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

- Every triple gluon vertex creates 6 terms:

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

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

\[ v_{3g}(p_1^{\mu,a}, p_2^{\nu,b}, p_3^{\rho,c}) = -i f^{abc} \left[ p_1^{\sigma} t_3^{\sigma \nu \rho \mu} - p_2^{\sigma} t_3^{\sigma \mu \rho \nu} \right] \]

\[ t_3^{\mu \nu \rho \sigma} = g_{\mu \rho} g_{\nu \sigma} + g_{\mu \sigma} g_{\nu \rho} - 2g_{\mu \nu} g_{\rho \sigma} . \]

- Only 1024 terms for time-consuming functions
PSLQ example: analytical fit of the constants of a simple Feynman master integral

\[ G_3 = -6.923045851761356912505617580735083517934776380710381211965 \\
027340374259906629690752260190170757759667710437231193300883 \\
722208056019674982728156634698268149690892037534175775971788 \\
180127966594635252125674083055745802190643143656847114850255 \\
771522900671424289953974155892404883578495065981138947009863 \\
989384112524078854075849081488184778622296031137031994015787 \\
355709435842042684144031744547454598728245967930947105337635 \\
47851433574980331386689370814658993873978915723856560738677 \\
037268647138423716829080649312360541511390097376323550066925 \\
885484197167310554001916363917752886054220736698992644253827 \\
491022344104861934092733258757240487753611243309219763024210 \\

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

Stefano Laporta
Elise de Doncker

Number-theoretic methods MC, QMC

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

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

$\Rightarrow$ 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:

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

DB new

Target Domain (unlabeled data)

Active Learning

What examples need labeling to guarantee a hypothesis with small predictive error?

Expert labels (few) examples

Learning System

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
Three features -

2. Automatic code generation, compilation, and relinking

\[
\int \frac{\phi^k e^{\frac{k^2}{2}}}{(2\pi)^d (k+p)^2 [(k+q)^2 - m^2]} k^2
\]

\[
\text{myIntegral} = \text{LoopIntegrate}[\{k, k \cdot k \cdot k \cdot p + k \cdot q + p \cdot q\}, k, \{k + p, 0\}, \{k + q, m\}, \{k, 0\}] /.
\]

\[
\begin{align*}
&\{p \cdot p \rightarrow m^2, q \cdot q \rightarrow 0, p \cdot q \rightarrow \frac{1}{2} (m^2 - t)\} \\
&\frac{3}{4} PVA[0, 0] + \frac{1}{4} PVA[0, m] + \left(\frac{m^2}{4} + \frac{1}{2} (m^2 - t)\right) PVB[0, 0, 0, 0, 0, m] + \\
&\left(-\frac{m^2}{4} + \frac{1}{2} (m^2 - t)\right) PVB[0, 0, m, 0, 0, 0] + \frac{1}{4} (m^2 - t) PVB[0, 1, 0, 0, 0, m] + \\
&\frac{1}{4} (m^2 - t) PVB[0, 1, m, 0, 0] + \frac{1}{4} (m^2 - t)^2 PVC[0, 0, 0, 0, m, t, 0, 0, 0, m]
\end{align*}
\]

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

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

Evaluates with machine-code speed!

\[
\text{Plot}[\{\text{Re}[f[t, 2.1]], \text{Im}[f[t, 2.1]]\}, \{t, -10, 10\}]
\]
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+ calculations

Panelists:
Walter Giele
Stephen Jones
Kiyoshi Kato
Takahiro Ueda
Track 3: Computations in Theoretical Physics

Round table discussion on computing issues for NNLO+ calculations

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
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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 (2 hosts)
  - 128GB mem
  - SuperMicro X10DRX
  - GbE for host connection
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Hiroshi Daisaka
Kiyoshi Kato

Table:

<table>
<thead>
<tr>
<th>Loops</th>
<th>Self energy</th>
<th>Vertex</th>
<th>Box</th>
</tr>
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<td>4</td>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>7</td>
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<td></td>
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<td>2</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
</tbody>
</table>

Peak performance
- 422 Gflops for quadruple
- 185 Gflops for hexuple
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3(6 hosts)
N-jettiness scheme

- Systematic to improve the convergence

- including power corrections substantially improves the convergence
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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)
Round table discussion on computing issues for NNLO+ calculations

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NNLO nTuple files

- Trade offs
  - Larger File size smaller
  - more Generality less
  - more intrusive less
  - more Efficient less
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- Computing in more formal physics
Four-point function: the basic simplex for $N = 4$

This slide requires 4-dim. imagination...

\[ D^{(4)} = \det \|c_{jl}\|, \quad \Lambda^{(4)} = \det \|(k_{j4} \cdot k_{l4})\|, \]

\[ V^{(4)} = \frac{m_1 m_2 m_3 m_4}{4!} \sqrt{D^{(4)}}, \quad \overline{V}_0^{(3)} = \frac{1}{3!} \sqrt{\Lambda^{(4)}}, \quad m_0 = m_1 m_2 m_3 m_4 \sqrt{\frac{D^{(4)}}{\Lambda^{(4)}}} \]
To answer this one should consider the complete family of abelian semigroups, i.e., to take into account the history of their classification:

<table>
<thead>
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<th>order</th>
<th># Of Semigroups</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>18</td>
</tr>
<tr>
<td>4</td>
<td>126</td>
</tr>
<tr>
<td>5</td>
<td>1,160</td>
</tr>
<tr>
<td>6</td>
<td>15,973</td>
</tr>
<tr>
<td>7</td>
<td>836,021</td>
</tr>
<tr>
<td>8</td>
<td>1,843,120,128</td>
</tr>
<tr>
<td>9</td>
<td>52,989,400,714,478</td>
</tr>
<tr>
<td>10</td>
<td>12,418,001,077,381,302,684</td>
</tr>
</tbody>
</table>

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


Carlos Inostroza
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)