High Performance Graph and Data Analytics Project

Alessandro La Conca - Pablo Giaccaglia

What we have done?

What we have done?

Acceleration of Personalized PageRank using GPUs

What is Personalized PageRank?

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briefly!

What is Personalized PageRank?

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- The algorithm originally behind Google Search
- Given a web page, it gives a score to the others
- A ranking is generated, according to pages' relevance

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Personalized PageRank works on graphs!

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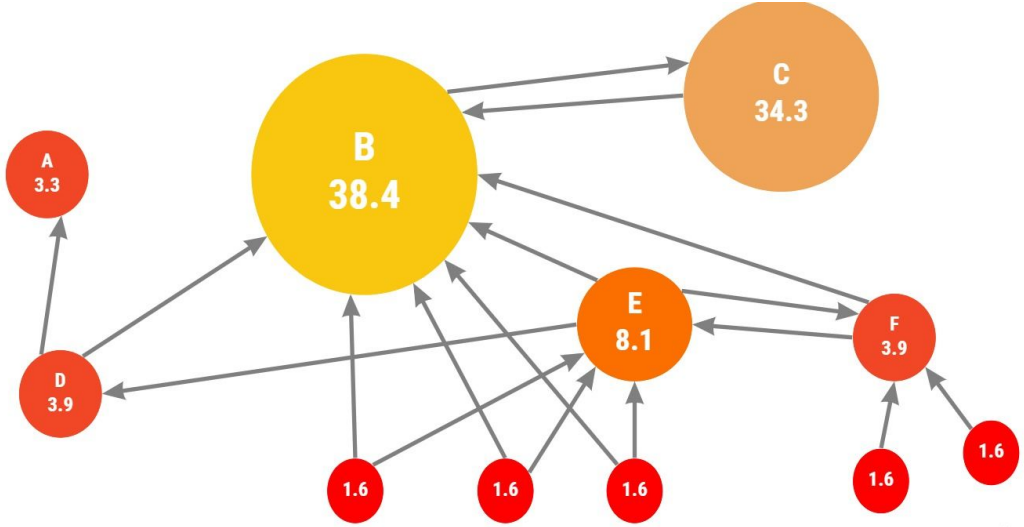

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Stochastic Matrix

1 for personalization vertex, 0 for other vertices

Personalized PageRank vector

1 for dangling vertices, 0 for other vertices

damping factor

Now, the fun part

Goals & Constraints

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- At least 80% precision on top-20 results
- Only ranking matters, not the score
- Tests run on NVIDIA Laptop GeForce RTX 3080 GPU

01
Naive Implementation

PPR with Power method

computed once

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Graph is stored in COO format

Implemented Kernels

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Just the meaningful ones!

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compute_dangling_factor_gpu(dangling_gpu, pr_old, pDanglingFact_gpu, *pV_gpu)

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    for(size_t i = blockIdx.x * blockDim.x + threadIdx.x; i < V; i += blockDim.x * gridDim.x){
        T2 val = (T2) dangling[i] * pr[i];
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- **Naive dot product kernel**

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- Naive dot product kernel
- Linear global memory access pattern
- atomicAdd synchronized for the whole GPU
- Many threads are stalled!

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```
template <typename T1, typename T2> __global__ void cooSPMV_math(
        const T1 *  __restrict__  x_gpu,
        const T1 *  __restrict__  y_gpu,
        const T2 * __restrict__ val_gpu,
        const T1 E,
        const T2 * __restrict__ pr_old,
        T2 * __restrict__ pr_temp)
{
    size_t index = blockIdx.x * blockDim.x + threadIdx.x;

    if (index < E){
        atomicAdd(&pr_temp[x_gpu[index]], val_gpu[index]*pr_old[y_gpu[index]]);

    }
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- Same inefficiencies of the previous kernel
- Works only with fixed number of threads
- Each thread does one load, computation and store
- Thread setup cost not properly “hided”

Implemented Kernels

compute_square_error_gpu(pr_old, pr_gpu, pSquareError_gpu, pPpr->V)

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```
template<typename T> __global__ void compute_square_error_gpu( T *old,  T *newVector, T *result, int V){
    for (size_t i = blockIdx.x * blockDim.x + threadIdx.x; i < V; i += blockDim.x * gridDim.x) {
        atomicAdd(result, (T)((old[i] - newVector[i]) * (old[i] - newVector[i])));
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- Computes only sum of square of the difference, square root on CPU
- Same inefficiencies of the first kernel

Performance

Instances	Average	Minimum	Maximum	Kernel
900	15,5 ms	15 ms	16 ms	**cooSPMV**
900	6,7 ms	6,5 ms	7,6 ms	**compute_square_error_gpu**
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- **Grid size k2 = (V + Block size - 1) / (Block size)**
- **Grid size k3 = (V + Block size - 1) / (Block size)**
- **Mean computation time (100 iterations, threshold 1e-6) = 1010 ms**
- **Mean accuracy (100 iterations, threshold 1e-6) = 100%**

After many optimizations...

02

Final coo Implementation

Some improvements

- Floats instead of doubles
- Usage of shared memory
- Some heuristics introduced
- Usage of single precision intrinsics
    - Device only
    - Compiler inline-able set of highly optimized instructions
    - Fast but has low numerical accuracy
    - Allows do things with a small instruction count

Implemented Kernels

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Just the meaningful ones!

Implemented Kernels

dangling_kernel(pDanglingIndexes_gpu, pr_old, pDanglingFact_gpu,dampingFract,danglingSize);

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    extern __shared__ T2 cache[];

    T2 temp = 0.0;
    while(index < n){

        temp = __fadd_rd(temp, y[x[index]]);
        index += stride;
    }

    cache[threadIdx.x] = temp;

    __syncthreads();

    // reduction
    unsigned int i = blockDim.x/2;
    while(i != 0){
        if(threadIdx.x < i){
            cache[threadIdx.x] = __fadd_rd(cache[threadIdx.x], cache[threadIdx.x + i]);
        }
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Intrinsic function

- Pseudo dot product
- Sum of 0s is avoided
- Shared memory to improve parallelism
- Reduction of partial results

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__spmv_coo_flat(x_gpu, y_gpu, val_gpu, pr_old, pr_gpu, pPpr->E, num_blocks, ...)

$$\left(\overline{\mathbf{d}}\mathbf{p}_{\mathbf{t}}\right)$$

- Adaptation from CUSP Library
- Flattens data irregularity (variable number of 0s per row)
- Works with COO format sorted by row to exploit parallelism

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  - Fetch rowIdx, colIdx, value of matrix, fetch vector value, compute product,store result in shared memory.
  - If a row extends over the 32 elements boundary, then the partial sum of a warp is carried over into the next warp, otherwise the result is written in global memory. The decision is taken by the first thread of the next warp.

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- (Example) Given interval of 16 and warp size of 32, for each thread:
  - Fetch rowIdx, colIdx, value of matrix, fetch vector value, compute product,store result in shared memory.
  - If a row extends over the 32 elements boundary, then the partial sum of a warp is carried over into the next warp, otherwise the result is written in global memory. The decision is taken by the first thread of the next warp.
  - Each warp conduct a segmented scan by looking if 2 values belong to the same row.

```
            0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15   # thread_lane
      idx [ 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2]  # row indices
      val [ 4, 6, 5, 0, 8, 3, 2, 8, 3, 1, 4, 9, 2, 5, 2, 4]  # M(i,j) * x(j)
→ result: val [ 4,10,15,15,23,26, 2,10,13,14, 4,13,15,20,22,26]  # A(i,j) * x(j)
```

How it works

__spmv_coo_flat(x_gpu, y_gpu, val_gpu, pr_old, pr_gpu, pPpr->E, num_blocks, ...)

- Each thread in a warp, except the last one, checks if it is the last of the row. The last thread writes the sum in the output vector

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- The last thread in each warp writes its row index and partial sum in 2 global arrays (at an index corresponding to that warp).
- These steps are repeated until the warp reaches the end of its interval
- Finally, the values to carry between warps are added to the result through reduction.

Implemented Kernels

euclidean_kernel_math(pr_old, pr_gpu, pSquareError_gpu, pPpr->V)

```
template<typename T> __global__ void euclidean_kernel_math(const T * __restrict__ x, const T * __restrict__ y, T * __restrict__ result, unsigned int n)
{
    size_t index = threadIdx.x + blockDim.x * blockIdx.x;
    size_t stride = blockDim.x * gridDim.x;

    extern __shared__ T cache1[];

    T temp = 0.0;
    while (index < n) {
        temp =  __fadd_rd(temp, (
                                __fmul_rd(
                                        __fsub_rd(x[index],y[index]),
                                        __fsub_rd(x[index],y[index])
                                )
                        )
        );

        index += stride;
    }

    cache1[threadIdx.x] = temp;

    __syncthreads();

    // reduction
    size_t i = blockDim.x / 2;
    while (i != 0) {
        if (threadIdx.x < i) {
            cache1[threadIdx.x] = __fadd_rd(cache1[threadIdx.x], cache1[threadIdx.x + i]);
        }
        __syncthreads();
        i /= 2;
    }


    if (threadIdx.x == 0) {
        atomicAdd(result, cache1[0]); //
    }

}
```

Implemented Kernels

euclidean_kernel_math(pr_old, pr_gpu, pSquareError_gpu, pPpr->V)

- Adaptation of dot product kernel

```
template<typename T> __global__ void euclidean_kernel_math(const T * __restrict__ x, const T * __restrict__ y, T * __restrict__ result, unsigned int n)
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- Square root computed on CPU

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euclidean_kernel_math(pr_old, pr_gpu, pSquareError_gpu, pPpr->V)

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        index += stride;
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}
```

Implemented Kernels

euclidean_kernel_math(pr_old, pr_gpu, pSquareError_gpu, pPpr->V)

- Adaptation of dot product kernel
- Square root computed on CPU
- Shared memory to improve parallelism
- Reduction of partial results

```
template<typename T> __global__ void euclidean_kernel_math(const T * __restrict__ x, const T * __restrict__ y, T * __restrict__ result, unsigned int n)
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                                        __fsub_rd(x[index],y[index])
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                        )
        );

        index += stride;
    }

    cache1[threadIdx.x] = temp;

    __syncthreads();

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    size_t i = blockDim.x / 2;
    while (i != 0) {
        if (threadIdx.x < i) {
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        }
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        i /= 2;
    }


    if (threadIdx.x == 0) {
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}
```

Performance

Instances	Average	StdDev	Minimum	Maximum	Kernel
900	8,5 ms	0,18 ms	8 ms	9 ms	**__spmv_coo_flat**
900	0,1 ms	0,09 ms	0,1 ms	0,13 ms	**euclidean_kernel_math**
900	0,015 ms	0,0098 ms	0,013 ms	0,018 ms	**dangling_kernel**

- **Block size = 128**

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- **Grid size k1 = (E + Block size - 1) / (Block size)**
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- **Grid size k3 = (D + Block size - 1) / (Block size) , D = |Dangling Vertexes|**
- **Mean computation time (100 iterations, threshold 1e-6) = 750 ms**
- **Mean accuracy (100 iterations, threshold 1e-6) = 100%**

Now, the heuristics

Some improvements

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Wikipedia top19 : {7030, 9008, 24716, 27566, 28020, 28196, 195101, 500469, 577659, 689491, 932394, 1518892, 1702309, 1835017, 2144742, 2257865, 2532493, 2979297, 2984189}

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Easily adaptable with different graphs

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- Pre-computed result on dangling indexes

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  - Adaptable with different threshold, depends on previous heuristic

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  - Adaptable with different threshold, depends on previous heuristic

Mean execution time: 100 ms **Mean accuracy: 95%**

Performance

Implementation	Mean total time (reset + exec)	Mean exec time	Accuracy
Naive	1023 ms	1010.62 ms	100%
Cublas coo, cusparse of dot	258 ms	255.081 ms	100%
Final implementation	103 ms	100 ms	>80%

Tested on rtx 3080 laptop

Performance

```
 Time (%)  Total Time (ns)  Instances    Avg (ns)      Med (ns)     Min (ns)    Max (ns)   StdDev (ns)                                          Name

 --------  ---------------  ---------  ------------  ------------  ----------  ----------  -----------  ----------------------------------------------------------------------------------------
--------
     92.0    4,818,817,005        300  16,062,723.4  16,025,571.5  15,933,219  20,742,032    401,228.2  void cooSPMV_math<int, float>(const T1 *, const T1 *, const T2 *, T2, const T2 *
, T2 *)
      6.0      314,028,668        300   1,046,762.2   1,044,380.0   1,038,236   1,440,922     32,342.9  void euclidean_kernel<float>(T1 *, T1 *, T1 *, unsigned int)

      0.6       29,358,324        300      97,861.1      97,504.0      97,216     128,736      3,080.1  void dot_product_kernel_math<int, float>(const T1 *, const T2 *, T2 *, T2, unsig
ned int)
      0.5       24,811,682        300      82,705.6      82,703.5      77,344      85,312        737.6  void vectorScalarAddAndIncrement_math<float>(T1, T1 *, int, int, T1)

      0.4       23,175,290        300      77,251.0      77,183.0      75,776      79,392        650.6  void copy_vector<float>(T1 *, T1 *, int)

      0.3       13,469,514         10   1,346,951.4   1,332,683.0   1,322,139   1,487,226     49,449.1  void vectorScalarMul<float>(T1, T1 *, int)

      0.2       12,004,502        300      40,015.0      39,968.0      39,296      41,344        324.3  void init_vector<float>(T1 *, int, T1)
```

For all the implementations seen until now the Time (%) were similar.
Can we skip the SPMV multiplication?

Performance

Implementation	Mean total time (reset + exec)	Mean exec time	Accuracy
Naive	1023 ms	1010.62 ms	100%
Cublas coo, cusparse of dot	258 ms	255.081 ms	100%
Final implementation	103 ms	100 ms	>80%
Monte Carlo complete path	17 ms	14.2666 ms	>80%

Tested on rtx 3080 laptop, 100 runs

03
Monte Carlo Implementation

Monte Carlo Complete path

- Simulate m random walks starting from the personalized vertex.
- At each step the walker can terminate with probability 1-alpha.
- At each step the walker move to a random vertex connected to an outgoing edge with probability alpha.

Let N_j be the number of visits by all walkers to vertex j, then the pr of vertex j is defined as following:

$$pr_j(personalized\,vertex, alpha) = (1 - alpha)\,\frac{1}{m} N_j\,(personalized\,vertex)$$

https://link.springer.com/content/pdf/10.1007/978-3-642-21286-4.pdf page 50

Monte Carlo Complete path

Since we don't care about the values we can skip the multiplication and division

$$pr_j(personalized\,vertex, alpha) = (1 - alpha)\,\frac{1}{m} N_j\,(personalized\,vertex)$$

$$\Downarrow$$

$$pr_j(personalized\,vertex, alpha) = N_j\,(personalized\,vertex)$$

MC Complete path on CPU

- Uses CSC (Compressed sparse column matrix format)
- Walkers run sequentially.

```
int walkLen = 0;
for (int run = 0; run < nWalkers; run++) {
    int vIdx = s;
    while (walkLen < maxWalkLen){
        pPpr->pr[vIdx]+=1.0f;
        bool terminate = dist(mt) < 1.0f-pPpr->alpha;//Terminate with probability 1-c
        if (terminate) {
            break;
        } else {
            int neighStartIdx = csc.xPtr_cpu[vIdx];
            int neighEndIdx = csc.xPtr_cpu[vIdx+1];
            int neighSize = neighEndIdx - neighStartIdx;
            if (neighSize == 0) {
                break;}

            //select a random connected vertex
            int rIdx = vJump(mt)%neighSize;
            vIdx=csc.x_cpu[neighStartIdx+rIdx];
        }
        walkLen++;
    }
    //std::cout << "Walk length: " << walkLen << std::endl;
    walkLen = 0;
}
```

MC Complete path on GPU naive

- 1 thread = 1 walker
- If we try to run the walkers in parallel we need an atomic add and in the first step each walker thread will add to the same position

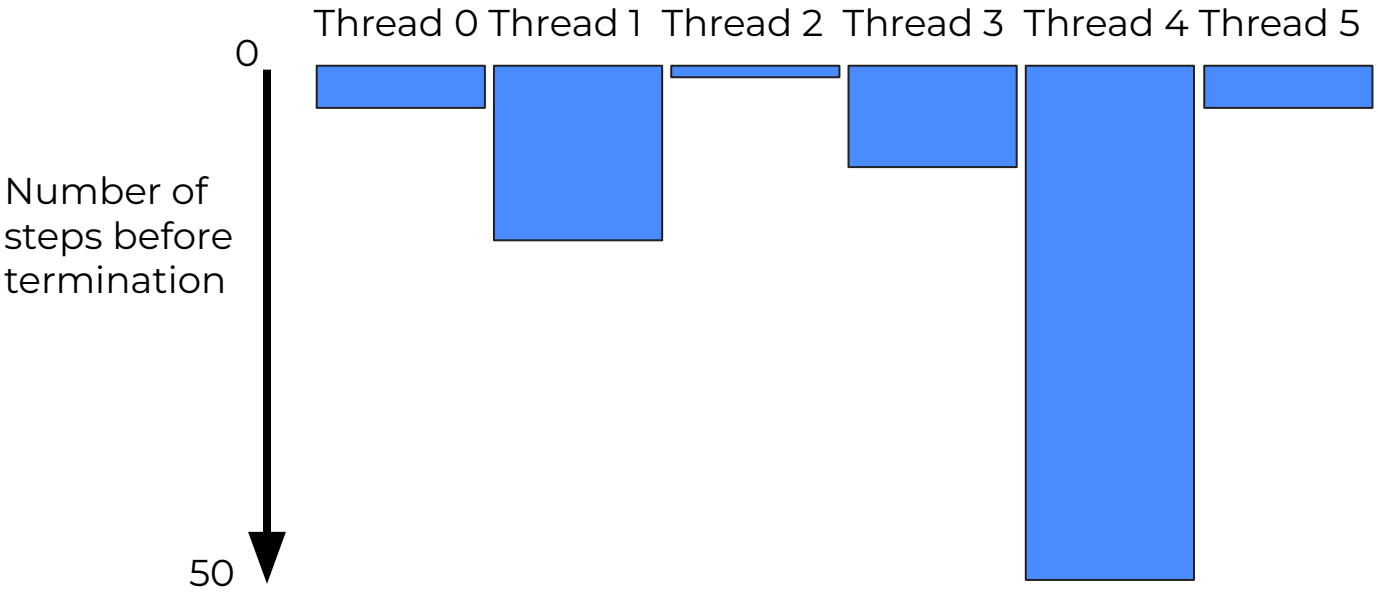
```
const unsigned int i = blockIdx.x * blockDim.x + threadIdx.x;
if (i < walkers) {
    int vIdx = s;
    while (walkLen < maxWalkLen){
        atomicAdd( address: &pr[vIdx],  val: 1.0f);//Add 1 to each visited node
        bool terminate = dist( &: mt) < 1.0f-pPpr->alpha;//Terminate with probability 1-c
        if (terminate) {
            break;
        } else {
            int neighStartIdx = csc.xPtr_cpu[vIdx];
            int neighEndIdx = csc.xPtr_cpu[vIdx+1];
            int neighSize = neighEndIdx - neighStartIdx;
            if (neighSize == 0) {
                break;}

            //select a random connected vertex
            int rIdx = vJump( &: mt)%neighSize;
            vIdx=csc.x_cpu[neighStartIdx+rIdx];
        }
        walkLen++;
    }
    walkLen = 0;
}
```

MC Complete path on GPU naive

- Solution:
  Each thread starts from a random vertex between the outgoing edges.
  In this way the atomic adds act on different memory locations

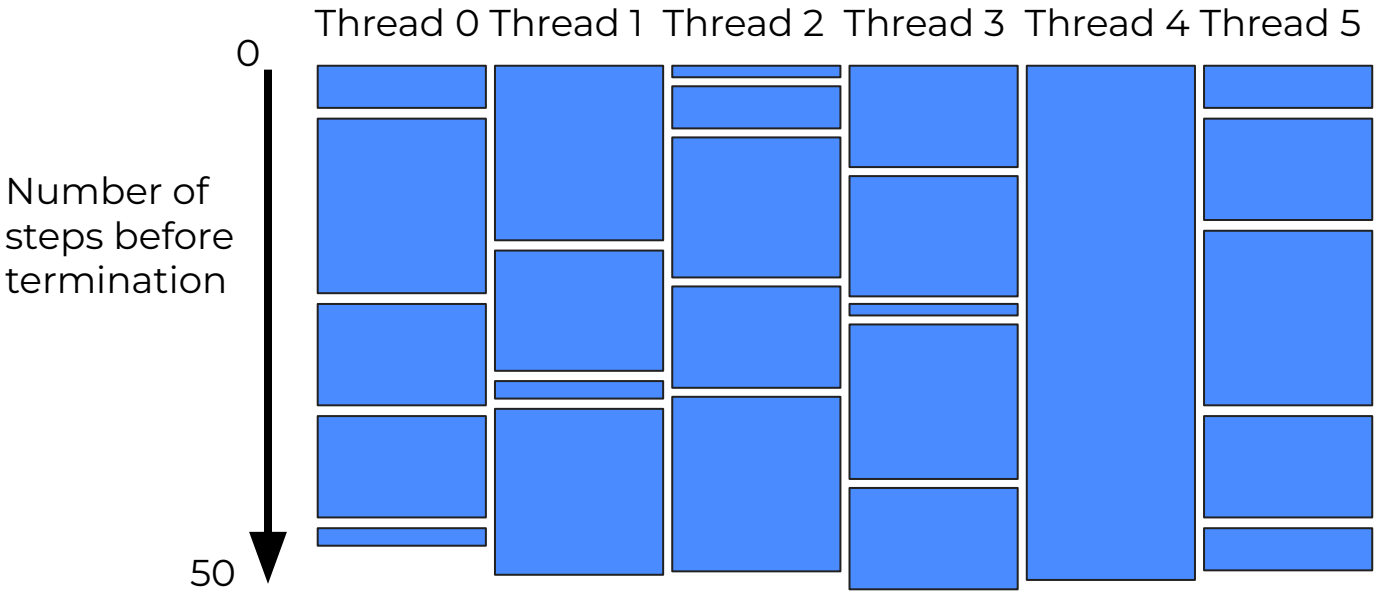
```
//Starting from neighbors of s
unsigned int rIdx0 = curand( state: &localState) % neighSizee[s];
int vIdx =  x[neighStartPos + rIdx0];
int cumulativeWalks = 1;
```

Thread utilization



Most threads do only a few steps and then terminate the random walk

Thread utilization solution



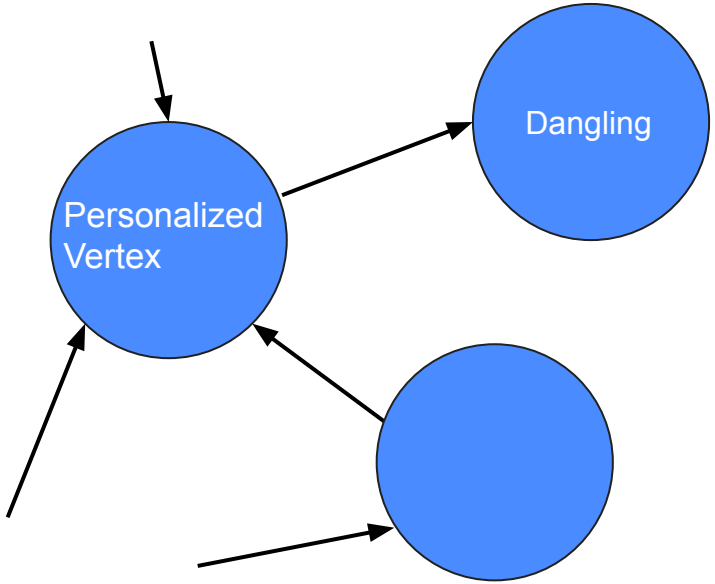
Use a thread that has terminated the computation as a new walker

```
if (cumulativeWalks<spawnWalkerThreshold)
    vIdx=s;
else
    break;
```

Leads to a much higher accuracy due to the larger number of samples

Dangling nodes in MC

We have to consider an additional case




```
error in value! (0) correct=1288741 (val=0.15), found=1288741 (val=7.68e+05)
error in value! (1) correct=975307 (val=0.1275), found=975307 (val=6.53e+05)
error in rank! (2) correct=1702309 (val=0.001989), found=3566906 (val=2.804e-07)
error in rank! (3) correct=500469 (val=0.0009716), found=3566905 (val=2.804e-07)
error in rank! (4) correct=1518892 (val=0.0009589), found=3566904 (val=2.804e-07)
error in rank! (5) correct=24716 (val=0.0008311), found=3566903 (val=2.804e-07)
error in rank! (6) correct=689491 (val=0.0008219), found=3566902 (val=2.804e-07)
error in rank! (7) correct=195101 (val=0.0007462), found=3566901 (val=2.804e-07)
error in rank! (8) correct=932394 (val=0.00071), found=3566900 (val=2.804e-07)
error in rank! (9) correct=2984189 (val=0.0006991), found=3566899 (val=2.804e-07)
error in rank! (10) correct=1835017 (val=0.0006721), found=3566898 (val=2.804e-07)
error in rank! (11) correct=577659 (val=0.0006673), found=3566897 (val=2.804e-07)
error in rank! (12) correct=28196 (val=0.0006478), found=3566896 (val=2.804e-07)
error in rank! (13) correct=7030 (val=0.0006427), found=3566895 (val=2.804e-07)
error in rank! (14) correct=2257865 (val=0.0006064), found=3566894 (val=2.804e-07)
error in rank! (15) correct=2532493 (val=0.0005939), found=3566893 (val=2.804e-07)
error in rank! (16) correct=28020 (val=0.0005909), found=3566892 (val=2.804e-07)
error in rank! (17) correct=2979297 (val=0.0005655), found=3566891 (val=2.804e-07)
error in rank! (18) correct=9008 (val=0.0004983), found=3566890 (val=2.804e-07)
error in rank! (19) correct=27566 (val=0.0004868), found=3566889 (val=2.804e-07)
```

Dangling nodes, MC

Correct first two places

Same ranking as dangling but shifted by one towards the bottom

```
error in value (0) correct=1288741 (val=0.15), found=1288741 (val=7.68e+05)
error in value (1) correct=975307 (val=0.1275), found=975307 (val=6.53e+05)
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error in rank! (5) correct=24716 (val=0.0008311), f
error in rank! (6) correct=689491 (val=0.0008219),
error in rank! (7) correct=195101 (val=0.0007462),
error in rank! (8) correct=932394 (val=0.00071), fo
error in rank! (9) correct=2984189 (val=0.0006991),
error in rank! (10) correct=1835017 (val=0.0006721)
error in rank! (11) correct=577659 (val=0.0006673),
error in rank! (12) correct=28196 (val=0.0006478),
error in rank! (13) correct=7030 (val=0.0006427), f
error in rank! (14) correct=2257865 (val=0.0006064)
error in rank! (15) correct=2532493 (val=0.0005939)
error in rank! (16) correct=28020 (val=0.0005909),
error in rank! (17) correct=2979297 (val=0.0005655)
error in rank! (18) correct=9008 (val=0.0004983), f
error in rank! (19) correct=27566 (val=0.0004868),
```

Initial pr values

Solution: Init pr with values for dangling

100% accuracy for vertices with outgoing edges towards dangling

100% accuracy and
2ms reset+execution time for danglings

Other MC optimizations

- Copy curand state in local memory
- Use an array to store outgoing edges size

Q&A

Additional slides

Performance of every implementation

Implementation	Mean total time (reset + exec)	Mean exec time	Accuracy
Naive	1023 ms	1010.62 ms	100%
Cublas bcr test	1304 ms	1215.45 ms	100%
Improved naive	814 ms	800.903 ms	100%
Cublas coo, cusparse of dot	258 ms	255.081 ms	100%
Final implementation	103 ms	100 ms	>80%
Monte Carlo complete path	17 ms	14.2666 ms	>80%

Tested on rtx 3080 laptop, 100 runs