Effect of round-off errors on the accuracy of randomized algorithms

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Outline

Characterize the accuracy of the result of a program

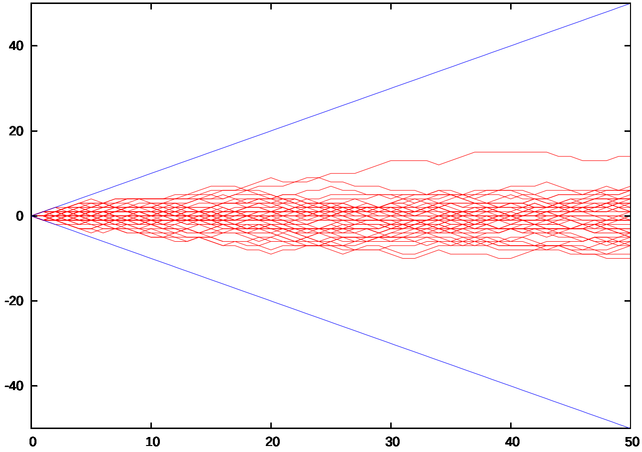
- Running on powerful systems
  - peta-flops ($10^{15} \approx 2^{45}$ operations each second)
  - exa-flops ($10^{18} \approx 2^{54}$ operations each second)
- Using hardware accelerators
  - ClearSpeed (PetaPath in WP8 of PRACE FP7 project)
  - GPU (GENCI joint call for projects with Caps Entreprises)
- Operating in
  - Single-precision (ulp $= 2^{-23}$)
  - Double precision (ulp $= 2^{-52}$)
- Based on Monte-Carlo method
  - Description containing 2,315,737 items

Route from Narita INTL to Paris Charles de Gaulle

Waypoint		N°xE°	Dist (nm)	Worst case error (1kHz)	Significant bits
Narita INTL	JP	36x140	0	0	25
Niigata	JP	38x139	180	0.04	4.6
Khabarovsk	RU	49x135	851	0.19	2.4
Neryungri	RU	57x125	1479	0.33	1.6
Igarka	RU	67x087	2698	0.60	0.7
Naryan-Mar	RU	68x053	3458	0.77	0.4
Josie	FI	63x030	4117	0.91	0.1
Marie	FI	60x020	4433	0.98	None
Dunker	SE	59x017	4538	1.01	None
Sveda	SE	56x013	4769	1.06	None
Alsie	DK	55x010	4885	1.08	None
Paris CDG	F	49x003	5342	1.18	None

Use almost certain bounds when worst case analysis fails

Random walks with probability of moving up or down equal to 1/2



Propose theoretical strong results

- Control software errors due to round-off and truncation errors
- We continue and use a theory
  - For extremely rare failures of very long processes
  - That can be applied to numerical analysis and hybrid systems (heat transfers, aircraft, nuclear power plants)
- Formal developments
  - Using PVS (SRI + NASA) and a previously published theory
  - Force explicit statement of all hypotheses
  - Prevent incorrect uses of theorems
- We assume in this work that round-off errors are
  - Independent variables
  - Independent of the Monte-Carlo variables

Outline

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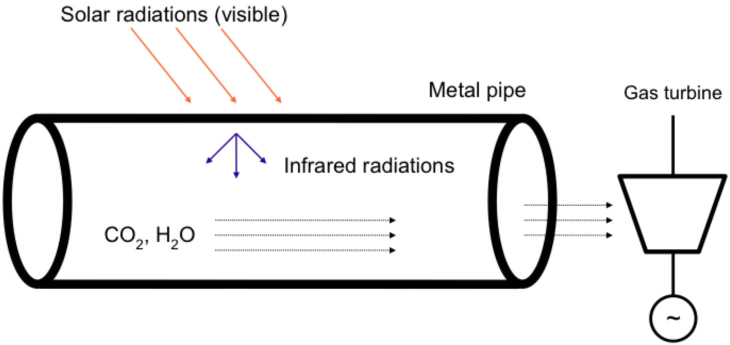
First application: solar power plant

Simulations for the design of high performance solar receptors

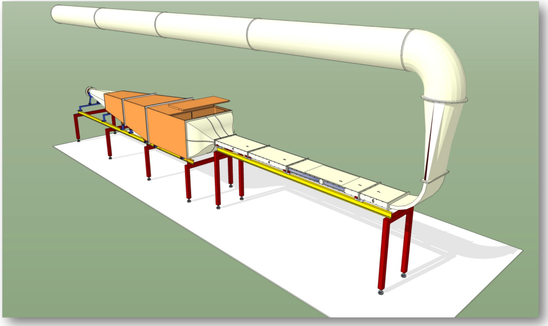
Courtesy of Philippe Égéa (CNRS-PROMES)

Simplified geometry



Experimental validation

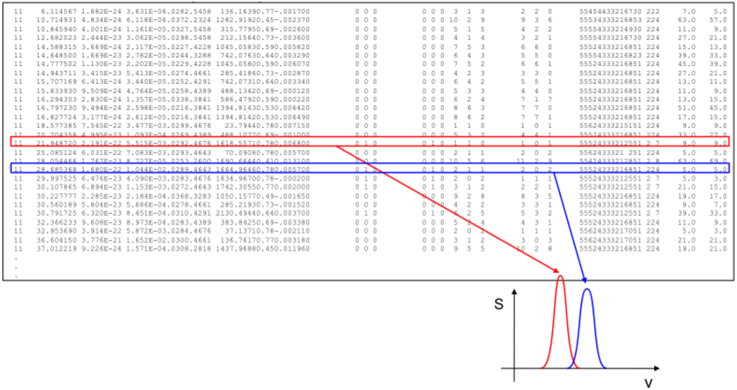
Moyen d'Essais des Écoulements Turbulents pour l'Intensification des transferts de Chaleur



Project supervised by Gabriel Olalde (CNRS-PROMES)

HITRAN-HITEMP molecular spectroscopic database

One record per spectral line



11	6.114567	1.682E-24	3.631E-06.0282.5458	136.16390.77-.001700	0 0 0	0 0 0 3 1 3	2 2 0	55454433216730	222	7.0	5.0
11	10.714931	4.834E-24	6.118E-06.0372.2324	1282.91920.45-.002370	0 0 0	0 0 0 10 2 9	9 3 6	55534333216853	224	63.0	57.0
11	10.845940	4.001E-24	1.161E-05.0327.5458	315.77950.69-.002600	0 0 0	0 0 0 5 1 5	4 2 2	55554333214930	224	11.0	9.0
11	12.682023	2.444E-23	3.062E-05.0298.5458	212.15640.73-.003600	0 0 0	0 0 0 4 1 4	3 2 1	55554333216730	224	27.0	21.0
11	14.588315	3.669E-24	2.117E-05.0227.4228	1045.05830.590.005820	0 0 0	0 0 0 7 5 3	6 6 0	55524333216851	224	15.0	13.0
11	14.648500	1.669E-23	2.782E-05.0244.3288	742.07630.640.003290	0 0 0	0 0 0 6 4 3	5 5 0	55554333216823	224	39.0	33.0
11	14.777502	1.130E-23	2.202E-05.0229.4228	1045.05800.590.006070	0 0 0	0 0 0 7 5 2	6 6 1	55524333216851	224	45.0	39.0
11	14.943711	3.415E-23	5.413E-05.0274.4661	285.41860.73-.002870	0 0 0	0 0 0 4 2 3	3 3 0	55524333216851	224	27.0	21.0
11	15.707169	6.413E-24	3.440E-05.0252.4291	742.07310.640.003340	0 0 0	0 0 0 6 4 2	5 5 1	55524333216851	224	13.0	11.0
11	15.833930	9.509E-24	4.764E-05.0258.4389	488.13420.69-.000120	0 0 0	0 0 0 5 3 3	4 4 0	55524333216851	224	11.0	9.0
11	16.294303	2.830E-24	1.357E-05.0338.3841	586.47920.590.000220	0 0 0	0 0 0 6 2 4	7 1 7	55524333216851	224	13.0	15.0
11	16.797230	9.494E-24	2.598E-05.0216.3841	1394.81430.530.006420	0 0 0	0 0 0 8 6 3	7 7 0	55524333216851	224	51.0	45.0
11	16.827724	3.177E-24	2.612E-05.0216.3841	1394.81420.530.006490	0 0 0	0 0 0 8 6 2	7 7 1	55524333216851	224	17.0	15.0
11	18.577385	7.545E-22	3.477E-03.0299.4676	23.79440.780.007150	0 0 0	0 0 0 1 1 0	1 0 1	55624333215151	224	9.0	9.0
11	20.704358	4.995E-23	1.093E-04.0269.4389	488.10770.69-.001000	0 0 0	0 0 0 5 3 2	4 4 1	55524333216851	224	33.0	27.0
11	21.948720	2.191E-22	5.515E-03.0292.4676	1618.55710.780.006800	0 1 0	0 1 0 1 1 0	1 0 1	55524333212551	2 7	9.0	9.0
11	25.085124	6.031E-22	7.083E-03.0293.4643	70.09080.780.005700	0 0 0	0 0 0 2 1 1	2 0 2	5562433321 251	224	5.0	5.0
11	28.054466	1.767E-23	8.727E-05.0253.2600	1690.66440.410.013100	0 0 0	0 0 0 10 5 6	11 2 9	55424333212851	2 8	63.0	69.0
11	28.685368	1.680E-22	1.044E-02.0289.4643	1664.96460.780.005700	0 1 0	0 1 0 2 1 1	2 0 2	55524333216851	224	5.0	5.0
11	29.997525	6.476E-23	4.090E-03.0283.4676	1634.96700.78-.000200	0 1 0	0 1 0 2 0 2	1 1 1	55524333212551	2 7	5.0	3.0
11	30.107865	6.894E-23	1.153E-03.0272.4643	1742.30550.770.002000	0 1 0	0 1 0 3 1 2	2 2 1	55524333212551	2 7	21.0	15.0
11	30.227777	2.285E-23	2.184E-04.0368.3283	1050.15770.49-.001650	0 0 0	0 0 0 9 2 8	8 3 5	55524333216851	224	19.0	17.0
11	30.560189	5.804E-23	5.686E-04.0278.4661	285.21930.73-.001520	0 0 0	0 0 0 4 2 2	3 3 1	55524333216851	224	9.0	7.0
11	30.791725	6.320E-23	8.451E-04.0310.4291	2130.49440.640.003700	0 1 0	0 1 0 6 2 5	5 3 2	55524333212551	2 7	39.0	33.0
11	32.366233	9.608E-23	8.973E-04.0283.4389	383.84250.69-.003380	0 0 0	0 0 0 5 2 4	4 3 1	55524333216851	224	11.0	9.0
11	32.953690	3.914E-22	5.872E-03.0284.4676	37.13710.78-.002110	0 0 0	0 0 0 2 0 2	1 1 1	55624333217051	224	5.0	3.0
11	36.604150	3.776E-21	1.652E-02.0300.4661	136.76170.770.003180	0 0 0	0 0 0 3 1 2	3 0 3	55624333217051	224	21.0	21.0
11	37.012219	9.226E-24	1.571E-04.0308.2818	1437.96880.450.011960	0 0 0	0 0 0 9 5 5	10 2 8	55524333216851	224	19.0	21.0
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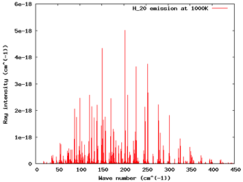
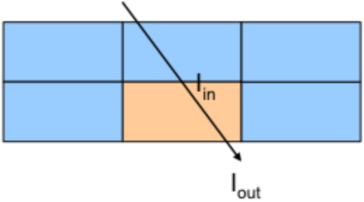
Line-by-line radiative heat transfers

- Use Monte-Carlo method to estimate combined heat transfers



- Compute optical depth with backward ray tracing



Second application: greenhouse gazes

Evolution of net effect of radiative heat transfers between clouds and Earth surface

Courtesy of NASA

Outline

Probability of an inaccurate results

- Truncation error of Monte Carlo quadratures bounded by

$$\mathbb{P}\left(\left|\frac{1}{N}\sum_{n=1}^{N} f(x_n) - \int d^d u f(u_1, \ldots, u_d)\right| \geq \epsilon\right) \leq 2\exp\left(-\frac{N\epsilon^2}{2M^2}\right)$$

- where M bounds $f(u_1, \ldots, u_d)$
- M/ϵ represents the significant digits of the quadrature
- We focus on cases where $N \gg M^2/\epsilon^2$

Fixed and floating point numbers

- Floating point: $v = m \times 2^e$
  - e is an integer called the exponent
  - m is the signed mantissa
- IEEE 754 standard on floating-point arithmetic uses
  - Sign-magnitude notation for the mantissa
  - An implicit first bit ($b_0 = 1$) for the mantissa in most cases

$$v = (-1)^s \times b_0.b_1 \cdots b_{p-1} \times 2^e$$

- Some circuits such as the TMS320 use two's complement

$$v = (b_0.b_1 \cdots b_{p-1} - 2 \times s) \times 2^e$$

- Fixed point: e is a constant and b_0 cannot be forced to 1

Individual measurement errors of physical constants

- v is a constant obtained from a database
- It is commonly admitted that
  - Natural constants follow a logarithmic distribution
  - Trailing digits are approximately uniformly distributed
- The difference between v and the actual value $\overline{v}$ is
  - In the range $\pm \mathrm{ulp}(v)/2$ with

$$\mathrm{ulp}(v) = 2^{e-p+1} \quad \text{(unit in the last place)}$$

  - Modeled by a uniformly distributed random variable X
- Less accurate constants use larger ranges $\pm u/2$

Individual errors of fixed or floating point operations

- Round-off errors created by operators ($+$, $\times$, $\div$, $\sqrt{\ }$) are discrete
- Distributions are very specific (not necessarily uniform)
- We may have to bound
  - Their ranges
  - Their moments

Accumulated round-off error of Monte-Carlo simulation

- Round-off errors δ_n are between $\pm Mu/2$
- Monte Carlo averages the values and the errors
- Probability of a large accumulation is bounded by

$$\mathbb{P}\left(\left|\frac{1}{N}\sum_{n=1}^{N}\delta_n\right| \geq \epsilon\right) \leq 2\exp\left(-\frac{N\epsilon^2}{2M^2u^2}\right)$$

- We focus on cases where $\epsilon / Mu \ll 1$

Accumulated round-off error of Monte-Carlo simulation

- First application sums only positive numbers
  - Various orders of magnitude
  - Partial absorption of small floating point numbers
  - Total absorption of $f(x_n)$ is not permitted
    - $\delta_n = f(x_n)$ would be correlated with the Monte Carlo process
- Second application sums positive and negative numbers
  - Transfers increase during daytime and decrease at night with the quantity of greenhouse gazes in the atmosphere
  - Magnifying effect of cancellations between night and day.

Outline

Validity of the hypotheses

- On the random variables
  - Law (uniform or logarithmic), parameters, symmetry
  - Identity (sometimes) and independence
- Impossible to set beforehand (build counter-example)
- A posteriori estimation (instrument the code)
- High quality level
  - Proofs validated by PVS
  - Very low probability of failure (10^{-9})

Develop and instrument real size applications

- Manage huge sets of data
  - GPU
  - ClearSpeed
- Converging problematic with BioWIC project of the ANR
- Theoretical and applied work

Outline

Working with formal methods

- Positioning a theory is a key issue
  - Too simple, we will be blocked by its limitations
  - Too evolved, we may not be able to use it (never finished)
- Its maturation is also a key issue
  - Formal tools block on any shadow area of a proof
  - Lester (among others) decided to follow textbooks
- Some decisions relate only to educational methods
  - Separate discrete and continuous variables
  - Use sections $[X \leq x]$ instead of the inverse image of Borel sets
- **Milestone:** Results proved but not fully certified formally yet

Formal proof assistants

- Used in areas where
  - Common misunderstandings can falsify key assumptions
  - Errors can cause loss of life
  - Errors can cause significant financial damage
- Used for floating-point arithmetic and probabilistic or randomized algorithms
- Proof assistants include
  - ACL2 (UT Austin)
  - HOL (Cambridge)
  - Coq (INRIA)
  - PVS (SRI and NASA)

Example of an increasingly common misunderstanding

- Attribute to articles the bibliometric properties of their journal
- One example from the American Mathematical Society
  - "Quantitative Assessment of Research Citation Statistics"
  - `//www.awm-math.org/CitationStatistics-FINAL.PDF`
  - Numbers of citations follow power laws
  - Impact factor is
    - 0,434 for the Proceedings (short articles less than 10 pages)
    - 0,846 for the Transactions (longer articles)
  - Probability of a random article of the Proceedings to have no less citations than a random article of the Transactions: **62%**

Conclusions and future work

- Worst case error analysis provides exponential bounds $O(A^n)$ suitable for small and toy applications
- Backward error analysis used to provide linear bounds $O(n)$ suitable for high performance computing
- We provide in this work sublinear bounds $O(\sqrt{n})$ suitable for peta- and exa-scale computing
- Our scheme is suitable to obtain the highest assurance level (EAL) of the ISO 15408 and 18045 standards establishing the Common Criteria for Information Technology Security Evaluation

Wider picture

- Most (all ?) recent applications of high performance computing are randomized algorithms
  - Countless references
- This work is about discrete probabilities...
  - Work of Joe Hurd
  - Work of Philippe Audebaud & Christine Paulin
- ... and continuous and general probabilities
  - Work with David Lester
  - Work with David Lester, Erik Martin-Dorel and Annick Truffert

Acknowledgment

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Many thanks for you attention

- Any question?