xHam: a *Mathematica* package for Hamiltonian analysis

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Meeting day GdR Gravitational Waves, 27/05/2026

Plan

Context and motivations

The Dirac's recipe

The code

Conclusion and perspectives

Context and motivations

GR is not enough

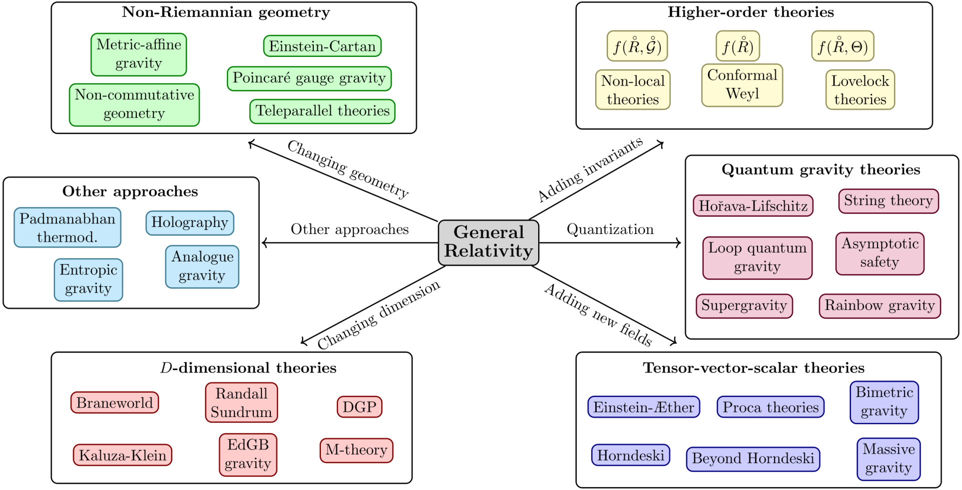
Einstein-Hilbert action :

$$S = \int d^4x\sqrt{-g}\left(\frac{1}{2\kappa}R + \mathcal{L}_m\right) \Longrightarrow R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \kappa T_{\mu\nu} \tag{1}$$

- Singularities
- Cosmological tensions
- Closed time-like geodesics
- Incompatible with quantum mechanics

Going Beyond

Sebastian Bahamonde et al 2023 Rep. Prog. Phys. 86 026901



General Relativity

Changing geometry →

Non-Riemannian geometry
- Metric-affine gravity
- Einstein-Cartan
- Poincaré gauge gravity
- Non-commutative geometry
- Teleparallel theories

Adding invariants →

Higher-order theories
- $f(\mathring{R},\mathring{\mathcal{G}})$
- $f(\mathring{R})$
- $f(\mathring{R},\Theta)$
- Non-local theories
- Conformal Weyl
- Lovelock theories

Other approaches →

Other approaches
- Padmanabhan thermod.
- Holography
- Entropic gravity
- Analogue gravity

Quantization →

Quantum gravity theories
- Hořava-Lifschitz
- String theory
- Loop quantum gravity
- Asymptotic safety
- Supergravity
- Rainbow gravity

Changing dimension →

***D*-dimensional theories**
- Braneworld
- Randall Sundrum
- DGP
- Kaluza-Klein
- EdGB gravity
- M-theory

Adding new fields →

Tensor-vector-scalar theories
- Einstein-Æther
- Proca theories
- Bimetric gravity
- Horndeski
- Beyond Horndeski
- Massive gravity

A brief example

Let's consider $\mathcal{L} = \frac{1}{2}(\Box\phi)^2$. Thus the equation of motion is :

$$\Box^2\phi = 0$$

4 Cauchy data needed $\Longrightarrow$ 2 d.o.fs !

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4 Cauchy data needed $\implies$ 2 d.o.fs !

Moreover, the additional degree of freedom is unstable.

Hence, when introducing higher order derivatives/couplings, one needs to knows how many degrees of freedom are acutally propagating

Motivations for a code

- Hamiltonian analysis (HA) is robust but hard to perform by hand. Computers are way more reliable.
- *Mathematica* : powerful and very efficient CAS, with a wide and popular family of packages for modified gravity calculations : **xAct**. But the software is not free...
- No such code exists for now (almost...)
- HA is one of the most used tools in modified gravity papers.

⟶ **There is something to try here !**

The Dirac’s recipe

Dirac-Bergmann algorithm

The recipe is very simple in theory, but experimentaly awful. Here is how to do :

First step : Primary constraints

Take a Lagrangian $\mathcal{L}$, and computes the hessian with respect to velocities of fields $\{\dot{\phi}_A\}$:

$$\mathcal{K}_{AB} \equiv \frac{\partial^2 \mathcal{L}}{\partial \dot{\phi}_A \partial \dot{\phi}_B} \tag{2}$$

If $\det \mathcal{K} = 0$, then the system is degenerate : there are constraints.

Note : For covariant Lagrangian, this requires a $3+1$ decomposition.

Dirac-Bergmann algorithm

Second step : Total Hamiltonian

Since we have some primary constraints ψ_A, the Hamiltonian is no longer unique on-shell. We need to introduce the **total Hamiltonian** :

$$H_T = \int_{\Sigma_3} d^3x \, \mathcal{H}_c + \sigma^A \psi_A \tag{3}$$

with σ^A being some arbitray functions (for now !) of phase space variables.

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⟶ How to uniquely determine the system's evolution if we have some arbitrariness in our Hamiltonian ?

Dirac-Bergmann algorithm

Third step : Consistency conditions

For now, nothing guarantees that $\psi_A \approx 0$ remains true with time... This has to be imposed :

$$\dot{\psi}_A \equiv \partial_t \psi_A + \{\psi_A ; H_T\} \approx 0 \tag{4}$$

We fall in one of this cases :

- $\dot{\psi}_A \approx 0$ fixes one of the σ^A ;
- $\dot{\psi}_A \approx 0$ is a linear combination of already known constraints ;
- $\dot{\psi}_A \approx 0$ gives an additional relation phase space variables must satisfy ⇒ **secondary constraints**

Some subtleties must be managed, like the presence of distributions

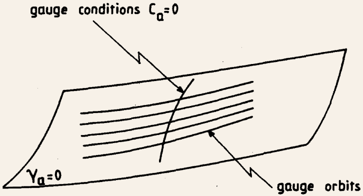
Then, we simply repeat until no new constraint emerges.

Dirac-Bergmann algorithm

Last step : Dirac constraint matrix

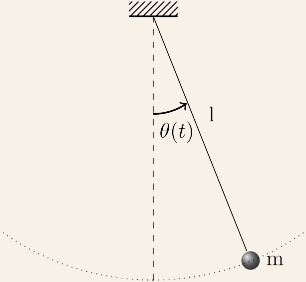
Is the dynamics on sub-manifold defined by the set of constraints well defined ? → Maybe not. There may be some degeneracy because of the so called first class constraints !

First class constraints



“Quantization of Gauge Systems”, M. Henneaux & C. Teitelboim

Second class constraints



Dirac-Bergmann algorithm

Last step : Dirac constraint matrix

Is the dynamics on sub-manifold defined by the set of constraints well defined ? → Maybe not. There may be some degeneracy because of the so called first class constraints !

$$M_{AB} \equiv \{C_A, C_B\} \tag{5}$$

The kernel of the dirac matrix M gives the first class constraints in the system.

Dirac-Bergmann algorithm

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The kernel of the dirac matrix M gives the first class constraints in the system.

This is the hard part !

A quick example : GR

We first perform an ADM decomposition of the Einstein-Hilbert Lagrangian :

$$\mathcal{L} = \sqrt{-g}R = N\sqrt{\gamma}\left(K_{ij}K^{ij} - K^2 + \mathcal{R} - 2\nabla_\mu(a^\mu - Kn^\mu)\right) \tag{6}$$

with $K_{ij} = -\frac{1}{2N}(\partial_t\gamma_{ij} - 2D_{(i}N_{j)})$. We find :

$$P_N = 0\ ;\ P_i = 0\ ;\ \Pi^{ij} = -\sqrt{\gamma}\left(K^{ij} - K\gamma^{ij}\right)$$

$$H_T = \int_{\Sigma_3} d^3x\, N\mathcal{H}_0 + N^i\mathcal{H}_i + \sigma P_N + \lambda^i P_i \tag{7}$$

with

$$\mathcal{H}_0 \equiv \frac{1}{\sqrt{\gamma}}\left(\Pi^{ij}\Pi_{ij} - \frac{1}{2}\Pi^2 - \gamma\mathcal{R}\right)\ ;\ \mathcal{H}_i \equiv D_j\Pi^j{}_i$$

A quick example : GR

Final set of constraints :

$$\{P_N \approx 0, P_i \approx 0, \mathcal{H}_0 \approx 0, \mathcal{H}_i \approx 0\}$$

They all (weakly) Poisson commute, *i.e* $M_{AB} \approx 0$. The eight constraints are first class. Since we started from $(1+3+6) \times 2 = 20$ phase space variables, we find that :

$$N_{\text{dof}} = \frac{20 - 2 \times 8 - 0}{2} = 2 \tag{8}$$

degrees of freedom are propagating in GR.

The code

What does xHam do ?

$$\mathcal{H}_C + \text{PS variables} + \text{Primaries} \;\longrightarrow \textbf{xHam} \;\longrightarrow \text{Constraints} \;+\; \text{Dirac matrix} + \text{D.O.Fs}$$

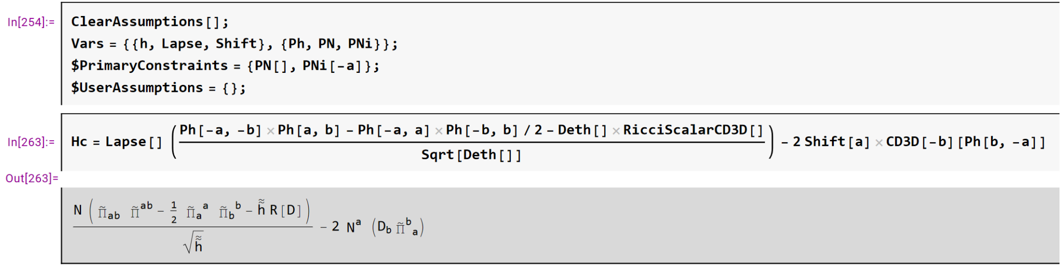
What does xHam do ?

$$\mathcal{H}_C + \text{PS variables} + \text{Primaries} \longrightarrow \textbf{xHam} \longrightarrow \text{Constraints} + \text{Dirac matrix} + \text{D.O.Fs}$$

- Reliable to find constraints
- Only detects obvious FCC in the Dirac matrix.
- Still a bit slow
- ADM decomposition has to be done by hand

GR

What about GR ?



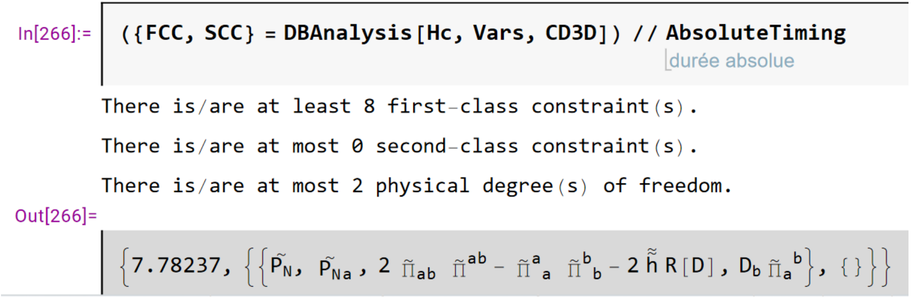
```
In[254]:= ClearAssumptions[];
          Vars = {{h, Lapse, Shift}, {Ph, PN, PNi}};
          $PrimaryConstraints = {PN[], PNi[-a]};
          $UserAssumptions = {};

In[263]:= Hc = Lapse[] ((Ph[-a, -b] × Ph[a, b] - Ph[-a, a] × Ph[-b, b] / 2 - Deth[] × RicciScalarCD3D[]) / Sqrt[Deth[]]) - 2 Shift[a] × CD3D[-b][Ph[b, -a]]
Out[263]=
```

$$\frac{N\left(\tilde{\Pi}_{ab}\;\tilde{\Pi}^{ab}-\frac{1}{2}\;\tilde{\Pi}_{a}{}^{a}\;\tilde{\Pi}_{b}{}^{b}-\tilde{\tilde{h}}\,R[D]\right)}{\sqrt{\tilde{\tilde{h}}}}-2\;N^{a}\;\left(D_{b}\,\tilde{\Pi}^{b}{}_{a}\right)$$

GR

What about GR ?



```
In[266]:= ({FCC, SCC} = DBAnalysis[Hc, Vars, CD3D]) // AbsoluteTiming
                                                     durée absolue
There is/are at least 8 first-class constraint(s).

There is/are at most 0 second-class constraint(s).

There is/are at most 2 physical degree(s) of freedom.
Out[266]=
```

$$\left\{7.78237, \left\{\left\{\tilde{P}_N, \tilde{P}_{Na}, 2\, \tilde{\Pi}_{ab}\, \tilde{\Pi}^{ab} - \tilde{\Pi}^{a}{}_{a}\, \tilde{\Pi}^{b}{}_{b} - 2\, \tilde{\tilde{h}}\, R[D], D_b\, \tilde{\Pi}_a{}^b\right\}, \{\}\right\}\right\}$$

Einstein-Maxwell (vacuum)

Let's now focus en Einstein-Maxwell Lagrangian without any charge :

$$\mathcal{L} = \sqrt{-g}\left(R - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\right) \tag{9}$$

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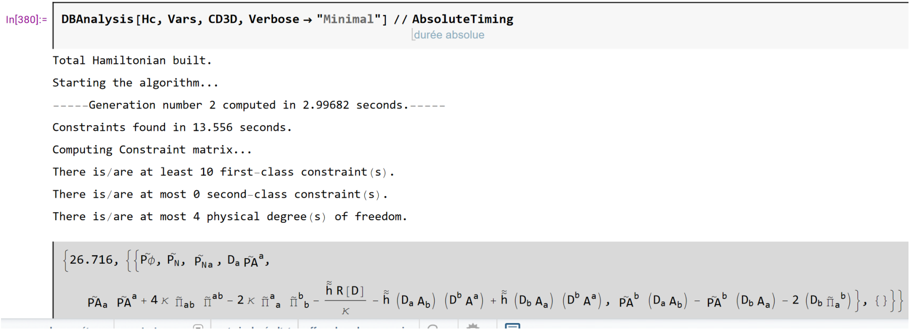

```
In[380]:= DBAnalysis[Hc, Vars, CD3D, Verbose → "Minimal"] // AbsoluteTiming
                                                          durée absolue
Total Hamiltonian built.
Starting the algorithm...
-----Generation number 2 computed in 2.99682 seconds.-----
Constraints found in 13.556 seconds.
Computing Constraint matrix...
There is/are at least 10 first-class constraint(s).
There is/are at most 0 second-class constraint(s).
There is/are at most 4 physical degree(s) of freedom.
```

$$\Big\{26.716, \Big\{\Big\{\tilde{P}\phi, \tilde{P}_N, \tilde{P}_{Na}, D_a \tilde{PA}^a, \tilde{PA}_a \tilde{PA}^a + 4\kappa\,\tilde{\pi}_{ab}\,\tilde{\pi}^{ab} - 2\kappa\,\tilde{\pi}^a{}_a\,\tilde{\pi}^b{}_b - \frac{\tilde{\tilde{h}}\,R[D]}{\kappa} - \tilde{\tilde{h}}\,(D_a A_b)\,(D^b A^a) + \tilde{\tilde{h}}\,(D_b A_a)\,(D^b A^a), \tilde{PA}^b\,(D_a A_b) - \tilde{PA}^b\,(D_b A_a) - 2\,(D_b \tilde{\pi}_a{}^b)\Big\}, \{\}\Big\}\Big\}$$

Other benchmarks

Let's now focus en Einstein-Maxwell Lagrangian without any charge :

Theory	Nb of DOFs	Time (s)	Correct ?
GR	2	~ 8	Yes
Einstein-Maxwell	4	~ 27	Yes
MCSF	3	~ 11	Yes
K-essence	3	~ 38	Almost
Mimetic gravity	3	~ 11	Almost
SME (Appendix)	3	~ 110	Yes
R+$(\Box\phi)^2$	4	~ 72	Almost
G3 Horndeski	?	?	Not anymore

Recents changes worsened the computation time...

Conclusion and perspectives

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- Automatic ADM decomposition
- Faddev-Jackiw method ?

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- **xHam** provides a reliable and "fast" way to follow Dirac's recipe. ⟶ but optimization is needed !
- Classification of constraints needs to be studied in depth
- Automatic ADM decomposition
- Faddev-Jackiw method ?

But the code **cannot** evade limitations intrinsic to HA...

Thank you !

Appendix 1 : K-essence

$$\mathcal{L} = \sqrt{-g}\left(\frac{1}{2\kappa}R + K(\phi, X)\right) \tag{10}$$

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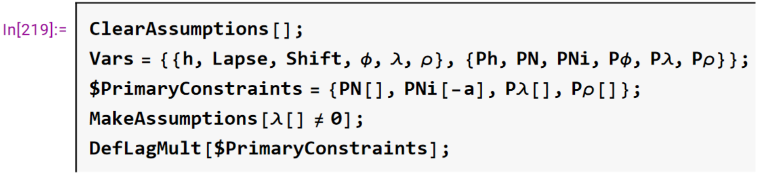

```
In[219]:= ClearAssumptions[];
          Vars = {{h, Lapse, Shift, ϕ, λ, ρ}, {Ph, PN, PNi, Pϕ, Pλ, Pρ}};
          $PrimaryConstraints = {PN[], PNi[-a], Pλ[], Pρ[]};
          MakeAssumptions[λ[] ≠ 0];
          DefLagMult[$PrimaryConstraints];
```

Appendix 1 : K-essence

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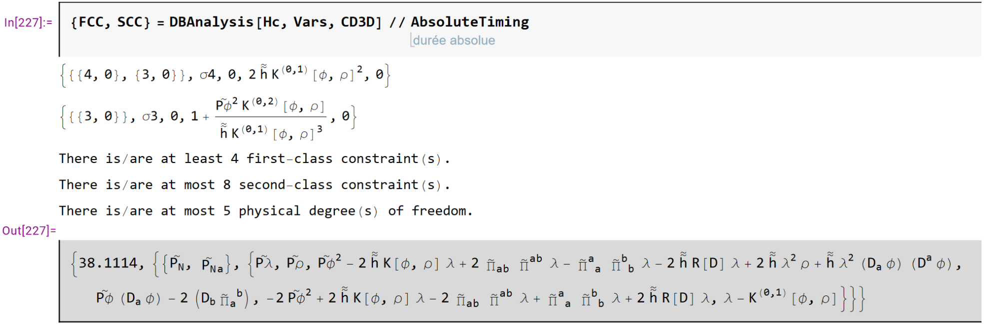

In[227]:=

```
{FCC, SCC} = DBAnalysis[Hc, Vars, CD3D] // AbsoluteTiming
```

$$\left\{\{\{4, 0\}, \{3, 0\}\}, \sigma 4, 0, 2\,\tilde{\tilde{h}}\,K^{(0,1)}[\phi, \rho]^2, 0\right\}$$

$$\left\{\{\{3, 0\}\}, \sigma 3, 0, 1 + \frac{\tilde{P\phi}^2\,K^{(0,2)}[\phi, \rho]}{\tilde{\tilde{h}}\,K^{(0,1)}[\phi, \rho]^3}, 0\right\}$$

```
There is/are at least 4 first-class constraint(s).
There is/are at most 8 second-class constraint(s).
There is/are at most 5 physical degree(s) of freedom.
```

Out[227]=

$$\Big\{38.1114, \big\{\{\tilde{P}_N, \tilde{P}_{Na}\}, \{\tilde{P\lambda}, \tilde{P\rho}, \tilde{P\phi}^2 - 2\,\tilde{\tilde{h}}\,K[\phi, \rho]\,\lambda + 2\,\tilde{\Pi}_{ab}\,\tilde{\Pi}^{ab}\,\lambda - \tilde{\Pi}^{a}{}_{a}\,\tilde{\Pi}^{b}{}_{b}\,\lambda - 2\,\tilde{\tilde{h}}\,R[D]\,\lambda + 2\,\tilde{\tilde{h}}\,\lambda^2\rho + \tilde{\tilde{h}}\,\lambda^2\,(D_a\phi)\,(D^a\phi),$$

$$\tilde{P\phi}\,(D_a\phi) - 2\left(D_b\,\tilde{\Pi}_a{}^{b}\right), -2\,\tilde{P\phi}^2 + 2\,\tilde{\tilde{h}}\,K[\phi, \rho]\,\lambda - 2\,\tilde{\Pi}_{ab}\,\tilde{\Pi}^{ab}\,\lambda + \tilde{\Pi}^{a}{}_{a}\,\tilde{\Pi}^{b}{}_{b}\,\lambda + 2\,\tilde{\tilde{h}}\,R[D]\,\lambda, \lambda - K^{(0,1)}[\phi, \rho]\}\big\}\Big\}$$

Appendix 1b : degenerate K-essence

$$\mathcal{L} = \sqrt{-g}\left(\frac{1}{2\kappa}R + K(\phi)\right) \tag{11}$$

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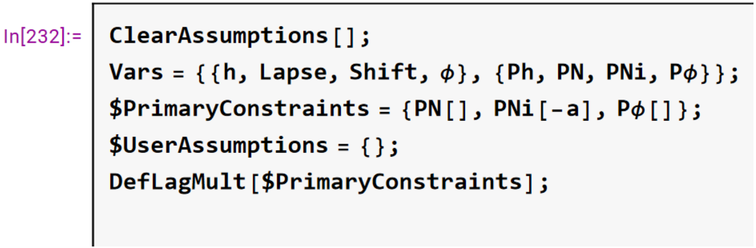

```
In[232]:= ClearAssumptions[];
          Vars = {{h, Lapse, Shift, ϕ}, {Ph, PN, PNi, Pϕ}};
          $PrimaryConstraints = {PN[], PNi[-a], Pϕ[]};
          $UserAssumptions = {};
          DefLagMult[$PrimaryConstraints];
```

Appendix 1b : degenerate K-essence

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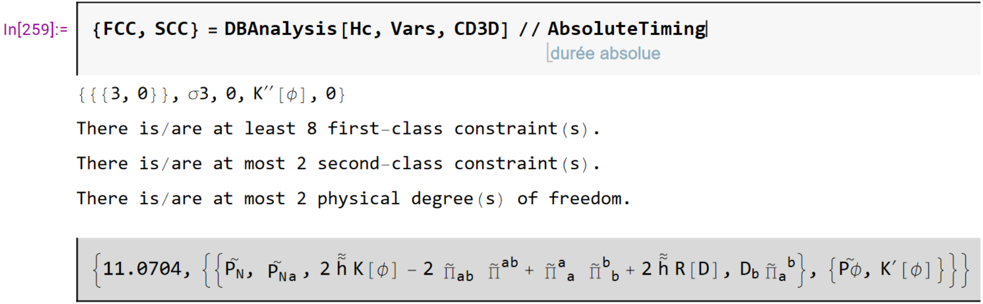


```
In[259]:= {FCC, SCC} = DBAnalysis[Hc, Vars, CD3D] // AbsoluteTiming
                                                    durée absolue

{{{3, 0}}, σ3, 0, K''[ϕ], 0}

There is/are at least 8 first-class constraint(s).

There is/are at most 2 second-class constraint(s).

There is/are at most 2 physical degree(s) of freedom.

{11.0704, {{P̃N, P̃Na, 2 h̃̃ K[ϕ] - 2 π̃ab π̃ab + π̃aa π̃bb + 2 h̃̃ R[D], Db π̃ab}, {P̃ϕ, K′[ϕ]}}}
```

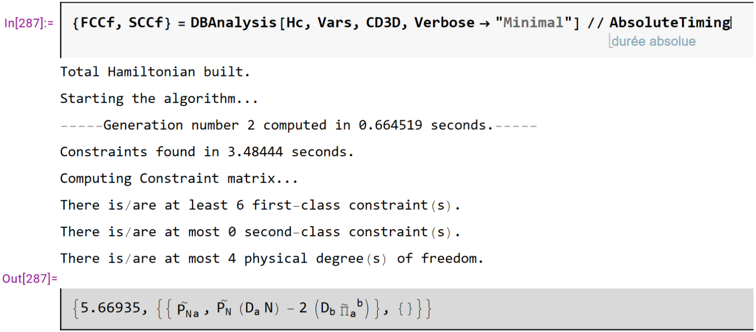
Appendix 2 : SME models

In the paper [2009.00949] (K. O'Neal-Ault, Q.G. Bailey, and N.A. Nilsson, Phys. Rev. D 103, 044010 (2021)), they consider the Lagrangian :

$$\begin{aligned}\mathcal{L}_1 = \frac{N\sqrt{\gamma}}{2\kappa}\Big[\mathcal{R} &+ \frac{N^2 - s_{00}}{N^2}\left(K^{ij}K_{ij} - K^2\right) + K\left(\frac{2}{N^4}s_{00}\left(\dot{N} - NN^i a_i\right) - \frac{1}{N^3}\left(\dot{s}_{00} - N^i \partial_i s_{00}\right)\right) \\ &+ \frac{2}{N^2}s_{00}a^i a_i - \frac{1}{N^2}a^i \partial_i s_{00}\Big] + \mathcal{L}_M \end{aligned} \qquad (12)$$

Appendix 2 : SME models

$$
\begin{aligned}
\mathcal{L}_1 = \frac{N\sqrt{\gamma}}{2\kappa}\Big[\mathcal{R} + \frac{N^2 - s_{00}}{N^2}\left(K^{ij}K_{ij} - K^2\right) + K\left(\frac{2}{N^4}s_{00}\left(\dot{N} - NN^i a_i\right) - \frac{1}{N^3}\left(\dot{s}_{00} - N^i\partial_i s_{00}\right)\right) \\
+ \frac{2}{N^2}s_{00}a^i a_i - \frac{1}{N^2}a^i\partial_i s_{00}\Big] + \mathcal{L}_M
\end{aligned}
\tag{12}
$$



In[287]:=

```
{FCCf, SCCf} = DBAnalysis[Hc, Vars, CD3D, Verbose → "Minimal"] // AbsoluteTiming
```

```
Total Hamiltonian built.

Starting the algorithm...

-----Generation number 2 computed in 0.664519 seconds.-----

Constraints found in 3.48444 seconds.

Computing Constraint matrix...

There is/are at least 6 first-class constraint(s).

There is/are at most 0 second-class constraint(s).

There is/are at most 4 physical degree(s) of freedom.
```

Out[287]=

$$\left\{5.66935, \left\{\left\{\tilde{P}_{Na}, \tilde{P}_N\,(D_a N) - 2\left(D_b\,\tilde{\Pi}_a{}^b\right)\right\}, \{\}\right\}\right\}$$