

The ComPWA project

Speeding up amplitude analysis
with a Computer Algebra System

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Ruhr University Bochum

11 May 2023
CHEP2023

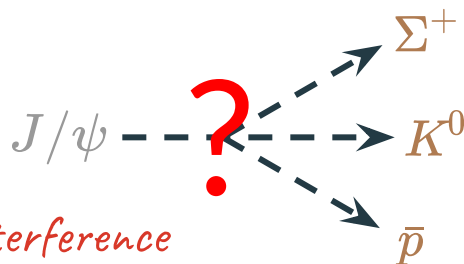
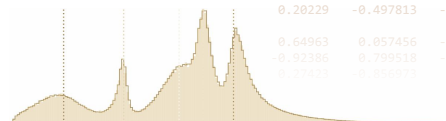
Amplitude analysis software

Aim: study of intermediate hadronic states

Input data

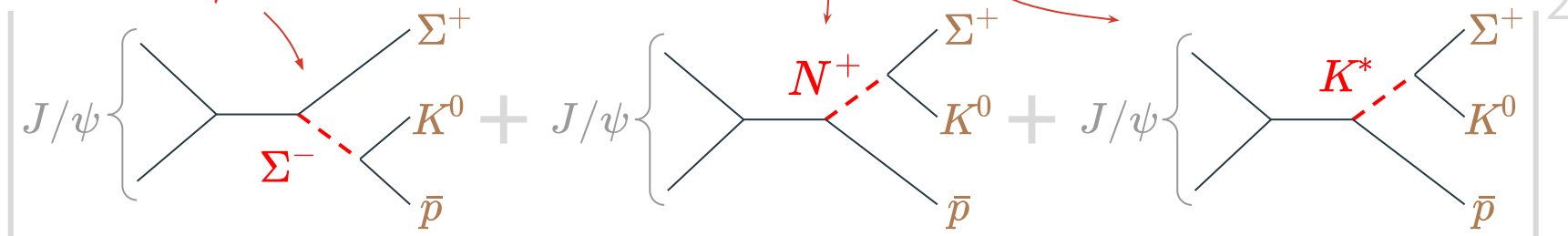
3 four-momenta per collision

E	p_x	p_y	p_z
0.05325	-0.102226	-0.271504	0.29496
1.30563	-0.324557	0.223228	1.37042
-1.35888	0.426783	0.048276	1.43152
-0.23327	0.509333	0.499320	0.75044
-0.68438	-0.801269	0.281889	1.09914
0.91766	0.291936	-0.781209	1.24733
-0.30031	0.284337	-0.255063	0.48589
-1.02024	-0.026281	0.630984	1.20746
1.32055	-0.258056	-0.375920	1.40356
0.55522	0.0865535	0.825067	0.99824
-0.75750	0.411259	0.234126	0.90331
0.20229	-0.497813	-1.059190	1.19534
0.64963	0.057456	-0.008806	0.65223
-0.92386	0.799518	-0.581799	1.35995
0.27423	-0.856973	-0.590605	1.08473



Interference
between amplitudes

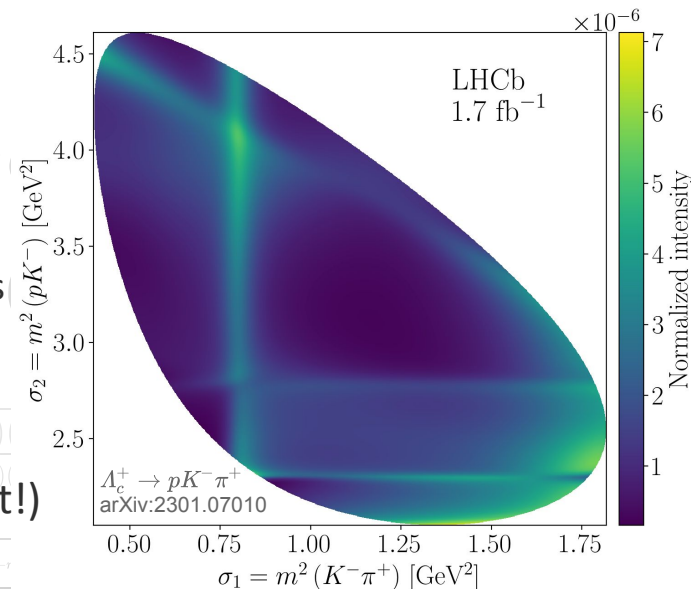
Find models that correctly
describe the observed
intensity distributions



Amplitude analysis software

What makes it so difficult?

- Unbinned, multidimensional problem set
- Complicated parametrizations and estimators
 - need to quickly try out different parameterizations
 - fits can take several weeks
- Theory is hard to get into
- Relatively small community (but growing interest!)

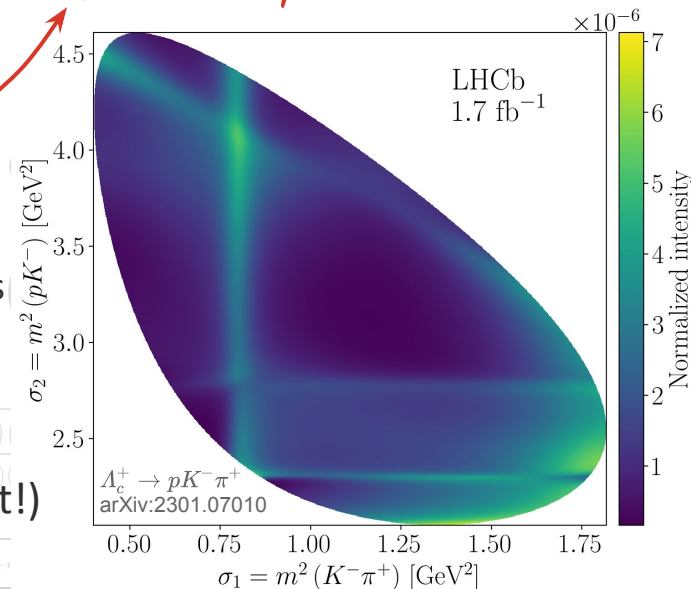


Amplitude analysis software

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fast computations



flexibility

documentation

Amplitude analysis software

Has led to a large number of analysis packages and scripts

PWA frameworks

GPUPWA

TFPWA

Laura++



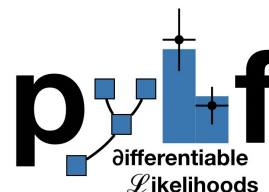
Pawian



TensorFlowAnalysis



AMPGEN



Scripts using fitter packages

Amplitude analysis software

Has led to a large number of analysis packages and scripts

Trend: many frameworks try to become more modular

- Designed as a library
- Python/Julia bindings
- Flexibility through scripts instead of config files

→ Results in a more **flexible workflow** that can easily integrate new theories

PWA frameworks

Scripts using fitter packages



AMPGEN

Coofit
CUDA/OpenMP
Fitting Framework
for C++ & Python

pylf
differentiable
Likelihoods

zfit

HYDRA
Multithreaded Data
Analysis Framework

RooFit

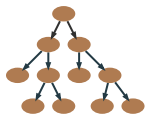
Laura++

GPUPWA

TFPWA

PYPWA

TensorFlowAnalysis



Differentiable programming

Additional trend: several specialised packages
from the ML and data science communities

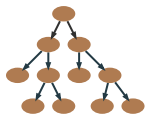


*e.g. gradient
descent algorithm*



Not just Machine Learning!

Can be used for any fast numerical computations



Differentiable programming

Some of the techniques these back-ends offer:

- Vectorization
- Just-in-time compilation
- XLA (Accelerated Linear Algebra)
- Automatic differentiation
- Support for multithreading, GPUs, ...

```
@tf.function(jit_compile=True)
def my_expression(x, y, z):
    return x + y * z
```

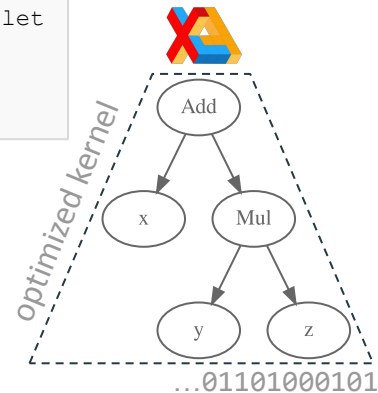
*Converted to
device-agnostic XLA code*

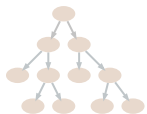


```
{ lambda ; a:i32[] b:i32[] c:i32[] . let
  d:i32[] = mul b c
  e:i32[] = add a d
in (e,) }
```

```
for (i = 0; i < rows; i++): {
  for (j = 0; j < columns; j++): {
    c[i][j] = a[i][j]*b[i][j];
  }
}
```

*Heavy lifting by
optimized backend*





Differentiable programming

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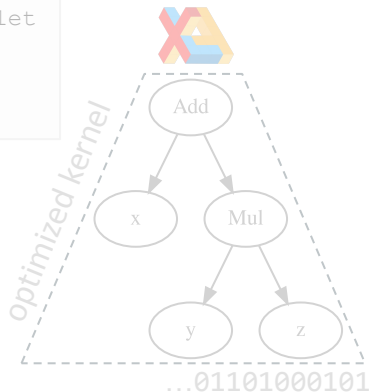
*Converted to
device-agnostic XLA code*

*Usually all that the
user needs to do*

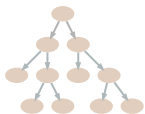
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  }
}
```

*Heavy lifting by
optimized backend*



How to bring code closer to theory?



High performance through **computational back-ends** from ML and data science



$$ax^2 + by^2$$

Flexibility through a **Computer Algebra System**



Academic continuity through **living documentation**



Symbolic amplitude models

A new technique: formulate your amplitude model with a Computer Algebra System

- Transparency: inspect the math as you formulate the model
- Flexibility: modify the model with analytic substitutions
- Code generation: symbolic model as template to computational back-ends (SSoT)
- Improve computational performance with algebraic simplifications

```
import sympy as sp
N, s, m0, w0 = sp.symbols("N s m0 Gamma0")
N / (m0**2 - sp.I * m0 * w0 - s)
```



$$\frac{N}{m_0^2 - im_0\Gamma_0 - s}$$

Quite common already for theoreticians:
quickly inspect and visualize some lineshape
with Maple, Mathematica, Matlab, etc...



Symbolic amplitude models

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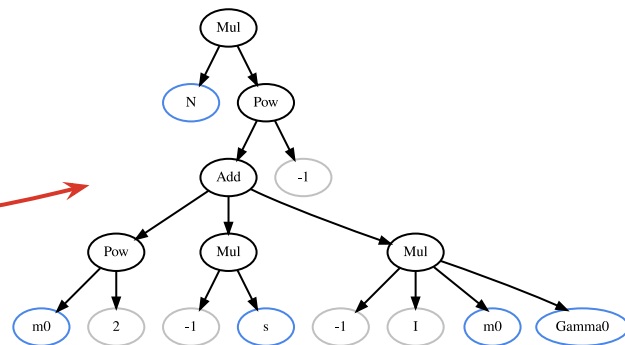
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```



$$\frac{N}{m_0^2 - im_0\Gamma_0 - s}$$

*CAS represents
expression as a tree*

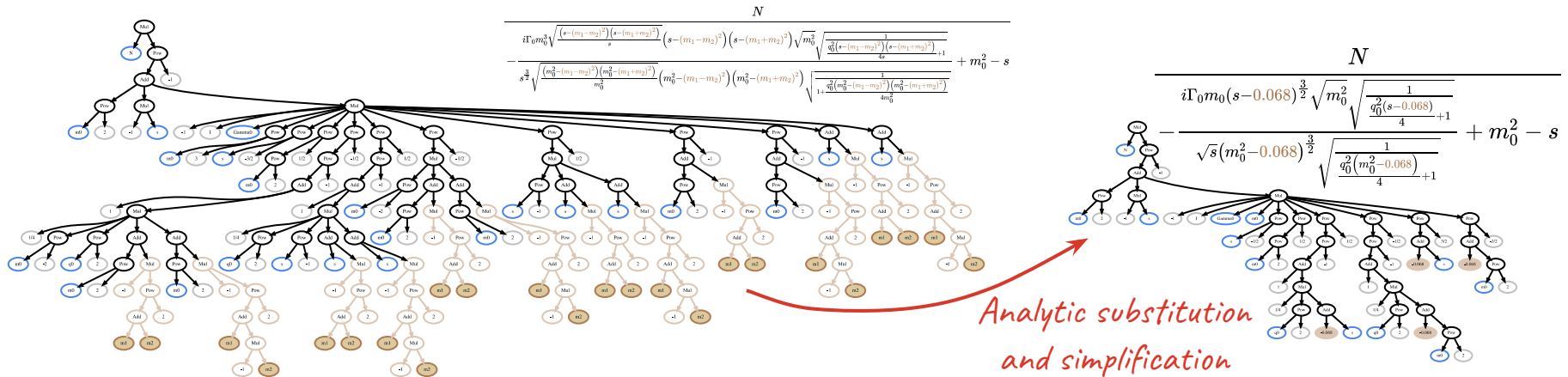




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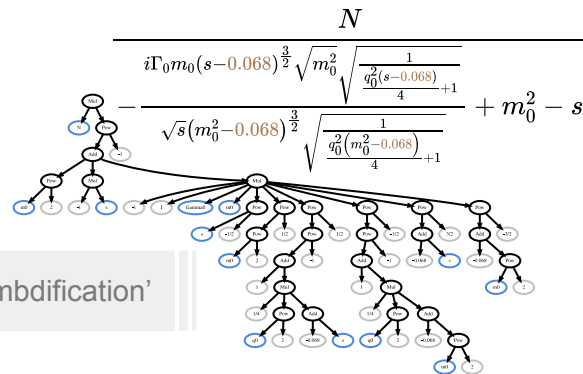
```
function out1 = my_expr(Gamma0, N, m0, s)
```

```
    out1 = N./(-1i*Gamma0.*m0.^3.*sqrt((s - 0.25).*(s -  
0.01)./s).*(1 + (m0.^2 - 0.25).*(m0.^2 - 0.01)./(4*m0.^2)).*(s  
- 0.25).*(s - 0.01).*sqrt(m0.^2)./(s.^(3/2).*sqrt((m0.^2 -  
0.25).*(m0.^2 - 0.01)./m0.^2).*(1 + (s - 0.25).*(s -  
0.01)./(4*s))).*(m0.^2 - 0.25).*(m0.^2 - 0.01)) + m0.^2 - s);
```

```
end
```



SymPy 'lambdification'





Symbolic amplitude models

A new technique: formulate your amplitude model with a Computer Algebra System

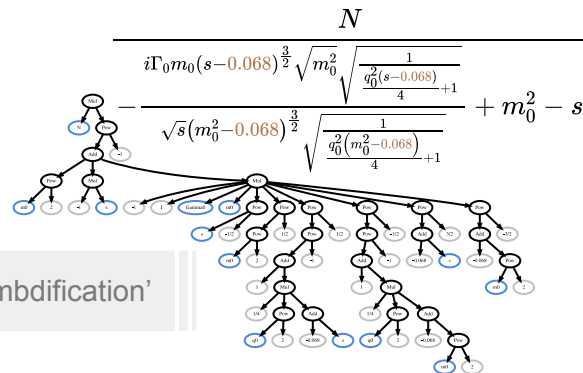
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```
REAL*8 function my_expr(Gamma0, N, m0, s)
implicit none
REAL*8, intent(in) :: Gamma0
REAL*8, intent(in) :: N
REAL*8, intent(in) :: m0
REAL*8, intent(in) :: s
```

```
my_expr = N/(-cmplx(0,1)*Gamma0*m0**3*sqrt((s - 0.25d0)*(s - 0.01d0)/s)* & (1 +
(1.0d0/4.0d0)*(m0**2 - 0.25d0)*(m0**2 - 0.01d0)/m0**2)*(s - & 0.25d0)*(s -
0.01d0)*sqrt(m0**2)/(s**(3.0d0/2.0d0)*sqrt((m0**2 - & 0.25d0)*(m0**2 -
0.01d0)/m0**2)*(1 + (1.0d0/4.0d0)*(s - 0.25d0)*( & s - 0.01d0)/s)*(m0**2 -
0.25d0)*(m0**2 - 0.01d0)) + m0**2 - s)
end function
```



SymPy 'lambdification'





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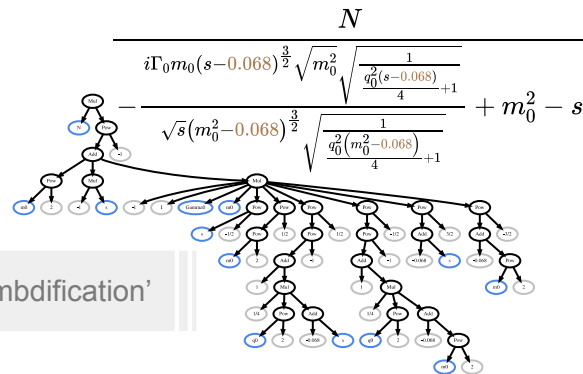
```
// my_expr.h
#ifndef PROJECT_MY_EXPR_H
#define PROJECT_MY_EXPR_H
double my_expr(double Gamma0, double N, double m0, double s);
#endif

// my_expr.c
#include "my_expr.h"
#include <math.h>

double my_expr(double Gamma0, double N, double m0, double s) {
    double my_expr_result;
    return N/(-I*Gamma0*pow(m0, 3)*sqrt((s - 0.25)*(s - 0.01)/s)*(1 + (1.0/4.0)*(pow(m0, 2) -
    0.25)*(pow(m0, 2) - 0.01)/pow(m0, 2))*(s - 0.25)*(s - 0.01)*sqrt(pow(m0, 2))/ (pow(s,
    3.0/2.0)*sqrt((pow(m0, 2) - 0.25)*(pow(m0, 2) - 0.01)/pow(m0, 2)))*(1 + (1.0/4.0)*(s -
    0.25)*(s - 0.01)/s)*(pow(m0, 2) - 0.25)*(pow(m0, 2) - 0.01)) + pow(m0, 2) - s);
}
```



SymPy 'lambdification'





Symbolic amplitude models

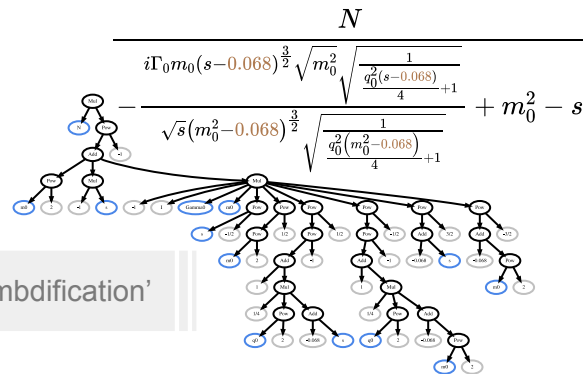
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```
@jax.jit
def _lambdifysymgenerated(Gamma0, N, m0, s):
    return N / (
        -1j
        * Gamma0
        * m0
        * ((1 / 4) * m0**2 + 0.9831)
        * (s - 0.0676) ** (3 / 2)
        * sqrt(m0**2)
        / (sqrt(s) * (m0**2 - 0.0676) ** (3 / 2) * ((1 / 4) * s + 0.9831))
        + m0**2
        - s
    )
```



SymPy 'lambdification'





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```
@jax.jit
```

```
def lambdaify(generatedGamma0, N, m0, s):
```

Physics separated from

the 'number crunching'

```
-1j
```

```
* Gamma0
```

```
m0
```

```
* (1 / 4) * m0**2 + 0.9831)
```

```
* (s - 0.0676) ** (3 / 2)
```

```
* sqrt(m0**2)
```

```
/ (sqrt(s) * (m0**2 - 0.0676) ** (3 / 2) + (s - 0.0676) ** (3 / 2))
```

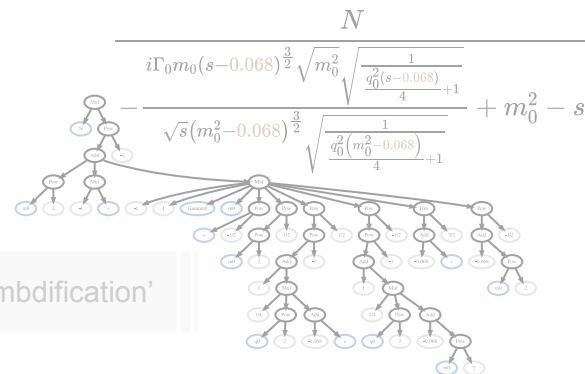
```
+ m0**2
```

```
- s
```

```
)
```



*Works just as well for models
with tens of thousands of nodes*

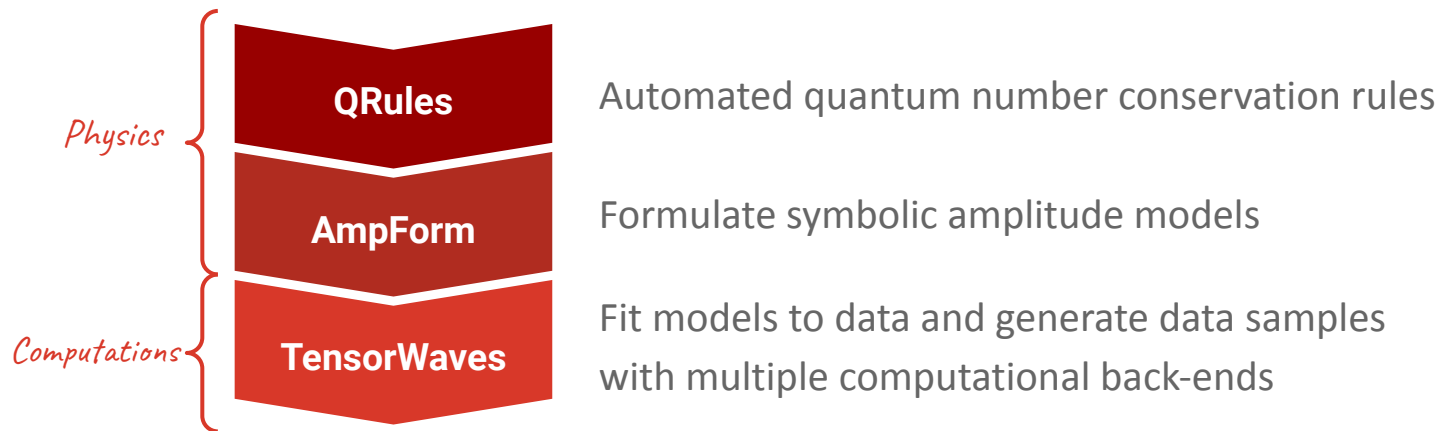


SymPy 'lambdification'

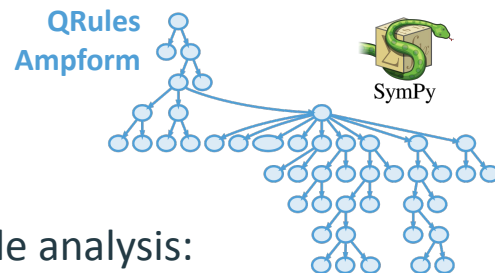
The ComPWA project

Common Partial Wave Analysis

Three main Python packages that together cover a full amplitude analysis:

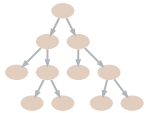


All are designed as **libraries**, so they can be used by other packages by installing through pip or Conda



*Demo in
backup slides*

How to bring code closer to theory?



High performance through **computational back-ends** from ML and data science



Flexibility through a **Computer Algebra System**



Academic continuity through **living documentation**



Living documentation

```
@implement_doit_method
class EnergyDependentWidth(UnevaluatedExpression):
    r"""Mass-dependent width, coupled to the pole position of the resonance.
```

```
See :pdg-review:`2020; Resonances; p.6` and
:cite:`asnerDalitzPlotAnalysis2006`, equation (6). Default value for
:code:`phsp_factor` is :meth:`PhaseSpaceFactor`.
```

```
Note that the `BlattWeisskopfSquared` of AmpForm is normalized in the
sense that equal powers of :math:`z` appear in the nominator and the
denominator, while the definition in the PDG (as well as some other
sources), always have :math:`1` in the nominator of the Blatt-Weisskopf.
In that case, one needs an additional factor :math:`\left(q/q_0\right)^{2L}`
in the definition for :math:`\Gamma_{\text{BlattWeisskopf}}(s)`.
```

Codebase

```
def evaluate(self) -> sp.Expr:
    s, mass0, gamma0, m_a, m_b, angular_momentum, meson_radius = self.args
    q_squared = BreakupMomentumSquared(s, m_a, m_b)
    q0_squared = BreakupMomentumSquared(mass0**2, m_a, m_b)
    form_factor_sq = BlattWeisskopfSquared(
        angular_momentum,
        z=q_squared * meson_radius**2,
    )
    form_factor0_sq = BlattWeisskopfSquared(
        angular_momentum,
        z=q0_squared * meson_radius**2,
    )
    rho = self.phsp_factor(s, m_a, m_b)
    rho0 = self.phsp_factor(mass0**2, m_a, m_b)
    return gamma0 * (form_factor_sq / form_factor0_sq) * (rho / rho0)

def _latex(self, printer: LatexPrinter, *args) -> str:
    s, _, width, *_ = self.args
    s = printer._print(s)
    subscript = _indices_to_subscript(_determine_indices(width))
    name = Rf"\Gamma_{subscript}" if self._name is None else self._name
    return Rf"{name}\left({s}\right)"
```

Search the docs ...



Contents

Launch interactive examples

^ Pole parametrization

After all these matrix definitions, the final challenge is to choose a correct parametrization for the elements of \mathbf{K} and \mathbf{P} that accurately describes the resonances we observe.^[3] There are several choices, but a common one is the following summation over the poles R :^[4]

$$K_{ij} = \sum_R \frac{g_{R,i} g_{R,j}}{m_R^2 - s} + c_{ij}$$

$$\hat{K}_{ij} = \sum_R \frac{g_{R,i}(s) g_{R,j}(s)}{(m_R^2 - s) \sqrt{\rho_i \rho_j}} + \hat{c}_{ij}$$

Jupyter notebooks

- Dynamic code allows for interactivity
- Can be rendered as web pages
- Serves as integration test

with $\gamma_{R,i}$ some *real* constants and $\Gamma_{R,i}^0$ the **partial width** of each pole. In the Lorentz-invariant form, the fixed width Γ^0 is replaced by an “energy dependent” **CoupledWidth** $\Gamma(s)$.^[5] The **width** for each pole can be computed as $\Gamma_R^0 = \sum_i \Gamma_{R,i}^0$.

The production vector \mathbf{P} is commonly parameterized

Physics

Partial wave expansion
Transition operator
Ensuring unitarity
Lorentz-invariance
Production processes
Pole parametrization
Implementation
Interactive visualization



Living documentation

```
@implement_doit_method
class EnergyDependentWidth(UnevaluatedExpression):
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    See :pdg-review:`2020; Resonances; p.6` and
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    sources), always have :math:`1` in the nominator of the Blatt-Weisskopf.
    In that case, one needs an additional factor :math:`\left(q/q_0\right)^{2L}`
    in the definition for :math:`\Gamma_{\text{BW}}(m)`.
    """

    def evaluate(self) -> sp.Expr:
        s, mass0, gamma0, m_a, m_b, angular_momentum, meson_radius = self.args
        q_squared = BreakupMomentumSquared(s, m_a, m_b)
        q0_squared = BreakupMomentumSquared(mass0**2, m_a, m_b)
        form_factor_sq = BlattWeisskopfSquared(
            angular_momentum,
            z=q_squared * meson_radius**2,
        )
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            angular_momentum,
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        rho = self.phsp_factor(s, m_a, m_b)
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        return gamma0 * (form_factor_sq / form_factor0_sq) * (rho / rho0)

    def _latex(self, printer: LatexPrinter, *args) -> str:
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        s = printer._print(s)
        subscript = _indices_to_subscript(_determine_indices(width))
        name = Rf"\Gamma{subscript}" if self._name is None else self._name
        return Rf"{name}\left({s}\right)"
```

Codebase

File Edit View Run Kernel Tabs Settings Help

k-matrix.ipynb

Python 3 (ipykernel)

Now again let's compare the compare this with a sum of two
{func}.relativistic_breit_wigner s, now with the two additional β -constants.

```
[31]: beta1, beta2 = sp.symbols("beta1 beta2")
      bw_with_phases = beta1 * bw1 + beta2 * bw2
      display(
        bw_with_phases,
        remove_residue_constants(f_vector),
      )
```

$$\frac{\Gamma_1 \beta_1 m_1}{-i \Gamma_1 m_1 + m_1^2 - s} + \frac{\Gamma_2 \beta_2 m_2}{-i \Gamma_2 m_2 + m_2^2 - s}$$
$$\frac{\Gamma_1 c_1 m_1 e^{i\phi_1}}{(-m^2 + m_1^2) \left(-i \left(\frac{\Gamma_1 m_1}{-m^2 + m_1^2} + \frac{\Gamma_2 m_2}{-m^2 + m_2^2} \right) + 1 \right)} + \frac{\Gamma_2 c_2 m_2 e^{i\phi_2}}{(-m^2 + m_2^2) \left(-i \left(\frac{\Gamma_1 m_1}{-m^2 + m_1^2} + \frac{\Gamma_2 m_2}{-m^2 + m_2^2} \right) + 1 \right)}$$

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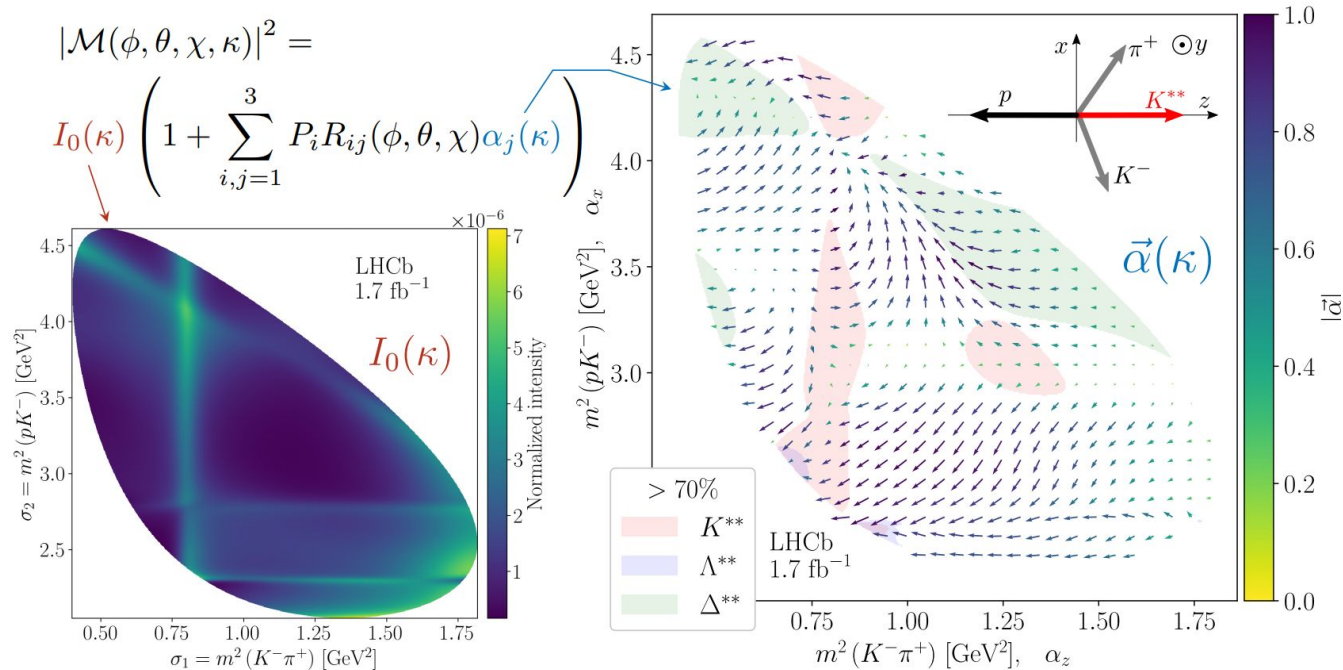
Im A (Breit-Wigner)

s-plane plot ☒ imag ☐ real ☐ abs



Living documentation

ComPWA recently enabled vector field computations for polarization studies



The self-documenting workflow allowed to publish the **full analysis as a website of notebooks**

Ongoing work and future ideas

- Main focus: Implement and test more symbolic spin formalisms and dynamics
Dalitz-plot decomposition, K-matrix, spin density, tensor formalism...
- Improve integration into other HEP python packages
e.g. standardise workflows, interfacing to zfit and scikit-hep package, ... → [PyHEP.dev](https://pyhep.dev)
- Benchmark comparisons between amplitude analysis frameworks?
Comparing workflows is hard and time-consuming, see e.g. [this meeting](#)

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e.g. standardise workflows, interfacing to zfit and scikit-hep package, ... → [PyHEP.dev](https://pyhep.dev)
- Benchmark comparisons between amplitude analysis frameworks?
Comparing workflows is hard and time-consuming, see e.g. [this meeting](#)

Thank you for your attention!



Back-up

The main ComPWA packages

`pip install grules`

`pip install ampform`

`pip install tensorwaves`





QRules

Quantum number conservation rules

Core: 'search engine' for quantum numbers

Get particle properties:*

```
PDG = qrules.load_pdg()
PDG.find("a(2) (1320) 0")
```

```
Particle(
  name='a(2) (1320) 0',
  pid=115,
  latex='a_{2} (1320)^{0}',
  spin=2.0,
  mass=1.3182,
  width=0.107,
  isospin=Spin(1, 0),
  parity=+1,
  c_parity=+1,
  g_parity=-1,
)
```

Find particles by quantum number:

```
selection = PDG.filter(
  lambda p: p.mass > 2.8
  and p.spin > 0
  and p.charge
  and p.charmness
  and p.parity == +1
)
selection.names
```

```
['Lambda(c) (2880)+', 'Xi(c) (2815)~-']
```

Check which conservation rules are violated:

```
qrules.check_reaction_violations (
  initial_state="pi0",
  final_state=["gamma", "gamma", "gamma"],
)
```

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```
{frozenset({'c_parity_conservation'})}
```

*Also a library of
conservation rules*

* PDG info computed from the
scikit-hep [particle](https://scikit-hep.org) package

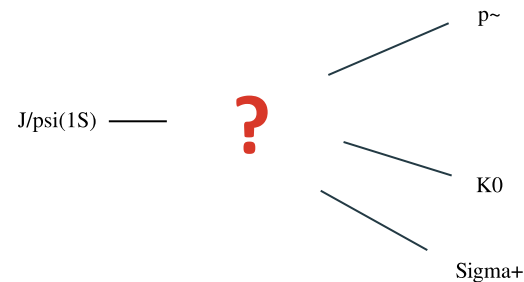


QRules

Quantum number conservation rules

PWA use case: compute which particle reactions are allowed between a given initial and final state

1. User specifies some boundary conditions
(particle names, allowed interactions, isobar model, etc.)



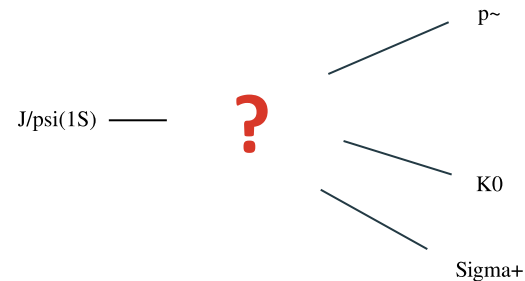


QRules

Quantum number conservation rules

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1. User specifies some boundary conditions
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2. QRules then:
 - determines all possible decay topologies,



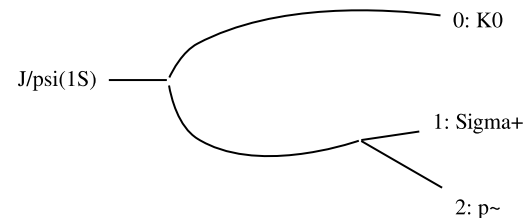
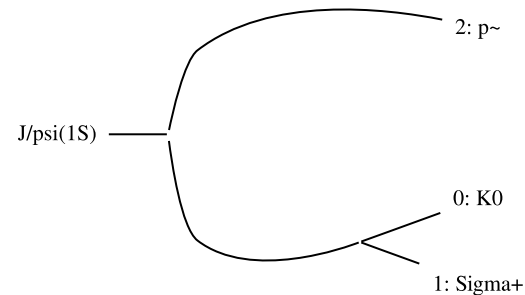
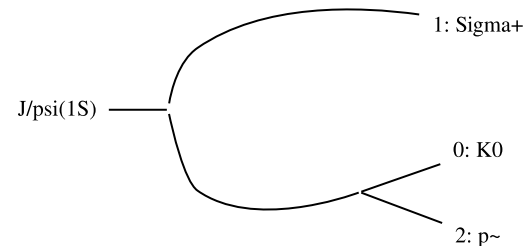


QRules

Quantum number conservation rules

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1. User specifies some boundary conditions
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 - determines all possible decay topologies,
 - gets corresponding particle properties from the PDG
(or any custom definitions),



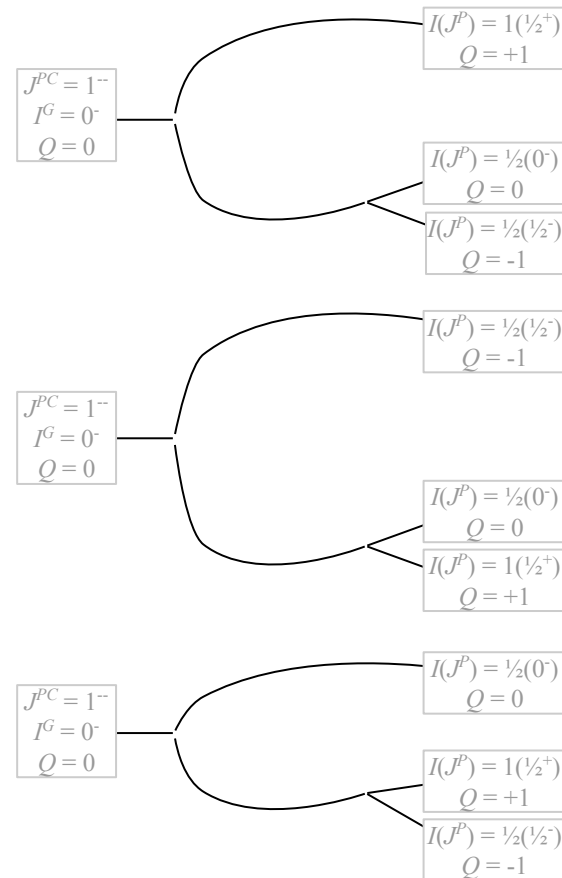


QRules

Quantum number conservation rules

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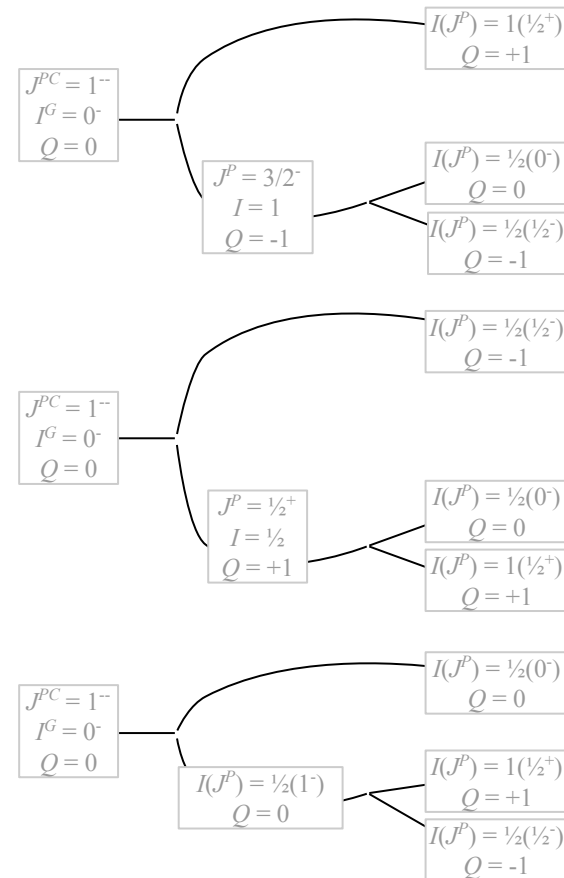


QRules

Quantum number conservation rules

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 - gets corresponding particle properties from the PDG (or any custom definitions),
 - propagates quantum numbers through intermediate edges,
 - and selects all allowed transitions with its conservation laws



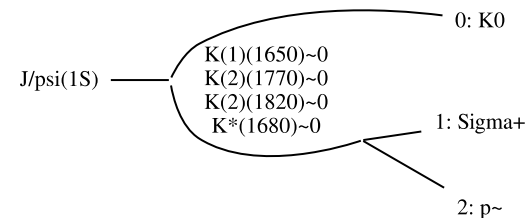
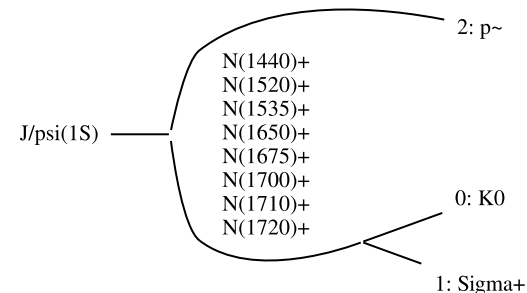
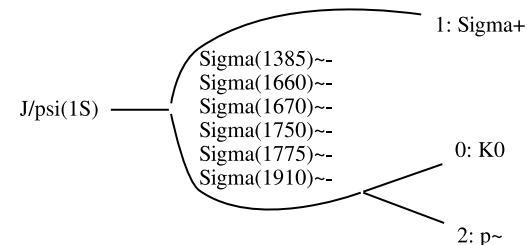


QRules

Quantum number conservation rules

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QRules

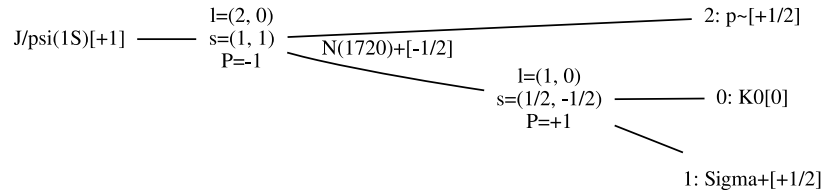
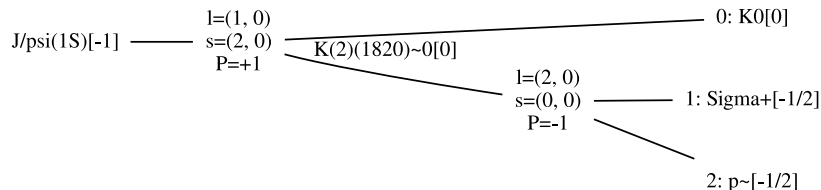
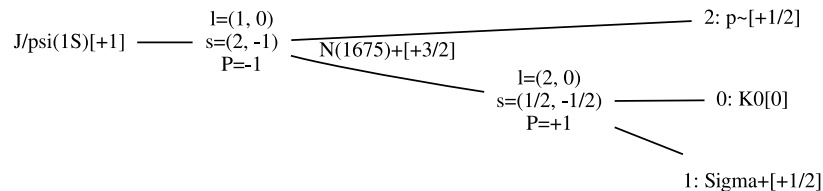
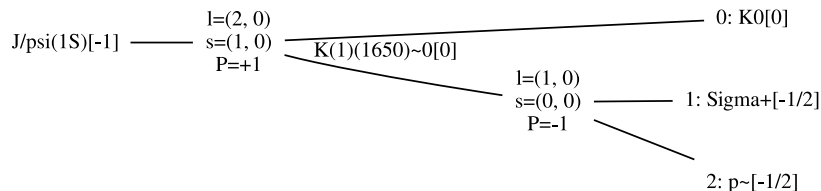
Quantum number conservation rules

The returned object contains **all information to formulate an amplitude model!**

```
reaction = qrules.generate_transitions(  
    initial_state="J/psi(1S)",  
    final_state=["K0", "Sigma+", "p~"],  
    allowed_interaction_types=["strong"],  
)
```

Selects conservation rules

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AmpForm

Symbolic amplitude model formulation

- Library of **spin formalisms** and **dynamics**
- Formulate QRules' state transitions as an amplitude model
- Formulated as **algebraic expressions** (SymPy)
- Serves as **template to a computational back-end** for fitting and generating data distributions

```
n = sp.Symbol("n_R")
matrix = RelativisticKMatrix .formulate (
    n_channels=1,
    n_poles=n,
)
matrix[0, 0]
```

$$\frac{\rho(s) \sum_{R=1}^{n_R} \frac{\Gamma(s) \gamma_{R,0}^2 m_R}{-s + m_R^2}}{-i \rho(s) \sum_{R=1}^{n_R} \frac{\Gamma(s) \gamma_{R,0}^2 m_R}{-s + m_R^2} + 1}$$

```
matrix = NonRelativisticKMatrix .formulate (
    n_channels=2,
    n_poles=1,
) .doit ()
matrix[0, 0].simplify ()
```

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$$-\frac{\Gamma_{1,0} \gamma_{1,0}^2 m_1}{s + i \Gamma_{1,0} \gamma_{1,0}^2 m_1 + i \Gamma_{1,1} \gamma_{1,1}^2 m_1 - m_1^2}$$



AmpForm

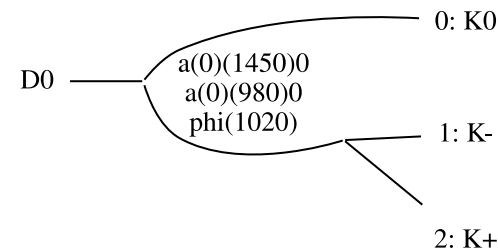
Symbolic amplitude model formulation

Example: amplitude model for $D^0 \rightarrow K^0 K^- K^+$ with 3 resonances

```
builder = ampform.get_builder(reaction)
resonances = reaction.get_intermediate_particles()
for p in resonances:
    builder.set_dynamics(p.name, create_relativistic_breit_wigner_with_ff)
builder.set_dynamics("a(0)(980)0", create_analytic_breit_wigner)
model = builder.formulate()
```



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$$\left| A_{D_0^0 \rightarrow K_0^0 \phi(1020)_0; \phi(1020)_0 \rightarrow K_0^+ K_0^-} + A_{D_0^0 \rightarrow K_0^0 a_0(1450)_0^0; a_0(1450)_0^0 \rightarrow K_0^+ K_0^-} + A_{D_0^0 \rightarrow K_0^0 a_0(980)_0^0; a_0(980)_0^0 \rightarrow K_0^+ K_0^-} \right|^2$$



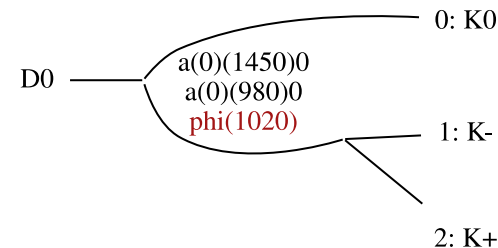
AmpForm

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```

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$$\left| A_{D^0 \rightarrow K^0_0 \phi(1020)_0; \phi(1020)_0 \rightarrow K^+_0 K^-_0} + A_{D^0 \rightarrow K^0_0 a_0(1450)_0; a_0(1450)_0 \rightarrow K^+_0 K^-_0} + A_{D^0 \rightarrow K^0_0 a_0(980)_0; a_0(980)_0 \rightarrow K^+_0 K^-_0} \right|^2$$

Each amplitude can be further inspected:

```
model.components[R"A_{D^{0}_{\{0\}} \to K^{+}_{\{0\}} \phi(1020)_{\{0\}}; \phi(1020)_{\{0\}} \to K^{+}_{\{+ \}_{\{0\}} K^{-}_{\{- \}_{\{0\}}}}"]
```

$$\frac{C_{D^0 \rightarrow K^0_0 \phi(1020)_0; \phi(1020)_0 \rightarrow K^+_0 K^-_0} \Gamma_{\phi(1020)} m_{\phi(1020)} \sqrt{B_1^2 \left(d_{\phi(1020)}^2 q_{122}^2(m_{12}^2) \right)} D_{0,0}^0(-\phi_0, \theta_0, 0) D_{0,0}^1(-\phi_1^{12}, \theta_1^{12}, 0)}{-m_{12}^2 + m_{\phi(1020)}^2 - im_{\phi(1020)} \Gamma_{1020}(m_{12}^2)}$$



TensorWaves

Fit and generate data with computational back-ends

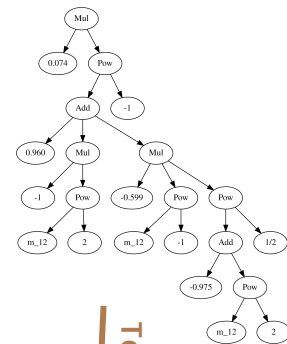
TensorWaves responsibilities:

- Express mathematical expressions in a computational back-end
- Generate (deterministic) amplitude-based Monte Carlo samples
- Perform unbinned fits with different back-ends
(TensorFlow, NumPy, JAX, ...)
- Also integrates different optimizers (Minuit2, SciPy, ...)

Any symbolic input

```
function = create_parametrized_function(expression, parameter_defaults, backend="jax")
estimator = UnbinnedNLL(function, data, phsp, backend="jax")
optimizer = Minuit2(callback=CSVSummary("fit_traceback.csv"))
fit_result = optimizer.optimize(estimator, initial_parameters)
```

 Open in Colab



TensorWaves



NumPy





TensorWaves

Fit and generate data with computational back-ends

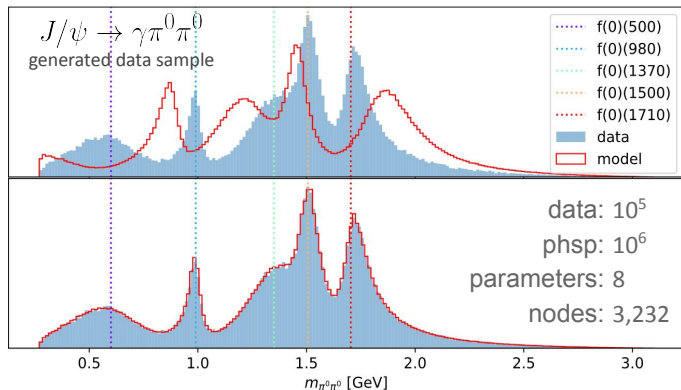
Does it work? JAX+Minuit2 example benchmark:

Intel Core i7-8750H CPU @ 2.20GHz 12 cores **56s**

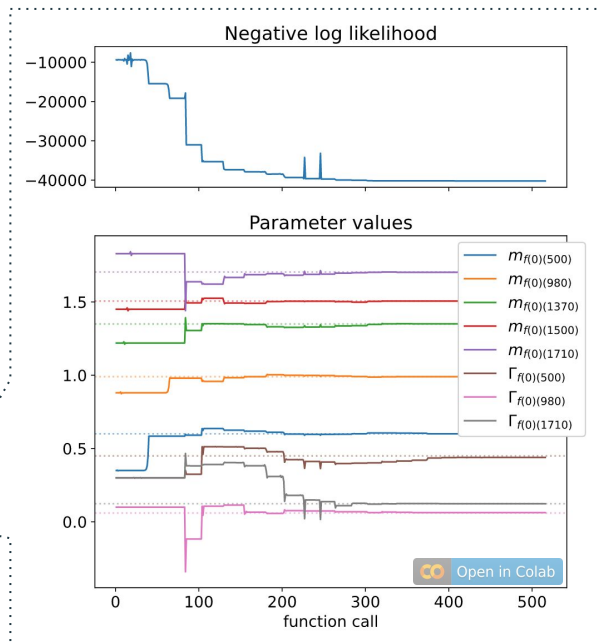
GeForce GTX 1050 Mobile GPU @ 1.35GHz **47s**

Tesla K80 GPU (Colab) **15s**

Intel Xeon CPU @ 2.20GHz 1 core (Colab) **3m20**



*optimise
parameters*





TensorWaves

Fit and generate data with computational back-ends

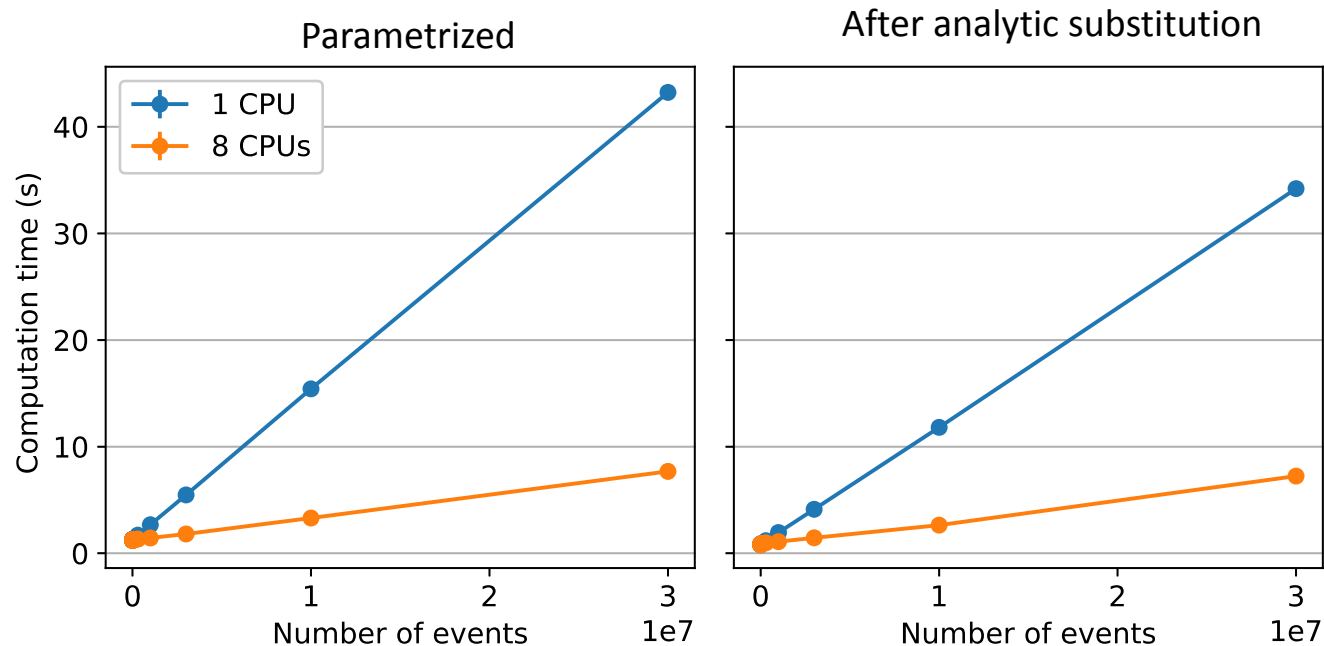
Amplitude model for $\Lambda_c \rightarrow p\pi K$
12 resonances, 59 parameters,
DPD alignment for 3 subsystems

Expression tree complexity:
parametrized: 43,198 nodes
substituted: 9,624 nodes

Backend: JAX

CPU: Intel i7-8750H 2.20GHz

→ computation time
decreases by 25%





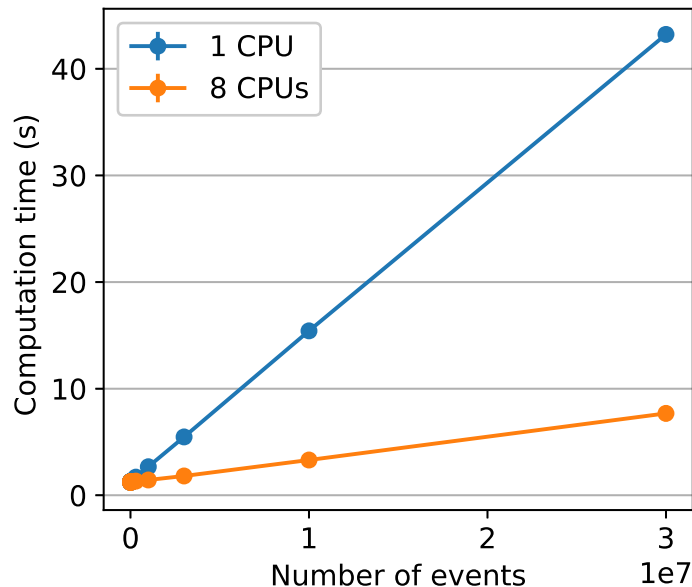
TensorWaves

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parametrized: 43,198 nodes
substituted: 9,624 nodes

SymPy+JAX (Python)



Julia

