

The Vienna Computing Library

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CG Libs - Smart Libraries for Computer Graphics 2013







Talk Overview

Session 1

Introduction to ViennaCL

How-To: ViennaCL Basics

Session 2

How-To: Advanced ViennaCL ViennaCL: Behind the curtain



Introduction to ViennaCL



Introduction to ViennaCL

What to expect

What is ViennaCL

OpenCL

History of ViennaCL

Goals of ViennaCL

Installation of ViennaCL



What Is ViennaCL?

What is it about the Name?

The beautiful city of **Vienna** Open**CL**



History of OpenCL

Prior to 2008

OpenCL developed by Apple Inc.



OpenCL

2008

OpenCL working group formed at Khronos Group OpenCL specification 1.0 released

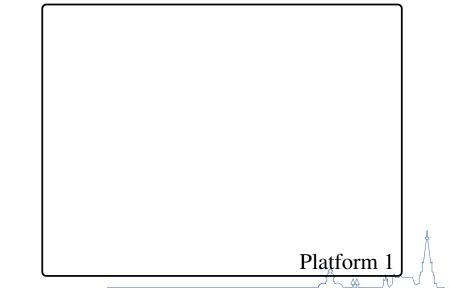
2010

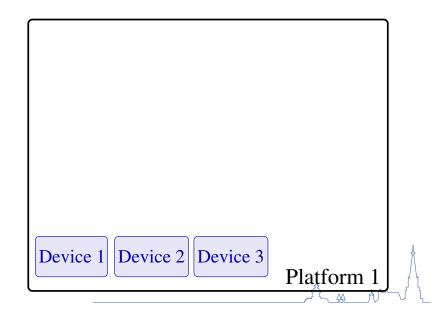
OpenCL 1.1 (multi-device, subbuffer manipulation)

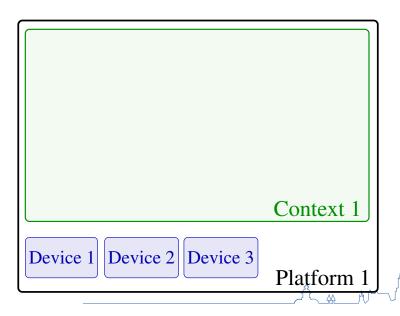
2011

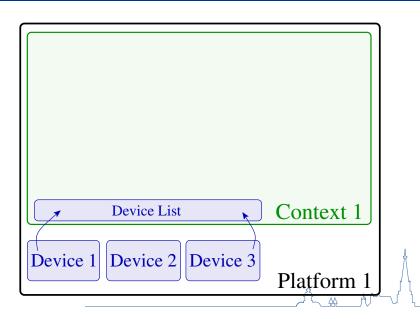
OpenCL 1.2 (device partitioning)

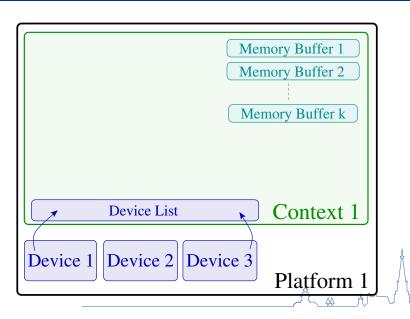


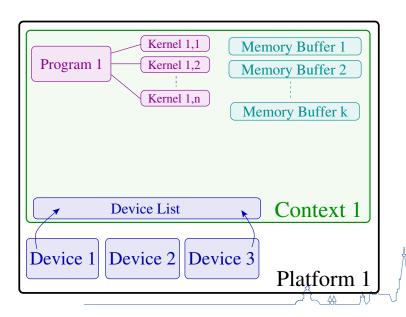


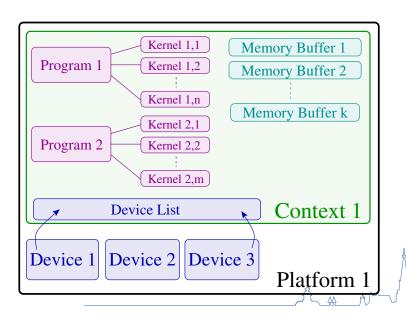


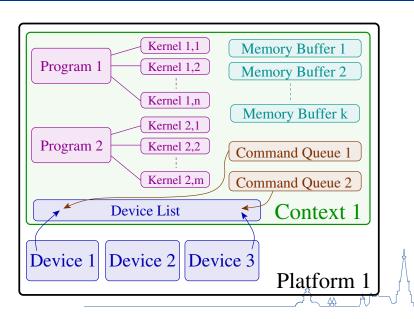












OpenCL Host API

```
context = clCreateContextFromType(NULL, CL DEVICE TYPE GPU, NULL, NULL,
    NULL);
queue = clCreateCommandOueue(context, NULL, 0, NULL);
memobis[0] = clCreateBuffer(context, CL MEM READ WRITE, sizeof(float) *2*
    num entries, NULL, NULL);
memobis[1] = clCreateBuffer(context, CL MEM READ ONLY |
    CL MEM COPY HOST PTR, sizeof(float) *2*num entries, srcA, NULL);
program = clCreateProgramWithSource(context, 1, &kernel src, NULL, NULL);
clBuildProgram(program, 0, NULL, NULL, NULL, NULL);
kernel = clCreateKernel(program, "my kernel", NULL);
clSetKernelArg(kernel, 0, sizeof(cl_mem), (void *) &memobjs[0]);
clSetKernelArg(kernel, 1, sizeof(cl_mem), (void *) &memobjs[1]);
clSetKernelArg(kernel, 2, sizeof(float)*(local work size[0]+1)*16, NULL);
global work size[0] = 128;
local work size[0] = 64;
clEnqueueNDRangeKernel(queue, kernel, 1, NULL, global_work_size,
    local_work_size, 0, NULL, NULL);
```

Issues

"Where is the error?"

Manage OpenCL handles



OpenCL Kernel Language

Sample Operation: Inplace Vector Addition

$$\begin{pmatrix} v_1^1 \\ v_1^2 \\ \vdots \\ v_1^n \end{pmatrix} + = \begin{pmatrix} v_2^1 \\ v_2^2 \\ \vdots \\ v_2^n \end{pmatrix}$$

OpenCL Kernel

2010

April: Roots in the Master's Thesis of Florian Rudolf

May 28th: ViennaCL 1.0.0 released

November: 1000th download December: ViennaCL 1.1.0

(BLAS level 3, refurbished OpenCL backend)



2010

April: Roots in the Master's Thesis of Florian Rudolf

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(BLAS level 3, refurbished OpenCL backend)

2011

March: Accepted for Google Summer of Code

December: ViennaCL 1.2.0

(AMG, SPAI, FFT, QR, graph algorithms, structured matrices)

2012

March: Accepted for Google Summer of Code

May: Tutorial at NVIDIA GTC 2012

May: ViennaCL 1.3.0

(ranges and slices, Automated OpenCL kernels, eigen values, ILU0,

SVD)

December: ViennaCL 1.4.0

(CUDA and host backend, initializer types)



2012

March: Accepted for Google Summer of Code

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May: ViennaCL 1.3.0

(ranges and slices, Automated OpenCL kernels, eigen values, ILU0,

SVD)

December: ViennaCL 1.4.0

(CUDA and host backend, initializer types)

2013

May: Accepted for Google Summer of Code

June: Tutorial at CGLibs



Goals of ViennaCL

About

High-level linear algebra C++ library
OpenMP, OpenCL, and CUDA backends
Header-only

API ViennaCL Core

Backend OpenMP OpenCL CUDA

Hardware CPU MIC GPU

Dissemination

Multi-platform

Free Open-Source MIT (X11) License http://viennacl.sourceforge.net/ 50-100 downloads per week

Design Rules

Reasonable default values

Compatible to Boost.uBLAS whenever possible

In doubt: clean design over performance



Goals of ViennaCL

Core features

Linear algebra, BLAS

Solver (direct and iterative)

Preconditioners

Additional features

Fast Fourier Transform

Eigenvalue computations

QR factorization

Bandwidth reduction

Nonnegative matrix factorization

_^________________

Goals of ViennaCL

Interfaces to other libraries

Boost.uBLAS

Eigen

MTL4

Backends

CPU

OpenCL

CUDA

C++ library

Generic free functions

Expression templates



Installation of ViennaCL

Three Steps

Download from http://viennacl.sourceforge.net/

Unzip

Copy source folder

Dynamic Library?

ViennaCL is header-only

Linking depends on used backend (OpenMP, OpenCL, CUDA)

Sample Applications

22 tutorials

7 benchmarks

about 35 tests



How-To: ViennaCL Basics



How-To: ViennaCL Basics

What to expect

From BLAS to Boost.uBLAS to ViennaCL

Basic Types

OpenCL Kernels

Basic Usage: Data Management

Basic Usage: Algebra Basic Usage: Solver

Summary



BLAS

Basic Linear Algebra Subprograms

De facto API standard

Low level interface

Boost.uBLAS

C++ API for BLAS

High level interface

Part of Boost libraries



Consider Existing CPU Code (Boost.uBLAS)

```
using namespace boost::numeric::ublas;
matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);
/* Fill A, x, rhs here */
rhs += 2.0 * x;
double val = inner_prod(x, rhs);
matrix += val * outer_prod(x, rhs);
x = solve(A, rhs, upper_tag()); // Upper triangular solver
std::cout << " 2-norm: " << norm_2(x) << std::endl;
std::cout << "sup-norm: " << norm_inf(x) << std::endl;</pre>
```

High-Level Code with Syntactic Sugar

Porting the previous code to GPU

"How much time will you need?"

1 minute?

1 hour?

1 day?

Quality Criteria

Working hours spent

Performance

Correctness

High-level description (Maintainability)

Consider Existing CPU Code (Boost.uBLAS)

```
using namespace boost::numeric::ublas;
matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);
/* Fill A, x, rhs here */
rhs += 2.0 * x:
double val = inner_prod(x, rhs);
matrix += val * outer_prod(x, rhs);
x = solve(A, rhs, upper_tag()); // Upper triangular solver
std::cout << " 2-norm: " << norm_2(x) << std::endl;
std::cout << "sup-norm: " << norm_inf(x) << std::endl;</pre>
```

Previous Code Snippet Rewritten with ViennaCL

```
using namespace viennacl;
using namespace viennacl::linalg;
matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);
/* Fill A, x, rhs here */
rhs += 2.0 * x;
double val = inner_prod(x, rhs);
matrix += val * outer_prod(x, rhs);
x = solve(A, rhs, upper_tag()); // Upper triangular solver
std::cout << " 2-norm: " << norm_2(x) << std::endl;
std::cout << "sup-norm: " << norm_inf(x) << std::endl;</pre>
```

ViennaCL in addition provides iterative solvers

```
using namespace viennacl;
using namespace viennacl::linalg;

compressed_matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);

/* Fill A, x, rhs here */

x = solve(A, rhs, cg_tag()); // Conjugate Gradient solver
x = solve(A, rhs, bicgstab_tag()); // BiCGStab solver
x = solve(A, rhs, gmres_tag()); // GMRES solver
```

No iterative solvers available in uBLAS...



Thanks to interface compatibility

```
using namespace boost::numeric::ublas;
using namespace viennacl::linalg;

compressed_matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);

/* Fill A, x, rhs here */

x = solve(A, rhs, cg_tag()); // Conjugate Gradient solver
x = solve(A, rhs, bicgstab_tag()); // BiCGStab solver
x = solve(A, rhs, gmres_tag()); // GMRES solver
```

OpenCL kernels

OpenCL kernels are needed for actual computation

Provided by ViennaCL Support for expression templates

Automatic kernel generation

Each of the following commands launches a separate OpenCL kernel

```
v1 = v2;
v1 += v2;
v1 -= v2;
v1 = alpha * v2;
v1 += alpha * v2;
v1 -= alpha * v2;
v1 *= alpha;
v1 /= alpha;
```

OpenCL kernels

OpenCL kernels have to be compiled at run time

OpenCL JIT compiler
Kernels can be grouped in programs

Compilation strategies

Each kernel individually: several milliseconds per kernel

All at once: Takes seconds

In groups: Compile groups of kernels whenever potentially needed



OpenCL kernels

Consider the following code

```
int main() {
  vector<double> x(100), y(100);
  matrix<double> A(100, 100), B(100, 100);
  matrix<double, column_major> C(100, 100);

  x += 3.1415 * y;
  C = prod(trans(A), B);
  y = prod(C, x);

  std::cout << y << std::endl;
}</pre>
```

OpenCL Kernels

Which kernels are compiled?

When are they compiled?

Hint: Program compiles and executes normally

OpenCL kernels

Consider the following code

```
int main() {
   vector<double> x(100), y(100);
   matrix<double> A(100, 100), B(100, 100);
   matrix<double, column_major> C(100, 100);

   x += 3.1415 * y;
   C = prod(trans(A), B);
   y = prod(C, x);

   std::cout << y << std::endl;
}</pre>
```

OpenCL Kernels

```
Which kernels are compiled? When are they compiled?
```

Hint: Program compiles and executes normally



OpenCL kernels

Consider the following code

```
int main() {
  vector<double> x(100), y(100);
  matrix<double> A(100, 100), B(100, 100);
  matrix<double, column_major> C(100, 100);

  x += 3.1415 * y;
  C = prod(trans(A), B);
  y = prod(C, x);

  std::cout << y << std::endl;
}</pre>
```

OpenCL Kernels

```
Which kernels are compiled?
```

When are they compiled?

Hint: Program compiles and executes normally

OpenCL kernel management

Special case: Matrix-Matrix product

Result matrix: Row/Column major memory layout First factor: Row/Column major, possibly transposed Second factor: Row/Column major, possibly transposed

Leads to 32 different kernels for matrix-matrix multiplication

Compiled separately on request



Supported types

Scalar

Vector

Dense matrix

Sparse matrix

Structured matrix

Numeric Types

float

double



Scalars

Represents a single scalar value on the computing device Behave like underlying type Implicit cast to underlying type Potentially expensive (Overhead!)

```
viennacl::scalar<NumericType> gpu_scalar;
viennacl::scalar<float> gpu_float;
viennacl::scalar<double> gpu_double;
```



Scalars

```
float cpu_float = 42.0f;
double cpu double = 13.7603;
viennacl::scalar<float> qpu_float(3.1415f);
viennacl::scalar<double> gpu_double = 2.71828;
// conversions and t
cpu_float = gpu_float;
// automatic transfer and conversion
gpu_float = cpu_double;
cpu_float = qpu_float * 2.0f;
cpu_double = gpu_float - cpu_float;
```

Vectors

Represents a vector on the computing device Operator overloading Alignment support

```
viennacl::vector<NumericType> gpu_vector;
viennacl::vector<float> gpu_float_vector;
viennacl::vector<double> gpu_double_vector;
```



Vectors

```
std::vector<ScalarType> stl_vec(10);
viennacl::vector<ScalarType> vcl_vec(10);
//fill the STL vector:
for (unsigned int i=0; i<vector_size; ++i)</pre>
  stl vec[i] = i;
//copy content to GPU vector (recommended initialization)
copy(stl_vec.begin(), stl_vec.end(), vcl_vec.begin());
//manipulate GPU vector here
vcl_vec *= 4.2;
//copy content from GPU vector back to STL vector
copy(vcl_vec.begin(), vcl_vec.end(), stl_vec.begin());
```

Vectors

```
std::vector<ScalarType> stl_vec(10);
viennacl::vector<ScalarType> vcl_vec(10);
//fill the STL vector:
for (unsigned int i=0; i<vector_size; ++i)</pre>
  stl vec[i] = i;
//copy content to GPU vector (recommended initialization)
copy(stl_vec, vcl_vec);
//manipulate GPU vector here
vcl_vec *= 4.2;
//copy content from GPU vector back to STL vector
copy(vcl_vec, stl_vec);
```

Alignment

Default = 1 Template parameter

In ViennaCL 1.5.0 deprecated (will be runtime parameter)

```
viennacl::vector<NumericType, Alignment>
    gpu_vector_with_alignment;

viennacl::vector<float, 4>
    gpu_float_vector_with_alignment;

viennacl::vector<double, 8>
    gpu_double_vector_with_alignment;
```



Vector initializer

```
	ext{unit\_vector} \Rightarrow \mathbf{u}_{N,i} = \left\{ egin{array}{ll} 1 & 	ext{if } i = N; \\ 0 & 	ext{else} \end{array} 
ight. 	ext{zero\_vector} \Rightarrow \mathbf{z}_i = 0 	ext{scalar\_vector} \Rightarrow \mathbf{s}_i = s
```

```
viennacl::unit_vector<NumericType>(size, index);
viennacl::zero_vector<NumericType>(size);
viennacl::scalar_vector<NumericType>(size, scalar);
```



Vector initializer

```
viennacl::vector<ScalarType> vcl_vec =
    viennacl::unit_vector<ScalarType>(10, 5);
// Creates the vector (0, 0, 0, 0, 1, 0, 0, 0, 0, 0)

viennacl::vector<ScalarType> vcl_vec =
    viennacl::zero_vector<ScalarType>(10);
// Creates the vector (0, 0, 0, 0, 0, 0, 0, 0, 0)

viennacl::vector<ScalarType> vcl_vec =
    viennacl::scalar_vector<ScalarType>(6, 1.5);
// Creates the vector (1.5, 1.5, 1.5, 1.5, 1.5, 1.5)
```



Dense matrix

Represents a dense matrix on the computing device

Dense matrix ⇒ zero elements are rare

Alignment support (same as vectors)

Row major or column major

```
viennacl::matrix<NumericType> gpu_matrix;
viennacl::matrix<NumericType, Scheme, Alignment>
    gpu_matrix_with_scheme_and_alignment;

viennacl::matrix<float> gpu_float_matrix;
viennacl::matrix<float, row_major, 4>
    row_major_gpu_float_matrix_with_alignment;

viennacl::matrix<double> gpu_double_matrix;
viennacl::matrix<double, column_major, 8>
    column_major_gpu_double_matrix_with_alignment;
```

Dense matrix

```
//set up a 3 by 5 matrix:
viennacl::matrix<float> vcl_matrix(4, 5);
//fill it up:
vcl_matrix(0,2) = 1.0
vcl_matrix(1,2) = -1.5;
vcl_matrix(2,0) = 4.2;
vcl_matrix(3,4) = 3.1415;
```



Matrix initializer

```
identity_matrix \Rightarrow \mathbf{I}_{i,j} = \begin{cases} d & \text{if } i = j; \\ 0 & \text{else} \end{cases}
\mathsf{zero\_matrix} \Rightarrow \mathbf{Z}_{i,j} = 0
\mathsf{scalar\_matrix} \Rightarrow \mathbf{S}_{i,i} = s
```



Matrix initializer

```
viennacl::matrix<ScalarType> vcl_mat =
   viennacl::identity_matrix<ScalarType>(4, 1);
```

Creates the following matrix: $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$



Matrix initializer

```
viennacl::matrix<ScalarType> vcl_mat =
   viennacl::zero_matrix<ScalarType>(3, 5);
```



Matrix initializer

```
viennacl::matrix<ScalarType> vcl_mat =
   viennacl::scalar_matrix<ScalarType>(4, 3, 4.2);
```

Creates the following matrix: $\begin{pmatrix} 4.2 & 4.2 & 4.2 \\ 4.2 & 4.2 & 4.2 \\ 4.2 & 4.2 & 4.2 \\ 4.2 & 4.2 & 4.2 \end{pmatrix}$



Sparse matrix

Represents a sparse matrix on the computing device

Sparse matrix ⇒ zero elements are frequent

Alignment support (same as vectors and dense matrices)

Sparse matrix types

Coordinate matrix

Compressed matrix

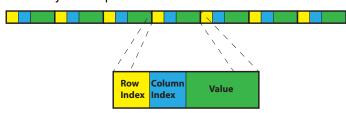
ELL matrix

Hybrid matrix





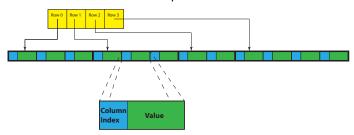
Easy to setup/extend



Compressed matrix

Less memory required

Fast matrix-vector multiplication



ELL matrix

Similar to compressed matrix Fixed number of non-zero values per row No row jumper array required

Hybrid matrix

Combination of compressed matrix and ELL matrix



Compressed matrix

```
//set up a sparse 4 by 5 matrix on the CPU:
std::vector< std::map< unsigned int, float> >
    cpu_sparse_matrix(4);
//fill it up:
cpu\_sparse\_matrix[0][2] = 1.0;
cpu_sparse_matrix[1][2] = -1.5;
cpu\_sparse\_matrix[3][0] = 4.2;
//set up a sparse ViennaCL matrix:
viennacl::compressed_matrix<float> sparse_matrix(4, 5);
//copy to OpenCL device:
copy(cpu_sparse_matrix, sparse_matrix);
//copy back to CPU:
copy(sparse_matrix, cpu_sparse_matrix);
```

Structured matrix

Dense matrices but with special structure

Access to one element might change other elements

Supported types

Circulant matrix

Hankel matrix

Toeplitz matrix



Structured matrix

Circulant matrix

Hankel matrix

Toeplitz matrix

$$\begin{pmatrix} c_0 & c_{n-1} & \dots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & & c_2 \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \dots & c_1 & c_0 \end{pmatrix}$$

Structured matrix

Circulant matrix

Hankel matrix

Toeplitz matrix

$$\left(\begin{array}{cccc}
a & b & c & d \\
b & c & d & e \\
c & d & e & f \\
d & e & f & g
\right)$$



Structured matrix

Circulant matrix

Hankel matrix

Toeplitz matrix

$$\left(\begin{array}{ccccc}
 a & b & c & d \\
 e & a & b & c \\
 f & e & a & b \\
 g & f & e & a
\end{array}\right)$$



Structured matrix

Circulant matrix

Hankel matrix

Toeplitz matrix

$$\begin{pmatrix} 1 & \alpha_1 & \alpha_1^2 & \dots & \alpha_1^{n-1} \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^{n-1} \\ 1 & \vdots & \vdots & \vdots \\ 1 & \alpha_m & \alpha_m^2 & \dots & \alpha_m^{n-1} \end{pmatrix}$$



How to access/transfer ViennaCL vectors/matrices elements?

Direct element access

```
vector<ScalarType> vcl(10);

for (int i = 0; i < 10; ++i)
    vcl(i) = i;

for (int i = 0; i < 10; ++i)
    std::cout << vcl(i) << std::endl;</pre>
```



How to access/transfer ViennaCL vectors/matrices elements?

Direct element access Iterator

```
vector<ScalarType> vcl(10);

ScalarType tmp = 0;
for (vector<ScalarType>::iterator it = vcl.begin();
   it != vcl.end(); ++it, tmp += 42.0)
   *it = tmp;

for (vector<ScalarType>::iterator it = vcl.begin();
   it != vcl.end(); ++it)
   std::cout << *it < std::endl;</pre>
```

How to access/transfer ViennaCL vectors/matrices elements?

Direct element access Iterator Copy functions

```
std::vector<ScalarType> cpu(10);
viennacl::vector<ScalarType> vcl(10);

for (int i = 0; i < 10; ++i)
    cpu[i] = i;

viennacl::copy( cpu.begin(), cpu.end(), vcl.begin() );
viennacl::copy( vcl.begin(), vcl.end(), cpu.begin() );</pre>
```

How to access/transfer ViennaCL vectors/matrices elements?

Direct element access Iterator Copy functions

```
std::vector<ScalarType> cpu(10);
viennacl::vector<ScalarType> vcl(10);

for (int i = 0; i < 10; ++i)
    cpu[i] = i;

viennacl::copy( cpu, vcl );
viennacl::copy( vcl, cpu );</pre>
```

Granularity of Operations

Filling a vector with data

```
viennacl::vector<double> v(10000);
for (size_t i=0; i<v.size(); ++i)
  v(i) = i;</pre>
```



Granularity of Operations

Filling a vector with data

```
viennacl::vector<double> v(10000);

for (size_t i=0; i<v.size(); ++i)
   v(i) = i;</pre>
```

GPU Computing Is Fast, Right?

Execution time: 1 sec (approx)

```
std::vector: < 1 ms
```

Granularity of Operations

Transfer is done for each element separately High overhead, similar to scalar operations

How to avoid the pitfall

Use temporary vector Use copy functions

```
viennacl::vector<double> v(10000);
std::vector<double> cpu_v( v.size() );

for (size_t i=0; i<cpu_v.size(); ++i)
   cpu_v(i) = i;

viennacl::copy(cpu_v, v);</pre>
```

How to access/transfer ViennaCL vectors/matrices elements?

Direct element access ⇒ Bad idea!

Iterator \Rightarrow Bad idea!

Copy functions ⇒ Good idea!

```
std::vector<ScalarType> cpu_vec(10);
viennacl::vector<ScalarType> vcl_vec(10);

for (int i = 0; i < 10; ++i)
    cpu_vec[i] = i;

viennacl::copy( cpu_vec, vcl_vec );
viennacl::copy( vcl_vec, cpu_vec );</pre>
```

Basic Usage: Data Management

Fast copy

copy does not require linear arrays ⇒ temporary required

```
std::list<ScalarType> cpu_vec(10);
viennacl::vector<ScalarType> vcl_vec(10);

for (int i = 0; i < 10; ++i)
    cpu_vec[i] = i;

viennacl::copy( cpu_vec, vcl_vec );

viennacl::copy( vcl_vec, cpu_vec );</pre>
```

Basic Usage: Data Management

Fast copy

copy does not require linear arrays \Rightarrow temporary required If container is linear memory \Rightarrow use fast_copy instead

Algebra operations

Trivial operations done by **operator overloading**Scalar multiplication support for vector and matrices
Inner product and norm support for vectors
Matrix transpose using function **trans**Matrix-vector and matrix-matrix multiplication using function **prod**



Scalar operations

```
NumericType s1, s2;
viennacl::scalar<NumericType> vcl_s1, vcl_s2, vcl_s3;
vcl_s1 = 5;
vcl_s2 = vcl_s1 * 3;
vcl_s3 -= vcl_s1 + (vcl_s2 / 4);
s1 = vcl_s3;
s2 = vcl_s1 - vcl_s2 * 2;
```



Vector operations

```
viennacl::scalar<NumericType> vcl_s1, vcl_s2;
viennacl::vector<NumericType> v1(10), v2(10), v3(10);
v2 = vcl_s1 * v1 + v2
v3 += vcl_s1 * v2;
v3 = 0.5 * v2 - v3;
```



Vector operations

```
NumericType s1, s2;
viennacl::scalar<NumericType> vcl_s1, vcl_s2;
viennacl::vector<NumericType> v10), v2(10), v3(10);

vcl_s1 = viennacl::linalg::inner_prod(v1, v2);
s1 = viennacl::linalg::inner_prod(v1, v2);

s1 = viennacl::linalg::norm_1(v1);
vcl_s2 = viennacl::linalg::norm_2(v2);
s2 = viennacl::linalg::norm_inf(v3);
```



Matrix operations

```
viennacl::scalar<NumericType> vcl_s1, vcl_s2;
viennacl::matrix<NumericType> M1(10, 10),
    M2(10, 10), M3(10,10);
M2 = vcl s1 * M1 + M2
M3 += vcl_s2 * M2;
M3 = 0.5 * M2 - M3;
M3 = viennacl::trans(M2); // Transposed matrix
// Matrix-matrix product
M1 = viennacl::linalg::prod( M2, M3 );
M1 = viennacl::linalq::prod( M2, viennacl::trans(M3) );
```

GEMM: ViennaCL vs. CUBLAS

```
// ViennaCL
M1 = vcl_s1 * prod(M2, trans(M3)) + vcl_s2 * M3;
// CUBLAS
cublasStatus_t cublasDgemm(handle,
    transa, transb,
    m, n, k,
    alpha,
    A, lda,
   B, ldb,
   beta,
   C, 1dc);
```



Matrix-vector operations

```
viennacl::vector<NumericType> v1(10), v210), v3(20);
viennacl::matrix<NumericType> M1(10, 10), M2(20, 10);

v1 = viennacl::linalg::prod( M1, v2 );
v1 = viennacl::linalg::prod( viennagrid::trans(M1), v2 );
v3 = viennacl::linalg::prod( M2, v2 );
v1 = viennacl::linalg::prod( M1, v3 );
// ERROR! dimension missmatch
```



Solving a system of linear equations

Ax = b

A and b given, x is unknown

Common problem in mathematics

Types of solver

Direct solver

Iterative solver



Direct solver

Solving the system directly e.g. Gaussian elimination with pivoting

Iterative solver

Solving using an iterative process

Convergence relies on matrix properties

Recommended for large and sparse systems

No write operation needed on matrix

(most only use matrix-vector multiplication)



Direct solver

LU factorization

No pivoting (work in progress)

```
using namespace viennacl::linalg;
viennacl::matrix<float> vcl_matrix;
viennacl::vector<float> vcl rhs, vcl result;
/* Set up matrix and vectors here */
//solution of an upper triangular system:
vcl_result = solve(vcl_matrix, vcl_rhs, upper_tag());
//solution of a lower triangular system:
vcl_result = solve(vcl_matrix, vcl_rhs, lower_tag());
//solution of a full system right into the vector vcl_rhs:
lu_factorize(vcl_matrix);
lu_substitute(vcl_matrix, vcl_rhs);
```

Iterative solver

Conjugate Gradient (CG)

Stabilized Bi-CG (BiCGStab)

Generalized Minimum Residual (GMRES)

Method	Matrix class	ViennaCL
Conjugate Gradient (CG)	symmetric positive definite	y = solve(A, x, cg_tag());
Stabilized Bi-CG (BiCGStab)	non- symmetric	y = solve(A, x, bicgstab_tag());
Generalized Minimum Residual (GMRES)	general	y = solve(A, x, gmres_tag());



Iterative solver

Solver configuration via tag

```
using namespace viennacl::linalg;

// conjugate gradient solver with tolerance 1e10
// and at most 100 iterations:
viennacl::linalg::cg_tag custom_cg(1e-10, 100);

vcl_result = solve(vcl_matrix, vcl_rhs, custom_cg);

//print number of iterations taken and estimated error:
cout << "No. of iters: " << custom_cg.iters() << endl;
cout << "Est. error: " << custom_cg.error() << endl;</pre>
```

Summary

What have we learned?

ViennaCL provides interface compatibility with Boost.uBLAS

Basic types of ViennaCL

How OpenCL kernels are used

How to transfer data to and from ViennaCL

How to work with ViennaCL types

Simple algebraic operations

Solver for systems of linear equations



How-To: Advanced ViennaCL



How-To: Advanced ViennaCL

What to expect

Subvectors and Submatrices

Escaping the Curse of Temporaries

Interface: Eigen

Performance

Summary



Important for Many Algorithms

LU, Cholesky QR, SVD

Two sub-types available

Range [a,b)

Slice a:inc:size

Ranges and slices are proxies

Read- and writeable



Range example

```
std::size_t lower_bound = 1;
std::size_t upper_bound = 7;
viennacl::range r(lower_bound, upper_bound);

typedef viennacl::vector<ScalarType> VectorType;
typedef viennacl::matrix<ScalarType> MatrixType;

// v[1:6]
viennacl::vector_range<VCLVectorType> v_sub(v, r);
// M[1:6,1:6]
viennacl::matrix_range<VCLMatrixType> M_sub(M, r, r);
```



Slice example

```
std::size_t start = 2;
std::size t stride = 3;
std::size_t size = 5
viennacl::slice s(start, stride, size);
typedef viennacl::vector<ScalarType> VectorType;
typedef viennacl::matrix<ScalarType> MatrixType;
// v[2, 5, 8, 11, 14]
viennacl::vector_slice<VCLVectorType> v_sub(v, r);
//M[2,2], \ldots, M[2,14], \ldots, M[14,2], \ldots, M[14,14]
viennacl::matrix_slice<VCLMatrixType> M_sub(M, r, r);
```

Convenience Functions

```
viennacl::vector<ScalarType> v1(4), v2(2);
viennacl::matrix<ScalarType> M1(4,4), M2(2,2);

range r(0, 2);
slice s(0, 2, 2);

v2 = project(v1, r);
project(v1, s) = v2;

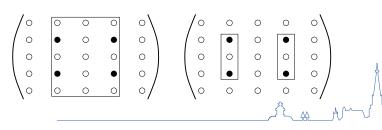
M2 = project(M1, r, r);
viennacl::copy(M2, project(M1, s, s));
```



Copy Headaches: Row-Major

$$\begin{pmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \bullet & \circ & \bullet & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \bullet & \circ & \bullet & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \end{pmatrix} \qquad \begin{pmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \bullet & \circ & \bullet & \circ \\ \circ & \bullet & \circ & \bullet & \circ \\ \circ & \bullet & \circ & \bullet & \circ \\ \circ & \bullet & \circ & \bullet & \circ \\ \bullet & \circ & \bullet & \circ & \circ \\ \end{pmatrix}$$

Copy Headaches: Column-Major



Simple BLAS Level 1 Operation

Consider

```
vec1 = vec2 + alpha * vec3 - beta * vec4;
```

With naive C++, this is equivalent to

```
tmp1 <- alpha * vec3
tmp2 <- beta * vec4;
tmp3 <- tmp1 - tmp2;
tmp4 <- vec2 + tmp3;
vec1 <- tmp4;</pre>
```

Temporaries Lead to Poor Performance

Costly on CPUs, extremely expensive on GPUs
Use expression templates for avoiding temporaries

Vector Addition

$$x = y + z;$$

Naive Operator Overloading

```
vector<T> operator+(vector<T> & v, vector<T> & w);
```

$$t \leftarrow y + z, x \leftarrow t$$

Temporaries are extremely expensive!



Expression Templates

```
vector_expr<vector<T>, op_plus, vector<T> >
operator+(vector<T> & v, vector<T> & w) { ... }

vector::operator=(vector_expr<...> const & e) {
   viennacl::linalg::avbv(*this, 1,e.lhs(), 1,e.rhs());
}
```

Allows to Avoid a Significant Amount of Temporaries

Covers most frequent cases
Influence on compilation times moderate

Expression templates have their limitations

```
viennacl::vector<NumericType> v;
viennacl::matrix<NumericType> M;
v = viennacl::linalg::prod(M, v);
```

Temporary object is required here!

ViennaCL detects such cases and takes care of it



Data transfer

Like transfer from and to std container Using provided copy functions

Interface compatibility

ViennaCL algorithms work with Eigen e.g.: iterative solver



Data transfer: vectors

```
#define VIENNACL HAVE EIGEN
Eigen::VectorXd eigen_vector(dim);
// fill Eigen objects in a very sophisticated way with
   numbers here
viennacl::vector<double> viennacl_vector(dim);
// copy data from Eigen objects to ViennaCL objects
viennacl::copy(eigen_vector, viennacl_vector);
// do some heavy linear algebra with ViennaCL here
// copy back to Eigen:
viennacl::copy(viennacl_vector, eigen_vector);
```

Data transfer: dense matrix

```
#define VIENNACL HAVE EIGEN
Eigen::MatrixXd eigen_densematrix(dim, dim);
// fill Eigen objects in a very sophisticated way with
   numbers here
viennacl::matrix<double> viennacl_densematrix(dim, dim);
// copy data from Eigen objects to ViennaCL objects
viennacl::copy(eigen_densematrix, viennacl_densematrix);
// do some heavy linear algebra with ViennaCL here
// copy back to Eigen:
viennacl::copy(viennacl_densematrix, eigen_densematrix);
```

Data transfer: sparse matrix

```
#define VIENNACL HAVE EIGEN
Eigen::SparseMatrix<double, Eigen::RowMajor>
   eigen_sparsematrix(dim, dim);
// fill Eigen objects in a very sophisticated way with
   numbers here
viennacl::compressed_matrix<double> viennacl_sparsematrix(
   dim, dim);
// copy data from Eigen objects to ViennaCL objects
viennacl::copy(eigen_sparsematrix, viennacl_sparsematrix);
// do some heavy linear algebra with ViennaCL here
// copy back to Eigen:
viennacl::copy(viennacl_sparsematrix, eigen_sparsematrix);
```

Interface Compatibility: iterative solver

```
#define VIENNACL HAVE EIGEN
using namespace viennacl::linalg;
Eigen::SparseMatrix<double, Eigen::RowMajor>
    matrix(dim, dim);
Eigen::VectorXd rhs(dim);
Eigen::VectorXd result(dim);
// fill eigen_matrix and eigen_rhs here
// Solve system using CG from ViennaCL
result = solve(matrix, rhs, cq_taq());
// Solve system using BiCGStab from ViennaCL
result = solve(matrix, rhs, bicgstab_tag());
// Solve system using GMRES from ViennaCL
result = solve(matrix, rhs, gmres_tag());
```

Granularity of Operations

Solving linear systems

```
viennacl::matrix<double> mat(N, N);
viennacl::vector<double> rhs(N);

for (size_t i=0; i<1000; ++i)
{
   viennacl::vector<double> result
   = solve(mat, rhs, bicgstab_tag());
   /* process result */
}
```

Why Is There No Speed-Up?



Granularity of Operations

Solving linear systems

```
viennacl::matrix<double> mat(N, N);
viennacl::vector<double> rhs(N);

for (size_t i=0; i<1000; ++i)
{
   viennacl::vector<double> result
   = solve(mat, rhs, bicgstab_tag());
   /* process result */
}
```

Why Is There No Speed-Up?

$$N = 3$$

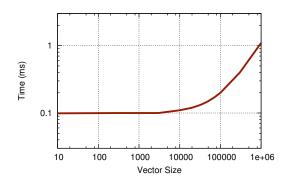


Lets take a look



Sample Operation

$$v_1 \leftarrow v_2$$

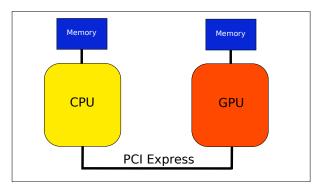


OpenCL Kernel Launch Overhead

 $10 - 100 \; \mu$ s

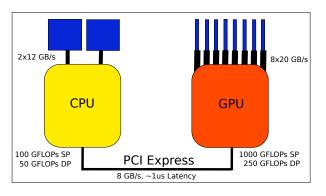


GPUs: Disillusion - Computing Architecture Schematic



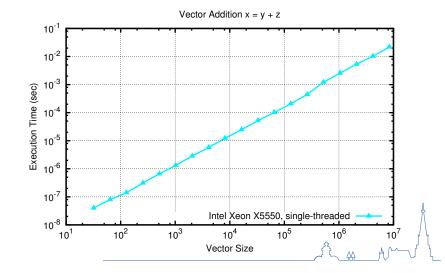


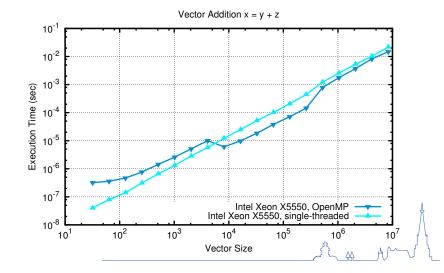
GPUs: Disillusion - Computing Architecture Schematic

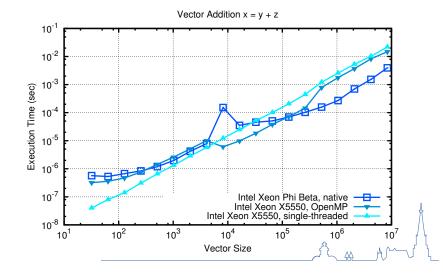


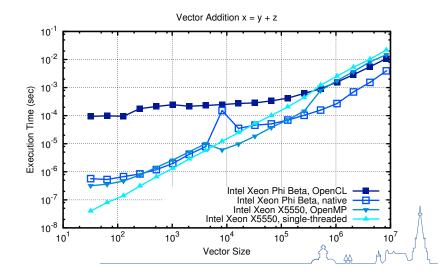
Good for large FLOP-intensive tasks, high memory bandwidth PCI-Express can be a bottleneck

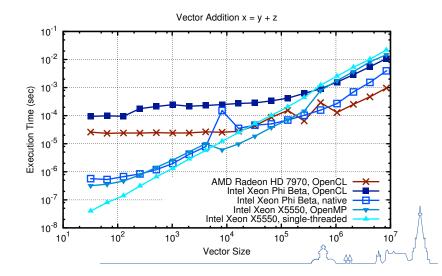
>> 10-fold speedups (usually) not backed by hardware

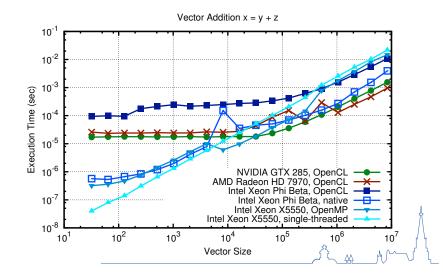


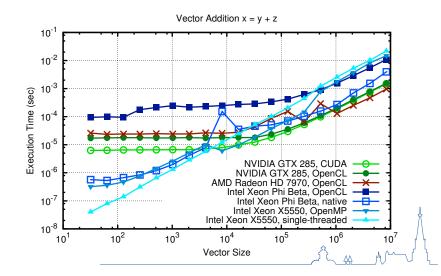


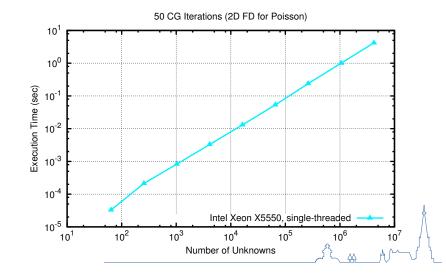


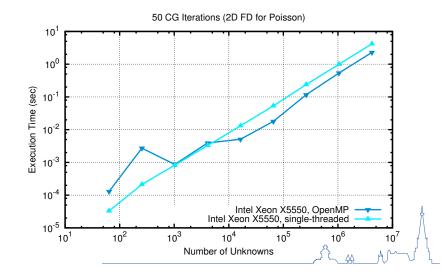


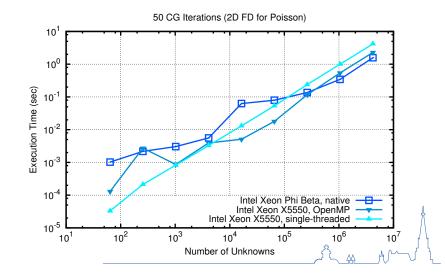


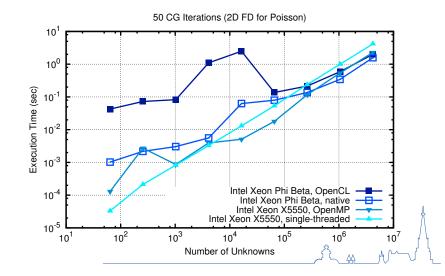


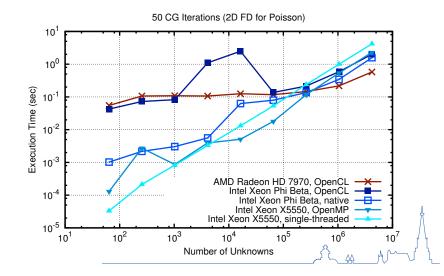


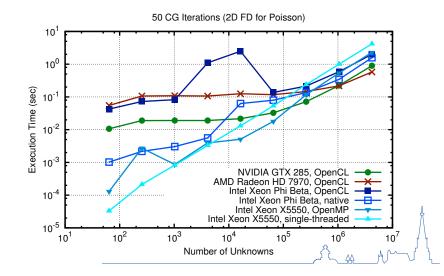


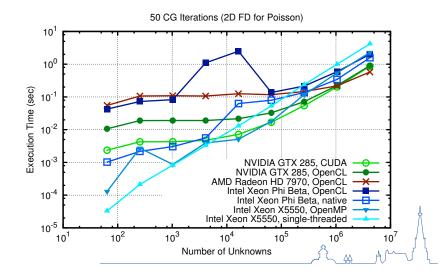








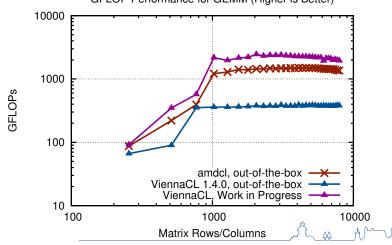




Some benchmarks - Matrix-Matrix Multiplication

Auto-tuning environment (AMD Radeon HD 7970, single precision)

GFLOP Performance for GEMM (Higher is Better)



Summary

What have we learned?

What are subvectors/submatrices and how to use them How to eliminate temporaries

Expression templates and when they help us

Interface to Eigen

ViennaCL isn't optimized for small vectors/matrices

Performance bottleneck

Overview of ViennaCL performance



ViennaCL: Behind the curtain



ViennaCL: Behind the curtain

What to expect

Backends

OpenCL kernel management

Extending ViennaCL

ViennaCL and OpenGL

Summary



ViennaCL: Behind the curtain

Backends

There is more than OpenCL

CUDA from NVIDIA

OpenACC

Each framework has advantages and disadvantages



OpenCL

```
const char *kernel string =
"__kernel void mykernel(__global double *buffer) {
  buffer[get global id(0)] = 42.0;
};":
int main() {
  cl_program my_prog = clCreateProgramWithSource(
         my_context, 1, &kernel_string, &source_len, &err);
  clBuildProgram (my_prog, 0, NULL, NULL, NULL, NULL);
  cl kernel my kernel = clCreateKernel(my prog,
                           "mykernel", &err);
  clSetKernelArg(my_kernel, 0, sizeof(cl_mem), &buffer);
  clEngueueNDRangeKernel(gueue, my kernel, 1, NULL,
                &global size, &local size, 0, NULL, NULL);
```

Additional boilerplate code required (low-level API)
Broad hardware support (separate SDKs)
No more development effort from NVIDIA

NVIDIA CUDA

```
// GPU kernel:
__global__ void kernel(double *buffer)
{
   int idx = blockIdx.x * blockDim.x + threadIdx.x;
   buffer[idx] = 42.0;
}

// host code:
int main()
{
   ...
   cudaMalloc((void**)&buffer,size);
   kernel<<<blooklocknum, blockdim>>>(buffer);
   ...
}
```

Almost no additional code required Vendor-lock Relies on nycc being available



OpenACC

Simple OpenMP-type pragma annotations

Compiler support?

Insufficient control over memory transfers?



What to use?

Why choose one when we can support all?

ViennaCL has a backend layer

Backend is responsible for hardware interaction Not only OpenCL anymore Since ViennaCL 1.4.0

Different backends supported

OpenCL OpenMP

CUDA



Backend support has to be enabled explicitly

```
viennacl::vector<float> v1, v2;
v1 += v2;
```

CPU used!



Backend support has to be enabled explicitly

```
#define VIENNACL_WITH_OPENCL
viennacl::vector<float> v1, v2;
v1 += v2;
```

Now we are using OpenCL



Lets take a look!



Vector Addition

Memory buffers can switch memory domain at runtime

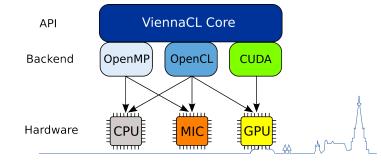
```
void avbv(...) { // x = y + z
  switch (active_handle_id(x))
    case MAIN MEMORY:
      host_based::avbv(...);
      break;
    case OPENCL_MEMORY:
      opencl::avbv(...);
      break;
    case CUDA_MEMORY:
      cuda::avbv(...):
      break;
    default:
      raise error();
```

Internals

Memory Buffer Migration

```
vector<double> x = zero_vector<double>(42);

memory_types src_memory_loc = memory_domain(x);
switch_memory_domain(x, MAIN_MEMORY);
/* do work on x in main memory here */
switch_memory_domain(x, src_memory_loc);
```



Memory buffer switching at runtime

```
#define VIENNACL_WITH_OPENCL
#define VIENNACL WITH OPENMP
viennacl::vector<float> v1, v2;
switch memory domain (v1, MAIN MEMORY);
switch_memory_domain(v2, MAIN_MEMORY);
v1 += v2; \\ working on CPU with OpenMP
switch memory domain (v1, OPENCL MEMORY);
switch_memory_domain(v2, OPENCL_MEMORY);
v1 += v2; \\ working on GPU with OpenCL
```

Best kernel implementations depend on target hardware NVIDIA, AMD, Intel

Best work group size depends on target hardware

					AMD			
	32	64	128	256	32	64	128	256
64	191	151	174	193	324	262	256	249
128	194	177	195	214	357	290	272	247
256	161	164	195	214	307	264	256	248
512	145	151 177 164 157	198	211	282	255	258	253

Execution times for sparse matrix-vector product in milliseconds

Kernel parameter tuning

Default number of work groups = 128 Default number of work items per work group = 128 Automatic tuning environment \Rightarrow XML file

How to use kernel parameters

```
using namespace viennacl;
using viennacl::io;

read_kernel_parameters< vector<float> >
    ("float_vector_parameters.xml");
read_kernel_parameters< matrix<float> >
    ("float_matrix_parameters.xml");
read_kernel_parameters< compressed_matrix<float> >
    ("float_sparse_parameters.xml");
```

ViennaCL expression template don't cover all operations

Sample operation: $\mathbf{x} = \mathbf{A} \times \left[(\mathbf{y} \cdot (\mathbf{y} + \mathbf{z}))\mathbf{y} + \mathbf{z} \right]$

Automated kernel generation

Supported since ViennaCL 1.3.0

Experimental support

Symbolic variables

Operation is defined with C++ symbolic variables

Custom kernel object is generated



Automated kernel generation

Sample operation: $\mathbf{x} = \mathbf{A} \times \left[(\mathbf{y} \cdot (\mathbf{y} + \mathbf{z}))\mathbf{y} + \mathbf{z} \right]$

```
// Instantiation of the symbolic variables
symbolic_vector<NumericType, 0> sX;
symbolic_matrix<NumericType, 1> sA;
symbolic_vector<NumericType, 2> sY;
symbolic_vector<NumericType, 3> sZ;

//Creation of the custom operation
custom_operation my_op(
   sX = prod(sA, inner_prod(sY, sY+sZ) * sY + sZ),
   "operation_name");
```

Automated kernel execution

```
viennacl::vector<NumericType> x, y, z;
viennacl::matrix<NumericType> A;

// fill data here

//Execution of the custom operation
viennacl::ocl::enqueue(my_op(x,A,y,z));
```



Extending ViennaCL

Not Everything Covered by ViennaCL

Complicated vector expressions in a single compute kernel

Direct OpenCL Kernel Handling is a Pain

```
const char * my_kernel_sources =
"__kernel void element_prod(\n"
           __global const float * vec1, \n"
           __global const float * vec2, \n"
           global float * result,\n"
           unsigned int size) \n"
"{ \n"
  for (unsigned int i = get_global_id(0); \n"
                     i < size; \n"
                     i += get global size(0))\n"
     result[i] = vec1[i] * vec2[i]; \n"
"};\n";
```

Extending ViennaCL

The OpenCL Way (error checks and casts omitted)

Issues

Access my_kernel at some other location in an application? What to do with my_proq?

Extending ViennaCL

The ViennaCL Way (namespaces omitted)

At any other Location within the Application

```
kernel & my_kernel = get_kernel(
    "my_program", "element_prod");
viennacl::ocl::enqueue(
    my_kernel(vec1, vec2, result, vec1.size()));
```

Allows for Adding Missing Functionality Easily

A bit of OpenCL knowledge required

Extending ViennaCL

Integrate ViennaCL into User-Environment

User-provided context, queue and device

```
cl_context my_context = ...; //a context
cl_device_id my_device = ...; //a device in my_context
cl_command_queue my_queue = ...; //a queue for my_device
// supply existing context 'my_context' with one device
// and one queue to ViennaCL using id '0':
viennacl::ocl::setup_context(0, my_context, my_device,
    my_queue);
```

Wrapping Memory Buffers

```
cl_mem my_memory = ...;
viennacl::vector<float> my_vec(my_memory, 10);
```

Use ViennaCL operations as usual



ViennaCL and OpenGL

Since OpenCL 1.1: OpenGL interoperability

With own OpenCL context: easy task

Workflow

Setup OpenGL and OpenCL

Create OpenGL buffer and OpenCL memory object

Pass OpenCL memory object to ViennaCL

Do ViennaCL magic

Use data in OpenGL



Setup OpenGL context (simple glut-glew magic)

```
glutInit(&argc, argv);

glutInitDisplayMode(...);
glutInitWindowPosition(100,100);
glutInitWindowSize(1600,800);
glutCreateWindow("CL - GL");

glewInit();
```



Setup OpenCL context with OpenGL interoperability support

```
cl_context_properties properties[] = {
    CL_GL_CONTEXT_KHR, (cl_context_properties)
        glXGetCurrentContext(),
    CL_GLX_DISPLAY_KHR, (cl_context_properties)
        glXGetCurrentDisplay(),
    CL_CONTEXT_PLATFORM, (cl_context_properties)
        viennacl::ocl::get_platforms()[0].id(),
    0 };
cl_device_id my_device =
    viennacl::ocl::current_device().id();
cl_context my_context = clCreateContext(properties, 1,
    &my_device, NULL, NULL, &err);
cl_command_queue my_queue = clCreateCommandQueue(
    my_context, my_device, 0, &err );
```

Setup OpenCL context with OpenGL interoperability support

```
cl_context_properties properties[] = {
    CL_GL_CONTEXT_KHR, (cl_context_properties)
        glXGetCurrentContext(),
    CL_GLX_DISPLAY_KHR, (cl_context_properties)
        glXGetCurrentDisplay(),
    CL_CONTEXT_PLATFORM, (cl_context_properties)
        viennacl::ocl::get_platforms()[0].id(),
    0 };
cl_device_id my_device =
    viennacl::ocl::current device().id();
cl_context my_context = clCreateContext(properties, 1,
    &my_device, NULL, NULL, &err);
cl_command_queue my_queue = clCreateCommandQueue(
    my_context, my_device, 0, &err );
```

Setting up ViennaCL for our context

Create OpenGL buffer and OpenCL memory object

```
glGenBuffers(1, &gl_buffer);
glBindBuffer(GL_PIXEL_UNPACK_BUFFER, gl_buffer);
glBufferData(GL_PIXEL_UNPACK_BUFFER, size, NULL,
    GL_DYNAMIC_COPY);

cl_mem cl_buffer = clCreateFromGLBuffer(my_context,
    CL_MEM_READ_WRITE, gl_buffer, &err);
```



ViennaCL magic

```
// Create viennacl vector from OpenCL memory
viennacl::vector<float> my_vec(cl_buffer, size);
// Acquire memory object for write read/write operation
clEnqueueAcquireGLObjects (my_queue, 1, &cl_buffer,
    O, NULL, NULL);
// copy CPU data to ViennaCL
viennacl::copy( tmp_vec, my_vec );
// doing some stuff
my_vec *= 0.5f;
// Release memory object
clEnqueueReleaseGLObjects (my_queue, 1, &cl_buffer,
    O, NULL, NULL);
```

ViennaCL magic

```
// Create viennacl vector from OpenCL memory
viennacl::vector<float> my_vec(cl_buffer, size);
// Acquire memory object for write read/write operation
clEnqueueAcquireGLObjects (my_queue, 1, &cl_buffer,
    O, NULL, NULL);
// copy CPU data to ViennaCL
viennacl::copy( tmp_vec, my_vec );
// doing some stuff
my_vec *= 0.5f;
// Release memory object
clEnqueueReleaseGLObjects(my_queue, 1, &cl_buffer,
    O, NULL, NULL);
```

Lets take a look at this example



Summary

What have we learned?

ViennaCL has different backends

How to enable and use backends

OpenCL management in ViennaCL

How to use an own OpenCL kernel with ViennaCL

How to provide own OpenCL contexts

ViennaCL works with OpenGL!

How to use ViennaCL to work with OpenGL



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Summary

High-Level C++ Approach of ViennaCL

Convenience of single-threaded high-level libraries (Boost.uBLAS) Header-only library for simple integration into existing code MIT (X11) license

http://viennacl.sourceforge.net/

Selected Features

Backends: OpenMP, OpenCL, CUDA

Iterative Solvers: CG, BiCGStab, GMRES Preconditioners: AMG, SPAI, ILU, Jacobi

BLAS: Levels 1-3

