thermoscientific

The Use of Multiple Detection Electrodes in Electrostatic Linear Ion Traps

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ABSTRACT

Purpose: Evaluate the behavior of Electrostatic Linear Ion Traps which use multiple detection electrodes and Fourier transform processing.

Methods: Synthesis of simulated signals followed by Fourier analysis.

Results: Multiple detectors do not by themselves increase the fundamental frequency of the detected signal. The additional detectors distort the time domain signal, which generally leads to harmonics and peak splitting in the resulting frequency domain spectra instead of the desired increase in resolution.

INTRODUCTION

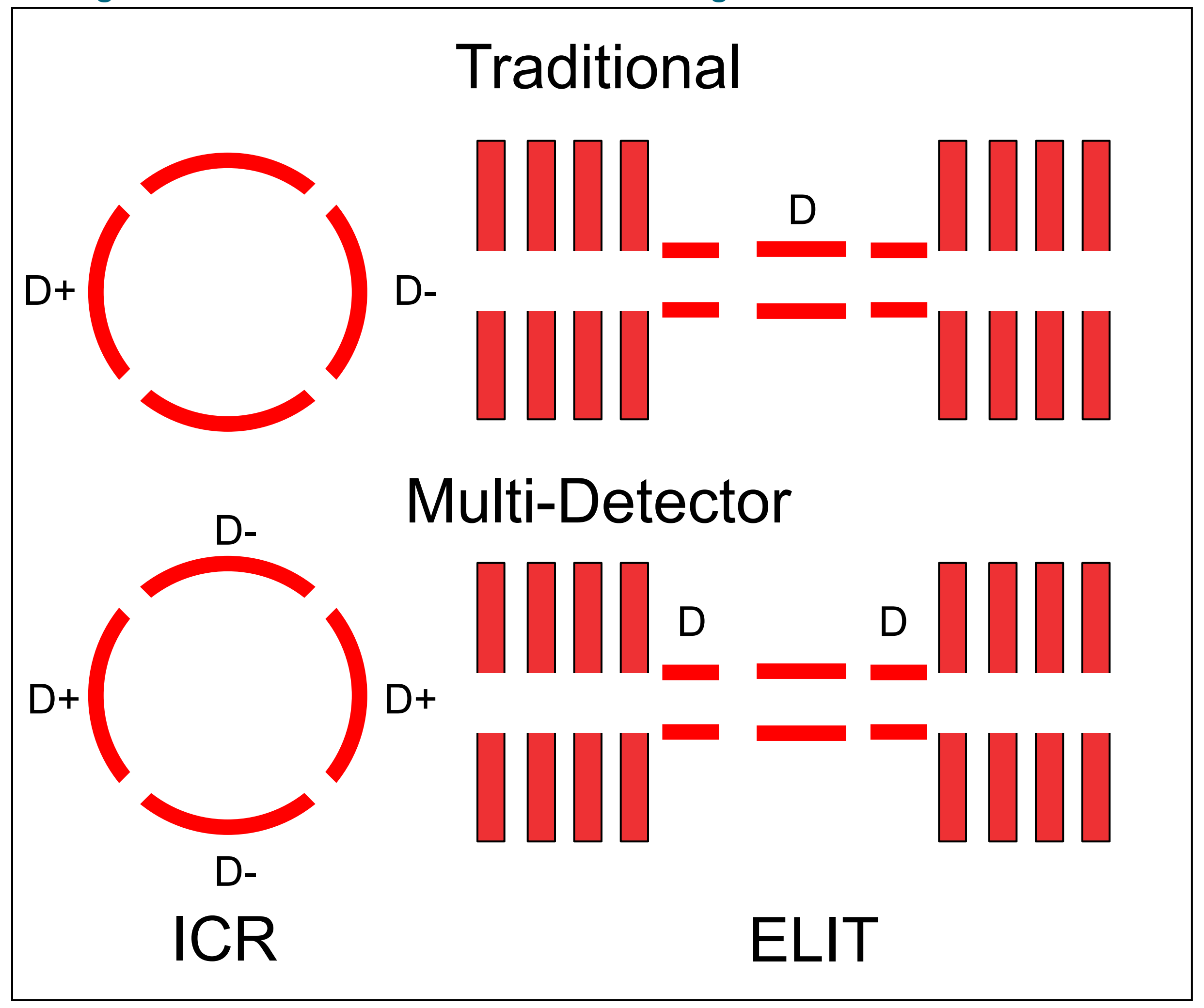
Electrostatic Linear Ion Traps (ELIT) have grown in popularity in the mass spectrometry community due to the high performance that can be obtained with a low level of instrumental complexity [1]. ELIT's are also the basis for many Charge Detection Mass Spectrometers (CDMS) [2-4], which are of expanding importance due to the ability to easily characterize complex biopharmaceuticals and drug delivery vehicles like adeno-associated viruses (AAV).

Although ELITs provide relatively high performance for a simple instrument, the achievable resolution falls short when compared to FTICR and Orbitrap instruments. To improve ELIT resolution, there have been attempts to use multiple detectors, which would allow the generation of a higher frequency signal than what is achieved with a single detector [5]. This is meant to mimic the successful use of multiple detectors with FTICR's [6,7].

MATERIALS AND METHODS

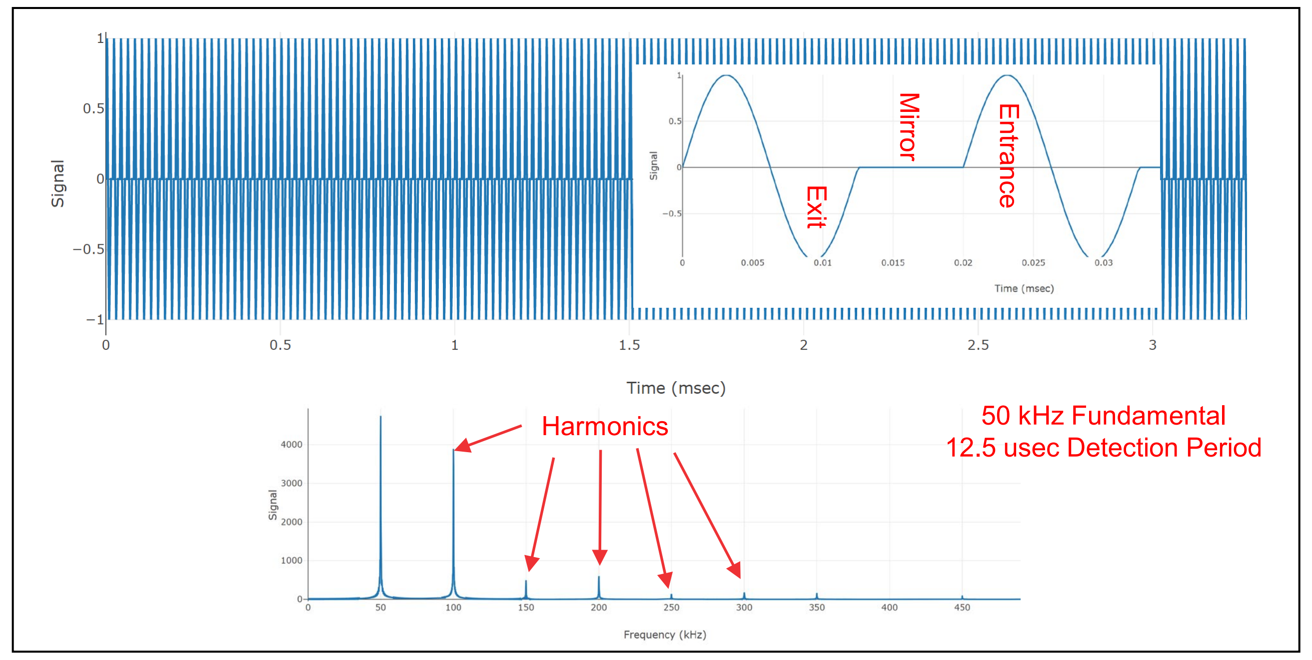
All simulations were performed in Lua. Synthetic time domain signals were generated without signal decay. Frequency domain spectra were generated by Fourier transform using one zero fill and no apodization.

Figure 1. Standard and Multi-detector configurations for ICR and ELIT



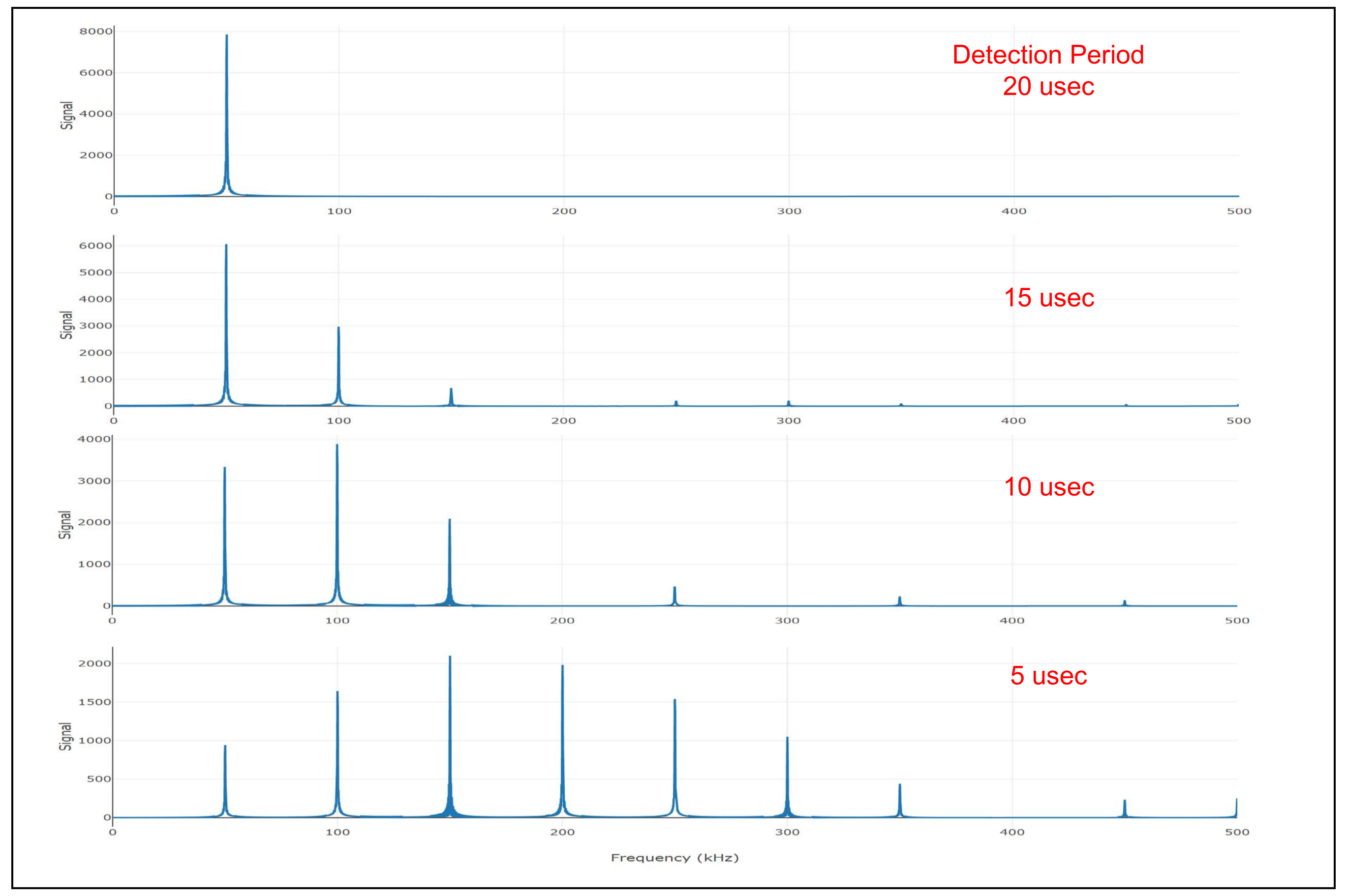
RESULTS

Figure 2. Synthetic Signal for Single Detector



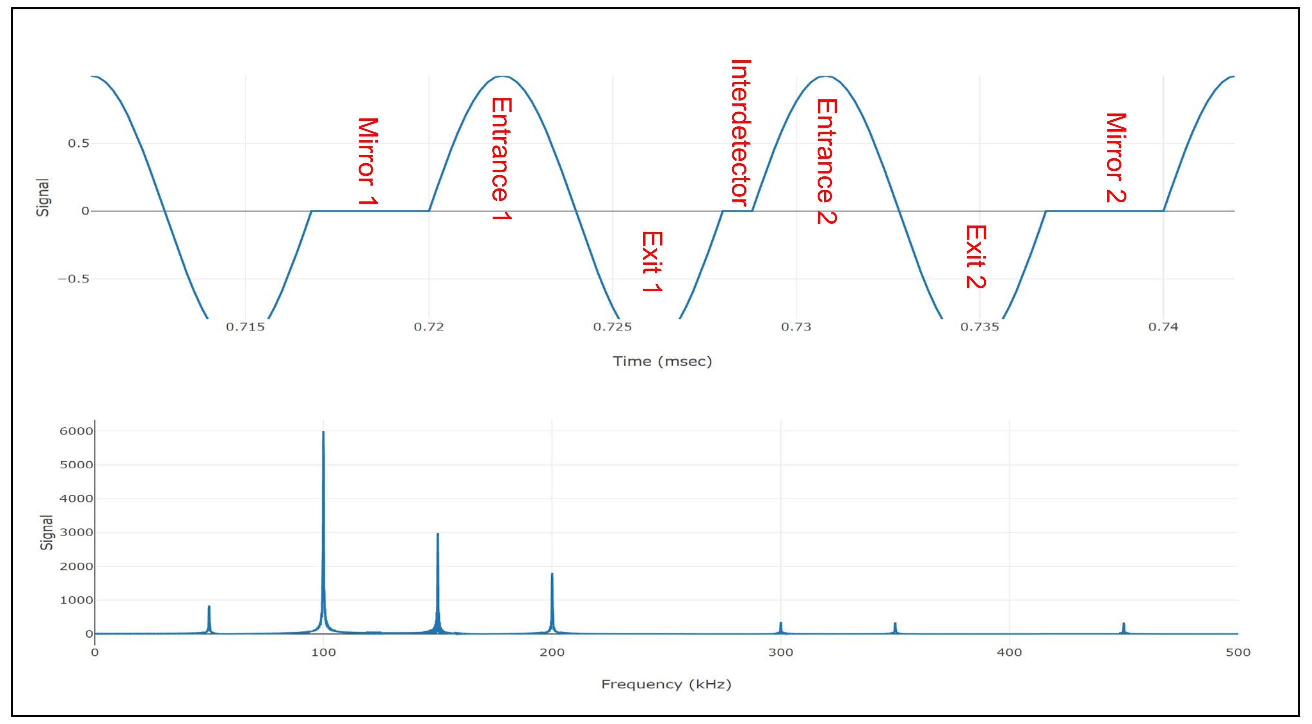
Shown in Figure 2 is a synthetic signal for an ELIT, where the ion packet passed through the detector every 20 usec, with 12.5 usec being spent in the vicinity of the detector, and 7.5 usec being spent ion the ion mirror. Since the signal is not a pure sine wave, the result of the Fourier transformation is a series of harmonics.

Figure 3. Effect of Detection Period on Harmonic Content



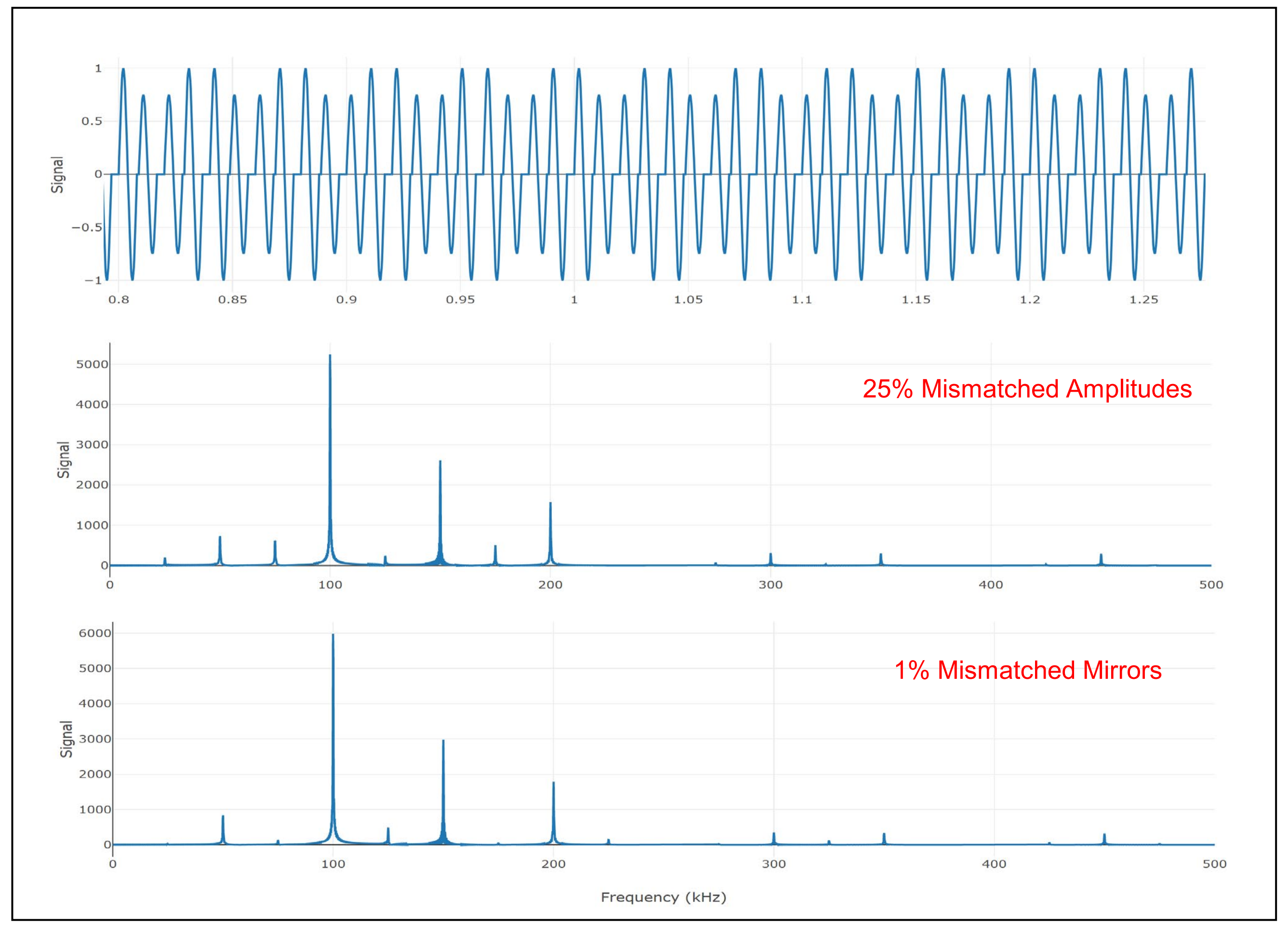
Shown in Figure 3 is the effect of the detection period on the harmonic content. When the detection period exactly matches the fundamental period, the result is a pure sine wave, with no harmonics. As the detector sees shorter signal pulses and the ions spend more time in the mirror, the amount of harmonic content increases. This can be exploited to improve resolution but comes at the cost of sensitivity and spectral complexity.

Figure 4. Synthetic Signal for Dual Detector



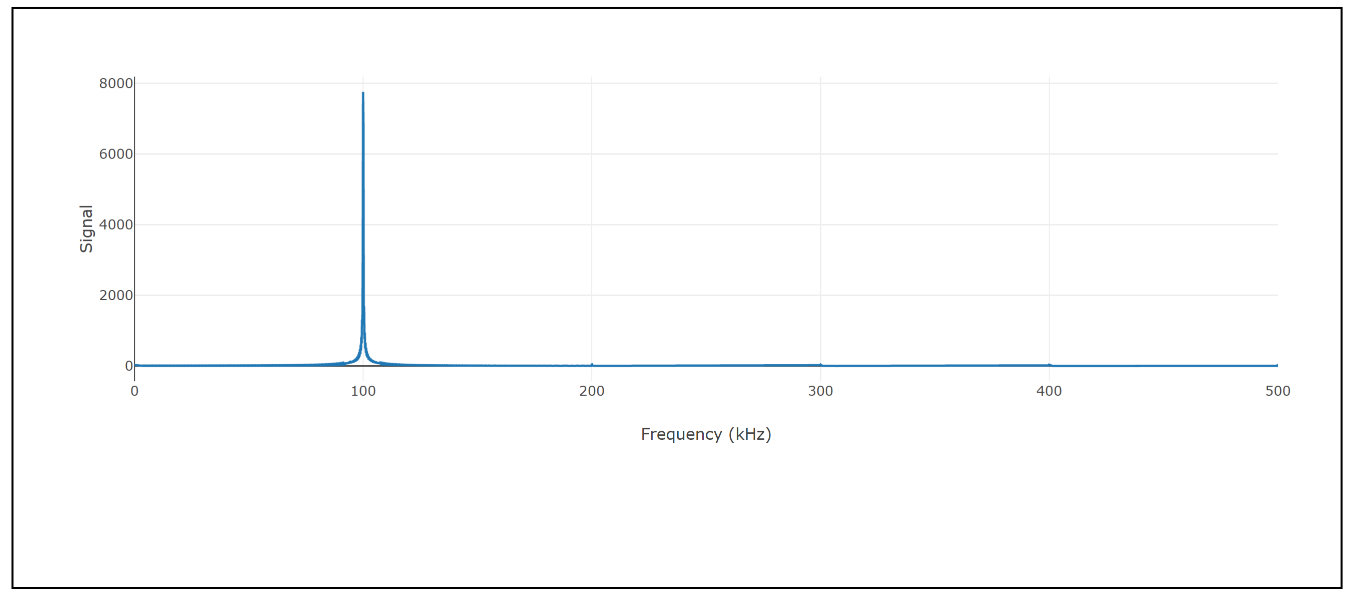
Shown in Figure 4 is the effect of using a second detector between the mirrors. This increases the harmonic content beyond what is observed for a similar single detector since the repetitive signal has less characteristics of the fundamental. This will only result in higher resolution if the spacing between mirrors does not increase significantly, which would result in a lower fundamental frequency. This is unlike an ICR, where additional detectors will not decrease the cyclotron frequency The second detector does increase the total signal, and under certain conditions, this will improve sensitivity, while multiple detectors in ICR generally reduce sensitivity.

Figure 5. Mismatched Detectors



Shown in Figure 5 is the effect of having detectors which don't produce identical signals. This is equivalent to amplitude modulation at half the fundamental frequency, and results in sidebands on each peak seen in Figure 4. This both steals signal from the primary peaks and adds to spectral complexity. The mismatch can be caused by either unequal gain of the detectors, or different mirror turn around times. An ideal ELIT with two detectors would result in perfect detection of twice the frequency (Figure 6), but this would require the two detector device to be the same size as the single detector device, and the precision required for construction and operation may be impractical.

Figure 6. Spectrum from an Ideal Dual Detector ELIT



CONCLUSIONS

Efforts with ELITs have produced limited success, due to a fundamental difference of the ion motion and detector geometries compared to ICR's. While the use of multiple detectors in ICR can generate integer multiples of the cyclotron frequency, detectors in ELITs generate stronger harmonics of the fundamental frequency, and non-ideal detectors will produce amplitude modulation. When using Fourier analysis, the modulation results in splitting, or sidebands of the fundamental, and not the desired multiplication that would provide higher resolution. ELITs with multiple detectors may still prove to be beneficial if they are combined with non-FT based processing techniques [8,9]

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ACKNOWLEDGEMENTS

I would like to acknowledge the San Jose Orbitrap Tribrid Science group for enlightening discussions.

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