PETSc Tutorial PETSc and Many-Core/GPU Architectures

Karl Rupp
me@karlrupp.net

Freelance Computational Scientist and Institute for Microelectronics, TU Wien



Boulder, Colorado June 14-16, 2017



Table of Contents

FLOPs and Bandwidth

Performance Modeling

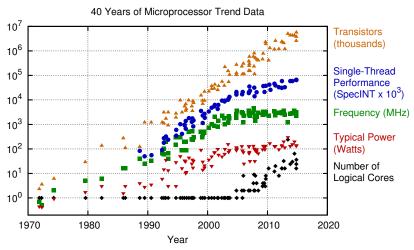
PETSc Profiling

PETSc and Threads

PETSc and GPUs

PETSc

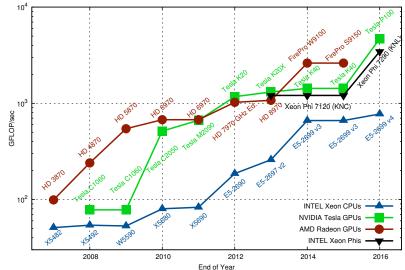
FLOPs and Bandwidth



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten New plot and data collected for 2010-2015 by K. Rupp

Theoretical Peak Performance

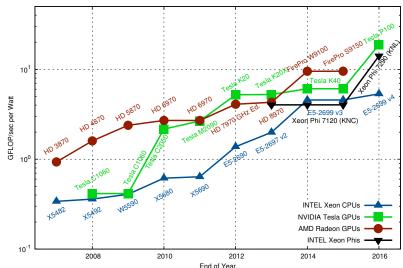
Theoretical Peak Performance, Double Precision



https://www.karlrupp.net/2013/06/cpu-gpu-and-mic-hardware-characteristics-over-time/

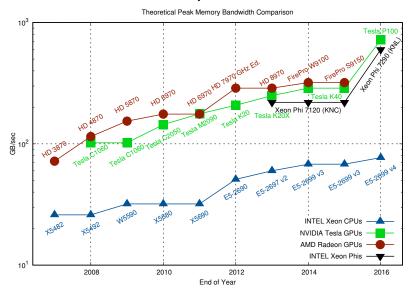
Theoretical Peak Performance per Watt

Theoretical Peak Floating Point Operations per Watt, Double Precision



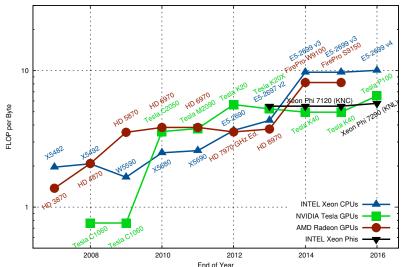
https://www.karlrupp.net/2013/06/cpu-gpu-and-mic-hardware-characteristics-over-time/

Memory Bandwidth



Theoretical Peak Performance (FLOPs) per Byte of Memory Bandwidth

Theoretical Peak Floating Point Operations per Byte, Double Precision



Typical PETSc Operations

Vector operations (add, dot, etc.)

Sparse matrix-vector products (Krylov solvers, smoothers, residuals, etc.)

Maximizing Memory Bandwidth

Read contiguous blocks of memory (contiguous access)

Avoid unordered reads whenever possible

Check Memory Bandwidth Yourself

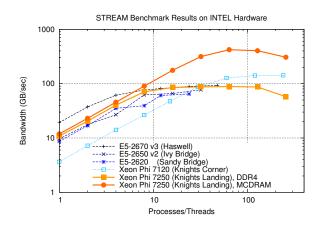
make streams

Performance question to petsc-maint, about 2h ago:

```
np speedup
1 1.0
2 1.85
3 2.25
4 2.37
(...)
39 2.47
40 2.45
Estimation of possible speedup of MPI programs based on Streams benchmark.
It appears you have 1 node(s)
```

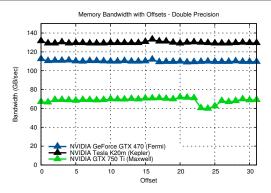
How does Memory Bandwidth Scale with Cores?

Usually saturates quickly 8-16 processes/threads usually suffice



Offset Memory Access

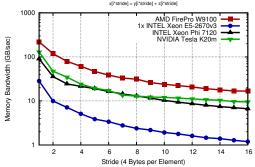
```
void work(double *x, double *y, double *z, int N, int k)
{
    for (size_t i=0; i<N; ++i)
        z[i+k] = x[i+k] + y[i+k];
}</pre>
```



Strided Memory Access

```
void work(double *x, double *y, double *z, int N, int k)
{
    for (size_t i=0; i<N; ++i)
        z[i*k] = x[i*k] + y[i*k];
}</pre>
```



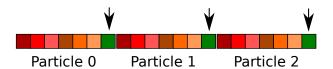


Strided Memory Access

Array of structs problematic

```
typedef struct particle
{
   double pos_x; double pos_y; double pos_z;
   double vel_x; double vel_y; double vel_z;
   double mass;
} Particle;

void increase_mass(Particle *particles, int N)
{
   for (int i=0; i<N; ++i)
      particles[i].mass *= 2.0;
}</pre>
```



Strided Memory Access

Workaround: Structure of Arrays

```
typedef struct particles
{
   double *pos_x; double *pos_y; double *pos_z;
   double *vel_x; double *vel_y; double *vel_z;
   double *mass;
} Particle;

void increase_mass(Particle *particles, int N)
{
   for (int i=0; i<N; ++i)
      particles.mass[i] *= 2.0;
}</pre>
```



PETSc

Mindlessly applying object-oriented programming all the way down to fine granularity is a recipe for a performance disaster.

PETSc Tutorial

Performance Modeling

Performance Modeling Mantra

At any given time during a run, at least one hardware component is operating at 100 percent capacity.

Bottleneck Potpourri

Latency

Bottleneck in strong scaling limit Ultimate limit for time stepping

Latency - Sources

Network latency (Ethernet $\sim 20\mu s$, Infiniband $\sim 5\mu s$) PCI-Express latency (Kernel launches, $\sim 10\mu s$)

Thread synchronization (barriers, locks, $\sim 1 - 100 \mu$ s)

Thread synchronization (barriers, locks, $\sim 1-100\mu {
m s}$

Memory latency ($\sim 100 \mathrm{ns}$)

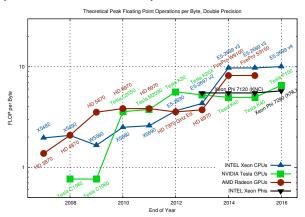
Bottleneck Potpourri

Arithmetic Intensity

Number of FLOPs per Byte

FLOP-limited: Arithmetic intensity larger than $\sim\!\!10$

Memory-limited: Arithmetic intensity smaller than \sim 1



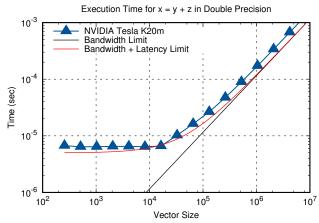
Performance Modeling: Vector Addition

Vector Addition

x = y + z with N elements each

1 FLOP per 24 byte in double precision

Limited by memory bandwidth $\Rightarrow T_2(N) \stackrel{?}{\approx} 3 \times 8 \times N/B$ andwidth + Latency



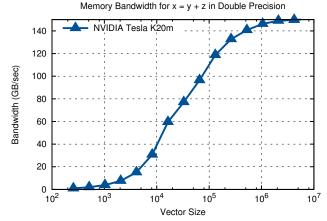
Performance Modeling: Vector Addition

Vector Addition

x = y + z with N elements each

1 FLOP per 24 byte in double precision

Limited by memory bandwidth $\Rightarrow T_2(N) \stackrel{?}{\approx} 3 \times 8 \times N/\text{Bandwidth} + \text{Latency}$



PETSc Tutorial

PETSc Profiling

First: Get the Math Right!

Choose an algorithm that gives robust iteration counts Choose an algorithm that really converges

Profiling

```
Use -log_view for a performance profile

Event timing
Event flops
Memory usage
MPI messages

Call PetscLogStagePush() and PetscLogStagePop()
User can add new stages

Call PetscLogEventBegin() and PetscLogEventEnd()
User can add new events

Call PetscLogFlops() to include your flops
```

Reading -log_view

```
Max/Min
                      Max
                                                     Total
                                             Avq
Time (sec):
                   1.548e+02
                                 1.00122 1.547e+02
Objects:
                   1.028e+03
                                 1.00000 1.028e+03
Flops:
                   1.519e+10
                                 1.01953 1.505e+10 1.204e+11
Flops/sec:
                  9.814e+07
                                 1.01829 9.727e+07 7.782e+08
                                 1.00556 8.819e+03 7.055e+04
MPI Messages:
                  8.854e+03
MPI Message Lengths: 1.936e+08
                                 1.00950 2.185e+04 1.541e+09
MPT Reductions:
                  2.799e+03
                                 1.00000
```

Also a summary per stage

Memory usage per stage (based on when it was allocated)

Time, messages, reductions, balance, flops per event per stage

Always send <code>-log_view</code> when asking performance questions on mailing list

VecNorm 3972 1.0 1.3021e+00 4.6 8.16e+07 1.0 0.0e+00 0.0e+00 1.7e+03 0 1 0 0 14 1 1 1 0 0 0 0 0 0 0 0 0 0 0	Event	Count		Time	(sec)	Flops	Flops					- G	lob	al			- St	tag	e -	
VecNot		Max Ra	atio	Max	Ratio	Max I	Ratio	Mess	Avg len	Reduct	%T	%F	%M	%L	%R	%T	%F	%М	%L	olo
VecNorm 3972 1.0 1.5460e+00 2.5 8.48e+07 1.0 0.0e+00 0.0e+00 1.7e+03 0 1 0 0 14 1 1 0 0 0 0 0 0 0 0 0 0 0 0	Event Stage 1:	Full s	solve	€																
VecNorm 3972 1.0 1.5460e+00 2.5 8.48e+07 1.0 0.0e+00 0.0e+00 0.0e+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	VecDot	43	1.0	4.8879e-	02 8.3	1.77e+0	5 1.0	0.0e+00	0.0e+00	4.3e+01	0	0	0	0	0	0	0	0	0	
VecScale VecScatterBegin VecScatterBegin VecScatterEnd 4503 1.0 4.040e-01 1.0 0.00e+00 0.0 e+00 0.0e+00 0.0e+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	VecMDot	1747	1.0	1.3021e+	00 4.6	8.16e+0	7 1.0	0.0e+00	0.0e+00	1.7e+03	0	1	0	0	14	1	1	0	0	2
VecScatterBegin 4503 1.0 4.0440e-01 1.0 0.00e+00 0.0 6.1e+07 2.0e+03 0.0e+00 0 0 50 26 0 0 0 96 52 VecScatterEnd 4503 1.0 2.8207e-00 6.4 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	VecNorm	3972	1.0	1.5460e+	00 2.5	8.48e+0	7 1.0	0.0e+00	0.0e+00	4.0e+03	0	1	0	0	31	1	1	0	0	6
VecScatterEnd 4503 1.0 2.8207e+00 6.4 0.00e+00 0.0 e+00 0.0e+00 0.0e+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	VecScale	3261	1.0	1.6703e-	01 1.0	3.38e+0	7 1.0	0.0e+00	0.0e+00	0.0e+00	0	0	0	0	0	0	0	0	0	
MatMultAdd 604 1.0 3.2634e-01 1.1 3.68e+09 1.1 4.9e+07 2.3e+03 0.0e+00 11 22 40 24 0 22 44 78 45 MatMultTranspose 676 1.0 1.3220e+00 1.6 6.59e+07 1.0 3.7e+06 1.3e+06 0.0e+00 0 0 3 3 0 0 0 1 1 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0	VecScatterBegin	4503	1.0	4.0440e-	01 1.0	0.00e+00	0.0	6.1e+07	2.0e+03	0.0e+00	0	0	50	26	0	0	0	96	53	
MatMultAdd 604 1.0 6.0195e-01 1.0 5.66e+07 1.0 3.7e+06 1.3e+02 0.0e+00 0 0 3 0 0 0 1 6 6 6 6 6 6 6 1.0 1.3220e+00 1.6 6.50e+07 1.0 4.2e+06 1.4e+02 0.0e+00 0 0 3 0 0 0 1 1 7 7 6 6 6 7 6 1.0 1.3220e+00 1.6 6.50e+07 1.0 4.2e+06 1.4e+02 0.0e+00 0 0 3 0 0 0 1 1 7 7 6 6 7 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8	VecScatterEnd	4503	1.0	2.8207e+	00 6.4	0.00e+00	0.0	0.0e+00	0.0e+00	0.0e+00	0	0	0	0	0	0	0	0	0	
Mathsolve 3020 1.0 2.5957e+01 1.0 3.25e+09 1.0 0.0e+00 0.0e+00 0.0e+00 0 0 0 3 0 0 1 1 7 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0	MatMult	3001	1.0	3.2634e+	01 1.1	3.68e+09	9 1.1	4.9e+07	2.3e+03	0.0e+00	11	22	40	24	0	22	44	78	49	
MatSolve 3020 1.0 2.5957e+01 1.0 3.25e+09 1.0 0.0e+00 0.0e+00 0.0e+00 0 0 0 0 0 18 41 0 0 0 MatCholFctrSym 3 1.0 2.8324e-04 1.0 0.00e+00 0.0e+00 0.0e+00 0.0e+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	MatMultAdd	604	1.0	6.0195e-	01 1.0	5.66e+0	7 1.0	3.7e+06	1.3e+02	0.0e+00	0	0	3	0	0	0	1	6	0	
MatCholFctrSym	MatMultTranspose	676	1.0	1.3220e+	00 1.6	6.50e+0	7 1.0	4.2e+06	1.4e+02	0.0e+00	0	0	3	0	0	1	1	7	0	
MatchsemblyBegin 119 1.0 2.8250e+00 1.5 0.00e+00 0.0 2.4e+05 5.4e+04 3.1e+02 1 0 0 0 4 4 9 0 0 0 4 4 9 0 0 0 0 0 0 0 0	MatSolve	3020	1.0	2.5957e+	01 1.0	3.25e+09	9 1.0	0.0e+00	0.0e+00	0.0e+00	9	21	0	0	0	18	41	0	0	
MatAssemblyBegin 119 1.0 2.8250e+00 1.5 0.00e+00 0.0 2.1e+06 5.4e+04 3.1e+02 1 0 2 24 2 2 0 3 47 MatAssemblyEnd 119 1.0 1.9689e+00 1.4 0.00e+00 0.0 2.8e+05 1.3e+03 6.8e+01 1 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0	MatCholFctrSym	3	1.0	2.8324e-	04 1.0	0.00e+00	0.0	0.0e+00	0.0e+00	0.0e+00	0	0	0	0	0	0	0	0	0	
MathasemblyEnd 119 1.0 1.9689e-00 1.4 0.00e+00 0.0 2.8e+05 1.3e+03 6.8e+01 1 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0	MatCholFctrNum	69	1.0	5.7241e+	00 1.0	6.75e+08	3 1.0	0.0e+00	0.0e+00	0.0e+00	2	4	0	0	0	4	9	0	0	
SNESSolve 4 1.0 1.4302e+02 1.0 8.1le+09 1.0 6.3e+07 3.8e+03 6.3e+03 51 50 52 50 50 99100 99100 SNESILneSearch 43 1.0 1.5116e+01 1.0 1.05e+08 1.1 2.4e+06 3.6e+03 1.8e+02 5 1 2 2 1 10 1 4 4 SNESFunctionEval 5 5 1.0 1.4930e+01 1.0 0.00e+00 0.0 1.8e+06 3.3e+03 8.0e+00 5 0 1 1 0 0 1 0 3 3 SNESFunctionEval 43 1.0 3.7077e+01 1.0 7.77e+06 1.0 4.3e+06 2.6e+04 3.0e+02 13 0 4 24 2 26 0 7 48 SPECMRESOrthog 1747 1.0 1.577e+00 2.9 1.63e+08 1.0 0.0e+00 0.0e+00 1.7e+03 1 1 0 0 14 1 2 0 0 SKSPSctup 24 1.0 2.1040e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 1.7e+03 1 1 0 0 10 4 1 2 0 0 SKSPSctup 43 1.0 8.9988e+01 1.0 7.99e+09 1.0 5.6e+07 2.0e+03 5.8e+03 32 49 46 24 46 62 99 88 48 PCSetUp 112 1.0 1.7354e+01 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 8.7e+01 6 4 0 0 1 12 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	MatAssemblyBegin	119	1.0	2.8250e+	00 1.5	0.00e+00	0.0	2.1e+06	5.4e+04	3.1e+02	1	0	2	24	2	2	0	3	47	
SNESIneSearch 43 1.0 1.5116e+01 1.0 1.05e+08 1.1 2.4e+06 3.6e+03 1.8e+02 5 1 2 2 1 10 1 4 4 4 5 1.0 1.4930e+01 1.0 0.00e+00 0.0 1.8e+06 3.3e+03 8.0e+00 5 0 1 1 0 10 10 0 3 3 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	MatAssemblyEnd	119	1.0	1.9689e+	00 1.4	0.00e+00	0.0	2.8e+05	1.3e+03	6.8e+01	1	0	0	0	1	1	0	0	0	
SNESFunctionEval 55 1.0 1.4930e+01 1.0 0.00e+00 0.0 1.8e+06 3.3e+03 8.0e+00 5 0 1 1 0 0 10 0 3 3 3 3 5 5 5 1.0 1.4930e+01 1.0 7.77e+06 1.0 4.3e+06 2.6e+04 3.0e+02 13 0 4 24 2 26 0 7 4 5 5 5 1.0 1.47 1.0 1.5737e+00 2.9 1.63e+08 1.0 0.0e+00 0.0e+00 1.7e+03 1 1 0 0 14 1 2 0 0 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	SNESSolve	4	1.0	1.4302e+	02 1.0	8.11e+09	9 1.0	6.3e+07	3.8e+03	6.3e+03	51	50	52	50	50	99	100	99	100	9
SNESJacobianEval 43 1.0 3.7077e+01 1.0 7.77e+06 1.0 4.3e+06 2.6e+04 3.0e+02 13 0 4 24 2 26 0 7 48 4 48 4 48 4 5 2 6 0 7 48 4 5 2 6 0 7 48 4 8 5 6 6 6 6 6 6 7 8 8 8 8	SNESLineSearch	43	1.0	1.5116e+	01 1.0	1.05e+08	3 1.1	2.4e+06	3.6e+03	1.8e+02	5	1	2	2	1	10	1	4	4	
KSPGMRESOrthog 1747 1.0 1.5737e+00 2.9 1.63e+08 1.0 0.0e+00 0.0e+00 1.7e+03 1 1 0 0 14 1 2 0 0 KSPSGUP 224 1.0 2.1040e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00 3.0e+01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	SNESFunctionEval	55	1.0	1.4930e+	01 1.0	0.00e+00	0.0	1.8e+06	3.3e+03	8.0e+00	5	0	1	1	. 0	10	0	3	3	
KSPSetup 224 1.0 2.1040e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 3.0e+01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	SNESJacobianEval	43	1.0	3.7077e+	01 1.0	7.77e+06	5 1.0	4.3e+06	2.6e+04	3.0e+02	13	0	4	24	2	26	0	7	48	
KSPSOIVe 43 1.0 8.9988e+01 1.0 7.99e+09 1.0 5.6e+07 2.0e+03 5.8e+03 32 49 46 24 46 62 99 88 48 PCSetUp 112 1.0 1.7354e+01 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 8.7e+01 6 4 0 0 1 12 9 0 0 PCSetUpOnBlocks 1208 1.0 5.8182e+00 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 8.7e+01 2 4 0 0 1 4 9 0 0	KSPGMRESOrthog	1747	1.0	1.5737e+	00 2.9	1.63e+08	3 1.0	0.0e+00	0.0e+00	1.7e+03	1	1	0	0	14	1	2	0	0	2
PCSetUp 112 1.0 1.7354e+01 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 8.7e+01 6 4 0 0 1 12 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	KSPSetup	224	1.0	2.1040e-	02 1.0	0.00e+00	0.0	0.0e+00	0.0e+00	3.0e+01	0	0	0	0	0	0	0	0	0	
PCSetUpOnBlocks 1208 1.0 5.8182e+00 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 8.7e+01 2 4 0 0 1 4 9 0 0	KSPSolve	43	1.0	8.9988e+	01 1.0	7.99e+09	1.0	5.6e+07	2.0e+03	5.8e+03	32	49	46	24	46	62	99	88	48	8
	PCSetUp	112	1.0	1.7354e+	01 1.0	6.75e+08	3 1.0	0.0e+00	0.0e+00	8.7e+01	6	4	0	0	1	12	9	0	0	
PCApply 276 1.0 7.1497e+01 1.0 7.14e+09 1.0 5.2e+07 1.8e+03 5.1e+03 25 44 42 20 41 49 88 81 39	PCSetUpOnBlocks	1208	1.0	5.8182e+	00 1.0	6.75e+08	3 1.0	0.0e+00	0.0e+00	8.7e+01	2	4	0	0	1	4	9	0	0	
	PCApply	276	1.0	7.1497e+	01 1.0	7.14e+09	9 1.0	5.2e+07	1.8e+03	5.1e+03	25	44	42	20	41	49	88	81	39	

Communication Costs

Reductions: usually part of Krylov method, latency limited

VecMDot

VecNorm

MatAssemblyBegin

Change algorithm (e.g. IBCGS)

Point-to-point (nearest neighbor), latency or bandwidth

VecScatter Mat.Mult.

PCApply

MatAssembly

SNESFunctionEval

SNESJacobianEval

Compute subdomain boundary fluxes redundantly Ghost exchange for all fields at once

Better partition

Adding a Logging Event (C)

```
PetscLogEvent USER_EVENT;
PetscClassId classid;
PetscLogDouble user_event_flops;

PetscClassIdRegister("class name",&classid);
PetscLogEventRegister("user event",classid,&USER_EVENT);

PetscLogEventBegin(USER_EVENT,0,0,0,0);
    /* code segment to monitor */
PetscLogFlops(user_event_flops);
PetscLogEventEnd(USER_EVENT,0,0,0,0);
```

Adding a Logging Event (Python)

```
with PETSc.logEvent('Reconstruction') as recEvent:
    # All operations are timed in recEvent
    reconstruct(sol)
    # Flops are logged to recEvent
    PETSc.Log.logFlops(user_event_flops)
```

Adding a Logging Stage (C)

```
PetscLogStage stage;
PetscLogStageRegister("name", &stage);
PetscLogStagePush(stage);
/* Code to Monitor */
PetscLogStagePop();
```

```
Count Time (sec) Flops --- Global --- --- Stage --
Event
                  Max Ratio Max Ratio Max Ratio Mess Avg len Reduct %T %F %M %L %R %T %F %M %L
--- Event Stage 0: Main Stage
MatMult
                    178 1.0 7.8040e+01 1.0 2.59e+11 1.0 4.4e+02 2.0e+05 0.0e+00 33 41 6 11 0 51 89 20 24
MatPtAP
                    10 1.0 2.4870e+01 1.0 5.45e+09 1.0 2.1e+02 3.1e+05 1.8e+02 10 1 3 8 1 16 2 9 18
MatPtAPSymbolic 10 1.0 1.8828e+01 1.0 0.00e+00 0.0 1.2e+02 2.7e+05 8.2e+01
                                                                                 8 0 2 4 0 12 0 5 9
Mat Pt APNumeric
                    10 1.0 6.0428e+00 1.0 5.45e+09 1.0 9.4e+01 3.7e+05 1.0e+02
                                                                                            0
                                                                                                4 2 4 9
SNESSolve
                    2 1.0 1.9059e+02 1.0 6.22e+11 1.0 6.6e+03 9.3e+04 3.4e+03
                                                                                 79 99 92 75 16 123213292168
KSPSolve
                 2 1.0 1.8230e+02 1.0 6.07e+11 1.0 6.5e+03 9.1e+04 3.2e+03
                                                                                 76 97 89 72 15 118208285161
                    8 1.0 1.6138e+01 1.0 4.81e+09 1.1 1.2e+03 8.1e+04 2.5e+03
                                                                                7 1 17 12 11 10 2 55 28
PCSetUp
                  46 1.0 1.2586e+02 1.0 4.43e+11 1.0 6.3e+03 8.5e+04 2.7e+03
PCApply
                                                                                 52 70 87 65 12 81152277146
KSPSolve FS 0 46 1.0 1.0038e+02 1.0 3.42e+11 1.0 6.2e+03 8.2e+04 2.6e+03
                                                                                 42 54 86 62 12 65117273138
(...)
--- Event Stage 1: MG Apply
MatMultMFA11
                   296 1.0 4.3461e+01 1.0 2.82e+11 1.0 1.2e+03 3.0e+05 0.0e+00 18 45 16 43 0 51 84 24 78
                   230 1.0 7.2581e+01 1.0 2.87e+11 1.0 4.5e+03 8.5e+04 2.6e+02
                                                                                 30 46 62 47 1 85 85 91 841
KSPSolve
PCApply
                    642 1.0 1.0269e+01 1.0 1.40e+10 1.1 3.0e+03 8.7e+03 1.8e+02
                                                                                4 2 42 3 1 12 4 61 6
MGSmooth Level 1 92 1.0 2.4177e+01 1.0 3.17e+10 1.0 5.0e+03 8.3e+03 1.7e+02 MGResid Level 1 46 1.0 4.3231e+101 1.0 5.77e+10 1.0 5.0e+02 1.2e+05 4.6e+01
                 46 1.0 7.8169e+00 1.0 1.06e+10 1.1 3.0e+03 8.3e+03 1.7e+02
                                                                                                 9 3 61 5
                                                                                 10 5 7 7
MGInterp Level 1 92 1.0 3.5063e-01 1.1 1.09e+08 1.0 9.2e+01 1.5e+04 0.0e+00
MGSmooth Level 2 92 1.0 4.0886e+01 1.0 2.44e+11 1.0 1.0e+03 3.0e+05 4.6e+01 17 39 14 37 0 MGResid Level 2 46 1.0 6.8277e+00 1.0 4.39e+10 1.0 1.8e+02 3.0e+05 0.0e+00 3 7 3 7 0
                                                                                 17 39 14 37 0 48 73 20 66
MGInterp Level 2 92 1.0 1.0898e+00 1.4 8.47e+08 1.0 9.2e+01 3.8e+04 0.0e+00
                                                                               0 0 1 0 0 1 0 2 1
```

PETSc Tutorial

PETSc and Threads

PETSc and Threads

Competing Threading Approaches

pthread

OpenMP

C++11 threads

Compiler magic

...

Issues with Threads

Problematic across compilers

Data locality

Thread ownership

Software interface

Assumption for Subsequent Discussion

Primary Goal: Get the science done!

10 percent performance difference is **not significant**

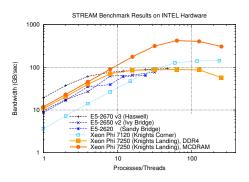
PETSc and Threads

When to Use Threads After All?

Distributed Memory: Need MPI anyway

Shared Memory: MPI for multi-socket systems for NUMA reasons

1-Socket Machines: If a 2-5x gain is critical, use a cluster!



```
numactl --membind 0 ./stream # DDR4
numactl --membind 1 ./stream # MCDRAM
```

Threads and Library Interfaces

Attempt 1

Library spawns threads

```
void library_func(double *x, int N) {
    #pragma omp parallel for
    for (int i=0; i<N; ++i) x[i] = something_complicated();
}</pre>
```

Problems

Call from multi-threaded environment?

```
void user_func(double **y, int N) {
    #pragma omp parallel for
    for (int j=0; j<M; ++j) library_func(y[j], N);
}</pre>
```

Incompatible OpenMP runtimes (e.g. GCC vs. ICC)

Threads and Library Interfaces

Attempt 2

Use pthreads/TBB/etc. instead of OpenMP to spawn threads Fixes incompatible OpenMP implementations (probably)

Problems

Still a problem with multi-threaded user environments

```
void user_func(double **y, int N) {
    #pragma omp parallel for
    for (int j=0; j<M; ++j) library_func(y[j], N);
}</pre>
```

Threads and Library Interfaces

Attempt 3

Hand back thread management to user

```
void library_func(ThreadInfo ti, double *x, int N) {
  int start = compute_start_index(ti, N);
  int stop = compute_stop_index(ti, N);
  for (int i=start; i<stop; ++i)
    x[i] = something_complicated();
}</pre>
```

Implications

Users can use their favorite threading model

API requires one extra parameter

Extra boilerplate code required in user code

Threads and Library Interfaces

Reflection

Extra thread communication parameter

```
void library_func(ThreadInfo ti, double *x, int N) {...}
```

Rename thread management parameter

```
void library_func(Thread_Comm c, double *x, int N) {...}
```

Compare:

```
void library_func(MPI_Comm comm, double *x, int N) {...}
```

Conclusion

Prefer flat MPI over MPI+OpenMP for a composable software stack MPI automatically brings better data locality

PETSc

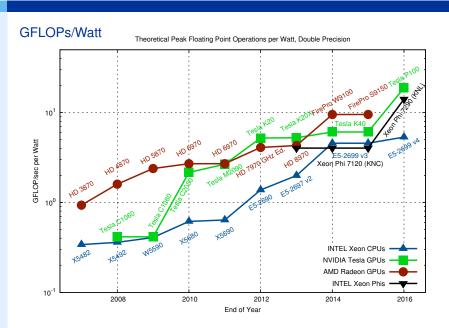
PETSc and GPUs

Why bother?

Don't believe anything unless you can run it

Matt Knepley

Why bother?



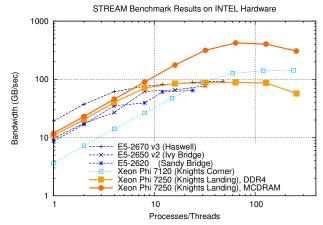
Why bother?

Procurements

Theta (ANL, 2016): 2nd generation INTEL Xeon Phi

Summit (ORNL, 2017), Sierra (LLNL, 2017): NVIDIA Volta GPU

Aurora (ANL, 2018): 3rd generation INTEL Xeon Phi



Current Status

PETSc on GPUs and MIC:

Current Status

Available Options

Native on Xeon Phi

Cross-compile for Xeon Phi

CUDA

CUDA-support through CUSP

-vec_type cusp -mat_type aijcusp

-vec_type cuda -mat_type aijcusparse

Only for NVIDIA GPUs

CUDA/OpenCL/OpenMP

CUDA/OpenCL/OpenMP-support through ViennaCL

-vec_type viennacl -mat_type aijviennacl

OpenCL on CPUs and MIC fairly poor







Configuration

CUDA (CUSP)

CUDA-enabled configuration (minimum)

```
./configure [..] --with-cuda=1
--with-cusp=1 --with-cusp-dir=/path/to/cusp
```

Customization:

```
--with-cudac=/path/to/cuda/bin/nvcc
--with-cuda-arch=sm_60
```

OpenCL (ViennaCL)

OpenCL-enabled configuration

```
./configure [..] --download-viennacl
   --with-opencl-include=/path/to/OpenCL/include
   --with-opencl-lib=/path/to/libOpenCL.so
```

How Does It Work?

Host and Device Data

Possible Flag States

How Does It Work?

Fallback-Operations on Host

Data becomes valid on host (PETSC_CUSP_CPU)

```
PetscErrorCode VecSetRandom_SeqCUSP_Private(..) {
   VecGetArray(...);
   // some operation on host memory
   VecRestoreArray(...);
}
```

Accelerated Operations on Device

Data becomes valid on device (PETSC_CUSP_GPU)

```
PetscErrorCode VecAYPX_SeqCUSP(..) {
   VecCUSPGetArrayReadWrite(...);
   // some operation on raw handles on device
   VecCUSPRestoreArrayReadWrite(...);
}
```

Example

KSP ex12 on Host

```
$> ./ex12
    -pc_type ilu -m 200 -n 200 -log_summary
```

```
KSPGMRESOrthog 228 1.0 6.2901e-01
KSPSolve 1 1.0 2.7332e+00
```

KSP ex12 on Device

```
$> ./ex12 -vec_type cusp -mat_type aijcusp
   -pc_type ilu -m 200 -n 200 -log_summary
```

```
[0]PETSC ERROR: MatSolverPackage petsc does not support
    matrix type seqaijcusp
```

Example

KSP ex12 on Host

```
$> ./ex12
-pc_type none -m 200 -n 200 -log_summary
```

```
KSPGMRESOrthog 1630 1.0 4.5866e+00
KSPSolve 1 1.0 1.6361e+01
```

KSP ex12 on Device

```
$> ./ex12 -vec_type cusp -mat_type aijcusp
-pc_type none -m 200 -n 200 -log_summary
```

```
MatCUSPCopyTo 1 1.0 5.6108e-02
KSPGMRESOrthog 1630 1.0 5.5989e-01
KSPSolve 1 1.0 1.0202e+00
```

Pitfalls

Pitfall: Repeated Host-Device Copies

PCI-Express transfers kill performance Complete algorithm needs to run on device Problematic for explicit time-stepping, etc.

Pitfall: Wrong Data Sizes

Data too small: Kernel launch latencies dominate

Data too big: Out of memory

Pitfall: Function Pointers

Pass CUDA function "pointers" through library boundaries?

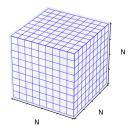
OpenCL: Pass kernel sources, user-data hard to pass

Composability?

Pitfalls

Pitfall: GPUs are too fast for PCI-Express

Latest GPU peaks: 720 GB/sec from GPU-RAM, 16 GB/sec for PCI-Express 40x imbalance (



Compute vs. Communication

Take N = 512, so each field consumes 1 GB of GPU RAM

Boundary communication: $2 \times 6 \times N^2$: 31 MB

Time to load field: 1.4 ms

Time to load ghost data: 1.9 ms (!!)

PETSc and GPUs

Many PETSc Operations do NOT benefit from modern high-end GPUs in a substantial way! (Exception: OpenPower systems)

50

Current GPU-Functionality in PETSc

Current GPU-Functionality in PETSc

	CUSP/CUDA	ViennaCL
Programming Model	CUDA	CUDA/OpenCL/OpenMP
Operations	Vector, MatMult	Vector, MatMult
Matrix Formats	CSR, ELL, HYB	CSR
Preconditioners	SA-AMG, BiCGStab	SA/Agg-AMG, Par-ILU0
MPI-related	Scatter	-

Additional Functionality

MatMult via cuSPARSE

OpenCL residual evaluation for PetscFE

Current Directions

PETSc on GPUs and MIC:

Current Directions

Current: CUDA

Split CUDA-buffers from CUSP

Vector operations by cuBLAS

MatMult by different packages

CUSP (and others) provides add-on functionality

More CUSP Functionality in PETSc

Relaxations (Gauss-Seidel, SOR) Polynomial preconditioners Approximate inverses

Current: PETSc + ViennaCL

API

Backend

ViennaCL

CUDA, OpenCL, OpenMP backends Backend switch at runtime CUDA, OpenCL and OpenMP exposed in PFTSc

Focus on shared memory machines

ViennaCL Core OpenMP OpenCl CUDA Hardware CPU MIC

Recent Advances

Pipelined Krylov solvers Fast sparse matrix-vector products Fast sparse matrix-matrix products Fine-grained algebraic multigrid

Fine-grained parallel ILU

Current: PETSc + ViennaCL

Current Use of ViennaCL in PETSc

```
$> ./ex12 -vec_type viennacl -mat_type aijviennacl ...
```

Executes on OpenCL device

New Use of ViennaCL in PETSc

```
$> ./ex12 -vec_type viennacl -mat_type aijviennacl
-viennacl_backend openmp ...
```

Pros and Cons

Use CPU + GPU simultaneously

Non-intrusive, use plugin-mechanism

Non-optimal in strong-scaling limit

Gather experiences for best long-term solution

GPU Summary and Conclusion

Currently Available

CUSP/CUDA for CUDA, ViennaCL for CUDA/OpenCL/OpenMP Automatic use for vector operations and SpMV Smoothed Agg. AMG via CUSP and ViennaCL ViennaCL as CUDA/OpenCL/OpenMP-hydra

Current Activities

GPU-acceleration for GAMG Better support for n > 1 processes Use of cuBLAS and cuSPARSE



Conclusions

PETSc can help You

solve algebraic and DAE problems in your application area rapidly develop efficient parallel code, can start from examples develop new solution methods and data structures debug and analyze performance advice on software design, solution algorithms, and performance

petsc-{users, dev, maint}@mcs.anl.gov

You can help PETSc

report bugs and inconsistencies, or if you think there is a better way tell us if the documentation is inconsistent or unclear consider developing new algebraic methods as plugins, contribute if your idea works