Beauty And The Beast

Exploiting GPUs In Haskell

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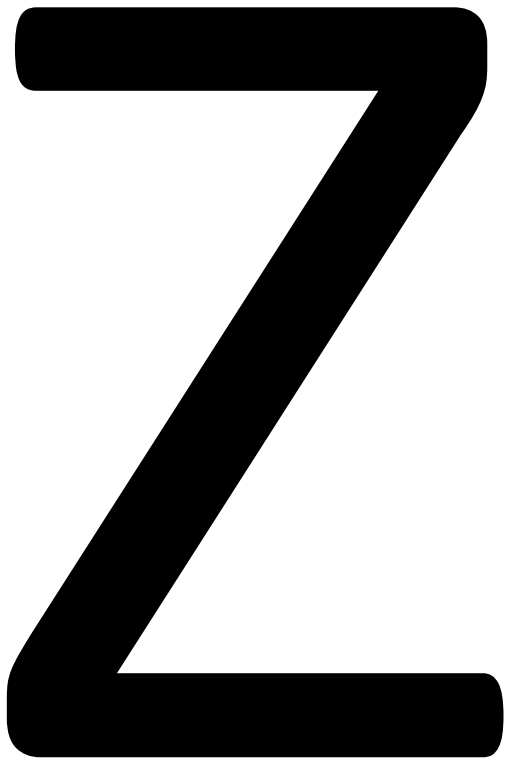

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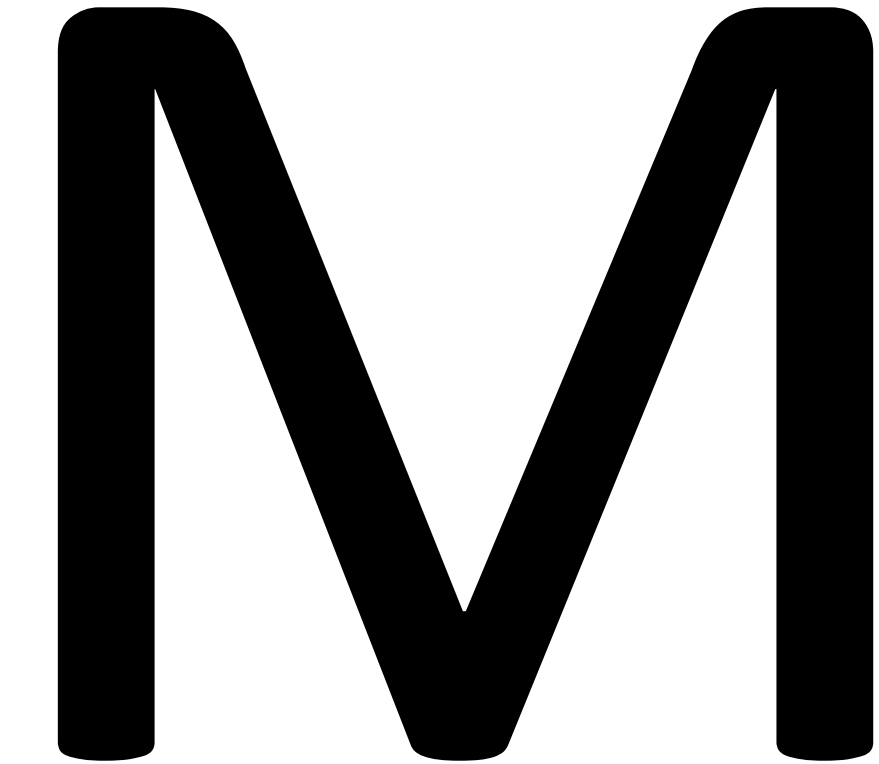
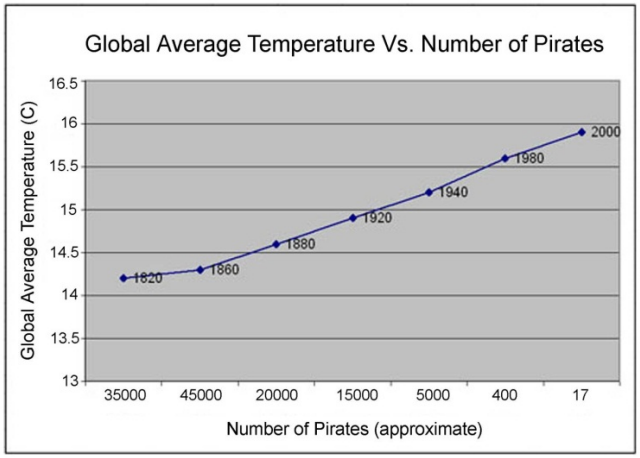
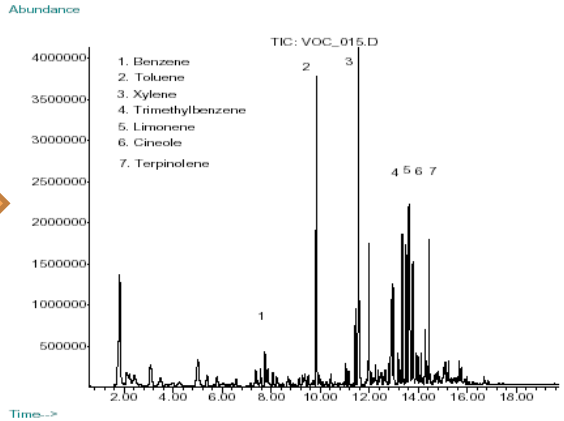



micrOTOF


Global Average Temperature Vs. Number of Pirates
Global Average Temperature (C)
16.5
16
15.5
15
14.5
14
13.5
13
1820
1860
1880
1920
1940
1980
2000
35000
45000
20000
15000
5000
400
17
Number of Pirates (approximate)


The Future
NEXT EXIT

1st Weight Reading	2nd Weight Reading	3rd Weight Reading	Average Weight	1st Weight Reading	2nd Weight Reading	3rd Weight Reading	Average Weight	Body Mass Index
1.600	1.620	1.610	1.610	69.90	68.00	66.00	67.967	17.753
1.650	1.660	1.670	1.660	50.40	50.30	50.30	50.333	18.266
1.690	1.650	1.650	1.653	62.00	61.50	61.50	61.667	22.585
1.700	1.710	1.720	1.710	78.00	78.00	78.10	78.033	26.698
1.620	1.610	1.610	1.613	56.80	57.00	57.00	56.933	21.674
1.680	1.670	1.670	1.673	58.00	57.80	57.90	57.900	20.678
1.690	1.695	1.694	1.693	66.60	66.50	66.50	66.533	23.307
1.564	1.565	1.565	1.565	45.40	45.50	45.40	45.433	18.556
1.654	1.655	1.656	1.655	61.60	61.50	61.50	61.533	15.894
1.691	1.692	1.692	1.892	56.10	56.00	56.00	56.033	19.580
1.673	1.674	1.676	1.674	50.00	50.10	50.00	50.033	17.847
1.650	1.652	1.651	1.651	65.00	65.20	65.00	65.067	23.871
1.700	1.720	1.725	1.703	60.90	61.20	61.00	61.033	20.314
1.750	1.750	1.755	1.752	57.80	57.90	57.50	57.667	18.729
1.800	1.805	1.820	1.808	71.80	71.70	72.00	71.833	21.987
1.780	1.783	1.782	1.783	75.00	75.00	74.80	74.933	24.145
1.850	1.852	1.852	1.851	76.00	76.00	76.00	76.000	23.780
1.790	1.791	1.792	1.791	69.00	69.10	69.00	69.033	21.521
1.771	1.773	1.773	1.772	67.10	67.00	67.00	67.033	21.340
1.810	1.811	1.812	1.811	72.00	72.00	72.20	72.067	21.973
1.770	1.771	1.770	1.770	70.00	69.90	70.00	69.967	22.324
1.700	1.701	1.702	1.701	66.80	67.00	67.00	66.933	22.133
1.821	1.822	1.822	1.822	67.00	66.90	67.00	66.967	20.180
1.675	1.674	1.675	1.674	58.00	58.10	58.00	58.033	20.709
1.670	1.673	1.670	1.672	70.10	70.20	70.30	70.200	25.121
1.765	1.765	1.768	1.763	66.80	66.70	67.00	66.833	21.494
1.720	1.700	1.720	1.710	64.90	64.80	65.00	64.900	22.195
1.590	1.600	1.610	1.600	48.80	49.00	48.80	48.867	19.089
1.680	1.690	1.690	1.693	50.40	50.40	50.50	50.433	18.450
1.570	1.575	1.580	1.575	44.80	45.00	45.10	44.967	18.127
1.790	1.780	1.735	1.795	69.80	70.00	70.00	69.933	22.232
1.890	1.870	1.880	1.880	79.80	80.00	79.90	79.900	22.686
1.780	1.730	1.735	1.755	90.10	90.00	90.00	90.033	19.940
1.780	1.750	1.760	1.763	55.00	54.80	55.00	54.933	18.075
1.690	1.691	1.692	1.891	58.00	58.00	58.00	58.000	20.283
1.700	1.733	1.732	1.732	83.00	83.10	83.00	83.033	27.690
1.550	1.551	1.550	1.550	68.00	68.10	68.00	68.033	19.984
1.640	1.642	1.641	1.841	55.00	55.00	54.90	54.967	20.412
1.651	1.650	1.650	1.850	58.90	59.00	59.10	59.000	21.693
1.840	1.841	1.842	1.841	71.00	71.00	71.30	71.067	20.968
1.750	1.750	1.751	1.750	79.00	79.00	78.90	78.967	25.775
1.720	1.720	1.720	1.720	86.00	84.00	84.10	84.033	28.405
1.540	1.540	1.540	1.540	45.20	45.50	45.40	45.367	19.129
1.531	1.532	1.533	1.532	48.00	48.00	48.10	48.033	19.412
1.790	1.790	1.792	1.791	84.00	84.00	83.80	83.933	26.170
1.670	1.671	1.671	1.671	56.00	56.00	56.00	56.000	20.064
1.520	1.523	1.520	1.521	36.00	36.20	36.00	36.067	15.590
1.690	1.690	1.681	1.680	55.00	55.10	55.00	55.033	19.491
1.701	1.702	1.730	1.701	50.00	50.10	50.00	50.033	16.898
1.780	1.781	1.782	1.781	88.10	88.50	88.20	88.133	28.484



1st Weight Reading	2nd Weight Reading	3rd Weight Reading	Average Weight	1st Weight Reading	2nd Weight Reading	3rd Weight Reading	Average Weight	Body Mass Index
1.680	1.620	1.610	1.637	45.90	66.00	66.00	45.967	17.753
1.650	1.660	1.670	1.660	50.40	50.30	59.30	53.333	18.266
1.680	1.650	1.650	1.653	42.00	61.50	61.50	61.667	22.590
1.700	1.710	1.720	1.710	78.00	78.00	78.10	78.033	26.688
1.620	1.610	1.610	1.613	56.80	57.00	57.00	56.933	21.874
1.680	1.670	1.670	1.673	58.00	57.90	57.90	57.900	20.678
1.690	1.695	1.694	1.693	66.60	66.50	66.50	66.533	23.317
1.564	1.545	1.565	1.565	45.40	45.30	45.40	45.433	18.556
1.654	1.655	1.656	1.655	61.80	61.50	61.50	61.533	15.494
1.691	1.692	1.892	1.892	56.10	56.00	56.00	56.033	19.780
1.673	1.674	1.678	1.674	50.00	50.10	50.00	50.033	17.847
1.650	1.652	1.651	1.651	45.00	45.20	45.00	45.067	21.871
1.730	1.735	1.735	1.733	60.90	61.20	61.00	61.033	20.314
1.750	1.750	1.755	1.752	57.40	57.50	57.50	57.467	18.729
1.800	1.805	1.820	1.808	71.80	71.70	72.00	71.833	21.967
1.760	1.763	1.762	1.762	75.00	75.00	74.80	74.933	24.165
1.850	1.852	1.852	1.851	76.00	76.00	76.00	76.000	23.390
1.790	1.791	1.792	1.791	69.00	69.10	69.00	69.033	21.521
1.771	1.773	1.771	1.772	67.10	67.00	67.00	67.033	23.340
1.810	1.811	1.812	1.811	72.00	72.00	72.20	72.067	21.973
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1.675	1.674	1.673	1.674	58.00	58.10	58.00	58.033	20.709
1.670	1.675	1.670	1.672	70.10	70.20	70.20	70.167	25.131
1.785	1.785	1.780	1.783	66.80	66.70	67.00	66.833	21.494
1.710	1.700	1.720	1.710	66.90	64.90	65.00	64.900	22.199
1.790	1.690	1.810	1.805	48.80	49.00	48.80	48.867	19.099
1.690	1.690	1.650	1.653	50.40	50.40	50.50	50.433	18.450
1.570	1.575	1.580	1.575	44.80	45.00	45.10	44.967	18.127
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1.890	1.870	1.880	1.880	79.80	80.00	79.90	79.900	22.906
1.780	1.790	1.785	1.785	80.10	80.00	80.00	80.033	19.943
1.760	1.750	1.760	1.763	55.00	54.80	55.00	54.933	18.075
1.890	1.890	1.892	1.891	56.00	56.00	56.00	56.000	20.283
1.750	1.733	1.732	1.732	83.00	83.10	83.00	83.033	27.690
1.700	1.701	1.705	1.702	48.00	48.10	48.00	48.033	19.994
1.640	1.642	1.641	1.641	55.00	55.00	54.90	54.967	20.412
1.651	1.650	1.650	1.650	59.90	59.90	59.10	59.000	21.693
1.840	1.841	1.842	1.841	71.00	71.00	71.20	71.067	20.968
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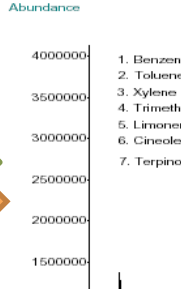
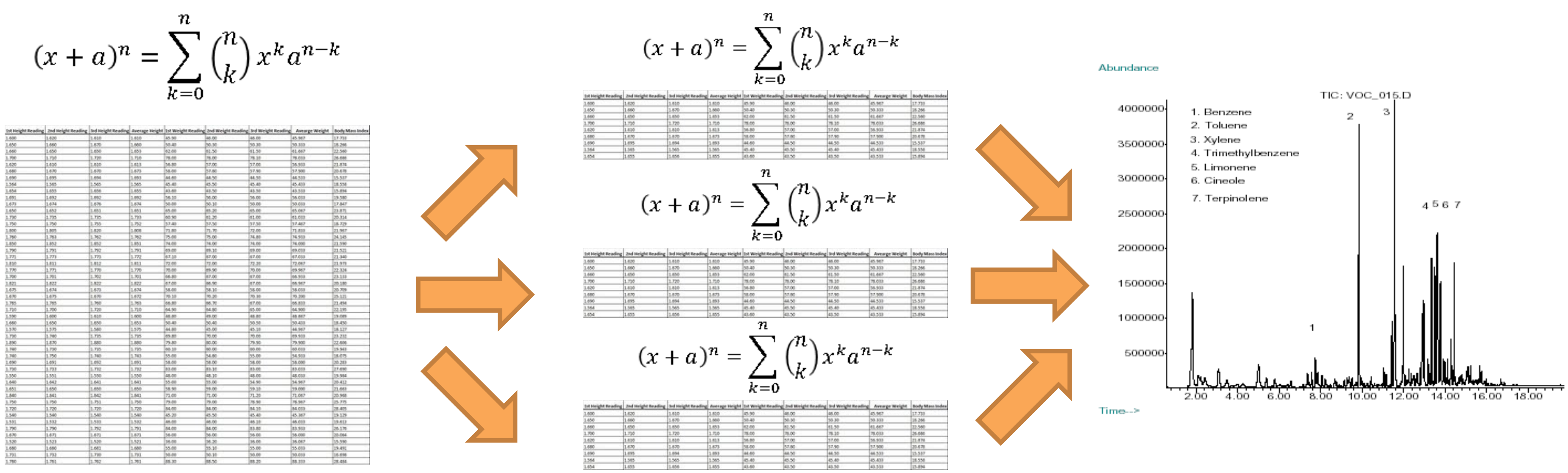
1.720	1.720	1.720	1.720	86.00	84.00	86.10	86.033	28.405
1.540	1.540	1.540	1.540	45.20	45.50	45.40	45.367	19.129
1.533	1.532	1.533	1.532	49.00	48.00	48.10	48.033	19.813
1.790	1.790	1.792	1.791	84.00	84.00	83.80	83.933	26.176
1.670	1.671	1.671	1.671	56.00	56.00	56.00	56.000	20.064
1.520	1.523	1.520	1.521	36.00	36.20	36.00	36.067	15.590
1.680	1.680	1.681	1.680	55.00	55.10	55.00	55.033	19.491
1.701	1.702	1.700	1.701	50.00	50.10	50.00	50.033	16.698
1.780	1.781	1.782	1.781	88.30	88.50	88.20	88.333	28.484




$(x+a)^n = \sum_{k=0}^{n} \binom{n}{k} x^k a^{n-k}$
$(x+a)^n = \sum_{k=0}^{n} \binom{n}{k} x^k a^{n-k}$
$(x+a)^n = \sum_{k=0}^{n} \binom{n}{k} x^k a^{n-k}$
$(x+a)^n = \sum_{k=0}^{n} \binom{n}{k} x^k a^{n-k}$
Abundance
TIC: VOC_015.D
1. Benzene
2. Toluene
3. Xylene
4. Trimethylbenzene
5. Limonene
6. Cineole
7. Terpinolene
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
Time-->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ATI
RADEON

[Only] a few of the proposed approaches […] are currently used in practice due to the unavailability of the software or due to difficulties with incorporating the new tools in the existing data analysis pipelines.

- Nesvizhskii10

Hypotheses

- Haskell is easy
- But performance (lists) stinks
- Using a DSL we can recover some “C” performance
- We think the trade-off is acceptable
- Based on this, we can address the richer MS computation domain with ease and performance.

Whole Array / Index .

- Shift .<<<
- Add .+
- Multiply .*

Per-Element ^

- Shift ^<<<
- Add ^+
- Multiply ^*

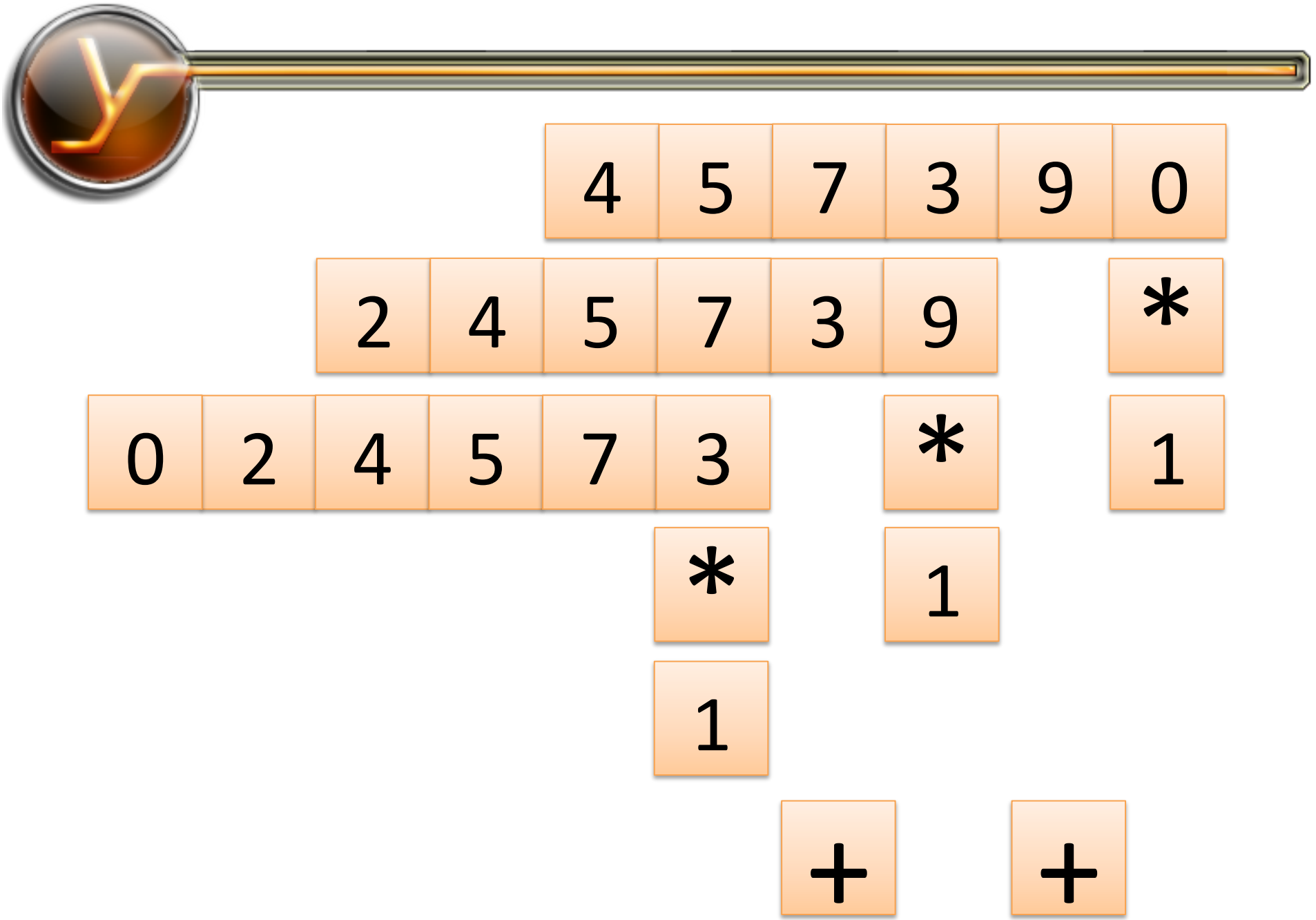
2	4	5	7	3	9

*

1	3	1

=

10	19	18	29	25	30


4 5 7 3 9 0
2 4 5 7 3 9 *
0 2 4 5 7 3 * 1
* 1
1
+ +

```
-- Sum up all the parts for the final answer.
convolve filter input = sum convolvedParts
    where
        -- Convolve the whole array with o      t an      ly.
        oneFilterElement shift mul = (inp .<<< hif      1
        -- Get the filter radius.
        r = length filter `div` 2
        -- Do all the shifts and multiplies separately.
        convolvedParts = zipWith oneFilterElement [-r..r] filter
```

.<<<

^*

- Using Lists:

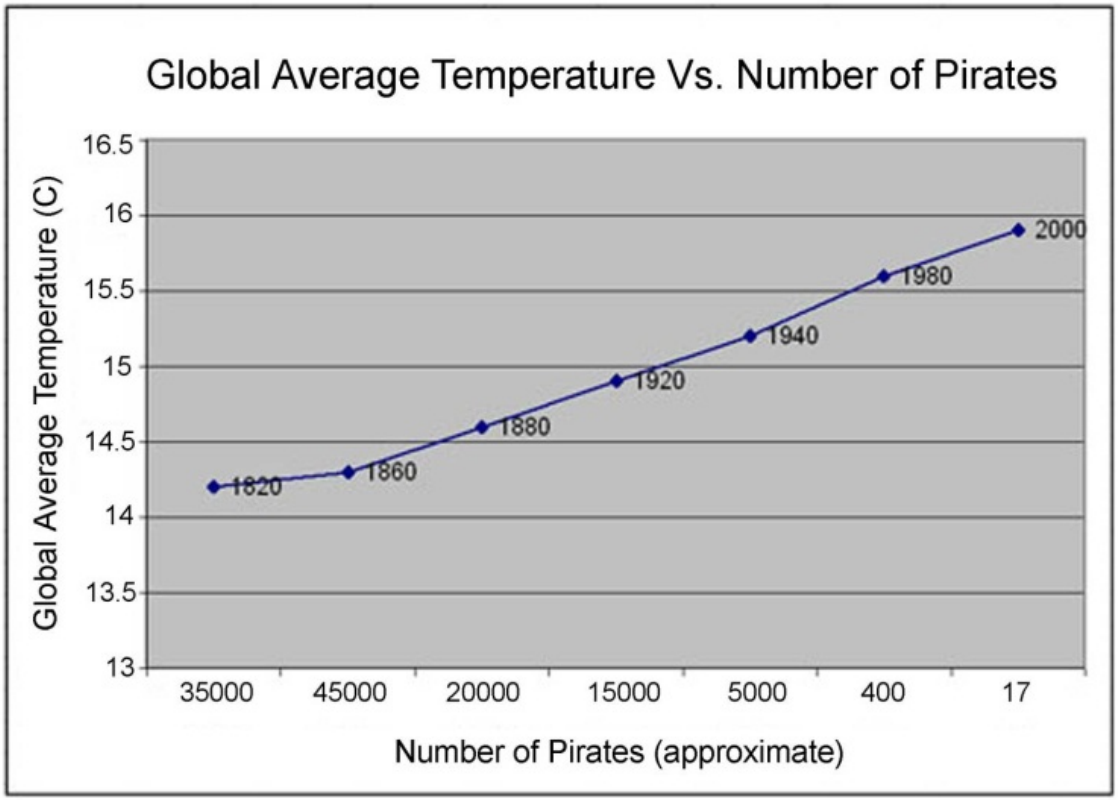
```
convolve :: [Float] -> [Float] -> [Float]
```

- Using PEGGY:

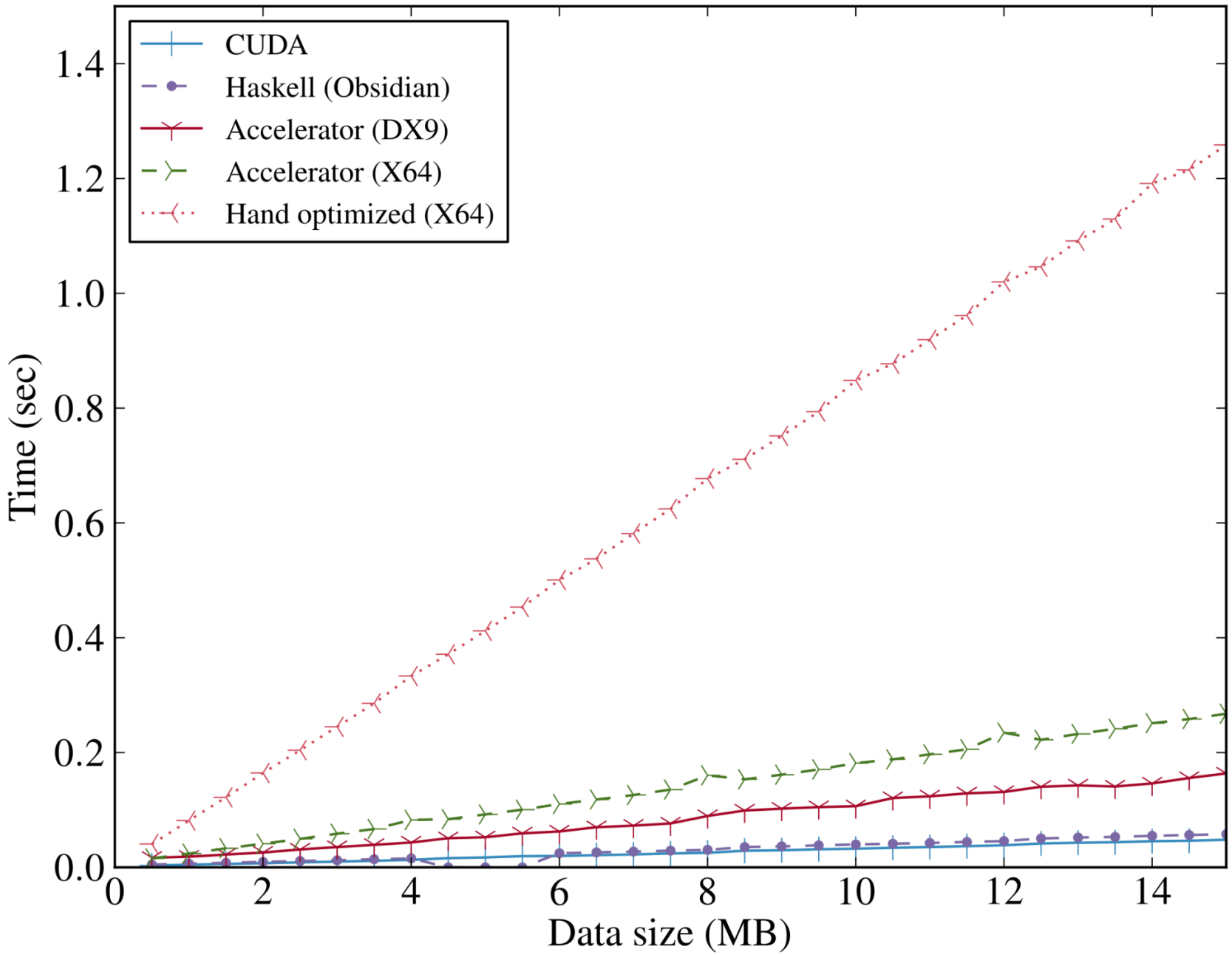
```
convolve :: [Float] -> PYExpr Float target -> PYExpr Float target

-- Convert the old input to PEGGY GPU data.
peggyInput = toArray listInput
```

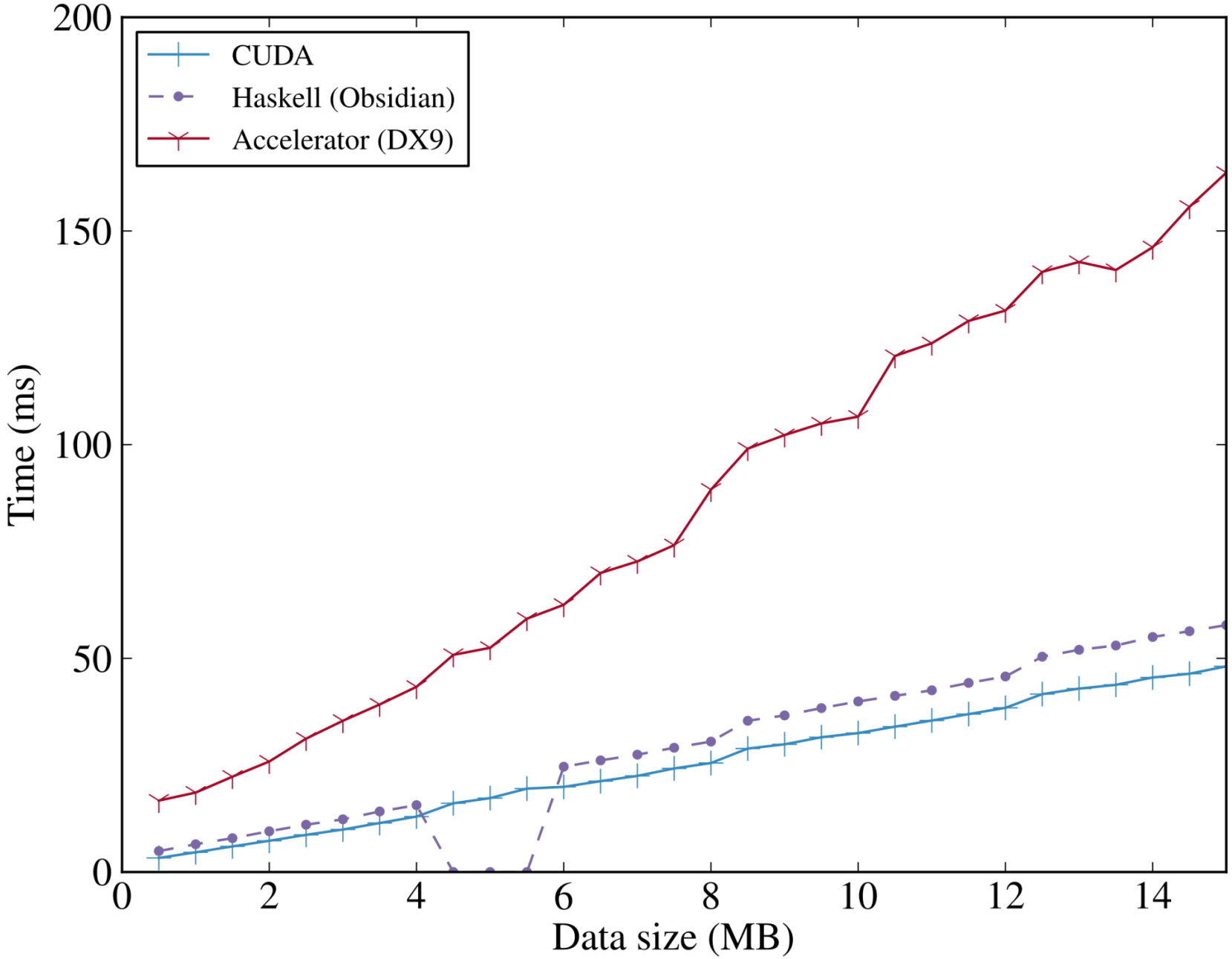
```
data PYExpr a b = (PYCode a b) (PYMem a b)

data instance PYMem a TargetHaskell = [a]

instance PYCode a TargetHaskell where
        (^+) x y = zipWith (+) x y
```

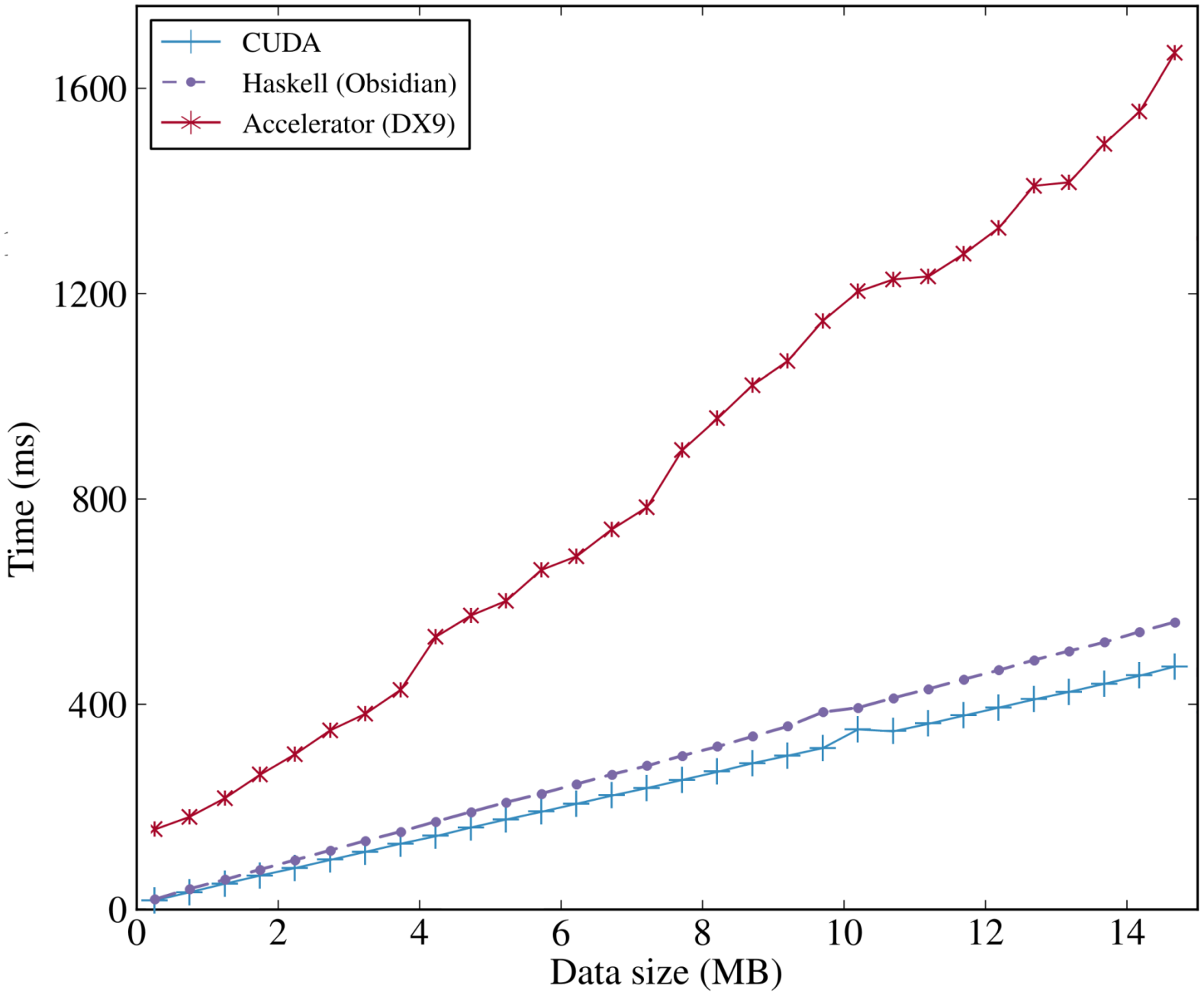
STOP GLOBAL WARMING: BECOME A PIRATE

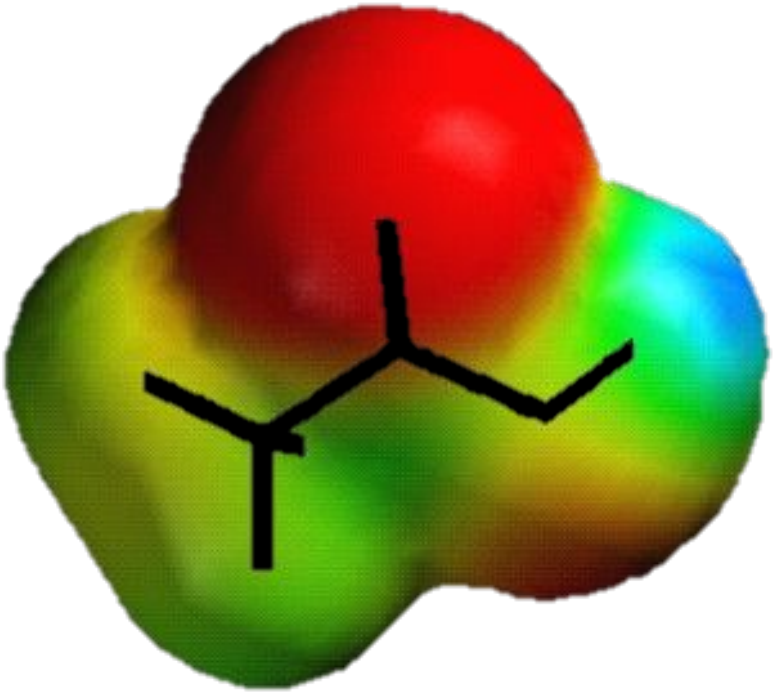


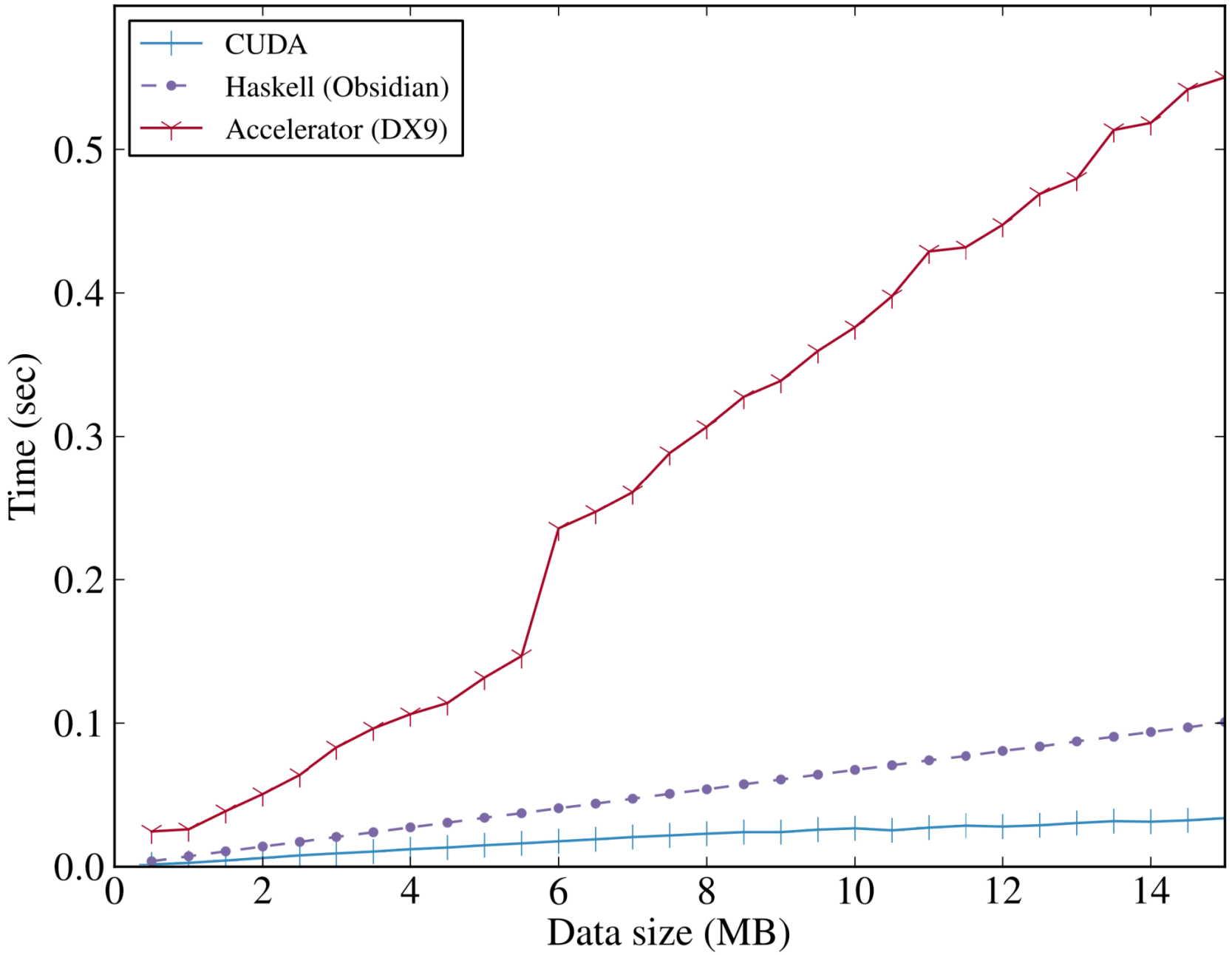
WWW.VENGANZA.ORG


CUDA
Haskell (Obsidian)
Accelerator (DX9)
Accelerator (X64)
Hand optimized (X64)
Time (sec)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
2
4
6
8
10
12
14
Data size (MB)


CUDA
Haskell (Obsidian)
Accelerator (DX9)
Time (ms)
Data size (MB)
0
50
100
150
200
0
2
4
6
8
10
12
14


CUDA
Haskell (Obsidian)
Accelerator (DX9)
Time (ms)
0
400
800
1200
1600
0
2
4
6
8
10
12
14
Data size (MB)




CUDA
Haskell (Obsidian)
Accelerator (DX9)
Time (sec)
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
10
12
14
Data size (MB)

DATA

* f1 =

* f2 =

LOW FREQUENCY

HIGH FREQUENCY

* f1 =

* f2 =

LOW FREQUENCY

HIGH FREQUENCY

* f1 =

* f2 =

LOW FREQUENCY

HIGH FREQUENCY

f1

f2

LOW FREQUENCY

HIGH FREQUENCY

LOW FREQUENCY

HIGH FREQUENCY

HIGH FREQUENCY

HIGH FREQUENCY

HIGH FREQUENCY

CUT OFF FILTER

DATA

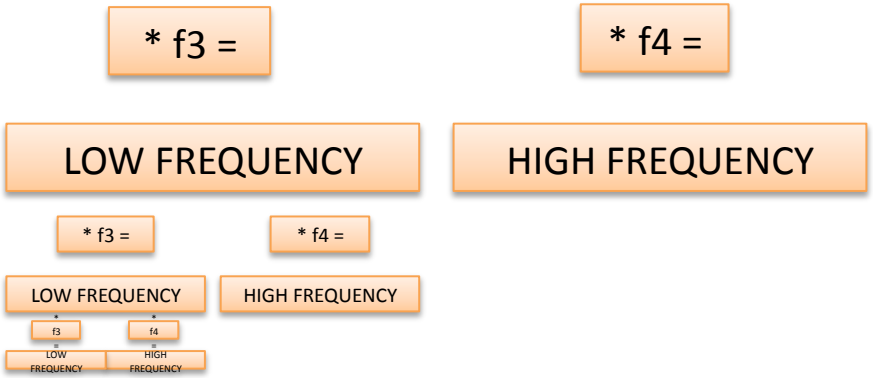
DATA

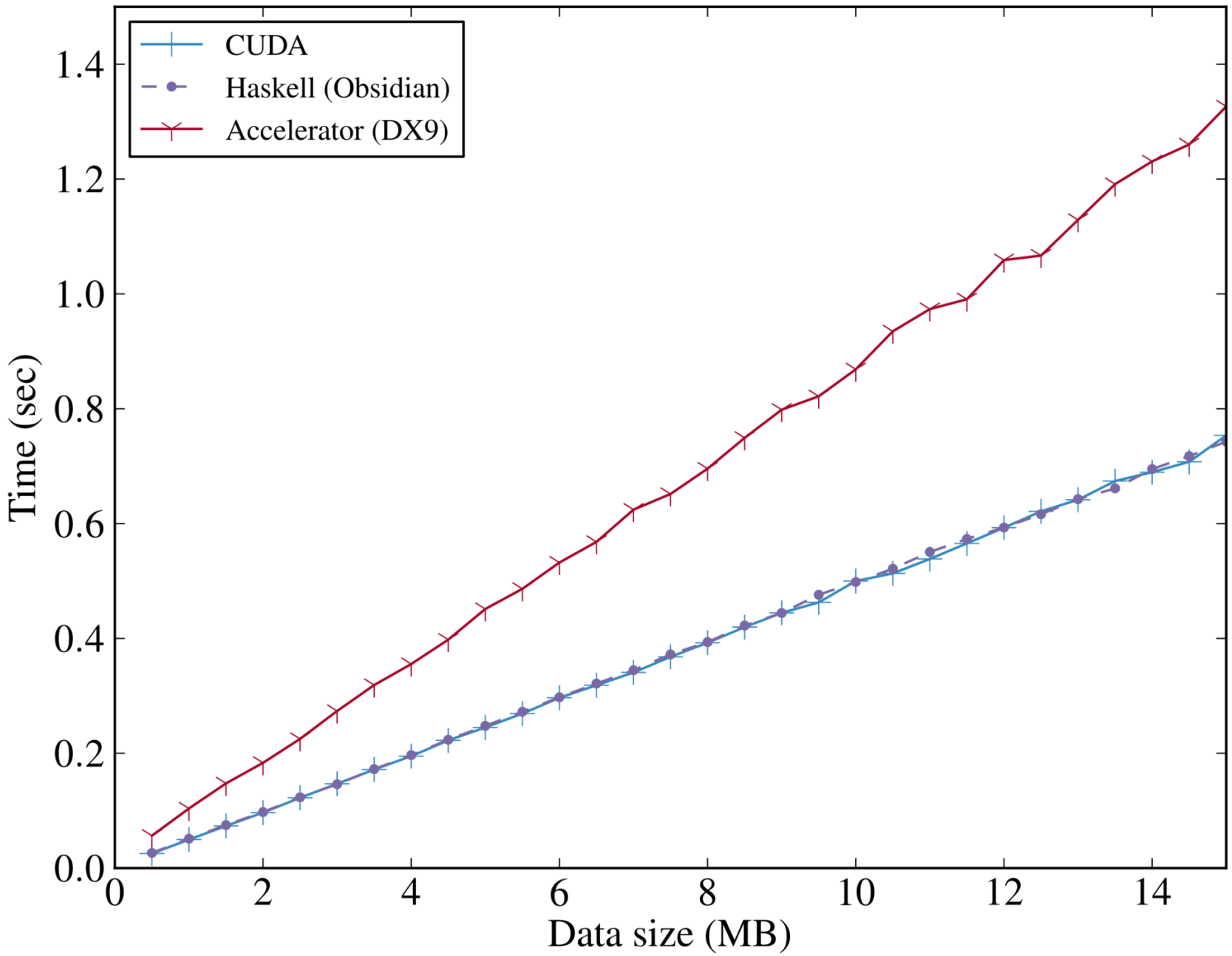
* f3 =

* f4 =

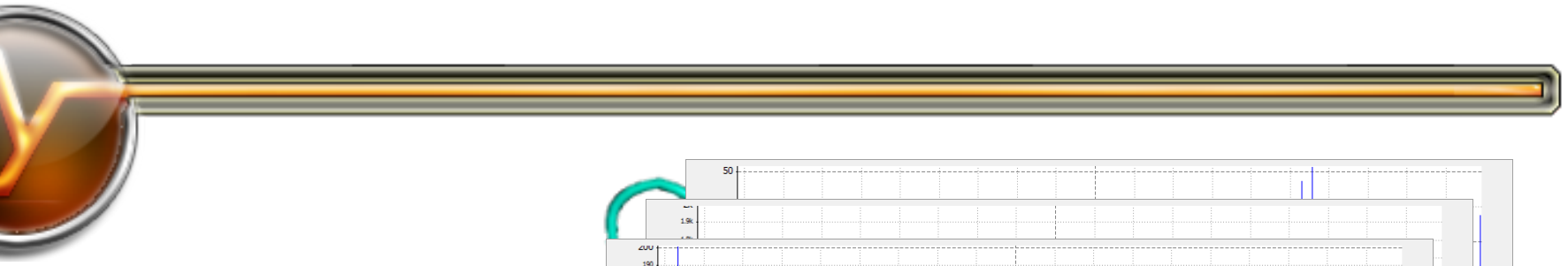
LOW FREQUENCY

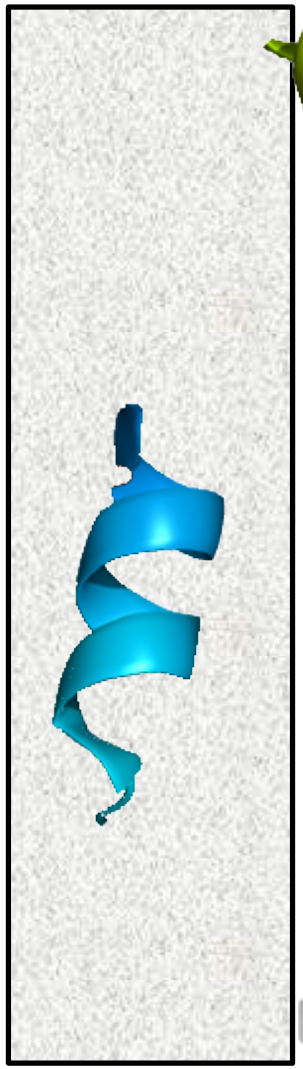
HIGH FREQUENCY

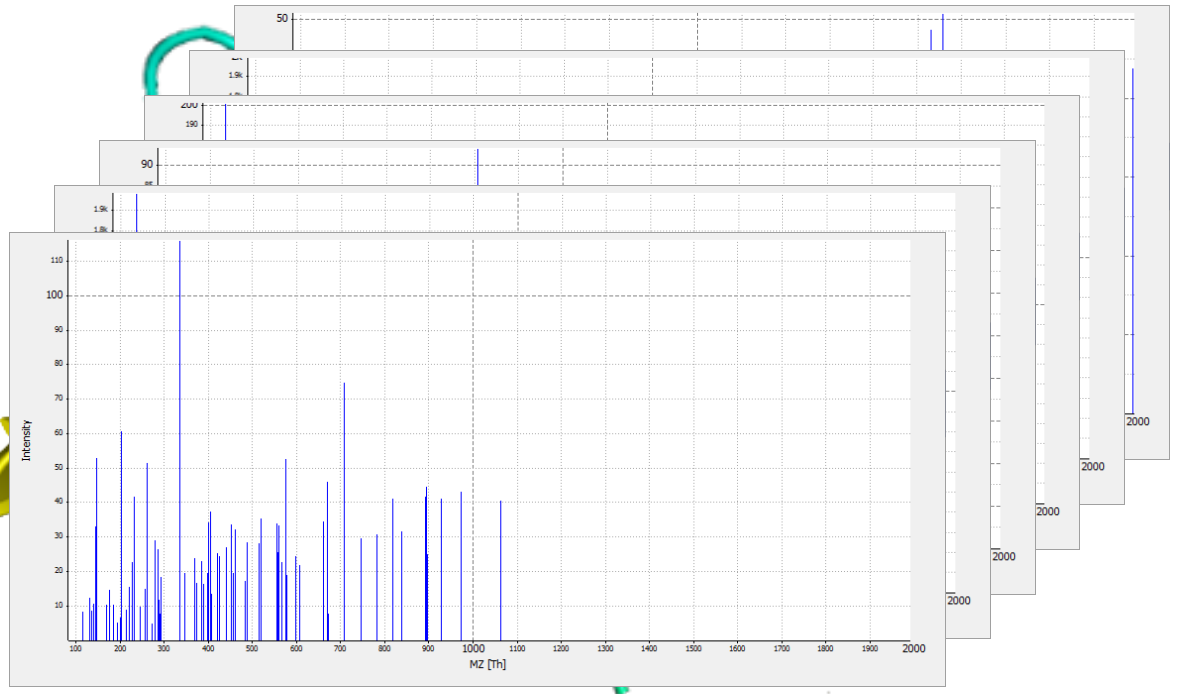



CUDA
Haskell (Obsidian)
Accelerator (DX9)
Time (sec)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
2
4
6
8
10
12
14
Data size (MB)


The Future
NEXT EXIT






Intensity
MZ [Th]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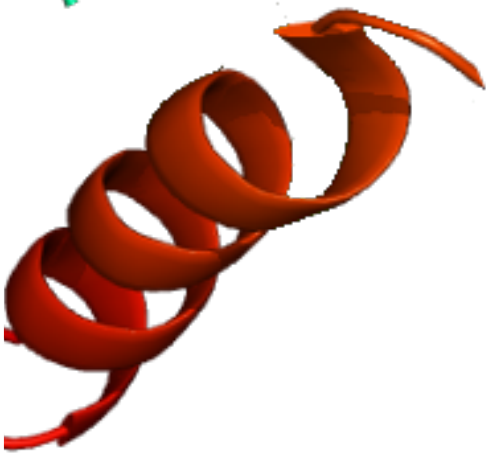
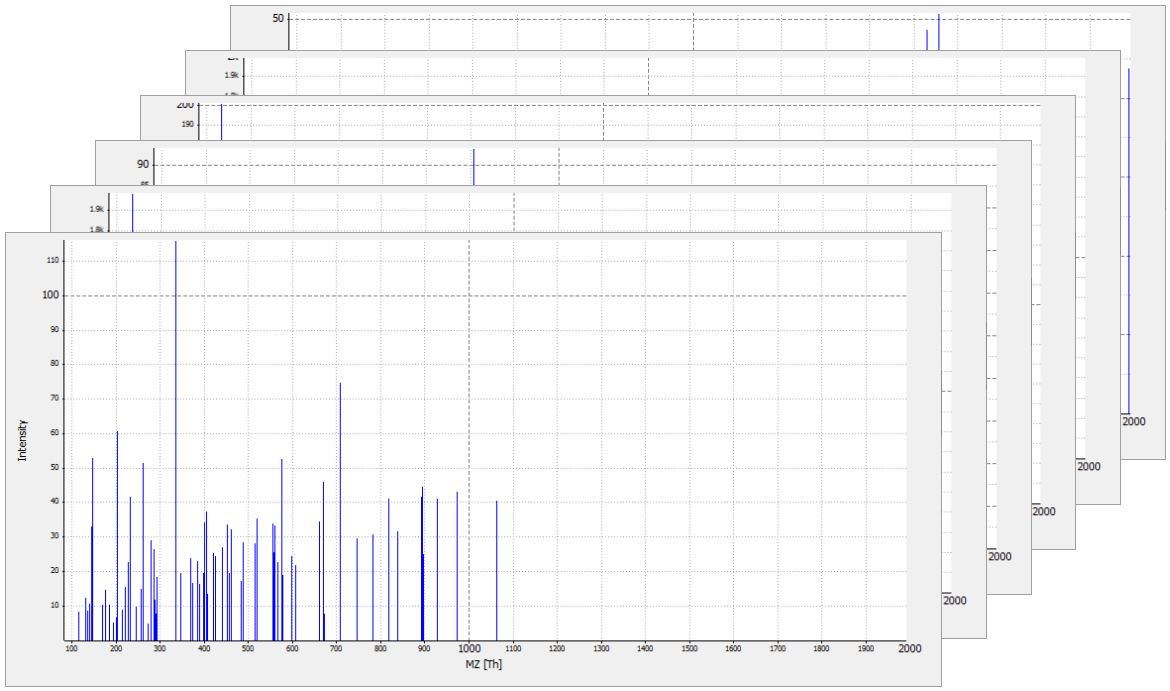
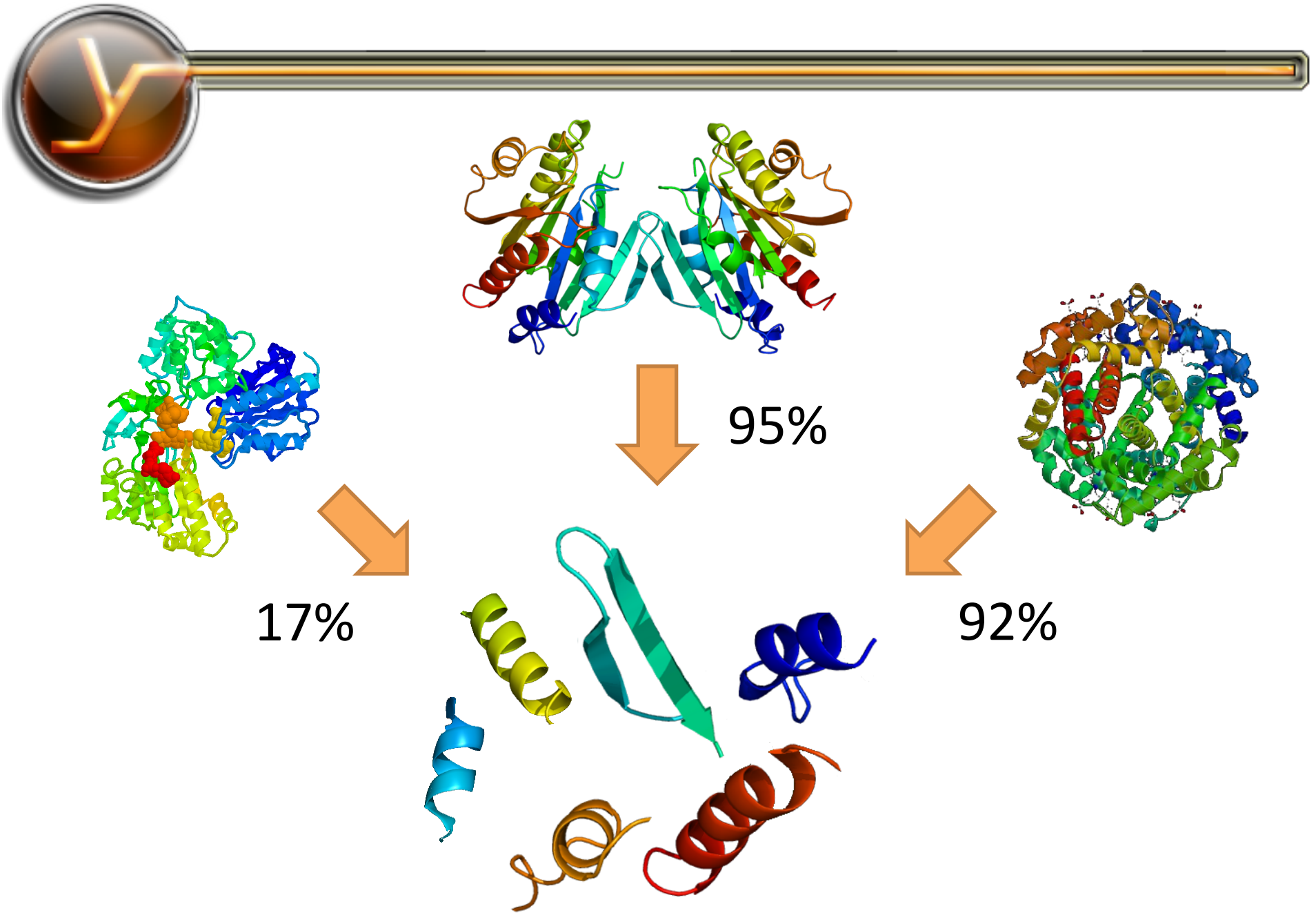


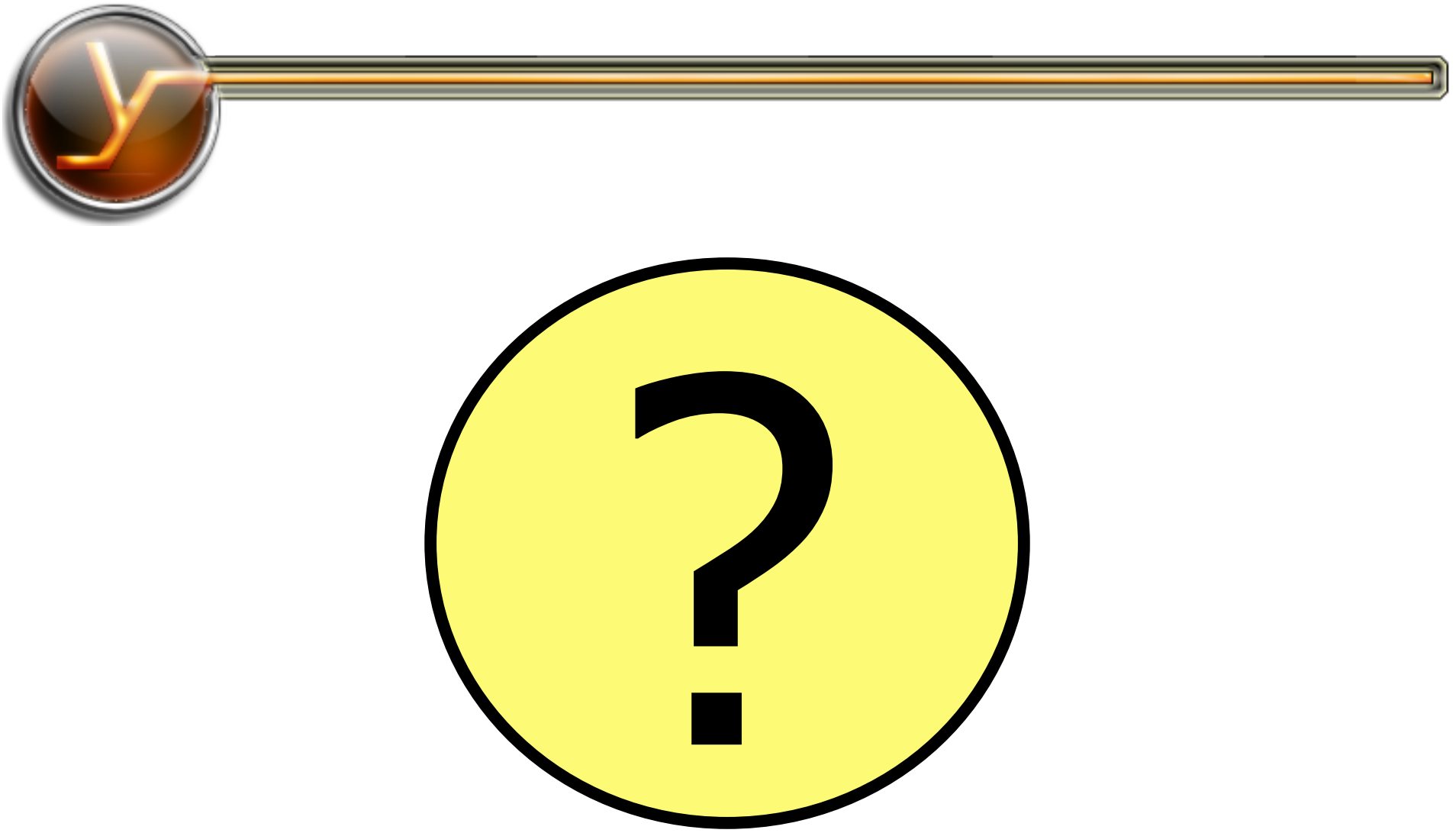

Intensity
MZ [Th]


micrOTOF


95%
17%
92%

Overview

- Backend with proven potential
- Complete MS analysis implementation
- Abstract to a DSL
- Improved performance



Nesvizhskii10:

"A survey of computational methods and error rate estimation procedures for peptide and protein identification in shotgun proteomics." Alexey Nesvizhskii, *Journal Of Proteomics*, 2010