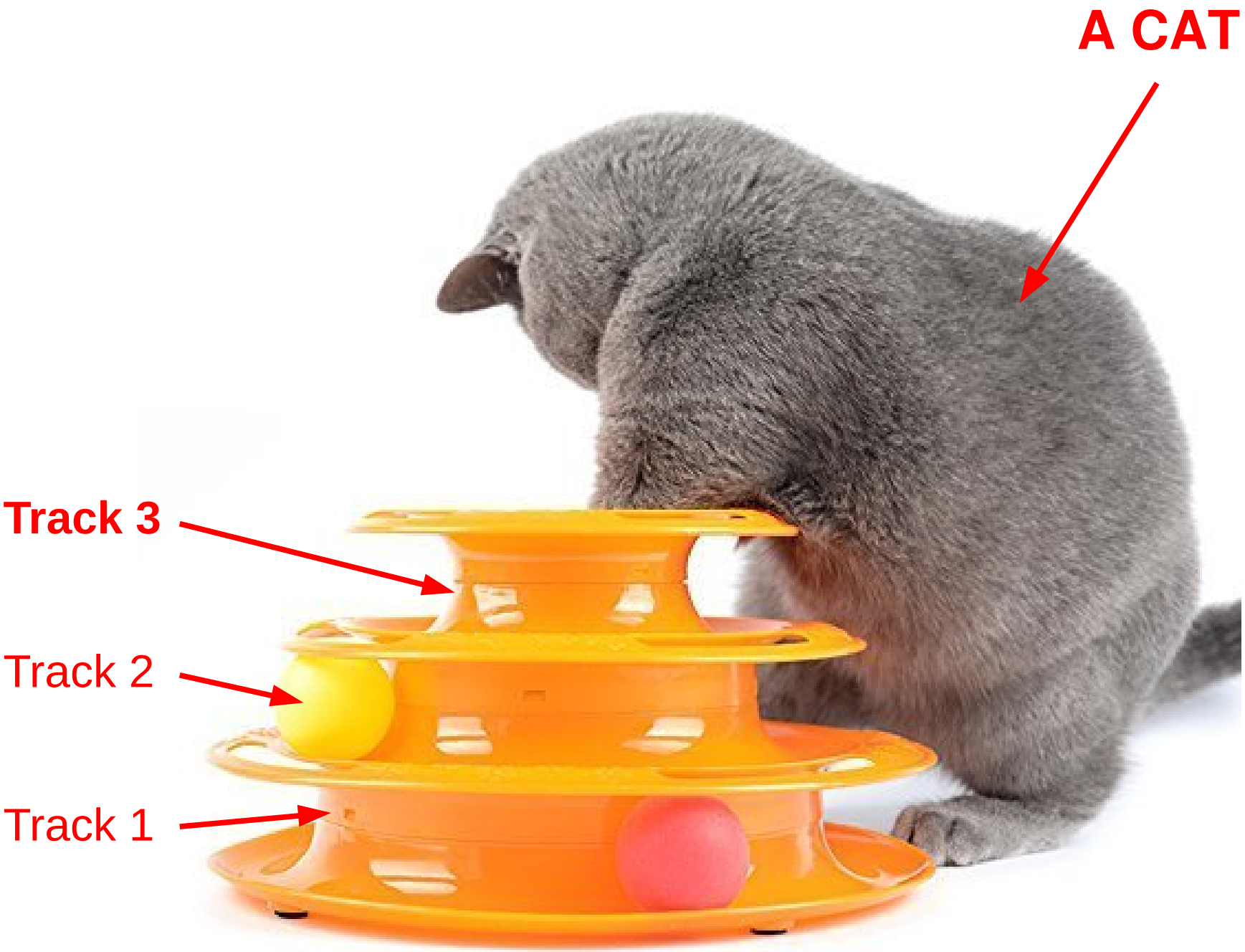

A CAT
Track 3
Track 2
Track 1

Track 3: Computations in Theoretical Physics

- Theorists use computers

Track 3: Computations in Theoretical Physics

- Theorists use computers

- Theorists want to be in the driver's seat...
  (*understand* what the computer is doing)

Track 3: Computations in Theoretical Physics

- Theorists use computers
- Theorists want to be in the driver's seat... (*understand* what the computer is doing)
- ...but they have to go where everybody goes

Track 3: Computations in Theoretical Physics

- Theorists use computers
- Computers help ...
- ... but insightful ideas are equally (more?) important

Computational blow-up

Ben Ruijl

- Every triple gluon vertex creates 6 terms:

$$v_{3g}(p_1^{\mu,a}, p_2^{\nu,b}, p_3^{\rho,c}) = -if^{abc}\Big[(p_1 - p_2)^\rho g_{\mu\nu} + (2p_2 + p_1)^\mu g_{\nu\rho} + (-2p_1 - p_2)^\nu g_{\mu\rho}\Big]$$

- Subgraph finding and Taylor expansions are invariant under momentum contraction, so rewrite the rule:

$$v_{3g}(p_1^{\mu,a}, p_2^{\nu,b}, p_3^{\rho,c}) = -if^{abc}\left[p_1^\sigma t_3{}^{\sigma\nu\rho\mu} - p_2^\sigma t_3{}^{\sigma\mu\rho\nu}\right]$$
$$t_3{}^{\mu\nu\rho\sigma} = g_{\mu\rho}g_{\nu\sigma} + g_{\mu\sigma}g_{\nu\rho} - 2g_{\mu\nu}g_{\rho\sigma}\ .$$

- Only 1024 terms for time-consuming functions

PSLQ example: analytical fit of the constants of a simple Feynman master integral

$$G_3 = -6.9230458517613569125056175807350835179347763807103812119650273403742599066296907522601901707577596677104372311933008837222080560196749827281566346982681496908920375341757759717881801279665946352521256740830557458021906431436568471148502557715229006714242899539741558924048835784950659811389470098639893841125240788540758490814881847786222960311370319940157873557094358420426841440317445474545987282459679309471053376354785143357498033138668937081465899387397891572388565607386770372686471384237168290806493123605415113900973763235506692588548419716731055400191636391775288605422073669899264425382749102234410486193409273325875724048775361124330921976302421 0$$

$$= -\frac{449}{96} - \frac{1}{6}\pi^2 - \frac{1}{2}\zeta(3)$$

Stefano Laporta

Number-theoretic methods MC, QMC

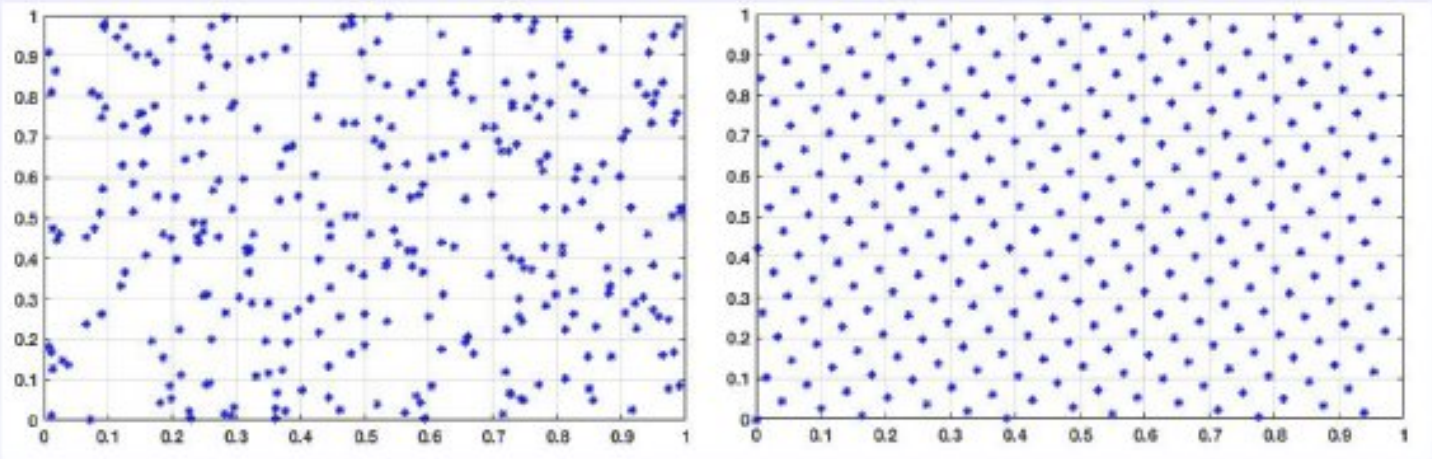
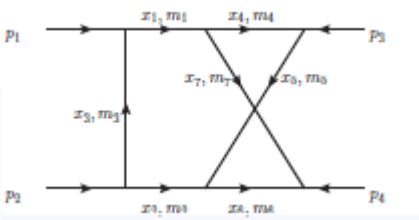


Figure: [MC-QMC] (left) 300 random points; (right) 300 points of 2-dimensional lattice constructed with generator vector z = (1, 129)

Elise de Doncker

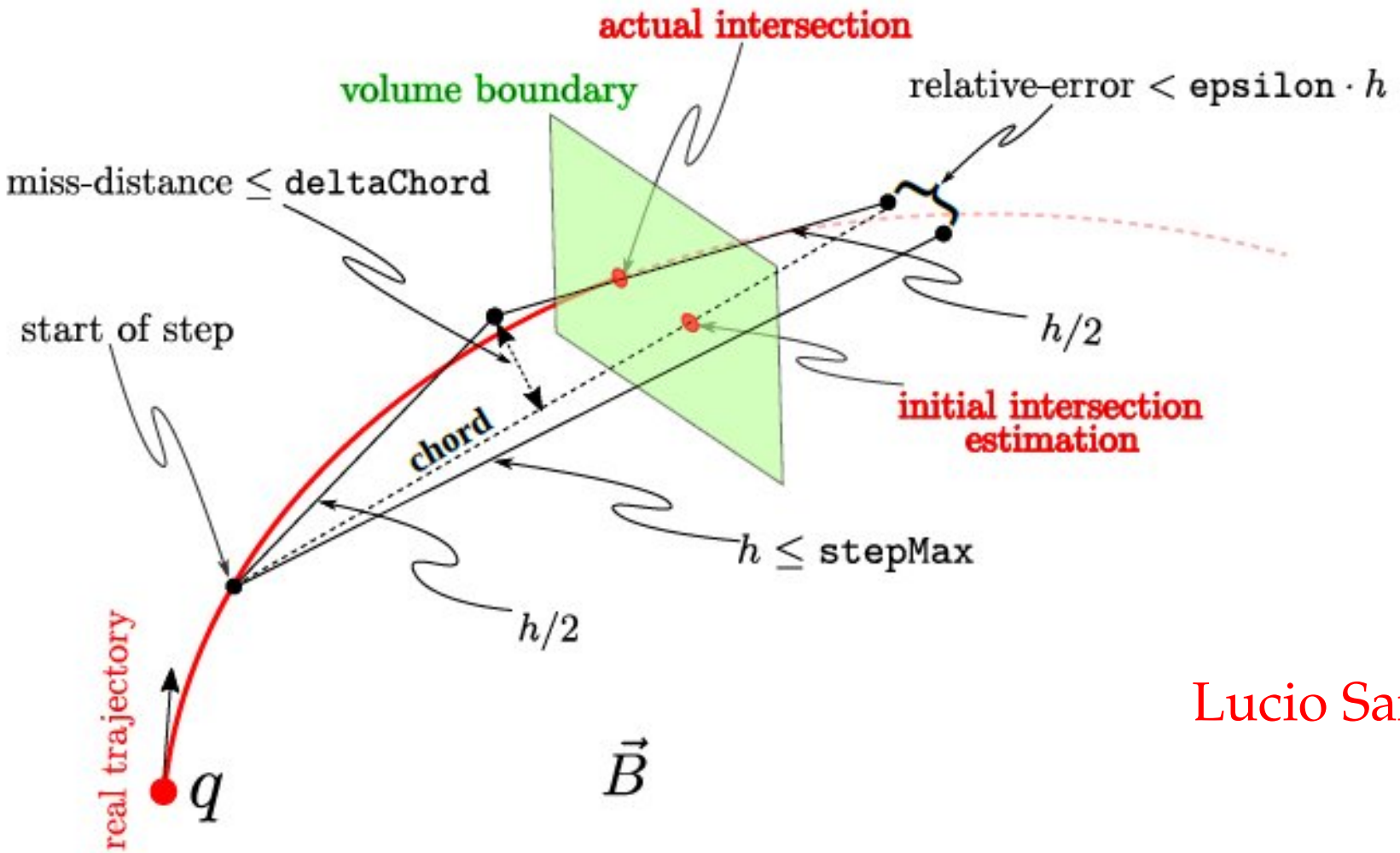


7	200M	0.0853513985005	3.47 e-10	0.591
	350M	0.0853513981538	4.28 e-14	1.115
	Exact:	0.0853513981538		

Table: [2lb] Performance of LR integration with tanh transformation for 2-loop box diagrams on (Kepler-20) GPU, on system with Intel(R) Xeon(R) E5-2670, 2.6 GHz dual

Geant4: particle transport

Transportation of a charged particle q along a step of length h proposed by a physics process:

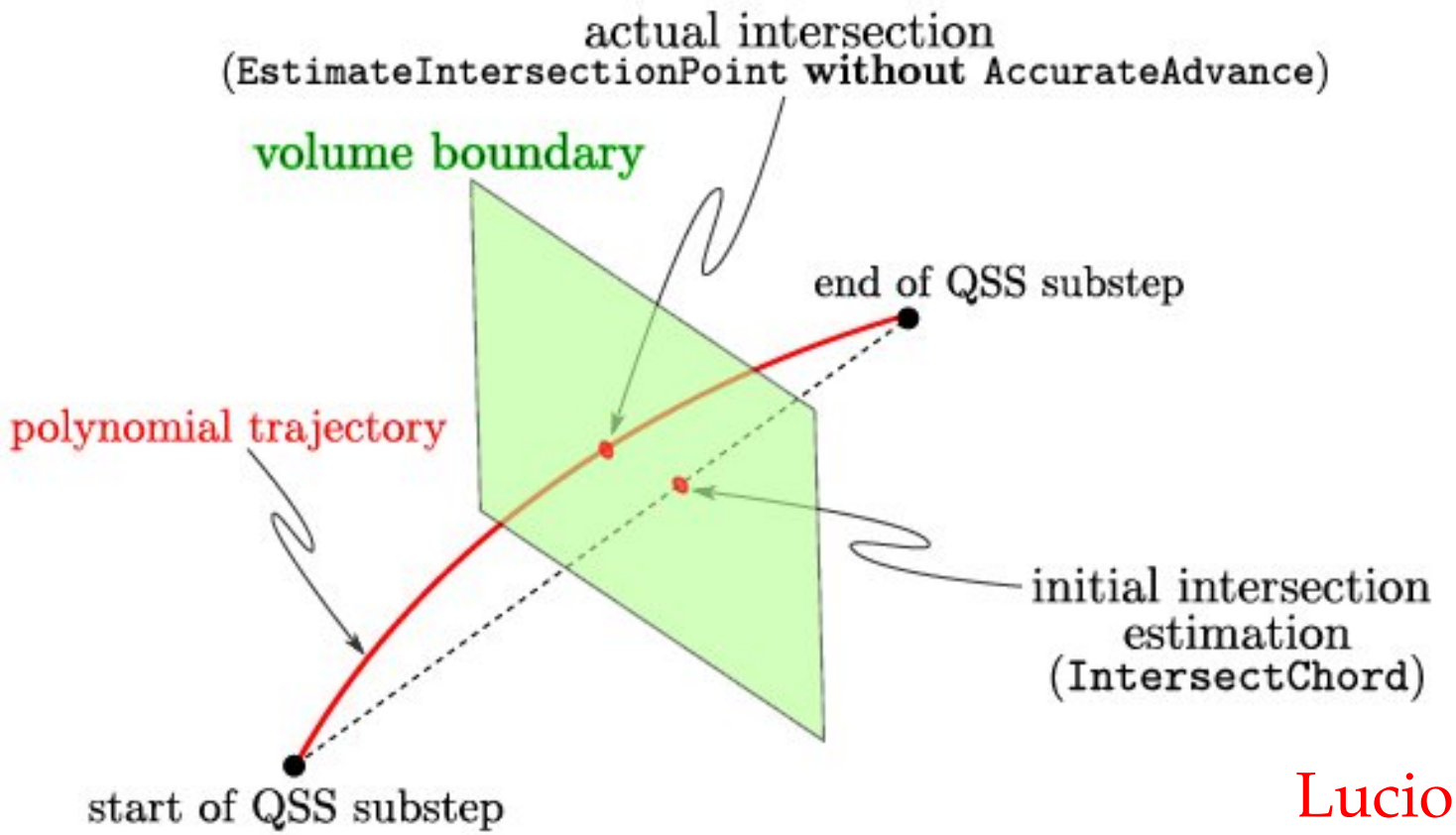


Lucio Santi

⇒ a total of 11 RHS evaluations involved for the 4th order Runge-Kutta.

Detection of boundary crossings

Cheaper particle transport until the crossing point using QSS polynomial dense output instead of iterative procedures:

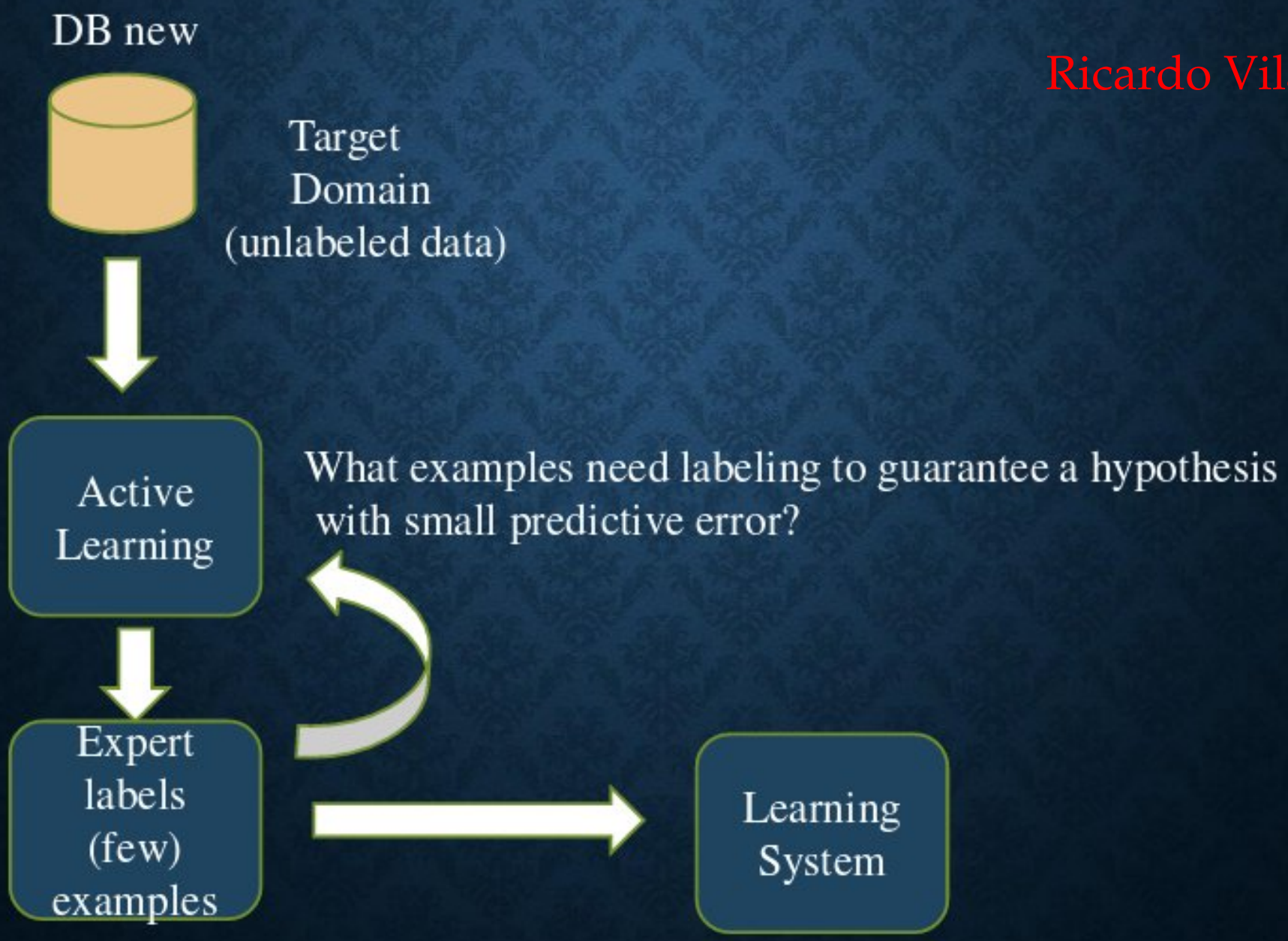


Lucio Santi

- QSS dense output not fully exploited yet for boundary crossing detection ⇒ main goal driving our current work.

ACTIVE LEARNING

Ricardo Vilalta



Track 3: Computations in Theoretical Physics

- Theorists use computers
- Computers help ...
- ... but insightful ideas are equally (more?) important
- Computer tools needs to be convenient

CollierLink

Hiren Patel

Three features -

2. *Automatic code generation, compilation, and relinking*

$$\int \frac{d^d k}{(2\pi)^d} \frac{(k^2 + k.p + k.q + p.q)^2}{(k+p)^2 \left[(k+q)^2 - m^2\right] k^2}$$

```
myIntegral = LoopIntegrate[(k.k + k.p + k.q + p.q)^2, k, {k + p, 0}, {k + q, m}, {k, 0}] /.
  {p.p → m^2, q.q → 0, p.q → 1/2 (m^2 - t)}
```

$$\frac{3}{4}\,\mathrm{PVA}[0,0] + \frac{1}{4}\,\mathrm{PVA}[0,m] + \left(\frac{m^2}{4} + \frac{1}{2}(m^2-t)\right)\mathrm{PVB}[0,0,0,0,m] + \left(-\frac{m^2}{4} + \frac{1}{2}(m^2-t)\right)\mathrm{PVB}[0,0,m^2,0,0] + \frac{1}{4}(m^2-t)\,\mathrm{PVB}[0,1,0,0,m] + \frac{1}{4}(m^2-t)\,\mathrm{PVB}[0,1,m^2,0,0] + \frac{1}{4}(m^2-t)^2\,\mathrm{PVC}[0,0,0,m^2,t,0,0,0,m]$$

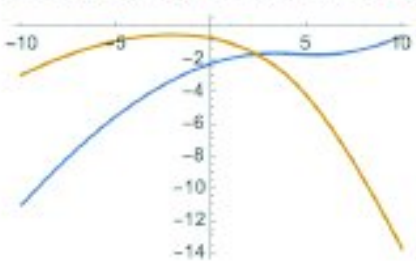
pretend this is many pages long…

```
f = CollierCompile[{t, m}, Evaluate[myIntegral]]
```

```
CollierCompiledFunction[ Variables (2): {t, m}  Denom: 3 (triangle)  Rank: 1 ]
```

Evaluates with machine-code speed!

```
Plot[{Re[f[t, 2.1]], Im[f[t, 2.1]]}, {t, -10, 10}]
```



under the hood…

- **Optimize expression** (Experimental`OptimizeExpression) — makes abbreviations for common subexpressions
- ↓ **Convert expression to pseudocode**
- ↓ **Translate pseudocode to C code**
- ↓ **Compile with available compiler (clang or gcc)** — creates temporary ccf1Lib-xxxx.dylib
- ↓ **Relink**
- ↓ **Prime COLLIER cache system** — evaluate at few random points

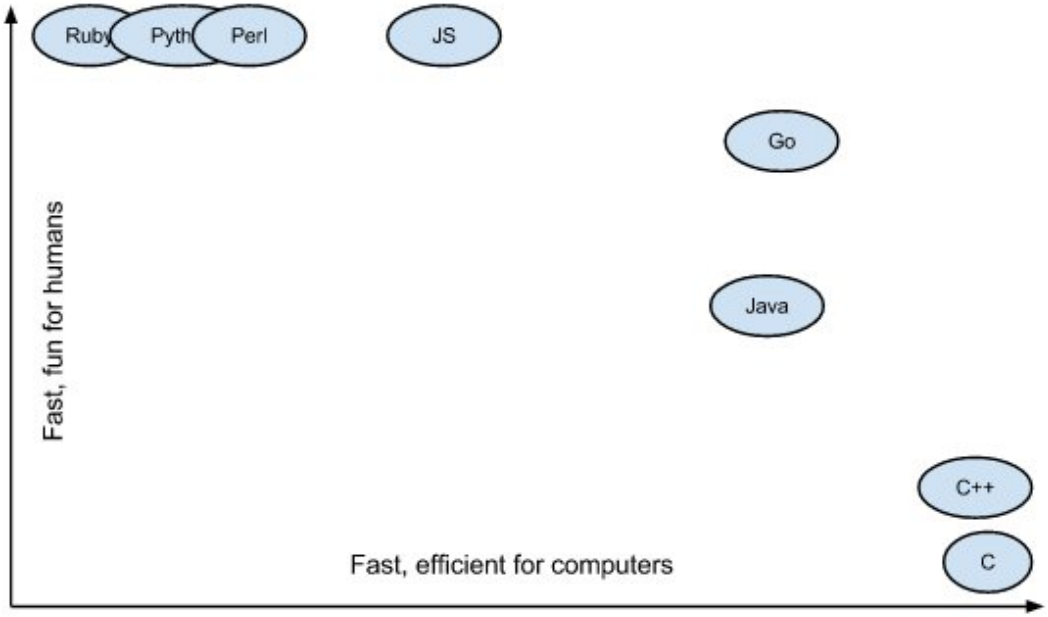
temporary dylib

UMASS AMHERST | ACFI

Sebastien Binet

Conclusions

Go is great at writing small and large (concurrent) programs.
Also true for **science-y** programs, even if the amount of libraries can still be improved.



Write your next tool/analysis/simulation/software in Go?

Track 3: Computations in Theoretical Physics

Round table discussion on computing issues for NNLO+ calcultions

Panelists:
Walter Giele
Stephen Jones
Kiyoshi Kato
Takahiro Ueda

Track 3: Computations in Theoretical Physics

Round table discussion on computing issues for NNLO+ calcultions

Panelists:
Walter Giele
Stephen Jones
Kiyoshi Kato
Takahiro Ueda

Main themes:

- New calculations are numerically more expensive (need to control)
- Results/programs need to be made available (in some form)
- Need standard for interfacing loop calculators

Track 3: Computations in Theoretical Physics

Round table discussion on computing issues for NNLO+ calcultions

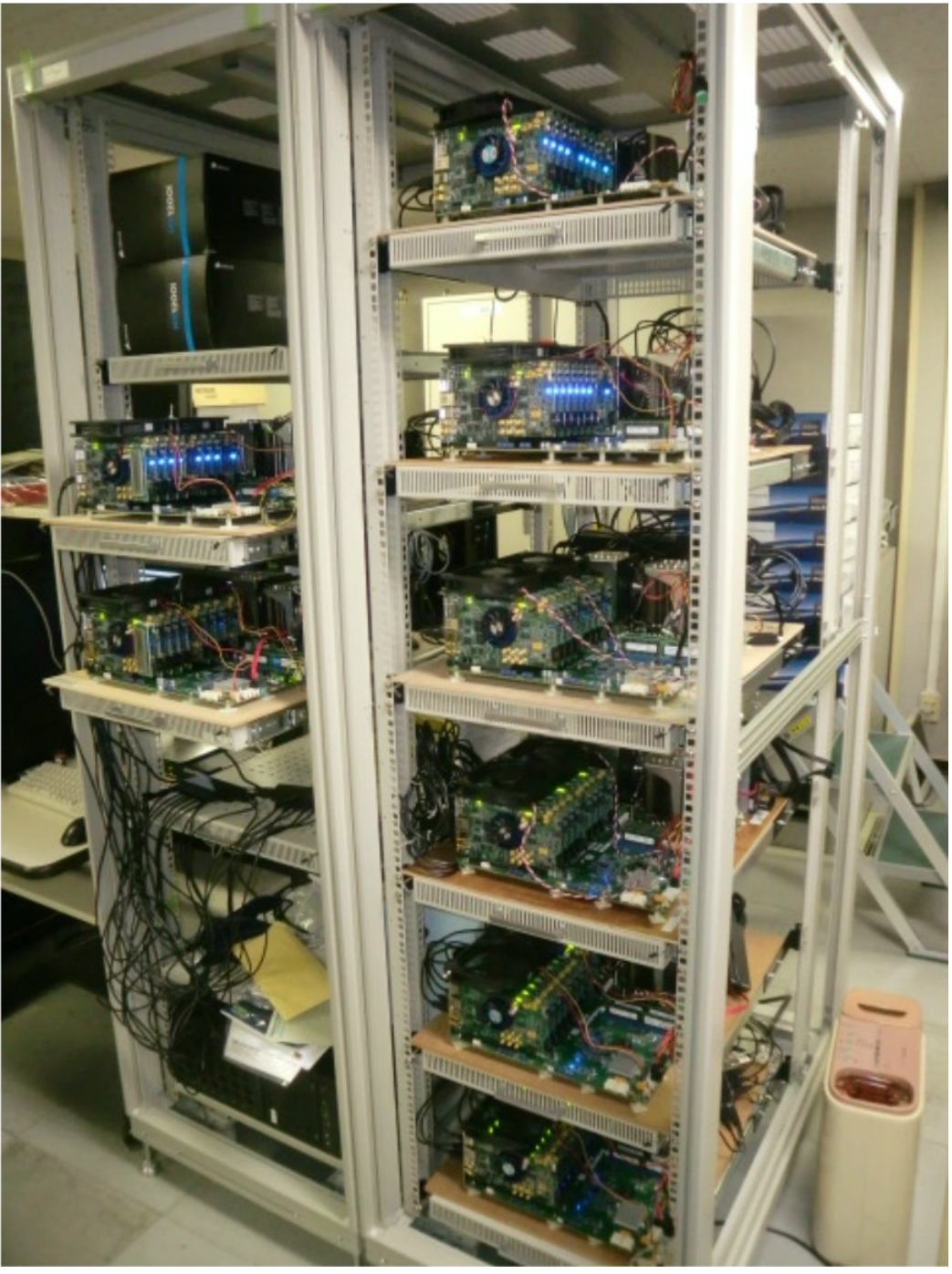
Panelists:
Walter Giele
Stephen Jones
Kiyoshi Kato
Takahiro Ueda

Main themes:

- New calculations are numerically more expensive (need to control)
- Results/programs need to be made available (in some form)
- Need standard for interfacing loop calculators

GRAPE9-MPX cluster system

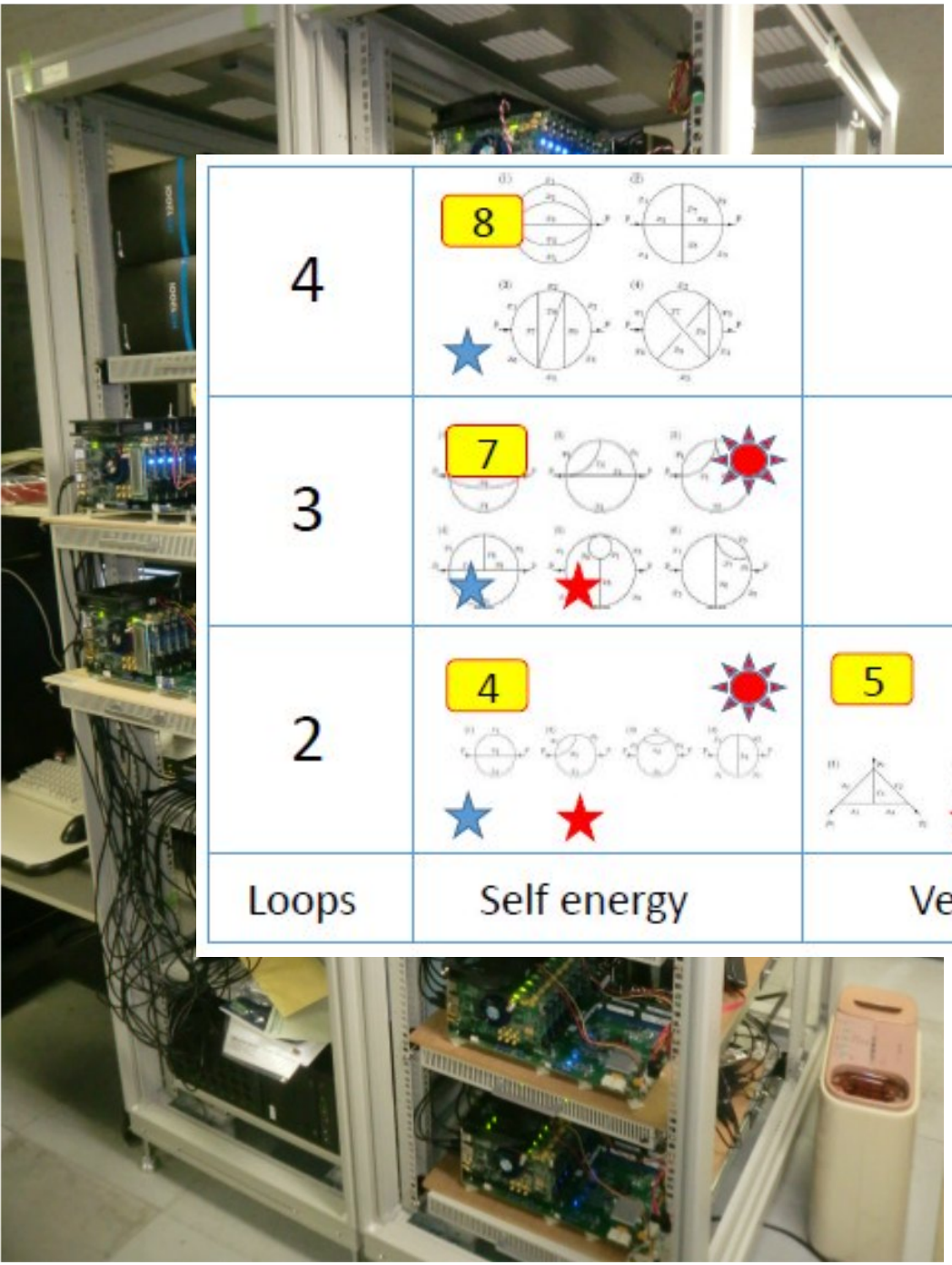
Hiroshi Daisaka



- 64 FPGA boards (Altera ArriaV) on 8 host computers
  - 8 FPGA boards per host
  - connected via PCIe
- Peak performance
  - 422 Gflops for quadruple
  - 185 Gflops for hexuple
  - 96 Gflops for octuple
- specifications of host PC
  - Intel Xeon 2687W v3(6 hosts) 2687w v4 (2hosts)
  - 128GB mem
  - SuperMicro X10DRX
  - GbE for host connection

GRAPE9-MPX cluster system

Hiroshi Daisaka



- 64 FPGA boards (Altera ArriaV) on 8 host computers

Kiyoshi Kato

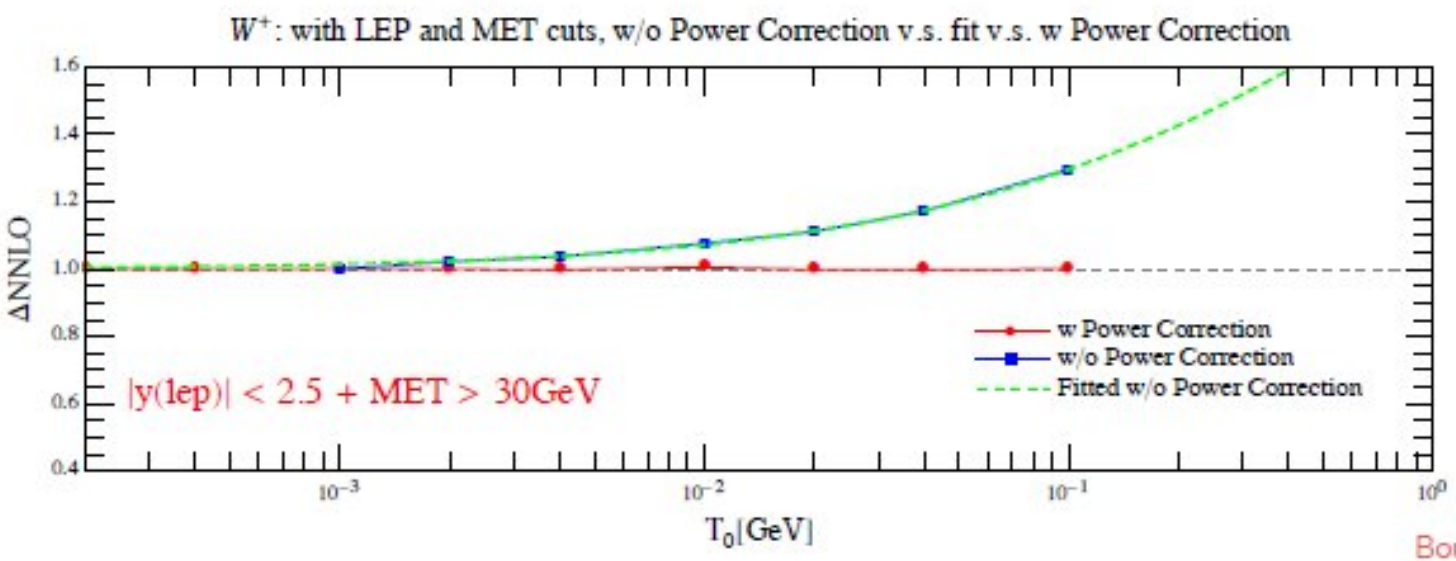
4	8		
3	7		
2	4	5	6
Loops	Self energy	Vertex	Box

- 128GB mem
- SuperMicro X10DRX
- GbE for host connection

Xiaohui Liu

N-jettiness scheme

- Systematic to improve the convergence
  - including power corrections substantially improves the convergence



Bougezhal, XL, Petriello

Track 3: Computations in Theoretical Physics

Round table discussion on computing issues for NNLO+ calcultions

Panelists:
Walter Giele
Stephen Jones
Kiyoshi Kato
Takahiro Ueda

Main themes:

- New calculations are numerically more expensive (need to control)
- Results/programs need to be made available (in some form)
- Need standard for interfacing loop calculators

pySecDec

pySecDec: a program to numerically evaluate dimensionally regulated parameter integrals

Stephen Jones

https://github.com/mppmu/secdec/releases

S. Borowka, G. Heinrich, S. Jahn, SPJ, M. Kerner, J. Schlenk, T. Zirke

Rewrite of SecDec in python & c++ using only open source software

Supports: Contour deformation (evaluate integrals in physical region)

Soper 99; Binoth, Guillet, Heinrich, Pilon, Schubert 05; Nagy, Soper 06; Anastasiou, Beerli, Daleo 07; Beerli 08; Borowka, Carter, Heinrich 12; Borowka 14;

Arbitrary loops/legs (within reason)

General parameter integrals (not restricted to loop integrals)

Thomas Hahn

Multiple Upload (expert)

Loopedia

Ex.: Edge list [(1,2),(2,3),(2,3),(3,4)] or 1 2 2 3 2 3 3 4 — Nickel index e11|e|

Enter your graph by its edge list (adjacency list) or Nickel index

or browse:

Loops = any Legs = any Scales = any

Fulltext must contain: must not contain:

Search Reset

If you wish to add a new integral to the database, start by searching for its graph first.

The Loopedia Team is C. Bogner, S. Borowka, T. Hahn, G. Heinrich, S. Jones, M. Kerner, A. von Manteuffel, M. Michel, E. Panzer, V. Papara.
Software version of 15 Aug 2017 15:05 UTC. In case of technical difficulties with this site please contact Thomas Hahn or Viktor Papara.
This Web site uses the GraphState library [arXiv:1409.8227] for all graph-theoretical operations
and the neato component of Graphviz for drawing graphs.

Loopedia is free and open to everyone. To acknowledge and support the work put into keeping Loopedia up to date, please cite arXiv:loop.edia.

Track 3: Computations in Theoretical Physics

Round table discussion on computing issues for NNLO+ calcultions

Panelists:
Walter Giele
Stephen Jones
Kiyoshi Kato
Takahiro Ueda

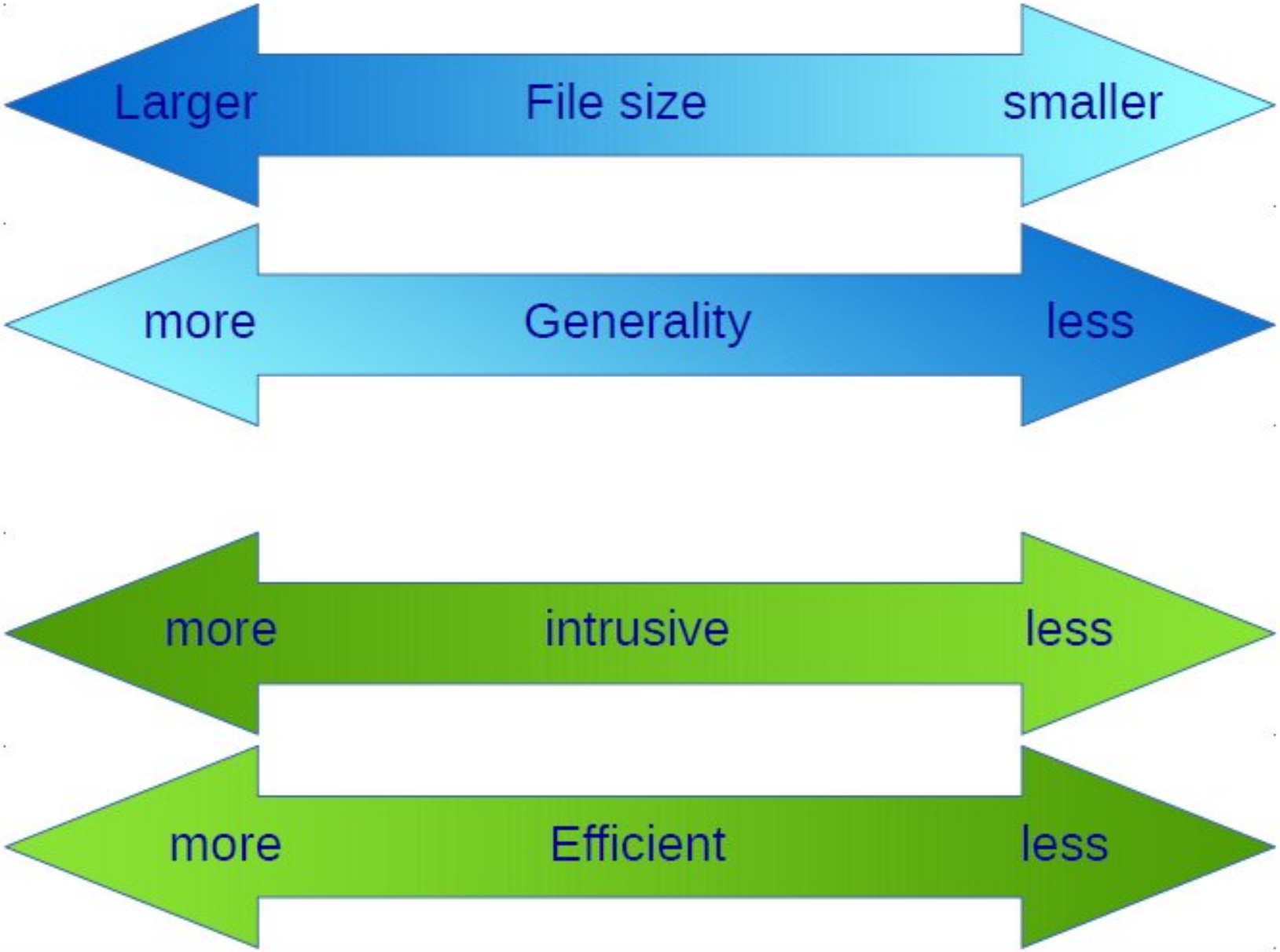
Main themes:

- New calculations are numerically more expensive (need to control)
- Results/programs need to be made available (in some form)
- Need standard for interfacing loop calculators

NNLO nTuple files

- Trade offs

Daniel Maitre

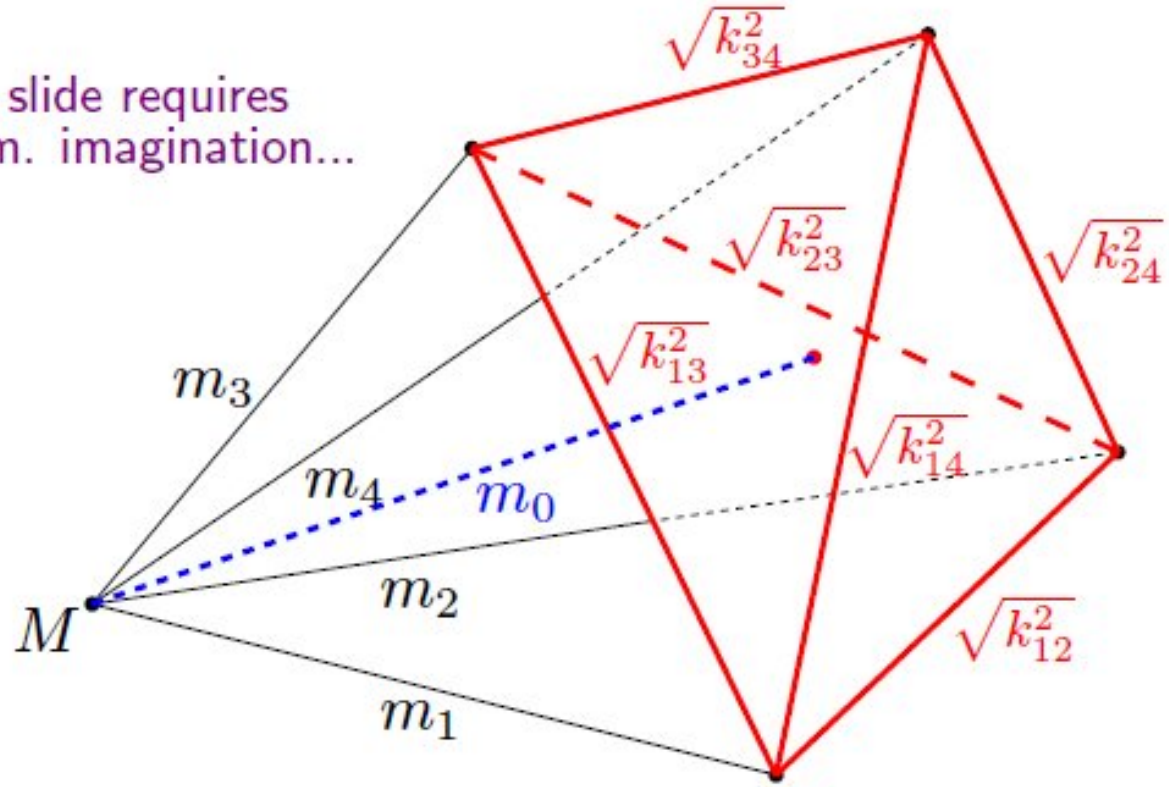


Track 3: Computations in Theoretical Physics

- Computing in more formal physics

Four-point function: the basic simplex for $N = 4$

This slide requires
4-dim. imagination...



Andrei
Davydychev

$$D^{(4)} = \det \|c_{jl}\| \,, \qquad \Lambda^{(4)} = \det \|(k_{j4} \cdot k_{l4})\| \,,$$

$$V^{(4)} = \frac{m_1 m_2 m_3 m_4}{4!} \sqrt{D^{(4)}}, \qquad \overline{V}_0^{(3)} = \frac{1}{3!} \sqrt{\Lambda^{(4)}}, \qquad m_0 = m_1 m_2 m_3 m_4 \sqrt{\frac{D^{(4)}}{\Lambda^{(4)}}}$$

To answer this one should consider the complete family of abelian semigrops, i.e., to take into account the history of their classification:

order	# Of Semigroups	
1	1	
2	4	
3	18	
4	126	[Forsythe '54]
5	1.160	[Motzkin, Selfridge '55]
6	15.973	[Plemmons '66]
7	836.021	[Jurgensen, Wick '76]
8	1.843.120.128	[Satoh, Yama, Tokizawa '94]
9	52.989.400.714.478	[Distler, Kelsey, Mitchell '09]
10	12.418.001.077.381.302.684	[Distler, Jefferson, Kelsey, Kotthoff '16]

and find a way to implement the S-expansion procedure.

[2] John A. Hildebrant, *Handbook of finite semigroup programs*.

Track 3: Computations in Theoretical Physics

Apologies for all the work that could not be properly mentioned in a 20 min. summary!

Track 3 coordinators: F. Yuasa (KEK), S. Jones (MPI Munich), A. Freitas (U. Pitt)