Standard Algorithms

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Recap I - Horner algorithm

Evaluating high order polynomial can be computationally expensive in terms of floating point operations.

Given a polynomial $p(x) = \sum_{i=0}^{n} a_i x^i$, instead of directly evaluating all the monomials at x_0, we compute the following sequence:

$$\begin{aligned} b_n &= a_n, \\ b_{n-1} &= a_{n-1} + b_n x_0, \\ &\vdots \\ b_0 &= a_0 + b_1 x_0. \end{aligned}$$

The Horner rule exploits the already computed informations to reduce the number of floating point operations.

Curiosity: *Horner's rule is optimal when evaluating scalar polynomials sequentially.*

Recap II - Horner algorithm

1. Implement the `eval()` and `eval_horner()` functions to compute:

$$p_{\text{eval}}(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \ldots + a_n x^n,$$
$$p_{\text{Horner}}(x) = a_0 + x\,(a_1 + x\,(a_2 + x\,(a_3 + \ldots + x\,(a_{n-1} + x\,a_n)\ldots))).$$

2. Implement an `evaluate_poly()` function by manually looping over the input points.
3. → Modify `evaluate_poly()` to use **std::transform**.
4. → Implement an `evaluate_poly_parallel()` that makes use of the **parallel execution policies** of `std::transform` (available since `C++17`).
5. Convert `eval` and `eval_horner` from function pointers to `std::function`.
6. (*Homework*) Let the user choose from a json parameters file the degree of the polynomial and the discretization interval. The `json` library can be installed by running `./install_PACS.sh` from `${PACS_ROOT}/Extras/json`

NB: the parallel version requires to link against the Intel Threading Building Blocks (`TBB`) library (preprocessor flags `-I${mkTbbInc}`, linker flags `-L${mkTbbLib} -ltbb`).

A dive into std::algorithms & execution policies

Ingredients:

- lambdas & function objects
- C++17 standard algorithms and execution policies
- gcc toolchain and tbb module (or equivalent in the course docker/podman container)
- extra: ad-hoc compilers for offloading execution to devices (eg GPU, but works also on CPU), such as nvhpc container*.

*Can be built with:
`sudo docker run --gpus all -it --rm nvcr.io/nvidia/nvhpc:25.1-devel-cuda_multi-ubuntu24.04`
or
`singularity build nvhpc.sif docker://nvcr.io/nvidia/nvhpc:25.1-devel-cuda_multi-ubuntu24.04`
Requires proper drivers for GPU execution.

It takes some minutes to download, so, if you want to use it, it might be better to start the build now

Lambdas and Functors recap

1. Lambdas are un-named function objects

```
vector<real_t> v = {0, 1, 2, 3};
real_t a = 4.;
auto f = [&v,a](idx_t i) { return v[i] * a; };
cout << "4 = " << f(1) << endl;

struct __unnamed
{
 real_t s;
 vector <real_t>& v;
 real_t operator()(int i) { return v[i] * a;}
};
__unnamed f{a, v};
cout << "4 = " << f(1) << endl;
```

2. You can pass vectors also copying pointers (gpu safe, see last slides)

```
vector<real_t> v = {0, 1, 2, 3};
real_t a = 4.;
auto f = [v = v.data (), a](idx_t i) { return v[i] * a; };
cout << "4 = " << f(1) << endl;
```

C++17 Algorithms Recap

From for loops

```
vector <real_t> u (3), v = {0, 1, 2};
for (idx_t i = 0; i < u.size () ; ++i)
  u[i] =  v[i];
```

to std::algorithm

```
transform (v.cbegin (), v.cend (), u.begin (), [](const real_t & vi){return vi;});
```

That takes an optional `ExecutionPolicy&& policy` as first parameter

C++17 - C++20 Execution Policies - I

The execution policy types:

```
std::execution::sequenced_policy
std::execution::parallel_policy
std::execution::parallel_unsequenced_policy
std::execution::unsequenced_policy
```

have the following respective instances:

```
std::execution::seq,
std::execution::par,
std::execution::par_unseq, and
std::execution::unseq.
```

These instances are used to specify the execution policy of parallel algorithms, i.e., the kinds of parallelism allowed.

C++17 - C++20 Execution Policies - II

1. **seq**: requires that a parallel algorithm's execution may not be parallelized.
2. **par**: indicates that a parallel algorithm's execution may be parallelized. The invocations of element access functions in parallel algorithms invoked with this policy are permitted to execute in either the invoking thread or in a thread implicitly created by the library to support parallel algorithm execution.
3. **par_unseq**: indicates that a parallel algorithm's execution may be parallelized, vectorized, or migrated across threads. The invocations of element access functions in parallel algorithms invoked with this policy are permitted to execute in an unordered fashion in unspecified threads, and unsequenced with respect to one another within each thread.
4. **unseq** (C++20): indicates that a parallel algorithm's execution may be vectorized, e.g., executed on a single thread using instructions that operate on multiple data items.

Remark When using any parallel execution policy, it is the programmer's responsibility to avoid data races and deadlocks.

Indexing

In for loops we can use plain indices; given some functional `f` and vector v, we have

```
1 for (idx_t i = 0; i < v.size (); ++i)
2     v[i] = f(i);
```

In std::algorithms we can use:

- raw pointers (error prone, not suggested)
- index vectors (memory inefficient, not suggested)
- counting iterators (external library required)
- C++20 std::ranges and std::views (full support from C++23, eg, for n-dimensional arrays)

Raw pointers

Compute index as difference between each element memory address and raw pointer to vector data

```
1  std::transform (v.begin (), v.end (),
2                  [v = v.data(), f](real_t vi)
3                  {
4                    auto i = &vi - v;
5                    return f(i);
6                  });
```

Vectors of indices

Easiest solution, highly inefficient

```
1  std::vector <idx_t> indices (v.size ());
2  std::iota (indices.begin (), indices.end (), 0);
3  // now indices is {0,1,2...v.size()-1}
4  std::for_each (indices.begin (), indices.end (),
5                 [v = v.data()](idx_t i)
6                 {
7                   v[i] = f(i);
8                 });
```

Almost equal to the traditional for loop: ease of porting, but we are allocating a full vector of indices

Remark Avoid using vector of indices, it is shown here only for didactic purposes, to help giving an operational definition of counting iterators and views in this realm.

Counting iterators

One of the best available solutions, requires:

- C++17
- a library (boost and thrust are header only, it is enough to include them; boost is in the mk modules)

```
1 boost::counting_iterator <idx_t> first(0), last(v.size ());
2 std::for_each (first, last,
3                [v = v.data(), f](idx_t i)
4                {
5                  v[i] = f(i);
6                });
```

Remark: compile with `g++ -std=c++20 -I$mkBoostInc boost_example.cpp`

Ranges and views

One of the best available solutions; features:

- C++20 required, 23 for full support
- no external dependencies needed

C++20:

```
auto indices = std::views::iota (0, v.size ());
std::for_each (indices.begin (), indices.end (),
               [v = v.data()](idx_t i)
               {
                 v[i] = f(i);
               });
```

From C++23*

```
std::views::cartesian_product(std::views::iota (0, m), std::views::iota (0, n));
...
```

Remark: remember to `#include <ranges>` for the definition of `std::views::iota`

*In previous standards you could rely on proposals for missing features, eg https://github.com/ericniebler/range-v3, but, in case, it becomes competitive with boost

Example application: Single/Double precision A $\times$ X + Y

SAXPY and DAXPY stands for Single and Double-Precision A $\times$ X + Y
It is a basic operation in linear algebra and is commonly used in numerical computing.
We will use it to show examples of:

- basic std algoritghms usage
- efficient std algorithms usage
- parallel std algorithms usage and performance metrics (bandwidth)
- possible effects of floats precision

Saxpy - slow

Using STL defined std::algorithms only

```
1  void saxpy_slow (float a, std::vector <float> & x, std::vector <float> & y)
2  {
3    std::vector <float> temp (x.size ());
4    std::fill (temp.begin (), temp.end (), a);
5    std::transform (x.begin (), x.end (), temp.begin (), temp.begin (), std::
         multiplies <float> ());
6    std::transform (temp.begin (), temp.end (), y.begin (), y.begin (), thrust::plus
         <float> ());
7  }
```

Saxpy - fast - full example I

Using user-defined function object and `std::for_each`

```
1  #include <algorithm>
2  #include <iostream>
3  #include <vector>
4  #ifdef USE_BOOST
5    #include <boost/iterator/counting_iterator.hpp>
6  #else
7    #include <ranges>
8  #endif
9
10 using idx_t = size_t;
11 using real_t = float;
12
13 int main()
14 {
15   std::vector <real_t> x{0,1,2,3,4}, y{0,1,2,3,4};
16   real_t a (5.);
17
18   auto saxpy = [x = x.data (), y = y.data (), a]
19                (idx_t i)
20                { y[i] += a * x[i];};
21
22
```

Saxpy - fast - full example II

```
23    #ifdef USE_BOOST
24      boost::counting_iterator <idx_t> first(0), last(x.size ());
25      std::for_each (first, last, saxpy);
26    #else
27      auto indices = std::views::iota (static_cast<std::vector<real_t>::size_type>
            (0),  x.size ());
28      std::for_each (indices.begin (), indices.end (), saxpy);
29    #endif
30
31    for (idx_t i=0; i<x.size(); ++i)
32      std::cout << 5 << "x" << x[i] << "+" << x[i] << "=" << y[i] << std::endl;
33    return 0;
34  }
```

Compile with `g++ -std=c++20 -Wall saxpy.cpp -o views` , or:

```
1  source /u/sw/etc/bash.bashrc
2  module load gcc-glibc
3  module load boost
4  g++ -std=c++20 -Wall -I$mkBoostInc -DUSE_BOOST saxpy.cpp -o boost
```

and test with `./views` or `./boost`

Notes on parallel execution - I

- you can modify the above saxpy.cpp to run in parallel, adding `#include <execution>` and `std::execution::par_unseq` in the `for_each`
- if you use g++ (or clang++), you have to link against a parallel library, such as tbb. In our case, eg with boost, besides the above steps, we have:

```
1 module load tbb
2 g++ -std=c++20 -Wall -I$mkBoostInc -I$mkTbbInc -L$mkTbbLib -ltbb -DUSE_BOOST
      saxpy.cpp -o boost+tbb
3 ./boost+tbb
```

- if you have nvhpc sdk (software development toolkit), you can compile also with
  - cpu: `nvc++ -stdpar=multicore -std=c++20 -O4 -fast -march=native -Mllvm-fast -DNDEBUG -o saxpy saxpy.cpp`
  - NVIDIA gpu: `nvc++ -stdpar=gpu -std=c++20 -O4 -fast -march=native -Mllvm-fast -DNDEBUG -o saxpy saxpy.cpp`

Notes on parallel execution - II

- mind that GPUs are not CPUs with more threads; the hardware solutions introduced to achieve their parallelism and memory bandwidth requires constraints on the code, which currently, for nvc++, can be translated in the following recommendations:
  - prefer declaring and defining functions to be run on device in the same file (eg, define a full functor in a .hpp)
  - prefer dynamically allocated containers, such as std::vectors instead of std::arrays
  - avoid function pointers
  - avoid references in lambda captures
  - avoid exeptions

Notes on parallel execution - III

- for performance metrics, check the uploaded "bandwidth.cpp" example. You can compile with
  - `g++ -std=c++20 -Wall -Ofast -march=native -DNDEBUG -o daxpy_g++_tbb bandwidth.cpp -ltbb`
  - `clang++ -std=c++20 -Wall -O3 -ffast-math -march=native -DNDEBUG -o daxpy_clang++_tbb bandwidth.cpp -ltbb`
  - `nvc++ -stdpar=multicore -std=c++20 -Wall -O4 -fast -march=native -Mllvm-fast -DNDEBUG -o daxpy_nvc++_multicore bandwidth.cpp`
  - `nvc++ -stdpar=gpu -std=c++20 -Wall -O4 -fast -march=native -Mllvm-fast -DNDEBUG -o daxpy_nvc++_gpu bandwidth.cpp`
- and compare the results of, eg
  - `./daxpy_g++_tbb 1000000` and `./daxpy_nvc++_gpu 1000000`
  - `./daxpy_g++_tbb 100000000` and `./daxpy_nvc++_gpu 100000000`

  for `real_t=float` and `real_t=double`

Exercise (homework)

Return to our Horner - std::transform solution, and try to apply the new material.

References

- https://en.cppreference.com/
- https://developer.nvidia.com/
- https://www.boost.org/
- https://github.com/ericniebler