Generic Programming for High Performance Numerical Linear Algebra

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Overview

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Introduction & Motivation

- Scientific software can benefit from software engineering methodologies
  - Development
  - Maintenance
- Perpetual interest in using C++ (e.g.) in scientific computing
- Common perception: Abstraction is the enemy of performance

Introduction & Motivation

- C++ can be used effectively in scientific computing (with concomitant software engineering benefits)
- Generic programming has some particular benefits in this domain
- Follow the theme of STL
- Keep high-performance always in mind

Combinatorial Explosion

- Four precision types
- Several dense storage types
- A multitude of sparse storage types
- Row and column oriented matrices
- Scaling and striding

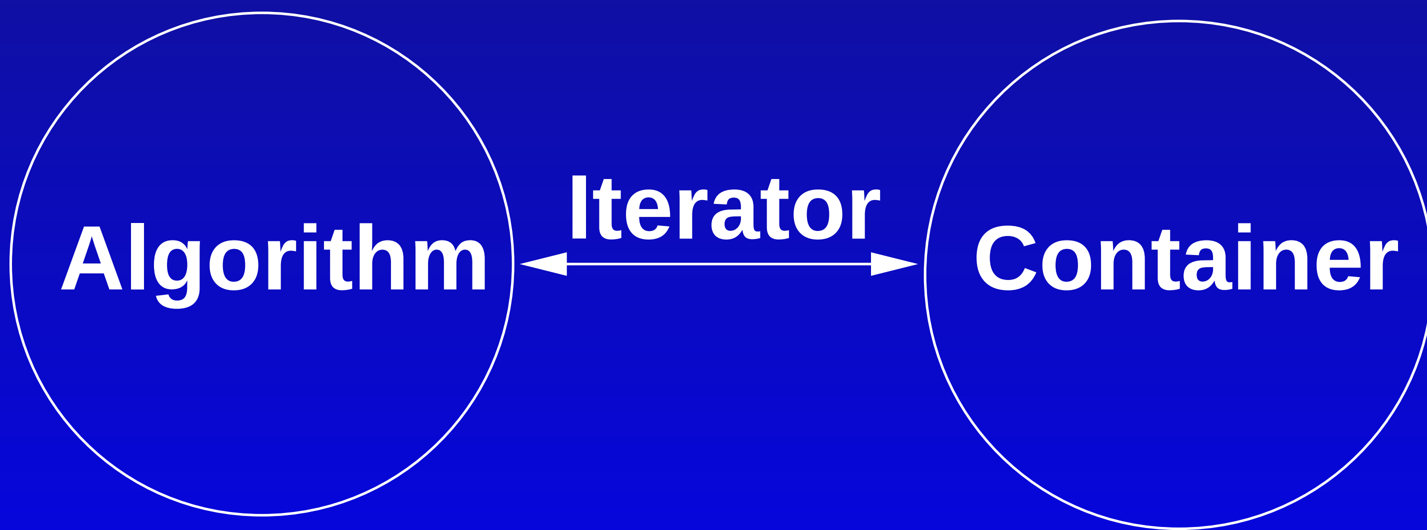
Combinatorial Explosion

- Unnecessary artifact of certain programming languages
- Algorithm expression also includes data type information
- Not necessary in certain other languages (most notably, C++)

Generic Programming

- Algorithms can be expressed independently of data storage formats
- Define standard *interfaces* for data storage components
- *iterators* are the interface between *containers* and algorithms
- E.g., The Standard Template Library
- High performance linear algebra *is* amenable to generic programming

Iterator Bridge Between Algorithms and Containers



Example of Generic Programming

```
template <class InIter, class T>
T accumulate(InIter first, InIter last, T init)
{
  while (first != last)
    init = init + *first++;
  return init;
}
// how it is used:
vector<double> x(10,1.0);
double sum = accumulate(x.begin(),x.end(),0.0);
```

Generic Algorithms for Linear Algebra

- Extend the generic style of programming to domain of linear algebra
- A matrix can be abstractly thought of as a *container of containers*
- Use *iterators* and *2-dimensional iterators* to traverse the matrix
- A large class of matrix types can be implemented with this interface.

The MTL Generic Algorithms

- Encompasses BLAS functionality
- A *single* algorithm typically used for all matrix and numeric types
- Index-less algorithms
- Sparse and dense algorithms unified
- Transpose, scaling, and striding handled by adapters, not the algorithm

Index-less Algorithms

- Iterate from `begin()` to `end()` of a vector.
- Iterate from `begin_rows()` to `end_rows()` (or columns) of a 2-D container.
- This side-steps traditional annoyances such as the difference between Fortran (from 1) and C (from 0) indexing.

Unifying Sparse and Dense

- Iterators hides difference in traversal
- `index()` method hides difference in indexing
- An example from a matrix-vector multiply.

```
for(j = i->begin(); not_at(j, i->end()); ++j)
  tmp += *j * x[j.index()];
```

A Generic Matrix-Vector Multiply

```
template <class Matrix,class IterX,class IterY>
void matvec::mult(Matrix A, IterX x, IterY y) {
  typename Matrix::row_2Diterator i;
  typename Matrix::RowVector::iterator j;
  for (i = A.begin_rows();
       not_at(i, A.end_rows()); ++i) {
    typename Matrix::PR tmp = y[i.index()];
    for(j=i->begin(); not_at(j,i->end()); ++j)
      tmp += *j * x[j.index()];
    y[i.index()] = tmp;
  }
}
```

Transpose, Scaling, and Striding

- Matrix and vector adapters
- An adapter wraps up an object an modifies its behavior

```
// y <- A' * alpha x

matvec::mult(trans(A),
             scale(x, alpha),
             stride(y, incy));
```

The MTL Components

- Iterators
- 1-D Containers
- 2-D Containers
- Orientation Adapter: Row and Column
- Shape Adapter: Banded, Triangle, Symmetric

```
triangle<row<array2D<dense1D<double>>>,lower>
```

The MTL Iterators

- For sparse vectors
- For dense vectors
- Strided iterator adapter
- Scaled iterator adapter
- Block iterator

The MTL 1-D Containers

- `dense1D` similar to STL's `vector` class
- `sparse1D` index-value pairs
- `compressed1D` separate index and value arrays
- `scaled1D` adapter class
- `strided` adapter class

```
triangle<row<array2D<dense1D<double>>>,lower>
```

The MTL 2-D Containers

- `array2D` composes 1-D containers into a matrix
- `dense2D` contiguous dense matrix
- `compressed2D` contiguous sparse matrix
- `scaled2D` adapter class

```
triangle<row<array2D<dense1D<double>>>,lower>
```

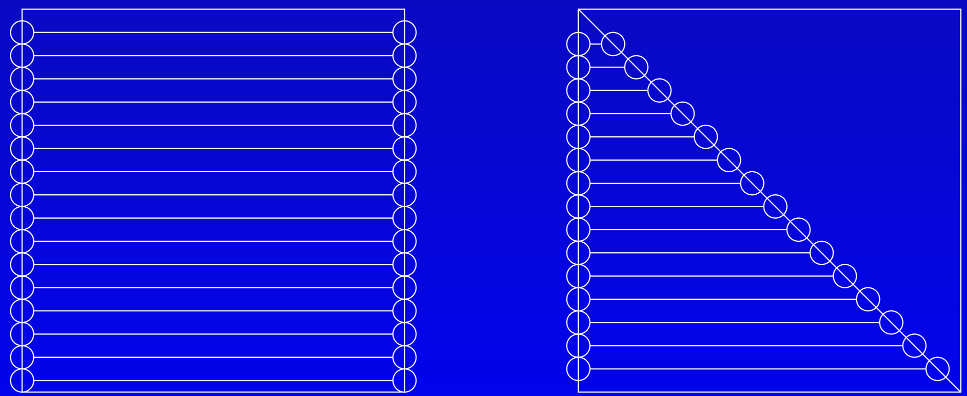
The MTL Orientation Classes

- Row Orientation
  - Maps row to *major*
  - Maps column to *minor*
- Column Orientation
  - Maps column to *major*
  - Maps row to *minor*
- All 2-D methods and typedefs are mapped.

```
triangle<row<array2D<dense1D<double>>>,lower>
```

The MTL Shape Adapters

- `banded`, `triangle`
- `symmetric`, `hermitian`



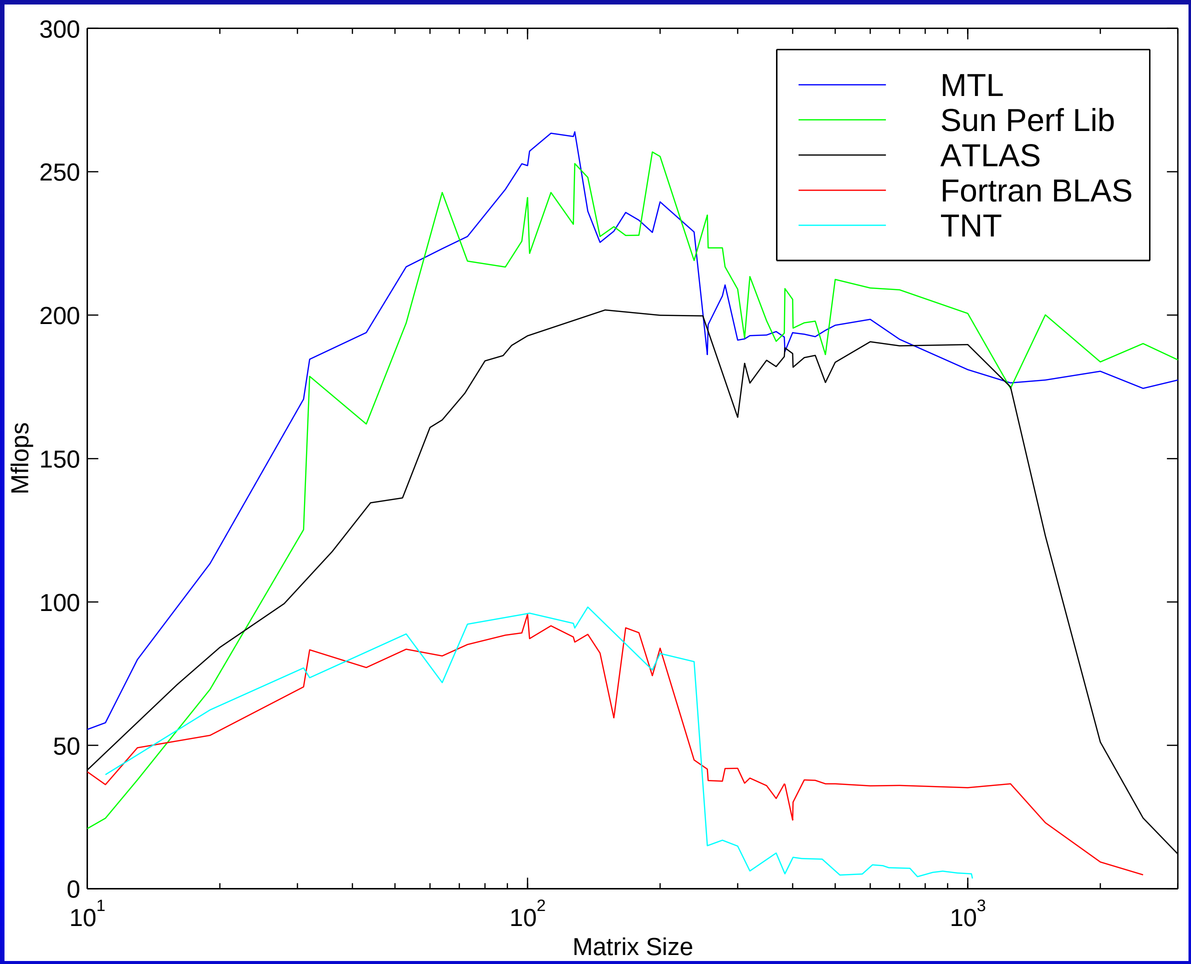
`triangle<row<array2D<dense1D<double>>>,lower>`

High Performance with C++

- Explicit unrolling and blocking in C++ using the BLAIS.
- Use a good optimizing compiler to remove layers of abstraction: lightweight object optimization and inlining.
- Follow a set of coding guidelines to ensure the above optimizations can be made, and double check the intermediate C code.
- Don't interfere with backend compiler unrolling and scheduling.

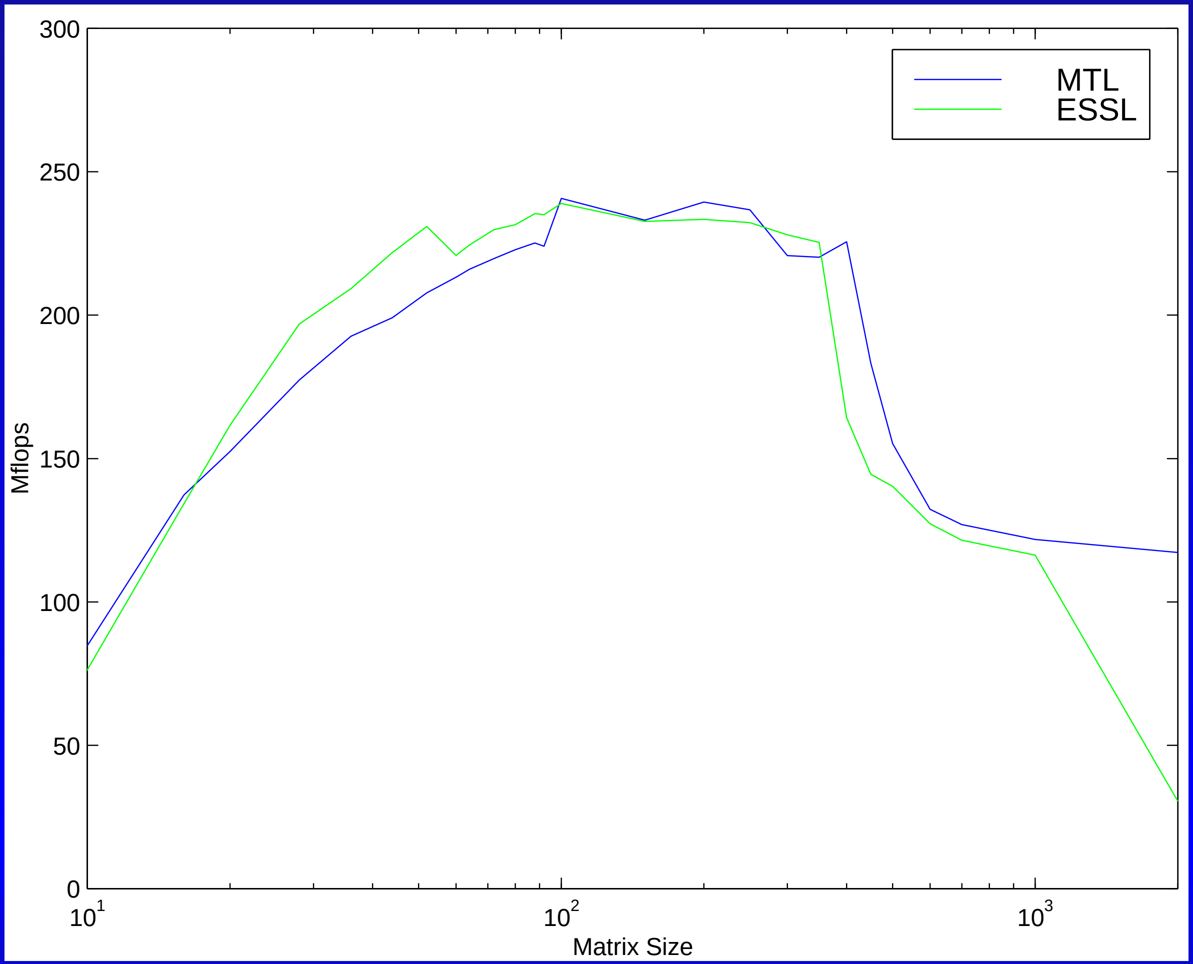
Dense Matrix-Matrix Performance

(UltraSPARC 170E)



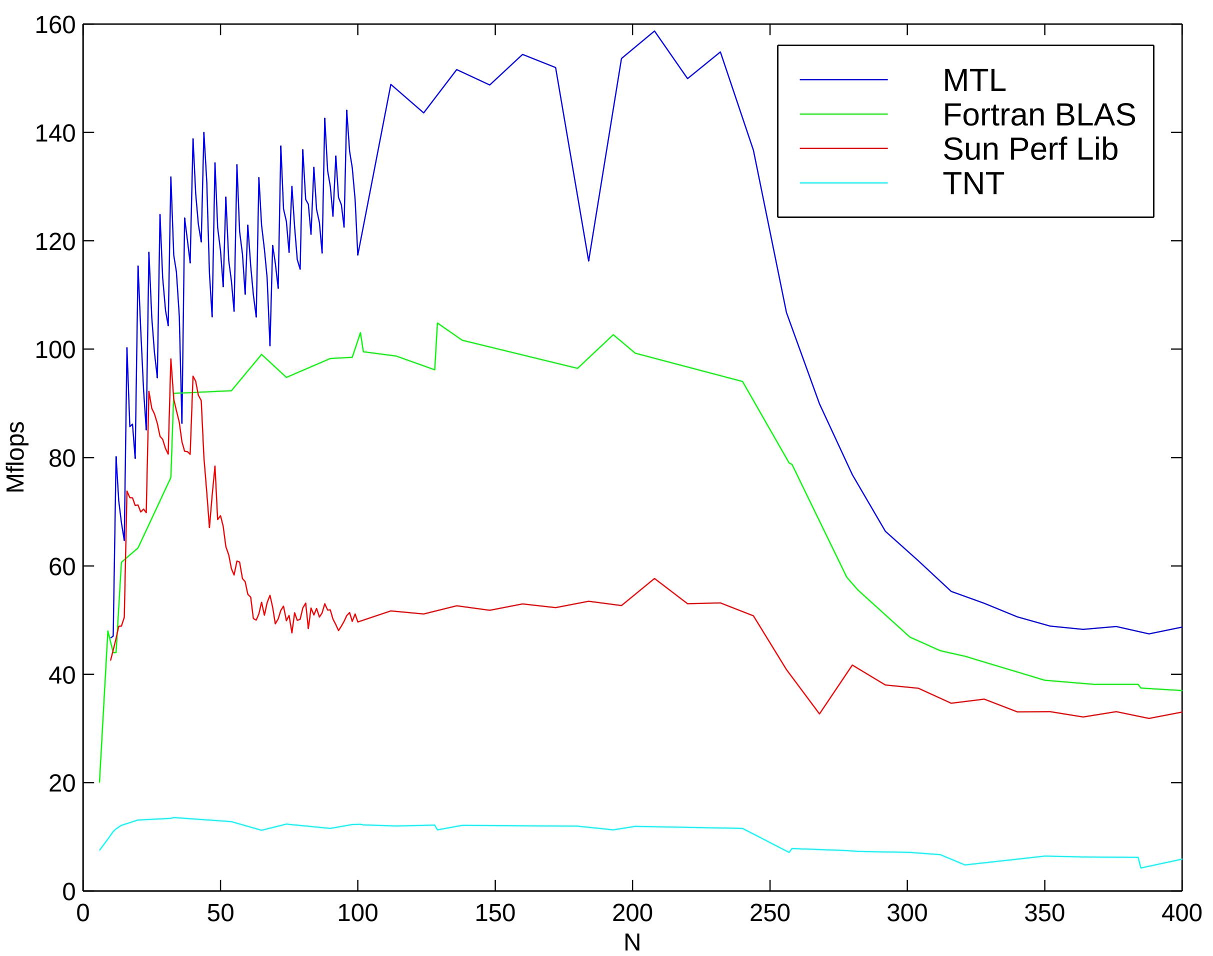
Dense Matrix-Matrix Performance

(RS6000 590)



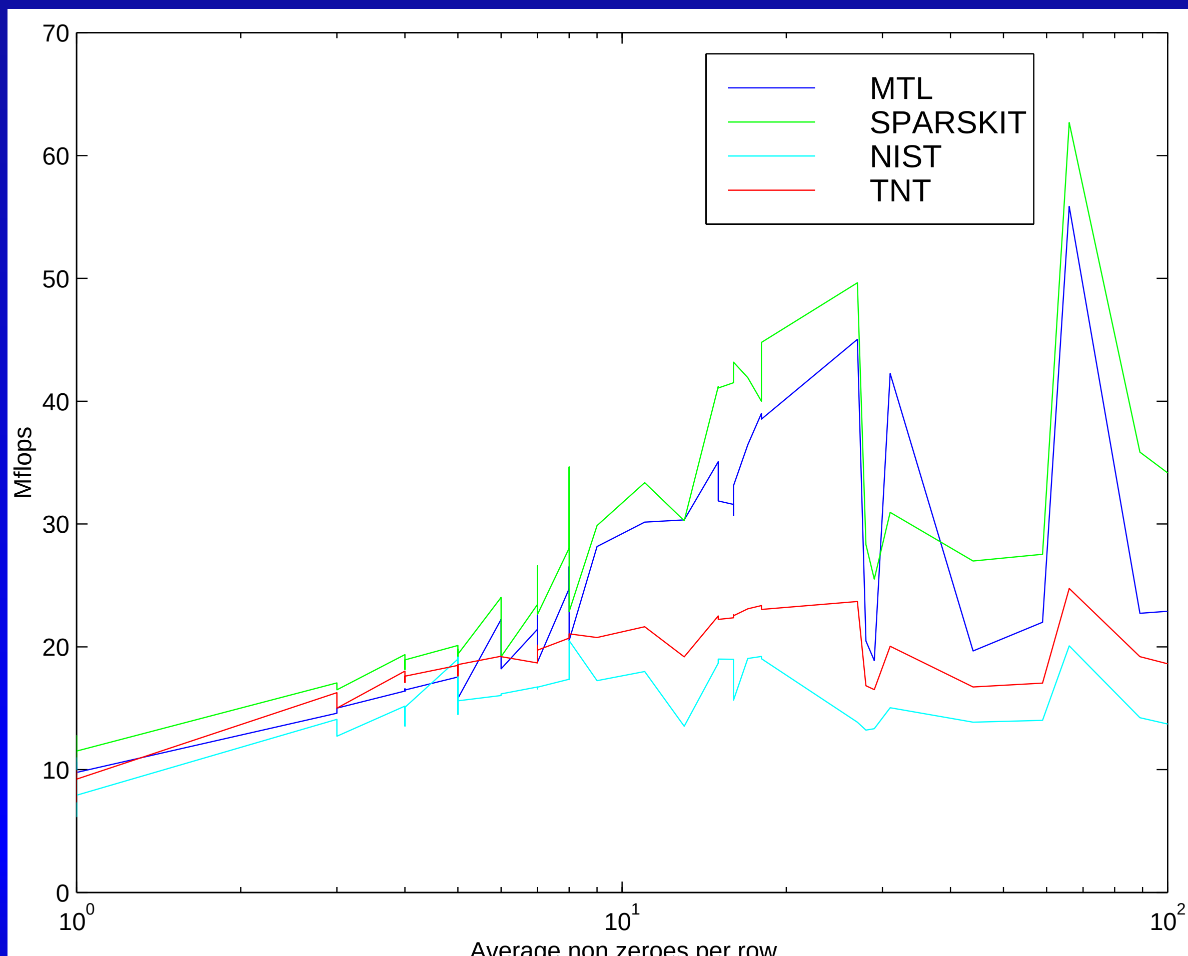
Dense Matrix-Vector Performance

(UltraSPARC 170E)



Sparse Matrix-Vector Performance

(UltraSPARC 170E)



Conclusion

- High performance linear algebra
- Comprehensive (sparse, dense, etc.) and orthogonal
- Only 25,000 lines of code
- 150,000 lines for Fortran BLAS