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PROGRAMMING CUDA AND OPENCL: A CASE STUDY USING MODERN C++ LIBRARIES[*]

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Abstract. We present a comparison of several modern C++ libraries providing high-level interfaces for programming multi- and many-core architectures on top of CUDA or OpenCL. The comparison focuses on the solution of ordinary differential equations (ODEs) and is based on odeint, a framework for the solution of systems of ODEs. Odeint is designed in a very flexible way and may be easily adapted for effective use of libraries such as MTL4, VexCL, or ViennaCL, using CUDA or OpenCL technologies. We found that CUDA and OpenCL work equally well for problems of large sizes, while OpenCL has higher overhead for smaller problems. Furthermore, we show that modern high-level libraries allow us to effectively use the computational resources of many-core GPUs or multicore CPUs without much knowledge of the underlying technologies.

Key words. GPGPU, OpenCL, CUDA, C++, Boost.odeint, MTL4, VexCL, ViennaCL

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1. Introduction.

Recently, general purpose computing on graphics processing units (GPGPU) has acquired considerable momentum in the scientific community. This is confirmed both by increasing numbers of GPGPU-related publications and GPU-based supercomputers in the TOP500[1] list. Major programming frameworks are NVIDIA's CUDA and OpenCL. The former is a proprietary parallel computing architecture developed by NVIDIA for general purpose computing on NVIDIA graphics adapters, and the latter is an open, royalty-free standard for cross-platform, parallel programming of modern processors and GPUs maintained by the Khronos group. By nature, the two frameworks have their distinctive pros and cons. CUDA has a more mature programming environment with a larger set of scientific libraries but is available for NVIDIA hardware only. OpenCL is supported on a wide range of hardware, but its native application programming interface (API) requires a much larger amount of boilerplate code from the developer. Another problem with OpenCL is that it is generally difficult to achieve performance portability across different hardware architectures.

Both technologies are able to provide scientists with the vast computational resources of modern GPUs at the price of a steep learning curve. Programmers need to familiarize themselves with a new programming language and, more importantly,

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[1] http://top500.org.

with a new programming paradigm. However, the entry barrier may be lowered with the help of specialized libraries. The CUDA Toolkit includes several such libraries (BLAS implementations, fast Fourier transform, Thrust, and others). OpenCL lacks standard libraries, but there are a number of third-party projects aimed at developing both CUDA and OpenCL programs.

This paper presents a comparison of several modern C++ libraries aimed at easing GPGPU development. We look at both the convenience and the performance of the libraries under consideration in the context of solving ordinary differential equations (ODEs). The comparison is based on odeint,[2] a modern C++ library for solving ODEs numerically [2, 3] which has been included in the Boost libraries[3] recently. It is developed in a generic way using template metaprogramming techniques, which leads to extraordinary high flexibility at the utmost performance. The numerical algorithms are implemented independently of the underlying arithmetic. This results in a broad applicability of the library, especially in nonstandard environments. For example, odeint supports matrix types and arbitrary precision arithmetic and can be easily adapted to use either CUDA or OpenCL frameworks.

The GPGPU libraries considered in this work are MTL4, VexCL, and ViennaCL. We also employ Thrust[4] in order to provide a reference point for the comparison of the considered libraries. Thrust is a parallel algorithms library which resembles the C++ Standard Template Library [6]. Its high-level interface greatly enhances developer productivity while enabling performance portability between GPUs and multicore CPUs. Thrust is distributed with the NVIDIA CUDA Toolkit since version 4.1.

MTL4 (The Matrix Template Library)[5] is a C++ linear algebra library providing an intuitive interface by establishing a domain-specific language embedded in C++ [12]. The library aims for maximal performance achievable by high-level languages using compile-time transformations. Currently, three versions exist: the open-source edition supporting single- and multicore CPUs, the supercomputing edition providing generic MPI-based parallelism, and the CUDA edition introduced in this paper. In the following, we will refer to the CUDA version of MTL4 as CMTL4.

VexCL is a vector expression template library[6] for OpenCL [11]. It has been created for ease of OpenCL development with C++. VexCL strives to reduce the amount of boilerplate code needed to develop OpenCL applications. The library provides a convenient and intuitive notation for vector arithmetic, reduction, sparse matrix-vector multiplication, etc. Multidevice and even multiplatform computations are supported.

ViennaCL (The Vienna Computing Library) is a scientific computing library[7] written in C++ [30]. CUDA and OpenMP compute backends were added recently, but only the initial OpenCL backend is considered in the remainder of this work. The programming interface is compatible with Boost.uBLAS[8] and allows for simple, high-level access to the vast computing resources available on parallel architectures such as GPUs. The library's primary focus is on common linear algebra operations (BLAS levels 1, 2, and 3) and the solution of large sparse systems of equations by means of iterative methods with optional preconditioners.

[2] http://odeint.com.

[3] http://boost.org.

[4] http://thrust.github.com.

[5] http://mtl4.org.

[6] https://github.com/ddemidov/vexcl.

[7] http://viennacl.sourceforge.net.

[8] http://www.boost.org/libs/numeric/ublas.

CUDA and OpenCL differ in their handling of compute kernel compilation. In NVIDIA's framework the compute kernels are compiled to PTX code together with the host program. PTX is a pseudoassembler language which is compiled at runtime for the specific NVIDIA device the kernel is launched on. Since PTX is already very low-level, this just-in-time kernel compilation has low overhead. In OpenCL the compute kernels are compiled at runtime from higher-level C-like sources, adding an overhead which is particularly noticeable for smaller sized problems. A portable precompilation to some low-level pseudocode as in CUDA is not feasible in OpenCL because of hardware agnosticism by design.

The approach taken for the generation and compilation of the compute kernels is one of the main differences between the OpenCL libraries we considered. VexCL generates and compiles an OpenCL program with a single kernel for each vector expression it encounters. This leads to potentially higher initialization overhead but should prove to be more effective in long program runs. On the other hand, ViennaCL uses a set of predefined kernels, which functionally overlaps with BLAS level 1 routines for vector operations. These kernels are compiled in batch at the program start to allow for faster initialization. However, due to this design decision, vector expressions with several operands may result in the launch of more than one kernel. It should be noted that because the main focus of ViennaCL is on iterative solvers for large sparse systems of equations, where complex vector expressions are rare, predefined kernels are favorable in such a setting.

The other difference between CUDA and OpenCL is that CUDA supports a subset of the C++ language in compute kernels, while OpenCL kernels are written in a subset of C99. Therefore, CUDA programmers may use template metaprogramming techniques which may lead to more efficient and compact code. The native OpenCL API does not provide such features, but the drawback is balanced by the ability of kernel source generation during runtime. Modern C++ libraries such as those considered in this work successfully use this approach and hide low-level details from their users.

2. Adapting odeint.

ODEs play a major role in many scientific disciplines. They occur naturally in the context of mechanical systems, such as granular [28] and molecular dynamics. In fact, the Newtonian and Hamiltonian mechanics are formulated as ODEs [21]. Many other applications can be found in such diverse fields as biology [8, 25], neuroscience [18], chemistry [4], and social sciences [16]. Furthermore, ODEs are also encountered in the context of the numerical solution of nonstationary partial differential equations (PDEs), where they occur after a discretization of the spatial coordinates [17].

Odeint solves the initial value problem (IVP) of ODEs given by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \dot{x} = f(x,t), \qquad x(0) = x_0. \tag{2.1}$$

Here, x is the dependent variable and is usually a vector of real or complex values. t is the independent variable. We will refer to t as the time throughout the paper and will denote the time derivative as $\mathrm{d}x/\mathrm{d}t = \dot{x}$. $f(x,t)$ is the system function and defines the ODE.

Typical use cases for solving ODEs on GPUs are large systems of coupled ODEs which occur as discretizations of PDEs, or ODEs defined on lattices or graphs. Another use case is parameter studies, where the dependence of an ODE on some parameters is of interest. Here, a high-dimensional ODE system consisting of many low-dimensional uncoupled ODEs, each with a different parameter set, is considered. This one large system is then solved at once; hence all low-dimensional ODEs are solved simultaneously.

Numerous methods for solving ODEs exist [13, 14, 29]; these are usually categorized in the field of numerical analysis. Odeint implements the most prominent of these methods—for example, the classical Runge–Kutta methods and Runge–Kutta–Fehlberg methods, multistep methods (Adams–Bashforth–Moulton), symplectic Runge–Kutta–Nyström methods, and implicit methods (Rosenbrock and implicit Euler). All of these methods work iteratively, starting from a given initial value $x(t_0)$ to calculate the next value $x(t + \Delta t)$. Δt is the step size and may be chosen either statically or adaptively. For reference, we note that the simplest method is the explicit Euler scheme

$$x\,(t + \Delta t) = x(t) + \Delta t\; f(x(t), t). \tag{2.2}$$

Its global accuracy is of first order, but the scheme is usually not used for real applications because of stability and accuracy issues.

One main feature of odeint is the decoupling of the specific algorithm for solving the ODE from the underlying arithmetic operations. This is achieved by a combination of a state type, an algebra, and operations. The state type represents the state of the ODE being solved and is usually a vector type like std :: vector<>, std :: array<>, or a vector residing on a GPU. The algebra is responsible for iterating through all elements of the state, whereas the operations are responsible for the elementary operations.

To see how the explicit Euler method (2.2) is translated to code in odeint, we briefly discuss its implementation:

```
template< class State, class Algebra, class Operations >
class euler {
    // ...
    template< class Ode >
    void do_step(Ode ode, State &x, time_type t, time_type dt) {
        ode(x, m_dxdt, dt);
        Algebra::for_each3( x, x, m_dxdt, Operations::scale_sum2(1.0, dt) );
    }
};
```

The state type, the algebra, and the operations enter the Euler method as template parameters; hence they are exchangeable. The function object ode represents the ODE and must be provided by the user. It calculates the right-hand side $f(x, t)$ of (2.1) and stores the result in m_dxdt. The call of for_each3 iterates simultaneously over all elements of three vectors and applies scale_sum2 to each triple. The operation is performed in place, meaning that x is updated to the new value. In the code-snippet above, the call to for_each3 is thus equivalent to the vector operation

```
x = 1.0 * x + dt * m_dxdt
```

which is just (2.2), since m_dxdt holds the values of $f(x(t), t)$.

An odeint algebra is a class consisting of for_each1, ..., for_eachN methods. For example, the for_each3 method in the range_algebra—the default algebra for most vector types—is similar to

```
struct range_algebra {
    // ...
    template< class R1, class R2, class R3, class Op >
    void for_each3(R1 &r1, R2 &r2, R3 &r3, Op op) {
        auto it1 = boost::begin(r1);
        auto it2 = boost::begin(r2);
        auto it3 = boost::begin(r3);
        while( it1 != boost::end(r1) ) op(*it1++, *it2++; *it3++);
    }
    // ...
};
```

The operations are represented by a struct with public member classes defining the operations used by the algebras. There is only one default operations class implementation in odeint, which uses the arithmetic operators as usual:

```
struct default_operations {
    // ...
    template< class Fac1, class Fac2 >
    struct scale_sum2 {
        Fac1 m_fac1;
        Fac2 m_fac2;
        scale_sum2( Fac1 fac1, Fac2 fac2 ) : m_fac1(fac1), m_fac2(fac2) { }
        template< class S1, class S2, class S3 >
        void operator()( S1 &s1, const S2 &s2, const S3 &s3 ) const {
            s1 = m_fac1 * s2 + m_fac2 * s3;
        }
    };
    // ...
};
```

The main reason for the separation of algebra and operations is that all arithmetic calculations and iterations are completely encapsulated in the algebra and the operations. Therefore, the numerical algorithms to solve the ODEs are independent from the underlying arithmetic. Note that the algebra and the operations must be chosen such that they interact correctly with the state type.

Many libraries for vector and matrix types provide expression templates [33, 34, 35] for the elementary operations using operator overload convenience. Such libraries do not need to define their own algebra but can instead be used with a default algebra and a default operation set included in odeint, which simply call the operations directly on the matrix or vector type.

We describe the adaptation of odeint for the GPGPU libraries under consideration in the following. The adaptations are now part of odeint; thus native support for these libraries is available. Implementation details such as the resizing of vectors are accomplished in a straightforward manner and are not further addressed for the sake of conciseness.

To adapt Thrust to odeint, we need to provide both an algebra and operations. The algebra needs to define the for_each family of algorithms. All of these operations follow the same pattern, so we consider for_each3 only:

```
struct thrust_algebra {
    template<class StateType1, class StateType2, class StateType3, class Op>
    static void for_each3(StateType1 &s1, StateType2 &s2, StateType3 &s3, Op op) {
        thrust::for_each(
                thrust::make_zip_iterator( thrust::make_tuple(
                    s1.begin(), s2.begin(), s3.begin() ) ),
                thrust::make_zip_iterator( thrust::make_tuple(
                    s1.end(), s2.end(), s3.end() ) ),
                op);
    }
};
```

Here, thrust::make_zip_iterator is used in combination with make_tuple to pack several device vector iterators into a single iterable sequence. The sequence is then processed by the thrust::for_each algorithm, applying the function object op to each entry.

The operations called via the function object op are defined in thrust_operations and are actually function objects executed on the respective CUDA device:

```
struct thrust_operations {
    template<class Fac1 = double, class Fac2 = Fac1>
    struct scale_sum2 {
        const Fac1 m_alpha1;
        const Fac2 m_alpha2;

        scale_sum2(const Fac1 alpha1, const Fac2 alpha2)
            : m_alpha1(alpha1), m_alpha2(alpha2) { }

        template< class Tuple >
        __host__ __device__ void operator()( Tuple t ) const {
            thrust::get<0>(t) = m_alpha1 * thrust::get<1>(t)
                                      + m_alpha2 * thrust::get<2>(t);
        }
    };
};
```

The device function object uses thrust::get<> functions to unpack the zip iterator into separate values. This approach is heavily used with Thrust and allows the processing of several vectors in a single efficient sweep.

CMTL4, VexCL, and ViennaCL libraries provide convenient expression templates that may be directly used with odeint's vector_space_algebra and default_operations. This combination proved to be effective with CMTL4 and VexCL, where each expression results in a single kernel. For ViennaCL, however, default operations involving more than two terms result in multiple kernel launches. Moreover, temporary vectors are allocated and deallocated for each such composite operation, resulting in a dramatic decline in performance. To address such problems, ViennaCL provides a kernel generator [32], which is able to generate specialized operations for ViennaCL. For example, the scale_sum2 operation is defined as

```
struct viennacl_operations {
    template<class Fac1 = double, class Fac2 = Fac1>
    struct scale_sum2 {
        // ...
        template<class T1, class T2, class T3>
        void operator()( viennacl::vector<T1> &v1,
                    const viennacl::vector<T2> &v2,
                    const viennacl::vector<T3> &v3) const
        {
                typedef viennacl::generator::vector<T1> vec;

                viennacl::generator::custom_operation op;
                op.add( vec(v1) = m_alpha1 * vec(v2) + m_alpha2 * vec(v3) );
                op.execute();
            }
        };
};
```

Here, a custom OpenCL kernel is automatically generated from symbolic vector expression in the first call of the **operator**() and is then buffered and reused for all subsequent calls. The objects of type vec are used to distinguish direct ViennaCL statements from symbolic specifications for the kernel generation facility.

3. Numerical experiments.

As shown in the previous section, all four GPGPU libraries considered in our comparison could be adapted to odeint without getting in contact with low-level CUDA or OpenCL code. The purpose of this section is to evaluate the performance of the GPGPU libraries and whether there is a price to pay for the high-level interface.

3.1. Lorenz attractor ensemble.

In the first example we consider the Lorenz system [23]. The Lorenz system is a system of three coupled ODEs which shows chaotic behavior for a large range of parameters. It is one of the most frequently used ODEs for evaluation purposes in the nonlinear dynamics community. The equations for the Lorenz system read

$$\dot{x} = -\sigma\left(x - y\right), \quad \dot{y} = Rx - y - xz, \quad \dot{z} = -bz + xy. \tag{3.1}$$

Solutions of the Lorenz system usually furnish very interesting behavior in dependence on one of its parameters. For example, one might want to study the chaoticity in dependence on the parameter R. Therefore, one would create a large set of Lorenz systems (each with a different parameter R), pack them all into one system, and solve them simultaneously. In a real study of chaoticity one may also calculate the Lyapunov exponents [26], which requires solving the Lorenz system and their linear perturbations.

The Thrust version of the system function object for the Lorenz attractor ensemble example is presented below. It holds the model parameters and provides the necessary **operator**() with a signature required by the odeint library. The state type is represented by thrust::device_vector<**double**>:

```
typedef thrust::device_vector<double> state_type;

struct lorenz_system {
    size_t N;
    const state_type &R;
    lorenz_system( size_t n, const state_type &r) : N(n), R(r) { }
    void operator()(const state_type &x, state_type &dxdt, double t) const;
};
```

The X, Y, and Z components of the state are held in the continuous partitions of the vector. **operator**() uses the standard technique of packing the state components into a zip iterator and passes the composite sequence to the thrust::for_each algorithm together with the provided device function object:

```
struct lorenz_functor;

void lorenz_system::operator()(const state_type &x, state_type &dxdt,
                               double t) const
{
    thrust::for_each(
        thrust::make_zip_iterator( thrust::make_tuple(
            R.begin(),
            x.begin(), x.begin() + N, x.begin() + 2 * N,
            dxdt.begin(), dxdt.begin() + N, dxdt.begin() + 2 * N ) ),
        thrust::make_zip_iterator( thrust::make_tuple(
            R.end(),
            x.begin() + N, x.begin() + 2 * N, x.end(),
            dxdt.begin() + N, dxdt.begin() + 2 * N, dxdt.end() ) ),
        lorenz_functor() );
}
```

The device function object unpacks the individual components and applies the required operations to the derivative part, essentially leading to a one-to-one translation of (3.1) into code:

```
struct lorenz_functor {
  template< class T >
  __host__ __device__ void operator()( T t ) const {
    double R = thrust::get<0>(t);
    double x = thrust::get<1>(t);
    double y = thrust::get<2>(t);
    double z = thrust::get<3>(t);
    thrust::get<4>(t) = sigma * ( y - x );
    thrust::get<5>(t) = R * x - y - x * z;
    thrust::get<6>(t) = -b * z + x * y ;
  }
};
```

The system function object for the CMTL4 version of the Lorenz attractor example is more compact than the Thrust variant because CMTL4 supports a rich set of vector expressions. CMTL4 provides the type multi_vector that allows for expressing the operations directly:

```
typedef mtl::dense_vector<double>    vector_type;
typedef mtl::multi_vector<vector_type> state_type;

struct lorenz_system {
  const vector_type &R;
  explicit lorenz_system(const vector_type &R) : R(R) { }

  void operator()(const state_type& x, state_type& dxdt, double t) {
     dxdt.at(0) = sigma * (x.at(1) - x.at(0));
     dxdt.at(1) = R * x.at(0) - x.at(1) - x.at(0) * x.at(2);
     dxdt.at(2) = x.at(0) * x.at(1) - b * x.at(2);
  }
};
```

In this context, the class multi_vector is used in two ways: expressing operations on subvectors and expressing operations on entire vectors. Each operation on subvectors of x and dxdt causes a kernel call.

There is potential for optimization when the three operations are performed by one kernel. This can be achieved with the following formulation:

```
    ( lazy(dxdt.at(0)) = sigma * (x.at(1) - x.at(0)) ) ||
    ( lazy(dxdt.at(1)) = R * x.at(0) - x.at(1) - x.at(0) * x.at(2) ) ||
    ( lazy(dxdt.at(2)) = x.at(0) * x.at(1) - b * x.at(2) );
```

The vector assignments are not performed immediately, but their evaluation is delayed and can be fused with other expressions, denoted by operator ||. This formulation has yet another advantage: the three vector operations are performed in one single loop, which provides much better data locality for vector x. For the sake of performance, the multivectors are constructed with contiguous memory whenever the types allow for it. Then, expressions on multivectors can be evaluated with one kernel call. Especially for small vectors, the overhead of calling multiple kernels is significant: we observed 150 % overhead with a 3-component vector with 4K entries compared to one vector of size 12K.

The VexCL implementation of the Lorenz attractor ensemble example is as compact as that of CMTL4. Here, the state is represented by the vex::multivector<**double**,3> type, which holds three instances of vex::vector<**double**> and transparently dispatches all operations to the underlying components. The code for the body of **operator**() practically coincides with the problem statement (3.1):

```
typedef vex::multivector<double, 3> state_type;

struct lorenz_system {
    const vex::vector<double> &R;
    lorenz_system(const vex::vector<double> &r) : R(r) {}

    void operator()(const state_type &x, state_type &dxdt, double t) const {
        dxdt(0) = sigma * (x(1) - x(0));
        dxdt(1) = R * x(0) - x(1) - x(0) * x(2);
        dxdt(2) = x(0) * x(1) - b * x(2);
    }
};
```

However, the drawback of this variant is that it leads to three kernel launches, namely, one per each vector assignment. As we have discussed previously for the CMTL4 variant, this results in suboptimal performance. A direct use of arithmetic operations for multivectors is not possible due to mixed components in the right-hand side expressions. These additional kernel launches can be eliminated in VexCL by assigning a tuple of expressions to a multivector. The required implementation is only slightly less intuitive than the above variant:

```
    dxdt = std::tie( sigma * (x(1) - x(0)),
                     R * x(0) - x(1) - x(0) * x(2),
                     x(0) * x(1) - b * x(2)          );
```

The performance gain of these fused expressions is a bit larger (25 % for large systems) compared to CMTL4. The reason might be the larger kernel launch overhead for OpenCL kernels.

For the ViennaCL version of the Lorenz attractor example a boost::fusion::vector is used to pack the coordinate components of the state vector into a single type. Individual components are instances of the viennacl::vector<**double**> type. The ViennaCL kernel generation facility already used in section 2 is then used to avoid multiple kernel launches. Even though a custom_operation object is instantiated in each call to **operator**(), the kernel is created only once and then is buffered internally for further reuse.

```
typedef fusion::vector<
    viennacl :: vector<double>, viennacl::vector<double>, viennacl::vector<double>
    > state_type;

struct lorenz_system {
    const viennacl::vector<double> &R;
    lorenz_system(const viennacl::vector<double> &r) : R(r) {}

    void operator()(const state_type &x, state_type &dxdt, double t) const {
        typedef viennacl::generator :: vector<value_type> vec;

        const auto &X = fusion::at_c<0>(x);
        const auto &Y = fusion::at_c<1>(x);
        const auto &Z = fusion::at_c<2>(x);

        auto &dX = fusion::at_c<0>(dxdt);
        auto &dY = fusion::at_c<1>(dxdt);
        auto &dZ = fusion::at_c<2>(dxdt);

        viennacl :: generator :: custom_operation op;
        op.add( vec(dX) = sigma * (vec(Y) − vec(X)) );
        op.add( vec(dY) = element_prod(vec(R), vec(X)) − vec(Y)
                          − element_prod(vec(X), vec(Z)) );
        op.add( vec(dZ) = element_prod(vec(X), vec(Y)) − b * vec(Z) );
        op.excecute()
    }
};
```

3.2. Chain of coupled phase oscillators. As a second example we consider a chain of coupled phase oscillators. A phase oscillator describes the dynamics of an autonomous oscillator [19]. Its evolution is governed by the phase φ, which is a 2π-periodic variable growing linearly in time, i.e., $\dot{\varphi} = \omega$, where ω is the phase velocity. The amplitude of the oscillator does not occur in this equation, so interesting behavior can be observed only if many such oscillators are coupled. In fact, such a system can be used to study such divergent phenomena as synchronization, wave and pattern formation, phase chaos, and oscillation death [20, 27]. It is a prominent example of an emergent system where the coupled system shows a more complex behavior than its constitutes.

The concrete example we analyze here is a chain of nearest-neighbor coupled phase oscillators [9]:

$$\dot{\varphi}_i = \omega_i + \sin(\varphi_{i+1} - \varphi_i) + \sin(\varphi_i - \varphi_{i-1}). \tag{3.2}$$

The index i here denotes the ith phase in the chain. Note that the phase velocity is different for each oscillator.

The Thrust version for the coupled phase oscillator chain is very similar to the Lorenz attractor example. Again, a zip iterator is used to pack the required components and to process the resulting sequence with a single sweep of the for_each algorithm. The only difference here is that values of neighboring vector elements are needed. In order to access these values, we use Thrust's permutation iterator, so that **operator**() of the system function object becomes

```
thrust::for_each(
    thrust::make_zip_iterator(
        thrust::make_tuple(
            x.begin(),
            thrust::make_permutation_iterator( x.begin(), prev.begin() ),
            thrust::make_permutation_iterator( x.begin(), next.begin() ),
            omega.begin() , dxdt.begin() ) ),
    thrust::make_zip_iterator(
        thrust::make_tuple(
            x.end(),
            thrust::make_permutation_iterator( x.begin(), prev.end() ),
            thrust::make_permutation_iterator( x.begin(), next.end() ),
            omega.end(), dxdt.end() ) ),
     phase_oscillators_functor ()
    );
```

Here, prev and next are vectors of type thrust::device_vector<size_t> and hold the indices to the left and right vector elements. The function object phase_oscillators_functor implements (3.2) similarly to the lorenz_functor above and is thus omitted for brevity.

The stencil operator in CMTL4 is a minimalistic matrix type. Its application is expressed by a matrix-vector product that is assigned to, or is used to either increment or decrement, the vector:

```
y = S * x;       y += S * x;      y -= S * x;
```

The user must provide a function object that applies the stencil on the ith element of a vector and its neighbors. For the sake of performance the function object has to provide two methods: one that checks indices near the beginning and the end of the vector and one that does not check indices. For the considered example, the function object is

```
struct stencil_kernel {
    static const int start = -1, end = 1;
    int n;

     stencil_kernel (int n) : n(n) {}

    template <typename Vector>
     __device__ __host__ double operator()(const Vector& v, int i) const {
        return sin(v[i+1] - v[i]) + sin(v[i] - v[i-1]);
    }

    template <typename Vector>
     __device__ __host__
    double outer_stencil(const Vector& v, int i, int offset = 0) const {
        double s1 = i > offset? sin(v[i] - v[i-1]) : sin(v[i]),
               s2 = i+1 < n + offset? sin(v[i+1] - v[i]) : sin(v[i]);
```

```
            return s1 + s2;
        }
    };
```

The parameter offset is needed when vector parts are cached so that the addressing is shifted. For the sake of backward (and forward) compatibility the nonportable keywords __device__ and __host__ should be replaced by a macro that is defined suitably for the according platform, e.g., to an empty string on regular compilers. This makes the user code entirely platform-independent.

The stencil function object is passed as a template argument to the stencil matrix:

```
typedef mtl::dense_vector<double> state_type;

struct phase_oscillators {
    const state_type& omega;
    mtl::matrix::stencil1D<stencil_kernel> S;

    phase_oscillators (const State& w) : omega(w), S(num_rows(w)) {}

    void operator()(const State &x, State &dxdt, double t) const {
        dxdt = S * x;
        dxdt += omega;
    }
};
```

The stencil matrix S in the system function above uses shared memory to benefit from reaccessing vector entries and to avoid noncoalesced memory accesses.

The VexCL version of the example is the most concise variant. The sum of sines in (3.2) is encoded using the VEX_STENCIL_OPERATOR preprocessor macro. Its parameters are the names of the resulting function object, the return type, the stencil width, the center, and the body string for the generated OpenCL function encoding the required operation. Once the stencil operator is defined, **operator**() of the system function object is implemented with a single line of code:

```
typedef vex::vector<double> state_type;

struct phase_oscillators {
    const state_type &omega;
    phase_oscillators (const state_type &w) : omega(w) { }
    void operator()(const state_type &x, state_type &dxdt, double t) const {
        static VEX_STENCIL_OPERATOR(S, double, 3, 1,
                "return sin(X[1] - X[0]) + sin(X[0] - X[-1]);", omega.queue_list());
        dxdt = omega + S(x);
    }
};
```

The stencil operations are implemented in ViennaCL using the shift () operation, which shifts the indices of a vector by a certain offset. New shifted values at the beginning or at the end of the vector are by default the same as the first or last entry of the vector, respectively, which is just the required behavior for this example:

```
typedef viennacl::vector<double> state_type;

struct phase_oscillators {
    const state_type &omega;
     phase_oscillators (const state_type &w) : omega(w) { }

    void operator()(const state_type &x, state_type &dxdt, double t) const {
        typedef viennacl::generator::vector<value_type> vec;

        viennacl::generator::custom_operation op;
        op.add( vec(dxdt) = vec(omega) + sin(shift(vec(x),  1) − vec(x))
                                       + sin(vec(x) − shift(vec(x), −1)) );
        op.execute();
    }
};
```

3.3. Disordered Hamiltonian lattice. The last example in our performance and usage study is a nonlinear disordered Hamiltonian lattice [24]. Its equations of motion are governed by

$$\dot{q}_{i,j} = p_{i,j}, \qquad \dot{p}_{i,j} = -\omega_{i,j}^2 q_{i,j} - \beta q_{i,j}^3 + \Delta_d q_{i,j}. \tag{3.3}$$

Here, $\Delta_d q_{i,j}$ denotes the two-dimensional discrete Laplacian $\Delta_d q_{i,j} = q_{i+1,j} + q_{i-1,j} + q_{i,j+1} + q_{i,j-1} - 4q_{i,j}$. Such systems are widely used in theoretical physics to study phenomena like Anderson localization [31] and thermalization [10].

An important property of (3.3) is its Hamiltonian nature. Equation (3.3) can be obtained from the Hamilton equations, and it can be shown that both energy and phase volume are conserved during the time evolution. To account for these properties, a special class of solvers exists, namely, symplectic solvers. Odeint implements three different variants of such solvers, all of the Runge–Kutta–Nyström type [15, 22]. The implementation of these solvers requires only the second part of (3.3) with $\dot{p}_{i,j}$ to be specified by the user.

The natural choice for the implementation of (3.3) is a sparse matrix-vector product. Since Thrust provides neither sparse matrix types nor sparse matrix-vector products, Thrust was combined with the CUSPARSE library in order to implement this example. CUSPARSE contains a set of basic linear algebra subroutines used for handling sparse matrices and is included in the CUDA Toolkit distribution together with the Thrust library [1].

For better comparison, all libraries considered in our study use the hybrid ELL format for storing the sparse matrices on GPUs, since this is one of the most efficient formats for sparse matrices on these devices [5]. The standard compressed sparse row format is used for CPU runs. As the construction of the sparse matrix for $-\omega_{i,j}^2 q_i + \Delta_d q_{i,j}$ is straightforward, we provide code only for the system function object interface.

The relevant code for the Thrust version of the system function object is

```
typedef thrust::device_vector<double> state_type;

void operator()(const state_type &q , state_type &dp) const {
    static double one = 1;
    thrust::transform(q.begin(), q.end(), dp.begin(), scaled_pow3_functor(−beta) );

    cusparseDhybmv(handle, CUSPARSE_OPERATION_NON_TRANSPOSE,
            &one, descr, A, thrust::raw_pointer_cast(&q[0]), &one,
            thrust::raw_pointer_cast(&dp[0]) );
}
```

Here, handle, descr, and A are CUSPARSE data structures holding the CUSPARSE context and sparse matrix data. The thrust::transform() algorithm is used in line 5 to compute the scaled third power of the input vector q. Lines 7–9 call the sparse matrix-vector product kernel in CUSPARSE, where thrust::raw_pointer_cast() is used to convert the thrust device vector iterator to a raw device pointer.

The CMTL4 implementation reads

```
typedef mtl::dense_vector<double> state_type;

void operator()(const state_type& q, state_type& dp) {
    dp = A * q;
    dp -= beta * q * q * q;
}
```

Here A is an instance of a sparse matrix holding the discretization of the linear combination $-\omega_{i,j}^2 q_i + \Delta_d q_{i,j}$. The expression q ∗ q ∗ q computes the triple elementwise product of column vector q. Usually, products of column/row vectors among themselves are often program errors and therefore not allowed in CMTL4. Their use may be enabled by defining an according macro during compilation.

The VexCL version employs the user-defined OpenCL function pow3, which computes the third power of its argument and is used for the sake of best performance:

```
typedef vex::vector<double> state_type;
VEX_FUNCTION(pow3, value_type(value_type), ”return prm1 * prm1 * prm1;”);

void operator()(const state_type &q, state_type &dp) const {
    dp = (-beta) * pow3(q) + A * q;
}
```

Similar to CMTL4, the ViennaCL version of the system function object is split into two parts: first, the sparse matrix-vector product Aq is computed; second, the nonlinear term $-\beta q^3$ is added to the result by means of a custom operation:

```
typedef viennacl::vector<double> state_type;

void operator()(const state_type &q, state_type &dp) const {
    typedef viennacl::generator::vector<value_type> vec;

    dp = viennacl::linalg::prod(m_A, q);
    viennacl::generator::custom_operation op;
    op.add( vec(dp) -= m_beta * element_prod(vec(q), element_prod(vec(q), vec(q))) );
    op.execute();
}
```

4. Results.

We present results obtained from our numerical experiments in this section. The complete source code for the experiments and the full set of results are freely available in a GitHub repository.[9]

All the libraries tested in this paper with the exception of CMTL4 and CUSPARSE allow for the use of both CPU and GPU devices. Thrust supports an OpenMP-based execution on the CPU, which is enabled by a compilation switch, while OpenCL libraries natively support CPUs provided that the respective runtime is installed. OpenCL implementations from AMD and from Intel were used on the

[9] https://github.com/ddemidov/gpgpu_with_modern_cpp.

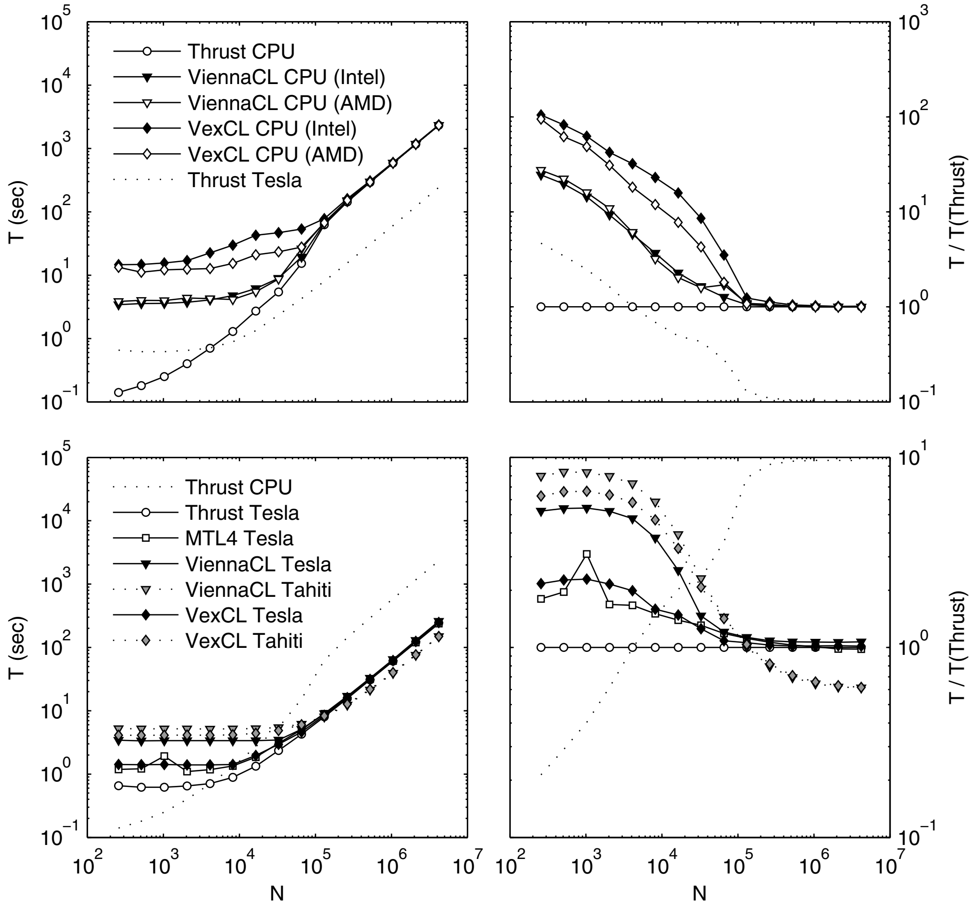


Fig. 4.1. *Lorenz attractor ensemble results.*

CPU, and those from AMD and NVIDIA were used on GPUs. The timings provided were obtained on a Gentoo Linux operating system for two GPUs, namely, an NVIDIA Tesla C2070 and an AMD Radeon HD 7970 (Tahiti), as well as for an Intel Core i7 930 CPU. All reported values are median values of execution times taken for ten runs.

Figures 4.1–4.3 show performance data for the three examples discussed in the previous section. The top row in each figure shows the performance obtained from CPU-based experiments, while the bottom row shows GPU-based data. On the GPU plots the graphs for NVIDIA Tesla and AMD Tahiti boards are correspondingly plotted with solid and dotted lines. The plots on the left show absolute solution time over the size of the problem being solved, while the plots on the right depict performances relative to the Thrust version with two exceptions, where ViennaCL is selected as the reference library. The first exception are GPU plots on Figure 4.2, where the Thrust library performs badly in case of the coupled phase oscillator chain example. The other exception is Figure 4.3, where the combination of Thrust and CUSPARSE is not able to run on a CPU.

Absolute execution times for the largest problem size for all of the considered libraries are given in Table 4.1. The table also provides the achieved memory

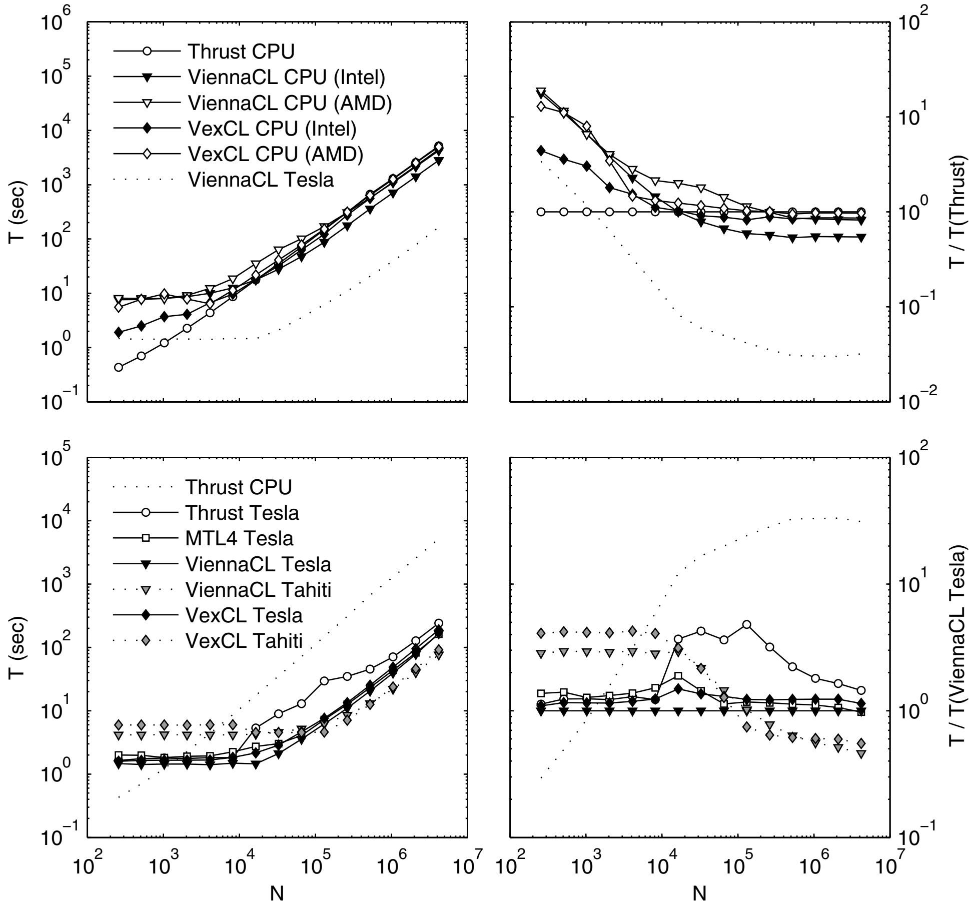


FIG. 4.2. *Coupled phase oscillator chain results.*

bandwidth in GB/sec and in fractions of the theoretical peak for each of the compute devices.

4.1. GPU performance. In general, all our experiments show up to 10× to 20× acceleration when run on a GPU as compared to the CPU path. This is the expected acceleration rate for the memory bandwidth bound examples that we looked at. However, both CUDA and OpenCL programs show considerable overhead at smaller problem sizes, thus requiring problems of sizes between 10^3 and 10^5 to see any significant acceleration on a GPU at all. The overhead for OpenCL libraries is larger than that for CUDA programs, which is mostly due to the additional kernel management logic required by the OpenCL runtime.

Performancewise, all of the considered libraries are close to each other when run on a GPU. VexCL and ViennaCL are in general slower than CMTL4 and Thrust by a few percent, which is usually negligible in practice. Apparently, the CUSPARSE implementation of the sparse matrix-vector product is more efficient than that of the rest of the libraries, since it outperforms the competitors by about 20–30% in the disordered Hamiltonian lattice experiment. The implementation of the phase oscillator chain example for Thrust is rather ineffective since it uses a permutation

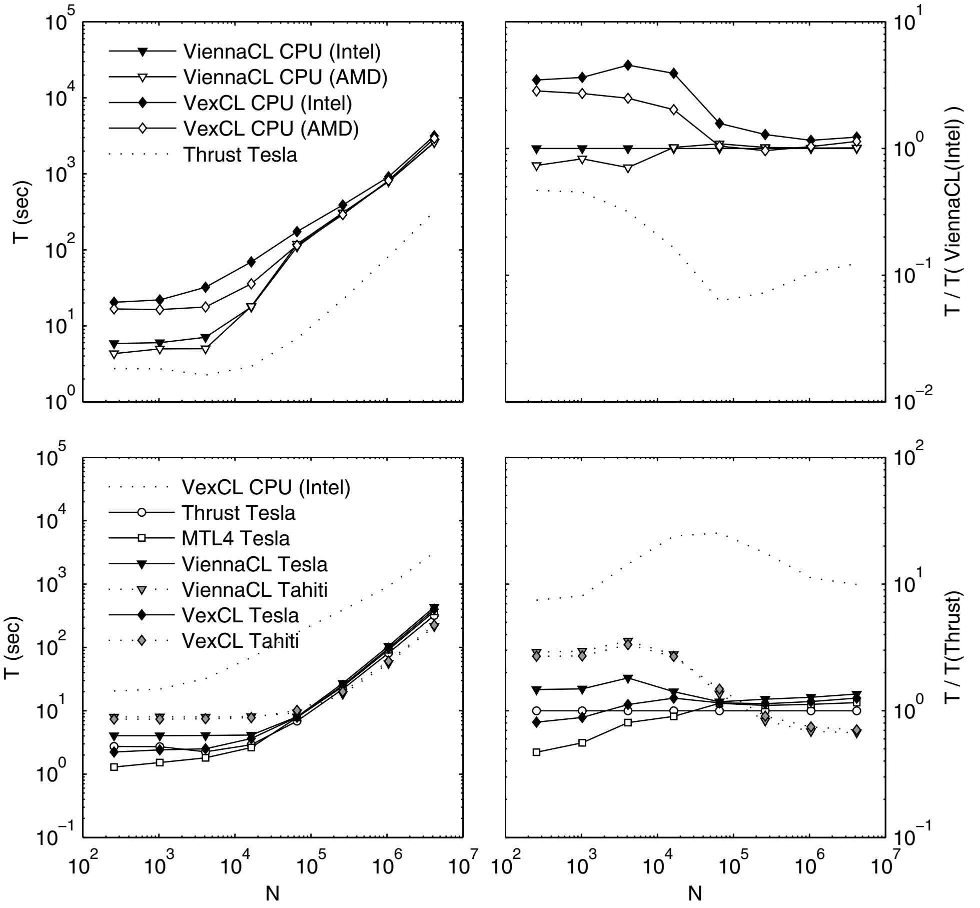


FIG. 4.3. *Disordered Hamiltonian lattice results.*

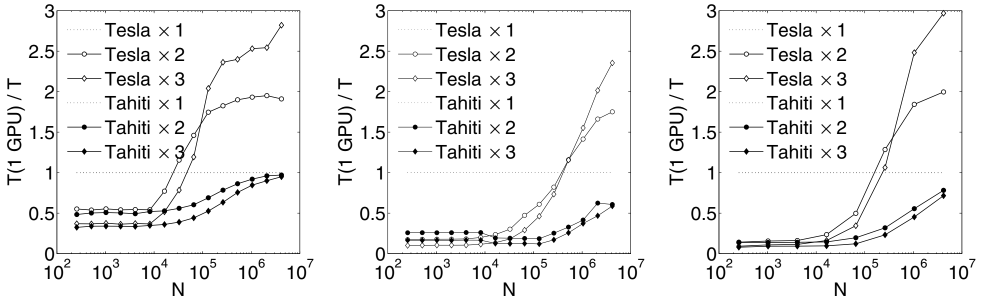
iterator requiring an additional global vector for storing indices. The implementations of stencil operations in CMTL4 and ViennaCL are slightly more efficient than those of VexCL.

Moreover, the overhead of using high-level libraries is negligible compared to the effort spent in getting familiar with the details of CUDA or OpenCL. Thus, we have successfully countered productivity concerns for GPU computing raised in the past [7].

4.2. CPU performance. Thrust, VexCL, and ViennaCL show very similar performance on the CPU for larger problem sizes. For smaller problems the difference between Thrust and OpenCL-based libraries is more pronounced, since Thrust uses an OpenMP backend which does not have any overhead such as OpenCL initialization and kernel compilation. The difference between the OpenCL implementations of AMD and the Intel is negligible in most cases. The only exception is the example of the chain of phase oscillators, where the implementation by Intel outperforms that of AMD by up to 50%. This might be explained by either a better implementation of trigonometric functions in Intel's version or the autovectorization feature of Intel's OpenCL SDK, which transparently compiles OpenCL kernels to fully utilize the SIMD processing on the underlying Intel CPU.

Table 4.1
Absolute run times (sec) and achieved throughput (GB/sec and percentage of theoretical peak) for the largest problem size.

	Lorenz attractor		Phase oscillators		Hamiltonian lattice	
	Time	T-put	Time	T-put	Time	T-put
NVIDIA Tesla C2070						
Thrust	242.78	105 (71%)	240.87	49 (33%)	319.60	120 (81%)
CMTL4	237.91	108 (73%)	161.96	73 (50%)	370.31	104 (70%)
VexCL	246.58	104 (70%)	189.38	63 (42%)	401.39	96 (65%)
ViennaCL	259.85	99 (66%)	166.20	71 (48%)	433.50	89 (60%)
AMD Radeon HD 7970 (Tahiti)						
VexCL	149.49	171 (65%)	91.60	130 (49%)	225.41	170 (65%)
ViennaCL	148.69	172 (65%)	76.55	155 (59%)	214.87	179 (68%)
Intel Core i7 930						
Thrust	2 336.14	11 (43%)	5 182.55	2 (9%)	N/A	
VexCL (AMD)	2 329.00	11 (43%)	5 011.66	2 (9%)	2 934.99	13 (51%)
VexCL (Intel)	2 372.70	11 (42%)	4 463.24	3 (10%)	3 171.74	12 (47%)
ViennaCL (AMD)	2 322.78	11 (43%)	4 246.24	3 (11%)	2 608.80	15 (58%)
ViennaCL (Intel)	2 322.39	11 (43%)	2 815.23	4 (16%)	2 580.47	15 (58%)



(a) Lorenz attractor ensemble.

(b) Coupled phase oscillator chain.

(c) Disordered Hamiltonian lattice.

Fig. 4.4. *VexCL scaling with multi-GPU computation.*

It has to be said that the overhead of OpenCL for small problem sizes is tremendous, if not embarrassing; hence OpenCL cannot be considered to be a competitive CPU programming model for a large area of applications in its present state. A considerable reduction in kernel launch overhead for CPU-based kernel execution is required to make OpenCL more attractive on this target.

Finally, results for multi-GPU usage as provided by VexCL in a transparent way are considered. Figure 4.4 shows scaling results for up to three GPUs. It can be seen that a notable speed-up for several Tesla GPUs over a single card is obtained only for problem sizes larger than 10^6. It seems that AMD's OpenCL implementation does not work very well with multiple GPUs employed. Still, the combined memory of several GPUs allows us to solve proportionally larger problems on the same system.

5. Conclusion.

Performancewise, there is almost no difference between various platforms and libraries when run on the same hardware for large problem sizes. As we have shown, various computational problems may be solved effectively in terms of both human and machine time with the help of modern high-level libraries. Hence, the differences in the programming interfaces of the libraries are more likely to determine the choice of a particular library for a specific application rather than raw performance.

The focus of Thrust is more on providing low-level primitives with an interface very close to the C++ Standard Template Library. Special purpose functionality is available via separate libraries such as CUSPARSE and can be integrated without a lot of effort. The rest of the libraries we looked at demonstrated that they are able to provide a more convenient interface for a scientific programmer than a direct implementation in CUDA or OpenCL. CMTL4 and VexCL have a richer set of elementwise vector operations and allow for the shortest implementations in the context of the ODEs considered in this work. ViennaCL requires two to three additional lines of code in each of the examples due to the use of the kernel generator facility. Still, this extra effort is acceptable considering that the library's focus is on sparse linear systems solvers, which are, however, beyond the scope of this paper.

Regarding a comparison of CUDA versus OpenCL, the main difference observed in this work is the wider range of hardware supported by OpenCL. Although the performance obtained via CUDA is a few percent better than that of OpenCL overall, the differences are mostly too small for us to decide in favor of CUDA based on performance only. Moreover, the slight performance advantage of CUDA can still turn into a disadvantage when taking the larger set of hardware supporting OpenCL into consideration.

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