Writing Performance-Portable Code for GPUs

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@karlrupp

with contributions from
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Josef Weinbub[1], Ansgar Jüngel[2], Tibor Grasser[1]
(based on stimuli from PETSc+ViennaCL users)

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Outline

Introduction

Conjugate Gradient - Standard Formulation

Conjugate Gradient - Kernel Parameters

Parameter Study for Portable Performance

Conjugate Gradient - Pipelining

BiCGStab and GMRES - Benchmark Results

Conclusion

Introduction

Positions

- PhD student at TU Wien (2009-2011)
- Postdoc at ANL (09/2012-09/2013)
- Postdoc at TU Wien (01/2012-09/2012, 09/2013-current)

Research Interests

- Semiconductor device simulation
- Numerical solution of PDEs
- Parallel computing

Software Development

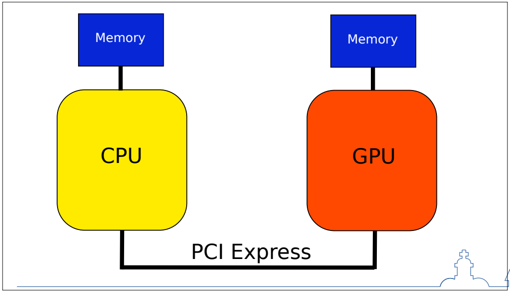
- PETSc
- ViennaCL
- ViennaSHE
- ...

Iterative Solvers

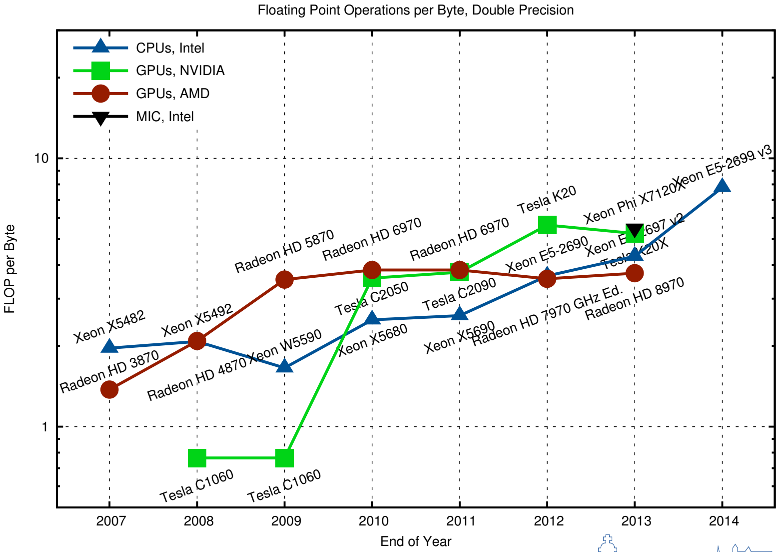
- Matrix-vector products and vector operations only
- Expose more fine-grained parallelism
- Preconditioners often desirable

Accelerators (CUDA, OpenCL)

- Graphics processing units (GPUs)
- Intel Xeon Phi



Introduction



Conjugate Gradients

Pseudocode

Choose x_0

$p_0 = r_0 = b - Ax_0$

For $i = 0$ until convergence

1. Compute and store Ap_i
2. Compute $\langle p_i, Ap_i \rangle$
3. $\alpha_i = \langle r_i, r_i \rangle / \langle p_i, Ap_i \rangle$
4. $x_{i+1} = x_i + \alpha_i p_i$
5. $r_{i+1} = r_i - \alpha_i A p_i$
6. Compute $\langle r_{i+1}, r_{i+1} \rangle$
7. $\beta_i = \langle r_{i+1}, r_{i+1} \rangle / \langle r_i, r_i \rangle$
8. $p_{i+1} = r_{i+1} + \beta_i p_i$

EndFor

BLAS-based Implementation

-

SpMV, AXPY

For $i = 0$ until convergence

1. SpMV
2. DOT
3. -
4. AXPY
5. AXPY
6. DOT
7. -
8. AXPY

EndFor

Conjugate Gradients

Pseudocode

Choose x_0
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8. $p_{i+1} = r_{i+1} + \beta_i p_i$

EndFor

BLAS-based Implementation

-
SpMV, AXPY
For $i = 0$ until convergence

1. SpMV
2. DOT $\leftarrow$ Global sync!
3. -
4. AXPY
5. AXPY
6. DOT $\leftarrow$ Global sync!
7. -
8. AXPY

EndFor

Conjugate Gradients

Pseudocode

Choose x_0
$p_0 = r_0 = b - Ax_0$
For $i = 0$ until convergence

1. Compute and store Ap_i
2. Compute $\langle p_i, Ap_i \rangle$
3. $\alpha_i = \langle r_i, r_i \rangle / \langle p_i, Ap_i \rangle$
4. $x_{i+1} = x_i + \alpha_i p_i$
5. $r_{i+1} = r_i - \alpha_i Ap_i$
6. Compute $\langle r_{i+1}, r_{i+1} \rangle$
7. $\beta_i = \langle r_{i+1}, r_{i+1} \rangle / \langle r_i, r_i \rangle$
8. $p_{i+1} = r_{i+1} + \beta_i p_i$

EndFor

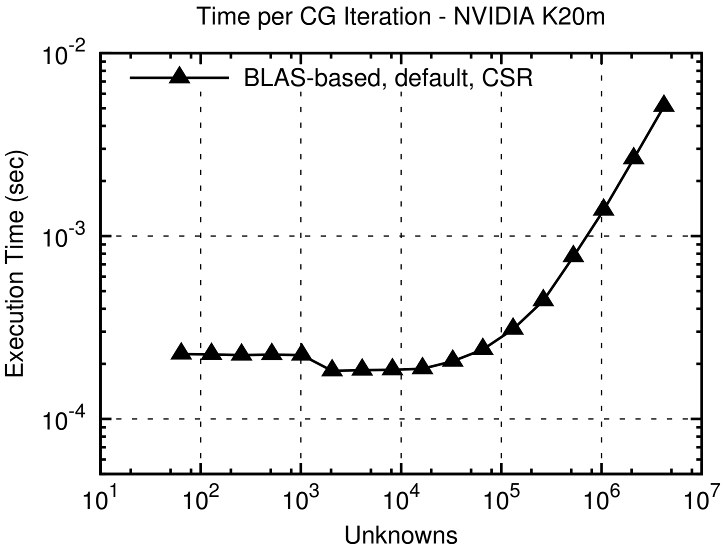
BLAS-based Implementation

-
SpMV, AXPY
For $i = 0$ until convergence

1. SpMV $\leftarrow$ No caching of Ap_i
2. DOT $\leftarrow$ Global sync!
3. -
4. AXPY
5. AXPY $\leftarrow$ No caching of r_{i+1}
6. DOT $\leftarrow$ Global sync!
7. -
8. AXPY

EndFor

Conjugate Gradients



(2D Finite Difference Discretization)

Conjugate Gradient

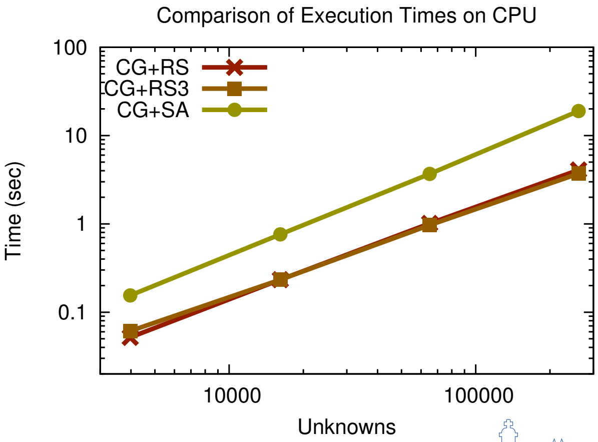
Implications

- Kernel launches expensive
- Delicate balance for preconditioners

Implications

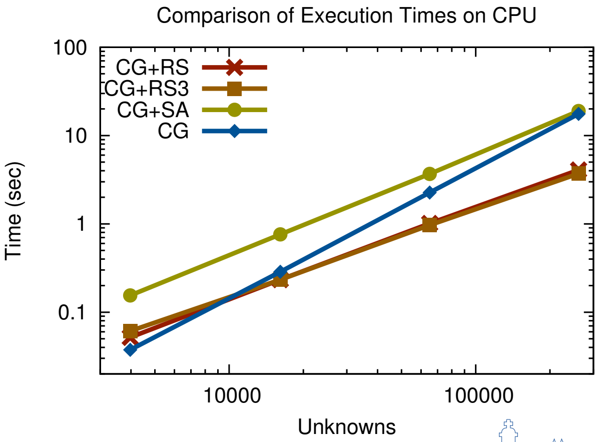
Kernel launches expensive

Delicate balance for preconditioners



Implications

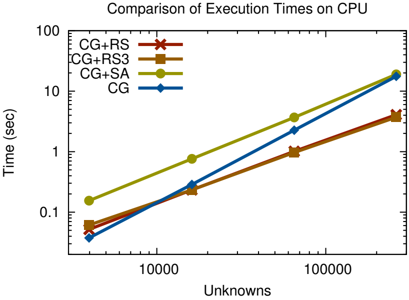
- Kernel launches expensive
- Delicate balance for preconditioners

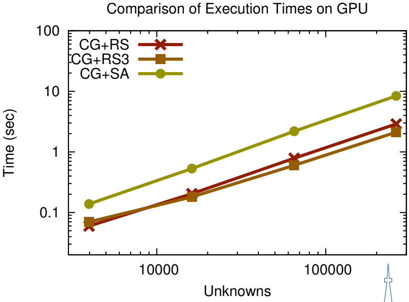


Implications

Kernel launches expensive

Delicate balance for preconditioners





Implications

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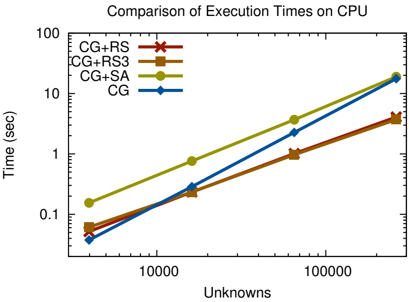
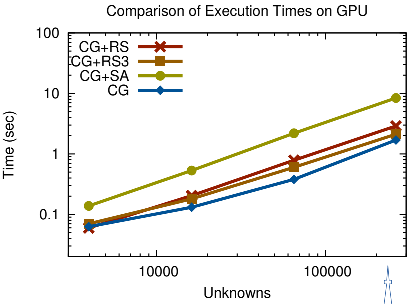




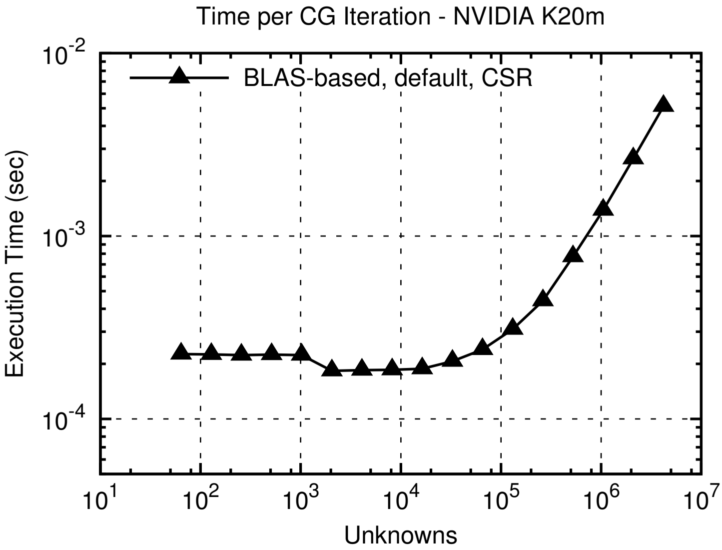
Conjugate Gradient Optimizations

Optimization 1

- Get best performance out of SpMV
- Compare different sparse matrix types

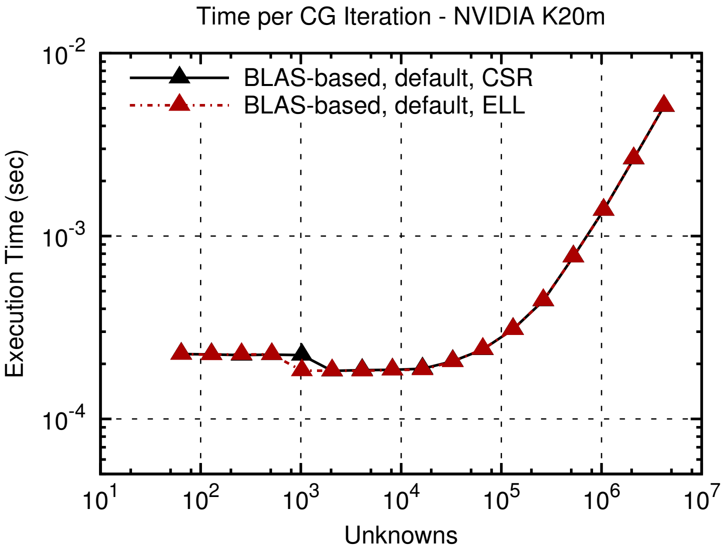
Cf.: N. Bell: Implementing sparse matrix-vector multiplication on throughput-oriented processors. *Proc. SC '09*

Conjugate Gradients



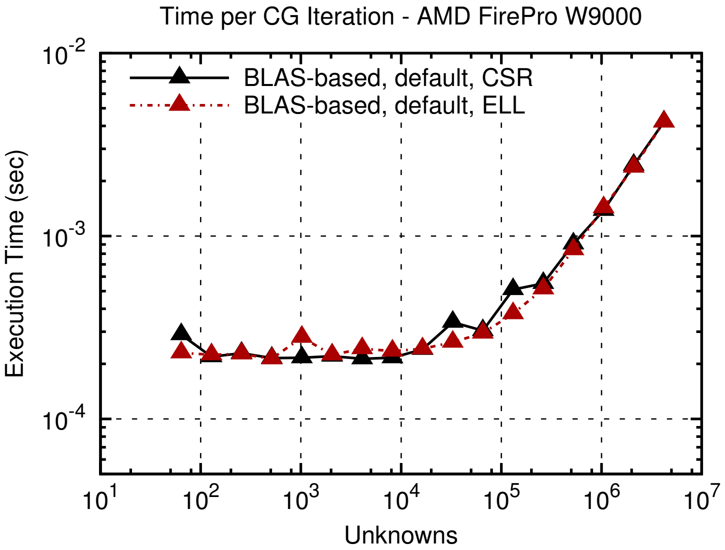
(2D Finite Difference Discretization)

Conjugate Gradients



(2D Finite Difference Discretization)

Conjugate Gradients



(2D Finite Difference Discretization)

Conjugate Gradient Optimizations

Optimization 2

Optimize kernel parameters for each operation

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Benchmark Setting

Scope for Portability Study

- Vector and matrix-vector operations (BLAS levels 1 and 2)
- Limited by memory bandwidth

Benchmark Setting

Scope for Portability Study

- Vector and matrix-vector operations (BLAS levels 1 and 2)
- Limited by memory bandwidth

Key Question (Memory-Bandwidth-Limited Kernels)

Good performance of complicated kernels by optimizing the simplest kernel?

Benchmark Setting

Vector Assignment (Copy) Kernel

$x \Leftarrow y$ for (large) vectors x, y

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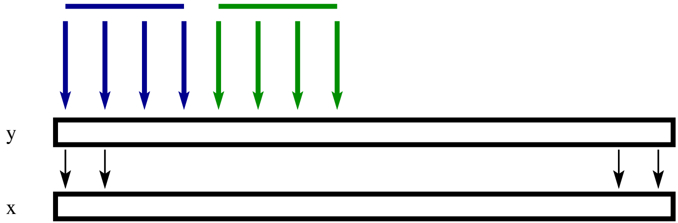

Benchmark Setting

Vector Assignment (Copy) Kernel

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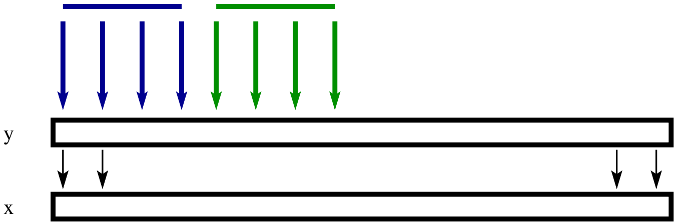


Parameters (1900 variations)

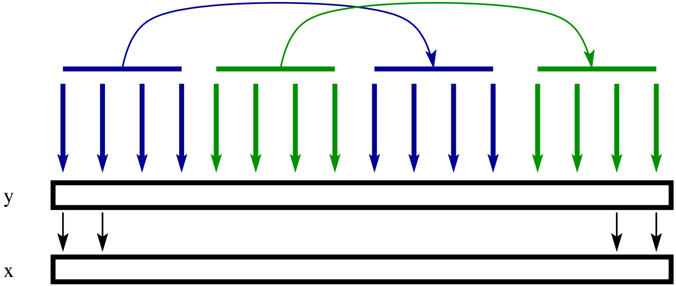
Local work size, global work size

Vector types (float1, float2, ... , float16)

Thread increment type

Vector Assignment (Copy) Kernel

$x \Leftarrow y$ for (large) vectors x, y



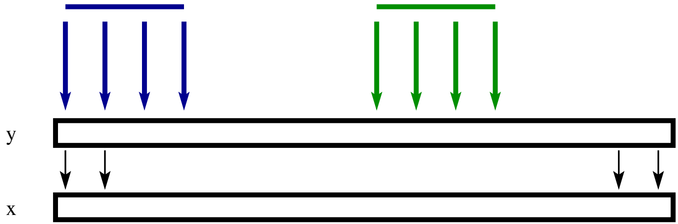
Parameters (1900 variations)

```
for (size_t i = get_global_id(0); i < N;
             i+= get_global_size(0))
  x[i] = y[i];
```

Benchmark Setting

Vector Assignment (Copy) Kernel

$x \Leftarrow y$ for (large) vectors x, y

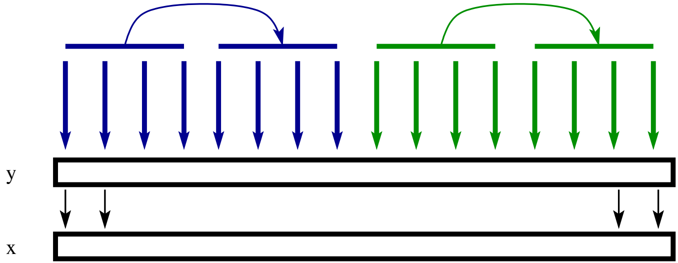


Parameters (1900 variations)

```
for (size_t i = group_start + get_local_id(0);
             i < group_end;
  i+= get_local_size(0)) x[i] = y[i];
```

Vector Assignment (Copy) Kernel

$x \Leftarrow y$ for (large) vectors x, y



Parameters (1900 variations)

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for (size_t i = group_start + get_local_id(0);
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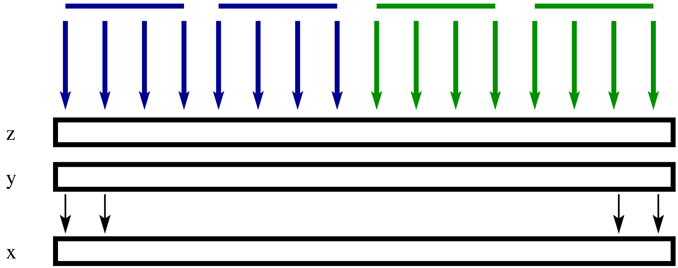
```

Benchmark Setting

Operations

Vector copy, vector addition, inner product

Matrix-vector product



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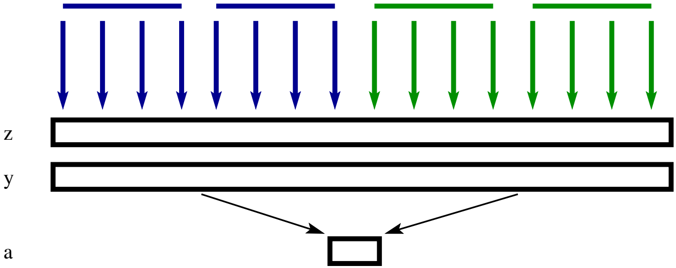

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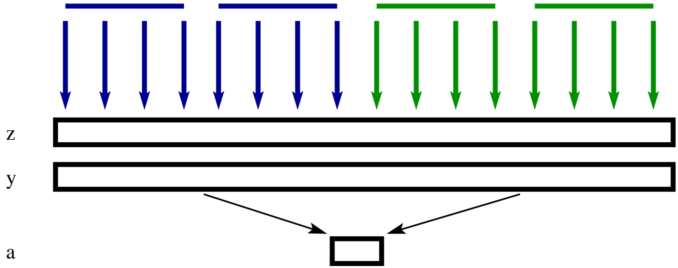


Devices

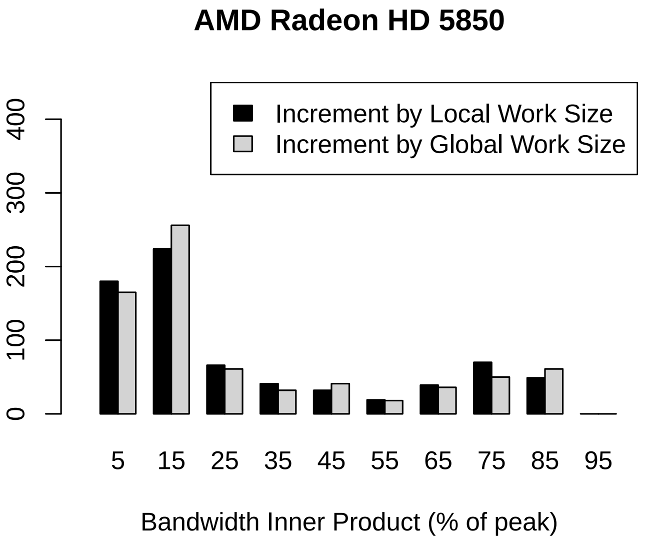
AMD: A10-5800 APU, HD 5850 GPU

INTEL: Dual Socket Xeon E5-2670, Xeon Phi

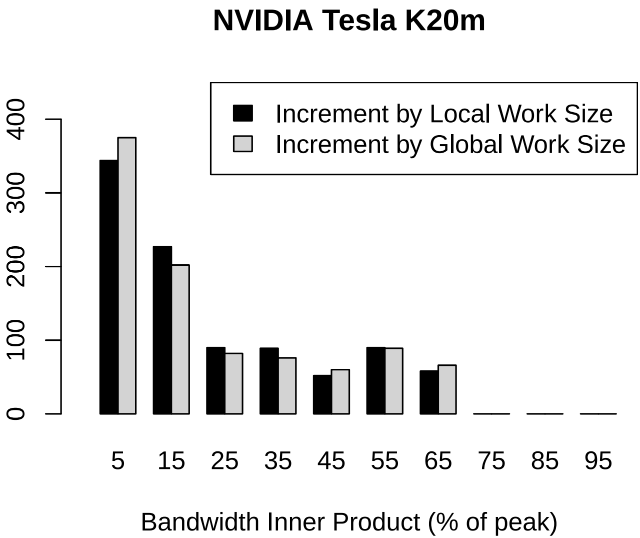
NVIDIA: GTX 285, Tesla K20m

Histograms

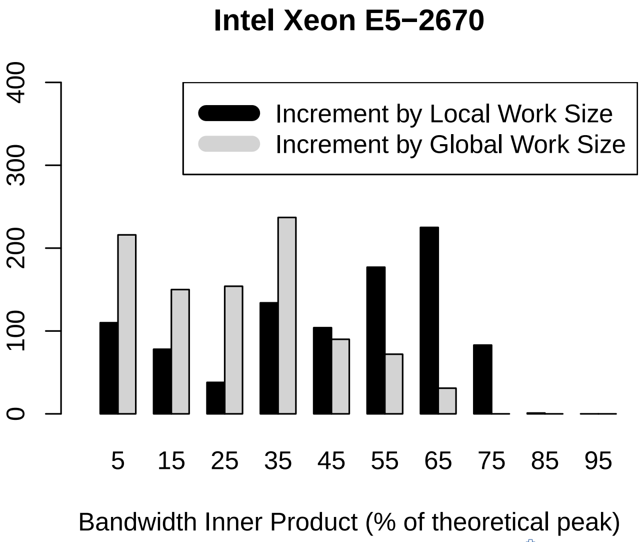
Benchmark



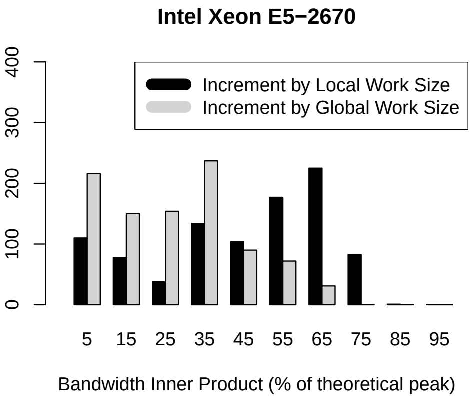
AMD Radeon HD 5850
Increment by Local Work Size
Increment by Global Work Size
0
100
200
300
400
5
15
25
35
45
55
65
75
85
95
Bandwidth Inner Product (% of peak)


NVIDIA Tesla K20m
Increment by Local Work Size
Increment by Global Work Size
0
100
200
300
400
5
15
25
35
45
55
65
75
85
95
Bandwidth Inner Product (% of peak)

Benchmark


Intel Xeon E5−2670
Increment by Local Work Size
Increment by Global Work Size
0
100
200
300
400
5
15
25
35
45
55
65
75
85
95
Bandwidth Inner Product (% of theoretical peak)

Benchmark


Intel Xeon E5−2670
Increment by Local Work Size
Increment by Global Work Size
0
100
200
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5
15
25
35
45
55
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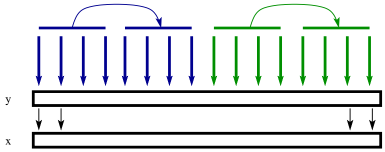
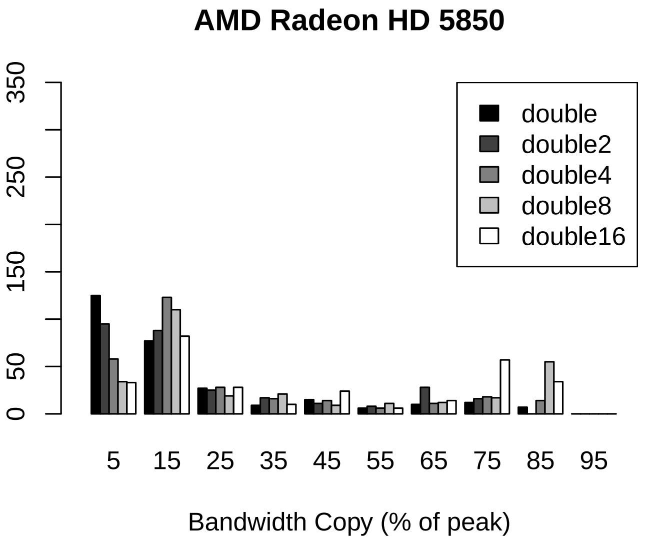
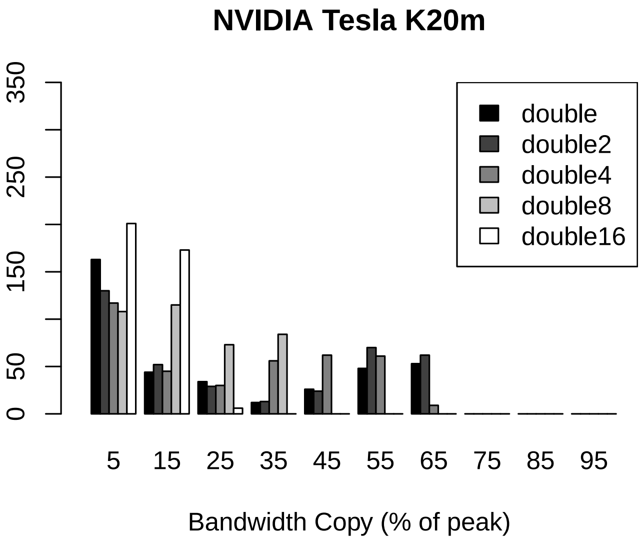
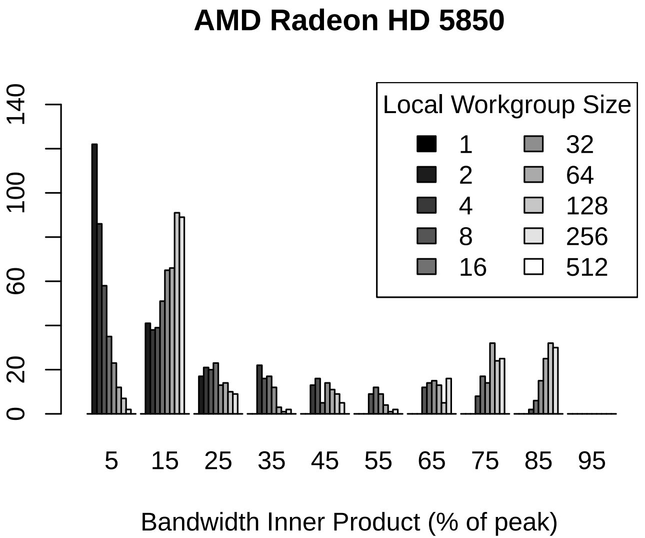
85
95
Bandwidth Inner Product (% of theoretical peak)


y
x

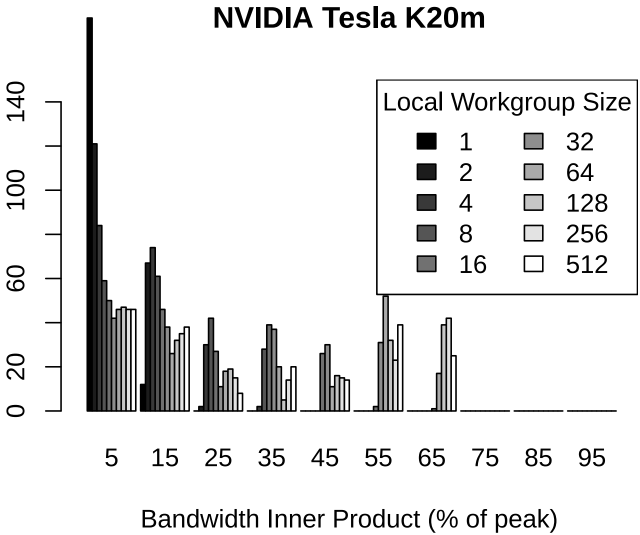

AMD Radeon HD 5850
350
250
150
50
0
double
double2
double4
double8
double16
5
15
25
35
45
55
65
75
85
95
Bandwidth Copy (% of peak)


NVIDIA Tesla K20m
0
50
150
250
350
double
double2
double4
double8
double16
5
15
25
35
45
55
65
75
85
95
Bandwidth Copy (% of peak)

Benchmark


AMD Radeon HD 5850
Local Workgroup Size
1
2
4
8
16
32
64
128
256
512
0
20
60
100
140
5
15
25
35
45
55
65
75
85
95
Bandwidth Inner Product (% of peak)

Benchmark


NVIDIA Tesla K20m
Local Workgroup Size
1
2
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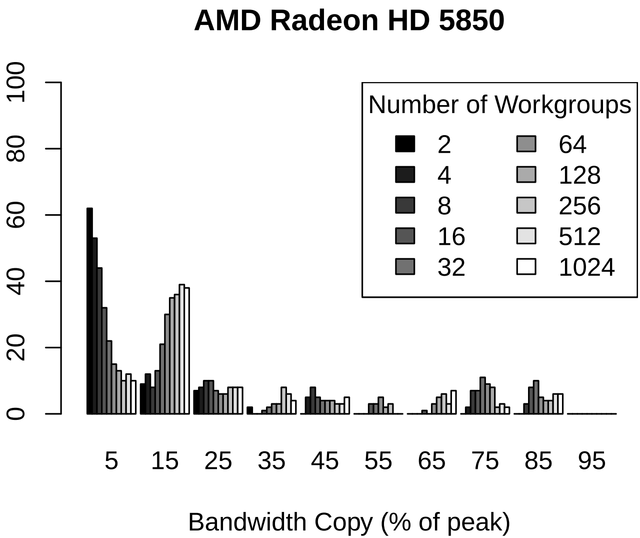
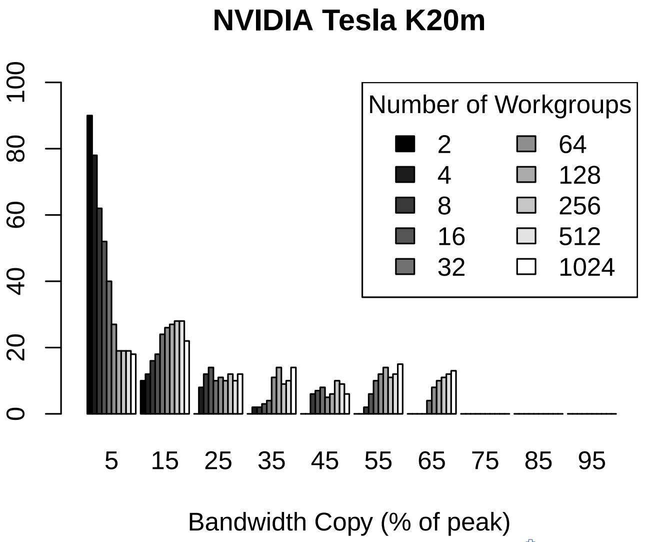
8
16
32
64
128
256
512
0
20
60
100
140
5
15
25
35
45
55
65
75
85
95
Bandwidth Inner Product (% of peak)

Benchmark



AMD Radeon HD 5850
Number of Workgroups
2
4
8
16
32
64
128
256
512
1024
0
20
40
60
80
100
5
15
25
35
45
55
65
75
85
95
Bandwidth Copy (% of peak)

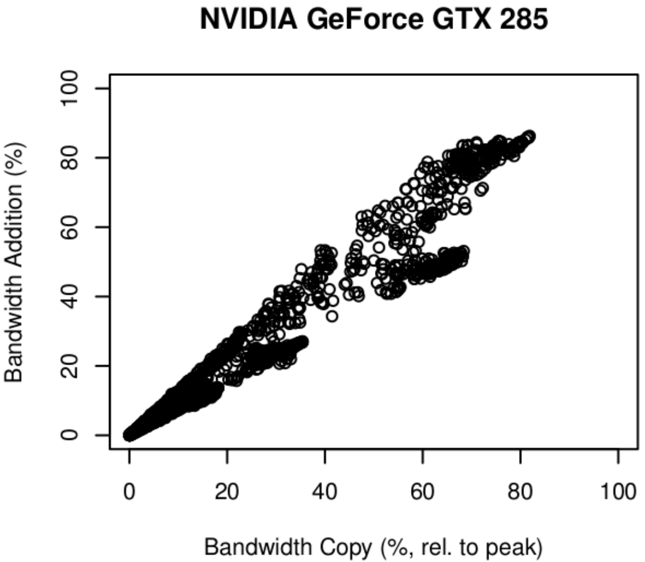
Benchmark


NVIDIA Tesla K20m
0
20
40
60
80
100
Number of Workgroups
2
4
8
16
32
64
128
256
512
1024
5
15
25
35
45
55
65
75
85
95
Bandwidth Copy (% of peak)

[Addition|Inner Product|Matrix-Vector] vs. Copy Kernel

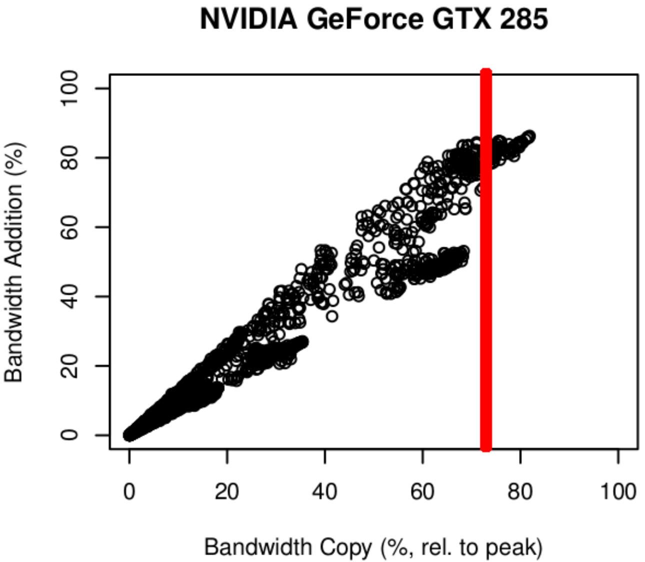
Same Device

Benchmark

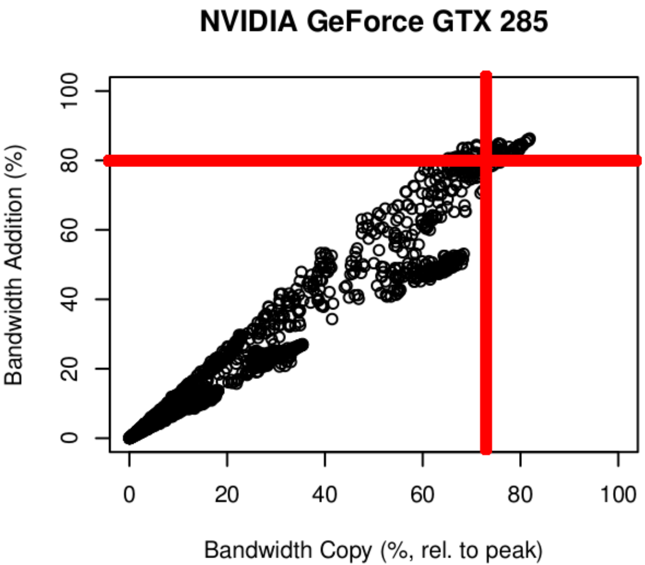


NVIDIA GeForce GTX 285
Bandwidth Addition (%)
0
20
40
60
80
100
Bandwidth Copy (%, rel. to peak)

Benchmark

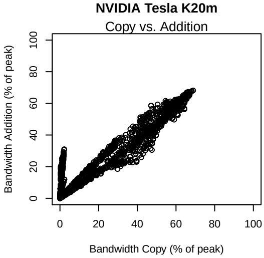

NVIDIA GeForce GTX 285
Bandwidth Addition (%)
0
20
40
60
80
100
Bandwidth Copy (%, rel. to peak)
0
20
40
60
80
100

Benchmark

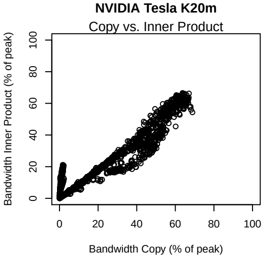

NVIDIA GeForce GTX 285
Bandwidth Addition (%)
0
20
40
60
80
100
0
20
40
60
80
100
Bandwidth Copy (%, rel. to peak)

NVIDIA Tesla K20m

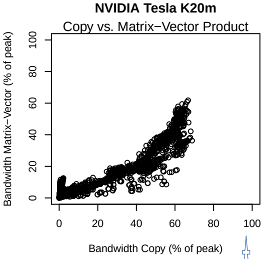
Addition



Inner Product

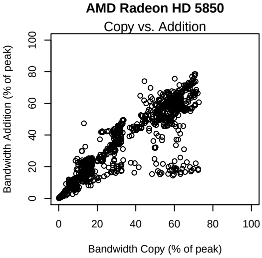


Mat-Vec Product

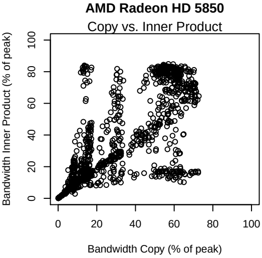


AMD Radeon HD 5850

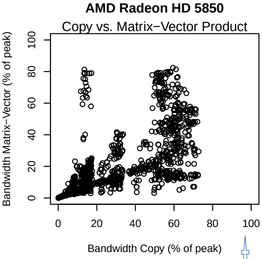
Addition



Inner Product



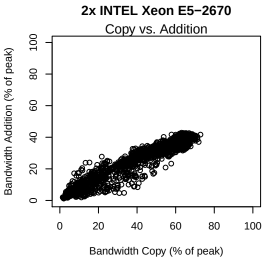
Mat-Vec Product



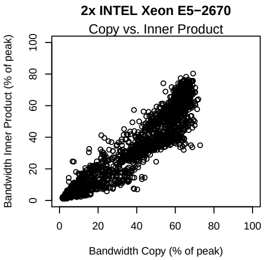
Benchmark

INTEL Dual Xeon E5-2670

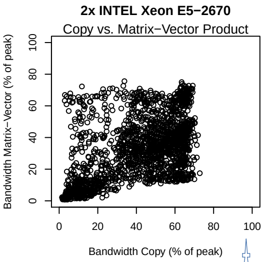
Addition



Inner Product

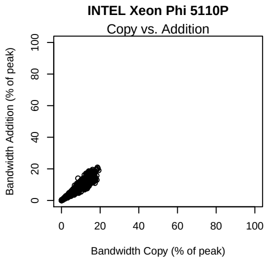


Mat-Vec Product

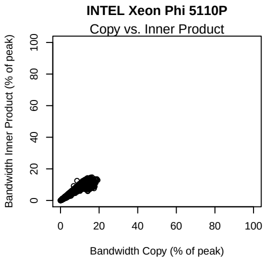


INTEL Xeon Phi

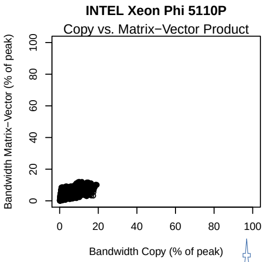
Addition



Inner Product



Mat-Vec Product



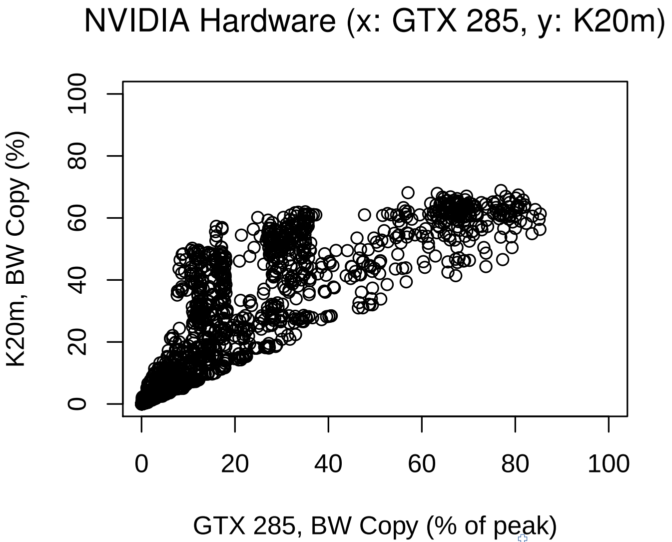
Conclusio:

Focus on fastest configurations for copy-kernel sufficient

[Copy|Addition|Inner Product|Matrix-Vector] vs. Copy Kernel

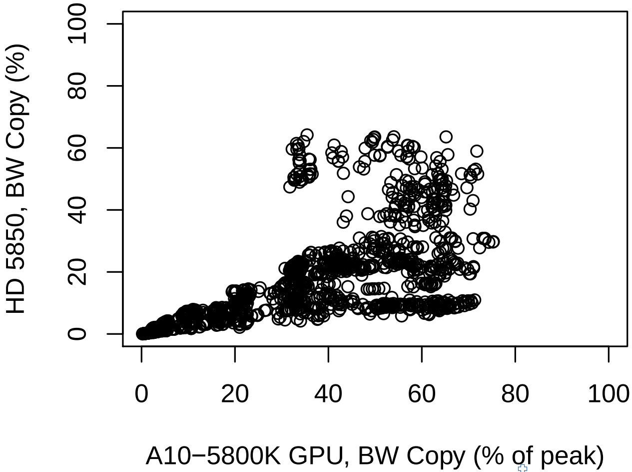
Different Device, Same Vendor

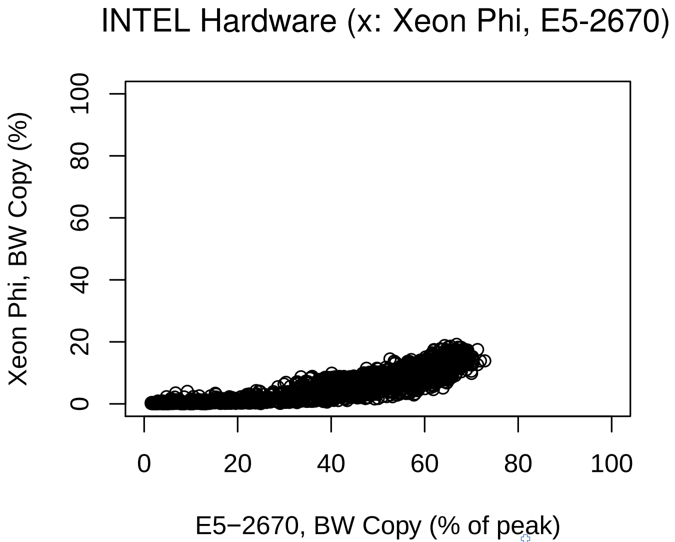
Benchmark



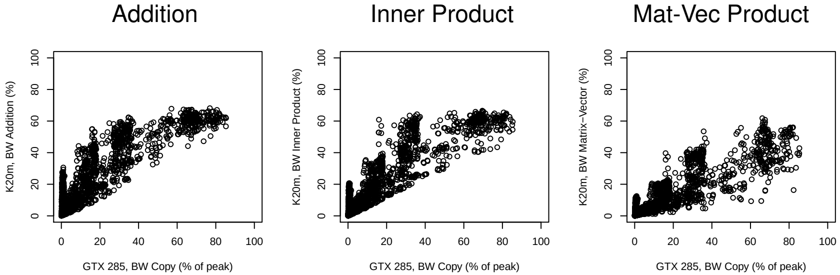
NVIDIA Hardware (x: GTX 285, y: K20m)
K20m, BW Copy (%)
0
20
40
60
80
100
GTX 285, BW Copy (% of peak)

AMD Hardware (x: A10-5800K GPU, y: HD 5850)

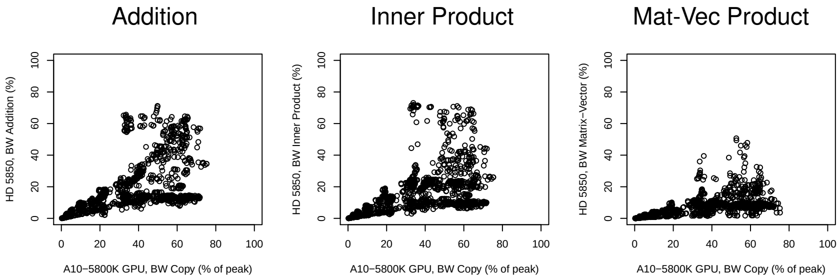



INTEL Hardware (x: Xeon Phi, E5-2670)
Xeon Phi, BW Copy (%)
0
20
40
60
80
100
E5−2670, BW Copy (% of peak)

NVIDIA Hardware (x: GTX 285, y: K20m)



AMD Hardware (x: A10-5800K GPU, y: HD 5850)

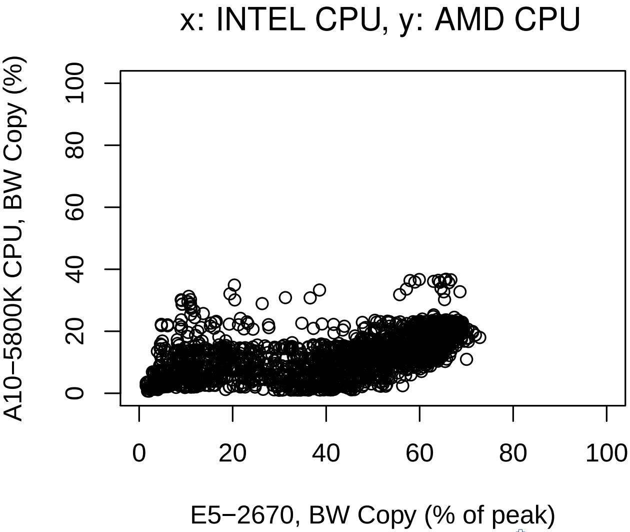


Conclusio:

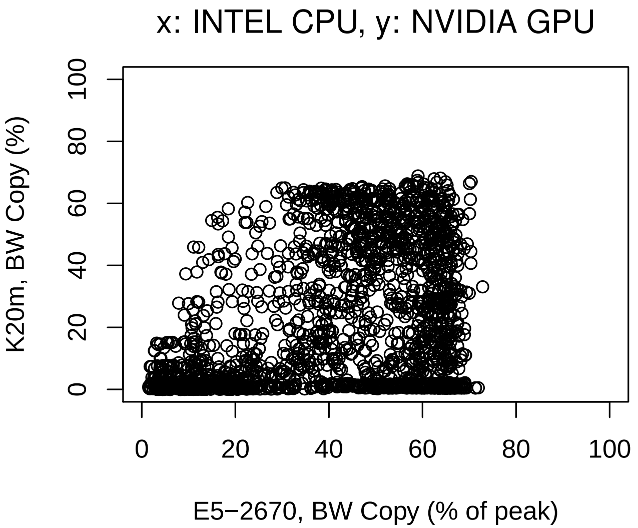
Certain Performance Portability per Vendor

[Copy|Addition|Inner Product|Matrix-Vector] vs. Copy Kernel

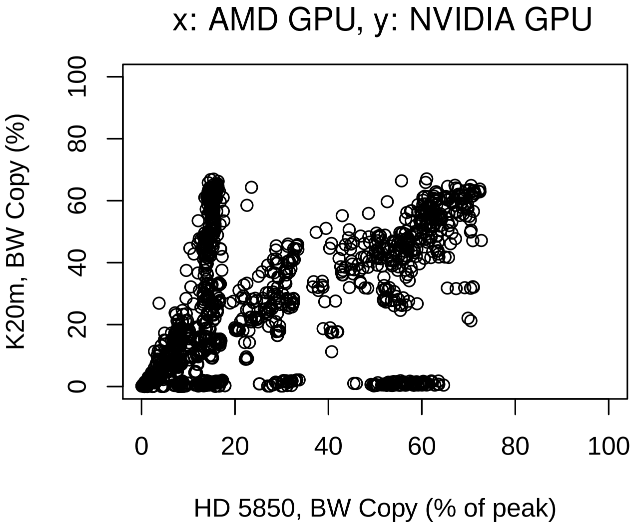
Different Device, Different Vendor


x: INTEL CPU, y: AMD CPU
A10−5800K CPU, BW Copy (%)
0
20
40
60
80
100
E5−2670, BW Copy (% of peak)

Benchmark


x: INTEL CPU, y: NVIDIA GPU
K20m, BW Copy (%)
0
20
40
60
80
100
E5−2670, BW Copy (% of peak)

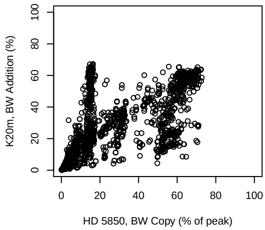
Benchmark


x: AMD GPU, y: NVIDIA GPU
K20m, BW Copy (%)
0
20
40
60
80
100
0
20
40
60
80
100
HD 5850, BW Copy (% of peak)

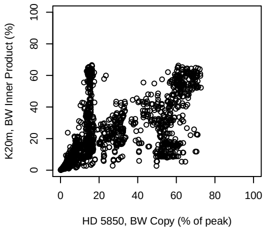
Benchmark

x: AMD HD 5850, y: NVIDIA K20m

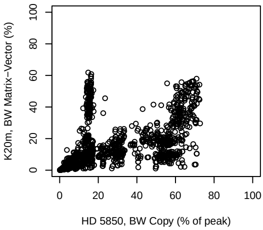
Addition



Inner Product



Mat-Vec Product



Benchmark

Conclusio:

Fast Configurations Across Vendors Exist

Outline

Introduction

Conjugate Gradient - Standard Formulation

Conjugate Gradient - Kernel Parameters

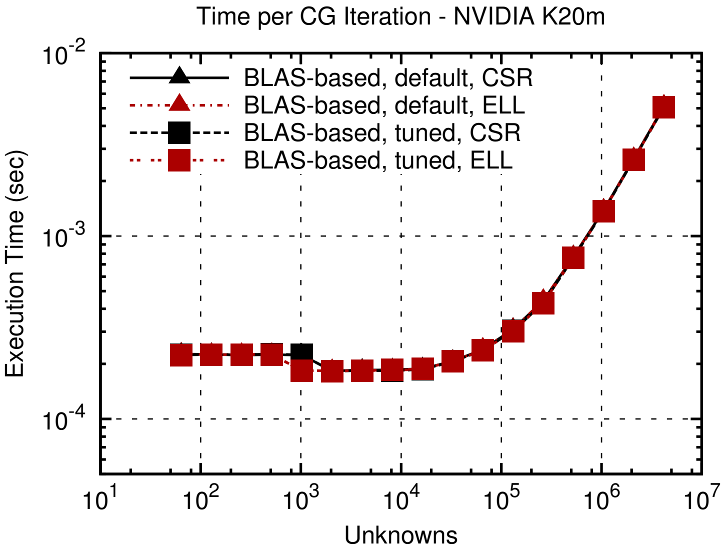
Parameter Study for Portable Performance

Conjugate Gradient - Pipelining

BiCGStab and GMRES - Benchmark Results

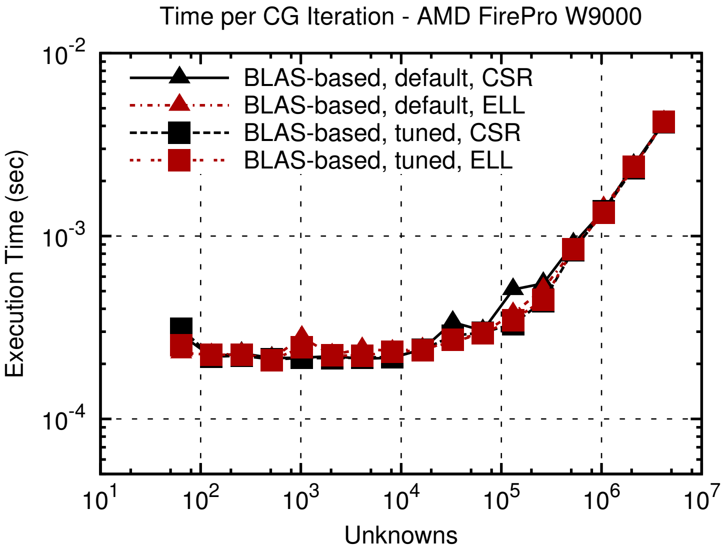
Conclusion

Conjugate Gradients



(2D Finite Difference Discretization)

Conjugate Gradients



(2D Finite Difference Discretization)

Optimization 3: Rearrange the algorithm

- Remove unnecessary reads
- Remove unnecessary synchronizations
- Use custom kernels instead of standard BLAS

Standard CG

Choose x_0
$p_0 = r_0 = b - Ax_0$
For $i = 0$ until convergence

1. Compute and store Ap_i
2. Compute $\langle p_i, Ap_i \rangle$
3. $\alpha_i = \langle r_i, r_i \rangle / \langle p_i, Ap_i \rangle$
4. $x_{i+1} = x_i + \alpha_i p_i$
5. $r_{i+1} = r_i - \alpha_i A p_i$
6. Compute $\langle r_{i+1}, r_{i+1} \rangle$
7. $\beta_i = \langle r_{i+1}, r_{i+1} \rangle / \langle r_i, r_i \rangle$
8. $p_{i+1} = r_{i+1} + \beta_i p_i$

EndFor

Conjugate Gradients

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EndFor

Pipelined CG

Choose x_0
$p_0 = r_0 = b - Ax_0$
For $i = 1$ until convergence

1. $i = 1$: Compute α_0, β_0, Ap_0
2. $x_i = x_{i-1} + \alpha_{i-1} p_{i-1}$
3. $r_i = r_{i-1} - \alpha_{i-1} Ap_i$
4. $p_i = r_i + \beta_{i-1} p_{i-1}$
5. Compute and store Ap_i
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7. $\alpha_i = \langle r_i, r_i \rangle / \langle p_i, Ap_i \rangle$
8. $\beta_i = (\alpha_i^2 \langle Ap_i, Ap_i \rangle - \langle r_i, r_i \rangle) / \langle r_i, r_i \rangle$

EndFor

Conjugate Gradients

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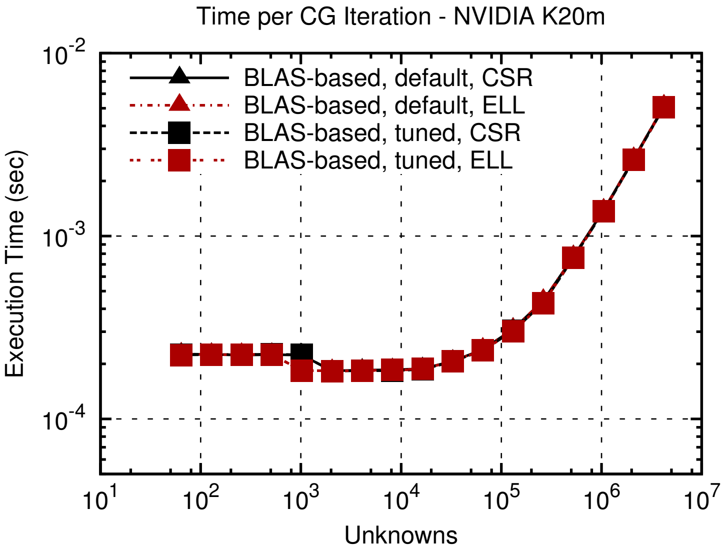
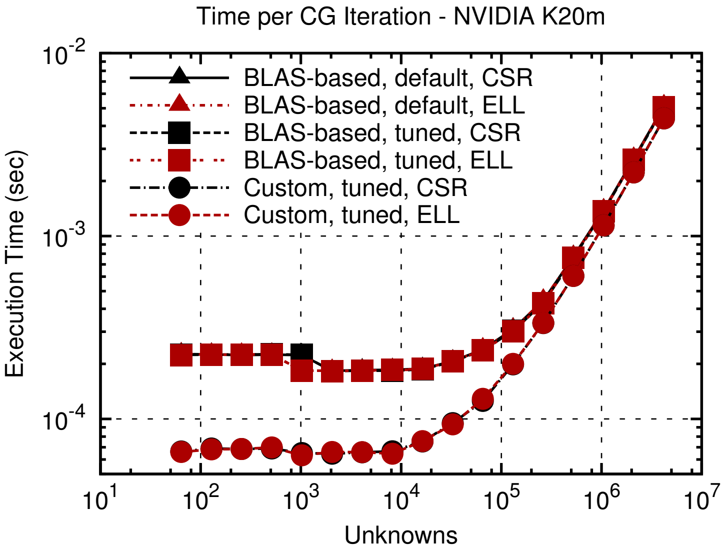
Conjugate Gradients



(2D Finite Difference Discretization)

Conjugate Gradients



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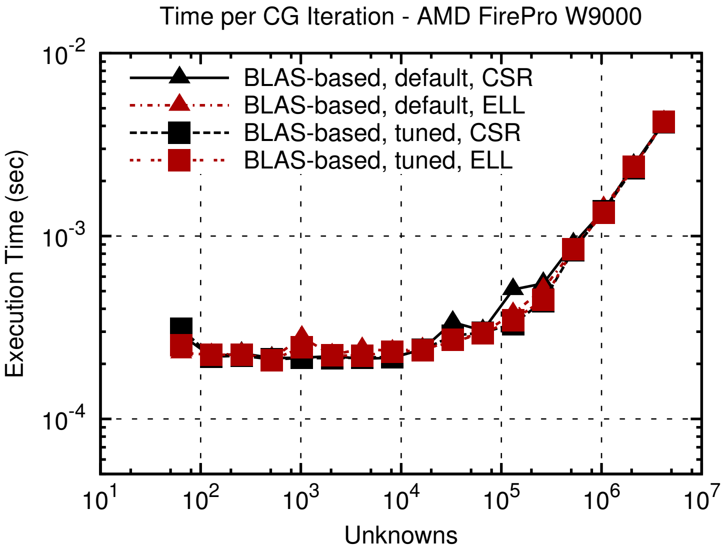

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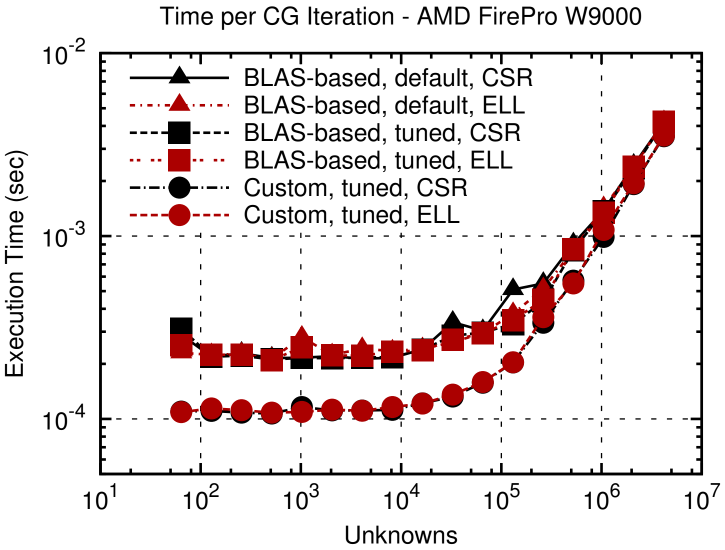

(2D Finite Difference Discretization)

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→ **Parameter Study** for Portable Performance

↓

Conjugate Gradient - Pipelining

↓

BiCGStab and GMRES - Benchmark Results

↓

Conclusion

BiCGStab and GMRES

BiCGStab

- Similar to CG
- Two SpMV per iteration
- Pipelining: 4 kernel launches instead of 12

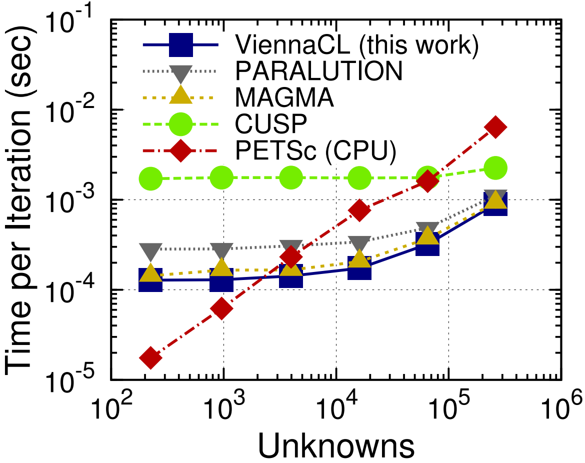
GMRES

- Store Krylov basis
- Orthonormalization in each step
- Pipelining: 3 kernel launches

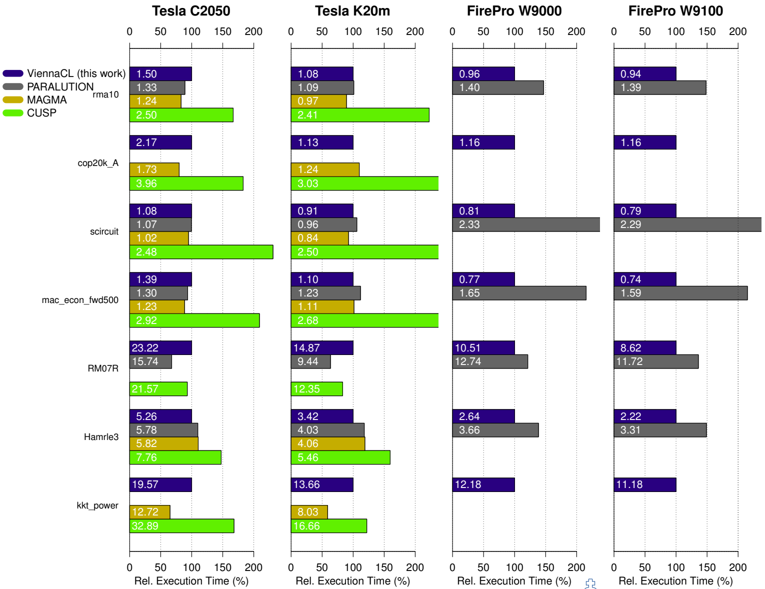
Benchmark Setup

- Poisson equation in 2D
- GPUs from NVIDIA and AMD

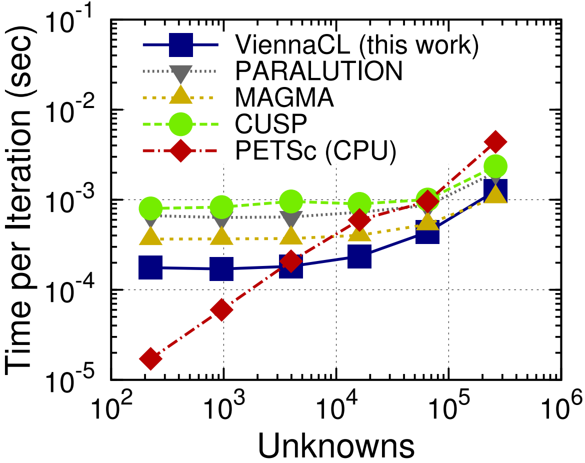
BiCGStab Benchmarks



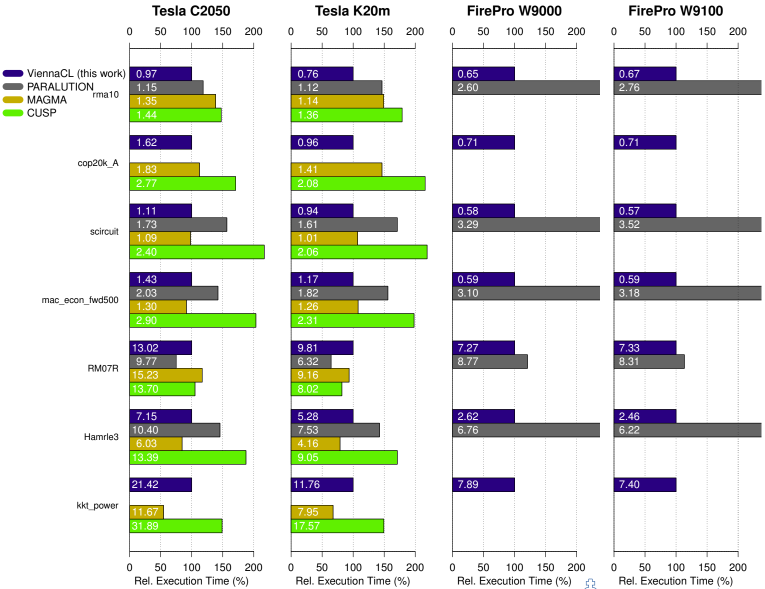
BiCGStab Benchmarks



GMRES Benchmarks



GMRES Benchmarks



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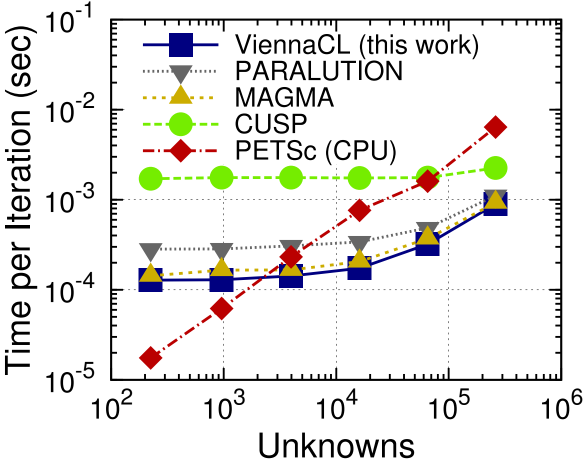

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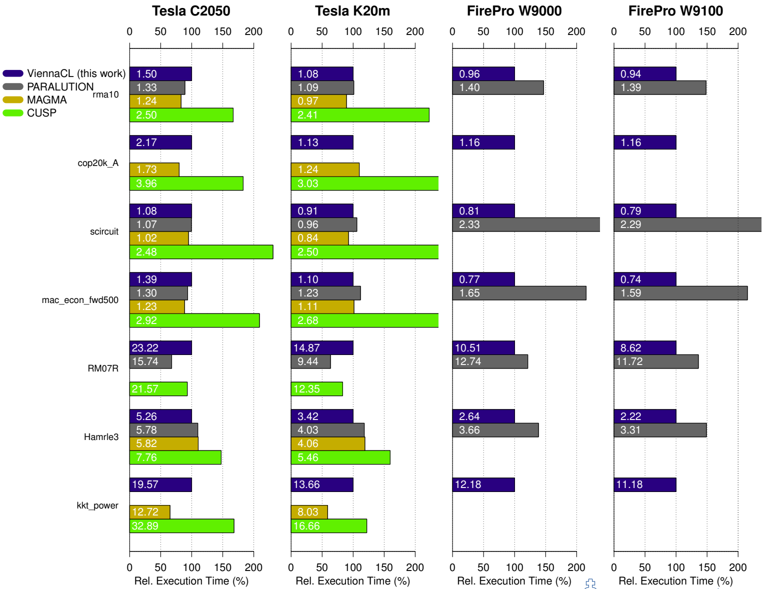

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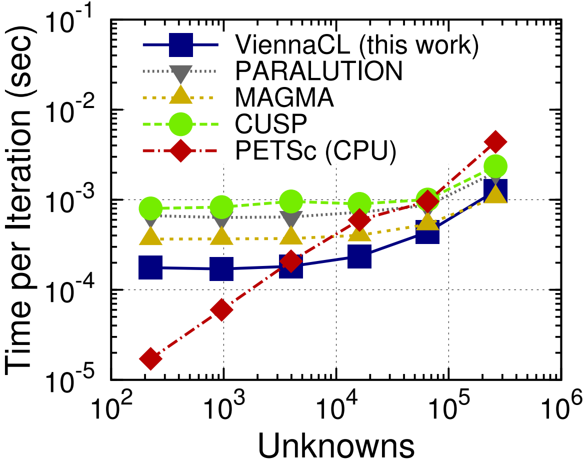
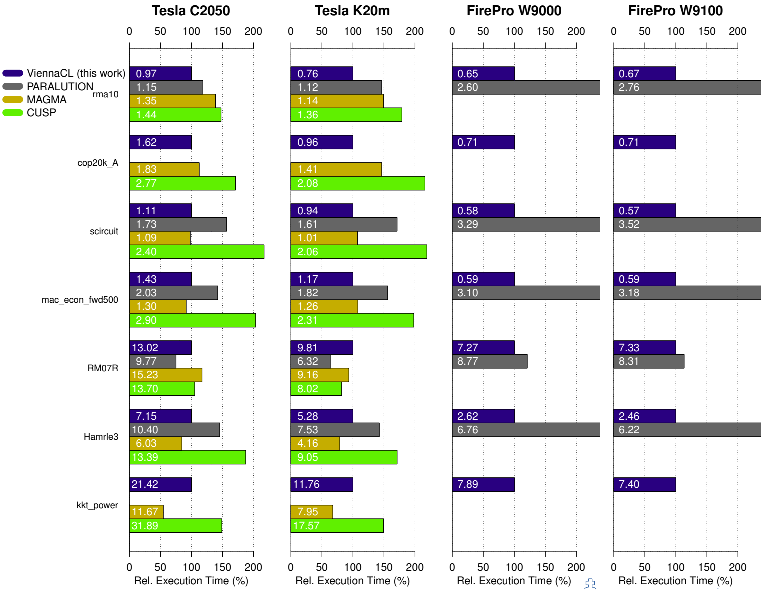


GMRES Benchmarks



Conclusion

Performance-Portable Code for GPUs

- Start with 128 work items
- Refrain from using vector datatypes
- Let each workgroup work on a contiguous piece of memory

Pipelined Iterative Solvers

- Reduced number of kernel launches
- On-chip data reuse
- Faster than BLAS-based implementations

Best Practices for GPU Computing

- FLOPs are (almost always) for free
- Work on large enough data
- Avoid unnecessary PCI-Express communication