Numerical approach to Feynman diagram calculations: Benefits from new computational capabilities

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Plan

- Introduction
- Numerical Computation
- Automatic systems and tools
- Control of numerical computation
  - Precision control
  - Speed control
- Summary

Introduction

- Feynman Diagram Calculation : Complicated and laborious calculations
  - Systems on computer appear to overcome the problems
    - Computer algebra systems manage the well-defined perturbative calculation in QFT
    - Numerical integration packages compute the multi-dimensional phase-space integral with required accuracy
    - Elaborated numerical algorithms perform efficient event generation
  - Thanks to emergence of powerful computing environments, a wide variety of systems achieve important results
  - This talk covers diagrammatic approaches only

Numbers of diagrams (QED)

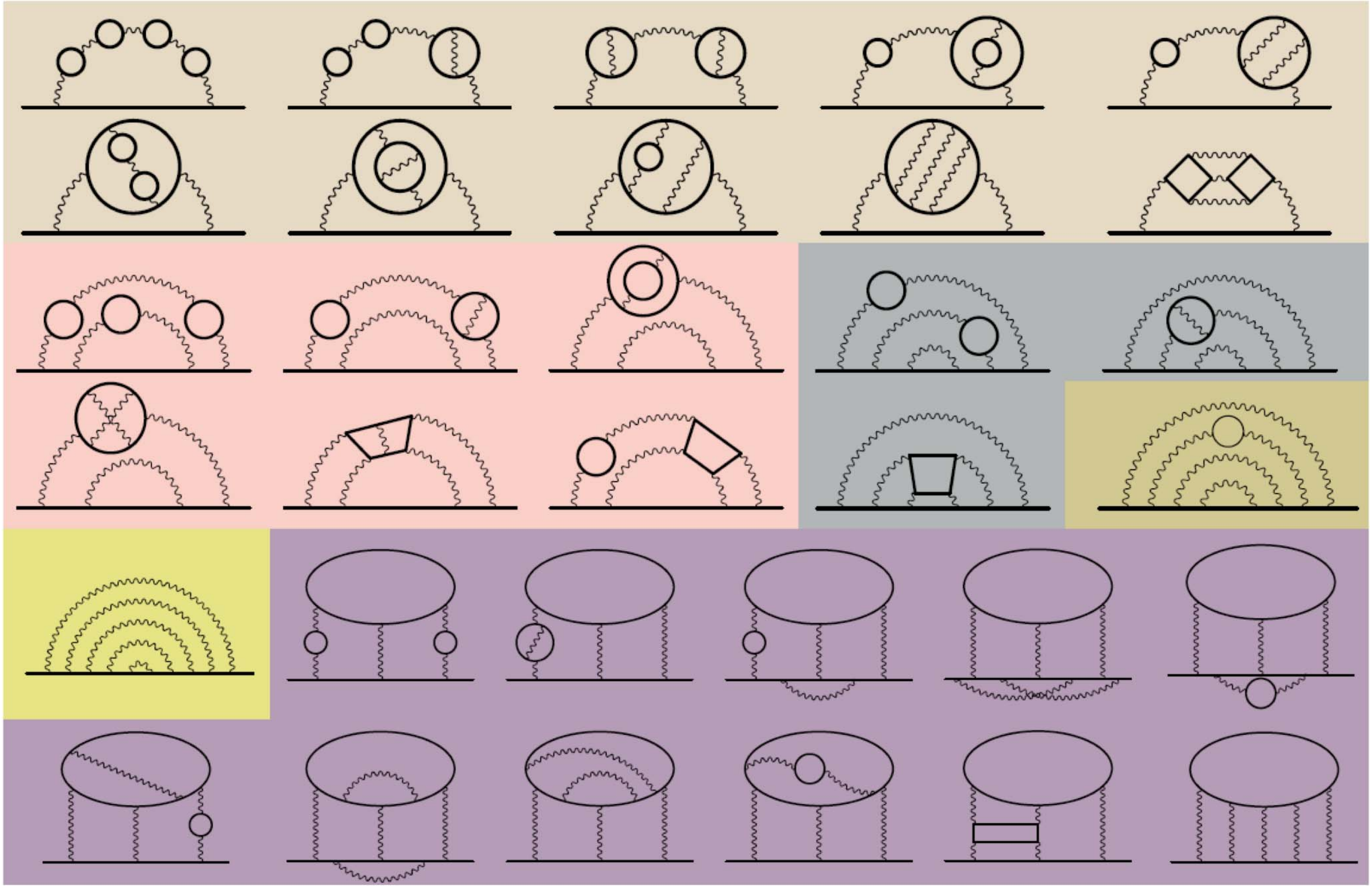
T.Kaneko, S.Kawabata, and Y.Shimizu CPC 43(1987)279.

1987

Process	Loop	diagrams	Process	Loop	diagrams
e-->e	1	1	e−e− ->e−e−	1	10
	2	3		2	94
	3	18	e+e− ->e+e−	1	10
	4	153		2	94
	5	1638		3	1136
	6	20898	e+e− ->e+e− γ	1	72
γ --> γ	1	1	e+e− ->e+e− γ γ	0	40
	2	3		1	564
	3	18	e+e− ->e+e−e+e−	0	36
	4	153		1	552
e+e− --> γ^*	1	1	e+e− ->e+e− $\mu+\mu-$	0	36
	2	7		1	552
	3	72	e+e− ->e+e− $\mu+\mu-\gamma$	0	252
	4	891	e+e− ->e+e−2($\mu+\mu-$)	0	1728
	5	12672	γ γ -> γ γ	1	6
	6	202770		2	60

5 loops, 10-th order (12672 diagrams), 32 gauge sets

Slide by T.Aoyama in JPS meeting 2009 fall



Numerical Computation

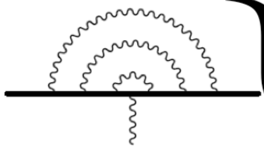
electron g-2 by T.Kinoshita et al.

Anomalous magnetic moment

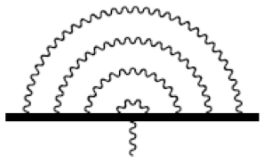
$$a_e \equiv (g-2)/2$$

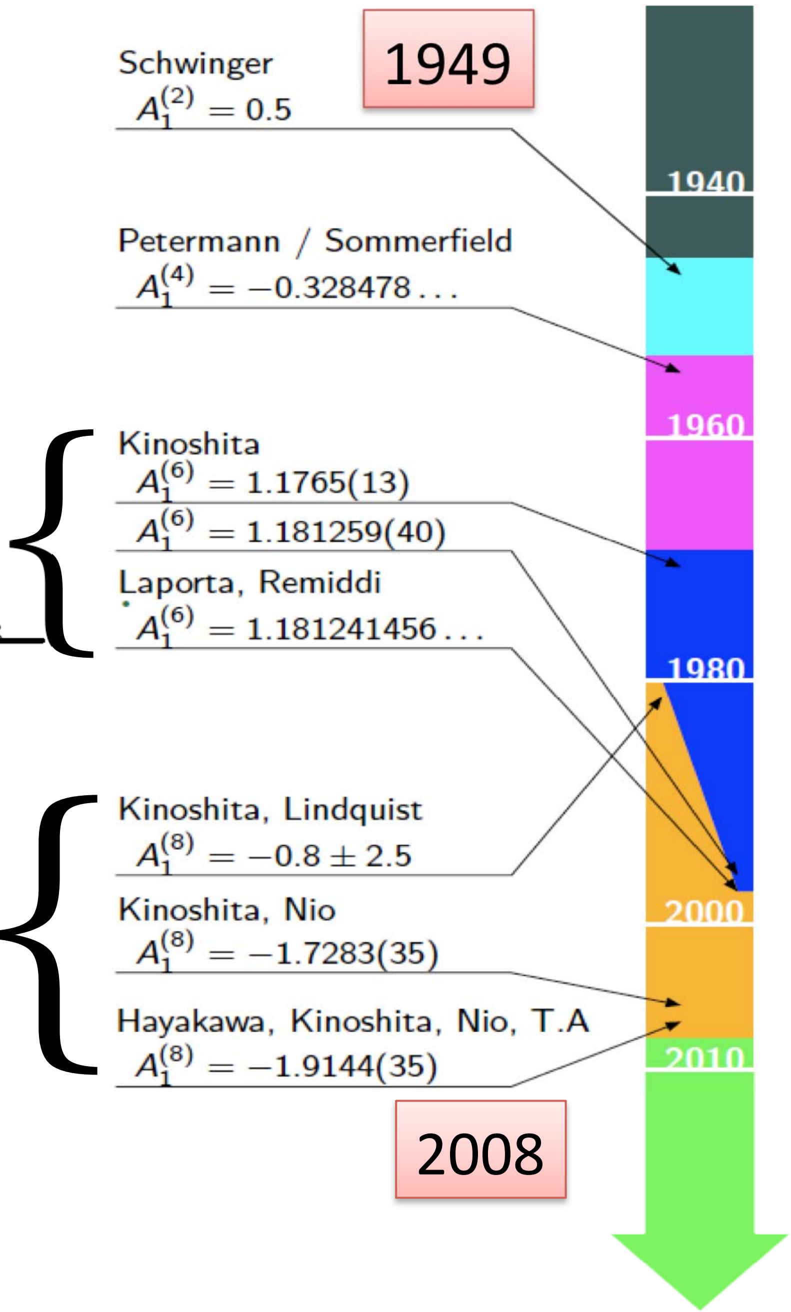
$$a_e(QED) = A^{(2)}\left(\frac{\alpha}{\pi}\right) + A^{(4)}\left(\frac{\alpha}{\pi}\right)^2 + A^{(6)}\left(\frac{\alpha}{\pi}\right)^3 + \cdots$$

- 3 loops, 6-th order (72 diagrams)
  - start in 1967 → end in 1995, 28 years
  - numerical and analytical method



- 4 loops, 8-th order (891 diagrams)
  - start in 1990 → end in 2006, 17 years
  - Kinoshita, Nio PRD 73 013003 ('06)
  - Revised in 2008
  - Numerical method

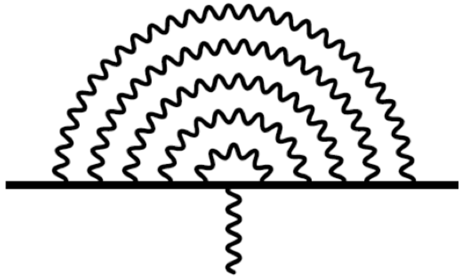




O(10^7) theoretical improvement
by 60-year hard work!

T.Aoyama, Hayakawa, Kinoshita PRD 77 053012 ('08)	Theory 1.15965218279 (7.71) x 10^{-3}
G.Hanneke, S.Forgwell, G.Gbrielse PRL 100 120801 ('08)	Experiment 1.15965218073 (28) x 10^{-3}

Numerical computation of 10-th order of electron g-2 is in progress since 2006 by Nio, Aoyama, Hayakawa, Kinoshita



- How large?
  - 12672 diagrams
  - $O(10^5)$ FORTRAN lines per diagram
  - 13 dim. Integration and 10^8 sampling points with 100 iteration by Monte Carlo integration package VEGAS (Lepage, 1978)
- How difficult?
  - human errors : Automatic system "gencode" has been developed
    - implemented in Perl with FORM and Maple
    - FORTRAN code generator
  - digit deficiency problem: extended precision arithmetic (quadruple or more) has been used

Development of Symbolic manipulation system in connection with HEP

- algebraic manipulation of matrix elements

  SCHOONSCHIP, REDUCE in 1960's.

  FORM (Vermaseren '84), GiNaC (GPL)

  Mathematica, Maple and so on

- Diagram generation algorithm

  Sasaki '76, QGRAF (Nogueira '91), grc (Kaneko '95)

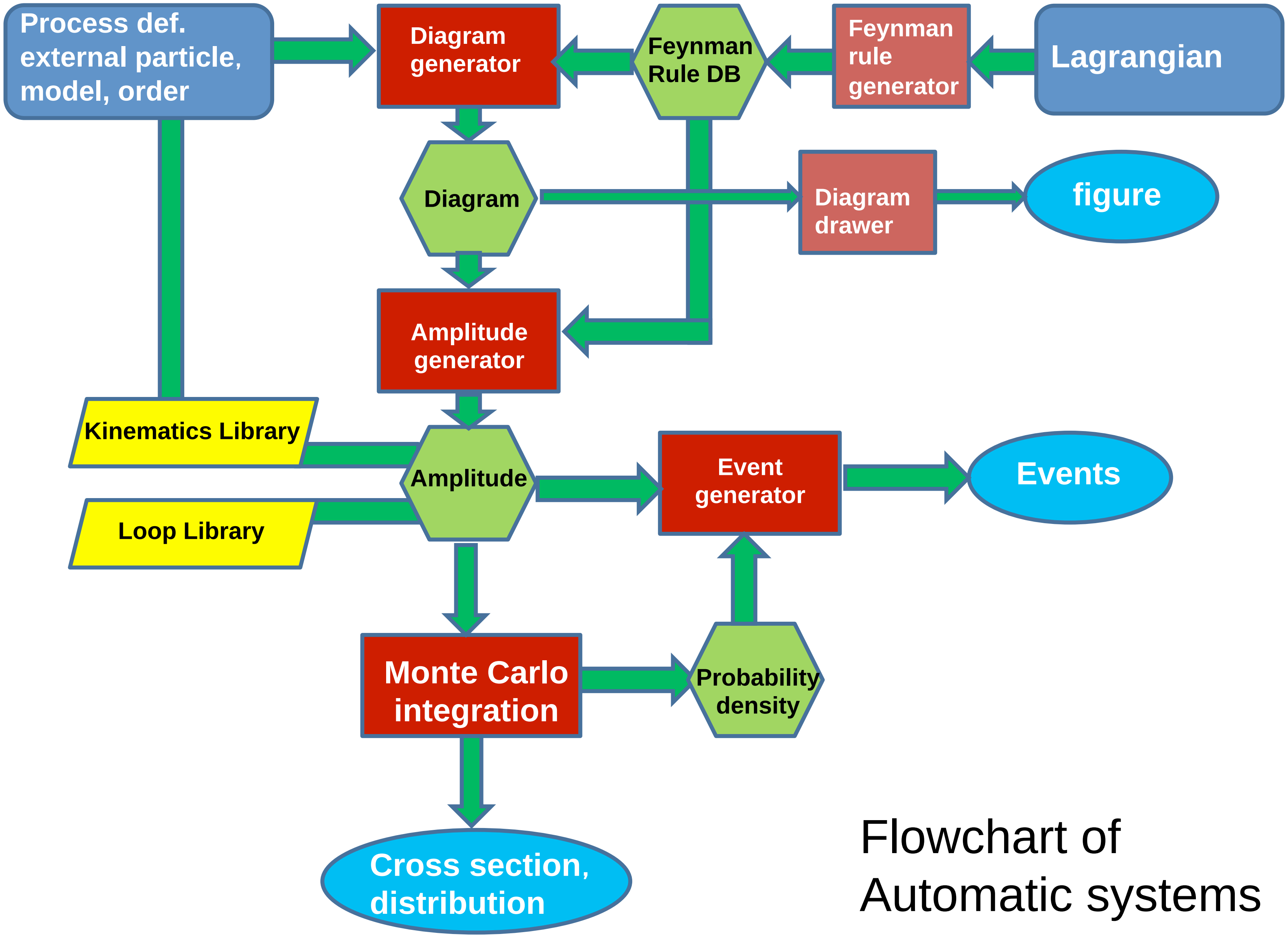
- Feynman rule generation from Lagrangian

  LanHEP (Semenov '98), gss (Kaneko '05), fdc (Wang '93),

  Feynrule (Christensen and Duhr '09)

→ Combined with numerical approach → Automatic system packages in HEP

Slide by K.Kato in JPS meeting 2009 fall



Flowchart of Automatic systems

Automatic Systems in HEP

- Packages
  - Tree level
    - GRACE, CompHEP, CalcHEP, FeynArts/FeynCalc/FormCalc, Madgraph, fdc and so on
  - one-loop level
    - FeynArts/FeynCalc/FormCalc with LoopTools, GRACE-1loop, SloopS, xloop, golem, DIANA, sanC, and so on
- two-loop and more level
  - Developments of tools or systems for multi-loop by many groups
    - Analytical approach , AMBRE, MB.m and so on..
    - Numerical approach, direct computation method and so on..

What is direct computation method ?

E. De Doncker, Y.Shimizu J.Fujimoto, FY CPC 159('04)145.

It can handle singularities without analytical treatment

In the analytic treatment, ε in the denominator is an infinitesimal number (in complex analysis) while we consider it a finite (sometimes rather large) number

$$I = \lim_{\varepsilon \to 0} \int_0^1 dx \int_0^{1-x} dy \frac{1}{D(x,y) - i\varepsilon}$$

Sometimes denominator becomes 0 in the integration region.

Change ε as $\varepsilon_l = \frac{\varepsilon_0}{c^l}, \quad c > 1$
Do integration
and get $\mathrm{I}(\varepsilon_l)$, $\varepsilon_l > 0$, $l = 0, 1, 2, \ldots$

$$\Re(I(\varepsilon_l)) = \int_0^1 dx \int_0^{1-x} dy \frac{D(x,y)}{D(x,y)^2 + \varepsilon_l^{\,2}},$$

$$\Im(I(\varepsilon_l)) = \int_0^1 dx \int_0^{1-x} dy \frac{\varepsilon_l}{D(x,y)^2 + \varepsilon_l^{\,2}}$$

Extrapolate $\mathrm{I}(\varepsilon_l)$
and get the result when ε becomes 0
using ε-algorithm by P.Wynn.

$$\Re(I) = \lim_{\varepsilon \to 0} \left\{ \Re(I(\varepsilon_l)) \right\},$$

$$\Im(I) = \lim_{\varepsilon \to 0} \left\{ \Im(I(\varepsilon_l)) \right\}$$

Integration package used in direct computation method

- DQAGE

R.Piessens E. De Doncker, C.W.Uberhuber, D.K.Kahaner;
" Quadpack – a subroutine package for automatic integration", Springer-Verlag, 1983

$$I = \int_a^b f(x)dx \approx \sum_{i=1}^{n} \omega_i f(x_i)$$

Gauss-Kronrod quadrature rule

- Double Exponential formulae

H.Takahashi and M.Mori;
"Double Exponential Formulas for Numerical Integration",
Bull.R.I.M.S.,Kyoto Univ.,9,pp. 721-741(1974).

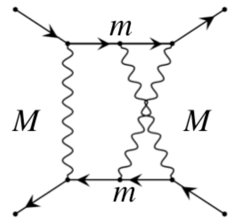
$$I = \int_{-1}^{1} f(x)dx = \int_{-\infty}^{\infty} f(g(t))g'(t)dt \approx h \sum_{j=-N}^{N} \omega_j f(x_j)$$

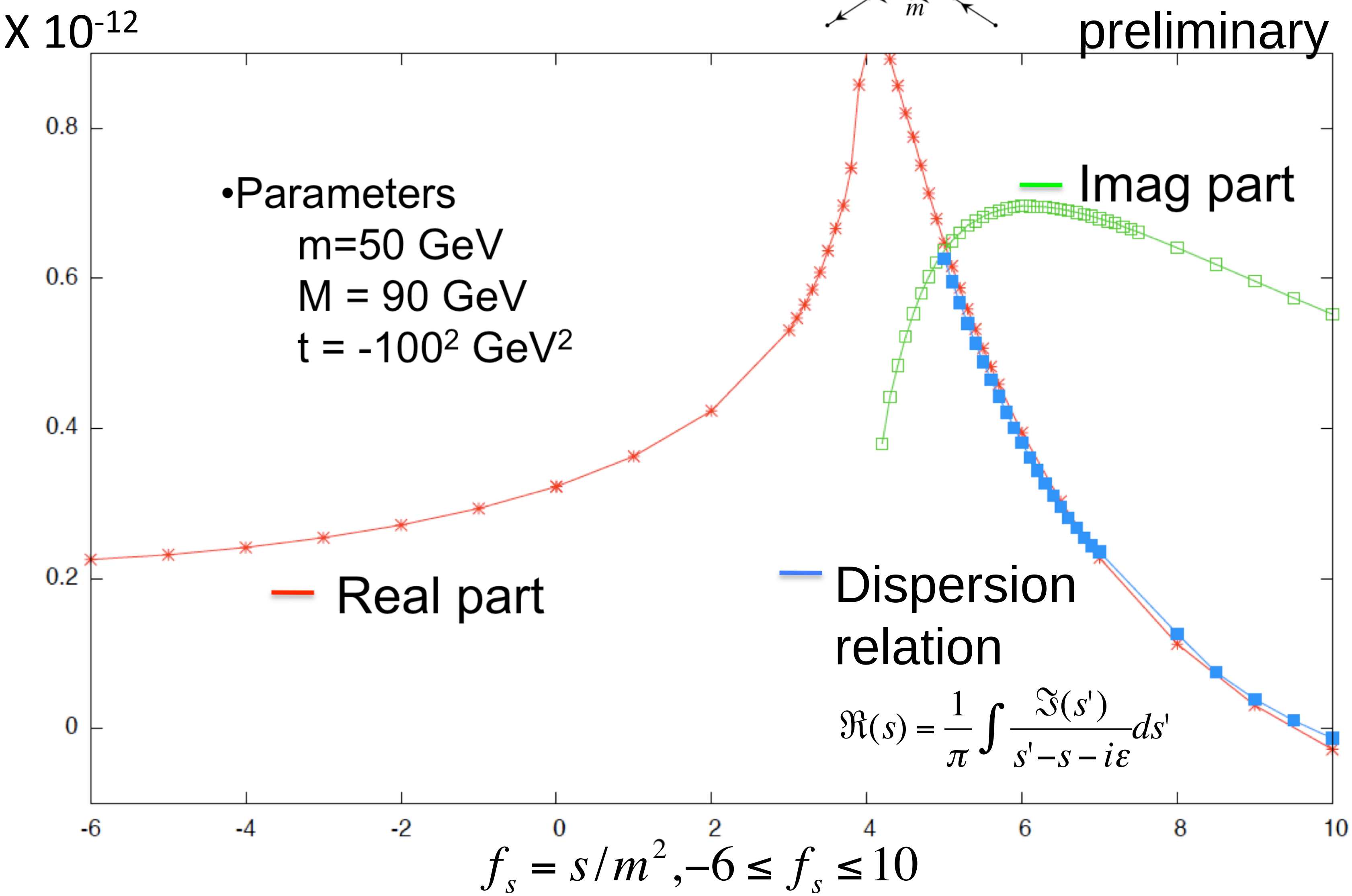
$$x = g(t) \qquad g(t) = \tanh\left(\frac{\pi}{2}\sinh(t)\right) \qquad g'(t) = \frac{\frac{\pi}{2}\cosh(t)}{\cosh^2\left(\frac{\pi}{2}\sinh(t)\right)}$$

$$x_j = g(hj) \qquad \omega_j = g'(hj)$$

DQAGE and DE (for 1dim) can be used iteratedly for multi-dimensional integral. Talk by E. de Doncker

Example of direct computation method
two-loop crossed box with masses





control of numerical computation

- How to keep the quality of the computation
  - Check using gauge invariance
    - Unitary gauge ←→ 'tHooft Feynman gauge
    - R_ξ gauge
    - Parameter check in non-linear gauge
  - Check using multi-precision arithmetic
    - Digit deficiency by cancellation
  - Comparison among systems

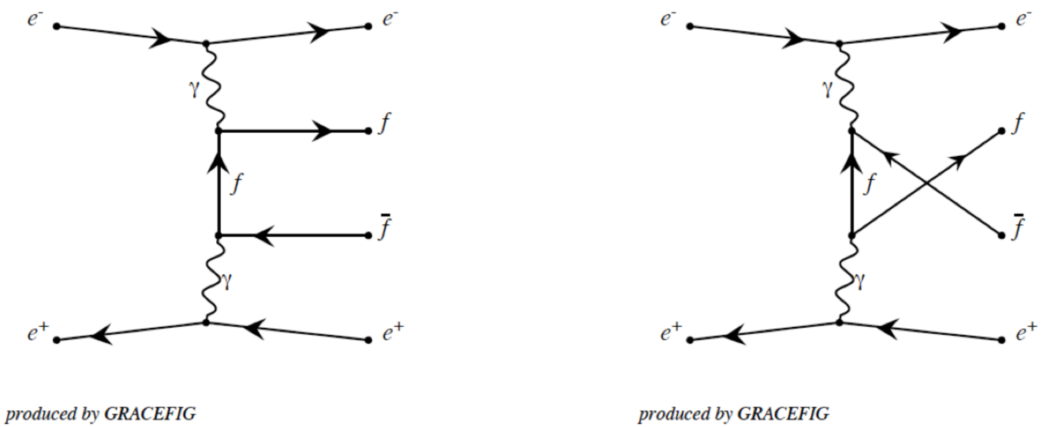
Precision control

- How to reduce the elapsed time for computation

Speed control

Precision control

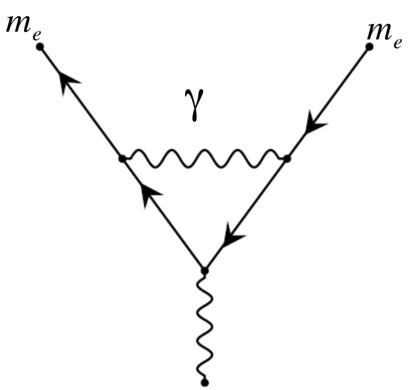
1^{st} Example : tree-level $e^+e^- \to e^+e^- f\bar{f}$



Large cancellation between diagrams

T.Ishikawa, T.kaneko. K.Kato, S.Kawabata, Y.Shimizu, H.Tanaka KEK Reports 92-19

m_f	Double precision (covariant gauge)	Quadruple precision (covariant gauge)	Special treatment to avoid cancellation
10.0	(1. 7372 +- 0. 0034) X 10^1	(1. 7657 +- 0. 0042) X 10^1	(1.7632 +- 0.0054) X 10^1
5.0	(8. 7012 +- 0. 0185) X 10^1	(9. 0786 +- 0. 0042) X 10^1	(9.0356 +- 0.0278) X 10^1
1.0	(2. 9527 +- 0. 0350) X 10^3	(3. 4108 +- 0. 0094) X 10^3	(3.3926 +- 0.0153) X 10^3
0. 10566	(6. 6538 +- 0. 5541) X 10^5	(4. 2900 +- 0. 0236) X 10^5	(4.2661 +- 0.0186) X 10^5



2^{nd} example :

Precision control

one-loop integral with infrared divergence by direct computation method

$$I=\int_0^1 dx \int_0^{1-x} dy \frac{1}{-xys+(x+y)^2 m_e{}^2+(1-x-y)\lambda^2}$$

$m_e = 0.5\times 10^{-3}$ GeV

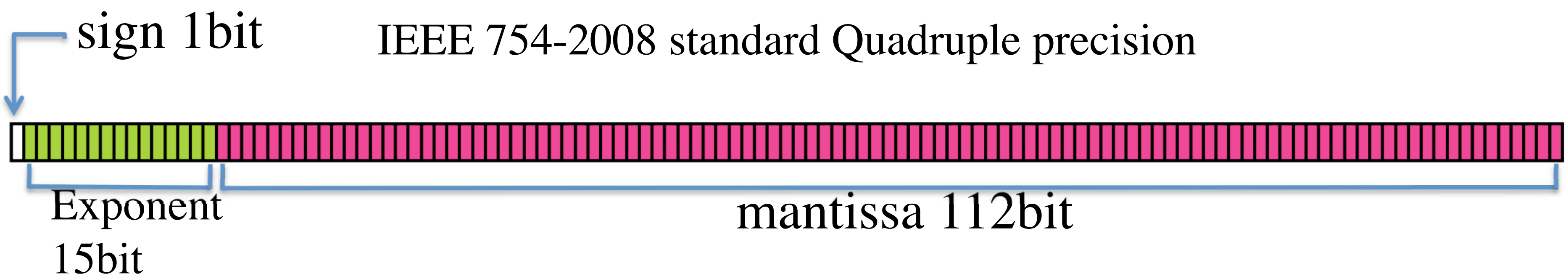
$\sqrt{s} = 500$ GeV

$\lambda = 10^{-n}$ GeV : A fictitious photon mass

Quadruple precision is not enough →

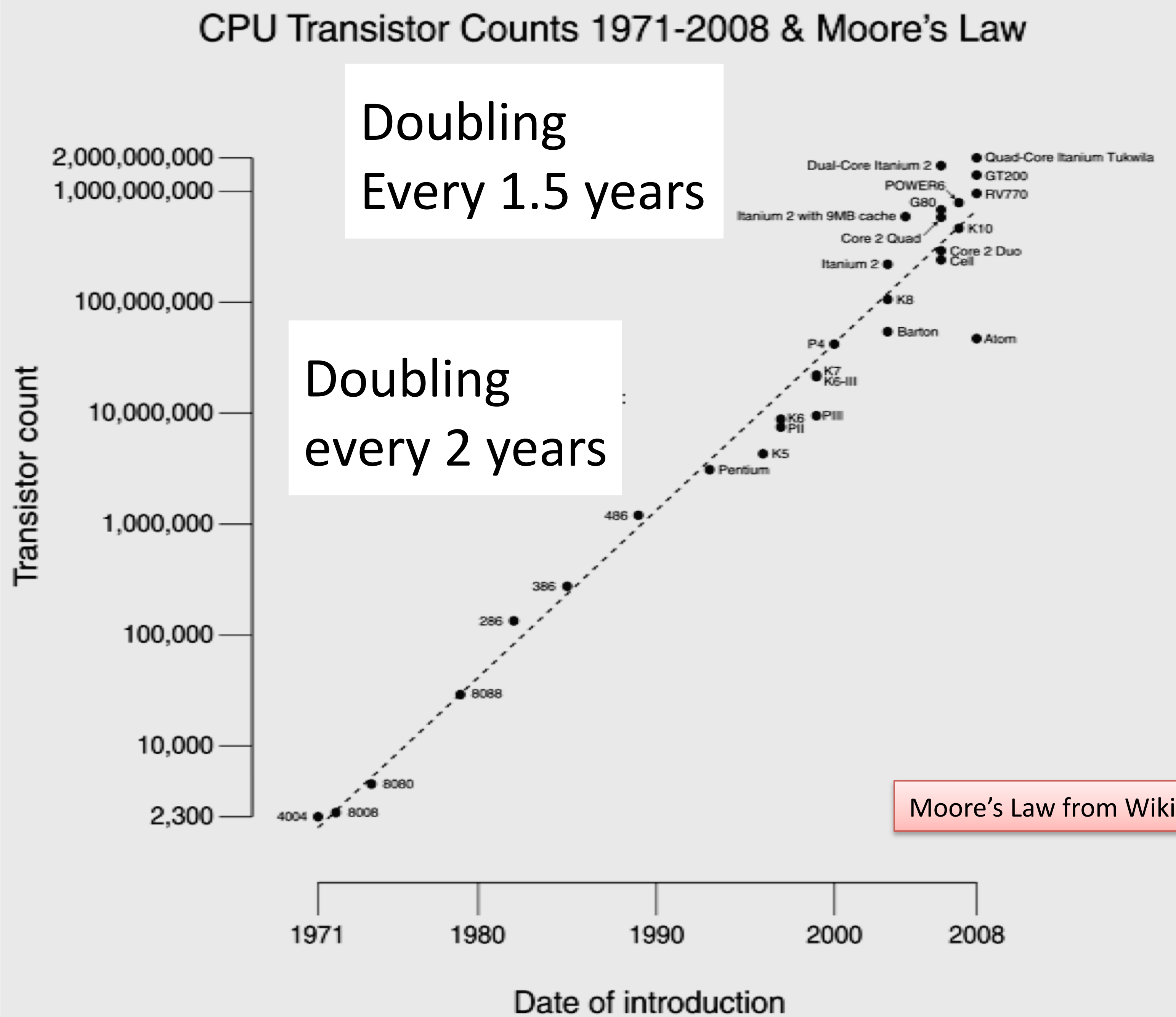
n	Av. Lost bit	Max. Lost bit
20	88	92
21	98	102
22	108	112

IEEE 754-2008 standard Quadruple precision



multi-precision arithmetic library

- MPFUN: http://crd.lbl.gov/~dhbailey/mpdist/
- QD: http://www.experimentalmath.info/
- GMP: http://gmplib.org/
- MPFR: http://www.mpfr.org/
- exflib: http://www-an.acs.i.kyoto-u.ac.jp/~fujiwara/exflib/
- HMLIB: Nuclear Instruments and Methods in Physics Research Section A: Volume 559, Issue 1, 1 April 2006, Pages 269-272
  Proceedings of the X International Workshop on Advanced Computing and Analysis Techniques in Physics Research - ACAT 05
- and so on ……



Doubling
Every 1.5 years

Doubling
every 2 years

Moore's Law from Wikipedia

Parallel computation in automatic systems

Speed control

- Symbolic manipulation part
  - FORM : TFOTM and ParFORM

  D.Fliegner, A. Retey, M.Tentyukov, J.A.M. Vermaseren
  arXiv:hep-ph/9906426, arXiv:hep-ph/0007221, arXiv:cs/0407066, arXiv:cs/0604052, arXiv:hep-ph/0702279
- Amplitude computation part
  - Parallel computation of diagrams in GRACE

  FY et al., AIHENP99 (arXiv:hep-ph/0006268)
- Numerical integration part (Monte Carlo Integration)
  - Parallelized BASES
  - Parallelized VEGAS

  R. Kreckel CPC 106 ('97) 258 and others
- Loop integration part

  FY et al., ACAT2008 (arXiv:0904.2823)

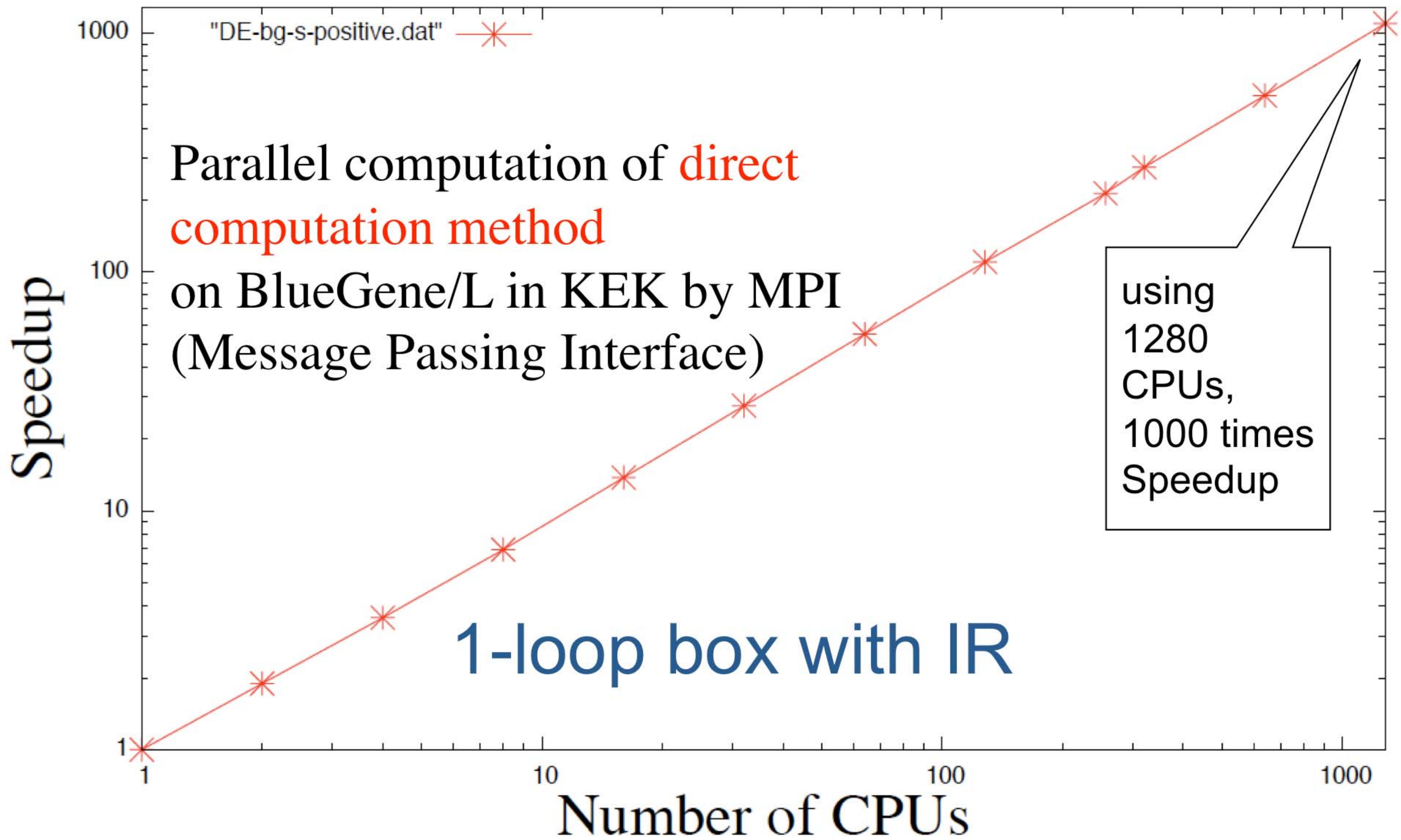
http://www.nikhef.nl/~form/aboutform/aboutform.html

97.94TFLOPS since 2009 in RIKEN
http://www.riken.jp/engn/r-navi/video/index.html

57.3TFLOPS since 2006 in KEK
http://scwww.kek.jp/index_e.html

Speed control

MPI(Message Passing Interface) approach



Accelerator-based Computing

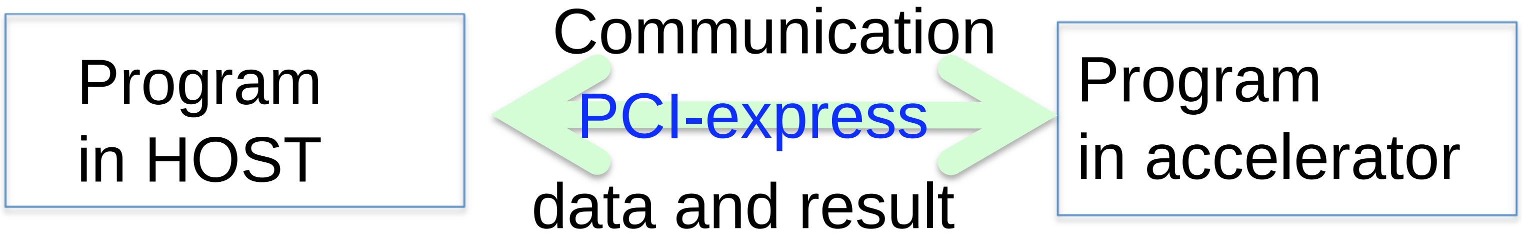
- Why GPGPU (General Purpose Graphics Processing Unit) ?
  - Performance, green computing, cost
- Commercial GPU
  - GeForce GTX200 series/Tesla 8/Tesla 10 by NVIDIA
    - CUDA since '07
  - RV (ATI RADEON) series by AMD/ATI
    - ATI Stream SDK since '08

Tianhe-1
ATI Radeon HD 4870 2
National SuperComputer Center in Tianjin/NUDT
http://www.top500.org/system/10186

vendor	Intel	AMD	NVIDIA	AMD/ATI
Model	Xeon X5570	opteron8435	Tesla C1060	FireStream9270
Number of cores	4	6	240	800
Clock [GHz]	2.93	2.6	1.3	0.75
Memory Bandwidth [GB/s]	25.6	12.8	102	108.0
Performance single/double [GFlops]	46.88/23.44	62.4/31.2	933/78	1200/240
Power consumption [GFops/W]	0.55	0.83	4.97	5.45

Accelerator-based computing

- How does acceleration work?



- Can any application be accelerated?

  Unfortunately no

- How much is GPU used in physics field?

  GPU keyword search in arXiv.org (on 19/Feb/2010)

Total	22
astro-ph	8
med-ph	4
cond-mat	3
hep-lat	3
comp-ph	2
hep-ph	1
others	1

2 papers are about the acceleration of HELAS (HELicity Amplitude Subroutines)

Acceleration of HELAS using GPU

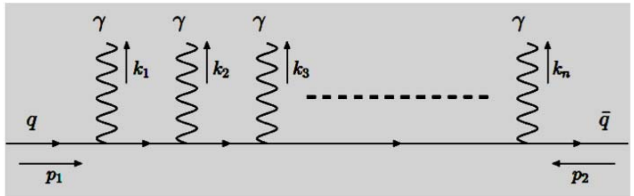
Speed control

K.Hagiwara, J.Kanzaki. N.Okamura, D.Rainwater and T.Stelzer

arXiv:0908.4403v1 [physics.comp-ph], arXiv:0909.5257 [hep-ph]

HEGET (HELAS Evaluation with GPU Enhanced Technology)

- QED: uu -> n-photons (n=2 to 8)
- QCD: gg -> n-gluons, uu -> n-gluons,
  uu -> uu + n-gluons (n=2 to 5)
- pp collisions @ 14TeV+CTEQ6L1
- single precision in GTX280 and so on



Program in HOST

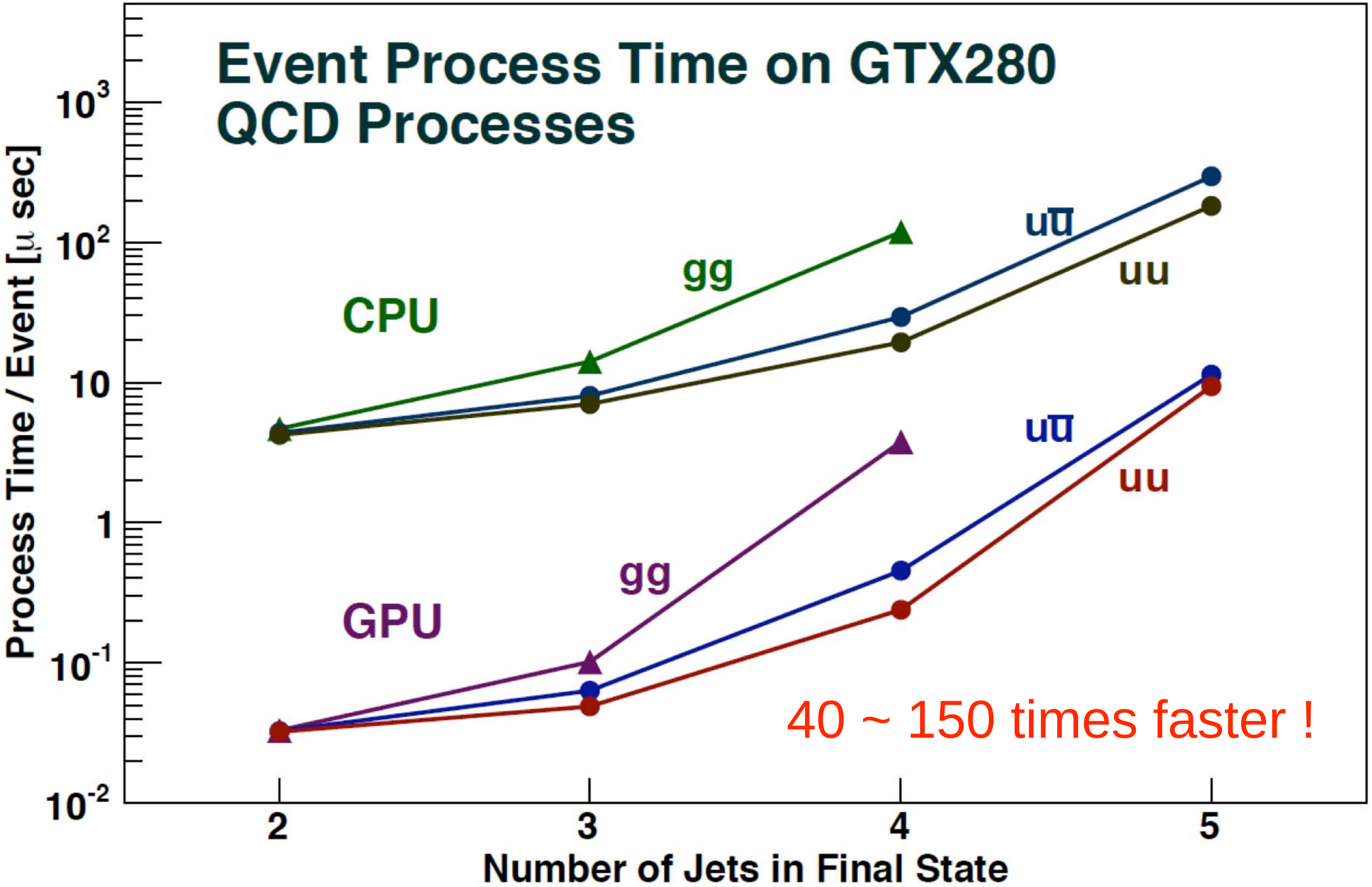
random numbers →

← momenta and helicities for external particles, squared amplitudes

Program in accelerator

Speedup of HELAS

Speed control



Accelerator-based Computing

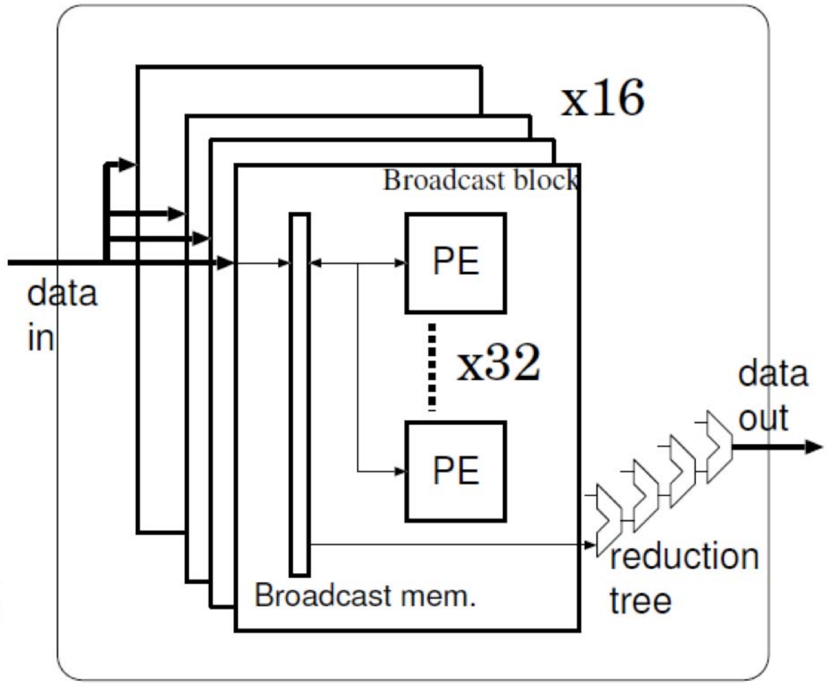
Speed control

Special purpose hardware Talk by N.Nakasato

– GRAPE (GRAvity PipE) since 1988
  - Developed for Gravitational N-body simulation
  - Gordon Bell prize ('95, '96, '99, '00, '01, '03, and '06)

– GRAPE-DR since 2006
  - 512 processors (PE)
  - 380 MHz
  - 390 GFlops (single)
  - 195 GFlops (double)

quadruple precision is available using Nakasato's compiler



GRAPE-DR Processor

Slide from Dr. Fukushige, GRAPE group

Speed control

Acceleration of computation of loop integral

- GRAPE-DR + direct computation method

  with double exponential formulae
- Some tests for loop integrals in quadruple precision
  - One-loop vertex with infrared divergence
  - One-loop box with infrared divergence

GRAPE-DR model450, PCI Express card

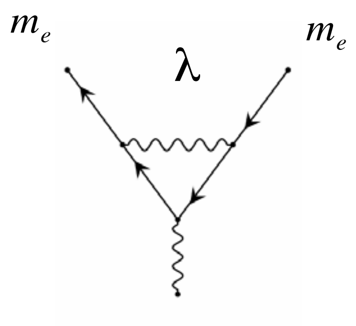
GRAPE-DR model1800

HOST

Speedup in quadruple precision

Speed control

$$I = \int_0^1 dx \int_0^{1-x} dy \frac{1}{-xys + (x+y)^2 m_e^{\ 2} + (1-x-y)\lambda^2}$$




```
LMEM xx, cnt2, cnt3;
BMEM x30, gw30;
RMEM res;
CONST lambda, fme, s, one, eps;
yy = x30*cnt2;

d = -xx*yy*s+(xx+yy)*(xx+yy)*fme*fme+(one-xx-yy)*lambda*lambda;

res += gw30/d;
```

$s = \pm 500^2$ GeV²

$m_e = 0.511 \times 10^{-3}$ GeV

$\lambda = 10^{-30}$ GeV

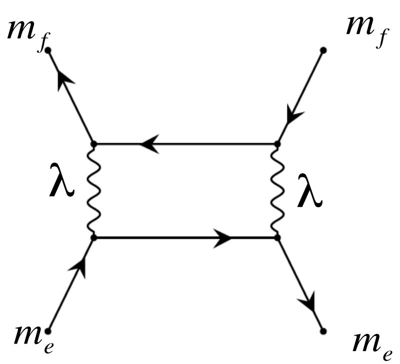
1 loop 3-point	Elapse time DR [sec]	Elapse time HOST [sec]	Speedup
S < 0	0.010830	0.501819	~ 46 times
S > 0	0.103304	11.729756	~114 times

Speedup in quadruple precision

Speed control

$$I = \int_0^1 dx \int_0^{1-x} dy \int_0^{1-x-y} dz \frac{1}{D^2}$$

$$D = -xys - tz(1-x-y-z) + (x+y)\lambda^2 + (1-x-y-z)(1-x-y)m_e{}^2 + z(1-x-y)m_f{}^2$$



$s = -500^2$ GeV²

$m_e = 0.511 \times 10^{-3}$ GeV

$m_f = 150$ GeV

$\lambda = 10^{-30}$ GeV

```
LMEM xx, yy, cnt4;
BMEM x30, gw30;
RMEM res;
CONST tt, lambda, fme, fmf, s, one;
zz = x30*cnt4;
d = -xx*yy*s-tt*zz*(one-xx-yy-zz)+(xx+yy)*lambda**2 +
(one-xx-yy-zz)*(one-xx-yy)*fme**2+zz*(one-xx-yy)*fmf**2;
res += gw30/d**2;
```

1 loop 4-point	Elapse time DR [sec]	Elapse time HOST [sec]	Speedup
S < 0	8.229714	701.962187	~ 85 times

Summary

- Some of important theoretical results have been produced and confirmed by the large scale of calculation.
- Thanks to the evolution of the hardware and software, automatic systems and software tools in HEP have evolved dramatically.
- The development of computer science is essential for HEP, such as parallel computing and extended precision arithmetic.
- These computer-based approach will contribute much in HEP to open new physics.