Heavy flavour measurements:
a theoretical perspective

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Workshop on the physics of HL-LHC
and perspectives at HE-LHC
Heavy Flavour in the QGP: the conceptual setup

- Description of soft observables based on hydrodynamics, assuming to deal with a system close to local thermal equilibrium (no matter why);
- Description of jet-quenching based on energy-degradation of external probes (high-$p_T$ partons);
- Description of heavy-flavour observables requires to employ/develop a setup (transport theory) allowing to deal with more general situations and in particular to describe how particles would (asymptotically) approach equilibrium.

Initial (off-equilibrium!) $Q\bar{Q}$ production occurs on a very short time-scale $\tau_{Q\bar{Q}} \sim 1/2M_Q \lesssim 0.1 \text{ fm/c} \ll \tau_{\text{QGP}}$

NB At high-$p_T$ the interest in heavy flavor is no longer related to thermalization, but to the study of the mass and color charge dependence of jet-quenching (last part of this talk)
Heavy quarks as probes of the QGP

A realistic study requires developing a multi-step setup:

- **Initial production**: pQCD + possible nuclear effects (nPDFs, \(k_T\)-broadening) \(\rightarrow\) QCD event generators, validated on p-p data;
- Description of the background medium (initial conditions, \(T(x), u^\mu(x)\)) \(\rightarrow\) hydrodynamics, validated on soft hadrons;
- **HQ-medium interaction** \(\rightarrow\) transport coefficients, in principle derived from QCD, but still far from a definite answer for the relevant experimental conditions;
- **Dynamics in the medium** \(\rightarrow\) transport calculations, in principle rigorous under certain kinematic conditions, but require transport coefficients;
- **Hadronization**: not well under control (fragmentation in the vacuum? recombination with thermal partons? validated on what?)
  - An item of interest in itself (change of hadrochemistry in A-A collisions? And also in p-p?)
  - However, a source of systematic uncertainty for studies of parton-medium interaction;
- **Hadronic rescattering** (e.g. \(D\pi \rightarrow D\pi\)), from effective Lagrangians, but no experimental data the on relevant cross-sections
Transport theory: general setup
Transport theory: the Boltzmann equation

Time evolution of HQ phase-space distribution $f_Q(t, x, p)$\textsuperscript{1}:

$$\frac{d}{dt} f_Q(t, x, p) = C[f_Q]$$

- **Total derivative** along particle trajectory
  
  $$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} + F \frac{\partial}{\partial p}$$

  Neglecting $x$-dependence and mean fields: $\partial_t f_Q(t, p) = C[f_Q]$

- **Collision integral**:
  
  $$C[f_Q] = \int dk [w(p + q, q)f_Q(p + q) - w(p, q)f_Q(p)]$$

  \text{gain term} \quad \text{loss term}

  $w(p, q)$: HQ transition rate $p \to p - q$

\textsuperscript{1}Approach adopted by Catania, Nantes, Frankfurt, LBL... groups
From Boltzmann to Fokker-Planck

Expanding the collision integral for small momentum exchange (Landau)

\[ C[f_Q] \approx \int d\mathbf{q} \left[ q^i \frac{\partial}{\partial p^i} + \frac{1}{2} q^i q^j \frac{\partial^2}{\partial p^i \partial p^j} \right] [w(p, q)f_Q(t, p)] \]

\(^2\text{In a relativistic gauge plasma } q \sim m_D \sim gT\)
Expanding the collision integral for small momentum exchange\(^2\) (Landau)

\[
C[f_Q] \approx \int d\mathbf{q} \left[ q^i \frac{\partial}{\partial p^i} + \frac{1}{2} q^i q^j \frac{\partial^2}{\partial p^i \partial p^j} \right] [w(p, q)f_Q(t, p)]
\]

the Boltzmann equation reduces to the Fokker-Planck equation

\[
\frac{\partial}{\partial t} f_Q(t, p) = \frac{\partial}{\partial p^i} \left\{ A^i(p)f_Q(t, p) + \frac{\partial}{\partial p^j}[B^{ij}(p)f_Q(t, p)] \right\}
\]

where

\[
A^i(p) = \int d\mathbf{q} q^i w(p, q) \quad \rightarrow \quad A^i(p) = A(p) p^i \quad \text{friction}
\]

\[
B^{ij}(p) = \frac{1}{2} \int d\mathbf{q} q^i q^j w(p, q) \quad \rightarrow \quad B^{ij}(p) = (\delta^{ij} - \hat{p}^i \hat{p}^j)B_0(p) + \hat{p}^i \hat{p}^j B_1(p) \quad \text{momentum broadening}
\]

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\]

momentum broadening

Problem reduced to the evaluation of *three transport coefficients*,
directly derived from the scattering matrix

\[^2\]In a relativistic gauge plasma \( q \sim m_D \sim gT \)
The FP equation can be viewed as a continuity equation for the phase-space distribution of the kind \( \partial_t \rho(t, \vec{p}) + \vec{\nabla}_p \cdot \vec{J}(t, \vec{p}) = 0 \)

\[
\frac{\partial}{\partial t} f_Q(t, \vec{p}) = \frac{\partial}{\partial p^i} \left\{ A^i(p) f_Q(t, \vec{p}) + \frac{\partial}{\partial p^j} [B^{ij}(p) f_Q(t, \vec{p})] \right\} = -J^i(t, \vec{p})
\]

admitting a steady solution \( f_{eq}(p) \equiv e^{-E_p/T} \) when the current vanishes:

\[
A^i(\vec{p}) f_{eq}(p) = -\frac{\partial B^{ij}(\vec{p})}{\partial p^j} f_{eq}(p) - B^{ij}(p) \frac{\partial f_{eq}(p)}{\partial p^j}.
\]

One gets then a constraint linking the three transport coefficients, which are not independent, but obey the Einstein fluctuation-dissipation relation

\[
A(p) = \frac{B_1(p)}{TE_p} - \left[ \frac{1}{p} \frac{\partial B_1(p)}{\partial p} + \frac{d-1}{p^2} (B_1(p) - B_0(p)) \right],
\]

quite involved due to the momentum dependence of the transport coefficients (measured HQ’s are relativistic particles!)
The relativistic Langevin equation

The Fokker-Planck equation can be recast into a form suitable to follow the dynamics of each individual quark arising from the pQCD Monte Carlo simulation of the initial $Q\bar{Q}$ production: the Langevin equation

$$\frac{\Delta p^i}{\Delta t} = -\eta D(p)p^i + \xi^i(t),$$

deterministic, stochastic

with the properties of the noise encoded in

$$\langle \xi^i(p_t) \rangle = 0 \quad \langle \xi^i(p_t)\xi^j(p_{t'}) \rangle = b^{ij}(p) \delta_{t t'} \quad b^{ij}(p) \equiv \kappa_L(p)\hat{p}^i\hat{p}^j + \kappa_T(p)(\delta^{ij} - \hat{p}^i\hat{p}^j)$$
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\]

*Transport coefficients* related to the FP ones:

- **Momentum diffusion**: $\kappa_T(p) = 2B_0(p)$ and $\kappa_L(p) = 2B_1(p)$
- **Friction** term, in the *Ito pre-point discretization scheme*,

\[
\eta^{Ito}_D(p) = A(p) = \frac{B_1(p)}{TE_p} - \left[ \frac{1}{p} \frac{\partial B_1(p)}{\partial p} + \frac{d-1}{p^2}(B_1(p) - B_0(p)) \right]
\]
A first check: thermalization in a static medium

(Test with a sample of $c$ quarks with $p_0 = 2$ GeV/c).

For $t \gg 1/\eta_D$ one approaches a relativistic Maxwell-Jüttner distribution

$$f_{MJ}(p) \equiv \frac{e^{-E_p/T}}{4\pi M^2 T K_2(M/T)}, \quad \text{with} \quad \int d^3p \ f_{MJ}(p) = 1$$

The larger $\kappa$ ($\kappa \sim T^3$), the faster the approach to thermalization.
Transport coefficients
One consider the non-relativistic limit of the Langevin equation for a HQ
\[
\frac{dp^i}{dt} = -\eta D p^i + \xi^i(t), \quad \text{with} \quad \langle \xi^i(t)\xi^j(t') \rangle = \delta^{ij}\delta(t - t')\kappa
\]
in which the strength of the noise is given by a single number, the momentum-diffusion coefficient $\kappa$. Hence, in the $p \to 0$ limit:
\[
\kappa = \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle \xi^i(t)\xi^i(0) \rangle_{\text{HQ}} \approx \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle F^i(t)F^i(0) \rangle_{\text{HQ}},
\]
\[
\equiv D^>(t)
\]
For a static ($M = \infty$) HQ the force is due to the color-electric field:
\[
F(t) = g \int dx Q^\dagger(t, x)t^a Q(t, x)E^a(t, x)
\]
Transport coefficients: non-perturbative definition

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The above non-perturbative definition, referring to the \(M \to \infty\) limit, is the starting point for a thermal-field-theory evaluation based on

- weak-coupling calculations (up to NLO);
- gauge-gravity duality (\(\mathcal{N} = 4\) SYM)
- lattice-QCD simulations
In the $M \to \infty$ limit the HQ exchange momentum $q^\mu = (0, \vec{q})$, with $q \sim gT$, with the medium partons. The exchanged soft gluon is dressed by the Debye mass $m_D \sim gT$, which screens IR divergences.

$$\kappa_{\text{LO}} \equiv \frac{g^4 C_F}{12\pi^3} \int_0^{\infty} k^2 dk \int_0^{2k} \frac{q^3 dq}{(q^2 + m_D^2)^2}$$

$$\times \left[ N_c n_B(k)(1+n_B(k)) \left(2 - \frac{q^2}{k^2} + \frac{q^4}{4k^2}\right) + N_f n_F(k)(1-n_F(k)) \left(2 - \frac{q^2}{2k^2}\right) \right]$$

Under the assumption that $q \ll k \sim T$ one can “expand” the results in a weak-coupling series

$$\kappa = \frac{C_F g^4 T^3}{18\pi} \left( \left[ N_c + \frac{N_f}{2} \right] \ln \frac{2T}{m_D} + \xi \right) + \frac{N_f \ln 2}{2} + \mathcal{O}(g)$$

with the structure $\kappa \sim g^4 T^3 (\# \ln(1/g) + \# + \mathcal{O}(g))$, clearly meaningful only as long as $g \ll 1$. 
The weak-coupling expansion for $\kappa$ receives $O(g)$ corrections of various origin (S. Caron-Huot and G.D. Moore, JHEP 0802 (2008) 081):

- one part is contained in the unexpanded tree-level result, arising from the region $k \sim gT$ in which $n_B(k) \sim T/k \sim 1/g$ and the approximation $q \ll k$ no longer holds;

- another part arises from a NLO correction to the screened gluon propagator, which can be easily inserted in the tree-level result;

- a last part comes from overlapping scatterings. Having a total scattering rate $\sim g^2T$ and the duration of a single scattering $\sim 1/q \sim 1/gT$ entails that a fraction $O(g)$ of scattering events overlap with each other (see diagrams).
Collecting together the various terms one gets, for $N_f = N_c = 3$,

$$\kappa = \frac{16\pi}{3} \alpha_s^2 T^3 \left( \ln \frac{1}{g} + 0.07428 + 1.9026g + \mathcal{O}(g^2) \right)$$

which shows that, for realistic values of the coupling $\alpha_s \sim 0.3$, NLO corrections to $\kappa$ are positive and large: what’s the guidance provided by weak-coupling calculations if NLO corrections are so large?
The \((p \to 0)\) HQ momentum-diffusion coefficient

\[\kappa = \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle \xi^i(t)\xi^i(0) \rangle_{\text{HQ}} = \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle F^i(t)F^i(0) \rangle_{\text{HQ}} \equiv D^>(t)\]

is given by the \(\omega \to 0\) limit of the FT of the electric-field correlator \(D^>\).

In a thermal ensemble, from the periodicity of the bosonic fields, one has \(\sigma(\omega) \equiv D^>(\omega) - D^<(\omega) = (1 - e^{-\beta\omega})D^>(\omega)\), so that

\[\kappa \equiv \lim_{\omega \to 0} \frac{D^>(\omega)}{3} = \lim_{\omega \to 0} \frac{1}{3} \frac{\sigma(\omega)}{1 - e^{-\beta\omega}} \sim \frac{1}{3} \frac{T}{\omega} \sigma(\omega)\]
The \((p \to 0)\) HQ momentum-diffusion coefficient

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\]

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\]

On the lattice one evaluates then the \textit{euclidean electric-field correlator} \((t = -i\tau)\)

\[
D_E(\tau) = -\frac{\langle \text{Re Tr}[U(\beta, \tau)gE^i(\tau, 0)U(\tau, 0)gE^i(0, 0)] \rangle}{\langle \text{Re Tr}[U(\beta, 0)] \rangle}
\]

and from the latter one extract the \textit{spectral density} according to

\[
D_E(\tau) = \int_{0}^{+\infty} d\omega \frac{\cosh(\tau - \beta/2)}{2\pi} \frac{1}{\sinh(\beta \omega/2)} \sigma(\omega)
\]
HQ momentum diffusion from lattice-QCD \((N_f = 0!)
\)

The direct extraction of the spectral density from the euclidean correlator

\[
D_E(\tau) = \int_0^\infty \frac{d\omega \cosh(\tau - \beta/2)}{2\pi} \frac{\sinh(\beta \omega/2)}{\sigma(\omega)}
\]

is an ill-posed problem, since the latter is known for a limited set \((\sim 20)\) of points \(D_E(\tau_i)\), and one wishes to obtain a fine scan of \(\sigma(\omega_j)\). A direct \(\chi^2\)-fit is not applicable. Possible strategies:

- Bayesian techniques (Maximum Entropy Method)
- Theory-guided ansatz for the behaviour of \(\sigma(\omega)\) to constrain its functional form (A. Francis et al., PRD 92 (2015), 116003)

From the different ansatz on the functional form of \(\sigma(\omega)\) one gets a systematic uncertainty band:

\[
\kappa/T^3 \approx 1.8 - 3.4
\]
Collisional broadening in the non-static case

In the case of experimental interest HQ’s have a large but finite mass and most of the $p_T$-bins for which data are available refer to quite fast, or even relativistic, HF hadrons: extending the estimates for the HQ transport coefficients to finite momentum is mandatory to provide theoretical predictions relevant for the experiment.

The effect of $2 \rightarrow 2$ collisions can be included in an “improved” tree-level calculation (W.M. Alberico et al., EPJC 73 (2013) 2481) with an Intermediate cutoff $|t|^* \sim m_D^2$ separating the contributions of

- hard collisions ($|t| > |t|^*$): kinetic pQCD calculation
- soft collisions ($|t| < |t|^*$): Hard Thermal Loop approximation (resummation of medium effects)

Transport coefficients $\kappa_{T/L}(p)$

When the exchanged 4-momentum is soft the t-channel gluon feels the presence of the medium and requires resummation. The blob represents the dressed gluon propagator, which has longitudinal and transverse components:

$$\Delta_L(z, q) = \frac{-1}{q^2 + \Pi_L(z, q)}, \quad \Delta_T(z, q) = \frac{-1}{z^2 - q^2 - \Pi_T(z, q)},$$

where medium effects are embedded in the HTL gluon self-energy.

NB In the corresponding static calculation only longitudinal gluon exchange, dressed simply by a Debye mass, without any energy and momentum dependence.
Transport coefficients: numerical results

Combining together the hard and soft contributions...

\[ m_c = 1.3 \text{ GeV}, \quad T = 400 \text{ MeV}, \quad \mu_{\text{soft}} = 1.5\pi T, \quad \mu_{\text{hard}} = |t|^{0.5} \]

\[ m_b = 4.8 \text{ GeV}, \quad T = 400 \text{ MeV}, \quad \mu_{\text{soft}} = 1.5\pi T, \quad \mu_{\text{hard}} = |t|^{0.5} \]

\[ \kappa_T, |t|^* = m_D^2 \]
\[ \kappa_T, |t|^* = 4m_D^2 \]
\[ \kappa_L, |t|^* = m_D^2 \]
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...the dependence on the intermediate cutoff \(|t|^*\) is very mild!

NB Notice, in the case of charm, the strong momentum-dependence of \(\kappa_L\), much milder in the case of beauty, for which \(\kappa_L \approx \kappa_T\) up to 5 GeV
**Spatial diffusion coefficient $D_s$**

In the *non-relativistic* limit an excess of HQ’s initially placed at the origin will diffuse according to

$$\langle \mathbf{x}^2(t) \rangle \sim 6 D_s t \quad \text{with} \quad D_s = \frac{2 T^2}{\kappa}.$$ 

For a strongly interacting system spatial diffusion is very small! Theory calculations for $D_s$ have been collected (F. Prino and R. Rapp, JGP 43 (2016) 093002) and are often used by the experimentalists to summarize the difference among the various models (BUT momentum dependence, not captured by $D_s$, is important!)

- **lattice-QCD**

  $$(2\pi T) D_s^{IQCD} \approx 3.7 - 7$$

- **$\mathcal{N} = 4$ SYM:**

  $$(2\pi T) D_s^{SYM} = \frac{4}{\sqrt{g_{SYM}^2 N_c}} \approx 1.2$$

  for $N_c = 3$ and $\alpha_{SYM} = \alpha_s = 0.3$. 
Although the Langevin approach is a very convenient numerical tool and allows one to establish a link between observables and transport coefficients derived from QCD...
Although the Langevin approach is a very convenient numerical tool and allows one to establish a link between observables and transport coefficients derived from QCD... it is nevertheless based on a soft-scattering expansion of the collision integral $C[f]$ truncated at second order (friction and diffusion terms), which may be not always justified, in particular for charm, possibly affecting the final $R_{AA}$ (V. Greco et al., Phys.Rev. C90 (2014) 044901)
The Langevin/FP approach: a critical perspective

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For beauty on the other hand Langevin≡Boltzmann!
In the presence of a medium, rather than fragmenting like in the vacuum (e.g. $c \rightarrow cg \rightarrow c\bar{q}q$), HQ’s can hadronize by recombining with light thermal quarks (or even diquarks) from the medium. This has been implemented in several ways in the literature:

- 2 → 1 (or 3 → 1 for baryon production) coalescence of partons close in phase-space: $Q + \bar{q} \rightarrow M$
- String formation: $Q + \bar{q} \rightarrow$ string → hadrons
- Resonance formation/decay $Q + \bar{q} \rightarrow M^{*} \rightarrow Q + \bar{q}$

In-medium hadronization may affect the $R_{AA}$ and $v_{2}$ of final D-mesons due to the collective (radial and elliptic) flow of light quarks. Furthermore, it can change the HF hadrochemistry, leading for instance to and enhanced productions of strange particles ($D_{s}$) and baryons ($\Lambda_{c}$): no need to excite heavy $s\bar{s}$ or diquark-antidiquark pairs from the vacuum as in elementary collisions, a lot of thermal partons available nearby!

Selected results will be shown in the following.
Experimental D-meson data show a peak in the $R_{AA}$ and a sizable $v_2$ one would like to interpret as a signal of *charm radial flow and thermalization* (green crosses: kinetic equilibrium, decoupling from FO hypersurface).
From quarks to hadrons: *kinematic* effect on $R_{AA}$ and $v_2$

Experimental D-meson data show a peak in the $R_{AA}$ and a sizable $v_2$ one would like to interpret as a signal of *charm radial flow and thermalization* (green crosses: kinetic equilibrium, decoupling from FO hypersurface).

However, at least part of the effect might be due to the radial and elliptic flow of the light partons from the medium picked-up at hadronization (POWL Lang results A.B. et al., in EPJC 75 (2015) 3, 121).
From quarks to hadrons: HF hadrochemistry

The abundance of strange quarks in the plasma can lead e.g. to an enhanced production of $D_s$ mesons wrt p-p collisions via $c + \bar{s} \rightarrow D_s$

ALICE data for $D$ and $D_s$ mesons (JHEP 1603 (2016) 082) compared with TAMU-model predictions (M- He et al., PLB 735 (2014) 445)

Langevin transport simulation in the QGP + hadronization modeled via

$$\left( \partial_t + \vec{v} \cdot \vec{\nabla} \right) F_M(t, \vec{x}, \vec{p}) = - (\Gamma/\gamma_p) F_M(t, \vec{x}, \vec{p}) + \beta(t, \vec{x}, \vec{p})$$

with

$$\sigma(s) = \frac{4\pi}{k^2} \frac{(\Gamma m)^2}{(s - m^2)^2 + (\Gamma m)^2}$$
Some new predictions

In the following, some new predictions by the POWLANG setup\textsuperscript{4} will be shown, mostly focused on

- HF observables in small systems
- Higher flow harmonic ($v_2, v_3$)

and compared to recent experimental data

\textsuperscript{4}A.B. et al., EPJC 75 (2015) no.3, 121 and JHEP 1603 (2016) 123 + work in progress
We display our predictions\(^5\), with different initializations (source smearing) and transport coefficients (HTL vs lQCD), compared to

- **HF-electron** \(R_{dAu}\) by PHENIX at RHIC (left panel)
- **D-mesons** \(R_{pPb}\) by ALICE at the LHC (right panel)

\(^5\) A.B. et al., JHEP 1603 (2016) 123
We also predict a non-vanishing $v_2$ of charmed hadrons, arising mainly from the elliptic flow inherited from the light thermal partons.
New results at 5.02 TeV: $D$-meson $v_2$ and $v_3$ in Pb-Pb

• CMS data for $D$-meson $v_{2,3}$ satisfactory described;

• Recombination with light quarks provides a relevant contribution;

• Further insight can come from event-shape engineering, selecting events with larger/smaller eccentricity within the same centrality class
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Theory-to-experiment comparison allows one to draw some robust qualitative conclusions: *c*-quarks interact significantly with the medium formed in heavy-ion collision, which affects both their propagation in the plasma and their hadronization. As a result, HF-hadron spectra are quenched at high-$p_T$, while at low-$p_T$ they display signatures of radial, elliptic and triangular flow.
Theory-to-experiment comparison allows one to draw some robust qualitative conclusions: $c$-quarks interact significantly with the medium formed in heavy-ion collision, which affects both their propagation in the plasma and their hadronization. As a result, HF-hadron spectra are quenched at high-$p_T$, while at low-$p_T$ they display signatures of radial, elliptic and triangular flow. A number of experimental challenges or theoretical questions remain to be answered:

- **Charm measurements down to $p_T \rightarrow 0$:** flow/thermalization and total cross-section (of relevance for charmonium supression!)
- **$D_s$ and $\Lambda_c$ measurements:** change in hadrochemistry and total cross-section
- **Beauty measurements in AA via exclusive hadronic decays:** better probe, due to $M \gg \Lambda_{QCD}$, $T$ (initial production, evaluation of transport coefficients and Langevin dynamics under better control)
- **Charm in p-A collisions:** which relevance for high-energy atmospheric muons/neutrinos (Auger and IceCube experiments)? Possible initial/final-state nuclear effects? Better measurements are needed!
Theory-to-experiment comparison allows one to draw some robust qualitative conclusions: \(c\)-quarks interact significantly with the medium formed in heavy-ion collision, which affects both their propagation in the plasma and their hadronization. As a result, HF-hadron spectra are quenched at high-\(p_T\), while at low-\(p_T\) they display signatures of radial, elliptic and triangular flow. A number of experimental challenges or theoretical questions remain to be answered:

- **Charm** measurements down to \(p_T \to 0\): flow/thermalization and total cross-section (of relevance for charmonium suppression!)
- **\(D_s\)** and \(\Lambda_c\) measurements: change in hadrochemistry and total cross-section
- **Beauty** measurements in AA via exclusive hadronic decays: better probe, due to \(M \gg \Lambda_{\text{QCD}}, T\) (initial production, evaluation of transport coefficients and Langevin dynamics under better control)
- **Charm in p-A** collisions: which relevance for high-energy atmospheric muons/neutrinos (Auger and IceCube experiments)? Possible initial/final-state nuclear effects? Better measurements are needed!

The challenge is to become more quantitative, with the extraction of HF transport coefficients from the data (like \(\eta/s\) in hydrodynamics), goal for which beauty is the golden channel.
The high-energy fronteer: b-tagged jets

b-tagging of jets/dijets allows in principle the study of the color-charge dependence of jet-quenching ($C_F$ vs $C_A$ for the Casimir factor). However nuclear-modification-factor and dijet asymmetry look similar for inclusive (gluon dominated) and b-tagged jets. Better study of gluon-splitting contribution (but should be negligible for back-to-back dijets!) is necessary. Error bars need to be reduced!