Assessing Performance Impact Of HPC in Vectorized Algorithms

[redacted]

```
library(ggplot2)
library(tidyverse)
```

Experiment Design

We implemented a PI estimation program based on the following reference implementation:

```
import numpy as np
points     = np.random.random((10000, 2))
points2    = np.square(points)
norm2      = np.sum(points2, axis=1)
num_inside = np.sum(norm2 <= 1.0)
4.0 * num_inside / 10000.0
```

```
## 3.1084
```

This is a monte-carlo approach where we estimated the ratio of the area of a circle with a radius of R over a square bounding that circle.

Since $S_{circle} = \pi * r^2$, $S_{square} = (2r)^2$, we have

$$\pi = 4 * \frac{S_{circle}}{S_{square}}$$

We can inspect the size and shape of these `ndarrays` by,

```
for v in ("points", "points2", "norm2"):
    d = locals()[v]
    print(f"{v}: size={d.size} shape={d.shape}")
```

```
## points: size=20000 shape=(10000, 2)
## points2: size=20000 shape=(10000, 2)
## norm2: size=10000 shape=(10000,)
```

Experiment Workflow

We defined two implementations(methods):

- `original`: Strictly reference Python implementation, create intermediate arrays for each step.
- `modified`: Complete all computations and reduction in one step.

This is implemented in source code:

```
...
if constexpr (original)
{
    result.method = "original";
    c2d<N, FP> coords_squared;

    // step1
    for (size_t i = 0; i < N; i++)
    {
        coords_squared.x[i] = coords.x[i] * coords.x[i];
        coords_squared.y[i] = coords.y[i] * coords.y[i];
    }

    FP norm2[N];
    // step2
    for (size_t i = 0; i < N; i++)
        norm2[i] = coords_squared.x[i] + coords_squared.y[i];

    // step3
    for (const FP &x : norm2)
        result.num_inside += x <= 1.0 ? 1 : 0;

    result.mem_footprint = (sizeof(coords) + sizeof(coords_squared) + sizeof(norm2));
}
else
{
    result.method = "modified";
    for (size_t i = 0; i < N; i++)
        result.num_inside += (coords.x[i] * coords.x[i] + coords.y[i] * coords.y[i]) <= 1.0 ? 1 : 0;

    result.mem_footprint = sizeof(coords);
}
...
```

We also defined three data locality modes:

- `none`: default NUMA binding, `numactl $argv`
- `local`: use the memory local to NUMA node, `numactl -N$i -m$i $argv`
- `shift`: use the memory next to the NUMA node, `numactl -N$i -m$((i+1)) $argv`

This is implemented in job script:

```
srun \
            -n1 -o out/$SLURM_JOBID/$output/none.out \
    parallel --lb -n0 -q numactl $argv ":::" (seq 0 $numa_bound) : \
            -n1 -o out/$SLURM_JOBID/$output/local.out \
    parallel --lb -q numactl -N{} -m{} $argv ":::" (seq 0 $numa_bound) : \
            -n1 -o out/$SLURM_JOBID/$output/shift.out \
    parallel -N2 --lb -q numactl -N{1} -m{2} $argv ":::" (seq 0 $numa_bound | line_shift)
```

We invoke the job script which requests a node for each of the 3 data locality modes, for we then spawn the program for each NUMA node (4 nodes on the `nvdimm` queue), the code will run both implementations in serial.

```
sbatch --wait job.sbatch.sh
./collect.sh
```

```
## Slurm JOBID=4957600
## 0: c100-010.frontera.tacc.utexas.edu
## 1: c100-011.frontera.tacc.utexas.edu
## 2: c100-012.frontera.tacc.utexas.edu
## Parallel over 4 NUMA nodes
## Running for upto N=50760940600
## Running with N= 1000
## Running with N= 10000
## Running with N= 100000
## Running with N= 1000000
## Running with N= 10000000
## Running with N= 100000000
## Running with N= 1000000000
## Running with N= 10000000000
```

After the job is complete we read in the output converted to CSV:

```
df <- read_csv("data.csv") %>%
    mutate(locality = recode(locality, "none" = "Default", "shift" = "Non-local", "local" = "Local"))
glimpse(df)
```

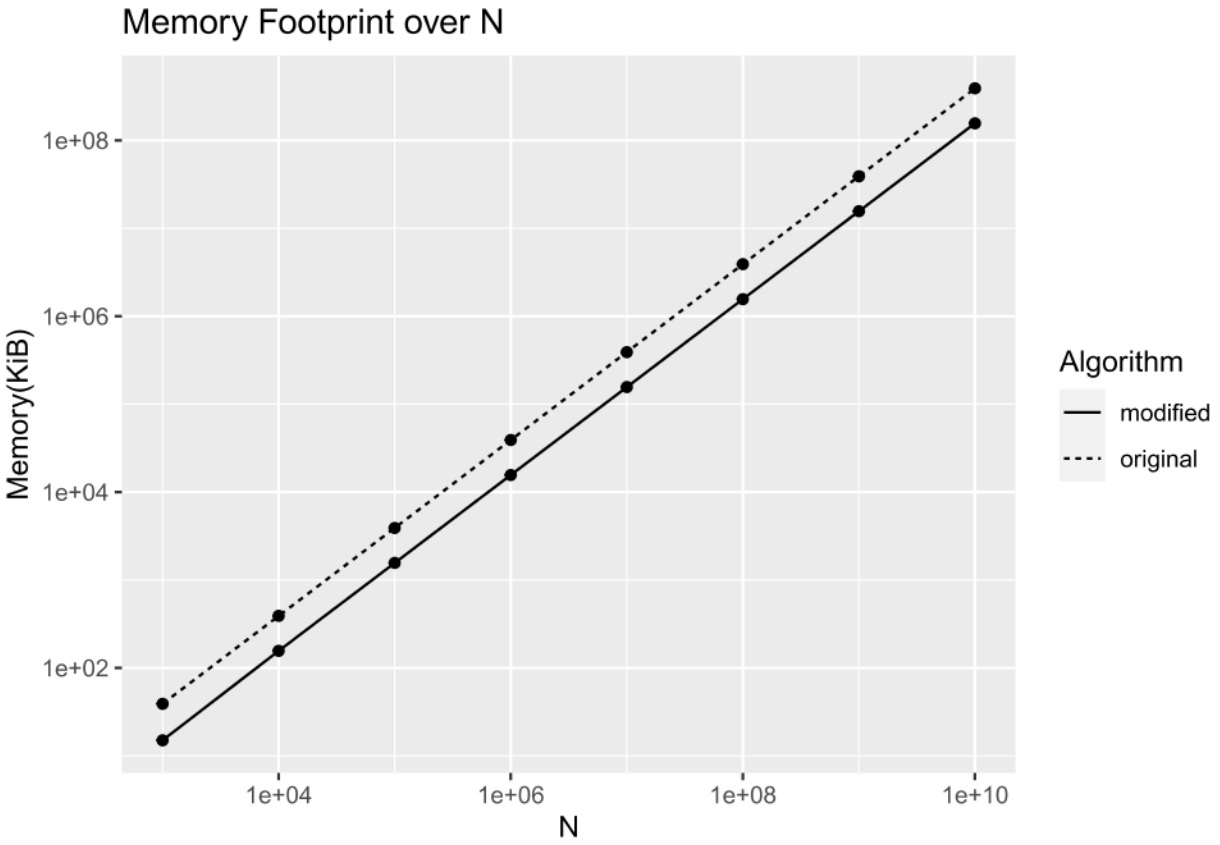
```
## Rows: 192
## Columns: 7
## $ jobid    <dbl> 4957600, 4957600, 4957600, 4957600, 4957600, 4957600, 4957600~
## $ locality <chr> "Local", "Local", "Local", "Local", "Local", "Local", "Local"~
## $ n        <dbl> 1000, 1000, 1000, 1000, 1000, 1000, 1000, 1000, 1000, 1000, 1~
## $ method   <chr> "modified", "modified", "modified", "modified", "original", "~
## $ pi       <dbl> 3.1280, 3.1280, 3.1280, 3.1280, 3.1280, 3.1280, 3.1280, 3.128~
## $ time_ms  <dbl> 0.0002689338, 0.0002680048, 0.0002680473, 0.0002680484, 0.000~
## $ data_kb  <dbl> 15, 15, 15, 15, 39, 39, 39, 39, 15, 15, 15, 15, 39, 39, 39, 3~
```

Discussion

Memory Footprint

```
df %>%
    ggplot(aes(x = n, y = data_kb, linetype = method)) +
    geom_point(stat = "summary") +
    geom_line(stat = "summary") +
    scale_x_log10() +
    scale_y_log10() +
    labs(title = "Memory Footprint over N", x = "N", y = "Memory(KiB)", linetype = "Algorithm")
```

```
## No summary function supplied, defaulting to `mean_se()`
## No summary function supplied, defaulting to `mean_se()`
```



The maximum memory footprint is 390.625 GB.

The modified method uses 60.1935238% less memory than the original reference implementation.

Access Pattern

In the original reference implementation:

- Step 1 (squaring): 2 Sequential Writes, 2 Sequential Reads, Cachable, Vectorizable
- Step 2 (normalizing): 1 Sequential Write, 2 Sequential Reads, Cachable, Vectorizable
- Step 3 (summing): 1 Scalar Write, 1 Sequential Read, Cachable, Vectorizable

In the modified implementation:

1 Sequential Write, 2 Sequential Reads, Cachable, Vectorizable

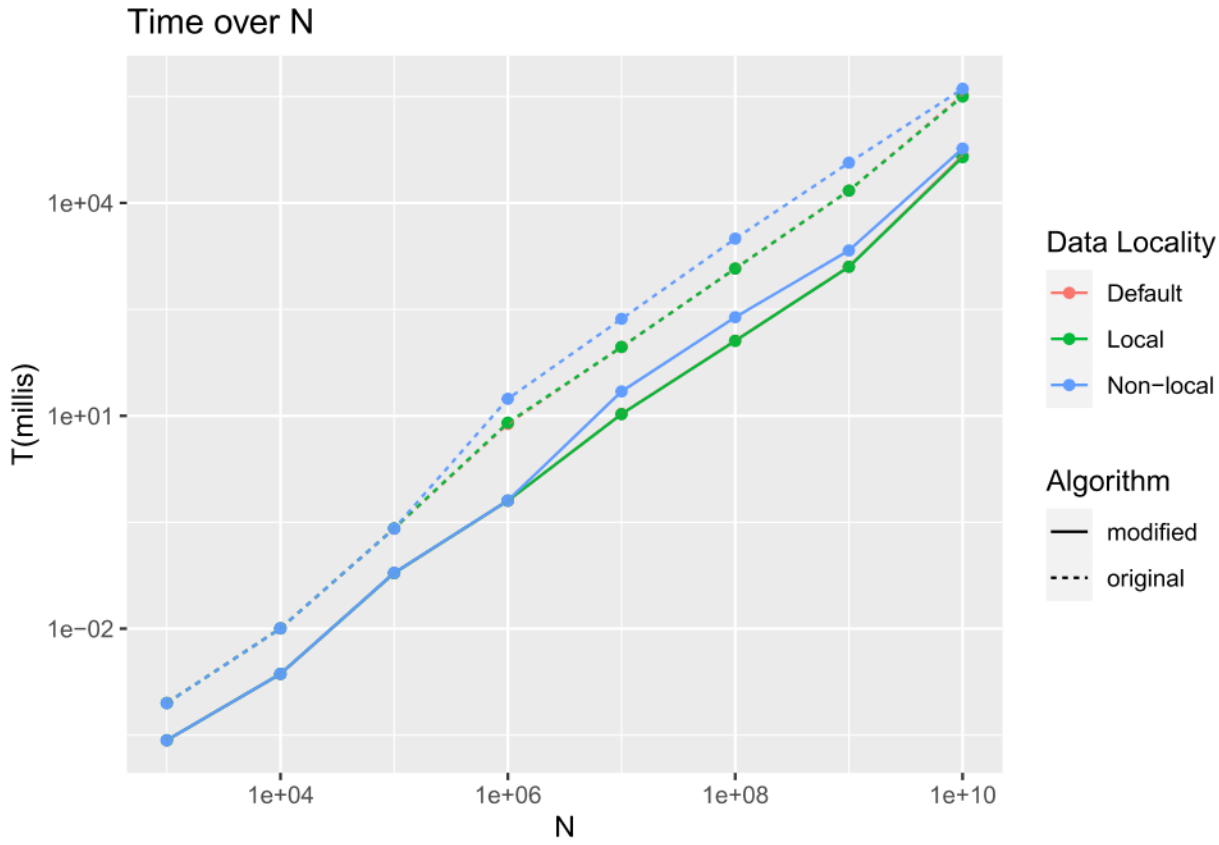
Rounding Errors

Since the variable `num_inside` is a floating point number, when N is large in later loop iterations `num_inside` may be so large that additional increments to `num_inside` may be discarded due to rounding errors which can result in the incorrect results.

Timing

```r
df %>%
    ggplot(aes(x = n, y = time_ms, color = locality, linetype = method)) +
    geom_point(stat = "summary") +
    geom_line(stat = "summary") +
    scale_x_log10() +
    scale_y_log10() +
    labs(
        title = "Time over N",
        x = "N", y = "T(millis)",
        color = "Data Locality", linetype = "Algorithm"
    )
```

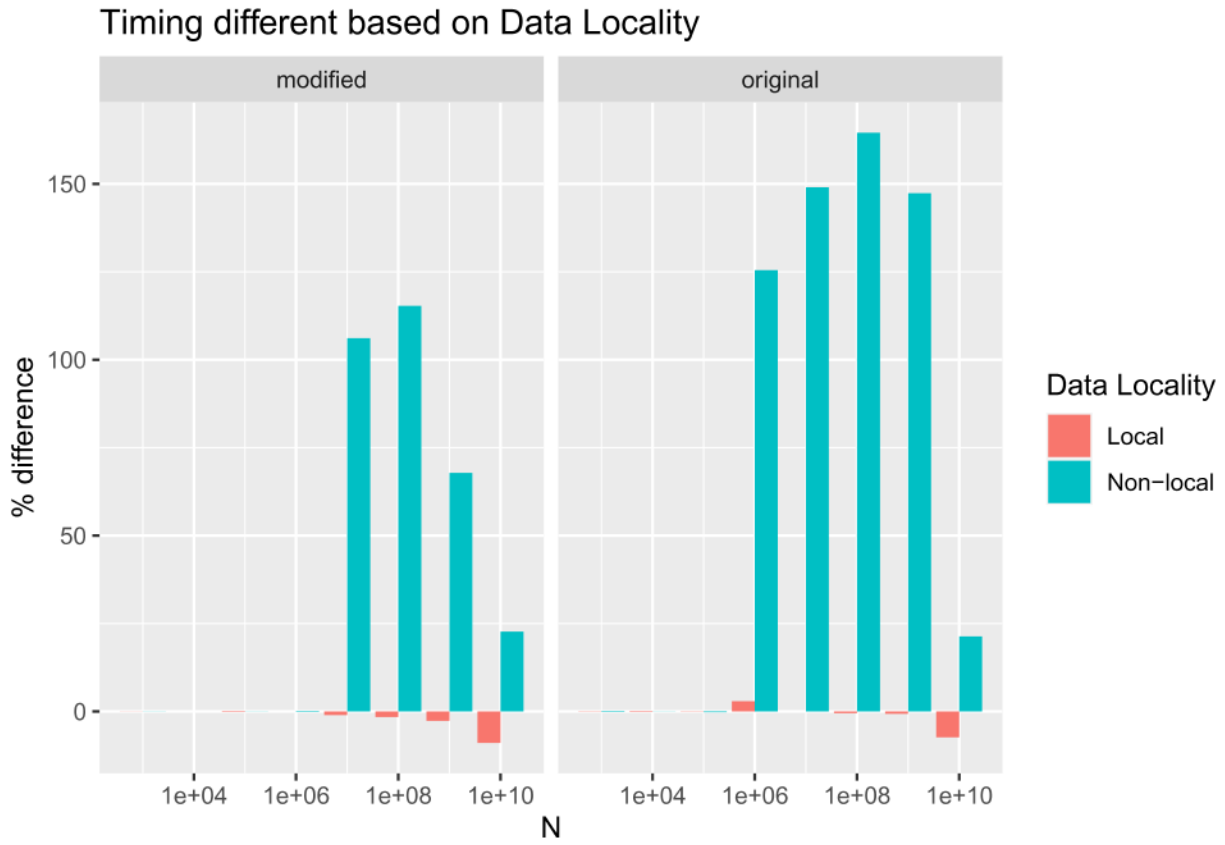
```
## No summary function supplied, defaulting to `mean_se()`
## No summary function supplied, defaulting to `mean_se()`
```



We see that the modified method is on average 84.7235219% quicker than the original reference implementation. This is largely attributed to less memory footprint and access and fewer loops.

```r
df %>%
    pivot_wider(
        id_cols = c(jobid, n, method),
        names_from = locality, names_prefix = "locality_",
        values_from = time_ms, values_fn = median
    ) %>%
    mutate(across(starts_with("locality_"), ~ (.x / locality_Default - 1))) %>%
    select(-locality_Default) %>%
```

```
    pivot_longer(
        names_prefix = "locality_", names_to = "locality",
        values_to = "diff", cols = starts_with("locality_")
    ) %>%
    ggplot(aes(x = n, y = diff * 100, fill = locality)) +
    geom_col(position = "dodge") +
    facet_wrap(~method) +
    scale_x_log10() +
    labs(
        title = "Timing different based on Data Locality",
        x = "N", y = "% difference", fill = "Data Locality"
    )
```



We see that running with explicitly non-local memory binding increases runtime by about 1 fold, with the original implementation being impacted more likely due to its higher demand on memory access.

Running with explicitly local memory binding may have slightly improved performance when N is large, the effect is not significant in smaller N's likely because caching and prefetching is sufficient in those cases to hide the latency of accessing non-local memory.

Appendix

Raw Output In Stdout and CSV

```
for i in out/4957600/*/*.out; do
    echo $i":"
    cat $i
    echo "-----"
done
```

```
out/4957600/1000/local.out:
N: 1000 Precision: 64
N: 1000 Precision: 64
N: 1000 Precision: 64
N: 1000 Precision: 64
modified                    | pi: 3.12800000000000011369     time: 0.00026893382587665028 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026800477504082380 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026804728917075553 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026804835350642732 ms     kb: 15
original                    | pi: 3.12800000000000011369     time: 0.00090055430093364944 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089091173829297806 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089529743072078139 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089743307731069896 ms     kb: 39
-----
out/4957600/1000/none.out:
N: 1000 Precision: 64
N: 1000 Precision: 64
N: 1000 Precision: 64
N: 1000 Precision: 64
modified                    | pi: 3.12800000000000011369     time: 0.00026790930653954547 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026803291403609141 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026837386637209952 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026898835697494120 ms     kb: 15
original                    | pi: 3.12800000000000011369     time: 0.00089561796654419096 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00090767024621456226 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089063674187349849 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089848400563888493 ms     kb: 39
-----
out/4957600/1000/shift.out:
N: 1000 Precision: 64
N: 1000 Precision: 64
N: 1000 Precision: 64
N: 1000 Precision: 64
modified                    | pi: 3.12800000000000011369     time: 0.00026796094349039196 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026831816253586408 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026818436292206684 ms     kb: 15
modified                    | pi: 3.12800000000000011369     time: 0.00026801493057542402 ms     kb: 15
original                    | pi: 3.12800000000000011369     time: 0.00089338958843775205 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089435233443755995 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089631424498321877 ms     kb: 39
original                    | pi: 3.12800000000000011369     time: 0.00089700478507097326 ms     kb: 39
-----
out/4957600/10000/local.out:
```

```
N: 10000 Precision: 64
N: 10000 Precision: 64
N: 10000 Precision: 64
N: 10000 Precision: 64
modified                    | pi: 3.18719999999999981100     time: 0.00230601875714865493 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230676721048655433 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230503359699055048 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230717670076286763 ms     kb: 15
original                    | pi: 3.18719999999999981100     time: 0.01009825365176339820 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01010032810306341934 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01009128483634473897 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01009728024879590416 ms     kb: 39
-----
out/4957600/10000/none.out:
N: 10000 Precision: 64
N: 10000 Precision: 64
N: 10000 Precision: 64
N: 10000 Precision: 64
modified                    | pi: 3.18719999999999981100     time: 0.00230635544126295885 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230789759747977675 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230606840836318754 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230497303530062580 ms     kb: 15
original                    | pi: 3.18719999999999981100     time: 0.01010918665082895240 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01011923884357734081 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01010138296808473120 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01015998798075701953 ms     kb: 39
-----
out/4957600/10000/shift.out:
N: 10000 Precision: 64
N: 10000 Precision: 64
N: 10000 Precision: 64
N: 10000 Precision: 64
modified                    | pi: 3.18719999999999981100     time: 0.00230505359824539381 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230669362499163816 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230806090852123807 ms     kb: 15
modified                    | pi: 3.18719999999999981100     time: 0.00230429029767946665 ms     kb: 15
original                    | pi: 3.18719999999999981100     time: 0.01011364088029005973 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01017155077888591032 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01009117328980695810 ms     kb: 39
original                    | pi: 3.18719999999999981100     time: 0.01012281311812282883 ms     kb: 39
-----
out/4957600/100000/local.out:
N: 100000 Precision: 64
N: 100000 Precision: 64
N: 100000 Precision: 64
N: 100000 Precision: 64
modified                    | pi: 3.14676000000000000156     time: 0.05929138091426539026 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06147595798241839438 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06147386995543260846 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06130570990681706578 ms     kb: 15
original                    | pi: 3.14676000000000000156     time: 0.26063821514203805441 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25722083011831275989 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25931988694412033691 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25908627474093265386 ms     kb: 39
```

```
-----
out/4957600/100000/none.out:
N: 100000 Precision: 64
N: 100000 Precision: 64
N: 100000 Precision: 64
N: 100000 Precision: 64
modified                    | pi: 3.14676000000000000156     time: 0.06106861753839577800 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.05981399291204354818 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06151851176524868875 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06150317688120791187 ms     kb: 15
original                    | pi: 3.14676000000000000156     time: 0.25968056985198650910 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25892217359223301809 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25907228329015546953 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25528256566687940188 ms     kb: 39
-----
out/4957600/100000/shift.out:
N: 100000 Precision: 64
N: 100000 Precision: 64
N: 100000 Precision: 64
N: 100000 Precision: 64
modified                    | pi: 3.14676000000000000156     time: 0.06166943211741852254 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06161894593012508942 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06099024663800201029 ms     kb: 15
modified                    | pi: 3.14676000000000000156     time: 0.06097074096881383021 ms     kb: 15
original                    | pi: 3.14676000000000000156     time: 0.26079536106402401163 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25236804958990538550 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25945465001945777761 ms     kb: 39
original                    | pi: 3.14676000000000000156     time: 0.25746615742051742748 ms     kb: 39
-----
out/4957600/1000000/local.out:
N: 1000000 Precision: 64
N: 1000000 Precision: 64
N: 1000000 Precision: 64
N: 1000000 Precision: 64
modified                    | pi: 3.14045199999999979923     time: 0.63925977692553537235 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63269451359898798426 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63784586607142856884 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63794260395408164399 ms     kb: 15
original                    | pi: 3.14045199999999979923     time: 8.01687675199999993936 ms     kb: 39
original                    | pi: 3.14045199999999979923     time: 7.92543794861660000350 ms     kb: 39
original                    | pi: 3.14045199999999979923     time: 8.19396806122449028464 ms     kb: 39
original                    | pi: 3.14045199999999979923     time: 7.96284335714285695929 ms     kb: 39
-----
out/4957600/1000000/none.out:
N: 1000000 Precision: 64
N: 1000000 Precision: 64
N: 1000000 Precision: 64
N: 1000000 Precision: 64
modified                    | pi: 3.14045199999999979923     time: 0.63129397286210164886 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63834933599234211510 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63786601434948986267 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63796551929824563132 ms     kb: 15
original                    | pi: 3.14045199999999979923     time: 7.82770196093749959232 ms     kb: 39
original                    | pi: 3.14045199999999979923     time: 7.72949914285714267947 ms     kb: 39
```

```
original                    | pi: 3.14045199999999979923     time: 7.80106805058365804229 ms     kb: 39
original                    | pi: 3.14045199999999979923     time: 7.44431143494423785967 ms     kb: 39
-----
out/4957600/1000000/shift.out:
N: 1000000 Precision: 64
N: 1000000 Precision: 64
N: 1000000 Precision: 64
N: 1000000 Precision: 64
modified                    | pi: 3.14045199999999979923     time: 0.63969384905660375829 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63833385130823228071 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.64027869878361076683 ms     kb: 15
modified                    | pi: 3.14045199999999979923     time: 0.63798717352472089637 ms     kb: 15
original                    | pi: 3.14045199999999979923     time: 17.54843862280701927148 ms    kb: 39
original                    | pi: 3.14045199999999979923     time: 16.53648068595041209505 ms    kb: 39
original                    | pi: 3.14045199999999979923     time: 17.46502815652173978833 ms    kb: 39
original                    | pi: 3.14045199999999979923     time: 17.93238402678571574711 ms    kb: 39
-----
out/4957600/10000000/local.out:
N: 10000000 Precision: 64
N: 10000000 Precision: 64
N: 10000000 Precision: 64
N: 10000000 Precision: 64
modified                    | pi: 3.14195599999999978905     time: 10.52237169633507818389 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 10.65527423404255280559 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 10.72054911764705842359 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 10.42302299479166727281 ms    kb: 15
original                    | pi: 3.14195599999999978905     time: 93.27894140909091902358 ms    kb: 39
original                    | pi: 3.14195599999999978905     time: 93.23942581818181452036 ms    kb: 39
original                    | pi: 3.14195599999999978905     time: 93.70797240909091385674 ms    kb: 39
original                    | pi: 3.14195599999999978905     time: 93.62192209090909500446 ms    kb: 39
-----
out/4957600/10000000/none.out:
N: 10000000 Precision: 64
N: 10000000 Precision: 64
N: 10000000 Precision: 64
N: 10000000 Precision: 64
modified                    | pi: 3.14195599999999978905     time: 10.44410825000000109242 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 10.72074428342246044110 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 10.72468939572192425658 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 10.67769802659574374104 ms    kb: 15
original                    | pi: 3.14195599999999978905     time: 93.44223690909092283619 ms    kb: 39
original                    | pi: 3.14195599999999978905     time: 93.28253481818181569452 ms    kb: 39
original                    | pi: 3.14195599999999978905     time: 93.54321399999999187003 ms    kb: 39
original                    | pi: 3.14195599999999978905     time: 93.45609840909091303729 ms    kb: 39
-----
out/4957600/10000000/shift.out:
N: 10000000 Precision: 64
N: 10000000 Precision: 64
N: 10000000 Precision: 64
N: 10000000 Precision: 64
modified                    | pi: 3.14195599999999978905     time: 22.03000957142857174631 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 22.13338002197802367732 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 22.07506335164834965212 ms    kb: 15
modified                    | pi: 3.14195599999999978905     time: 21.93971932608695496469 ms    kb: 15
```

```
original                    | pi: 3.14199599999999978905     time: 230.55015977777779312419 ms   kb: 39
original                    | pi: 3.14199599999999978905     time: 232.85593599999998559724 ms   kb: 39
original                    | pi: 3.14199599999999978905     time: 232.55433533333336981741 ms   kb: 39
original                    | pi: 3.14199599999999978905     time: 233.95215100000001484659 ms   kb: 39
-----
out/4957600/100000000/local.out:
N: 100000000 Precision: 64
N: 100000000 Precision: 64
N: 100000000 Precision: 64
N: 100000000 Precision: 64
modified                    | pi: 3.14163319999999979260     time: 111.31773527777778554082 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 111.91731266666666044785 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 112.12438972222223299013 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 120.34560705882353204288 ms   kb: 15
original                    | pi: 3.14163319999999979260     time: 1179.58853150000004461617 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 1180.17774400000007517519 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 1186.22836499999993975507 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 1217.57128699999998389103 ms  kb: 39
-----
out/4957600/100000000/none.out:
N: 100000000 Precision: 64
N: 100000000 Precision: 64
N: 100000000 Precision: 64
N: 100000000 Precision: 64
modified                    | pi: 3.14163319999999979260     time: 113.32515272222221369702 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 114.35702138888889578539 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 122.81765658823529463461 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 108.28471252631578636283 ms   kb: 15
original                    | pi: 3.14163319999999979260     time: 1156.22462999999993371603 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 1184.35401049999995848339 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 1193.69194199999992633821 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 1228.06526549999989583739 ms  kb: 39
-----
out/4957600/100000000/shift.out:
N: 100000000 Precision: 64
N: 100000000 Precision: 64
N: 100000000 Precision: 64
N: 100000000 Precision: 64
modified                    | pi: 3.14163319999999979260     time: 245.08873399999998810017 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 245.76400411111112020990 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 244.71562544444446984926 ms   kb: 15
modified                    | pi: 3.14163319999999979260     time: 245.18381733333333727387 ms   kb: 15
original                    | pi: 3.14163319999999979260     time: 3100.55007500000010622898 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 3136.51683499999990090146 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 3154.82737499999984720489 ms  kb: 39
original                    | pi: 3.14163319999999979260     time: 3173.87970899999982066220 ms  kb: 39
-----
out/4957600/1000000000/local.out:
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
modified                    | pi: 3.14163219600000021003     time: 1226.68112449999989621574 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 1214.53661000000010972144 ms  kb: 15
```

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modified                    | pi: 3.14163219600000021003     time: 1236.59263699999996788392 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 1356.71280200000001059379 ms  kb: 15
original                    | pi: 3.14163219600000021003     time: 14609.46586000000024796464 ms     kb
original                    | pi: 3.14163219600000021003     time: 14735.04129500000090047251 ms     kb
original                    | pi: 3.14163219600000021003     time: 14780.29658399999971152283 ms     kb
original                    | pi: 3.14163219600000021003     time: 15657.03483000000051106326 ms     kb
-----
out/4957600/1000000000/none.out:
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
modified                    | pi: 3.14163219600000021003     time: 1238.29150299999992057565 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 1288.44060050000007322524 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 1242.25016249999998763087 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 1290.45400500000005195034 ms  kb: 15
original                    | pi: 3.14163219600000021003     time: 14777.01887300000089453533 ms     kb
original                    | pi: 3.14163219600000021003     time: 14833.94266099999913421925 ms     kb
original                    | pi: 3.14163219600000021003     time: 14890.75566799999978684355 ms     kb
original                    | pi: 3.14163219600000021003     time: 15079.04421299999921757262 ms     kb
-----
out/4957600/1000000000/shift.out:
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
N: 1000000000 Precision: 64
modified                    | pi: 3.14163219600000021003     time: 2104.84614300000021103187 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 2086.85004699999990407377 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 2142.55690000000004147296 ms  kb: 15
modified                    | pi: 3.14163219600000021003     time: 2243.40766699999994671089 ms  kb: 15
original                    | pi: 3.14163219600000021003     time: 36349.82852100000309292227 ms     kb
original                    | pi: 3.14163219600000021003     time: 36580.97853500000201165676 ms     kb
original                    | pi: 3.14163219600000021003     time: 36936.75686300000234041363 ms     kb
original                    | pi: 3.14163219600000021003     time: 37792.62428099999669939280 ms     kb
-----
out/4957600/10000000000/local.out:
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
modified                    | pi: 3.14160661320000000885     time: 41931.84925800000200979412 ms     kb
modified                    | pi: 3.14160661320000000885     time: 42265.49402099999861093238 ms     kb
modified                    | pi: 3.14160661320000000885     time: 44271.84391299999697366729 ms     kb
modified                    | pi: 3.14160661320000000885     time: 48064.56920499999978346750 ms     kb
original                    | pi: 3.14160661320000000885     time: 305191.85965699999360367656 ms    kb
original                    | pi: 3.14160661320000000885     time: 310099.25222600001143291593 ms    kb
original                    | pi: 3.14160661320000000885     time: 310010.83182700001634657383 ms    kb
original                    | pi: 3.14160661320000000885     time: 338491.56843500002287328243 ms    kb
-----
out/4957600/10000000000/none.out:
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
```

```
modified                    | pi: 3.14160661320000000885     time: 41654.51966499999980442226 ms     kb
modified                    | pi: 3.14160661320000000885     time: 45987.53476599999703466892 ms     kb
modified                    | pi: 3.14160661320000000885     time: 49057.06052900000213412568 ms     kb
modified                    | pi: 3.14160661320000000885     time: 49144.67263300000195158646 ms     kb
original                    | pi: 3.14160661320000000885     time: 312273.00098700000671669841 ms    kb
original                    | pi: 3.14160661320000000885     time: 332452.12425300001632422209 ms    kb
original                    | pi: 3.14160661320000000885     time: 336982.12616200000047683716 ms    kb
original                    | pi: 3.14160661320000000885     time: 338662.79603099997621029615 ms    kb
-----
out/4957600/10000000000/shift.out:
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
N: 10000000000 Precision: 64
modified                    | pi: 3.14160661320000000885     time: 53528.86811199999647215009 ms     kb
modified                    | pi: 3.14160661320000000885     time: 56222.09949400000186869875 ms     kb
modified                    | pi: 3.14160661320000000885     time: 60398.04417300000204704702 ms     kb
modified                    | pi: 3.14160661320000000885     time: 64569.40269499999703839421 ms     kb
original                    | pi: 3.14160661320000000885     time: 394963.80453800002578645945 ms    kb
original                    | pi: 3.14160661320000000885     time: 393595.82794400001876056194 ms    kb
original                    | pi: 3.14160661320000000885     time: 420188.93379199999617412686 ms    kb
original                    | pi: 3.14160661320000000885     time: 417159.51079700002446770668 ms    kb
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```
4957600,shift,10000000000,original,3.14160661320000000885,417159.51079700002446770668,390625000
```

Program Source

```cpp
#include <sys/time.h>
#include <sys/resource.h>
#include <iostream>
#include <random>
#include <algorithm>
#include <iomanip>
#include <chrono>

#ifndef PIMC_N
#define PIMC_N 1000
#endif

static void printrss(void)
{
    system("ps -opid,comm,rss,drs $PPID");
}

template <size_t N, typename FP = double>
struct c2d
{
    FP x[N];
    FP y[N];
};

template <size_t N, typename FP = double>
struct PiMC
{
    c2d<N, FP> coords;

    struct result_type
    {
        std::string method;
        FP num_inside = 0.;
        FP pi = 0.;
        size_t n = N;
        size_t mem_footprint;
    };

    static constexpr size_t precision()
    {
        return sizeof(FP);
    }

    PiMC(uint32_t seed = std::mt19937::default_seed)
    {
        std::mt19937 rd(seed);
        static std::uniform_real_distribution<FP> dist(0, 1);
```

```
        for (size_t i = 0; i < N; i++)
        {
            coords.x[i] = dist(rd);
            coords.y[i] = dist(rd);
        }
    }

    template <bool original = true>
    result_type estimate() const
    {
        result_type result;

        if constexpr (original)
        {
            result.method = "original";
            c2d<N, FP> coords_squared;

            // step1
            for (size_t i = 0; i < N; i++)
            {
                coords_squared.x[i] = coords.x[i] * coords.x[i];
                coords_squared.y[i] = coords.y[i] * coords.y[i];
            }

            FP norm2[N];
            // step2
            for (size_t i = 0; i < N; i++)
                norm2[i] = coords_squared.x[i] + coords_squared.y[i];

            // step3
            for (const FP &x : norm2)
                result.num_inside += x <= 1.0 ? 1 : 0;

            result.mem_footprint = (sizeof(coords) + sizeof(coords_squared) + sizeof(norm2));
        }
        else
        {
            result.method = "modified";
            for (size_t i = 0; i < N; i++)
                result.num_inside += (coords.x[i] * coords.x[i] + coords.y[i] * coords.y[i]) <= 1.0 ? 1

            result.mem_footprint = sizeof(coords);
        }

        result.pi = result.num_inside * 4. / N;
        return result;
    }
};

int main()
{

    auto eval = [](auto fun)
```

```
    {
        size_t nrep = 1;
        const auto t1 = std::chrono::high_resolution_clock::now();
        const auto result = fun();
        const auto t2 = std::chrono::high_resolution_clock::now();
        std::chrono::duration<double, std::milli> ms = t2 - t1;
        while (ms.count() < 2000)
        {
            (void)fun();
            const auto t3 = std::chrono::high_resolution_clock::now();
            ms = t3 - t1;
            nrep++;
        }
        std::cout << std::setw(28) << std::setprecision(20) << std::fixed << std::left << result.method
                  << result.pi << "\t time: " << ms.count() / nrep << " ms"
                  << "\t kb: " << result.mem_footprint / 1024 << std::endl;
        // printrss();
    };

    PiMC<PIMC_N> mc;
    std::cout << "N: " << PIMC_N << " Precision: " << mc.precision() * 8 << std::endl;
    eval([&]
         { return mc.estimate<false>(); });
    eval([&]
         { return mc.estimate<true>(); });

    return 0;
}
```

Job Script

```
#!/usr/bin/env fish
#SBATCH -J hw2_pi          # Job name
#SBATCH -p nvdimm
#SBATCH -o hw2_pi.o%j      # Name of stdout output file
#SBATCH -e hw2_pi.e%j      # Name of stderr error file
#SBATCH -N 3
#SBATCH -n 3
#SBATCH --ntasks-per-node 1
#SBATCH -t 00:30:00        # Run time (hh:mm:ss)
#SBATCH --mail-type=all    # Send email at begin and end of job
#SBATCH --mail-user[redacted]

echo "Slurm JOBID="$SLURM_JOBID "MEMBIND="$SLURM_MEM_BIND_TYPE

srun --label hostname

module load intel
module load gnuparallel

set -l numa_bound (numactl -s | \
    awk 'BEGIN {n_numa=255} /^(cpu|mem)bind/ { if ($(NF)<n_numa) n_numa=$(NF) } END{print n_numa}')
```

```
echo "Parallel over" (math $numa_bound + 1) "NUMA nodes"

function line_shift
    sed "p;" | awk 'NR==1{store=$0;next}1;END{print store}'
end

function srun_trybind -V output -V numa_bound
    set -q output
        or set -l output output

    mkdir -p out/$SLURM_JOBID/$output

    srun \
                -n1 -o out/$SLURM_JOBID/$output/none.out \
        parallel --lb -n0 -q numactl $argv ":::" (seq 0 $numa_bound) : \
                -n1 -o out/$SLURM_JOBID/$output/local.out \
        parallel --lb -q numactl -N{} -m{} $argv ":::" (seq 0 $numa_bound) : \
                -n1 -o out/$SLURM_JOBID/$output/shift.out \
        parallel -N2 --lb -q numactl -N{1} -m{2} $argv ":::" (seq 0 $numa_bound | line_shift)
end

function slurm_seconds -a fmt
    printf "0 %s+p" (echo $fmt | string replace "-" " 24*+" | string replace -a ":" " 60*+") | dc
end

set fish_trace on

lstopo binding_$SLURM_JOB_PARTITION.xml

set -l max_n (awk '/MemFree/ { printf "%d \n", $2 / (40000000/1000000000) }' /proc/meminfo)
echo "Running for upto N="$max_n

set -l cur_n 1000

while [ (math \
    (slurm_seconds (squeue -h -j $SLURM_JOBID -o "%L")) "/" \
    (slurm_seconds (squeue -h -j $SLURM_JOBID -o "%l"))
) -gt .90 -a $cur_n -lt $max_n ]

    echo "Running with N=" $cur_n

    icpc -std=c++17 -o pi.$cur_n.exec -DPIMC_N=$cur_n -xcore-avx512 -O2 pi.cxx
        or break

    output=$cur_n srun_trybind \
        pi.$cur_n.exec
        or break

    set cur_n (math $cur_n "*" 10)
end
```

AWK Script to Parse Stdout to CSV

```
#!/usr/bin/awk -f

BEGIN {
    OFS=","
    print "jobid,locality,n,method,pi,time_ms,data_kb"
}

BEGINFILE {
    split(FILENAME,FPARTS,"/")
    sub("\\.out$", "",FPARTS[4])
}

/^N:/ { n = $2 }
/pi:/ { print FPARTS[2],FPARTS[4],n,$1,$4,$6,$9 }
```