Implementation of PDE methods on GPUs

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GPUs

In the last 6 years, GPUs have emerged as a major new technology in computational finance, as well as other areas in HPC:

- over 1000 GPUs at JP Morgan, and also used at a number of other Tier 1 banks and financial institutions

- use is driven by both energy efficiency and price/performance, with main concern the level of programming effort required

- Monte Carlo simulations are naturally parallel, so ideally suited to GPU execution:
  - averaging of path payoff values using binary tree reduction
  - implementations exist also for Longstaff-Schwartz least squares regression for American options – STAC-A2 testcase
  - key requirement is parallel random number generation, and that is addressed by libraries such as CURAND

Finite Difference calculations

Focus of this work is finite difference methods for approximating Black-Scholes and other related multi-factor PDEs

- explicit time-marching methods are naturally parallel – again a good target for GPU acceleration
- implicit time-marching methods usually require the solution of lots of tridiagonal systems of equations – not so clear how to parallelise this
- key observation is that cost of moving lots of data to/from the main graphics memory can exceed cost of floating point computations
  - 288 GB/s bandwidth
  - 5.0 TFlops (single precision) / 1.7 TFlops (double precision)

$\Longrightarrow$ should try to avoid this data movement

1D Finite Difference calculations

In 1D, a simple explicit finite difference equation takes the form

$$u_j^{n+1} = a_j \, u_{j-1}^n + b_j \, u_j^n + c_j \, u_{j+1}^n$$

while an implicit finite difference equation takes the form

$$a_j \, u_{j-1}^{n+1} + b_j \, u_j^{n+1} + c_j \, u_{j+1}^{n+1} = u_j^n$$

requiring the solution of a tridiagonal set of equations.

What performance can be achieved?

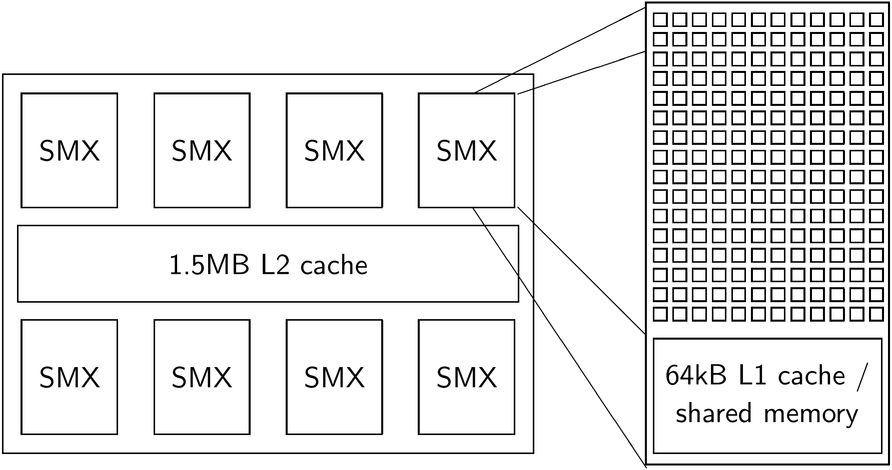
1D Finite Difference calculations

- grid size: 256 points
- number of options: 2048
- number of timesteps: 50000 (explicit), 2500 (implicit)
- K40 capable of 5 TFlops (single prec.), 1.7 TFlops (double prec.)

	single prec.		double prec.	
	msec	GFlops	msec	GFlops
explicit1	224	700	258	610
explicit2	52	3029	107	1463
implicit1	19	1849	57	892

How is this performance achieved?

NVIDIA Kepler GPU



1D Finite Difference calculations

Approach for explicit time-marching:

- each thread block (256 threads) does one or more options
- 3 FMA (fused multiply-add) operations per grid point per timestep
- doing an option calculation within one thread block means no need to transfer data to/from graphics memory – can hold all data in SMX

1D Finite Difference calculations

- `explicit1` holds data in shared memory
- each thread handles one grid point
- performance is limited by speed of shared memory access, and cost of synchronisation

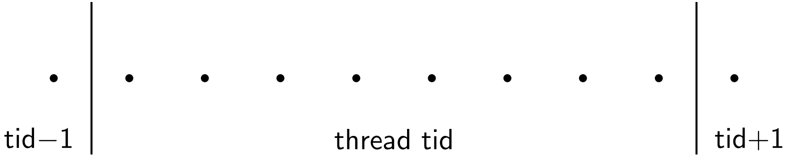
```
__shared__ REAL u[258];
...
utmp = u[i];

for (int n=0; n<N; n++) {
  utmp = utmp + a*u[i-1] + b*utmp + c*u[i+1];
  __syncthreads();
  u[i] = utmp;
  __syncthreads();
}
```

1D Finite Difference calculations

`explicit2` holds all data in registers

- each thread handles 8 grid points, so each warp (32 threads which act in unison) handles one option
- no block synchronisation required
- data exchange with neighbouring threads uses shuffle instructions (special hardware feature for data exchange within a warp)



1D Finite Difference calculations

```
for (int n=0; n<N; n++) {
  um = __shfl_up(u[7], 1);
  up = __shfl_down(u[0], 1);

  for (int i=0; i<7; i++) {
    u0   = u[i];
    u[i] = u[i] + a[i]*um + b[i]*u0 + c[i]*u[i+1];
    um   = u0;
  }

  u[7] = u[7] + a[7]*um + b[7]*u[7] + c[7]*up;
}
```

1D Finite Difference calculations

Bigger challenge is how to solve tridiagonal systems for implicit solvers.

- want to keep computation within an SMX and avoid data transfer to/from graphics memory
- prepared to do more floating point operations if necessary to avoid the data transfer
- need lots of parallelism to achieve good performance

Solving Tridiagonal Systems

On a CPU, the tridiagonal equations

$$a_i\, u_{i-1} + b_i\, u_i + c_i\, u_{i+1} = d_i, \quad i = 0, 1, \ldots, N-1$$

would usually be solved using the Thomas algorithm – essentially just standard Gaussian elimination exploiting all of the zeros.

- inherently sequential algorithm, with a forward sweep and then a backward sweep
- would require each thread to handle separate option
- threads don't have enough registers to store the required data – would require data transfer to/from graphics memory to hold / recover data from forward sweep
- not a good choice – want an alternative with reduced data transfer, even if it requires more floating point ops.

Solving Tridiagonal Systems

PCR (parallel cyclic reduction) is a highly parallel algorithm.

Starting with

$$a_i\, u_{i-1} + u_i + c_i\, u_{i+1} = d_i, \qquad i = 0, 1, \ldots, N\!-\!1,$$

where $u_j\!=\!0$ for $j\!<\!0, j\!\geq\!N$, can subtract multiples of rows $i\!\pm\!1$, and re-normalise, to get

$$a'_i\, u_{i-2} + u_i + c'_i\, u_{i+2} = d'_i, \quad i = 0, 1, \ldots, N\!-\!1,$$

Repeating with rows $i\!\pm\!2$ gives

$$a''_i\, u_{i-4} + u_i + c''_i\, u_{i+4} = d''_i, \quad i = 0, 1, \ldots, N\!-\!1,$$

and after $\log_2 N$ repetitions end up with solution because $u_{i\pm N} = 0$.

1D Finite Difference calculations

`implicit1` uses a hybrid Thomas / PCR algorithm:

- follows data layout of `explicit2` with each thread handling 8 grid points – means data exchanges can be performed by shuffles
- each thread uses Thomas algorithm to obtain middle values as a linear function of two (not yet known) "end" values

$$u_{J+j} = A_{J+j} + B_{J+j}\, u_J + C_{J+j}\, u_{J+7}, \quad 0 < j < 7$$

- the reduced tridiagonal system of size 2×32 for the "end" values is solved using PCR
- total number of floating point operations is approximately double what would be needed on a CPU using the Thomas algorithm (but CPU division is more expensive, so similar Flop count overall?)

1D Finite Difference calculations

$$
\left(\begin{array}{c|cccccccc|c}
 & & & & & & & & & \\ \hline
x & x & x & & & & & & & \\
 & x & x & x & & & & & & \\
 & & x & x & x & & & & & \\
 & & & x & x & x & & & & \\
 & & & & x & x & x & & & \\
 & & & & & x & x & x & & \\
 & & & & & & x & x & x & \\
 & & & & & & & x & x & x \\ \hline
 & & & & & & & & &
\end{array}\right)
$$

$$
\Longrightarrow \quad
\left(\begin{array}{c|cccccccc|c}
 & & & & & & & & & \\ \hline
x & x & & & & & & & x & \\
 & x & 1 & & & & & & x & \\
 & x & & 1 & & & & & x & \\
 & x & & & 1 & & & & x & \\
 & x & & & & 1 & & & x & \\
 & x & & & & & 1 & & x & \\
 & x & & & & & & 1 & x & \\
 & x & & & & & & & x & x \\ \hline
 & & & & & & & & &
\end{array}\right)
$$

1D Finite Difference calculations

For comparison, we have developed an implementation for two 8-core "Sandy Bridge" Xeon E5-2690 CPUs

- OpenMP used for multi-threading
- each core has two 256-bit AVX vector units (ADD and MUL)
- two CPUs are capable of 740 GFlops (single), 370 GFlops (double)
- a variety of possible vectorisation approaches
  - compiler auto-vectorisation
  - low-level vector intrinsics
  - OpenCL
  - Cilk Plus
- each core has a large 256kB L2 cache for temporary variables, so Thomas algorithm best for implicit solver

1D Finite Difference calculations

Performance on two 8-core "Sandy Bridge" Xeon E5-2690 CPUs

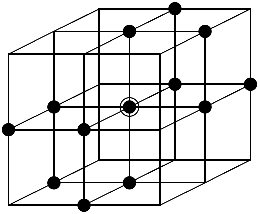
	single prec.		double prec.	
	msec	GFlop/s	msec	GFlop/s
explicit1	563	279	1188	132
explicit2	398	394	781	201
implicit1	187	139	470	48
implicit2	157	166	473	47

- `explicit1` uses compiler auto-vectorisation (data in L1 cache)
- `explicit2` uses low-level vector intrinsics and a similar approach to the GPU implementation (data in L1 cache)
- `implicit1` uses compiler auto-vectorisation (data in L2 cache)
- `implicit2` uses low-level vector intrinsics (data in L2 cache)

3D Finite Difference calculations

What about a 3D extension on a 256^3 grid?

- memory requirements imply one kernel with multiple thread blocks to handle a single option
- kernel will need to be called for each timestep, to ensure that the entire grid is updated before the next timestep starts
- 13-point stencil for explicit time-marching



- implementation uses a separate thread for each grid point in 2D x-y plane, then marches in z-direction

3D Finite Difference calculations

- grid size: 256^3 points
- number of timesteps: 500 (explicit), 100 (implicit)
- K40 capable of 5.0 TFlops (single prec.), 1.7 TFlops (double prec.) and 288 GB/s

	single prec.			double prec.		
	msec	GFlops	GB/s	msec	GFlops	GB/s
explicit1	747	597	100	1200	367	127
explicit2	600	760	132	923	487	144
implicit1	447	406	146	889	243	144

Performance as reported by nvprof, the NVIDIA Visual Profiler

3D Finite Difference calculations

`explicit1` relies on L1/L2 caches for data reuse – compiler does an excellent job of optimising loop invariant operations

```
u2[indg] = t23                                * u1[indg-KOFF-JOFF]
        +  t13                                * u1[indg-KOFF-IOFF]
        + (c1_3*S3*S3 - c2_3*S3 - t13 - t23) * u1[indg-KOFF]
        +  t12                                * u1[indg-JOFF-IOFF]
        + (c1_2*S2*S2 - c2_2*S2 - t12 - t23) * u1[indg-JOFF]
        + (c1_1*S1*S1 - c2_1*S1 - t12 - t13) * u1[indg-IOFF]
        + (1.0f - c3 - 2.0f*( c1_1*S1*S1 + c1_2*S2*S2 + c1_3*S3*S3
                   - t12 - t13 - t23 ) ) * u1[indg]
        + (c1_1*S1*S1 + c2_1*S1 - t12 - t13) * u1[indg+IOFF]
        + (c1_2*S2*S2 + c2_2*S2 - t12 - t23) * u1[indg+JOFF]
        +  t12                                * u1[indg+JOFF+IOFF]
        + (c1_3*S3*S3 + c2_3*S3 - t13 - t23) * u1[indg+KOFF]
        +  t13                                * u1[indg+KOFF+IOFF]
        +  t23                                * u1[indg+KOFF+JOFF];
```

3D Finite Difference calculations

`explicit2` uses extra registers to hold values which will be needed again

```
u =       t23                            * u1_om
       +  t13                            * u1_mo
       + (c1_3*S3*S3 - c2_3*S3 - t13 - t23) * u1_m;

u1_mm = u1[indg-JOFF-IOFF];
u1_om = u1[indg-JOFF];
u1_mo = u1[indg-IOFF];
u1_pp = u1[indg+IOFF+JOFF];

u = u  +  t12                            * u1_mm
       + (c1_2*S2*S2 - c2_2*S2 - t12 - t23) * u1_om
       + (c1_1*S1*S1 - c2_1*S1 - t12 - t13) * u1_mo
       + (1.0f - c3 - 2.0f*( c1_1*S1*S1 + c1_2*S2*S2 + c1_3*S3*S3
                        - t12 - t13 - t23 ) ) * u1_oo
       + (c1_1*S1*S1 + c2_1*S1 - t12 - t13) * u1_po
       + (c1_2*S2*S2 + c2_2*S2 - t12 - t23) * u1_op
       +  t12                            * u1_pp;

indg += KOFF;
u1_m  = u1_oo;
u1_oo = u1[indg];
u1_po = u1[indg+IOFF];
u1_op = u1[indg+JOFF];

u = u  + (c1_3*S3*S3 + c2_3*S3 - t13 - t23) * u1_oo
       +  t13                            * u1_po
       +  t23                            * u1_op;
```

3D Finite Difference calculations

The implicit ADI discretisation requires the solution of tridiagonal equations along each coordinate direction.

The `implicit1` code has the following structure:

- kernel similar to explicit kernel to produce r.h.s.
- separate kernel for tridiagonal solution in each coordinate direction
- very important to ensure each warp loads a contiguous vector of data (coalesced read) as much as possible
- requires some careful transposition of data using shared memory

Distinctly non-trivial, so check out the paper and the code on my webpage!

3D Finite Difference calculations

Performance on two 8-core "Sandy Bridge" Xeon E5-2690 CPUs, with combined 100 GB/s bandwidth to main memory (66 GB/s observed)

Dual-socket Intel Xeon E5-2690						
	single prec.			double prec.		
	msec	GFlop/s	GB/s	msec	GFlop/s	GB/s
explicit1	1903	233	34	3911	114	33
implicit1	2561	82	23	4966	42	23

- `explicit1` uses compiler auto-vectorisation
- `implicit1` uses compiler auto-vectorisation

Final GPU / CPU comparison

Best explicit/implicit one-factor (1F) and three-factor (3F) times (ms) on one K40 GPU versus two Intel E5-2690 Xeon CPUs

	K40 GPU		2 Xeon CPUs	
	SP	DP	SP	DP
1F explicit	52	107	398	781
1F implicit	19	57	157	473
3F explicit	600	923	1903	3911
3F implicit	447	889	2561	4966

Conclusions

- GPUs can deliver excellent performance for financial finite difference calculations, as well as for Monte Carlo
- some parts of the implementation are straightforward, but others require a good understanding of the hardware and parallel algorithms to achieve the best performance
- some of this work will be built into NVIDIA CUSPARSE library
- results show one K40 GPU is $7\!-\!8\times$ (1F) and $3\!-\!5.5\times$ (3F) faster than two 8-core Xeon E5-2690 CPUs

For further info, see software and other details at
`http://people.maths.ox.ac.uk/gilesm/codes/BS_1D/`
`http://people.maths.ox.ac.uk/gilesm/codes/BS_3D/`
`http://people.maths.ox.ac.uk/gilesm/cuda_slides.html`