Fernando Febres Cordero
Department of Physics, Florida State University

Snowmass CSS, University of Washington, Seattle, 7/22/2022

Based on the Snowmass White Paper [arXiv:2204.04200]
With Andreas von Manteuffel and Tobias Neumann
References From the Snowmass Process

- **Snowmass reports**
  
  - **Energy Frontier**: Narain, Reina, Tricoli, (& contributors)
  
  - **EF05-07 – QCD Report**: Begel, Höche, Lin, Mukherjee, Nadolsky, Royon, Schmitt, (& contributors)
  
  - **TF04 – Scattering Amplitudes and their Applications**: Bern, Trnka, (& contributors)
  
  - **TF06 – Theory Techniques for Precision Physics**: Boughezal, Ligeti, (& contributors)
  
  - **TF07 – Theory of Collider Phenomena**: Maltoni, Su, Thaler, (& contributors)

- **Snowmass white papers**
  
  - **Computational challenges for multi-loop collider phenomenology**: FFC, von Manteuffel, Neumann [arXiv:2204.04200]
  
  - **The Path forward to N^3LO**: Caola, Chen, Duhr, Liu, Mistlberger, Petriello, Vita, Weinzierl [arXiv:2203.06730]
  
  - See also: Special funcs [arXiv:2203.07088], Coll factorization [arXiv:2207.06507]

And references therein!
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And references therein!

*Apologies in advance for not covering all the impressive related activity!*
Outline

Introduction

State-of-the-art and future needs

A touch on techniques

Our survey & outlook
20-fold increase in data sets at the LHC experiments in the next decades

Reaching few-percent uncertainties in cross sections for processes with 3 (or more) objects in the final state
Snowmass Projections for Higgs Couplings

HL-LHC can achieve $\mathcal{O}(\text{few \%})$ errors for Higgs coupling measurements

Critical input from multi-scale theory predictions, typically in processes involving 3 (or more) FS objects
Hadron Collider Event Simulation

- Factorization
- Hard scattering
- Parton evolution
- Simulation underlying event and hadronization
- Particle decays and radiation

\[ \sigma_{h_1 h_2 \rightarrow H} = \sum_{a,b} \int dxa \, dx_b \, f_{a/h_1}(x_a, \mu_F) \, f_{b/h_2}(x_b, \mu_F) \hat{\sigma}_{ab \rightarrow H + X}(\mu_F, \mu_R) \]

Snowmass contribution: Sterman [arXiv:2207.06507]
**Uncertainties in Perturbative Predictions**

Parametric: determination of model’s parameters

couplings, PDFs, masses

\[ \hat{\sigma}_{ab \rightarrow H} = \alpha_s^\kappa \left( \sigma_{LO} + \alpha_s \sigma_{NLO} + \alpha_s^2 \sigma_{NNLO} + \alpha_s^3 \sigma_{N^3LO} + \cdots \right) \]

From G. Salam
Truncation and Underlying Amplitudes

\[ \sigma_{h_1 h_2 \rightarrow H} = \alpha_s^k \left( \sigma_{\text{LO}} + \alpha_s \sigma_{\text{NLO}} + \alpha_s^2 \sigma_{\text{NNLO}} + \alpha_s^3 \sigma_{\text{N^3LO}} + \cdots \right) \]
NNLO Progress in Time

Slide by L. Cieri, inspired by G. Salam
N^3LO Progress in Time

N^3LO AT THE LHC OVER TIME

Slide inspired by G. Salam / L. Cieri...

Higgs Threshold Exp. [Anastasiou, Duhr, Dulat, Herzog, BM, 15]
Higgs Jet Veto [Banfi, et al. 15]
Higgs VBF [Dreyer, Karlberg, 16]
Higgs Diff. Threshold App. [Dulat, BM, A. Pelloni, 17]
Higgs, [BM, 18]
Higgs Diff. qT [Cieri, Chen, Gehrmann, Glover, Huss, 18]
HH (VBF) [Dreyer, Karlberg, 18]
Higgs (Y approx.) [Dulat, BM, Pelloni, 18]
bb->H [Dulat, Duhr, BM, 19]
ggF->HH [Chen, Li, Shoa, Wang]
Drell-Yan [Dulat, Duhr, BM, 20]
bbH 4FS+5FS [Dulat, Duhr, Hirschi, BM, 20]
CCDY [Dulat, Duhr, BM, 20]
Fully differential Higgs -> 2Photons [Chen, BM, et al. 20]
Fiducial Higgs and DY [Billis, Tackmann, et al., 21]
Fiducial DY [Camarda, Cieri, Ferrera, 21]

Slide by B. Mistlberger

(Better) Theory Uncertainties

- Probabilistic definition of the perturbative theoretical uncertainty, Bonvini [arXiv:2006.16293]
- Bayesian estimates for missing higher orders in perturbative calculations, Duhr, Huss, Mazeliauskas, Szafron [arXiv:2106.04585]
Squeezing the physics from collider data
Outline

- Introduction
- State-of-the-art and future needs
- A touch on techniques
- Our survey & outlook
## Five+ Scales at Two Loops

### Integrals

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<th>Scale</th>
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<td>5pt 0M P</td>
<td>Papadopoulos et al.</td>
<td>[arXiv:1511.09404]</td>
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<td>Gehrmann et al.</td>
<td>[arXiv:1807.09812]</td>
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<td>[arXiv:1910.06275]</td>
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<td>Abreu et al.</td>
<td>[arXiv:2005.04195]</td>
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<td>Canko et al.</td>
<td>[arXiv:2009.13917]</td>
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<td>Chicherin et al.</td>
<td>[arXiv:2009.07803]</td>
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<td>Papadopoulos et al.</td>
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<td>[arXiv:2107.14180]</td>
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<td>Kardos et al.</td>
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### Amplitudes (analytic)

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<td>[arXiv:1904.00945]</td>
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<tr>
<td>5 gluon all-plus</td>
<td>Badger et al.</td>
<td>[arXiv:1905.03733]</td>
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<td>Abreu et al.</td>
<td>[arXiv:2010.15834], Chawdhry et al.</td>
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<td>3-p 2-γ LC</td>
<td>Agarwal et al.</td>
<td>[arXiv:2102.01820], Chawdhry et al.</td>
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<td>[arXiv:2102.13609]</td>
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<td>3-p 2-γ</td>
<td>Agarwal et al.</td>
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<td>4-p 2-l LC</td>
<td>Abreu et al.</td>
<td>[arXiv:2110.07541]</td>
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<td>3-p γ 2-l LC</td>
<td>Badger et al.</td>
<td>[arXiv:2201.04075]</td>
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By now all three-loop four-parton and two-parton two-photon amplitudes have been computed.

- **Integrals**
  - 4-point massless, Henn, Mistlberger, Smirnov, Wasser [arXiv:2002.09492]
  - 4-point 1-mass tennis-court, Canko, Syrrakos [arXiv:2112.14275]

- **Amplitudes**
  - 4-quark, Caola, Chakraborty, Gambuti, von Manteuffel, Tancredi [arXiv:2108.00055]
  - 2-gluon 2-\(\gamma\), Bargiela, Caola, von Manteuffel, Tancredi [arXiv:2111.13595]
  - 4-gluon, Caola, Chakraborty, Gambuti, von Manteuffel, Tancredi [arXiv:2112.11097]
Related Progress at Four+ Loops

- **Four-loop form factors for \(2 \rightarrow 1\) processes**
  - Henn, Smirnov, Smirnov, Steinhauser [arXiv:1604.03126]
  - Lee, von Manteuffel, Schabinger, Smirnov, Smirnov, Steinhauser [arXiv:2202.04660]
  - Chakraborty, Huber, Lee, von Manteuffel, Schabinger, Smirnov, Smirnov, Steinhauser [arXiv:2204.02422]

- **Progress on four-loop splitting functions**
  - Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:1707.08315]
  - Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:2111.15561]
  - (See the recent usage in the “aN^3LO” set from the MSHT PDF set! [arXiv:2207.04739])

- **Five-loop beta functions**
  - Herzog, Ruijl, Ueda, Vermaseren, Vogt [arXiv:1701.01404]
  - Luthe, Maier, Marquard, Schroder [arXiv:1709.07718]
The Future: Immediate Needs

Summary of the Les Houches precision wishlist for hadron colliders.

HTL stands for calculations in heavy top limit, VBF* stands for structure function approximation.

<table>
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<th>process</th>
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Huss, Huston, Josh, Pellen [arXiv:2207.02122]
Outline

Introduction

State-of-the-art and future needs

A touch on techniques

Our survey & outlook
Computing Scattering Amplitudes

\[ \mathcal{A} = \sum_\kappa D_\kappa \rightarrow \sum_i c_i F_i \rightarrow \sum_j C_j \mathcal{I}_j \rightarrow \sum_k r_k h_k \]

Many recent advances make possible recent progress: more optimal techniques for different steps or as shortcuts.
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- Deeper understanding of function spaces \[\text{arXiv:2203.07088}\] allow for analytic expressions and more efficient numerical evaluations
- Numerical approaches based on sector decomp automated in public codes \text{pySecDec} and \text{Fiesta}
- Building finite bases of master integrals have been automated (see e.g. \[\text{arXiv:1701.06583}\])
- Numerically solving diff equations through generalized series expansions \[\text{arXiv:1907.13234}\] has gained momentum, with public implementations appearing (e.g. \text{DiffExp})
- Promising technique for boundary values: the auxiliary mass flow method \[\text{arXiv:2107.01864}\], implemented in the package \text{AMFlow}
Computing Scattering Amplitudes

Feynman diags

\[ A = \sum_{\kappa} D_{\kappa} \rightarrow \sum_{i} c_{i} F_{i} \rightarrow \sum_{j} C_{j} I_{j} \rightarrow \sum_{k} r_{k} h_{k} \]

Projectors

Form factors

Master ints

Special functs

Many recent advances make possible recent progress: more optimal techniques for different steps or as shortcuts

- Usage of method of differential equations for integration spread out, in particular in canonical form [arXiv:1304.1806]

- Deeper understanding of function spaces [arXiv:2203.07088] allow for analytic expressions and more efficient numerical evaluations

- Numerical approaches based on sector decomp automated in public codes pySecDec and Fiesta

- Building finite bases of master integrals have been automated (see e.g. [arXiv:1701.06583])

- Numerically solving diff equations through generalized series expansions [arXiv:1907.13234] has gained momentum, with public implementations appearing (e.g. DiffExp)

- Promising technique for boundary values: the auxiliary mass flow method [arXiv:2107.01864], implemented in the package AMFlow

- Advanced one-loop tools available in programs like Helac-NLO, MG5_aMC@NLO, NLOX, OpenLoops, Recola

- Multi-loop analytic integrands aided by better projector methods [arXiv:1906.03298]


- Major advances in tools for IBP reduction, like for example Fire, Reduze, LiteRed and Kira

- Methods based on numerical evaluations in finite fields and functional reconstruction [arXiv:1406.4513] [arXiv:1608.01902] have become standard

- Many advances in simplifications of complex expressions, e.g. by developing multivariate partial fraction algorithms [arXiv:1904.00945]
Two-Loop Numerical Unitarity

Decompose $\mathcal{A}$ in terms of master integrals:

$$\mathcal{A}^{(L)} = \sum_{\Gamma \in \Delta} \sum_{i \in M_{\Gamma}} c_{\Gamma,i} \mathcal{I}_{\Gamma,i}$$

Drop the integral symbol, introducing the integrand ansatz:

$$\mathcal{A}^{(L)}(\ell_l) = \sum_{\Gamma \in \Delta} \sum_{k \in Q_{\Gamma}} c_{\Gamma,k} \frac{m_{\Gamma,k}(\ell_l)}{\prod_{j \in P_{\Gamma}} \rho_j(\ell_l)}$$

Functions $Q_{\Gamma} = \{ m_{\Gamma,k}(\ell_l) | k \in Q_{\Gamma} \}$ parametrize every possible integrand (up to a given power of loop momenta). E.g.:

- **Tensor Basis**: construct $Q$ from monomials of loop momenta (parameters). Easy to build for general integrands, non-trivial relation to master integrals. Easy to extract function-space dim

- **Master-Surface Basis**: a clever choice of parametrization makes mapping to master integrals straightforward [Ita, arXiv:1510.05626]. Break $Q_{\Gamma} = M_{\Gamma} \cup S_{\Gamma}$, where $S_{\Gamma}$ integrate to zero and $M_{\Gamma}$ correspond to master integrands
Consider the integration by parts (IBP) relation on $\Gamma$

$$0 = \int \prod_i d^D \ell_i \frac{\partial}{\partial \ell_j^\nu} \left[ \frac{u_j^\nu}{\prod_{k \in \Gamma} \rho_k} \right]$$

making it unitarity compatible (controlling the propagator structure) [Gluza, Kadja, Kosower '10; Schabinger '11]

$$u_j^\nu \frac{\partial}{\partial \ell_j^\nu} \rho_k = f_k \rho_k$$

Write ansatz for $u_j^\nu$ expanded in external and loop momenta, and find solution to the polynomial equations using the CAS SINGULAR

Build a full set of surface terms and fill the rest of the space with master integrands

Related [Boehm, Georgoudis, Larsen, Schulze, Zhang '16 - '19] [Agarwal, von Manteuffel '19]
A 1-loop Example for Surface Terms: Part 1

Consider the 1-loop 1-mass triangle with

\[ \rho_1 = (\ell + p_1)^2, \quad \rho_2 = \ell^2, \quad \rho_3 = (\ell - p_2)^2 \]

and we construct \( u^\nu \partial / \partial \ell^\nu \) by parametrizing

\[ u^\nu = u^\text{ext}_1 p_1^\nu + u^\text{ext}_2 p_2^\nu + u^\text{loop}_\ell \]

We then get the syzygy equation (polynomial equation):

\[
\left( u^\text{ext}_1 p_1^\nu + u^\text{ext}_2 p_2^\nu + u^\text{loop}_\ell \right) \frac{\partial}{\partial \ell^\nu} \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} - \begin{pmatrix} f_1 \rho_1 \\ f_2 \rho_2 \\ f_3 \rho_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}
\]

We can then show that we have the solution for the IBP-generating vector:

\[
u^\nu \frac{\partial}{\partial \ell^\nu} = \left[ (\rho_3 - \rho_2) p_1^\nu + (\rho_1 + \rho_2) p_2^\nu + (-s + 2\rho_3 - 2\rho_2) \ell^\nu \right] \frac{\partial}{\partial \ell^\nu}
\]
Now we have the surface term:

$$0 = \int d^D \ell \frac{\partial}{\partial l^\nu} \frac{u^\nu}{\rho_1 \rho_2 \rho_3} = \int d^D \ell \frac{1}{\rho_1 \rho_2 \rho_3} \left[ -(D-4)s - 2(D-3)\rho_2 + 2(D-3)\rho_3 \right]$$

The scalar triangle integrand can be replaced by a surface term, though commonly it is kept, the corresponding “master” integral in OPP reduction.

The IBP relation between the triangle and the $s = (p_1 + p_2)^2$ bubble is:

$$-(D-4)sI_{\text{tri}} - 2(D-3)I_{s\text{-bub}} = 0$$

Similar manipulations can be carried out at two loops. More complicated syzygy equations (polynomial relations) need to be solved (e.g. with SINGULAR)
Unitarity Approach to Computing Integrand Coefficients

[Bern, Dixon, Dunbar, Kosower] [Britto, Cachazo, Feng]

- In on-shell configurations of \( \ell_i \), the integrand factorizes

\[
\sum_{\text{states } i \in T_\Gamma} \prod A_i^{\text{tree}}(\ell_i^\Gamma) = \sum_{\Gamma' \geq \Gamma} \frac{c_{\Gamma',k} m_{\Gamma',k}(\ell_i^\Gamma)}{\prod_{j \in (P_{\Gamma'/P_{\Gamma}})} \rho_j(\ell_i^\Gamma)} \quad (1)
\]

- Need efficient computation of (products of) tree-level amplitudes
  - On-shell recursions, Berends-Giele relations, etc
  - \( D_s \)-dimensional state sum

- Never construct analytic integrand, numerics for every phase-space point!
NUMERICAL STABILITY:

e.g. 4-gluon amplitudes

Function spaces with $O(10/50)$ dimensions

Function spaces with $O(100/1000)$ dimensions

*Relative precision of two-loop 4-gluon amp necessitates calculation*

*High-precision floating point arithmetic a remedy*

[Abreu, FFC, Ita, Jaquier, Page, Zeng, '17]
**Modular Algebra:** [von Manteuffel, Schabinger, 2014]

* Integral reduction can be performed exactly in CAS if kinematical info is **RATIONAL** \((x_i \in \mathbb{Q}^n)\).

* Nevertheless, **RATIONAL** computer algebra reflects the numerical complexity of corresponding **analytic structure** (computational algorithm).

\[
X_i \quad \rightarrow \quad f(X_i) \quad \rightarrow \quad \frac{P}{Q}
\]

"Simple" input \(\rightarrow\) "Complicated" function \(\Rightarrow\) "Heavy" calculation \(\rightarrow\) Even if result is "simple"
**Finite (Number) Fields**: \[\text{von Manteuffel, Schabinger, 2014}\]

* MAP $\mathbb{Q}^m$ into $\mathbb{F}_p^m$ and try to reconstruct result!

* If cardinality $p$ is smaller than CPU's word size ($2^{64}$) operations will be very fast.

\[
\frac{m}{m} = l \mod p
\]

$X_i \rightarrow Y_i = I(X_i) \rightarrow f(Y_i) \rightarrow t \rightarrow \frac{p}{q}$

“Lift” back operation, or rational reconstruction works well if $\frac{p}{q}$ is “simple” enough (or more $\mathbb{F}_p$'s needed!).
INTEGRAL COEFFS AS FUNCTIONS $\neq \varepsilon$:

$$A(l_e) = \sum_{\Gamma, i} C_{\Gamma, i} \frac{m_{\Gamma, i}(l_e)}{\prod_{k \in \Gamma} \rho_k(l_e)} \rightarrow C_{\Gamma, i} \text{ are functions of } x_k \text{ and } D = 4 - 2\varepsilon$$

Indeed, $C_{\Gamma, i}$ appears as rational functions of $\varepsilon$

$$C_{\Gamma, i} = \frac{\sum_j f_j(x_k) \varepsilon^{j+N}}{\sum_j f_j \varepsilon^{j+M}}$$

$\varepsilon$ dependence comes from the structure of $m_{\Gamma, i}(l_e)$ and through linear algebra (”subtraction” procedure)
Thiéle's Interpolation Formula:

Every rational function can be written as a continued fraction.

\[
f(x) = \frac{\sum_{r=0}^{R} n_r x^r}{\sum_{r'=0}^{R'} d_r x^{r'}} = a_0 + \frac{x - y_0}{a_1 + \frac{x - y_1}{a_2 + \frac{x - y_2}{\ldots + \frac{x - y_{N-1}}{a_N}}}}
\]

* Determine \( a_i \) by evaluating \( f(y_i) \) (\( y_i \) random)
* Stop when \( f(y_{i+1}) \) matches interpolated value (+ extra check)
* Through only field operations recover rational function

(FF's result can be lifted to \( \mathbb{Q} \))

See also [Peraro, arXiv:1608.01902] for multi-variate case
Removing Lower-Order Information

\[ A_R^{(1)} = \frac{1}{\varepsilon^2} A_R^{(6)} + O(\varepsilon^0) \]

\[ A_R^{(2)} = \frac{1}{\varepsilon^2} A_R^{(1)} + \frac{1}{\varepsilon} A_R^{(2)} + O(\varepsilon) \]

Define Remainder:

\[ R^{(1)} = A_R^{(1)} - \frac{1}{\varepsilon} A_R^{(6)} + O(\varepsilon) \]

\[ R^{(2)} = A_R^{(2)} - \frac{1}{\varepsilon} A_R^{(1)} - \frac{1}{\varepsilon^2} A_R^{(2)} + O(\varepsilon) \]
By physical constraints:

\[ \gamma^+(s_{ij}) = \frac{\eta^+(s_{ij})}{\prod_{k} \frac{d\phi_k}{d\phi_k(s_{ij})}} \]

\[ \mapsto \text{Polynomial} \]

\[ \text{\rightarrow Special function's argument} \]

\[ \text{\rightarrow Alphabet letter} \]

Determining \( \prod_{k} \frac{d\phi_k}{d\phi_k(s_{ij})} \) can be achieved by

univariate reconstruction in curve \( s_{ij}(\tau) \)

and polynomial division!

Multivariate reconstruction reduced to determination of the polynomials \( \eta^+_{k}(s_{ij}) \)

\[ \rightarrow \text{Simplify by multivariate partial fractions!} \]

\[ \text{RELATED TO} \]

\[ \text{MULTIVARIATE ALGAPDT} \]

\[ \text{[Heller, M. Haubenfeld]} \]
Outline

Introduction

State-of-the-art and future needs

A touch on techniques

Our survey & outlook
As part of our white paper [arXiv:2204.04200] we performed a survey about resources needed to complete recent state-of-the-art calculations for precision collider phenomenology.

We received information about calculations appearing in 53 scientific publications.

Example questions:

- What computational resources did you employ?
- How many PhD/PD years went into this project?
- What kind of grow do you expect for the resources needed in your mid-term projects?
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Some of the Feedback

- **HPC usage** a standard in our community. For the first time **HPC systems** used for CAS!
- Typical project requires 2-5 PhD/PD years to complete, and often rely on a decade (or more) of developments
- Numerical and semi-numerical methods on the forefront, we forecast significant rise. **GPU usage** not spread out
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- Estimate of HPC usage:
Outlook

- Settling the SM status at the (under) 1% level will be one great achievement of the LHC, and we look forward to even more!

- After this Snowmass cycle we might expect as common place matched $2 \rightarrow 3$ NNLO studies, fixed order $2 \rightarrow 2$ N$^3$LO calculations and even N$^4$LO results

- Significant investment is required to deliver the techniques, algorithms and implementations needed to achieve that

- The amplitudes community is very vibrant and continuous advances in our understanding of field theory will keep driving progress in precision collider phenomenology
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