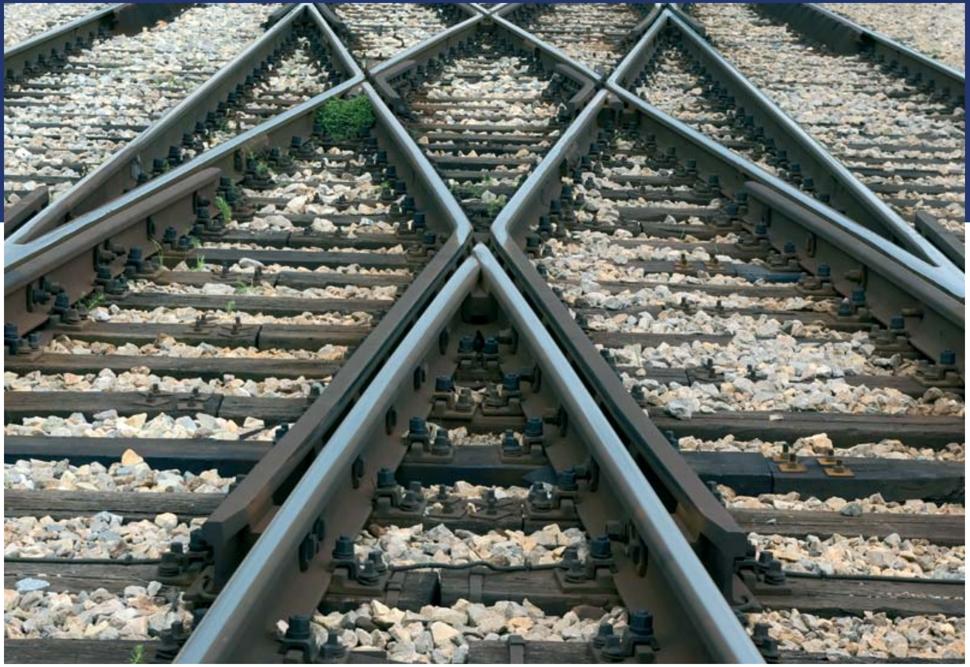
Advanced programming with OpenMP



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Programme of the lab

- OpenMP Tasks – parallel merge sort, parallel evaluation of expressions
- OpenMP SIMD – parallel integration to calculate π
- User-defined reduction – parallel summation of the matrix with collapsed for loops
- The sequential code of examples is available on Course Ware.

Sequential merge sort

```
...
void mergeSortRecursive(vector<double>& v, unsigned long left, unsigned long right)    {
        if (left < right)       {
                unsigned long mid = (left+right)/2;
                mergeSortRecursive(v, left, mid);
                mergeSortRecursive(v, mid+1, right);
                inplace_merge(v.begin()+left, v.begin()+mid+1, v.begin()+right+1);
        }
}

void mergeSort(vector<double>& v)       {
        mergeSortRecursive(v, 0, v.size()-1);
}
...
```

Sorting algorithm	Runtime
Sequential STL sort	20.981 s
Sequential Merge Sort	39.859 s

Number of elements to sort: 160000000
2 x Intel Xeon E5-2620 v2 @ 2.10GHz (in total 12 cores + HT)

Sequential merge sort

```
...
void mergeSortRecursive(vector<double>& v, unsigned long left, unsigned long right)     {
        if (left < right)       {
                if (right-left >= 32)   {
                        unsigned long mid = (left+right)/2;
                        mergeSortRecursive(v, left, mid);
                        mergeSortRecursive(v, mid+1, right);
                        inplace_merge(v.begin()+left, v.begin()+mid+1, v.begin()+right+1);
                } else {
                        sort(v.begin()+left, v.begin()+right+1);
                }
        }
}

void mergeSort(vector<double>& v)       {
        mergeSortRecursive(v, 0, v.size()-1);
}
...
```

Use fast O(n^2) algorithm to decrease the deepness of the recursion. Typically, Insert Sort performs very well for small arrays.

The sort from the C++ standard library is used to keep the code simple.

Sorting algorithm	Runtime
Sequential STL sort	20.981 s
Sequential Merge Sort	29.210 s (previously 39.9 s)

Number of elements to sort: 160000000
2 x Intel Xeon E5-2620 v2 @ 2.10GHz (in total 12 cores + HT)

Parallel sort in 5 minutes

```
...
void mergeSortRecursive(vector<double>& v, unsigned long left, unsigned long right)    {
        if (left < right)      {
                if (right-left >= 32)   {
                        unsigned long mid = (left+right)/2;
                         #pragma omp taskgroup
                         {
                                 #pragma omp task shared(v)
                                 mergeSortRecursive(v, left, mid);
                                mergeSortRecursive(v, mid+1, right);
                         }

                        inplace_merge(v.begin()+left, v.begin()+mid+1, v.begin()+right+1);
                } else {
                       sort(v.begin()+left, v.begin()+right+1);
                }
        }
}

void mergeSort(vector<double>& v)      {
        #pragma omp parallel
        #pragma omp single
        mergeSortRecursive(v, 0, v.size()-1);
}
...
```

Vector *v* is shared by all the tasks.

Wait for inner tasks.

Create pool of threads and start with one of them.

Sorting algorithm	Runtime
Sequential STL sort	20.981 s
Sequential Merge Sort	29.210 s
Parallel Merge Sort v1	25.569 s (1.14 x)

Parallel sort in 5 minutes

```
...
void mergeSortRecursive(vector<double>& v, unsigned long left, unsigned long right)    {
        if (left < right)      {
                if (right-left >= 32)   {
                        unsigned long mid = (left+right)/2;
                        #pragma omp taskgroup
                        {
                                #pragma omp task shared(v) untied if(right-left >= (1<<14))
                                mergeSortRecursive(v, left, mid);
                               mergeSortRecursive(v, mid+1, right);
                        }

                        inplace_merge(v.begin()+left, v.begin()+mid+1, v.begin()+right+1);
                } else {
                       sort(v.begin()+left, v.begin()+right+1);
                }
        }
}

void mergeSort(vector<double>& v)      {
        #pragma omp parallel
        #pragma omp single
        mergeSortRecursive(v, 0, v.size()-1);
}
...
```

Do not bind the task to CPUcore.

Create a new task only if the amount of work is sufficient.

Sorting algorithm	Runtime
Sequential STL sort	20.981 s
Sequential Merge Sort	29.210 s
Parallel Merge Sort v1	25.569 s (1.14 x)
Parallel Merge Sort v2	4.74 s (6.16 x)

Parallel sort in 5 minutes

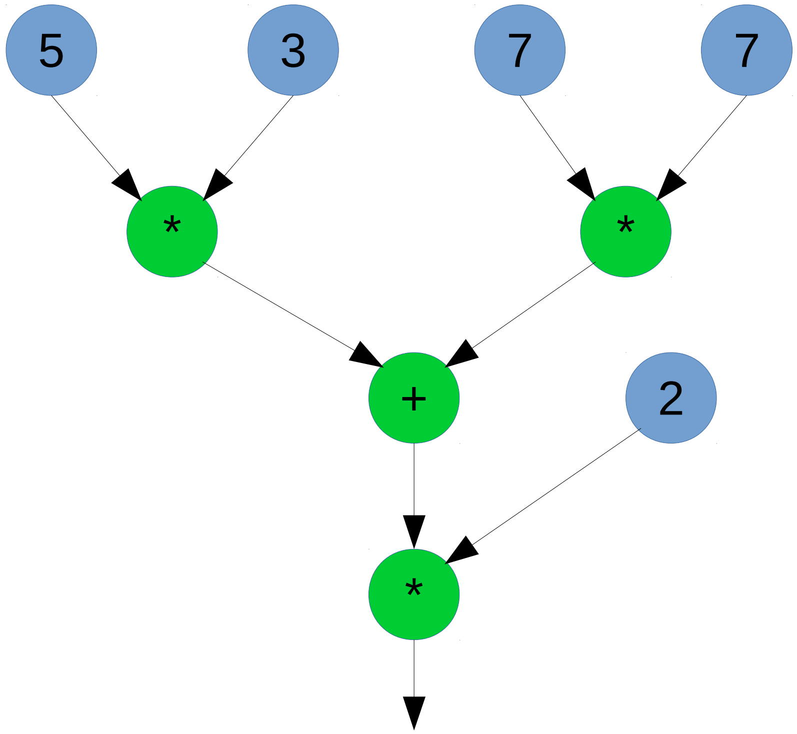
```
...
void mergeSortRecursive(vector<double>& v, unsigned long left, unsigned long right)     {
        if (left < right)       {
                if (right-left >= 32)   {
                        unsigned long mid = (left+right)/2;
                         #pragma omp taskgroup
                         {
                                 #pragma omp task shared(v) untied if(right-left >= (1<<14))
                                 mergeSortRecursive(v, left, mid);
                                 #pragma omp task shared(v) untied if(right-left >= (1<<14))
                                mergeSortRecursive(v, mid+1, right);
                                 #pragma omp taskyield
                         }

                        inplace_merge(v.begin()+left, v.begin()+mid+1, v.begin()+right+1);
                } else {
                        sort(v.begin()+left, v.begin()+right+1);
                }
        }
}

void mergeSort(vector<double>& v)       {
        #pragma omp parallel
        #pragma omp single
        mergeSortRecursive(v, 0, v.size()-1);
}
...
```

The current thread can be suspended.

Sorting algorithm	Runtime
Sequential STL sort	20.981 s
Sequential Merge Sort	29.210 s
Parallel Merge Sort v1	25.569 s (1.14 x)
Parallel Merge Sort v2	4.74 s (6.16 x)
Parallel Merge Sort v3	4.83 s (6.05 x)
Parallel Merge Sort v3 (48 threads)	4.42 s (6.61 x)

Tasks with dependencies

```
...
cout<<"Evaluating expression: 2*(5*3+7*7)"<<endl;
int term1 = 0, term2 = 0, total = 0;

#pragma omp parallel
#pragma omp single
{

    #pragma omp task depend(out: term1)
    {
        this_thread::sleep_for(seconds(2));
        term1 = 5*3;
    }

    #pragma omp task depend(out: term2)
    {
        this_thread::sleep_for(seconds(2));
        term2 = 7*7;
    }

    #pragma omp task depend(in: term1, term2) depend(out: total)
    {
        this_thread::sleep_for(seconds(1));
        total = term1+term2;
    }

    #pragma omp task depend(in: total)
    {
        this_thread::sleep_for(seconds(2));
        total *= 2;
    }

    #pragma omp taskwait
    cout<<"Final value of the expression: "<<total<<endl;
}
...
```



What is the sequential (parallel) evaluation time?

Calculation of pi

$$4 * \arctan(1) = \pi \qquad \int \frac{1}{1+x^2} = \arctan(x)$$

$$4 \int_0^1 \frac{1}{1+x^2} = 4\left(\arctan(1) - \underbrace{\arctan(0)}_{= 0}\right) = \pi$$

Calc of π	Runtime
Sequential version	5.41 s

10^9 of steps; 2 x Intel Xeon E5-2620 v2

```
...
double piIntStepTrapezoidalRule(int i, const double& step)      {
        double x = (i+0.5)*step;
        return 1.0/(1.0+x*x);
}
...
        ...
        double sum = 0.0, step = 1.0/nsteps;
        for (unsigned long i = 0; i < nsteps; ++i)
                sum += piIntStepTrapezoidalRule(i, step);

        double pi = 4.0*step*sum;
        ...
```

Calculation of pi - vectorization

```
...
#pragma omp declare simd
double piIntStepTrapezoidalRule(int i, const double& step)      {
        double x = (i+0.5)*step;
        return 1.0/(1.0+x*x);
}
...
        ...
        double sum = 0.0, step = 1.0/nsteps;
         #pragma omp simd reduction(+: sum)
        for (unsigned long i = 0; i < nsteps; ++i)
                sum += piIntStepTrapezoidalRule(i, step);

        double pi = 4.0*step*sum;
         ...
```

Calc of π	Runtime
Sequential version	5.41 s
Vectorized version	2.71 s (2.0 x)

10^9 of steps; 2 x Intel Xeon E5-2620 v2

The parallel processing of multiple data is hidden in hardware, the program behaves like a sequential version from the programmer point of view.

To verify that code was vectorized, you can compile with ‘**-fopt-info-vec**’ argument (GCC).

```
$ g++ -fopenmp -fopt-info-vec -std=c++11 -march=native -O2 -o
CalcOfPi CalcOfPi.cpp
CalcOfPi.cpp:36:42: note: loop vectorized
CalcOfPi.cpp:10:15: note: loop vectorized
```

Not all the code is vectorizable (loop dependencies)!

Calculation of pi - parallelization

```
...
#pragma omp declare simd
double piIntStepTrapezoidalRule(int i, const double& step)     {
        double x = (i+0.5)*step;
        return 1.0/(1.0+x*x);
}
...
        ...
        double sum = 0.0, step = 1.0/nsteps;
         #pragma omp parallel for simd reduction(+: sum)
        for (unsigned long i = 0; i < nsteps; ++i)
                sum += piIntStepTrapezoidalRule(i, step);

        double pi = 4.0*step*sum;
         ...
```

Calc of π	Runtime
Sequential version	5.41 s
Vectorized version	2.71 s (2.0 x)
Parallel SIMD version	0.26 s (20.8 x)

10^9 of steps; 2 x Intel Xeon E5-2620 v2

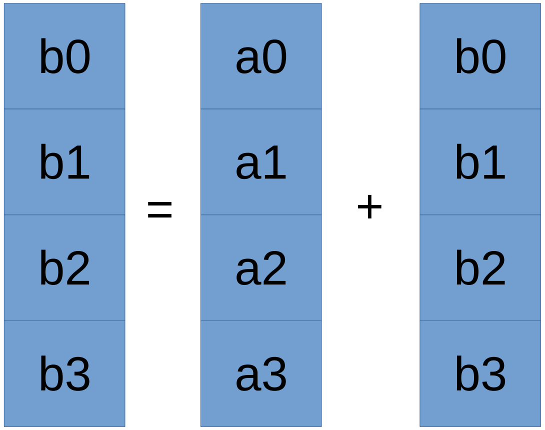
- Two/three dimensional integration can be significantly accelerated. To improve the accuracy other integration rules (e.g. Simpson rule) are used in practice
- How many arithmetical operations are performed per integration step? What is the slowest operation?
- Although the speedup is amazing the algorithm achieves only 23 GFlops/s (10 % of the peak), how is it possible?

OpenMP - user-defined reduction

```
...
// User defined reduction for vectors.
#pragma omp declare reduction(+ : MatrixColumn : transform(omp_in.cbegin(),  omp_in.cend(),\
                omp_out.begin(), omp_out.begin(), plus<double>())) initializer(omp_priv(omp_orig))

// Sum all the entries in the matrix.
MatrixColumn sumOfRows(M, 0.0);
#pragma omp parallel for collapse(2) reduction(+: sumOfRows) if(M*N > 10e6)
for (int i = 0; i < M; ++i)     {
        for (int j = 0; j < N; ++j)
                sumOfRows[i] += m[i][j];
}

double totalSum = 0.0;
for (int i = 0; i < M; ++i)
        totalSum += sumOfRows[i];
...
```

It works effectively for all the shapes of the input matrix!

Illustration of vector reduction:



OpenMP – other topics.

- **Affinity of threads**
  - Threads are fixed to cores, especially useful for NUMA systems.
  - Since threads are not migrated between cores, the number of cache invalidations is reduced.
- **Device offloading** (Intel Xeon Phi, NVIDIA)
  - Extension of pragmas to support offloading of work to coprocessors, graphics cards, etc.
  - You can check a trivial demonstration on http://industrialinformatics.cz/xeon-phi-installation-gentoo-linux
- To get more information on the aforementioned topics you can check slides from Intel: http://www.lrz.de/services/compute/courses/x_lecturenotes/MIC_GPU_Workshop/Intel-03-OpenMP-in-a-Nutshell.pdf

That’s all!

Thanks you for your attention.