

# Sequence Alignment with GPU: Performance and Design Challenges

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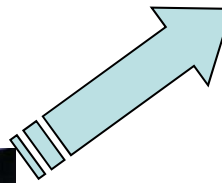
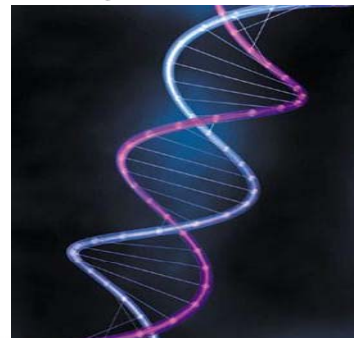
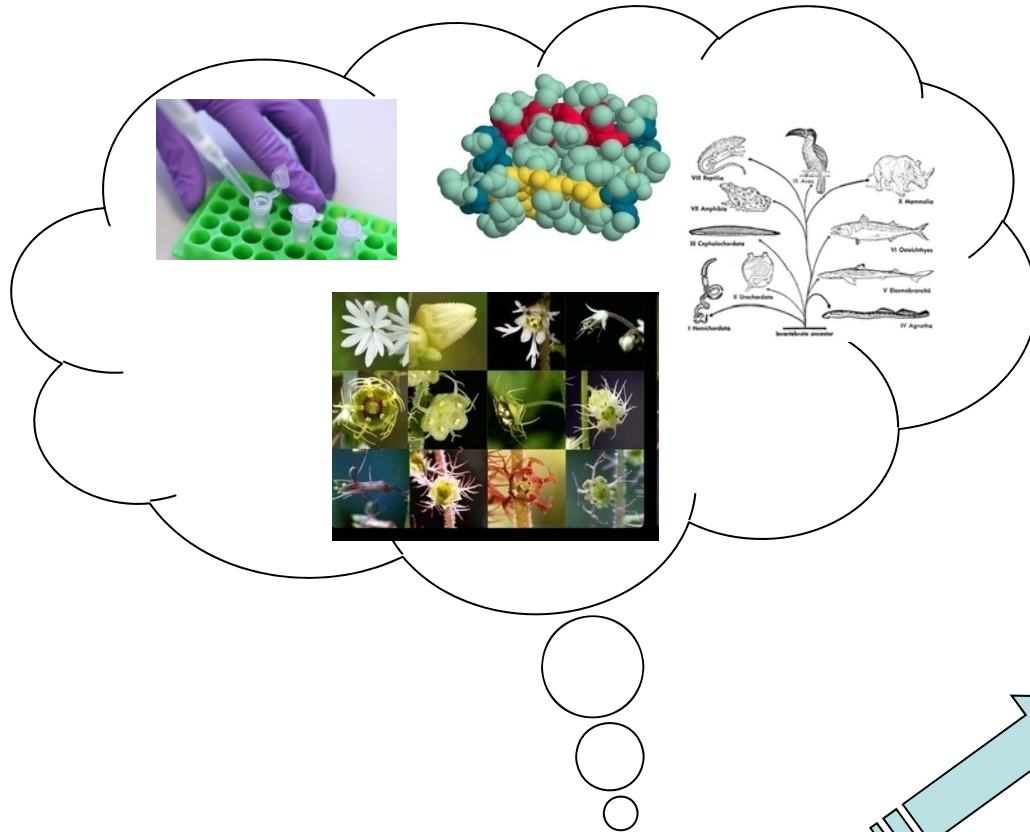
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- Motivation
- Project Goals
- Hardware Architecture (Tesla GPU)
- Software Architecture (Smith-Waterman)
- Parallelization Strategy
- Results



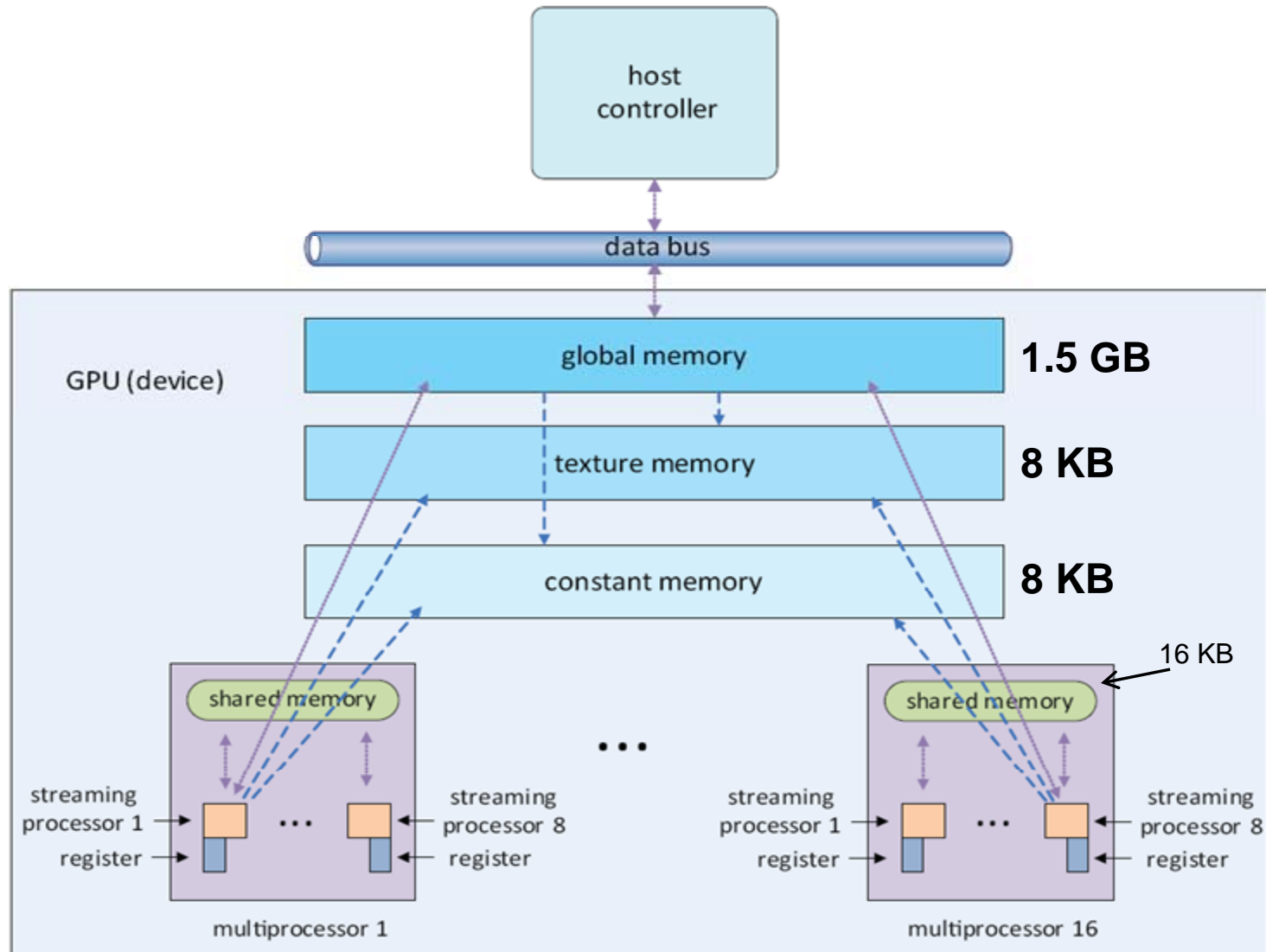
# Motivation



- Explore the GPU as a massively parallelized scientific computing device
  - Learn the GPU architecture and its intricacies
  - Study how programs must be parallelized to work with the GPU architecture
  - Find ways to exploit GPU memory hierarchy
- Mapping software architecture onto hardware architecture
  - Demonstrate the feasibility of mapping software architectures to the GPU and the drawbacks
  - Explore what makes software architectures suitable for the GPU
- Run software purely on the GPU
  - Design software mapping to be scalable



# Hardware Architecture



# Sequence Alignment

$$H_{ij} = \max \left\{ \begin{array}{l} H_{i-1,j-1} + S_{ij}, \\ H_{i-1,j} - G, \\ H_{i,j-1} - G, \\ 0 \end{array} \right\} \quad //G = 10$$

		Database Sequence			
		A	C	D	W
Query Sequence	A	0	0	0	0
	C	0	0	18	8
	F	0	0	8	13
	W	0	0	0	3
	0	0	0	0	0
	0	5	0	0	0

Arrows indicate alignment path from (A, W) to (C, D) to (F, C) to (A, A).

	A	B	C	D	F	W
A	5	-2	-1	-2	-3	-3
B	-2	5	-3	-3	-4	-5
C	-1	-3	13	-4	-2	-5
D	-2	-3	-4	8	-5	-5
F	-3	-4	-2	-5	8	4
W	-3	-5	-5	-5	4	15

Substitution Matrix



Manavski

- Poor memory utilization of GPU
  - Query Sequences are limited to 356 characters in length.
- Highly CPU Dependent
- Not scalable
- Requires large amounts of memory to store substitution table created from substitution matrix and query sequence

Farrar

- CPU must have SSE2 SIMD support.  
Not compatible with AMD
- Does not utilize larger register size supported by SSE3
- Requires large amounts of memory to store substitution table created from substitution matrix and query sequence



# Cost Function

## New Cost Function

$$S_{ij} = ( \text{ascii}(B) - 65, \text{ascii}(D) - 65 )$$

$$S_{ij} = ( 66 - 65, 68 - 65 )$$

$$S_{ij} = ( 1, 3 ) = -3$$

$$S_{ij} = -3$$

\*Does not use modulo

## Sorted Substitution Table

	A	B	C	D	...	Z
A	5	-2	-1	-2	...	-3
B	-2	5	-3	-3	...	-5
C	-1	-3	13	-4	...	-5
D	-2	-3	-4	8	...	-5
...	...	...	...	...	...	...
Z	-3	-5	-5	-5	...	15

Only need space for 26x26 matrix

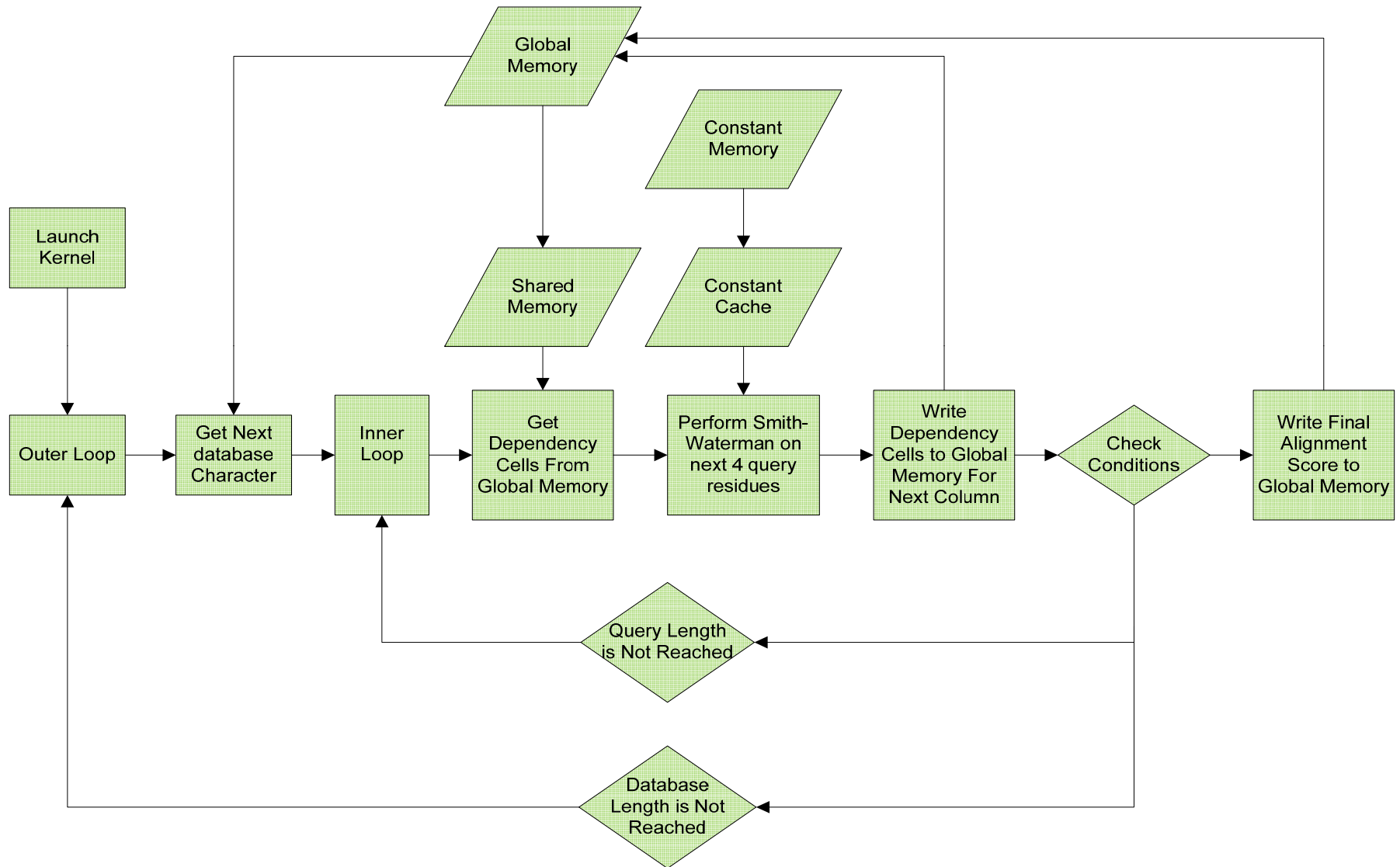
## Previous Methods

Computed new table from substitution matrix with substitution characters for top row and query sequence for column

	A	R	N	D	...	X
Q	-1	1	0	0	...	-1
U	-1	-1	-1	-1	...	-1
E	-1	0	0	2	...	-1
R	-1	5	0	-2	...	-1
Y	-2	-2	-2	-3	...	-1
...	...	...	...	...	...	...

Space needed is 23x(Query Length)





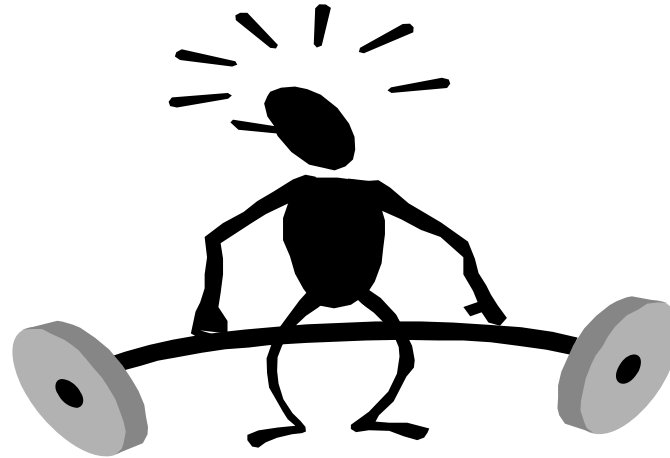
Alignment Database: Swissprot (Aug 2008), containing 392,768 sequences. GSW vs SSEARCH.

Protein Length	GPU (1.35GHz) Time (s)	SSEARCH (3.2GHz) Time(s)	Speedup	GPU Cycles (Billions)	SSEARCH Cycles (Billions)	Cycles Ratio
4	1.3	10	8	1.69	32.00	<b>18.96</b>
8	1.8	12	<b>6.8</b>	2.38	38.40	<b>16.11</b>
16	2.8	26	<b>9.2</b>	3.83	83.20	<b>21.71</b>
32	5.8	47	<b>8.1</b>	7.79	150.40	<b>19.30</b>
64	11.2	99	<b>8.8</b>	15.17	316.80	<b>20.89</b>
128	22.0	212	<b>9.7</b>	29.64	678.40	<b>22.88</b>
256	43.8	428	<b>9.8</b>	59.14	1369.60	<b>23.16</b>
512	92.4	886	<b>9.6</b>	124.78	2835.20	<b>22.72</b>
768	144.6	1292	<b>8.9</b>	195.15	4134.40	<b>21.19</b>
1024	279.7	1807	<b>6.5</b>	377.55	5782.40	<b>15.32</b>

Alignment Database: Swissprot (Aug 2008), containing 392,768 sequences. GSW vs Farrar.

Protein Length	GPU (1.35GHz) Time (s)	Farrar (2.4GHz) Time(s)	Speedup	GPU Cycles (Billions)	Farrar Cycles (Billions)	Cycles Ratio
4	1.3	2.78	<b>2.14</b>	1.69	6.67	<b>3.95</b>
8	1.8	2.81	<b>1.56</b>	2.38	6.74	<b>2.83</b>
16	2.8	2.96	<b>1.06</b>	3.83	7.10	<b>1.85</b>
32	5.8	3.35	<b>0.58</b>	7.79	8.04	<b>1.03</b>
64	11.2	4.46	<b>0.40</b>	15.17	10.70	<b>0.71</b>
128	22.0	6.50	<b>0.30</b>	29.64	15.60	<b>0.53</b>
256	43.8	12.77	<b>0.29</b>	59.14	30.65	<b>0.52</b>
512	92.4	23.37	<b>0.25</b>	124.78	56.09	<b>0.45</b>
768	144.6	26.61	<b>0.18</b>	195.15	63.86	<b>0.33</b>
1024	279.7	37.47	<b>0.13</b>	377.55	89.93	<b>0.24</b>

# Questions



## Farrar's SIMD Implementation

### Execution Time vs Sequence Length

