Numerical Accuracy and Reliability Issues in HPC

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Towards a Reliable Performance Evaluation of Accurate Summation Algorithms

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How to manage accuracy and speed?

A new "better" algorithm every year since 1999

1965 Møller, Ross
1969 Babuska, Knuth
1970 Nickel
1971 Dekker, Malcolm
1972 Kahan, Pichat
1974 Neumaier
1975 Kulisch/Bohlender
1977 Bohlender, Mosteller/Tukey
1981 Linnaimaa
1982 Leuprecht/Oberaigner
1983 Jankowski/Semoktunowicz/-Wozniakowski
1985 Jankowski/Wozniakowski
1987 Kahan
1991 Priest
1992 Clarkson, Priest
1993 Higham
1997 Shewchuk
1999 Anderson
2001 Hlavacs/Uberhuber
2002 Li et al. (XBLAS)
2003 Demmel/Hida, Nievergelt, Zielke/Drygalla
2005 Ogita/Rump/Oishi, Zhu/Yong/Zeng
2006 Zhu/Hayes
2008 Rump/Ogita/Oishi
2009 Rump, Zhu/Hayes
2010 Zhu/Hayes

Accurate or faithful floating point summation

Limited accuracy for backward stable sums

- Accuracy of the computed sum $\leq (n-1) \times \mathit{cond} \times \mathbf{u}$
- No more significant digit in IEEE-b64 for large cond, *i.e.* $> 10^{16}$

Accurate but still conditioning dependent

- Accuracy of the computed sum $\lesssim \mathbf{u} + \mathit{cond} \times \mathbf{u}^K$
- double-double, compensated sums: Kahan(72), Sum2(05), SumK(05)

Faithfully or correctly rounded sums

- Accuracy of the computed sum $\leq \mathbf{u}$
- Kahan (87), . . . , Rump *et al.*: AccSum (SISC-08), FastAccSum (SISC-09)
  Zhu-Hayes: iFastSum, HybridSum (SISC-09), OnLineExact (TOMS-10)

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  Zhu-Hayes: iFastSum, HybridSum (SISC-09), OnLineExact (TOMS-10)
- Run-time and memory efficiencies are now the choice factors

Reliable and significant measure of the time complexity?

Flop count vs. run-time measures: which one trust?

Metric	Sum	DDSum	Sum2
Flop count	$n-1$	$10n$	$7n$
Flop count ratio vs. Sum (approx.)	1	10	7
Measured #cycles ratio (approx.)	1	7.5	2.5

- Flop counts and measured run-times are not proportional
- Run-time measure is a very difficult experimental process

How to trust non-reproducible experiment results?

Measures are mostly non-reproducible

- The execution time of a binary program varies, even using the same data input and the same execution environment.

Why? Experimental uncertainty (even) of the hardware performance counters

- Spoiling events: background tasks, concurrent jobs, OS interrupts
- Non predictable issues: instruction schedul., branch pred., cache mng.
- Timing in seconds depends on external conditions: temperature of the room
- Timing in cycles difficult: 1 core cycle $\neq$ 1 bus cycle on modern processors

Uncertainty increases as computer system complexity does

- Architecture and micro-architecture issues: multicore, hybrid, speculation
- Compiler options and its effects

Software and system performance experts' point of view

The limited *Accuracy of Performance Counter Measurements*

> *We caution performance analysts to be suspicious of cycle counts . . . gathered with performance counters.*
>
> *D. Zaparanuks, M. Jovic, M. Hauswirth (2009)*

Can Hardware Performance Counters Produces Expected, Deterministic Results?

> *In practice counters that should be deterministic show variation from run to run on the x86_64 architecture. . . . it is difficult to determine known "good" reference counts for comparison.*
>
> *V.M. Weaver, J. Dongarra (2010)*

How to trust the current literature?

Numerical results in S.M. Rump et al. contributions (for summation)

- 26% for Sum2-SumK (SISC-05) : 9 pages over 34
- 20% for AccSum (SISC-08) : 7 pages over 35
- 20% for AccSumK-NearSum (SISC-08b) : 6 pages over 30
- **less that 3%** for FastAccSum (SISC-09) : 1 page over 37

Lack of proof, or at least of reproducibility

> *Measuring the computing time of summation algorithms in a high-level language on today's architectures is more of a hazard than scientific research.* *S.M. Rump (SISC, 2009)*

. . . in the paper entitled *Ultimately Fast Accurate Summation*

Outline

ILP and the performance potential of the algorithm

Instruction Level Parallelism (ILP) describes the potential of the instructions of a program that can be executed simultaneously

Hennessy-Patterson's ideal machine (H-P IM)

- every instruction is executed one cycle after the execution one of the producers it depends
- no other constraint than the true instruction dependency (RAW)

Our ideal run measures : C=#cycles, I=# instruc. and I/C

- ideal run = maximal exploitation of the program ILP
- ILP measures the potential of the algorithm performance
- processor and ILP in practice: superscalar out-of-order executions

The ideal execution of Sum: hand-made analysis

The ideal execution of Sum takes n cycles

Sum		iter.	1	2	3	...	$n-1$
	`s = x[0];`		0				
	`for(i=1; i<n; i++)`						
a	`  s = s + x[i];`		1	2	3	$\cdots$	n-1
	`return(s);`						n

No ILP in Sum

- $C_{\text{Sum}} = n$
- $I = n$
- ILP=1

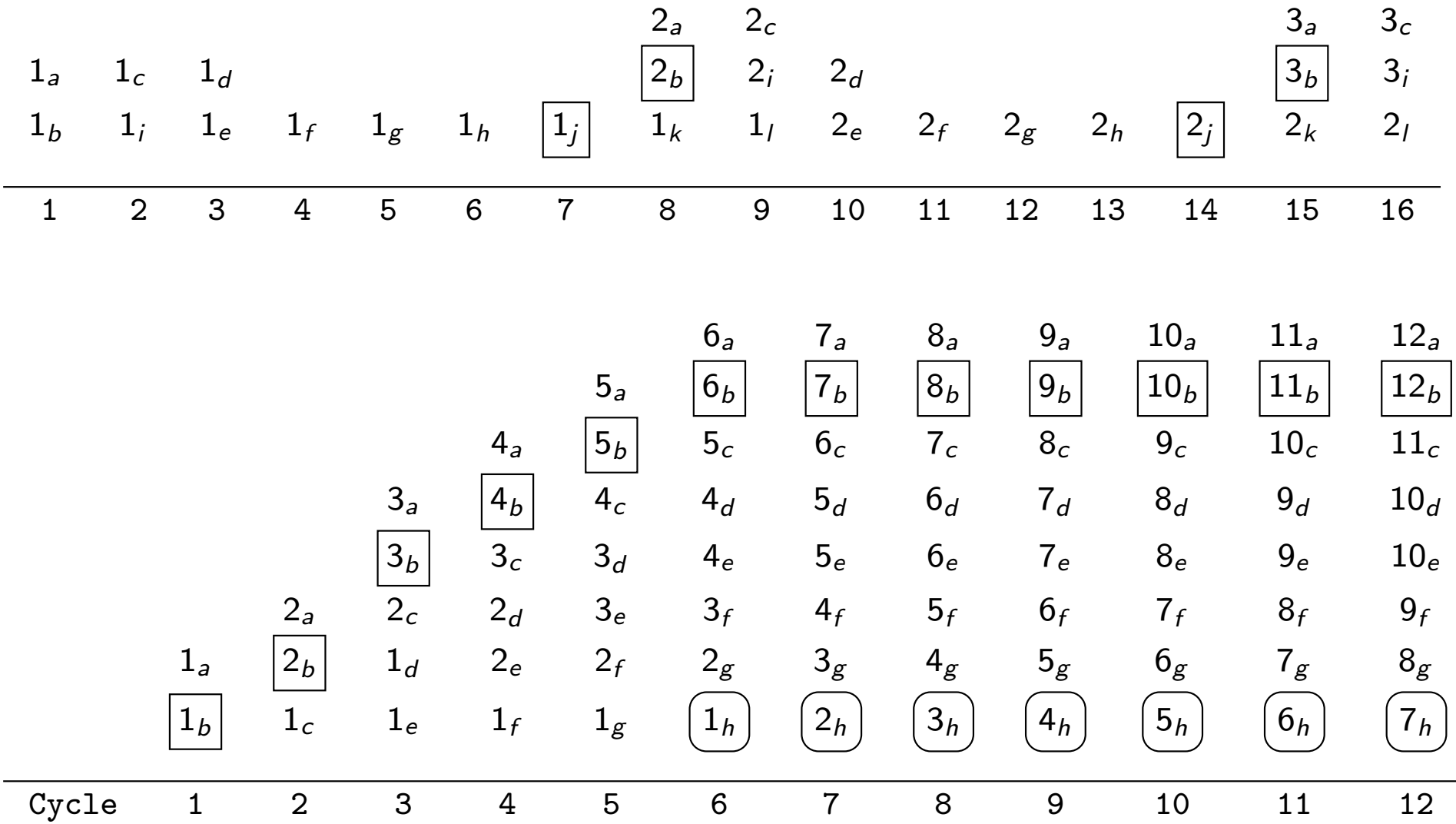
DDSum ideally runs in $7n - 5$ cycles

DDSum		iter.	1	2	3	...	$n-1$
	`s = x[0];`		0				
	`for(i=1; i<n; i++){`						
a	`  s_ = s;`		1	8	15	···	7n-13
b	`  s = s + x[i];`		1	8	15	···	7n-13
c	`  t = s - s_;`		2	9	16	···	7n-12
d	`  t2 = s - t ;`		3	10	17	···	7n-11
e	`  t3 = x[i] - t;`		3	10	17	···	7n-11
f	`  t4 = s_ - t2;`		4	11	18	···	7n-10
g	`  t5 = t4 + t3;`		5	12	19	···	7n-9
h	`  s_l = s_l + t5;`		6	13	20	···	7n-8
i	`  s_ = s;`		2	9	16	···	7n-12
j	`  s = s + s_l;`		7	14	21	···	7n-7
k	`  e = s_ - s;`		8	15	22	···	7n-6
l	`  s_l = s_l + e;`		9	16	23	···	7n-5
	`}`						
	`return(s);`						7n-4

Sum2 ideally runs in $n + 7$ cycles

Sum2		iter.	1	2	3	...	$n-1$
	`s = x[0];`		0				
	`for(i=1; i<n; i++){`						
a	`  s_ = s;`		1	2	3	···	n-1
b	`  s = s + x[i];`		1	2	3	···	n-1
c	`  t = s - s_;`		2	3	4	···	n
d	`  t2 = s - t ;`		3	4	5	···	n+1
e	`  t3 = x[i] - t;`		3	4	5	···	n+1
f	`  t4 = s_ - t2;`		4	5	6	···	n+2
g	`  t5 = t4 + t3;`		5	6	7	···	n+3
h	`  c = c + t5;`		6	7	8	···	n+4
	`}`						
	`return(s+c);`						n+6

Less ILP in DDSum(top) than in Sum2 (bottom)



ILP hand-made analysis: conclusion

Metric	Sum	DDSum	Sum2
Flop count (approx. ratio)	1	10	7
Measured #cycles (approx. ratio)	1	7.5	2.5
Flop count / measured #cycles (approx.)	1	1.4	2.8
Ideal C (approx. ratio)	1	7	1
Ideal flop count / C (approx.)	1	1.7	8

- DDSum actually run as fast as it can
- Current architectures exploit only 30% of Sum2's ILP
- Huge potential in Sum2 which can run as fast as Sum

The PerPI Tool automatizes this ILP analysis

PerPI: a pintool to analyse and visualise the ILP of x86-coded algorithms

- Pin (Intel) tool (http://www.pintool.org)
- Outputs: ILP measure (#C, #I), IPC histogram, data-dependency graph
- Input: x86_64 binary file
- Developed and maintained by B. Goossens and D. Parello (DALI)
- In progress: `http://perso.univ-perp.fr/david.parello/perpi/`

Seven recent accurate and fast summation algorithms

Recursive summation (not accurate)

- Sum

Accurate sums: twice more precision

- Sum2
- DDSum

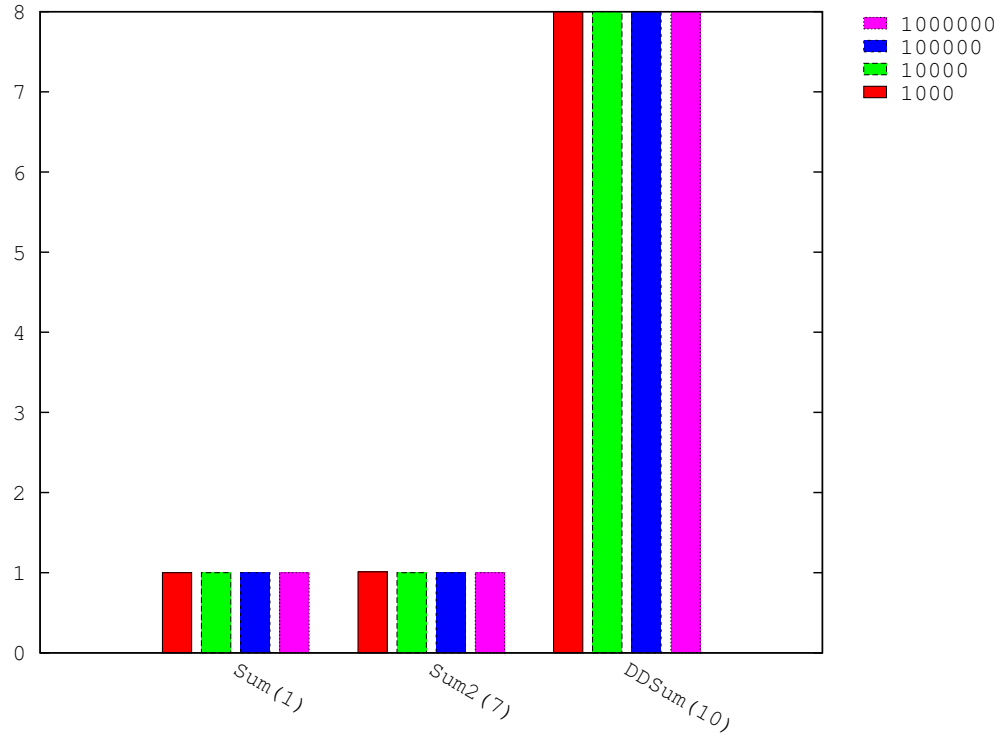
Faithfully or exactly rounded sums

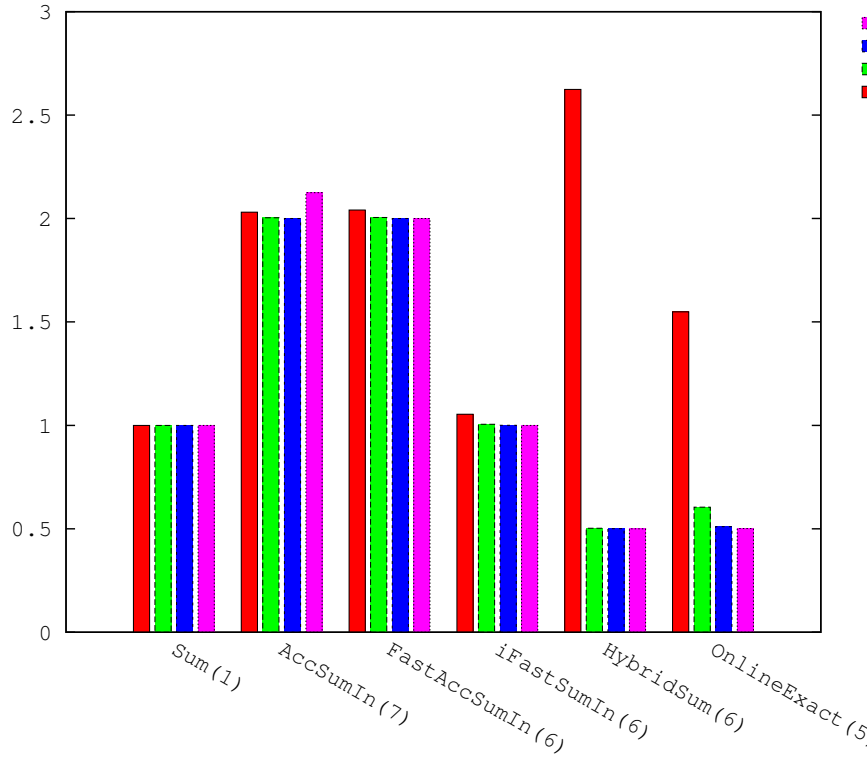
- iFastSum
- AccSum
- FastAccSum
- HybridSum
- OnLineExactSum

PerPI and reproducibility: one run is enough

```
start : <main>   (depth: 2, lcid: 104)
  stop  : <Sum>   (depth: 3, lcid: 10201)(cid: 10201)    I[13781]::C[10000]::ILP[1.3781]
  stop  : <Sum>   (depth: 3, lcid: 10203)(cid: 10203)    I[13781]::C[10000]::ILP[1.3781]
  stop  : <Sum>   (depth: 3, lcid: 10205)(cid: 10205)    I[13781]::C[10000]::ILP[1.3781]
  stop  : <iFastSumIn>   (depth: 3, lcid: 10207)(cid: 10207)    I[696088]::C[18043]::ILP[38.5794]
  stop  : <iFastSumIn>   (depth: 3, lcid: 10241)(cid: 10241)    I[696076]::C[18043]::ILP[38.5787]
  stop  : <iFastSumIn>   (depth: 3, lcid: 10275)(cid: 10275)    I[696076]::C[18043]::ILP[38.5787]
  start : <OnlineExactSum>   (depth: 3, lcid: 10309)
    stop  : <iFastSumIn>   (depth: 4, lcid: 10320)(cid: 10320)    I[29704]::C[611]::ILP[48.6154]
  stop  : <OnlineExactSum>   (depth: 3, lcid: 10309)(cid: 10309)    I[301467]::C[10607]::ILP[28.4215]
 stop  : <main>   (depth: 2, lcid: 104)(cid: 104)    I[2884900]::C[49320]::ILP[58.4935]
Global ILP (cid: 0)    I[2895541]::C[49572]::ILP[58.4108]
```

PerPI # cycle ratio: accurate (left) and faithful sums (right)

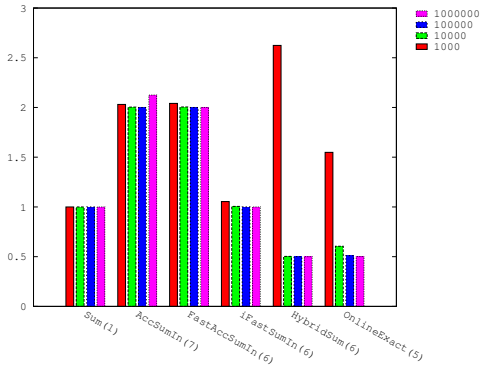




- $cond = 10^{32}$ and $n = 10^3, 10^4, 10^5, 10^6$.
- Twice more precision "free" with the compensated sum
- Faithful sum for even less

How to trust it? PerPI bug vs. reality?

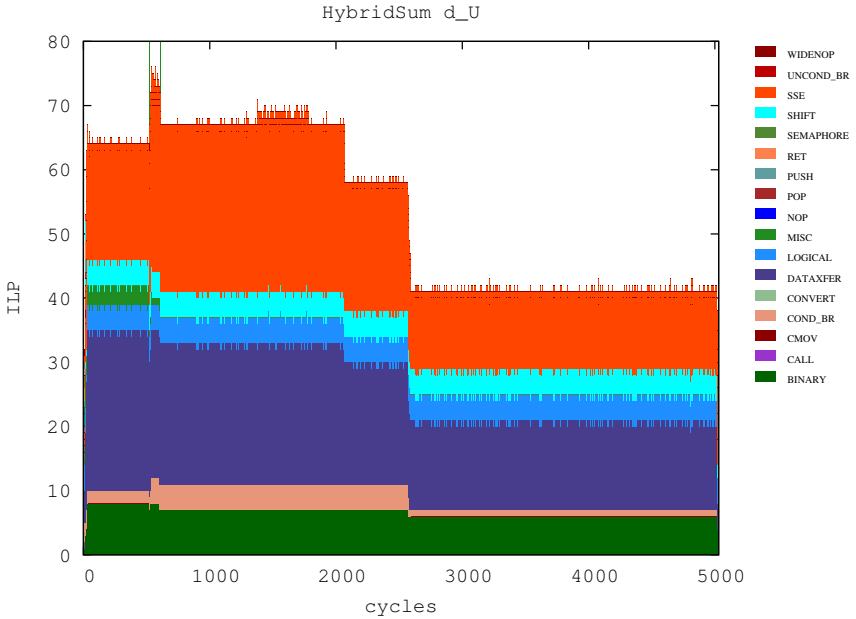
Huge ILP of HybridSum and OnLineExact

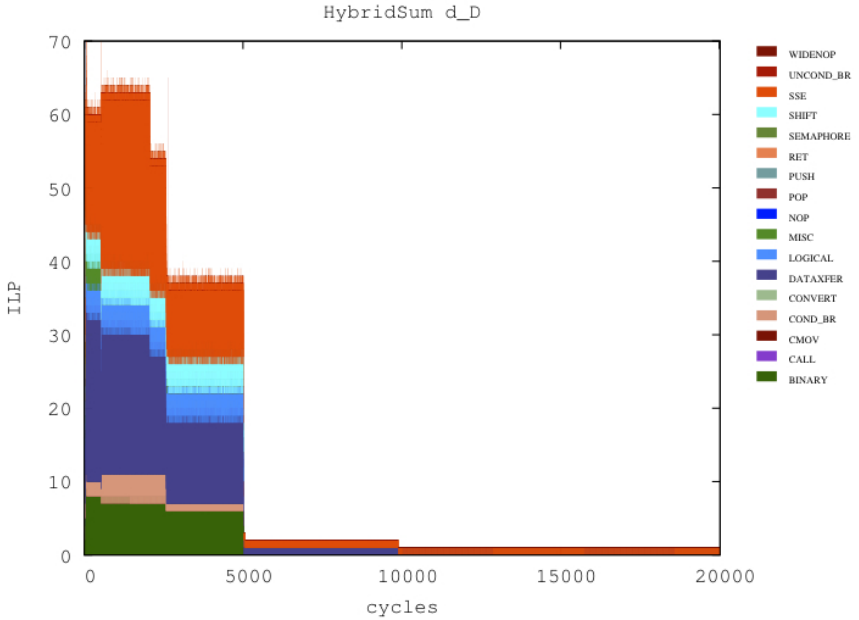


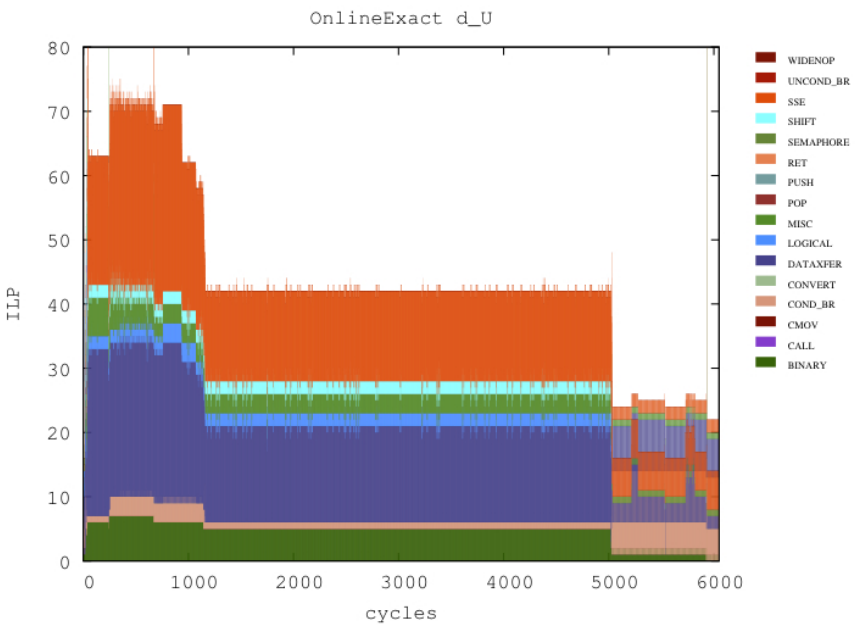
PerPI helps to highlight many details . . . but not all

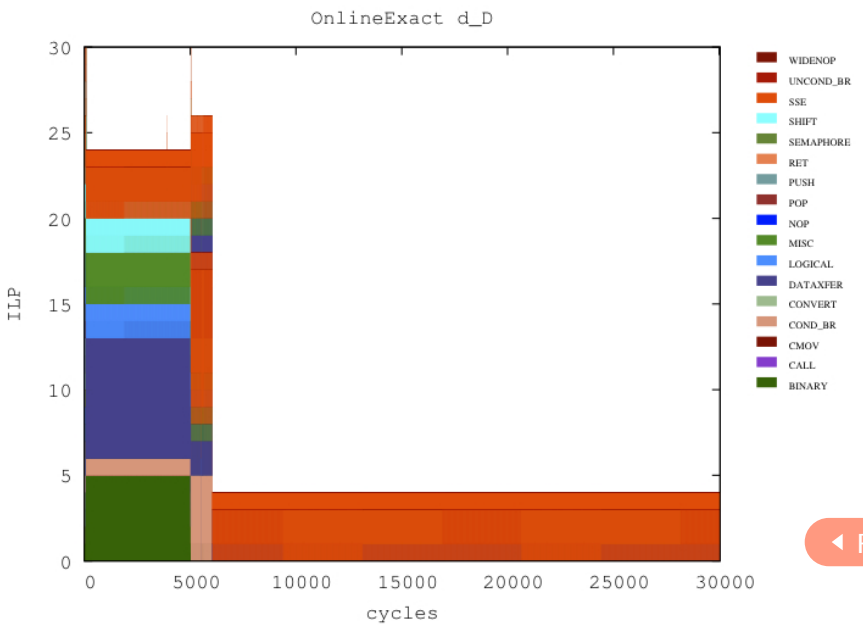
- PerPI measures and exhibits C=$n/2$ ▸ histograms
- Assembly code analysis confirms C=$n/2$
- Floating-point consistency: Sum does not benefit from loop unrolling
- Faithfulness consistency: use as much as possible optimisations
- Loop unroll ($\times 2$) in the exponent extraction step
- Short vector summation starts as soon as possible . . .
- . . . depending on the distribution of the data exponent even for a given exponent range ▸▸ Skip ▸ x86 peculiarities

PerPI histograms for HS (↑) and OLE (↓) for d_U: left, d_D: right



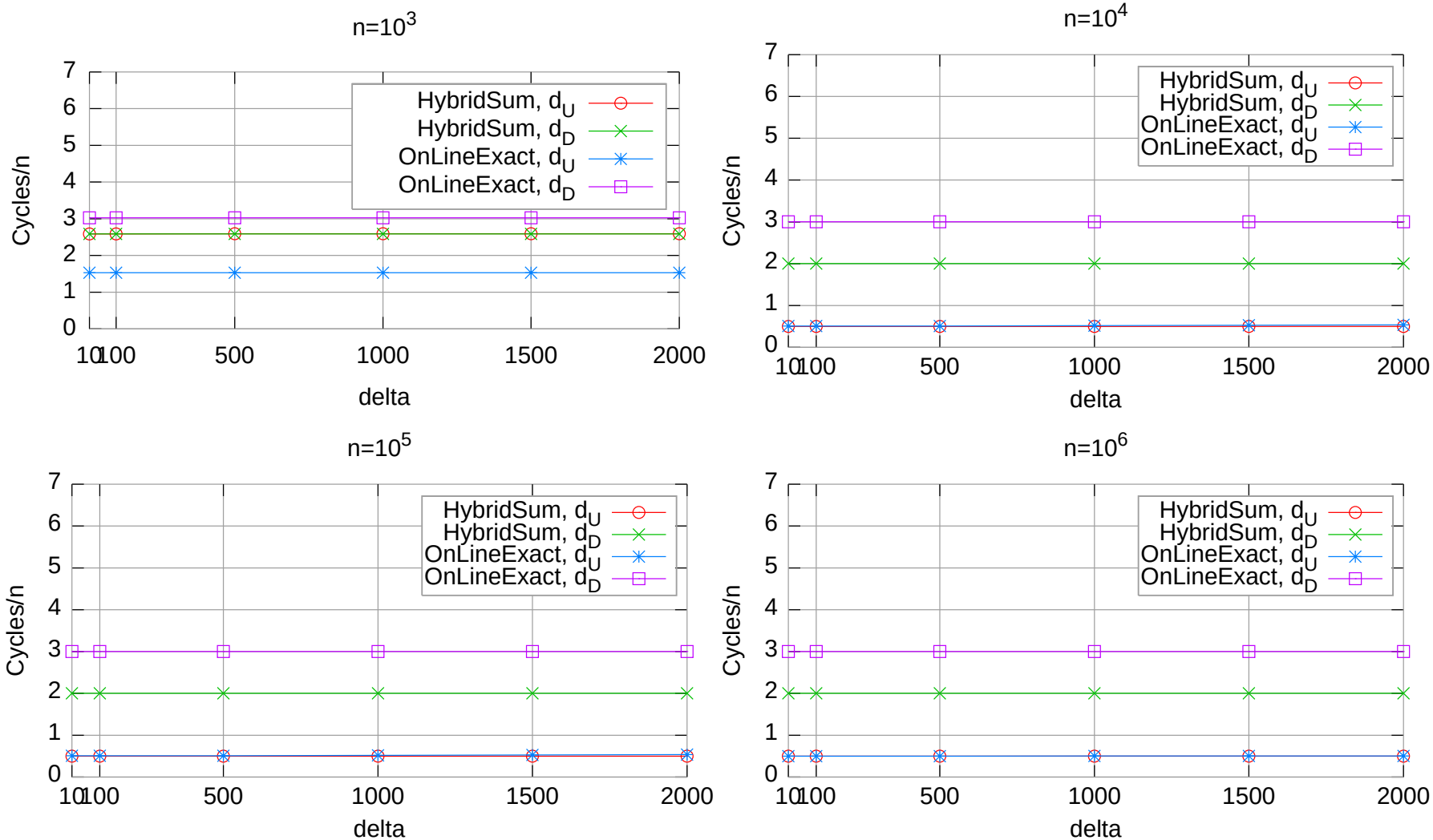






◀ Ret.

Exponent distribution at $\delta = cst$ for HS and OLE



d_U: uniform dist. in $[-\delta/2, \delta/2]$ vs. d_D: Dirac-like distr.: one $-\delta/2$, n-1 $\delta/2$

Zooming and understanding the worst measures (d_D)

```
start : <HybridSum>
  start : <iFastSumIn>
  stop  : <iFastSumIn>      I[62719]::C[2580]::ILP[24.3097]
stop  : <HybridSum>       I[267980]::C[20020]::ILP[13.3856]
start : <OnlineExact>
  start : <iFastSumIn>
  stop  : <iFastSumIn>      I[334]::C[32]::ILP[10.4375]
stop  : <OnlineExact>     I[229263]::C[30026]::ILP[7.63548]
```

Explanation: extraction step and x86 ISA peculiarities

- Cycles between two iterations: 2 in HS vs. 3 in OLE

Conclusion

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- Highly accurate algorithm needs reliable performance evaluation
- PerPI provides reproducible measures of the performance potential
- PerPI highlights how the algorithm and the architecture interact
- PerPI may help to improve the algorithm or its implementation
- Hand-made vs. PerPI analysis: the ideal machine vs. one ISA machine
- Towards a dynamic reference repository for accurate sums and other core routines

▸ exponent distribution ▸ x86 peculiarities

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