Technical Report about implementation in CUDA of Monte Carlo Linear Solvers (MCLS)

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Abstract

In this report timings are presented as concerns Monte Carlo Linear Solvers (MCLS) with different configurations. Different test cases are used to get quite a general overview of the behavior. In particular various options to generate random numbers as well as handling of data storage are tested for the sake of efficiency. All the test cases have been run three times to filter the fluctuations due to hardware issues.

Introduction

In this report different approaches are tested in order to maximize the performance of Monte Carlo linear solvers algorithms in GPU environment. Both Forward and Adjoint method are analyzed, pointing out the different implementation issues and pinpointing the different viable options to improve timings. Four different numerical test cases are employed with different properties in terms of spectral radius of the iteration matrix, sparsity pattern, degrees of freedom and number of histories employed. The study is accomplished both by using a weight cutoff to kill the histories and by using a fixed number of steps for each of those, in order to discriminate the actual effectiveness of the different modifications introduced. An attempt to justify the improvements sometimes detected is provided, however a deeper understanding of the behaviors still has to be carried out.

1 Adjoint method - Different random number generation techniques

The generation of random numbers plays an important role in the calculation of the solution to a linear system through a Monte Carlo procedure, since a new random number must be generated to either step ahead in a random walk or to kink off a new one. Since this operation must be repeated very frequently in the code, it is recommendable to decrease its cost as much as possible, not to affect the efficiency of the overall performance. Two viable options to initialize random number generators are:

1. Having the same seed but different sequence number generates a number guaranteed to be 2^{67} away from each other, but the downside is the heavy computations to advance the 2^{67} position

   ```
   __global__ void initialize_rng(curandState *state, int seed, int offset)
   {
   ```

```
        int  tid  =  threadIdx.x  +  blockIdx.x  *  blockDim.x;

        curand_init(seed,tid,offset,&state[tid]);

    }
```

2. Giving different seeds, and just keeping the sequence number at 0, it is a lot faster but
   there might be correlation between threads, since there is no guarantee on the separation
   between each threads. In this case the different seeds can be picked accordingly to different
   criteria. In this report we explore two approaches:

   - picking the seeds with consecutive indices
   - picking the seeds with indices provided by a generator of integer random numbers

   In case seeds with consecutive indices are chosen the set of instructions employed to generate
   the seed vector is the following:

```
else  if  (  d_seed_type==SEED_TYPE::DIFF  )
{
    std::cout<<"Different  adjacent  seeds  instantiated"<<std::endl;

    thrust::device_vector<int>  seeds(  BLOCK_SIZE*num_blocks);
    thrust::sequence(seeds.begin(),  seeds.end(),  d_rng_seed);
    int*  seed_ptr  =  thrust::raw_pointer_cast(seeds.data());

    initialize_rng<<<num_blocks, BLOCK_SIZE>>>(rng_states,  seed_ptr,
        d_num_curand_calls,  d_seed_type);
}
```

Instead in the case of seeds chosen with random indices the set of instructions executed is:

```
else  if  (  d_seed_type==SEED_TYPE::RAND  )
{
    std::cout<<"Different  random  seeds  instantiated  from  0  to  "<<
    RAND_MAX<<std::endl;

    thrust::device_vector<int>  dev_seeds(  BLOCK_SIZE*num_blocks);
    thrust::host_vector<int>  host_seeds(  BLOCK_SIZE*num_blocks  );
    std::srand(std::time(0));
    thrust::generate(host_seeds.begin(),  host_seeds.end(),  std::rand);
    dev_seeds=host_seeds;
    int*  seed_ptr  =  thrust::raw_pointer_cast(dev_seeds.data());

    initialize_rng<<<num_blocks, BLOCK_SIZE>>>(rng_states,  seed_ptr,
        d_num_curand_calls,  d_seed_type);
}
```

The macro variable `RAND_MAX` is set to 2147483647. Therefore we have the guarantee that
a wide range of integers is spanned for the choice of the seeds.

In case as many seeds as the number of threads are employed, the kernel remains the same independently of the policy adopted for the selection of the seeds.

```
__global__ void initialize_rng(curandState *state, int *seed, int offset)
{
    int tid = threadIdx.x + blockIdx.x * blockDim.x;

    curand_init(seed[tid], 0, offset, &state[tid]);
}
```

Matrix	Size	Nb. Histories	% time rng	% time kernel	tot. time (ms)	rel. residual norm
2D Laplacian	900	10^7	36.0	64.0	299,563	0.0931241
1D shifted Laplacian	10^6	10^4	0.05	99.5	50,016	12.3509
1D shifted Laplacian	10^6	10^7	18.3	81.7	640,563	0.391686
SP_1	25,568	10^7	18.0	82.0	349,096	0.450792

Table 1: Adjoint method - Timings using same seed and different sequences.

Matrix	Size	Nb. Hist.	% time rng	% time kernel	tot. time (ms)	rel. res. norm	Rel. Timing
2D Laplacian	900	10^7	0.0	100.0	191,796	0.119588	0.64
1D shift Laplacian	10^6	10^4	0.0	100.0	36,123	12.3914	0.722
1D shift Laplacian	10^6	10^7	0.0	100.0	533,451	0.408134	0.833
SP_1	25,568	10^7	0.0	100.0	241,571	0.397887	0.692

Table 2: Adjoint method - Timings using different consecutive seeds and same sequence.

Matrix	Size	Nb. Hist.	% time rng	% time kernel	tot. time (ms)	rel. res. norm	Rel. Timing
2D Laplacian	900	10^7	0.0	100.0	193,381	0.112068	0.64
1D shift Laplacian	10^6	10^4	0.0	100.0	36,295	12.3404	0.726
1D shift Laplacian	10^6	10^7	0.0	100.0	549,992	0.408296	0.859
SP_1	25,568	10^7	0.0	100.0	241,817	0.383815	0.693

Table 3: Adjoint method - Timings using different seeds picked randomly and same sequence.

As it can be noticed from the previous Tables 1, 2 and 3, the second and third options provides better timings. However the payoff is an increase of the final relative residual, likely due to the correlation between the sequences generated by different seeds. The quantities "time rng" and "time kernel" are expressed in terms of percentage of the total time.

2 Adjoint method - Use of texture memory

The LDG instruction (exposed via the `__ldg` intrinsic) is a memory load that uses the texture path. It has the advantage that it does not require the explicit use of textures, since it does not explicitly bind one. Therefore `__ldg()` reads data through the texture path, without requiring a texture itself. It is an overloaded function with the prototype `__ldg(const *T)` where T is one

of CUDA's built-in types. The perk of using LDG instruction is that explicit uses of textures causes a certain amount of code clutter and overhead (e.g. for API calls to bind textures). Classical textures also use the texture load path, but in addition can transform both index (e.g. clamping modes) and data returned (e.g. interpolation) in various ways; the necessary control information is provided to the hardware during texture binding. Because the texture cache is non-coherent with respect to writes in the same kernel, use of the texture load path requires that the underlying data is read-only across the entire kernel.

3 Adjoint method - LDG calls into the code

LDG instructions have been introduced in the following functions of Profugus code:

1. `lower_bound`

2. `initialize_history`

3. `getNewState`

4. `tallyContribution`

All the instructions employed above provide a runtime decrease. However, some of them are more significant than the others. In particular the most effective calls are the ones located in 1) and 3). This is due to the fact that these functions are the ones called most frequently. The option of using LDG instruction at point 4) actually plays a role just when the expected value estimator is employed.

In the examples represented below the length of the history is set to 10000 steps. The simulations have been accomplished both with and without a weight cut off equal to 10^{-9}.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)
2D Laplacian	900	10^7	0.994869	0.99447	191,818
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	35,351
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	517,788
SP$_1$	25,568	10^7	0.977674	0.999836	241,671

Table 4: Adjoint method - Timings without LDG instructions and constant history length equal to 10,000.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	139,882	0.729
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	37,610	1.064
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	500,092	0.966
SP$_1$	25,568	10^7	0.977674	0.999836	157,545	0.652

Table 5: Adjoint method - Timings with LDG instructions at 1) and constant history length equal to 10,000.

In Tables 5-10 the relative timing is compared with the reference values in Table 4. Tables 12-17 contain relative timings with respect to the reference values in Table 11.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	193,336	1.008
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	37,759	1.068
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	548,909	1.060
SP_1	25,568	10^7	0.977674	0.999836	241,490	1

Table 6: Adjoint method - Timings with LDG instructions at 2) and constant history length equal to 10,000.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	105,010	0.547
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	36,340	1.028
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	519,408	1.003
SP_1	25,568	10^7	0.977674	0.999836	200,559	0.830

Table 7: Adjoint method - Timings with LDG instructions at 3) and constant history length equal to 10,000.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	140,347	0.732
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	36,344	1.028
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	499,007	0.964
SP_1	25,568	10^7	0.977674	0.999836	157,458	0.652

Table 8: Adjoint method - Timings with LDG instructions at 1), 2) and constant history length equal to 10,000.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	105,166	0.548
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	36,141	1.022
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	547,777	1.052
SP_1	25,568	10^7	0.977674	0.999836	200,325	0.829

Table 9: Adjoint method - Timings with LDG instructions at 2), 3) and constant history length equal to 10,000.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	105,331	0.549
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	34,616	0.979
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	520,762	1.006
SP_1	25,568	10^7	0.977674	0.999836	138,091	0.571

Table 10: Adjoint method - Timings with LDG instructions at 1), 2), 3) and constant history length equal to 10,000.

By comparing the values of Tables 4-11 it is pointed out that a benefit in terms of timings is achieved when `ldg` instructions are employed in all the three subroutines at issue. Moreover the improvement is more evident for the 2D laplacian and the SP_1 matrix. The reason of this might

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)
2D Laplacian	900	10^7	0.994869	0.99447	27,686
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	35,108
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	40,720
SP$_1$	25,568	10^7	0.977674	0.999836	4,919

Table 11: Adjoint method - Timings without LDG instructions and with weight cutoff.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	26,344	0.952
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	35,911	1.023
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	41,092	1.009
SP$_1$	25,568	10^7	0.977674	0.999836	4,759	0.967

Table 12: Adjoint method - Timings with LDG instructions at 1) and with weight cutoff.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	27,722	1.001
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	36,005	1.026
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	40,001	0.982
SP$_1$	25,568	10^7	0.977674	0.999836	5,585	1.135

Table 13: Adjoint method - Timings with LDG instructions at 2) and with weight cutoff.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	24,814	0.896
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	36,604	1.043
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	40,305	0.99
SP$_1$	25,568	10^7	0.977674	0.999836	5,065	1.03

Table 14: Adjoint method - Timings with LDG instructions at 3) and with weight cutoff.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	26,248	0.948
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	35,741	1.018
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	40,017	0.983
SP$_1$	25,568	10^7	0.977674	0.999836	4,701	0.956

Table 15: Adjoint method - Timings with LDG instructions at 1) and 2) and with weight cutoff.

be associated with the sparsity pattern. Indeed a higher number of nonzero entries induces the histories to run for longer, enhancing the utility of the texture memory might increase as well. For the 2D laplacian and the SP_1 matrix the employment of `__ldg` instructions almost halves the time for the computation. In particular the instruction which seems to be more effective is the one located in the `getNewState` subroutine. The time reduction gets weaker for the other test cases. In fact for the 1D laplacian it seems there is no benefit in terms of timings coming from the texture memory.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	27,184	0.982
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	36,141	1.029
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	40,727	1
SP$_1$	25,568	10^7	0.977674	0.999836	5,086	1.034

Table 16: Adjoint method - Timings with LDG instructions at 2), 3) and with weight cutoff.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	24,307	0.878
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	36,980	1.053
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	40,596	0.997
SP$_1$	25,568	10^7	0.977674	0.999836	4,921	1

Table 17: Adjoint method - Timings with LDG instructions at 1), 2) and 3) and with weight cutoff.

By looking at the results of the same test cases when a weight cutoff is used, we can see that the utility of `__ldg` instructions is almost vanished (see Tables 12-17). It still plays a significant role for the 2D Laplacian, plausibly because of the spectral radius $\rho(H) \approx 1$ which induces the histories to run for many steps even when the cutoff is employed. For the other cases instead the spectral radius is so small that the weight cutoff kills the histories too son for the texture memory to be effective.

4 Adjoint method - Generation of random numbers

Random numbers must be employed for each random walk to:

- determine what is the initial state

- determine the following state in the path accordingly to the current one

Essentially the generation of random numbers is located in the subroutines:

1. `initializeHistory`

2. `getNewState`

These two operations have to be repeated for all the random walks employed in the computations. In order to minimize the time spent in the generation of random numbers, it might be useful to gather the generation of many of these at the same time. Therefore a gathering of the random number generator's calls has been accomplished, partially modifying the subroutines `"initializeHistory"` and `"getNewState"`. The relationship one-to-one between the generation of a random number and a call to one of these two subroutines is broken. A group of random numbers is generated in advance before the call to the aforementioned functions. The size of the batch for this grouped random numbers is a parameter that can be tuned to find the optimal configuration, reducing the total time of execution.

The viable options that might be adopted are:

1. to call separately the random number generator once for the initializeHistory and then employ the batch for the successive steps

2. to start employing the batch even for the initial step of the history

Matrix	Size	Nb. Hist.	% time rng	% time kernel	tot. time (ms)	rel. res. norm	Rel. Timing
2D Laplacian	900	10^7	0.0	100.0	192,325	0.119588	1.003
1D shift Laplacian	10^6	10^4	0.0	100.0	36,602	12.3914	1.035
1D shift Laplacian	10^6	10^7	0.0	100.0	517,536	0.408134	1
SP$_1$	25,568	10^7	0.0	100.0	241,928	0.397887	1.001

Table 18: Adjoint method - Results for a single call of rng for both `initializeHistory` and `getNewState`.

Matrix	Size	Nb. Hist.	% time rng	% time kernel	tot. time (ms)	rel. res. norm	Rel. Timing
2D Laplacian	900	10^7	0.0	100.0	22,634	0.119588	0.818
1D shift Laplacian	10^6	10^4	0.0	100.0	37,002	12.3914	1.054
1D shift Laplacian	10^6	10^7	0.0	100.0	40,473	0.408134	0.994
SP$_1$	25,568	10^7	0.0	100.0	4,806	0.397887	0.977

Table 19: Adjoint method - Results for a single call of rng for both `initializeHistory` and `getNewState` with weight cut-off and use of ldg.

Overall, for a configuration where the length of the random walk is fixed, the two options seem to produce similar results (compare Tables 4 and 18). Slightly better results are obtained instead with the second approach (compare values in Tables 11 and 19) when a weight cutoff is used to terminate the histories.

The time reduction accomplished by grouping the generation of several random numbers has not produced significant effects though. Therefore from now on `initializeHistory` and `getNewState` will be employed by making an explicit call to the random number generator every time that is necessary to produce a new random number.

5   Adjoint method - Reorganization of data through `struct`

In order to attempt the reduction of GPU timings, a reorganization of the matrices used by the Monte Carlo linear solver is accomplished.

In particular the pursue is to increase the vicinity of data that are going to be consulted in adjacent time steps by the computer. Because of this a C++ `struct` has been introduced:

```
struct device_row_data{
        double H;
        double P;
        double W;
        int inds;
};
```

When a new state has to be taken by a random walk, corresponding values of the transition probability, iteration matrix and weight are picked from the memory storage, providing the motivation for this attempt. The integer `inds` is used to store the index of the state, while the double values `H`, `P` and `W` are employed to store the entries of the iteration matrix, probability and

weight respectively. This way, values of H, P, W associated with a particular entry are stored in contiguous cells of the memory.

This allows to reorganize the data necessary for the Monte Carlo linear solver in an array whose entries are `struct` elements. The length of the array corresponds to the number of nonzero entries of the iteration matrix.

In the following tables results associated with the employment of such data structure are presented, both by using a fixed length for the histories and by resorting to a weight cutoff of 10^{-9}.

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	105,093	0.998
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	27,404	0.792
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	422,197	0.811
SP_1	25,568	10^7	0.977674	0.999836	138,921	1.006

Table 20: Adjoint method - Timings with `struct` data used and without weight cutoff. LDG instructions at 1), 2) and 3)

Matrix	Size	Nb. Histories	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^7	0.994869	0.99447	24,669	1.015
1D shifted Laplacian	10^6	10^4	0.799972	0.639977	26,907	0.728
1D shifted Laplacian	10^6	10^7	0.799972	0.639977	30,773	0.758
SP_1	25,568	10^7	0.977674	0.999836	5,005	1.017

Table 21: Adjoint method - Timings with `struct` data used. LDG instructions at 1), 2) and 3) and with weight cutoff.

Looking at both results in Tables 20 and 21 it is pointed out that the reorganization of data does not introduce any benefits as regards the 2D Laplacian or the SP_1 matrix. However significant reduction of timings are obtained for the 1D shifted Laplacian.

6 Forward method - Assignment of tasks to threads

In the Adjoint method a single history contributes in the evaluation of different entries of the solution vector accordingly to the actual state visited. The Forward method instead is defined such that a single history always contributes on the same entry of the solution vector, depending on the state from which it has been initiated.

This typical property of the Forward method opens the way to different techniques to distribute the tasks between threads. In the problems at issue the concept of task coincide with a single history. Therefore the intent is to discover what is the best way to map histories to different threads accordingly to their index.

Regardless of the amount o histories employed for a single entry (when this number is bigger than one), two viable options to execute the assignment are:

- to employ different threads for the estimation of an entry of the solution vector

- create a one-to-one relationship between the entries of the solution vector and the threads initialized during the process.

The first option induces to deal with the issue of different threads trying to modify the value of the same entry (data concurrency). From the point of view of implementation different approaches can be use to cope with it. In the following dissertation we proceed storing the solution vector in global memory and executing an atomization of all those operation that access and modify values contained in the same memory cell. The second approach, instead, does not entail any data concurrency since each thread always accesses a memory cell which is never consulted by any other thread. However we have a restriction to the number of threads which actually do a job, since it is necessarily equal to the size of the linear system.

The goal is to compare the timings between these two settings, focusing on determining the effects of the serialization occurring in the execution of the kernel for the first option.

In the case when different threads are allowed to work on the same entry, a possible mapping might be the following one:

```
__global__ void run_forward_monte_carlo (...)
{

    ...

    int tid = threadIdx.x + blockIdx.x * blockDim.x;
    int entry = tid / entry_histories;

    ...

}
```

As already mentioned previously in the dissertation, this requires a serialization of the access by different threads to the same memory cell. This is accomplished by the following instruction:

```
__device__ void tallyContribution(int state, double wt, double * const x)
{
        // Collision estimator just adds weight
        atomicAdd(x+state,wt);
}
```

The one-to-one relationship between entries and threads instead induces instead the following mapping:

```
__global__ void run_forward_monte_carlo (...)
{

    ...

    int tid = threadIdx.x + blockIdx.x * blockDim.x;
    int entry = tid / entry_histories;

    ...

}
```

```
\hspace*{-2cm}
\begin{lstlisting}
__global__ void run_forward_monte_carlo(...)
{

    ...

    int tid = threadIdx.x + blockIdx.x * blockDim.x;
    if( tid < N )
    {
        ...
    }

    ...

}
```

In the last case obviously it is necessary to instantiate a number of threads bigger than the actual size of the problem to solve, since in general the size of the blocks is not a divisor of the number of degrees of freedom. However, the higher is the size of the problem, the less this is an issue.

For both the configurations the test cases are run both by using a fixed number of steps equal to 10,000 and by employing a weight cutoff equal to 10^{-9}. No texture memory instructions are employed.

Matrix	Size	Nb. Histories per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)
2D Laplacian	900	10^3	0.994869	0.99447	437,444
1D shifted Laplacian	10^6	5	0.799972	0.639977	78,767
SP$_1$	$25,568$	200	0.977674	1.99619	241,573

Table 22: Forward method - mapping of multiple threads to a single entry. Fixed number of steps equal to 10,000.

Matrix	Size	Nb. Hist. per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^3	0.994869	0.99447	79,306	0.181
1D shift Laplacian	10^6	5	0.799972	0.639977	74,621	0.947
SP$_1$	$25,568$	200	0.977674	1.99619	122,773	0.508

Table 23: Forward method - one-to-one mapping between threads and entries. Fixed number of steps equal to 10,000.

Even if the case of the SP_1 matrix does not converge, we are going to consider the behavior of the code for this test case anyway. Indeed the priority is to focus on the performance of the algorithm with respect to different instantiations of the threads rather than the accuracy of the final numerical result itself.

Comparing values in Tables 22 and 23, we can see that the atomization of the contribution coming from each tally affect the performance of the algorithm for all the test cases analyzed,

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in particular for the 2D Laplacian and the SP_1 matrix. The outstanding improvement for these cases can be explained with the small size of the problems. In the first approach for the distribution of tasks, indeed, the tasks are attributed to the same entry according to a rotation of the blocks. Therefore threads working on the same entry of the solution vector will always belong to different blocks. In fact for a fixed block size, the higher is the size of the problem the lower is the contention of memory resources between threads belonging to different blocks. This explains why results are pretty similar for the 1D shifted Laplacian, since its size is order of magnitudes bigger than for the other test cases analyzed.

Matrix	Size	Nb. Histories per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)
2D Laplacian	900	10^3	0.994869	0.99447	206,439
1D shifted Laplacian	10^6	5	0.799972	0.639977	39,295
SP_1	25,568	200	0.977674	1.99619	33,169

Table 24: Forward method - mapping of multiple threads to a single entry. Weight cutoff equal to 10^{-9}.

Matrix	Size	Nb. Hist. per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^3	0.994869	0.99447	11,572	0.056
1D shift Laplacian	10^6	5	0.799972	0.639977	38,484	0.976
SP_1	25,568	200	0.977674	1.99619	6,505	0.196

Table 25: Forward method - one-to-one mapping between threads and entries. Weight cutoff equal to 10^{-9}.

Looking at Tables 24 and 25, the employment of the one-to-one map still has a huge impact in terms of performance as concerns that 2D Laplacian and the SP_1 matrix. As regards the 1D shifted Laplacian, instead, the weight cutoff seems to have e dominant effect on the timing, eliding the utility of the different techniques for the assignment of the tasks to the threads instantiated. A plausible explanation for this phenomenon might be the sparsity pattern of the matrices analyzed. In fact the number of nonzero entries per row is much higher for the first and third problem than for the second. Moreover the spectral radii of H and $\hat{H}$ are much smaller for the shifted 1D Laplacian. Therefore the average number of steps per history is lower for the 1D shifted Laplacian than for the other cases, explaining why this particular problem is transparent to the employment of different mappings for the task distribution.

7 Forward method - Use of texture memory

We now focus on comparing the change of performance of the Forward method depending on whether texture memory instructions are used or not. The collocation of the texture memory instructions is the same as for the Adjoint method.

By default the one-to-one mapping for the execution of the tasks by different threads is employed. Results are shown both by resorting to a fixed length of the histories and also by using an adaptive weight cutoff.

Comparing results in Table 26 with the ones in Table 23, it is detected a significant improvement of the timings thanks to the employment of texture memory. Especially for the SP_1 matrix, supposedly for its sparsity pattern.

Matrix	Size	Nb. Hist. per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^3	0.994869	0.99447	52,077	0.657
1D shift Laplacian	10^6	5	0.799972	0.639977	63,353	0.849
SP$_1$	25,568	200	0.977674	1.99619	72,198	0.588

Table 26: Forward method - one-to-one mapping between threads and entries. Fixed number of steps equal to 10,000. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timings
2D Laplacian	900	10^3	0.994869	0.99447	9,316	0.805
1D shift Laplacian	10^6	5	0.799972	0.639977	40,005	1.04
SP$_1$	25,568	200	0.977674	1.99619	4,269	0.656

Table 27: Forward method - one-to-one mapping between threads and entries. Weight cutoff equal to 10^{-9}. LDG instructions employed.

By making a comparison between Tables 27 and 25 we discover a similar behavior to the one verified for the Adjoint method. In fact once the weight cutoff is employed, the use of `__ldg` instructions seem not to be effective for the reduction of the computational time.

8 Forward method - Reorganization of data through `struct`

In this section we focus on testing the efficiency of the employment of C++ `struct` objects to handle data, on the same lead as for the Adjoint method. The experiments are repeated both for a fixed length of histories equal to 10,000 and for the use of a weight cutoff equal to 10^{-9}, with and without `ldg` instructions as well. The one-to-one mapping between tasks and threads is employed.

Matrix	Size	Nb. Hist per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^3	0.994869	0.99447	80,059	1.009
1D shift Laplacian	10^6	5	0.799972	0.639977	79,807	1.069
SP$_1$	25,568	200	0.977674	1.99619	122,861	1

Table 28: Forward method - use of struct for data handling. One-to-one mapping between threads and entries. Fixed number of steps equal to 10,000. No LDG instructions.

Matrix	Size	Nb. Hist. per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^3	0.994869	0.99447	11,534	1.003
1D shift Laplacian	10^6	5	0.799972	0.639977	29,636	0.770
SP$_1$	25,568	200	0.977674	1.99619	6,247	0.960

Table 29: Forward method - use of struct for data handling. One-to-one mapping between threads and entries. Weight cutoff equal to 10^{-9}. No LDG instructions.

Results in Tables 28 (compared with Table 23) and 29 show (compared with Table 25) show that actually the employment of `struct` for the data storage does not provide improvements without using texture memory. However an interesting progress is detected for all the test cases

Matrix	Size	Nb. Hist. per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^3	0.994869	0.99447	50,159	0.627
1D shift Laplacian	10^6	5	0.799972	0.639977	67,993	0.852
SP$_1$	25,568	200	0.977674	1.99619	75,305	0.598

Table 30: Forward method - use of struct for data handling. One-to-one mapping between threads and entries. Fixed number of steps equal to 10,000. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	$\rho(H)$	$\rho(\hat{H})$	tot. time (ms)	Rel. Timing
2D Laplacian	900	10^3	0.994869	0.99447	8,950	1.041
1D shift Laplacian	10^6	5	0.799972	0.639977	30,314	0.758
SP$_1$	25,568	200	0.977674	1.99619	4,040	0.946

Table 31: Forward method - use of struct for data handling. One-to-one mapping between threads and entries. Weight cutoff equal to 10^{-9}. LDG instructions employed.

at hand when use of `struct` and texture memory are combined for a fixed length of the histories. Moreover, on the same lead as for the Adjoin method, the effectiveness of all the modifications shades with a weight cutoff to shut down the random walks adaptively (compare results in Tables 31 with the ones in Table 27).

9   Use of L1 global cache

Primary versions of NVIDIA graphic board were already garnered with L1 local cache memories. However they were not endowed with a similar memory to cache accesses to global memory which are known to cause the highest latency timings. Using a caching system for such accesses can provide evident advantages, relatively to the particular application at hand and t its implementation.

Recent versions of NVIDIA GPUs enable the use of L1 cache memories. Tesla K40m graphic boards, the ones installed in Titan, belong to this set of processors.

Even on Kepler GPUs that do support caching global memory in L1, the default behavior is to not cache global memory in L1. You have to opt-in to enable caching by passing `-Xptxas=-dlcm=ca` as an argument to NVCC when compiling your kernels. Kernels compiled in this fashion will still function on earlier Kepler devices though global memory operations will bypass the L1 cache.

You can programmatically query whether a GPU supports caching global memory operations using `cudaGetDeviceProperties` and examining the `globalL1CacheSupported` property.

In our code we have included the following commands in the main file in order to display the technical properties of GPUs at hand:

```
int nDevices;

cudaGetDeviceCount(&nDevices);
printf("The number of GPU devices is: %d\n", nDevices);
for (int i = 0; i < nDevices; i++) {
  cudaDeviceProp prop;
  cudaGetDeviceProperties(&prop, i);
```

```
printf("Device Number: %d\n", i);
printf("  Device name: %s\n", prop.name);
printf("  Memory Clock Rate (KHz): %d\n",
       prop.memoryClockRate);
printf("  Memory Bus Width (bits): %d\n",
       prop.memoryBusWidth);
printf("  Peak Memory Bandwidth (GB/s): %f\n\n",
       2.0*prop.memoryClockRate*(prop.memoryBusWidth/8)/1.0e6);
printf("  globalL1CacheSupported: %d\n", prop.globalL1CacheSupported);
printf("  localL1CacheSupported: %d\n", prop.localL1CacheSupported);
}
```

One we have verified the presence of L1 Global caches in the NVDIA GPUs available, we can still customize even more the use for the resources at hand. In fact the L1 cache and the shared memory use a single memory for their purposes, splitting a common physical resources in two equal parts. In the case when either the shared memory or the L1 global cache are not used, it is pointless to keep occupied a part of memory for something tat will never be employed. Therefore it is possible to recalibrate the amount of Kbytes dedicated to both the kind of memories. This is possible through the use of two functions named `cudaDeviceSetCacheConfig` and `cudaFuncSetCacheConfig`. Their definition is included in the `cuda_runtime_api.h` header file.

The subroutine `cudaDeviceSetCacheConfig` requires only an argument, since its action affect the way all the subsequent kernels are executed. Instead `cudaFuncSetCacheConfig` requires two arguments. The first one is the name of the kernel to which it has to be applied, since it changes the handling of hardware resources between L1 cache and shared memory just for the specific kernel declared. The argument of `cudaDeviceSetCacheConfig` and the second one of `cudaFuncSetCacheConfig` can attain one of the following values:

- `cudaFuncCachePreferShared`

- `cudaFuncCachePreferL1`

- `cudaFuncCachePreferEqual`

The third one corresponds to the default setting. The first one dedicate more memory cells to the shared memory, the second one instead shifts mos of it to the L1 cache use.

It is possible to monitor the amount of resources used at runtime by passing some parameter to the NVIDIA profiler (NVPROF or NVVP). In the case of `nvprof` the command line looks like the one presented below here:

```
 nvprof --metrics <type_of_counter> <executable_name>
<arguments_for_executable>
```

The kind of counters that can be used as metric tools are:

- `l1_cache_global_hit_rate` - percentage of reads that hit in L1 (Opt-In, K40/K80 only)

- `tex_cache_hit_rate` - percentage of reads that hit in texture cache (__ldg() or texture access only)

- `l2_l1_read_hit_rate` - percentage of l1 misses which hit in L2

- `l2_texture_read_hit_rate` - percentage of texture misses which hit in L2

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All these counters provide you information regarding the use of hardware resources for each separate kernel employed in the code.

For our current interest we use `l1_cache_global_hit_rate`. In the following treatise we present timings for the most important setting described before (for Adjoint and Forward MC), enabling the use of L1 global cache. Percentage of such resource used by the kernels are provided too. However, since the profiling affect the performance of the code, each configuration has been run twice for the sake of validity of the results presented: once without and once with the profiler.

As regards the Adjoint method, enabling L1 global cache does not provide evident improvements, as it can be verified with results in Tables 32-37. Sporadic time reductions occur for all the test cases considered but it is hard to find a correlation between the role played by the global cache memory and the other factors of the setting. In particular it is not possible to declare that such reductions are due to the global cache, since in most of the cases the profiler prompts out that no cache resources are actually employed.

Matrix	Size	Nb. Hist.	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^7	167,270	0 - 0	0.874
1D shift Laplacian	10^6	10^4	36,854	0 - 0	1.021
1D shift Laplacian	10^6	10^7	573,288	0 - 0	1.075
SP$_1$	25,568	10^7	306,248	0 - 0	1.268

Table 32: Adjoint method - Use of L1 global cache. Fixed number of steps equal to 10,000. No LDG instructions.

Matrix	Size	Nb. Hist.	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^7	32,460	0 - 0	1.172
1D shift Laplacian	10^6	10^4	38,002	0 - 0	1.082
1D shift Laplacian	10^6	10^7	40,910	0 - 0	1.005
SP$_1$	25,568	10^7	6,781	0 - 0	1.379

Table 33: Adjoint method - Use of L1 global cache. Weight cutoff equal to 10^{-9}. No LDG instructions.

Matrix	Size	Nb. Hist.	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^7	101,068	0 - 0	0.960
1D shift Laplacian	10^6	10^4	36,776	0 - 0	1.062
1D shift Laplacian	10^6	10^7	574,863	0 - 0	1.104
SP$_1$	25,568	10^7	118,604	0 - 0	0.859

Table 34: Adjoint method - Use of L1 global cache. Fixed number of steps equal to 10,000. LDG instructions employed.

Better results are obtained by activating L1 cache for the Forward method. In particular the combination of the use of `struct` and L1 global cache provides significant improvement of timings and cache resources are employed almost to the full for all the test cases considered. This phenomenon can be explained with the fact that the `struct` enables to reorder data so that values accessed in consecutive moments in time are physically close in the memory storage. Therefore caching information before using them helps in reducing the runtime effectively.

Matrix	Size	Nb. Hist.	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^7	28,222	0 - 0	1.161
1D shift Laplacian	10^6	10^4	36,042	0 - 0	0.975
1D shift Laplacian	10^6	10^7	41,473	0 - 0	1.022
SP_1	25,568	10^7	4,644	0 - 0	0.944

Table 35: Adjoint method - Use of L1 global cache. Weight cutoff equal to 10^{-9}. LDG instructions employed.

Matrix	Size	Nb. Hist.	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^7	101,004	0 - 0	0.961
1D shift Laplacian	10^6	10^4	27,351	0 - 21.37	0.998
1D shift Laplacian	10^6	10^7	413,696	0 - 0	0.980
SP_1	25,568	10^7	133,346	0 - 0	0.96

Table 36: Adjoint method - Use of `struct` for data handling. Use of L1 global cache. Fixed number of steps equal to 10,000. LDG instructions employed.

Matrix	Size	Nb. Hist.	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^7	28,986	0 - 74.29	1.175
1D shift Laplacian	10^6	10^4	26,838	0 - 0	0.997
1D shift Laplacian	10^6	10^7	30,671	0 - 0	0.997
SP_1	25,568	10^7	4,886	0 - 0	0.976

Table 37: Adjoint method - Use of `struct` for data handling. Weight cutoff equal to 10^{-9}. Fixed number of steps equal to 10,000. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^3	74,274	0 - 0	0.937
1D shift Laplacian	10^6	5	82,440	0 - 0	1.105
SP_1	25, 568	200	197,493	0 - 0	1.609

Table 38: Forward method. Fixed number of steps equal to 10,000. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^3	9,716	0 - 0	0.840
1D shift Laplacian	10^6	5	36,040	0 - 0	0.936
SP_1	25, 568	200	8,189	0 - 0	1.259

Table 39: Forward method. Weight cutoff equal to 10^{-9}. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^3	44,134	0 - 0	0.847
1D shift Laplacian	10^6	5	52,816	0 - 0	0.834
SP_1	25, 568	200	74,393	0 - 0	1.030

Table 40: Forward method. Fixed number of steps equal to 10,000. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^3	44,134	0 - 0	0.847
1D shift Laplacian	10^6	5	52,816	0 - 0	0.834
SP_1	25,568	200	74,393	0 - 0	1.030

Table 41: Forward method. Weight cutoff equal to 10^{-9}. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^3	42,610	0 - 0	0.849
1D shift Laplacian	10^6	5	58,473	0 - 0	0.860
SP_1	25,568	200	83,258	0 - 0	1.106

Table 42: Forward method - Use of `struct` for data handling. Fixed number of steps equal to 10,000. LDG instructions employed.

Matrix	Size	Nb. Hist. per entry	tot. time (ms)	% rng - % mc	Rel. Timing
2D Laplacian	900	10^3	7,713	0 - 94.16	0.862
1D shift Laplacian	10^6	5	29,512	0 - 82.14	0.974
SP_1	25,568	200	3,782	0 - 42.40	0.936

Table 43: Forward method - Use of `struct` for data handling. Weight cutoff equal to 10^{-9}. LDG instructions employed.