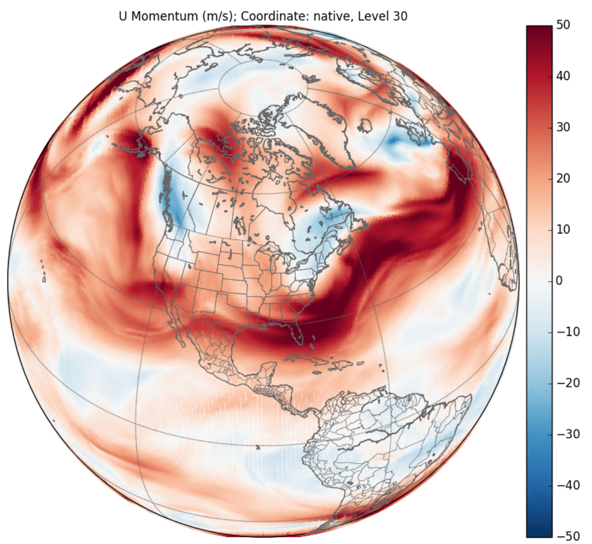
Example of Adaptive Grid tracking a severe event courtesy: Frank Giraldo, NPS

[1]***NEPTUNE: N****avy* ***E****nvironmental* ***P****rediction sys***T****em* ***U****tilizing the* ***N****UMA*[2] *cor***E**

[2]***NUMA****:* ***N****onhydrostatic* ***U****nified* ***M****odel of the* ***A****tmosphere (Giraldo et. al. 2013)*

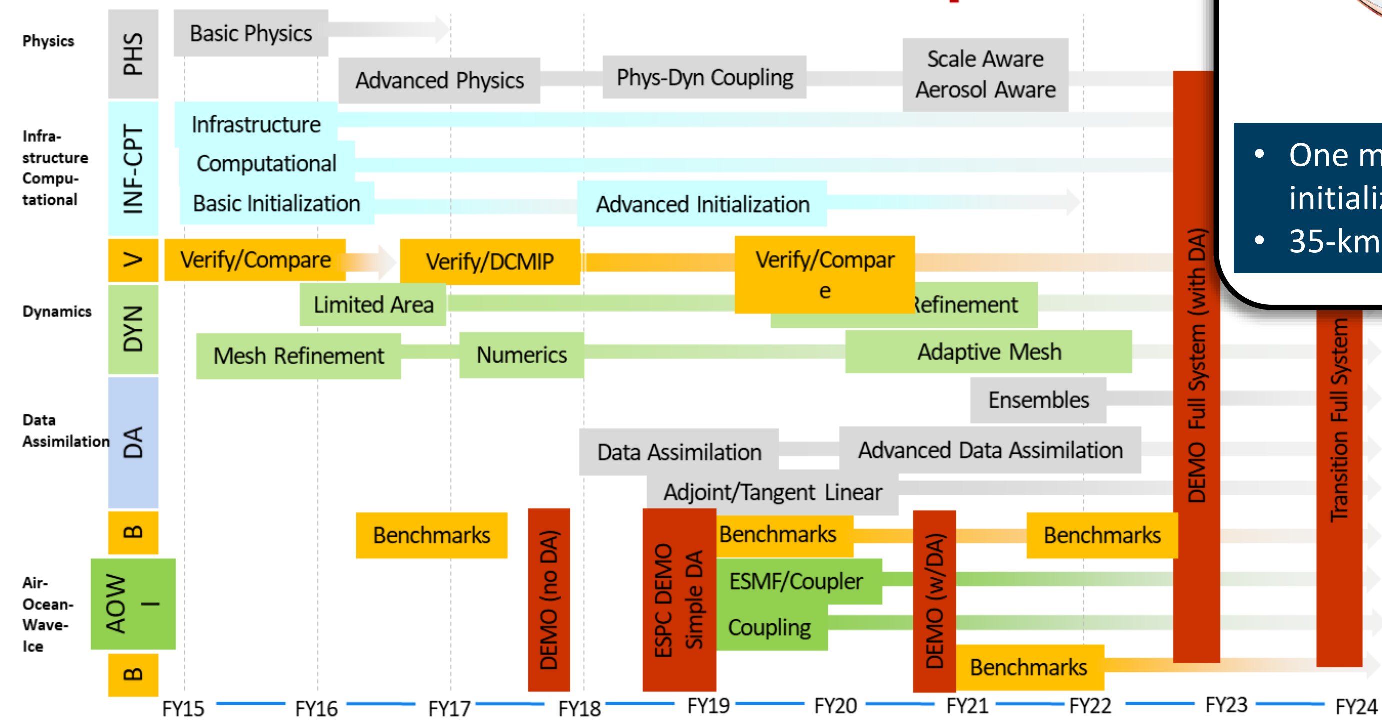
NEPTUNE/NUMA

- Navy's Next Generation Prediction System
  - Interoperable physics under NUOPC
  - Data assimilation development under JEDI framework
  - Coupling using ESMF framework
  - Conducting tests with real forecast data
  - Designing, testing and optimizing for next-gen HPC



- One month of real-data forecasts initialized with GFS analysis fields
- 35-km horizontal grid spacing

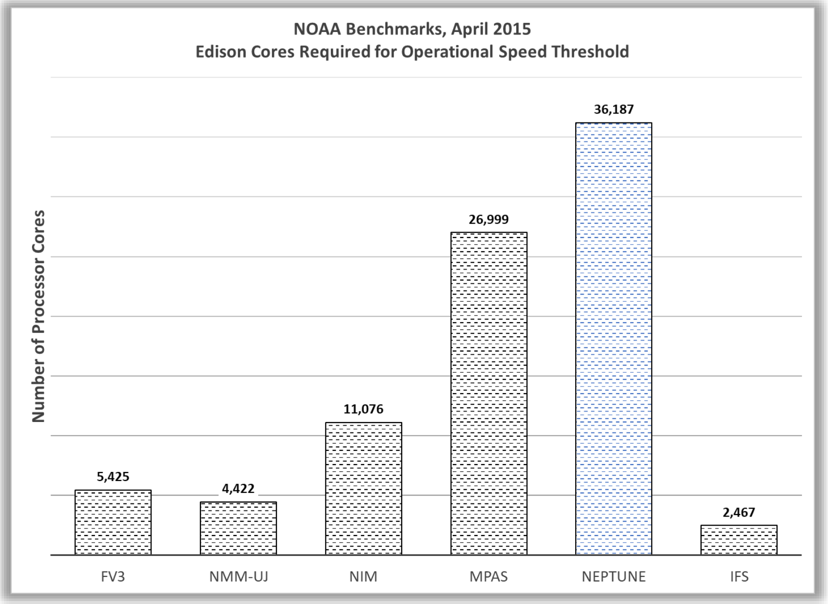
NEPTUNE Roadmap



Performance and Portability requirements

- **Performance** has lagged badly: good scaling but poor node speed
  - Insufficient fine-grain (vector) utilization
  - Low locality increases mem. latency
  - Excessive data movement lowers C.I.
- **Portability** limited by parallel programming model (MPI/OpenMP/vector) and code structure
  - ☑ Intel Xeon (Broadwell, Skylake, Knights Landing)
  - ☑ ARM64 (Cavium ThunderX2)
  - ☑ NEC VE
  - ☐ GPU (Nvidia) (NPS has a NUMA port using OCCA†)
- Solution likely to require major refactoring
  - Minimize one-time and recurring costs
  - Maximize performance benefit over time and range of architectures

Crucial: performance analysis and testing starting with kernels



NEPTUNE (blue) 6.6x slower than FV3 in NOAA benchmarks from 2015‡

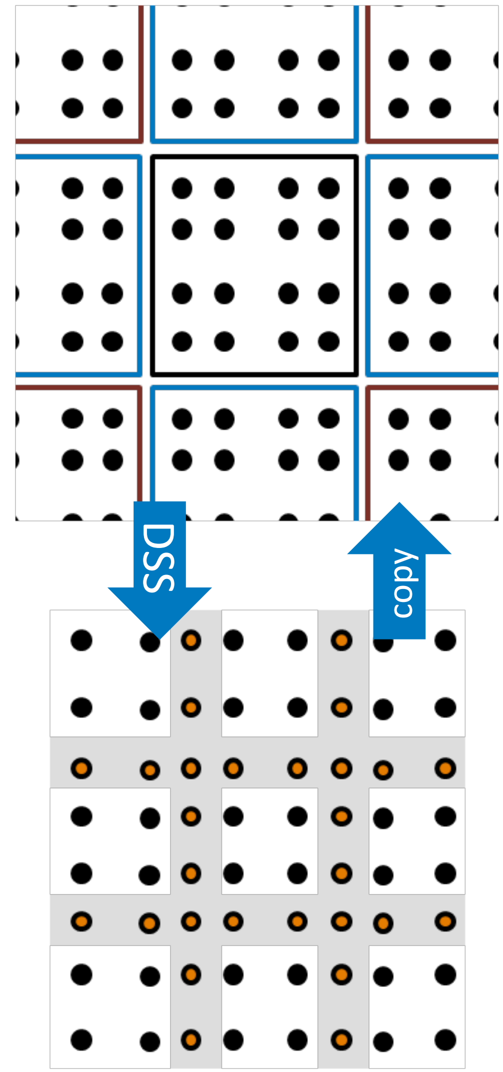
†Abdi, D. S., Wilcox, L. C., Warburton, T. C., & Giraldo, F. X. (2017). A GPU-accelerated continuous and discontinuous Galerkin non-hydrostatic atmospheric model. *The International Journal of High Performance Computing Applications*, 1094342017694427.

‡https://www.weather.gov/media/sti/nggps/AVEC%20Level%201%20Benchmarking%20Report%2008%2020150602.pdf

Diffusion kernel: create_laplacian

Purpose: Damp energy that cascades to frequencies higher than model can resolve

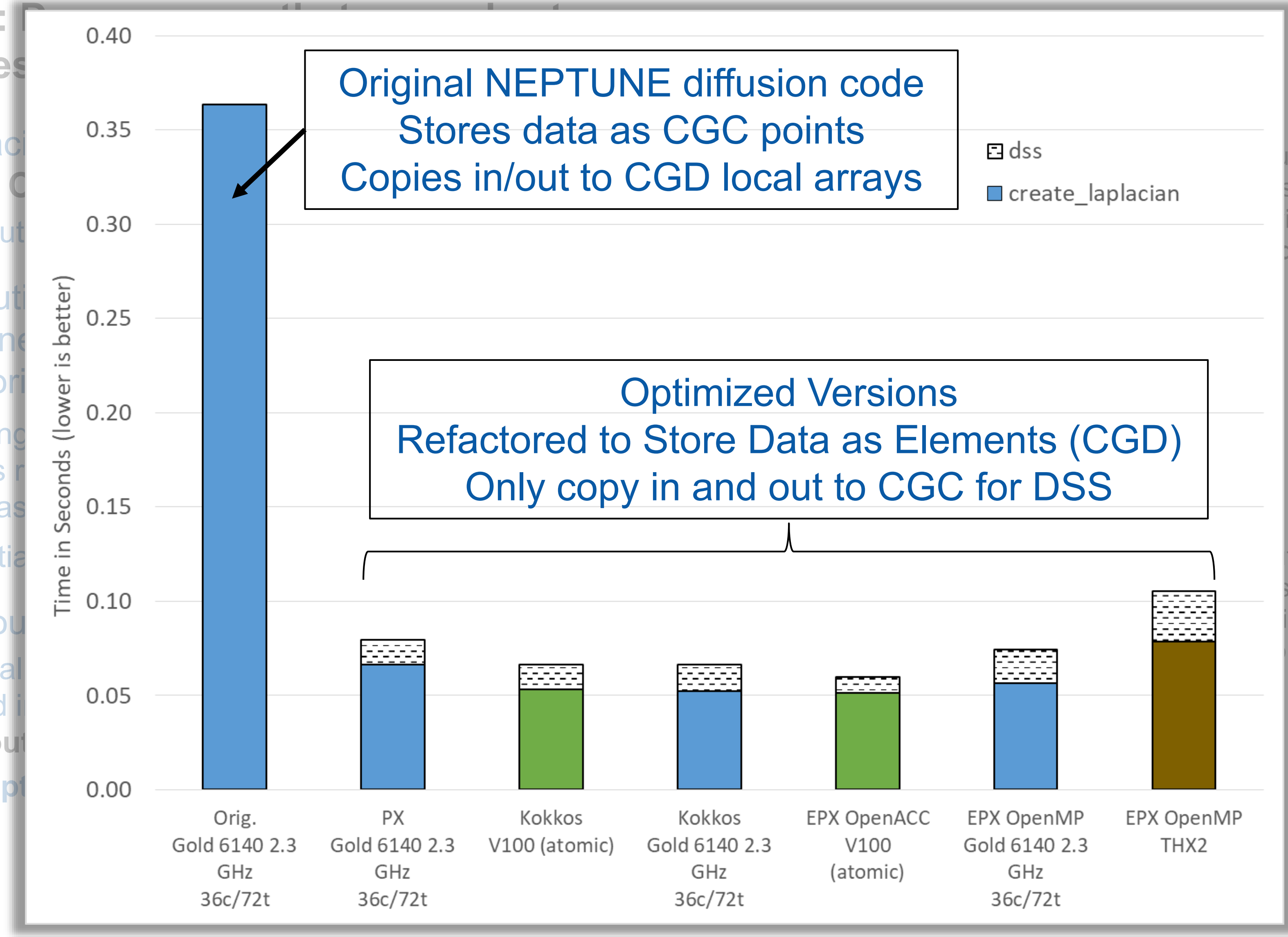
- Local laplacian computed and applied on each 3D element in **CGD layout**
  - + Computationally **dense**, **element-local**, **thread safe**
- Global solution computed on **CGC layout** using Direct Stiffness Summation (DSS) on points shared by neighboring elements
  - – Copying from CGC to CGD to accumulate face values requires transposition and non-unit strides that trash **data locality**
  - – Potential data races impede **thread parallelism**
- Hot spot routine in NEPTUNE
  - – Original implementation only stored CGC layout and copied into and out of local CGC arrays **for every subroutine in dycore**
  - – **Initial optimization: Pick a layout and stick with it**



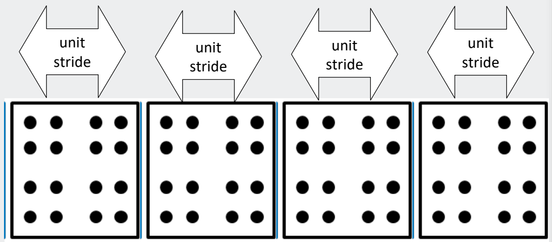
CGD layout: Continuous Galerkin with **Replicated** Points

CGC layout: Continuous Galerkin with **Shared** Points

Diffusion kernel: create_laplacian

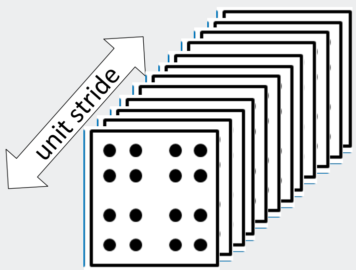


What can we control? Data layout and loops



element-**outer** arrays

dimension(np,nv,ne)



element-**inner** arrays

dimension(ne,np,nv)

Memory Layout

Inner/Outer
(null)

Outer/Outer
- \+ Cache-local elements, good locality
- • Vector dimension is limited to short, often non unit-stride accesses

Inner/Inner
- \+ Fine-grain dimension is unit-stride, dependency-free, and arbitrary length
- • Having fine-grain innermost requires array temporaries (cache, mem. pressure)

Outer/Inner
- \+ Fine-grain dimension is unit-stride, dependency-free, and arbitrary length
- \+ Coalesced accesses to memory by successive GPU threads

Element Loop Nesting

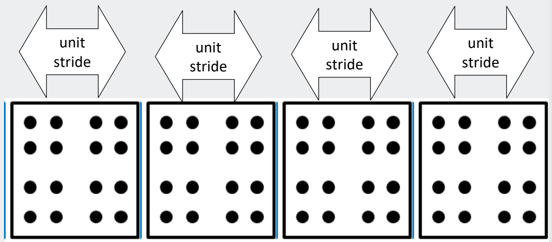
element-**inner** loops

```
do v ← 1,nv
  do p ← 1,np
    do e ← 1,ne
```

element-**outer** loops

```
do e ← 1,ne
  do v ← 1,nv
    do p ← 1,np
```

PX Optimization (element-outer)



element-**outer** arrays

dimension(np,nv,ne)

- NEPTUNE Prototype
- Ported to
  - Xeon
  - ARM
  - NEC VE

Memory Layout

Inner/Outer
(null)

Outer/Outer
+ Cache-local elements, good locality
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Element Loop Nesting

element-**outer** loops

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  do v ← 1,nv
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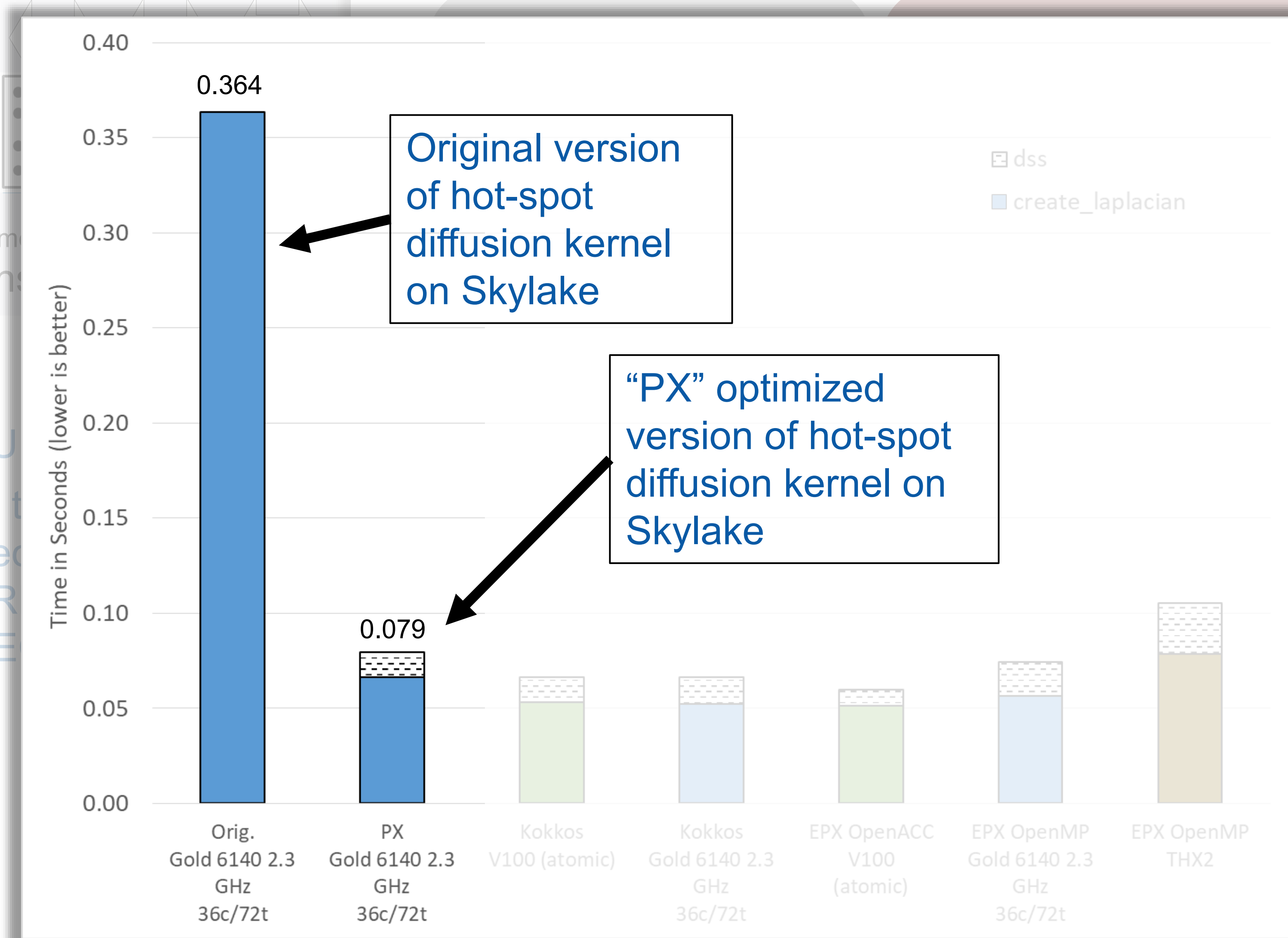
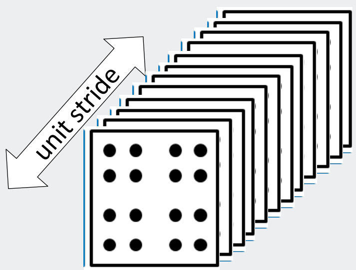
PX Optimization (element-outer)



EPX (element-inner) Optimization



element-**inner** arrays

dimension(ne,np,nv)

Memory Layout / Element Loop Nesting		
	Inner/Outer (null)	**Outer/Outer** + Cache-local elements, good locality • Vector dimension is limited to short, often non unit-stride accesses
	Inner/Inner + Fine-grain dimension is unit-stride, dependency-free, and arbitrary length • Having fine-grain innermost requires array temporaries (cache, mem. pressure)	**Outer/Inner** + Fine-grain dimension is unit-stride, dependency-free, and arbitrary length + Coalesced accesses to memory by successive GPU threads

Memory Layout

Element Loop Nesting

- Xeon, ARM & NEC VE
  OpenMP with vectorization
- Nvidia: OpenACC

  (Thanks Dave Norton, PGI)

element-**inner** loops

```
do v ← 1,nv
  do p ← 1,np
    do e ← 1,ne
```

element-**outer** loops

```
do e ← 1,ne
  do v ← 1,nv
    do p ← 1,np
```

EPX (element-inner) Optimization – GPU

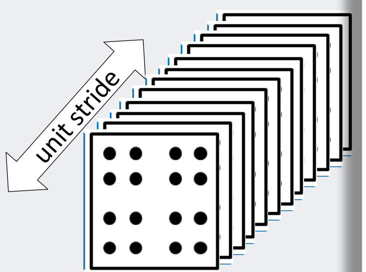
```
do ib = 1,neblk
  nrun = LEBLK
   (adjust nrun for partial blocks here)
!$acc loop
  do ie = 1, nrun, EVEC
    call create_laplacian_ep3( ib, ie, min(ie+EVEC-1,nrun)
```

extent of array in innermost element dimension (32 on GPU)

extent of vectorized-loops (array syntax) in routine (1, so outer loop partitioned over 32 threads)

```
subroutine create_laplacian_EPX( ib, es, ee, nvar &
    ...
    !KSI, ETA, ZETA Derivatives
    qq_e(es:ee,m) = qq_e(es:ee,m) + q_visc(es:ee,ipe,r
    qq_n(es:ee,m) = qq_n(es:ee,m) + q_visc(es:ee,ipn,r
    qq_c(es:ee,m) = qq_c(es:ee,m) + q_visc(es:ee,ipc,r
```

ee = es = +1 previous thread's index, GPU memory accesses coalesced



element-**inner** arrays

dimension(ne,np,nv)

mem. pressure)

Element Loop Nesting

element-**inner** loops	element-**outer** loops

do v ← 1,nv
  do p ← 1,np
    do e ← 1,ne
	do e ← 1,ne
	  do v ← 1,nv
	    do p ← 1,np

- Xeon, ARM & NEC VE
  OpenMP with vectorization
- Nvidia: OpenACC

  (Thanks Dave Norton, PGI)

EPX (element-inner) Optimization – CPU

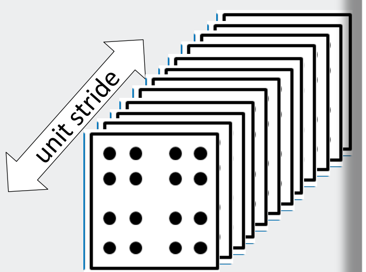
```
do ib = 1,neblk
  nrun = LEBLK
  (adjust nrun for partial blocks here)
!$acc loop
  do ie = 1, nrun, EVEC
    call create_laplacian_ep3( ib, ie, min(ie+EVEC-1,nrun)
```

extent of array in innermost element dimension (16 on CPU)

extent of vectorized-loops (array syntax) in routine (same as LEBLK, so outer loop executes only once)

```
subroutine create_laplacian_EPX( ib, es, ee, nvar &
   ...
   !KSI, ETA, ZETA Derivatives
   qq_e(es:ee,m) = qq_e(es:ee,m) + q_visc(es:ee,ipe,r
   qq_n(es:ee,m) = qq_n(es:ee,m) + q_visc(es:ee,ipn,r
   qq_c(es:ee,m) = qq_c(es:ee,m) + q_visc(es:ee,ipc,r
```

es = 1, ee = LEBLK – each statement vectorizes



element-**inner** arrays

dimension(ne,np,nv)

mem. pressure)

Element Loop Nesting

element-**inner** loops

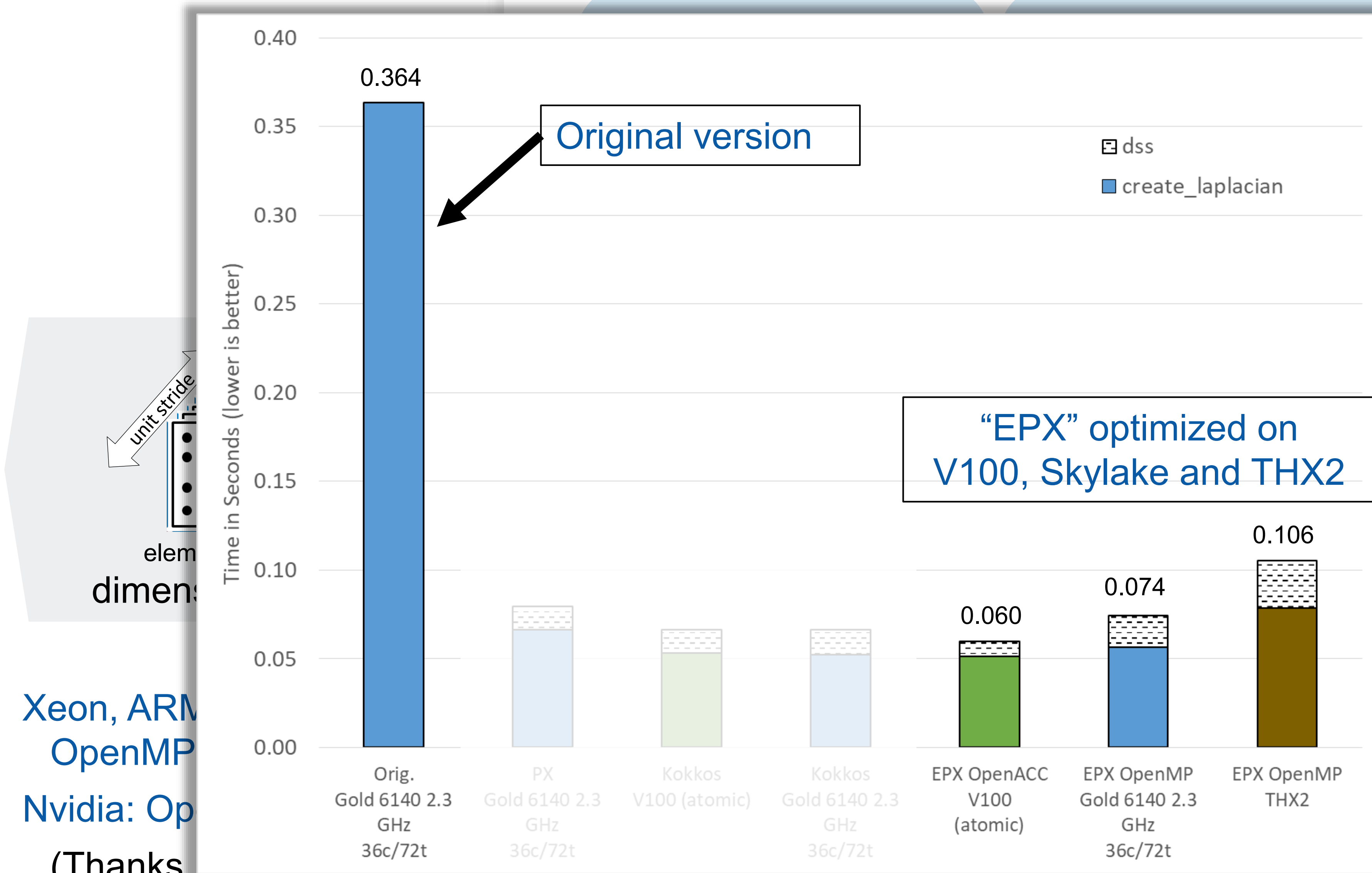
do v ← 1,nv
  do p ← 1,np
    do e ← 1,ne

element-**outer** loops

do e ← 1,ne
  do v ← 1,nv
    do p ← 1,np

- Xeon, ARM & NEC VE
  OpenMP with vectorization
- Nvidia: OpenACC
  (Thanks Dave Norton, PGI)

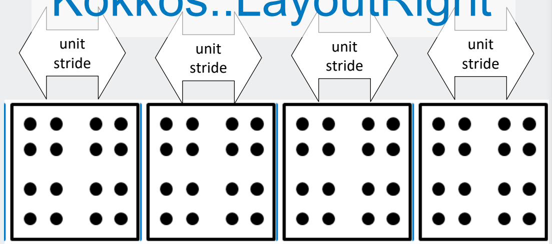
EPX (element-inner) Optimization



- Xeon, ARM OpenMP
- Nvidia: Op (Thanks

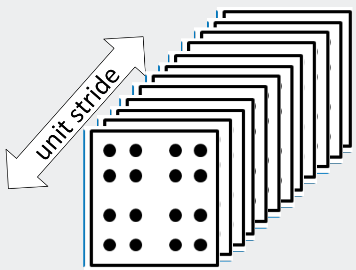
Kokkos Implementation

Kokkos::LayoutRight



element-**outer** arrays

dimension(np,nv,ne)



element-**inner** arrays

dimension(ne,np,nv)

- Template-meta programming lib.
- Single source (C++)
  - Xeon, ARM & NEC VE
  - Nvidia V100
- https://github.com/kokkos

(Thanks: C. Trott, Sandia NL)

Memory Layout / Loop Nesting

Inner/Outer
(null)

Outer/Outer
- \+ Cache-local elements, good locality
- • Vector dimension is limited to short, often non unit-stride accesses

Inner/Inner
- \+ Fine-grain dimension is unit-stride, dependency-free, and arbitrary length
- • Having fine-grain innermost requires array temporaries (cache, mem. pressure)

Outer/Inner
- \+ Fine-grain dimension is unit-stride, dependency-free, and arbitrary length
- \+ Coalesced accesses to memory by successive GPU threads

- GPU parallelizes outer loop over Gangs then SIMT threads
- CPU parallelizes outer loop over OpenMP threads option to vectorized inner loop using hierarchical parallelism

element-**outer** loops

```
do e ← 1,ne
  do v ← 1,nv
    do p ← 1,np
```

Kokkos Implementation

Kokkos::LayoutRight

unit stride

Outer/Outer

```
//  Define Functor Class and Operators
typedef Kokkos::View<double [nelem][nvar][npts]>    ViewNvarType ;
class CreateLaplacianFunctor {
  ViewNvarType  _q, _rhs ;
  KOKKOS_INLINE_FUNCTION
  CreateLaplacianFunctor(
                          const ViewNvarType q , const ViewNvarType rhs
                        ) : _q(q) , _rhs(rhs) {} ;
  KOKKOS_INLINE_FUNCTION
  void operator()(CreateLaplacianTag,const size_t ie) const{ // compute laplacian
    ...
  }
  KOKKOS_INLINE_FUNCTION
  void operator()(CreateGlobalTag, const size_t ie) const{ // DSS
    ...
  }
} ;

int main ( int argc, char *argv[] ){
 ViewNvarType  rhs("rhs"), q("q") ;   // construct views
// Executable
 Kokkos::initialize( argc, argv ) ;
 Kokkos::parallel_for(Kokkos::RangePolicy<CreateLaplacianTag>(0,nelem),CreateLaplacian) ;
 Kokkos::parallel_for(Kokkos::RangePolicy<CreateGlobalTag>(0,nelem),CreateLaplacian) ;
```

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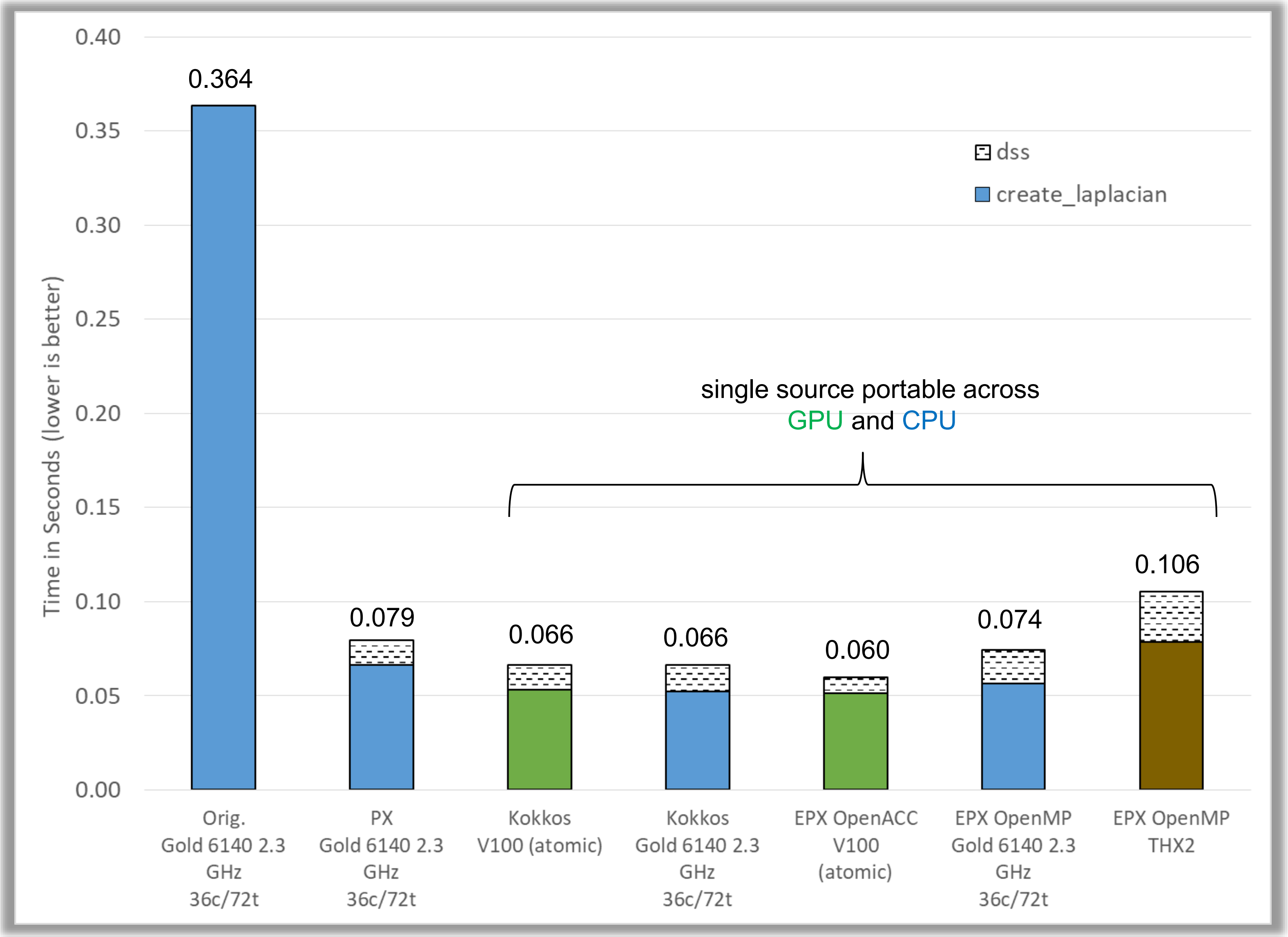
- Si
- https://github.com/kokkos

(Thanks: C. Trott, Sandia NL)

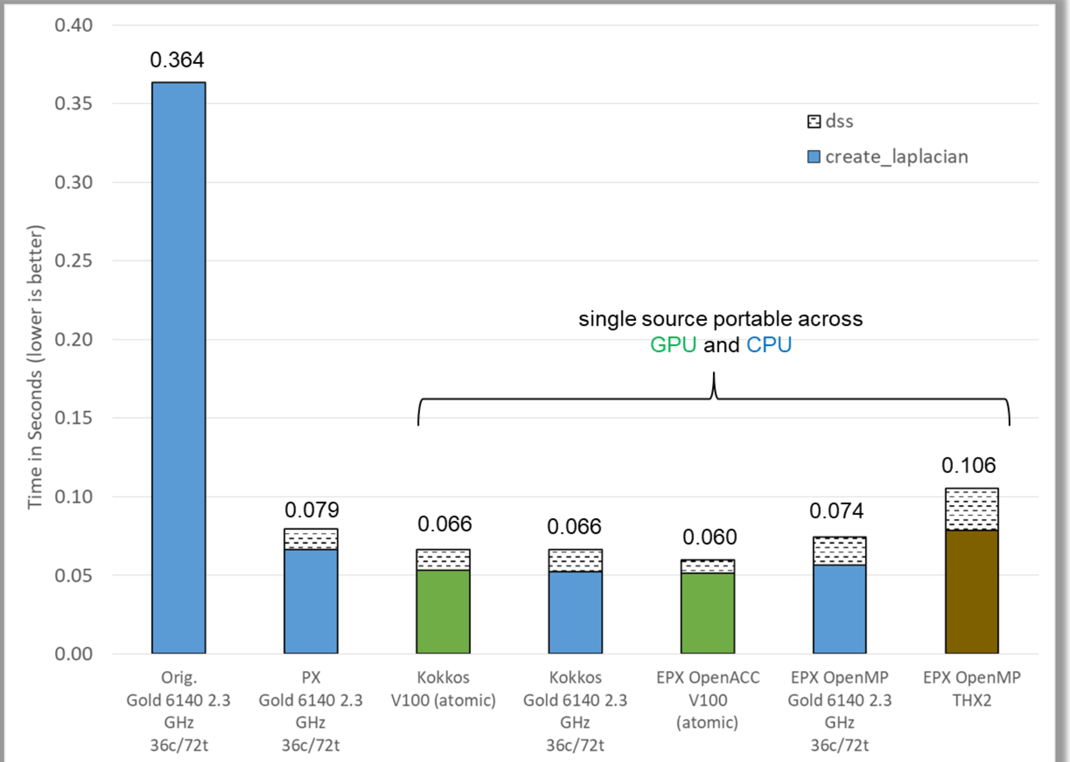
OpenMP threads option to vectorized inner loop using hierarchical parallelism

do p ← 1,np

Performance results



Performance results



Times for Diffusion Kernel
(Double Precision, Full Node)

		Orig	PX	EPX	KOKKOS
op counts	Scalar (M)	153	383	6	480
	128 (2 word) vector (M)	0	0	0	0
	256 (4 word) vector (M)	15	39	0	15
	512 (8 word) vector (M)	112	0	70	0
	Total instructions (M)	279	422	76	495
	DP ops (M)	**1,104**	**539**	**564**	**539**
	% vec	**0.75**	**0.22**	**0.87**	**0.08**
mem. sys.	L1 misses (M)	9.5	na	19.3	10.1
	L2 misses (M)	7.3	na	3.9	6.8
	L3 misses (M)	5.8	na	3.7	5.1
	r/w MB	414	na	294	399
	Comp. Intens.	2.66	na	1.91	1.35
	20 steps sec 1 thread	3.876	2.378	2.252	1.923
	GFLOPs	14.2	11.3	12.5	14.0
	% peak	0.19	0.15	0.17	0.19
	speedup rel orig	1.0	1.6	1.7	2.0

Skylake TAU/PAPI Performance Metrics
(Double Prec., Single Core)

SP over DP (Full Node)

Orig	PX	EPX	Kokkos
1.11	1.10	2.09	1.12

Effect of Floating Point Precision

Diffusion Kernel Performance Summary

Competitive Performance over Programming Models and Devices

performance portable

- ✓ Kokkos
  - GPU: Excellent fine-grained utilization on GPU
    - Good occupancy; 25% to 100%; moderate register pressure
  - CPU: Nearly identical performance to GPU
    - Failed to exploit vectorization on CPU (8%) because of strictly element-outer loops that only benefit OpenMP threading (hierarchical parallelism may improve)
    - The C++ compiler makes a difference: use icpc, not g++
  - Good environment, user support: https://github.com/kokkos/kokkos/issues
- ✓ Element-inner (EPX) Fortran
  - GPU: Best V100 performance with OpenACC
    - Lower occupancy: 18.8% to 31% occupancy; high register pressure
  - CPU: Skylake 20 percent slower than GPU
    - + Excellent 85% vector utilization on CPU (both AVX512 and ARM)
    - Large working set and L1 pressure and AVX-512 clock penalty
    - + Dramatic 2x benefit from single-precision
- Element-outer (PX, the current whole-code optimized prototype)
  - CPU-only, close to Kokkos CPU performance if vectorization disabled to avoid compiler-generated scatter gathers around non unit-stride loops

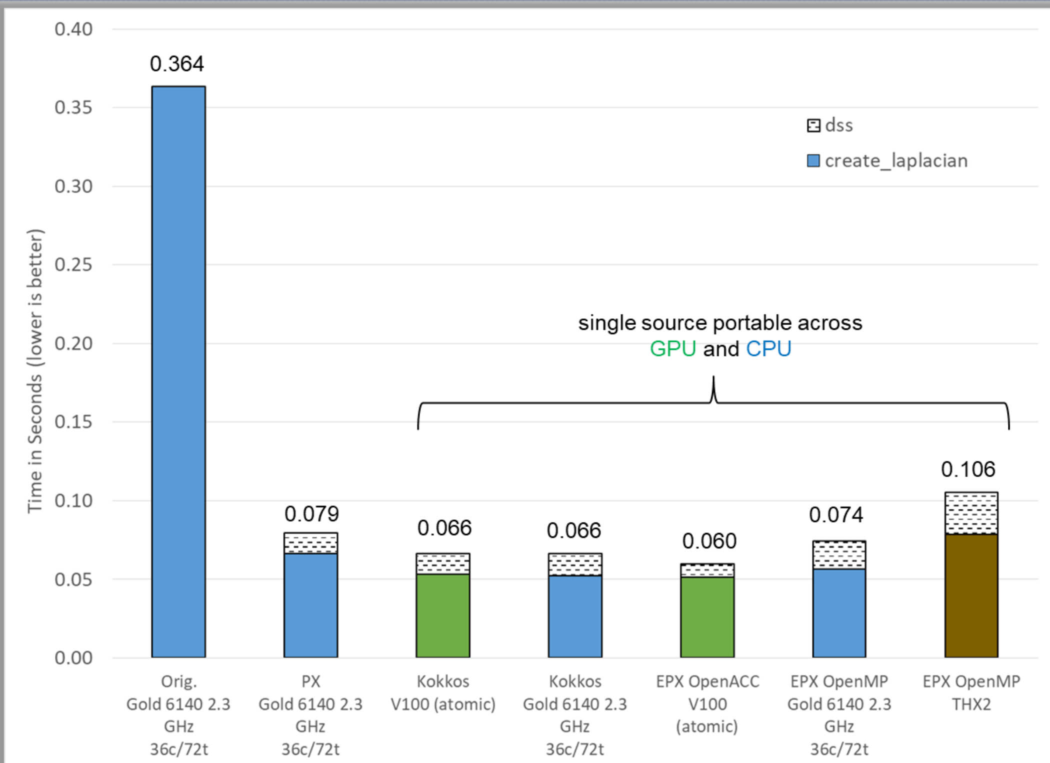
Should we refactor NEPTUNE and how?

- Need more information:
  - Additional kernels covering more of NEPTUNE dynamics
  - Whole code prototypes and testing
- Recommendation with costs, benefits and timelines for different options
- Decision by project management and sponsor, then implementation and testing

	Perf./Port.	Effort	Benefits
PX	Fortran CPU only Limited vectorization	Low: Already have this. Good modularity & object-orientedness	Good performance on CPU architectures
EPX	Fortran Fine-grain || Single-source CPU: OpenMP/Vector GPU: OpenACC	Moderate: Refactor data structures, loops; Preserve modularity, object-orientedness	Good performance on CPU and GPU; Application-level control over performance-critical factors; Positioned for next-gen architectures, but refactoring may be needed in future
Kokkos	C++ Fine-grain || Single-source GPU: native CUDA CPU: maybe vector?	Extreme: C++ rewrite!	Good performance on CPU and GPU; Piggyback DOE's Kokkos for future architectures; C++ resources and marketplace

extras

Performance results



Times for Diffusion Kernel
(Double Precision, Full Node)

SP over DP (Full Node)			
Orig	**PX**	**EPX**	**Kokkos**
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Effect of Floating Point Precision

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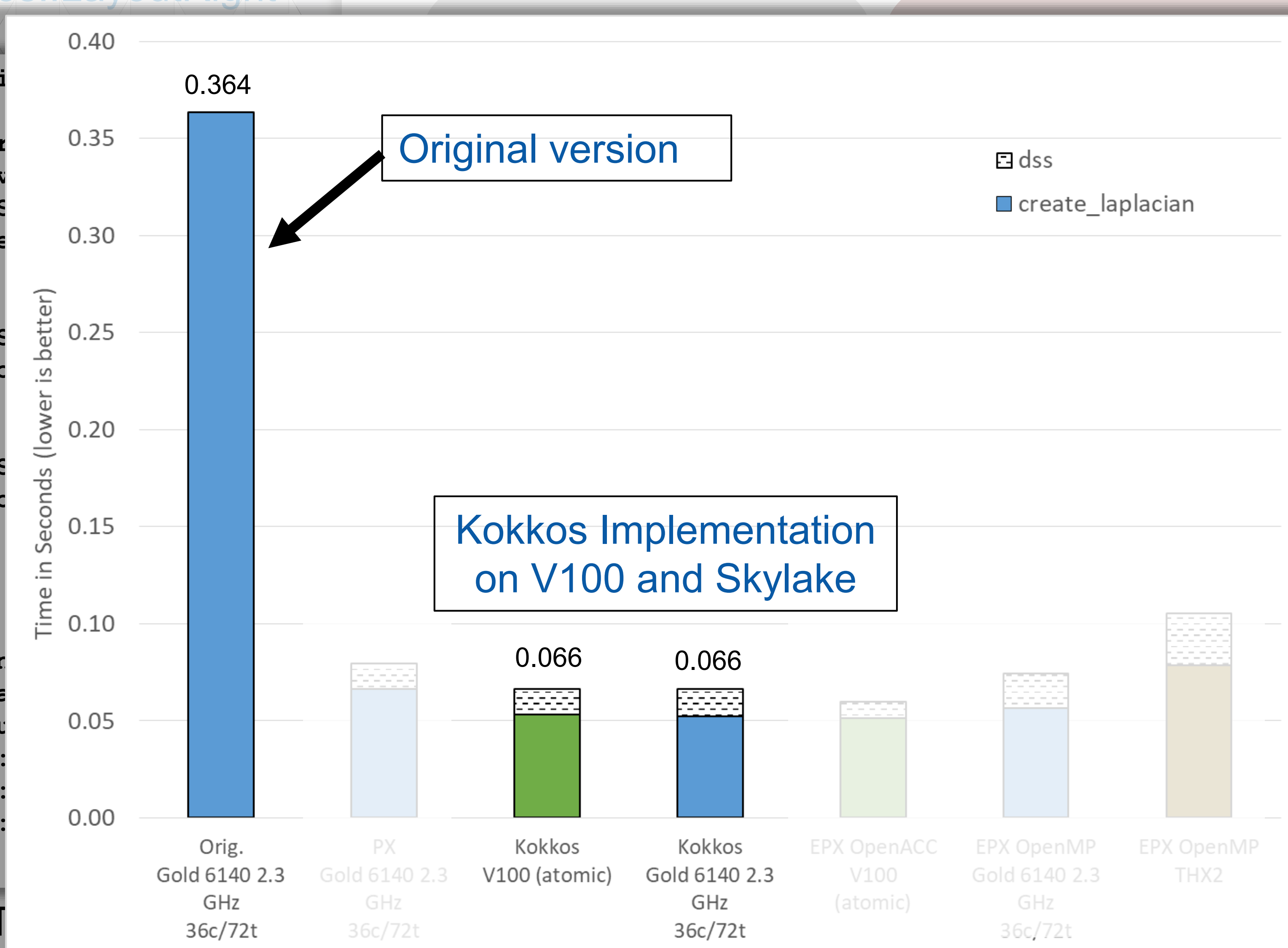
Skylake TAU/PAPI Performance Metrics
(Double Prec., Single Core)

Kokkos Implementation (Kernels Only)

Kokkos::LayoutRight

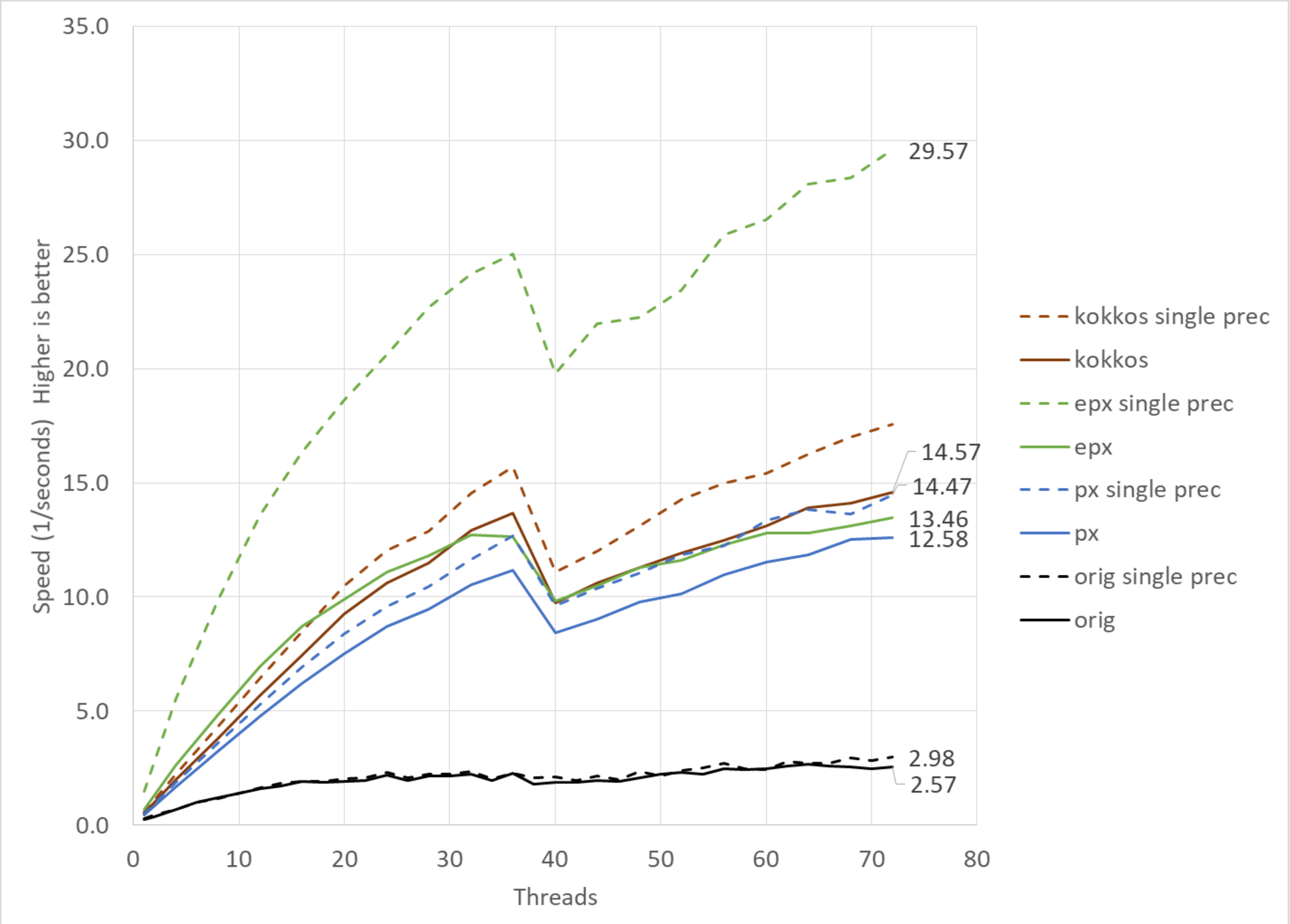
```
//  Defi
typedef
class Cr
  ViewNv
  KOKKOS
  Create


  KOKKOS
  void c
    ...
  }
  KOKKOS
  void c
    ...
  }
} ;

int mair
 ViewNva
// Execu
 Kokkos:
 Kokkos:
 Kokkos:
```

- Si



(Thanks: C. T

Scaling



35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
Speed (1/seconds) Higher is better
0
10
20
30
40
50
60
70
80
Threads
29.57
14.57
14.47
13.46
12.58
2.98
2.57
kokkos single prec
kokkos
epx single prec
epx
px single prec
px
orig single prec
orig

EPX (element-inner) Optimization

```
do ib = 1,neblk
  nrun = LEBLK
  (adjust nrun for partial blocks here)
!$acc loop
  do ie = 1, nrun, EVEC
    call create_laplacian_ep3( ib, ie, min(ie+EVEC-1,nrun)
```

Inner/Inner

Outer/Inner

```
subroutine create_laplacian_EPX( ib, es, ee, nvar &
   ...
   !KSI, ETA, ZETA Derivatives
   qq_e(es:ee,m) = qq_e(es:ee,m) + q_visc(es:ee,ipe,m)*dpsi(l,i)
   qq_n(es:ee,m) = qq_n(es:ee,m) + q_visc(es:ee,ipn,m)*dpsi(l,j)
   qq_c(es:ee,m) = qq_c(es:ee,m) + q_visc(es:ee,ipc,m)*dpsi(l,k)
```

- Xeon, ARM & NEC VE
  OpenMP with vectorization
- Nvidia: OpenACC

  (Thanks Dave Norton, PGI)

element-**inner** loops

```
do v ← 1,nv
  do p ← 1,np
    do e ← 1,ne
```

element-**outer** loops

```
do e ← 1,ne
  do v ← 1,nv
    do p ← 1,np
```