A Discussion of Selected Vienna-Libraries for Computational Science

Karl Rupp[1], Florian Rudolf[2], Josef Weinbub[2]

[1]MCS Division, Argonne National Laboratory, USA
[2]Institut für Mikroelektronik, TU Wien, Austria

C++Now, May 15th, 2013

Contents

Part 0: What is this all about?

Contents

Libraries

- ViennaCL
- ViennaData
- ViennaFEM
- ViennaGrid
- ViennaIPD
- ViennaMath
- ViennaMesh

Applications

- ViennaMOS
- ViennaProfiler
- ViennaSHE
- ViennaWD
- ViennaX

Contents

Covered In This Talk

Requirements in Computational Science

GPU Computing

Providing High-Level Interfaces

Avoiding Monolithic Code

Abstractions: From Math to Code (and back)

Not Covered

C++11

Maximize use of Boost

The Computational Scientist

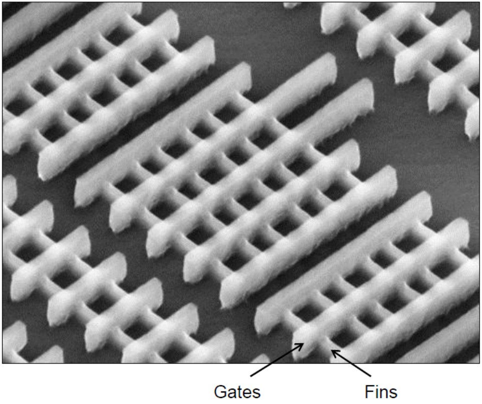
A Strange Animal

- Goal is science, not to execute software
- Codes seldomly designed for ’large scale’ upfront
- Scientists receive software training from scientists
- Performance vs. portability and maintainability
- Run code on clusters (headless, old software stack, ...)
- *Come and go*

Basili *et al.*, Understanding the High-Performance-Computing Community: A Software Engineer’s Perspective. IEEE Software, 2008.

Simulation Flow

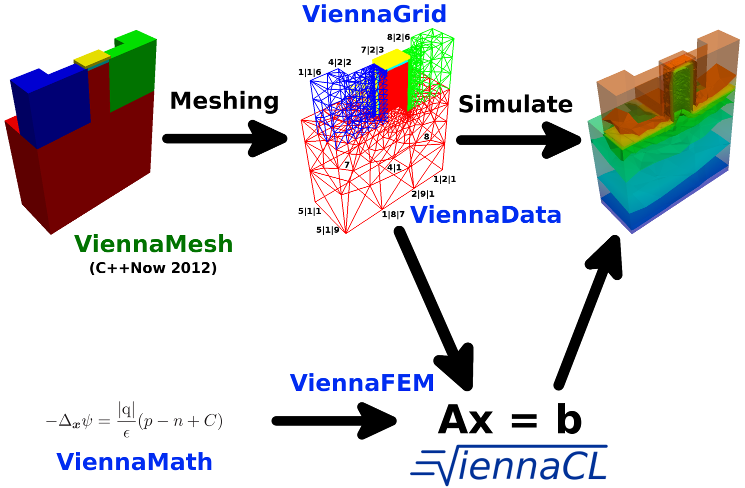
The Many Steps in Simulating a FinFET



(C) Intel, 2011

Simulation Flow

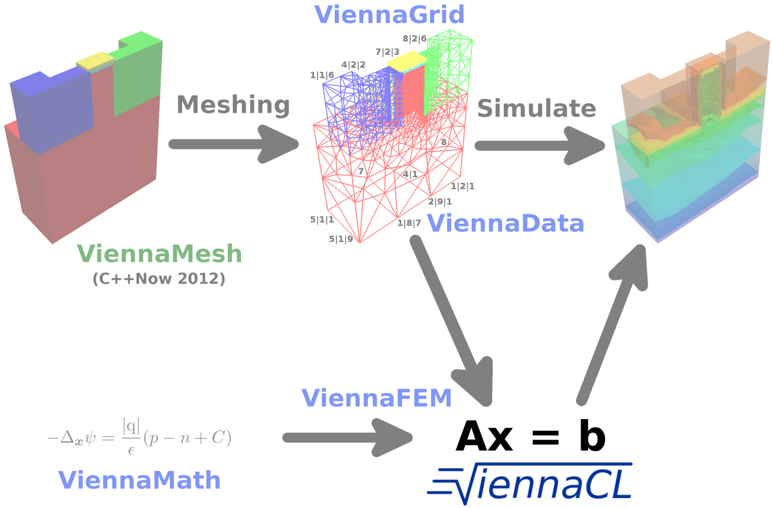
The Many Steps in Simulating a FinFET



Contents

Part 1: ViennaCL

Simulation Flow



From Boost.uBLAS to ViennaCL

Consider Existing CPU Code (Boost.uBLAS)

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


matrix<double> A(1000, 1000);
vector<double> x(1000), y(1000);

/* Fill A, x, y here */

double val = inner_prod(x, y);
y += 2.0 * x;
A += val * outer_prod(x, y);

x = solve(A, y, upper_tag()); // Upper tri. solver

std::cout << "  2-norm: " << norm_2(x) << std::endl;
std::cout << "sup-norm: " << norm_inf(x) << std::endl
    ;
```


High-level code with syntactic sugar

From Boost.uBLAS to ViennaCL

Previous Code Snippet Rewritten with ViennaCL

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

matrix<double> A(1000, 1000);
vector<double> x(1000), y(1000);

/* Fill A, x, y here */

double val = inner_prod(x, y);
y += 2.0 * x;
A += val * outer_prod(x, y);

x = solve(A, y, upper_tag()); // Upper tri. solver

std::cout << "  2-norm: " << norm_2(x) << std::endl;
std::cout << "sup-norm: " << norm_inf(x) << std::endl
    ;
```


High-level code with syntactic sugar

From Boost.uBLAS to ViennaCL

ViennaCL in Addition Provides Iterative Solvers

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

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

/* Fill A, x, y here */

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

No Iterative Solvers Available in Boost.uBLAS...

From Boost.uBLAS to ViennaCL

Thanks to Interface Compatibility

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

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

/* Fill A, x, y here */

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

Code Reuse Beyond GPU Borders

Eigen `http://eigen.tuxfamily.org/`

MTL 4 `http://www.mtl4.org/`

From Boost.uBLAS to ViennaCL

Generic CG Implementation (Sketch)

```
for (unsigned int i = 0; i < tag.max_iterations(); ++
    i)
{
  tmp = viennacl::linalg::prod(A, p);

  alpha     = ip_rr / inner_prod(tmp, p);
  result   += alpha * p;
  residual -= alpha * tmp;

  new_ip_rr = inner_prod(residual, residual);
  if (new_ip_rr / norm_rhs_squared < tag.tolerance())
    break;

  beta  = new_ip_rr / ip_rr;
  ip_rr = new_ip_rr;

  p = residual + beta * p;
}
```

About ViennaCL

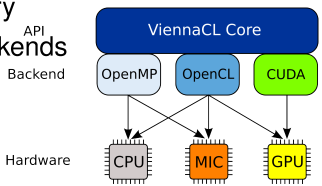
About

High-level linear algebra C++ library

OpenMP, OpenCL, and CUDA backends

Header-only

Multi-platform



Dissemination

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

About ViennaCL

Basic Types

scalar, vector

matrix, compressed_matrix, coordinate_matrix, ell_matrix, hyb_matrix

Data Initialization

```
     std::vector<double>      std_x(100);
   ublas::vector<double>    ublas_x(100);
viennacl::vector<double>      vcl_x(100);

for (size_t i=0; i<100; ++i)
  //   std_x[i] = rand();  // (1)
  // ublas_x[i] = rand();  // (2)
       vcl_x[i] = rand();  // (3)
```

(3) is slowest by orders of magnitude!

About ViennaCL

Basic Types

- scalar, vector
- matrix, compressed_matrix, coordinate_matrix, ell_matrix, hyb_matrix

Data Initialization

- Using viennacl::copy()

```
     std::vector<double>      std_x(100);
   ublas::vector<double>    ublas_x(100);
viennacl::vector<double>      vcl_x(100);

/* setup of std_x and ublas_x omitted */

viennacl::copy(std_x.begin(), std_x.end(),
               vcl_x.begin());   //to GPU
viennacl::copy(vcl_x.begin(), vcl_x.end(),
               ublas_x.begin()); //to CPU
```

About ViennaCL

Basic Types

- scalar, vector
- matrix, compressed_matrix, coordinate_matrix, ell_matrix, hyb_matrix

Data Initialization

- Using viennacl::copy()

```
     std::vector<std::vector<double> >    std_A;
   ublas::matrix<double>                ublas_A;
viennacl::matrix<double>                  vcl_A;

/* setup of std_A and ublas_A omitted */

viennacl::copy(std_A, vcl_A);    // CPU to GPU
viennacl::copy(vcl_A, ublas_A);  // GPU to CPU
```

- Iterator concept doesn't quite work on accelerators

Vector Addition

```
x = y + z;
```

Temporaries are costly (particularly on GPUs)

Expression Templates

Limited expansion

Map to a set of predefined kernels

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

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

Internals

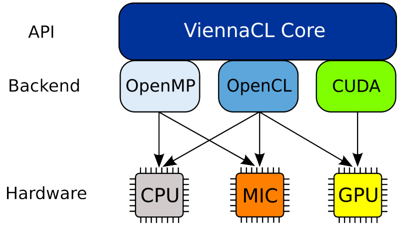
Vector Addition

```
// x = y + z
void avbv(...) {
  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();
  }
}
```

Memory buffers can switch memory domain at runtime

Memory Buffer Migration

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

memory_types src_memory_loc = memory_domain(x);
switch_memory_domain(x, MAIN_MEMORY);

/* work on x in main memory here */

switch_memory_domain(x, src_memory_loc);
```



Generalizing compute kernels

```
  // x = y + z
  __kernel void avbv(
    double * x,

    double * y,

    double * z, uint size)
{
  size_t i = get_global_id(0);
  for (; i<size; i += get_global_size())
    x[i] = y[i] + z[i];

}
```

Generalizing compute kernels

```
  // x = a * y + b * z
  __kernel void avbv(
    double * x,
    double a,
    double * y,
    double b,
    double * z, uint size)
{
  size_t i = get_global_id(0);
  for (; i<size; i += get_global_size())
    x[i] = a * y[i] + b * z[i];

}
```

Generalizing compute kernels

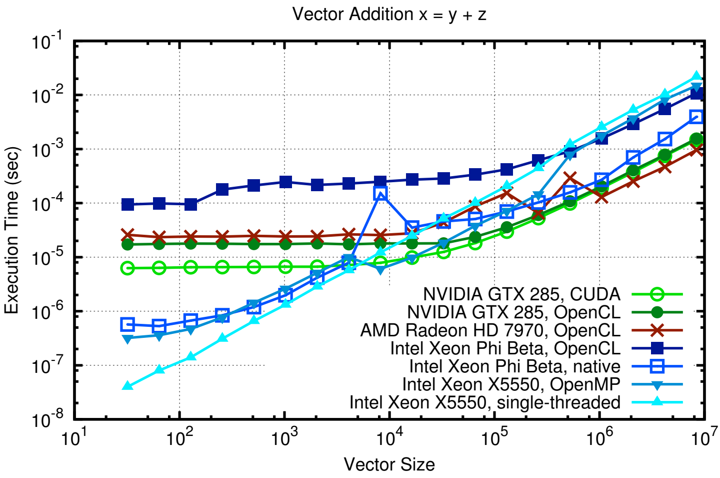
```
  // x[4:8] = a * y[2:6] + b * z[3:7]
  __kernel void avbv(
    double * x, uint off_x,
    double a,
    double * y, uint off_y,
    double b,
    double * z, uint off_z, uint size)
{
  size_t i = get_global_id(0);
  for (; i<size; i += get_global_size())
    x[off_x + i] = a * y[off_y + i] + b * z[off_z + i
        ];

}
```

Generalizing compute kernels

```
  // x[4:2:8] = a * y[2:2:6] + b * z[3:2:7]
  __kernel void avbv(
    double * x, uint off_x, uint inc_x,
    double a,
    double * y, uint off_y, uint inc_y,
    double b,
    double * z, uint off_z, uint inc_z, uint size)
{
  size_t i = get_global_id(0);
  for (; i<size; i += get_global_size())
    x[off_x + i * inc_x] =  a * y[off_y + i * inc_y]
                          + b * z[off_z + i * inc_z];
}
```

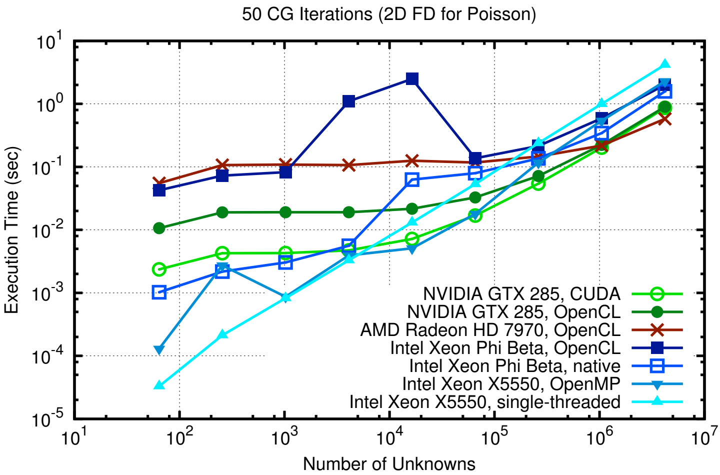
No penalty on NVIDIA GPUs because FLOPs are for free

Benchmarks



Vector Addition x = y + z
Execution Time (sec)
Vector Size
NVIDIA GTX 285, CUDA
NVIDIA GTX 285, OpenCL
AMD Radeon HD 7970, OpenCL
Intel Xeon Phi Beta, OpenCL
Intel Xeon Phi Beta, native
Intel Xeon X5550, OpenMP
Intel Xeon X5550, single-threaded

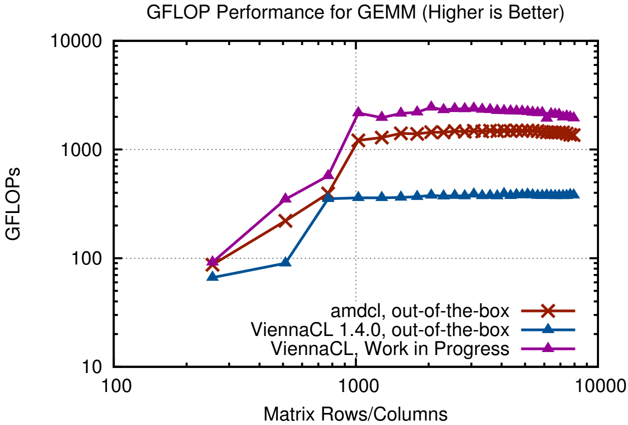
Benchmarks



50 CG Iterations (2D FD for Poisson)
Execution Time (sec)
Number of Unknowns
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
NVIDIA GTX 285, CUDA
NVIDIA GTX 285, OpenCL
AMD Radeon HD 7970, OpenCL
Intel Xeon Phi Beta, OpenCL
Intel Xeon Phi Beta, native
Intel Xeon X5550, OpenMP
Intel Xeon X5550, single-threaded

Matrix-Matrix Multiplication

Autotuning environment



(AMD Radeon HD 7970, single precision)

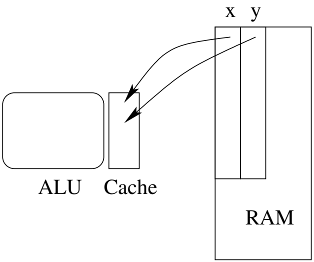
Expression Template Limitations

Expression Templates are Not Enough

Consider

```
u = x + y;
v = x - y;
```

Suboptimal performance with almost any library

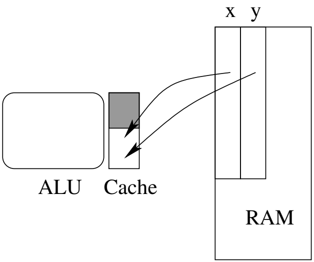


Expression Templates are Not Enough

Consider

```
u = x + y;
v = x - y;
```

Suboptimal performance with almost any library



Expression Template Limitations

Expression Templates are Not Enough

Consider

```
u = x + y;
v = x - y;
```

Suboptimal performance with almost any library

OpenCL Kernel Generation

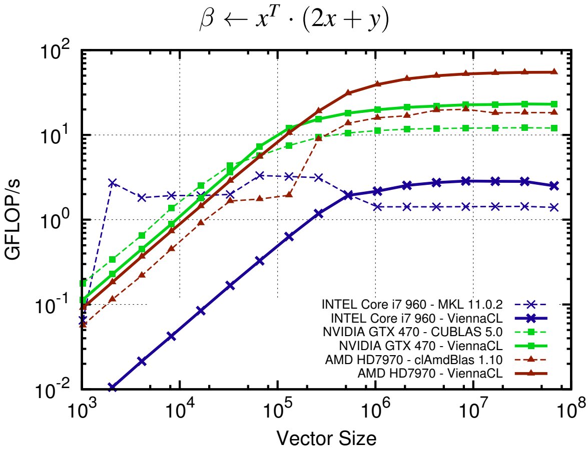
Separate temporary avoidance from operation execution

```
custom_operation op;
op.add( u = x + y );
op.add( v = x - y );
op.execute();          // OpenCL JIT
```

Fully transparent kernel fusion scheduled for release 1.5.0

Expression Template Limitations

Benchmark Results

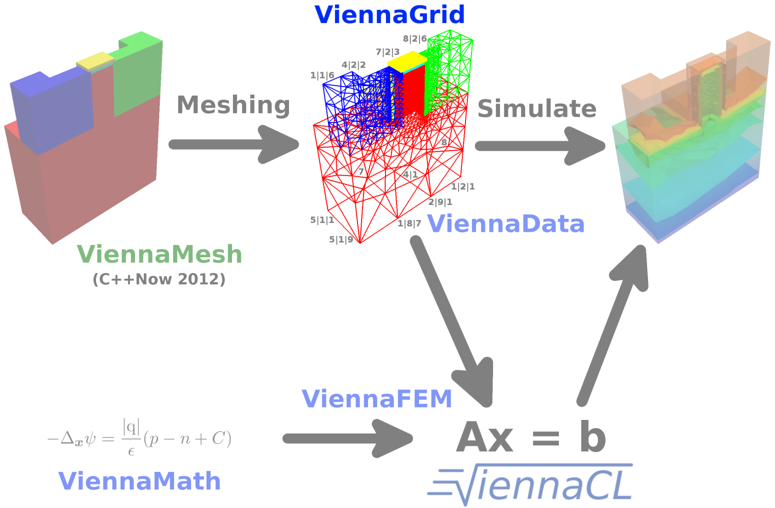


Tillet *et al.*, HotPar '13

Contents

Part 2: ViennaGrid

Simulation Flow



What about Boost.Geometry?

A Quick Look at Boost.Geometry

Concepts: Point, Segment, Linestring, Box, etc.

Algorithms: `distance()`, `intersects()`, `convex_hull()`, etc.

Central entity: Point

```
int a[3] = {1, 2, 3};
int b[3] = {2, 3, 4};

double d = boost::geometry::distance(a, b);
```

Why Boost.Geometry is Not Enough

What about 3D objects? Tetrahedra? Hexahedra?

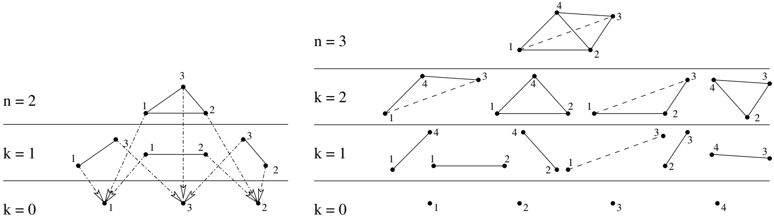
Traversal of boundary objects missing

No storage facilities for *many* objects

n-cell Concept

Concept of n-*cell*

Sub-k-cells of an n-cell



Separation of Geometry and Topology

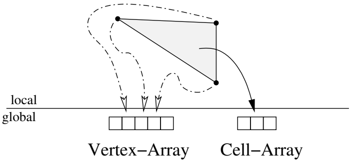
Geometry: Euclidian space, coordinate system

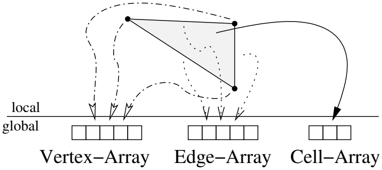
Topology: Connection between points (lines, triangles, etc.)

Datastructure Requirements

Don’t store boundary k-cells unnecessarily

Fast local iteration on k-cells





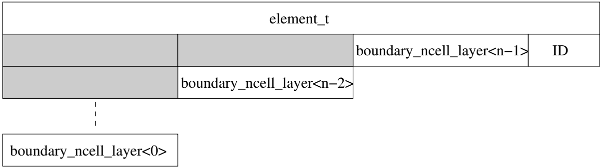
	Amount	Mem/Obj.	Total Mem.
Vertices	4913	24 B	115 KB
Edges	31024	16 B	485 KB
Facets	50688	48 B	2376 KB
Cells	24576	112 B	2688 KB
Total			**5664 KB**

	Amount	Mem/Obj.	Total Mem.
Vertices	4913	24 B	115 KB

n-cell Implementation

Implementation of `element_t`

- Recursive inheritance from boundary layer of dimension $n - 1$
- Tag dispatching to enable/disable topological layers




```
template <typename ConfigType, typename ElementTag>
class element_t :
  public boundary_ncell_layer<ConfigType, ElementTag, ElementTag::
      dim-1>,
  public result_of::element_id_handler<ConfigType, ElementTag>::
      type
```

Domain Configuration

Top Level Configuration of Domain

- Mostly a collection of tags
- Predefined configuration classes for common cases
- ViennaGrid 1.0.x: Supplemented by global customizations

```
struct triangular_3d
{
  typedef double              numeric_type;
  typedef cartesian_cs<3>    coordinate_system_tag;
  typedef triangle_tag        cell_tag;
};

result_of::domain<triangular_3d>::type     Domain;
```

- Work in progress: Everything in a single config class

User API Design Goals

- STL-style, reuse conventions
- Allow index-based traversal
- Avoid common C++ pitfalls (e.g. template member functions)

```
//iteration over all vertices in the domain:
typedef result_of::ncell_range<DomainType, 0>::type  VertexRange;
typedef result_of::iterator<VertexRange>::type       VertexIterator
     ;

VertexRange vertices = ncells<0>(domain);
for (VertexIterator it  = vertices.begin();
                    it != vertices.end();
                  ++it)
{
  // do something with each vertex here
}
```

- *Ranges* provide iterators over n-cells
- Extendible

ViennaGrid User API

User API Design Goals

- STL-style, reuse conventions
- Allow index-based traversal
- Avoid common C++ pitfalls (e.g. template member functions)

```
//iteration over all vertices in the domain:

for (std::size_t i = 0; i < ncells<0>(domain).size(); ++i)
{
  // do something with ncells<0>(domain)[i] here
}
```

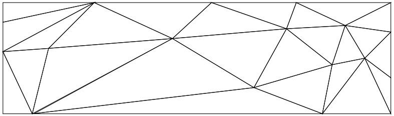
- OpenMP friendly
- `.size()` sometimes known at compiletime!

ViennaGrid User API

User API Design Goals

Boundary iteration: $k < n$

Coboundary iteration: $k > n$



```
//iteration over all triangles of a vertex
typedef result_of::ncell_range<VertexType, 2>::type  TriangleRange;
typedef result_of::iterator<TriangleRange>::type
     TriangleIterator;

TriangleRange triangles = ncells<2>(vertex, domain);
for (TriangleIterator it  = triangles.begin();
                      it != triangles.end();
                    ++it)
{
  // do something with each triangle here
}
```

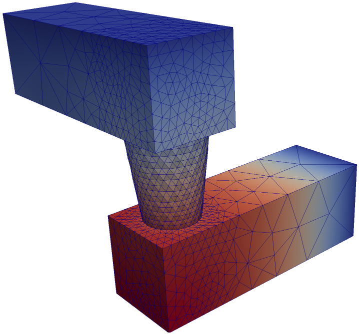
Coboundary information not a-priori available in datastructure

Built and cached at first request

ViennaGrid Features

Other Features

- Segments
- I/O: VTK, various mesh-format
- Voronoi information
- Refinement

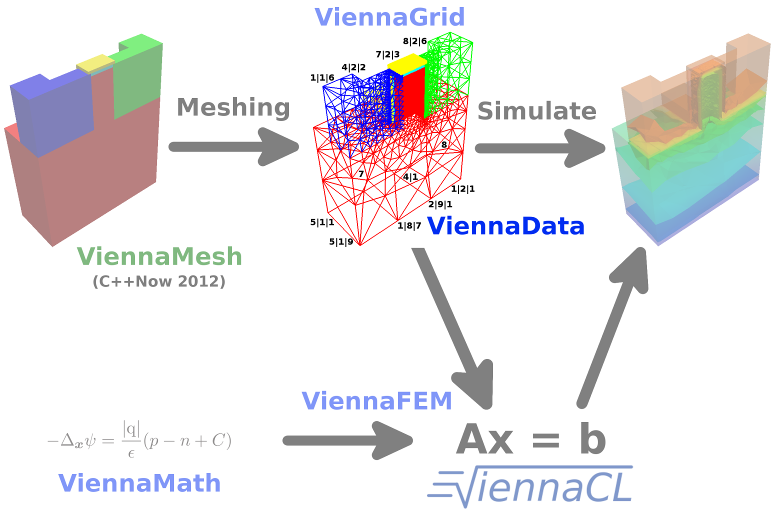


Work in Progress

- PLC, hybrid meshes, multigrid

Part 3: ViennaData

Simulation Flow



Data Storage

Plain Object-Oriented Approach?

```
struct Triangle {
 PointType a, b, c;
 bool is_on_boudary;
 double rho; };   //e.g. specific mass
```

Pros and Cons

- Data is directly stored with the object
- Each (!) triangle carries a boolean flag
- Reusability reduced ⇒ better rename to `TriangleWithMaterial`

Monolithic, don’t do this!

Data Storage

Store Data with Mesh:

```
class Mesh {
 vector<Triangle> triangles;
 std::map<size_t, bool>  boudary_map; //no memory
     wasted
 vector<double> rho_for_triangles;   };
```

Pros and Cons

`Triangle` is still reusable

`Mesh` class has to handle data storage complexity

Each additional data requires a change of `Mesh` class

`Mesh` object has to be passed to all modules

Monolithic, don’t do this!

Approach by ViennaData

- Introduction of a hidden data container
- Data is stored in a map-like manner using keys

```
//generic interface:
viennadata::access<KeyType, ValueType>(key)(obj);

//boundary flag and specific mass retrieval for triangle:
bool on_boundary = access<BoundaryKeyType, bool>(boundary_key)(
     triangle);
double       rho = access<MassKeyType,   double>(    mass_key)(
     triangle);
```

Pros and Cons

+ `Triangle` and `Mesh` are still reusable
+ Can be used with arbitrary objects (third-party libraries)
+ Unified interface for data access
– Global state

Generic Interface

```
viennadata::access<KeyType, ValueType>(key)(obj);
```

Default Storage Scheme

If nothing is known about the object:

```
std::map<ObjectType *,
         std::map<KeyType, ValueType> >
```

The compiler creates such a map for each of the following:

```
access<long, double>(42)(triangle);
access<char, double>('b')(triangle);
access<std::string, double>("mass")(triangle);
access<std::string, double>("mass")(vertex);
```

Performance Considerations

$\mathcal{O}(\log N) + \mathcal{O}(\log K)$ access time

N ... objects of same type (e.g. triangles)

K ... keys of same type

Usually too slow in a high-performance setting

Can We Do Better?

In general: No

In certain situations: Yes

Type-based Key Dispatch

- Only one key per type
- $\mathcal{O}(\log N)$ access time

```
access<mass_key, double>(mass_key())(triangle);

// or:
access<mass_key, double>()(triangle);
```

Internal Datastructure

```
std::map<ObjectType *, ValueType>
```

- Transparent to user
- One line of code for activation

Numeric IDs for Objects

- Only one key per type
- $\mathcal{O}(K)$ access time
- $\mathcal{O}(1)$ access time with type-based key dispatch

```
access<std::string, double>("mass")(triangle);

// with type-based key dispatch:
access<mass_key, double>()(triangle);
```

Internal Datastructure

```
std::vector<ValueType>
```

- Transparent to user
- One line of code for activation
- Overload generic `id()` accessor

Benchmarking ViennaData

- ID-based access to data via ViennaData (class `LightWeight`)
- OOP-style storage in classes with payload

```
template <size_t N>
struct FatClass {
  double data;
  char payload[N];
};
```

	10^3 Objects (us)	10^6 Objects (ms)
`LightWeight`	**4**	**5**
`FatClass<10>`	**1.3**	**4**
`FatClass<100>`	2.1	11
`FatClass<1000>`	2.5	11

Other Routines

Not further addressed:

```
viennadata::copy<KeyType, ValueType>(key)(
    src_obj, dst_obj);
viennadata::move<KeyType, ValueType>(key)(
    src_obj, dst_obj);
viennadata::find<KeyType, ValueType>(key)(obj);

viennadata::erase<KeyType, ValueType>(key)(obj);
viennadata::erase<KeyType, all>(key)(obj);
viennadata::erase<all, ValueType>(key)(obj);
```

Pitfalls

Inheritance

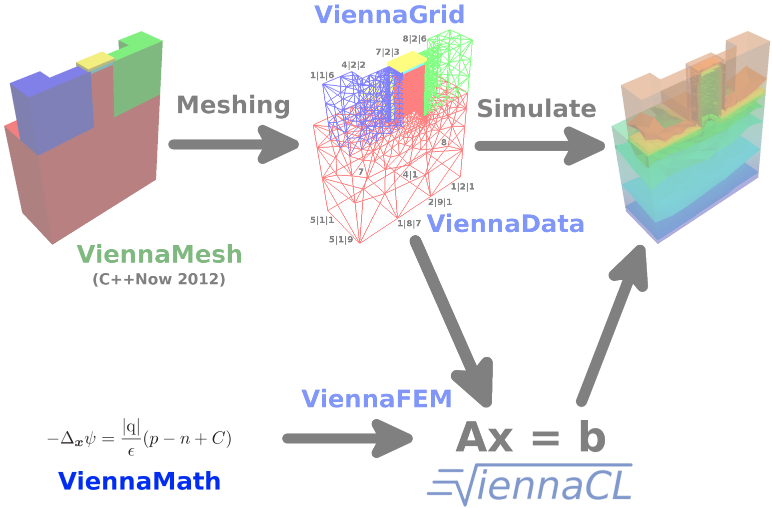
Limited lifetime of objects

Compilation units with different configuration

Contents

Part 4: ViennaMath

Simulation Flow



A Symbolic Math Library in C++

- Symbolic evaluation and manipulation of math expressions
- Unified run time and compile time interface
- Differentiation and integration provided
- LaTeX output

Example Usage

```
variable x(0);
variable y(1);
variable z(2);
expr f = x + y - z;
expr g = f * f;
eval(f, make_vector(1.0, 2.0, 4.0)); // returns
    -1.0
eval(g, make_vector(1.0, 2.0, 4.0)); // returns
    1.0
```


Run Time Evaluation

A Symbolic Math Library in C++

- Symbolic evaluation and manipulation of math expressions
- Unified run time and compile time interface
- Differentiation and integration provided
- LaTeX output

Example Usage

```
ct_variable<0> x;
ct_variable<1> y;
ct_variable<2> z;
ct_constant<1> c1;
ct_constant<2> c2;
ct_constant<4> c4;
eval(x + y - z, make_vector(c1, c2, c4)); //
    returns -1
```

- Compile Time Evaluation

Substitution and Differentiation (Run Time)

```
variable x(0);
variable y(1);
variable z(2);
substitute(x, y, x*y + z); // returns y*y+z
diff(x*y + z, x);          // returns y
```

Substitution and Differentiation (Compile Time)

```
ct_variable<0> x;
ct_variable<1> y;
ct_variable<2> z;
substitute(x, y, x*y + z); // returns y*y+z
diff(x*y + z, x);          // returns y
```

Numerical Integration (Run Time): $\int_0^1 x^2 \,\mathrm{d}x$

```
expr f = integral( make_interval(0, 1), x*x, x );

numerical_quadrature integrator(new gauss_quad_1())
    ;
integrator(f);                                    //
    method 1
integrator(make_interval(0, 1), x*x, x);          //
    method 2
```

Analytical Integration (Compile Time): $\int_0^1 x^2 \,\mathrm{d}x$, $\int_0^1 \int_0^{1-x} xy \,\mathrm{d}x\mathrm{d}y$

```
integrate(make_interval(c0, c1),
          x*y,
          x );    //returns y/2.0
integrate(make_interval(c0, c1),
          integrate( make_interval(c0, c1 - x), x*y
```

Function Symbols

Represent a function (not evaluable)

Differential Operators

Gradient, Divergence

Symbolic Integration Domain

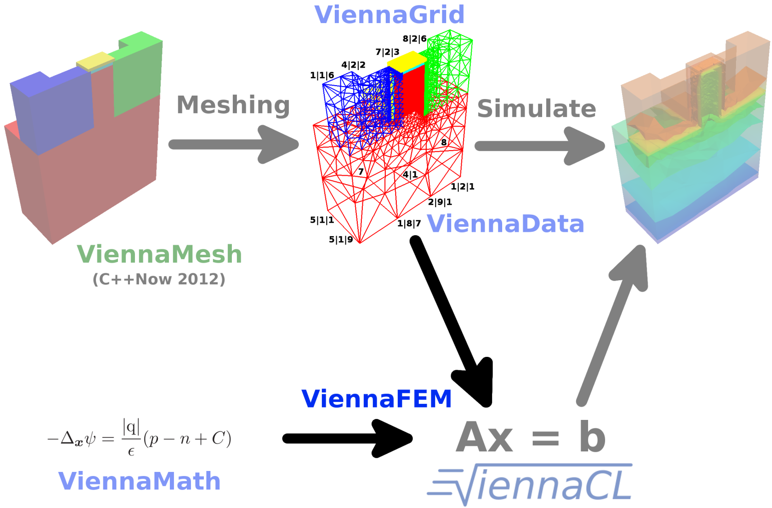
Specify actual integration domain and integration variables *later*

```
function_symbol u;
equation eq( laplace(u), 1.0 );  // Poisson
    equation

function_symbol v;
expr w = integral(symbolic_interval(),
                  grad(u) * grad(v));
```

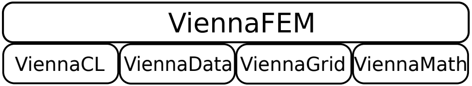
Contents

Part 5: ViennaFEM

Simulation Flow



Simulation Flow



Library-Centric Design

- ViennaCL for linear solver
- ViennaData for data storage
- ViennaGrid for mesh handling
- ViennaMath for symbolic math

Addresses Come&Go in Academia

- Focus on one package
- No in-depth knowledge of all packages required
- Additional emphasis on good interfaces

ViennaFEM

ViennaGrid deals with the Mesh

```
DomainType my_domain;
viennagrid::io::netgen_reader my_reader;
my_reader(my_domain, "mystructure.mesh");
```

Equation specification via ViennaMath: $\Delta u = -1$

```
equation poisson_eq = viennamath::make_equation(laplace(u), -1);
```

Assembly via ViennaFEM

```
viennafem::pde_assembler fem_assembler;
fem_assembler(viennafem::make_linear_pde_system(poisson_eq, u),
              my_domain,
              system_matrix, load_vector);
```

Linear solver provided by ViennaCL

```
VectorType pde_result
  = viennacl::linalg::solve(system_matrix, load_vector, cg_tag());
```

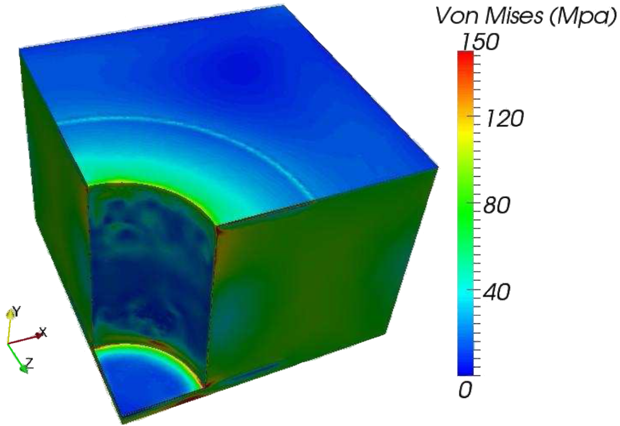
Lame equation for Linear Elasticity

$$\int_\Omega \varepsilon(u) : \sigma(v) \,\mathrm{d}\Omega = \int_\Omega F \cdot v \,\mathrm{d}\Omega \quad \forall v \in \mathcal{V}$$

With $F = (0, 0, 1)^\mathrm{T}$:

```
std::vector< Expression > strain = strain_tensor(u)
    ;
std::vector< Expression > stress = stress_tensor(v)
    ;

Equation weak_form_lame = make_equation(
           integral(symbolic_interval(),
                    tensor_reduce( strain, stress )
                        ),
           //=
           integral(symbolic_interval(),
                    constant(1.0) * v[2])
```

Solving Lame's Equation for a TSV



Summary

Software Packages

ViennaCL:	GPU-accelerated Linear Algebra
ViennaData:	Generic Data Storage
ViennaFEM:	Modular High-Level Finite Element Package
ViennaGrid:	Generic Mesh Datastructure
ViennaMath:	Symbolic Math Kernel

`http://vienna{cl,data,fem,grid,math}@sourceforge.ne`

Design Philosophy

- Orthogonal Software Design
- Convenient High-Level User API
- Avoid Unneeded Dependencies
- Free Open Source (MIT License)