LAL NR injections explained

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1 Introduction

In this brief document I will aim to present the main steps one should follow to convert their NR data into the HDF5 file following LAL conventions of Format 1. This file can then be directly used for injections into parameter estimation pipelines. If you are interested in finding out more about NR injections and how other higher Formats work, please refer to Ref. [1]. The source code of `LALsuite` can be found here: https://git.ligo.org/lscsoft/lalsuite.

2 Motivation and Theoretical Background

You may be wondering why it has to be so complicated to use numerically simulated waveforms as injections in data analysis codes (i.e. as 'synthetic' signals being injected into gravitational wave (GW) detector noise). The simple explanation is that typically waveform modeling requires at least two coordinate systems, a 'source-frame' in which it is convenient to specify properties of the source of GWs, and a 'wave-frame' which is adopted to wave-propagation to detectors on Earth. Now, you have your perfect NR simulation, what is your coordinate frame? It is essentially whatever was employed during the numerical simulation, so that now defines a third coordinate frame. Data analysis pipelines use a wave-frame, so one would need to convert their NR data to this particular frame in order to perform parameter estimation on numerically simulated signals. For this purpose, `XLALSimInspiralChooseTDWaveform` function was created to do the required frame transformations and this document tries to describe all all the technicalities related to its arguments and use.

Let us first start with the brief description of the different frames.

2.0.1 NR frame

This is just a generic coordinate system, with Cartesian basis-vectors

$$\hat{e}_x, \hat{e}_y, \hat{e}_z \tag{1}$$

By defining the spherical basis-vectors $(\hat{r}, \hat{\theta}, \hat{\phi})$, where $\hat{\theta}$ and $\hat{\phi}$ are the unit vectors of the polar and azimuthal directions respectively, the NR strain is given by

$$h_+^{\rm NR}(t) = \frac{1}{2}\left(\hat{\theta}_i\hat{\theta}_j - \hat{\phi}_i\hat{\phi}_j\right) h^{ij}(t), \tag{2}$$

$$h_\times^{\rm NR}(t) = \frac{1}{2}\left(\hat{\theta}_i\hat{\phi}_j + \hat{\phi}_i\hat{\theta}_j\right) h^{ij}(t). \tag{3}$$

2.0.2 Wave frame

The wave frame has basis-vectors given by

$$\hat{X}, \hat{Y}, \hat{Z}. \tag{4}$$

We note that it is adopted to the direction of the observer (i.e. Earth), such that its $\hat{Z}$-axis points toward the observer. $\hat{X}$ and $\hat{Y}$ represent basis-vectors orthogonal to the line-of-sight, i.e. they span the plane of the sky. It is then complemented by the following 3 angles:

- Φ – angle between the line of ascending node and $\hat{n}$, defining a vector pointing from the second body to the first,
- ι – inclination angle (i.e. angle between orbital angular momentum $\hat{L}$ and the line-of-sight $\hat{Z}$,
- Ω – angle between $\hat{X}$ and the line of ascending node. Note that changing Ω simply rotates the $\hat{X}$ and $\hat{Y}$ axes.

The strain modes are then found via:

$$h_{+}^{\mathrm{W}} = \frac{1}{2}\left(\hat{X}_i\hat{X}_j - \hat{Y}_i\hat{Y}_j\right)h^{ij}, \tag{5}$$

$$h_{\times}^{\mathrm{W}}(t) = \frac{1}{2}\left(\hat{X}_i\hat{Y}_j + \hat{Y}_i\hat{X}_j\right)h^{ij}. \tag{6}$$

2.0.3 Source frame (non-compulsory)

Even though we will not be dealing with the source frame, we define it here for completeness. It comprises of the following basis-vectors

$$\hat{x}, \hat{y}, \hat{z}, \tag{7}$$

where

- The $\hat{z}$-axis points along the orbital angular momentum of the binary: $\hat{z} \overset{\mathrm{ref}}{=} \hat{L}$,
- The $\hat{x}$-axis points along the vector $\hat{n}$ pointing from the second to the first body: $\hat{x} \overset{\mathrm{ref}}{=} \hat{n}$,
- The third vector just completes the triad as: $\hat{y} = \hat{z} \times \hat{x}$.

Note that $\overset{\mathrm{ref}}{=}$ indicates that a given quantity is specified at the reference point. Therefore, the above given expressions for $\hat{x}, \hat{z}$ define the source-frame at the reference point only. They are chosen such that the spin components $(s_1^{\mathrm{A}}, s_2^{\mathrm{A}}, s_3^{\mathrm{A}})$ of body A and $(s_1^{\mathrm{B}}, s_2^{\mathrm{B}}, s_3^{\mathrm{B}})$ of body B have coordinate-invariant meaning: s_1^{A} is the projection of $\vec{\chi}_1$ onto $\hat{n}$, s_3^{A} is the projection of $\vec{\chi}_1$ onto $\hat{L}$ and so on. A different reference point would lead to a different source-frame, related by some rotation.

2.0.4 So how do I get from NR frame to the wave frame?

Generally, you do not need to worry about this, as all of the calculations that are about to be mentioned are done internally through `LALsuite`. However, the key steps to be aware of are as follows:

1. Pick Φ and ι.
2. Compute $\hat{Z}_{\mathrm{ref}}$ at reference time using

$$\hat{Z} \overset{\mathrm{ref}}{=} \sin\iota(\sin\Phi\hat{n} + \cos\Phi\hat{L} \times \hat{n}) + \cos\iota\hat{L}. \tag{8}$$

3. Let us fix $\Omega = \pi/2$. Remember that $\hat{Z}$ points in the direction of emission of the GWs, so we must have:

$$\hat{Z}_{\mathrm{ref}} \overset{\mathrm{ref}}{=} \begin{pmatrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta \end{pmatrix} = \hat{r} \tag{9}$$

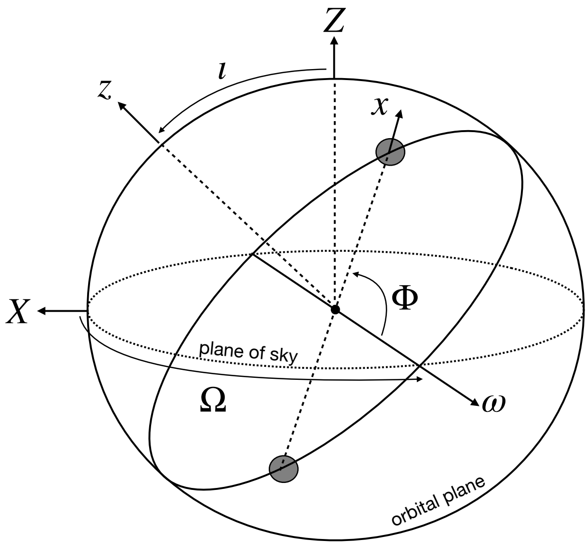

Figure 1: Relationship between the source frame (x, y, z) and the wave frame (X, Y, Z). Here by ω we denote the line of ascending node.

4. In the similar way we can relate $(\hat{X}, \hat{Y})$ to $(\hat{n}, \hat{L})$ using:

$$\hat{X} \overset{\text{ref}}{=} -\cos\iota(\sin\Phi\hat{n} + \cos\Phi\hat{L} \times \hat{n}) + \sin\iota\hat{L} \tag{10}$$

$$\hat{Y} \overset{\text{ref}}{=} \cos\Phi\hat{n} - \sin\Phi\hat{L} \times \hat{n}. \tag{11}$$

5. Note that $\hat{X}$ and $\hat{Y}$ are orthogonal to the direction of propagation of the GW, i.e. $\hat{r} = \hat{Z}$. In order to have the waveform in the wave frame, we then just need $(\hat{\theta}, \hat{\phi})$ of the NR frame to be rotated into $(\hat{X}, \hat{Y})$ of the wave frame through some rotation by an angle α:

$$\hat{X} = \cos\alpha\hat{\theta} - \sin\alpha\hat{\phi}, \tag{12}$$

$$\hat{Y} = \sin\alpha\hat{\theta} + \cos\alpha\hat{\phi}. \tag{13}$$

6. Finding this α is a just a task of taking the inner products of both sides of Eq.(12) and substituting relation for $(\hat{X}, \hat{Y})$ from Eq.(10):

$$\sin\alpha = \cos\Phi\hat{n} \cdot \hat{\theta} - \sin\Phi(\hat{L} \times \hat{n}) \cdot \hat{\theta}, \tag{14}$$

$$\cos\alpha = \cos\Phi\hat{n} \cdot \hat{\phi} - \sin\Phi(\hat{L} \times \hat{n}) \cdot \hat{\phi}. \tag{15}$$

7. As a dinal step, we substitute (θ, ϕ) into (2) and rotate the resulting polarisations by α using:

$$h_+^{\mathrm{W}}(t) = \cos(2\alpha)h_+^{\mathrm{NR}}(t) - \sin(2\alpha)h_\times^{\mathrm{NR}}(t) \tag{16}$$

$$h_\times^{\mathrm{W}}(t) = \sin(2\alpha)h_+^{\mathrm{NR}}(t) + \cos(2\alpha)h_\times^{\mathrm{NR}}(t) \tag{17}$$

This completes the transformation of the NR frame to the wave frame. The waveform can be used for injections.

3 What should I do to my NR data?

First, you should prepare all the modes that would be stored in the HDF5 file (be aware that higher modes can be contaminated with reflections and/or numerical noise, so check them first before injecting). Once you have done that, you should follow the steps below to post-process your NR data:

1. Choose your extraction radius – it may be useful to store the data for it in a separate file (unlike `GRChombo` conventions).
2. For each (lm)-mode, your Ψ_4 output should be scaled with the extraction radius, i.e. $R_{\text{ext}}\Psi_4$. Further it should be scaled with the mass, i.e. t/M and $M\Psi_4$, where M is the total mass.
3. For each (lm)-mode you wish to inject, convert your numerical Ψ_4 into strain (through the usual integration).
4. For each (lm)-mode compute amplitude A, phase ϕ and angular frequency ω of your strain.
5. Cut the junk radiation from all your modes. The time where you preformed a cut will now be referred to as the *start of your waveform*.
6. Shift your waveform. Typically, according to LAL conventions the waveform peak has to be aligned with $t = 0$ according to Eq.(4) of Ref. [1] (which is a fancy way of defining the largest peak of the amplitude). For my injections, I never did that – I simply shifted the start of all of my waveforms back to $t = 0$. The reasons of this would be described in the Remark of point 6 in Sec. 4.

4 How do I create the HDF5 file?

Once you have completed the steps above, you should next ask me for a python script that automatically generates the HDF5 file with all the information needed for a Format 1 waveform. In this script, you would need to provide some additional physical information through a simple `.ini` file, such as:

1. Initial masses and spins, m_1, m_2 and $\mathbf{s}_1, \mathbf{s}_2$.
2. Components of the Newtonian orbital angular momentum, $\hat{L}$ at the start of the waveform. Say you are simulating a non-precessing BH binary in the (xy)-plane, then your $\hat{L}$ is simply $(0, 0, 1)$.
3. Components of the orbital separation, $\hat{\mathbf{n}}$ at the start of the waveform:

$$\hat{\mathbf{n}} := \frac{\mathbf{c_1} - \mathbf{c_2}}{||\mathbf{c_1} - \mathbf{c_2}||}, \tag{18}$$

   where $\mathbf{c_1}, \mathbf{c_2}$ are the grid positions of the compact objects being simulated.

4. Dimensionless orbital frequency, Ω, where:

$$\mathbf{\Omega} = \hat{\mathbf{n}} \times \frac{\mathrm{d}\hat{\mathbf{n}}}{\mathrm{dt}}. \tag{19}$$

5. Eccentricity (I personally use the measure based on the phase, see Eq.(20) of Ref. [2]).
6. Angular frequency of the (22)-mode at the start of the waveform. This is then used for calculating the `f_lower_at_1MSUN` variable of Ref. [1] required by LAL, which corresponds to the frequency of the (22)-mode in Hz at the beginning of the waveform scaled to $1M_\odot$.

   Remark: `f_lower_at_1MSUN` variable is used to estimate the time elapsed in the reduced-order model (ROM) waveform from a given starting frequency until the ringdown. I guess this is useful if the waveform should be reconstructed from some frequency that is not `fStart`. The elapsed time, let's denote it by `est_start_time`, is returned via SimIMRSEOB-NRv4ROMTimeOfFrequency function. LAL also stores the start time of the waveform from the HDF5 file (i.e. the time where we have cut the junk radiation); let's denote it by `time_start_s`. If `(-1.1 * est_start_time) > time_start_s`, then the `est_start_time` is used for the start time, otherwise the routine falls back to using the start time of the HDF5 file. I always shift the start of my NR waveforms back to $t = 0$, so that `time_start_s` always equals to zero. Therefore, in this case, the approximated start time from SEOBNR is never used.

5 How to generate numerical relativity waveforms through LAL

Once you have generated the HDF5 file with all the metadata from your NR simulation, you can now reconstruct the waveform using `SimInspiralChooseTDWaveform` function. This function is dependent on some variables that you have to specify. In particular,

```
SimInspiralChooseTDWaveform(m1SI, m2SI, s1x, s1y, s1z, s2x, s2y, s2z, distance,
inclination, phiRef, longAscNodes, eccentricity, meanPerAno, deltaT, fStart, fRef,
params, approx)
```

What do they mean? Here:

1. `m1SI, m2SI` – masses of respective companions in kg,
2. `s1x, s1y, s1z, s2x, s2y, s2z` – Cartesian components of the dimensionless spin for both objects,
3. `distance` – distance to the source in m, i.e. luminosity distance,
4. `inclination` – inclination of the source in radians,
5. `phiRef` – reference orbital phase in radians, this is Φ angle in the wave frame,
6. `longAscNodes` – longitude of ascending nodes, degenerate with the polarization angle,
7. `eccentricity` - pretty self explanatory,
8. `meanPerAno` – mean anomaly of periastron,
9. `deltaT` – sampling interval in s,
10. `fStart` – starting GW frequency in Hz,
11. `fRef` – reference GW frequency in Hz,
12. `params` – LAL dictionary containing accessory parameters,
13. `approx` – post-Newtonian approximant to use for waveform production. In our case `approx = lalsim.NR_hdf5`.

Remark: Only formats 2 and above support the use of reference frequency, `fRef`. For formats < 2, we give the reference frequency as 0 or -1 to indicate that the start of the waveform should be used as the reference, i.e. `fRef` = `fStart`.

An example code calling this function can be found in Section III. A of Ref. [1]. But I will note a few steps you may need to undertake to use this function. Firstly, you may need to install `lalsuite` into your python environment: just run `pip install lalsuite`. Then, you should import the required libraries[1], in particular

```
import lalsimulation as lalsim
```

[1]For handling HDF5 formats I recommend using `h5py` package.

You should then create a dictionary for parameters that will store important information about our NR data

```
params = lal.CreateDict()
lalsim.SimInspiralWaveformParamsInsertNumRelData(params, filepath)
```

Additionally, define all the extrinsic parameters, e.g. total mass of the binary, inclination, etc., and extract the initial spins from the HDF5 file using:

```
spins = lalsim.SimInspiralNRWaveformGetSpinsFromHDF5File(fRef, mtotal, filepath)
```

Finally, you can then call our main function:

```
approx = lalsim.NR_hdf5
h_p, h_c = lalsim.SimInspiralChooseTDWaveform(m1SI, m2SI, s1x, s1y, s1z, s2x, s2y,
s2z, distance, inclination, phiRef, 0.0, 0.0, 0.0, deltaT, fStart, fRef, params, approx)
```

Note that I usually set $\Omega = \pi/2$ (this is a matter of choice). Further, eccentricity and mean-anomaly are not used for NR waveforms, so these can be safely set to zero.

You can access the array containing plus polarization by using `h_p.data.data` and similarly for the cross polarization. The time array can be reconstructed simply via:

```
np.arange(len(h_p.data.data))*h_p.deltaT
```

6 The inner-workings of LAL functions

So what happens when we call `XLALSimInspiralChooseTDWaveform`? Figure 2 shows the dependency of functions used in the waveform reconstruction with detailed descriptions on what they are doing exactly. However, below I will also summarise the relevant calls being made in the code:

1. The waveform driver routine `XLALSimInspiralNRWaveformGetHplusHcross`, that collects all the available modes and computes the angles necessary to rotate the intrinsic NR source frame into the LAL frame.

2. The function `XLALSimIMRNRWaveformGetModes` which performs consistency checks on the duration of the signal and spins. It further extracts information on phase and amplitude, and the amplitude gets re-scaled by $(\texttt{m1SI} + \texttt{m2SI})/r$.

3. The function `XLALSimInspiralNRWaveformGetRotationAnglesFromH5File` that performs the correct rotation of the NR strain into the wave frame described in Sec.2.0.4.

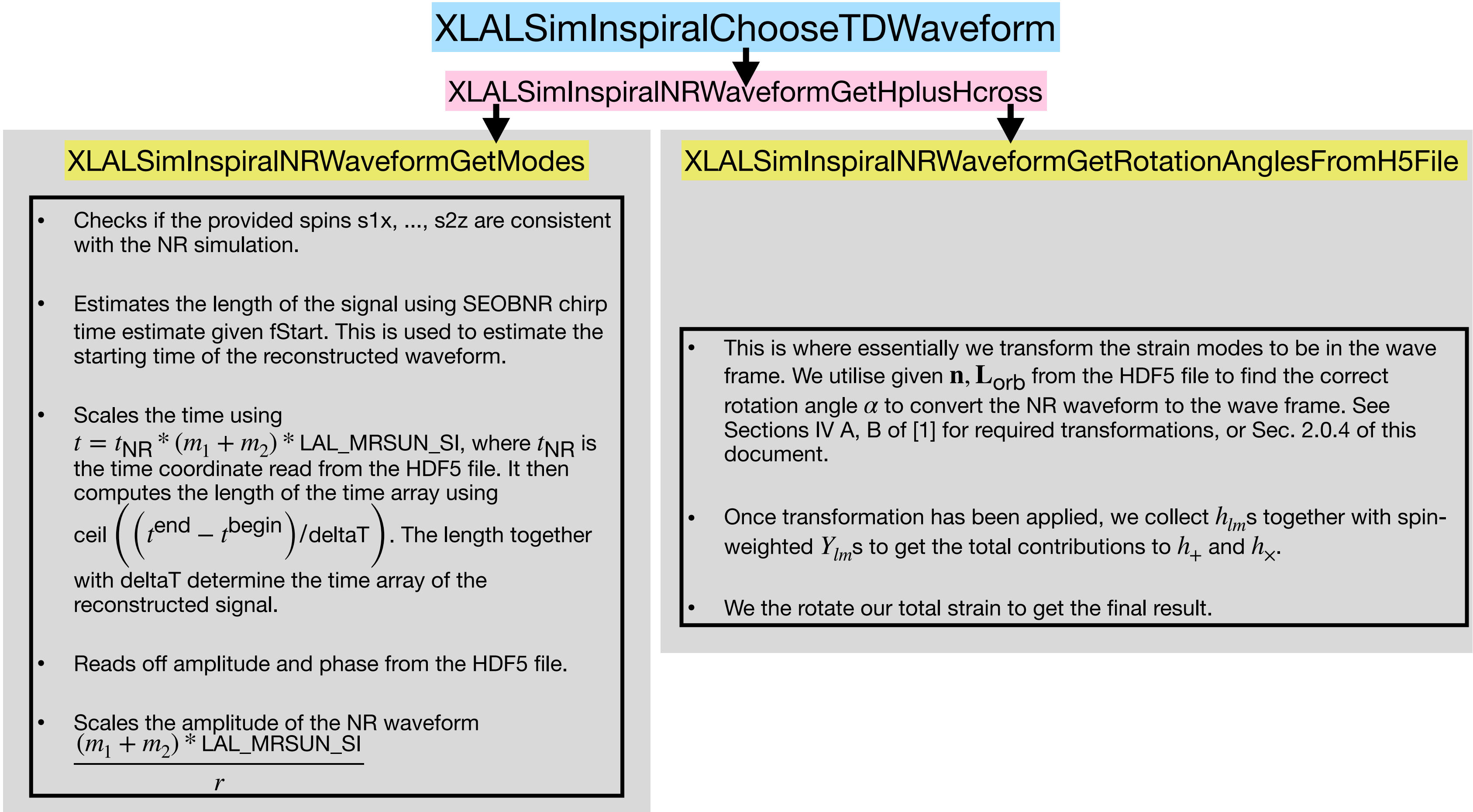

Figure 2: The flow-chart representing the function dependencies used in the waveform reconstruction. For an interested reader all these functions are located in the `lalsimulation` routine of `LALsuite`.

References

[1] Patricia Schmidt, Ian W. Harry, and Harald P. Pfeiffer. Numerical Relativity Injection Infrastructure. 3 2017.

[2] Abdul H. Mroue, Harald P. Pfeiffer, Lawrence E. Kidder, and Saul A. Teukolsky. Measuring orbital eccentricity and periastron advance in quasi-circular black hole simulations. *Phys. Rev. D*, 82:124016, 2010.