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CORRELATION ION MOBILITY SPECTROMETRY: THE INTERSECTION OF RADAR AND IMS

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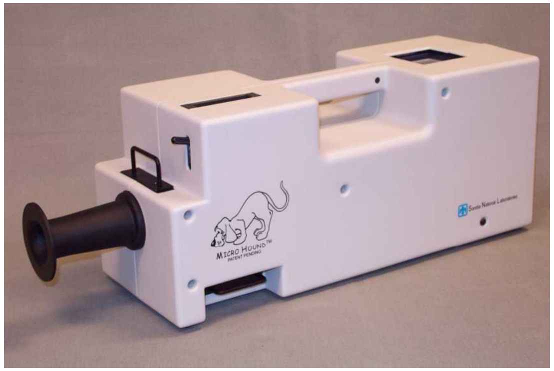
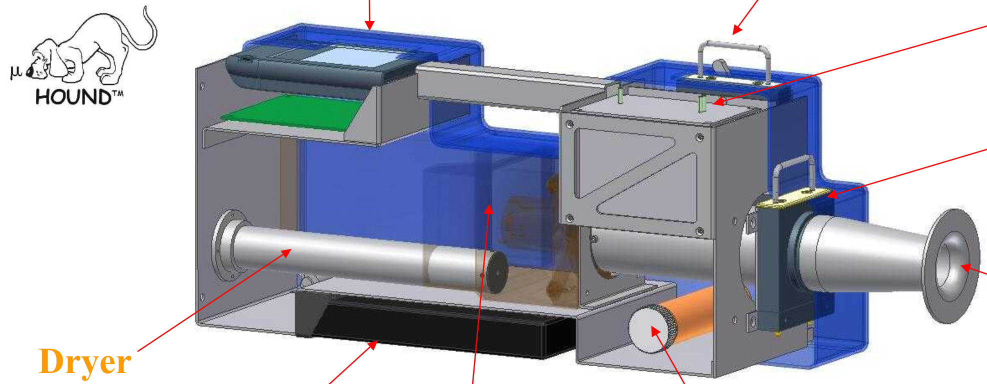
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

μ-Hound™ Concept

Handheld Explosives Detection System for First Responder Applications



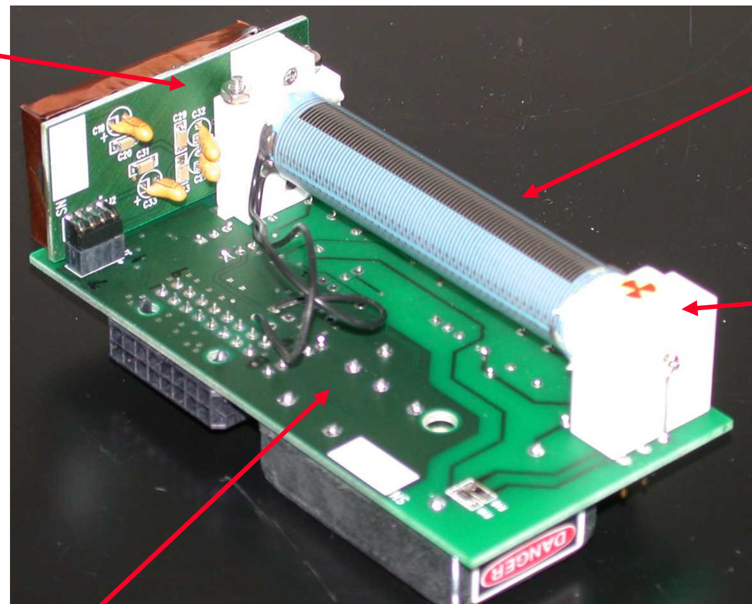


Prototype units are currently undergoing field trials with several agencies.

Sandia Miniature Rolled IMS

200 dB TIA
(10Hz-5kHz)

LTCC Drift Tube



20 μCi Am^{241}

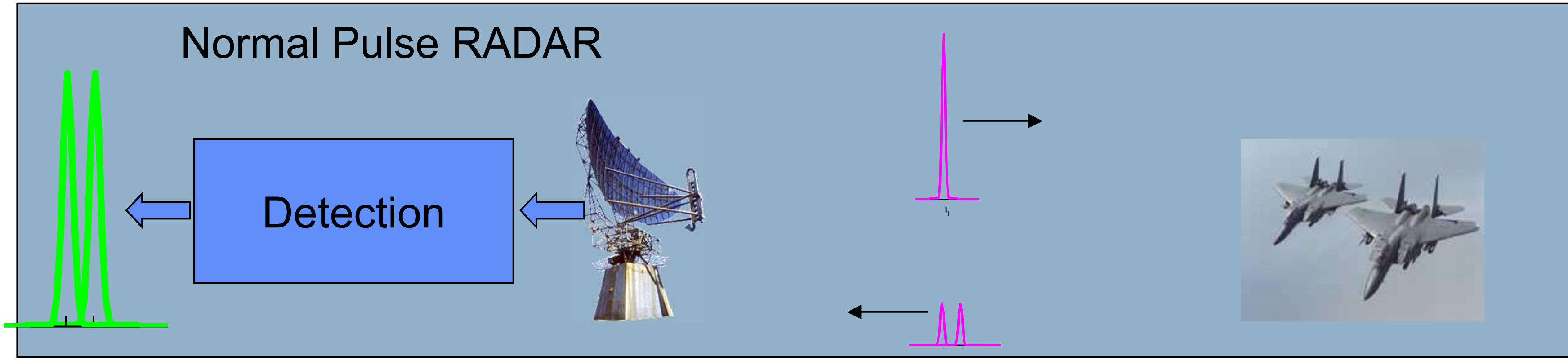
Tube Parameters

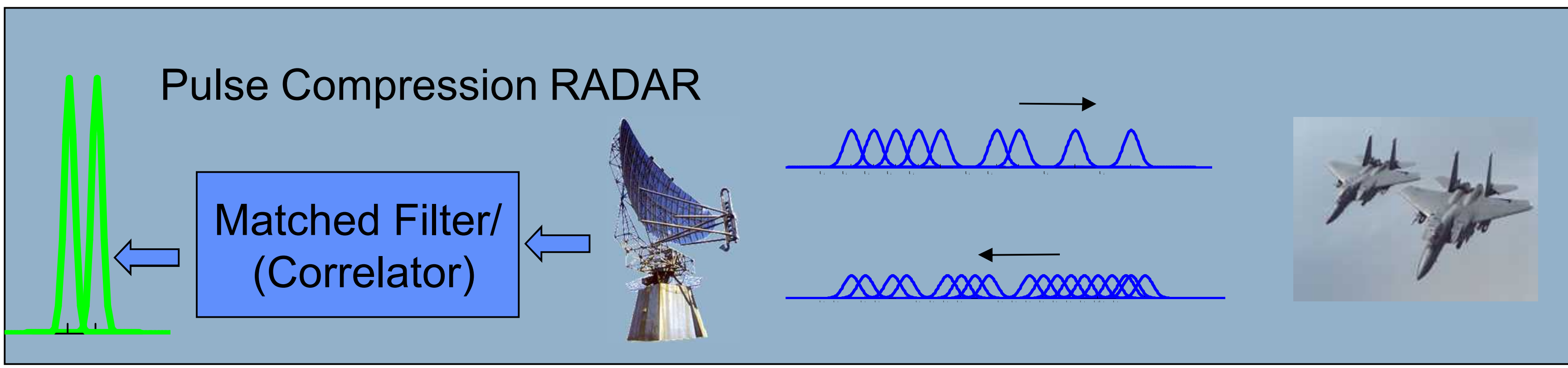
- 3-D LTCC
- 57mm Drift Length
- 12.5mm Diameter
- Nominal Res. 16

HV Switching/Supply

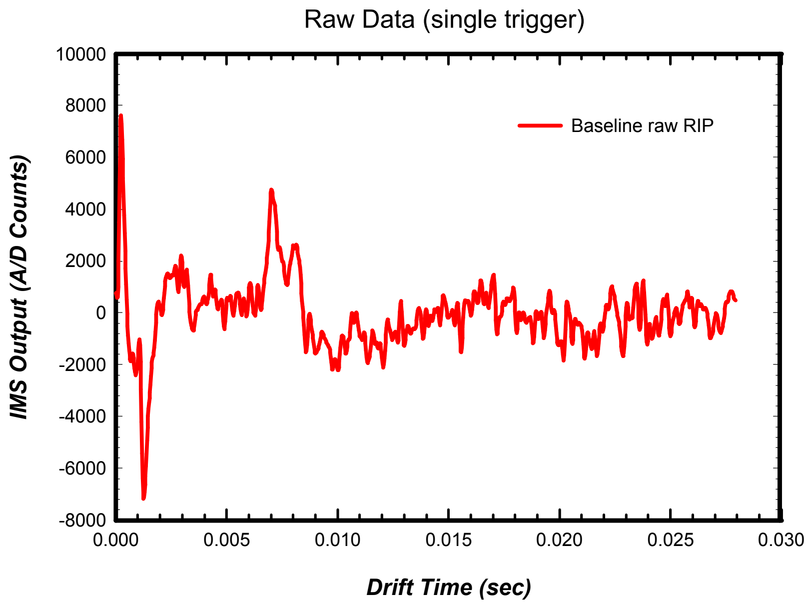
6cm x 6cm x 10 cm

Radar Analogy





Single Sweep S/N



$$SNR_{ave} = \sqrt{N}\, SNR_1$$

Detection requires chemical signature to remain constant during N sweeps.

Achievable SNR is limited in transient chemical systems such as μ-Hound™.

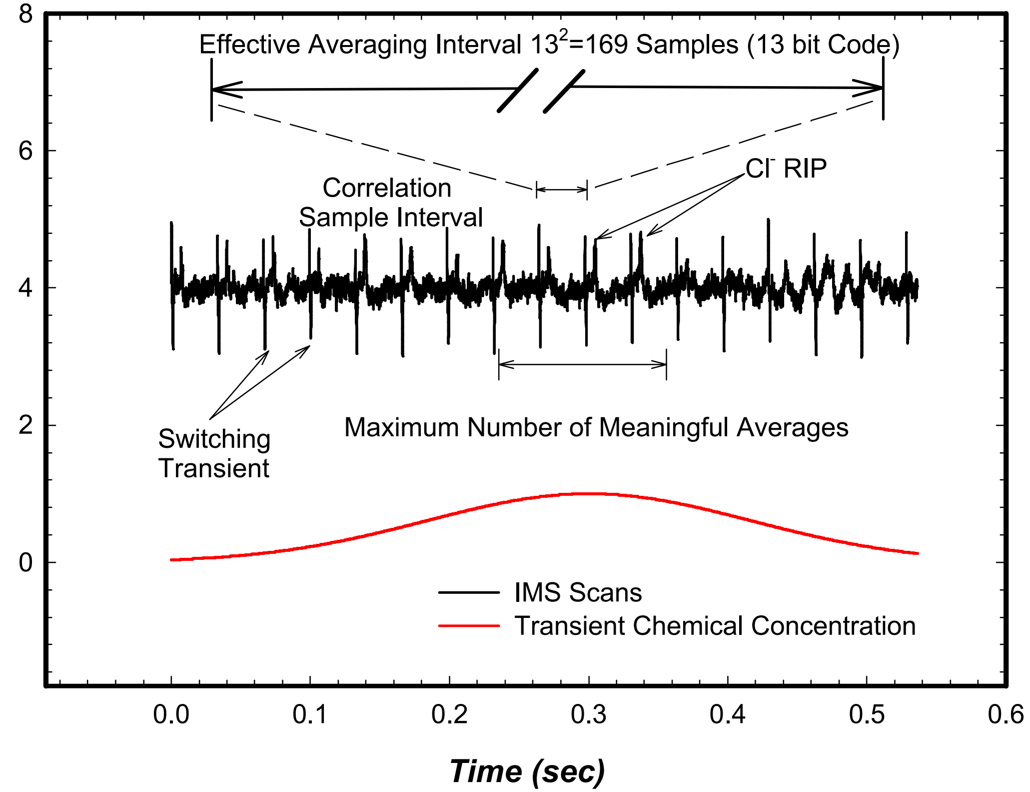
$$SNR_{peak} \leq \frac{2SignalEnergy}{MeanNoisePower}$$

Pulse Compression/ Barker Coding allows increase in signal energy while maintaining mean noise power. SNR is improved in ***SIMILAR MEASUREMENT TIME***!!

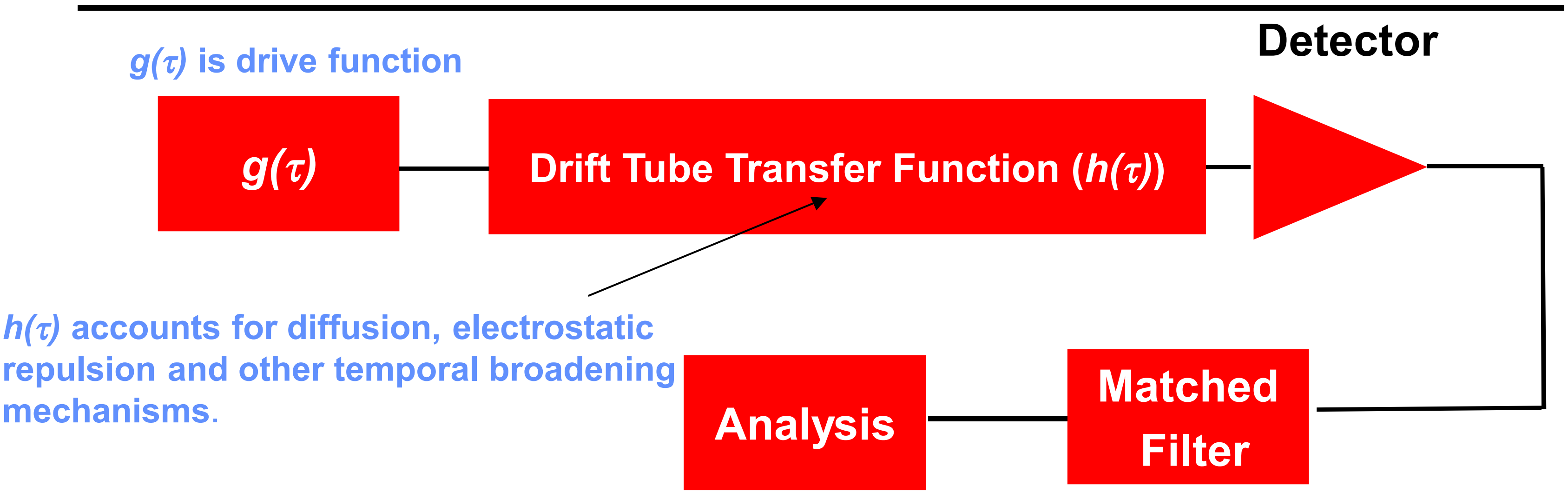
Advantage of Correlation IMS

By putting more information into a given IMS pulse, more SNR in a shorter interval can be obtained without risk of data "smear."

System requires more back end processing (matched filtering) to extract result.



Principle of Correlation IMS



Matched filter is designed to deconvolve the convolution of the drift tube transfer function ($h(\tau)$) with the drive function ($g(\tau)$). *A priori* knowledge of the drive function allows construction of the matched filter. Drive function ($g(\tau)$) can be any one of several binary or analog coding schemes including Barker-based codes or "chirped" sinusoidal drive signals.

CIMS Soapbox

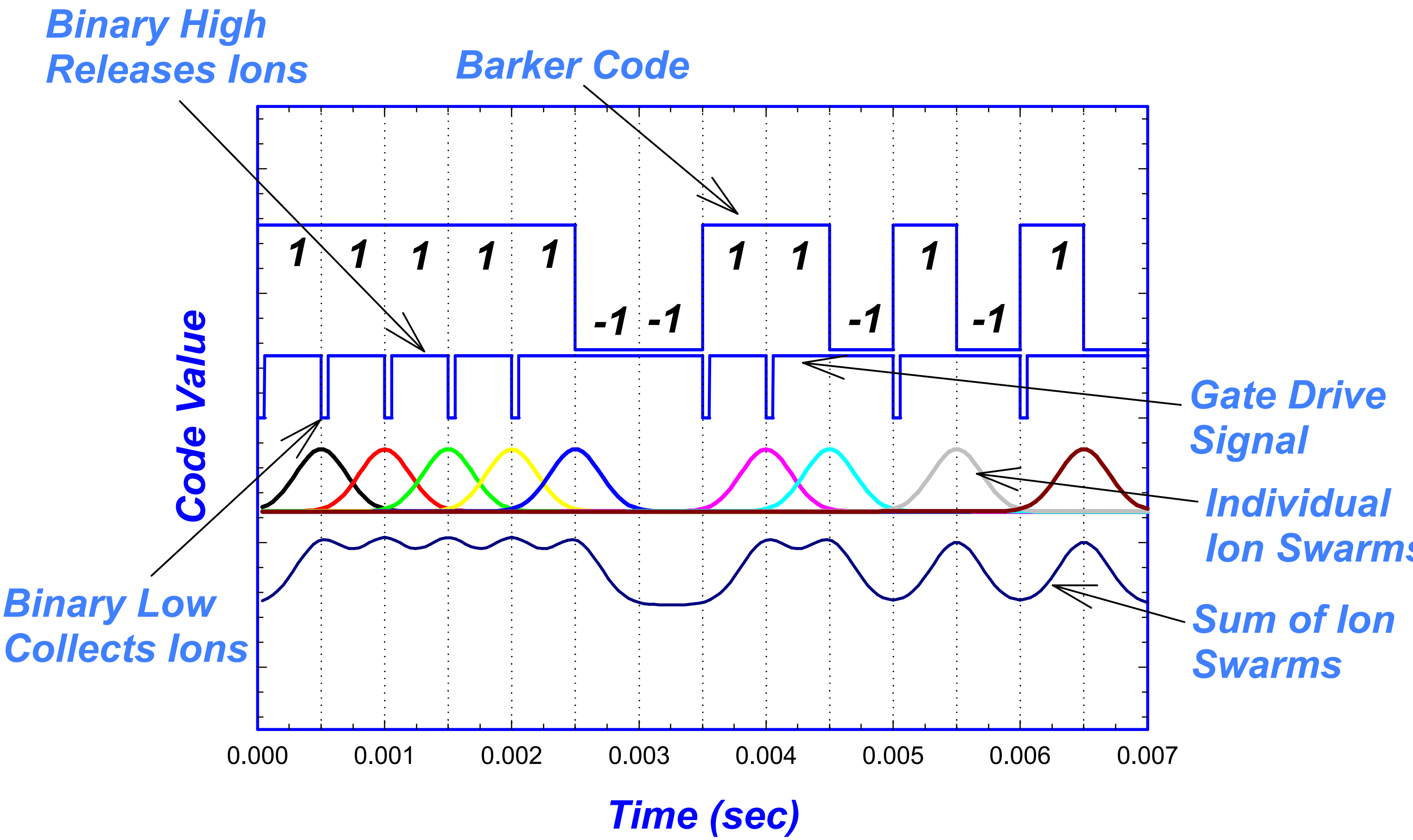
CIMS is <u>*NOT*</u> a Transform Technique

- Data is acquired in time domain and correlated in time domain.
  - FTIMS – data acquired in frequency domain and subsequently transformed back into time domain.
  - Hadamard – "Hadamard weights" acquired in binary "bin" domain and then transformed back into time domain.

Barker Codes are <u>*NOT*</u> a special case of Hadamard codes

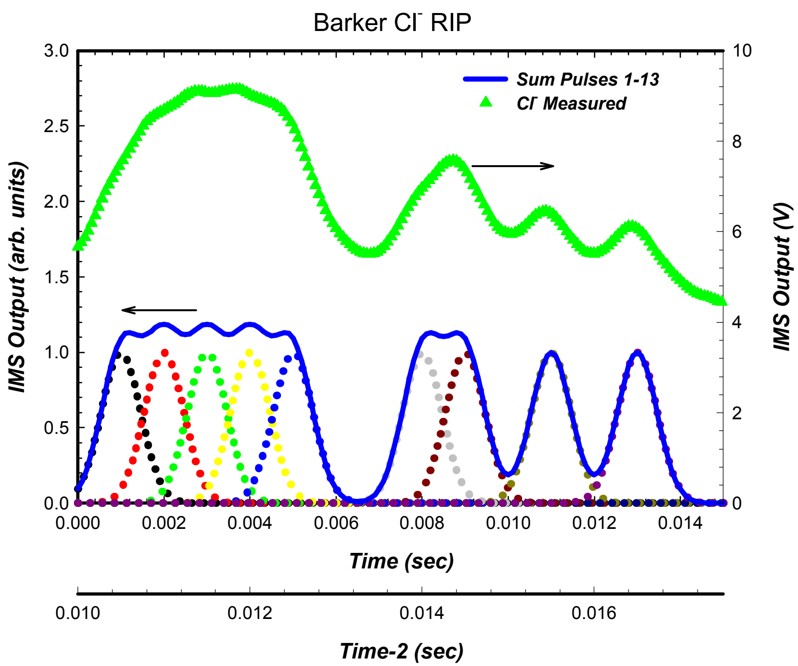
- Barker has equal side-lobe amplitude and maximum center to side-lobe ratio.
  - Hadamard codes have $\frac{N-1}{2}+1$ positive bits; Barker NO!
  - No known Barker codes greater than 13 bits; Hadamard known to hundreds of bits.

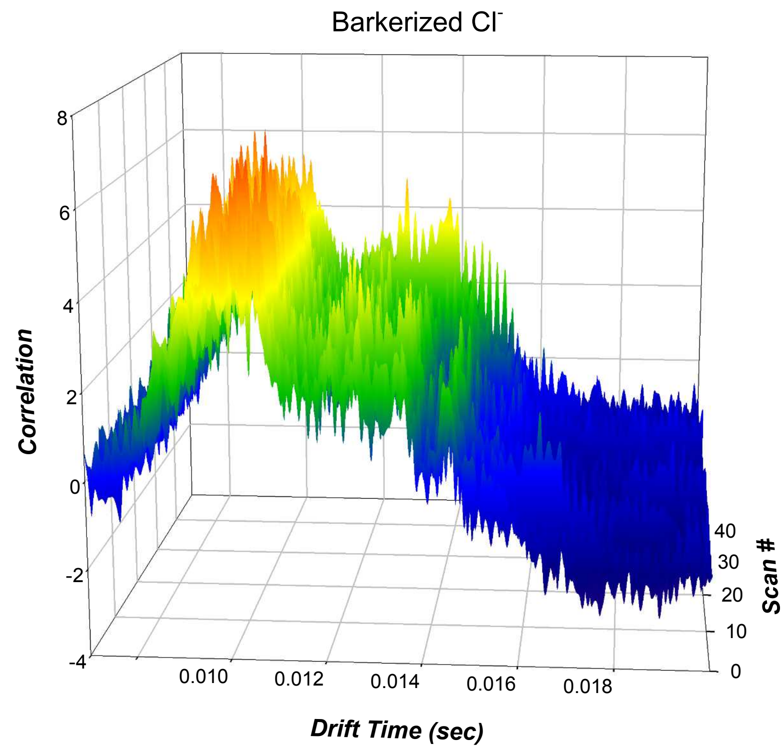
Barker Generation Approach



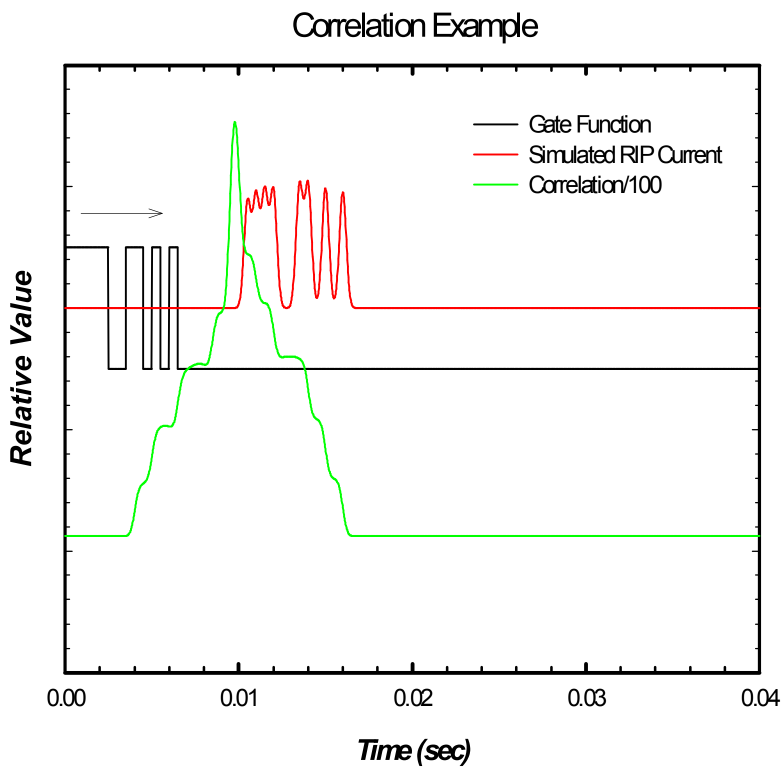
13-Bit Barkerized IMS Signal

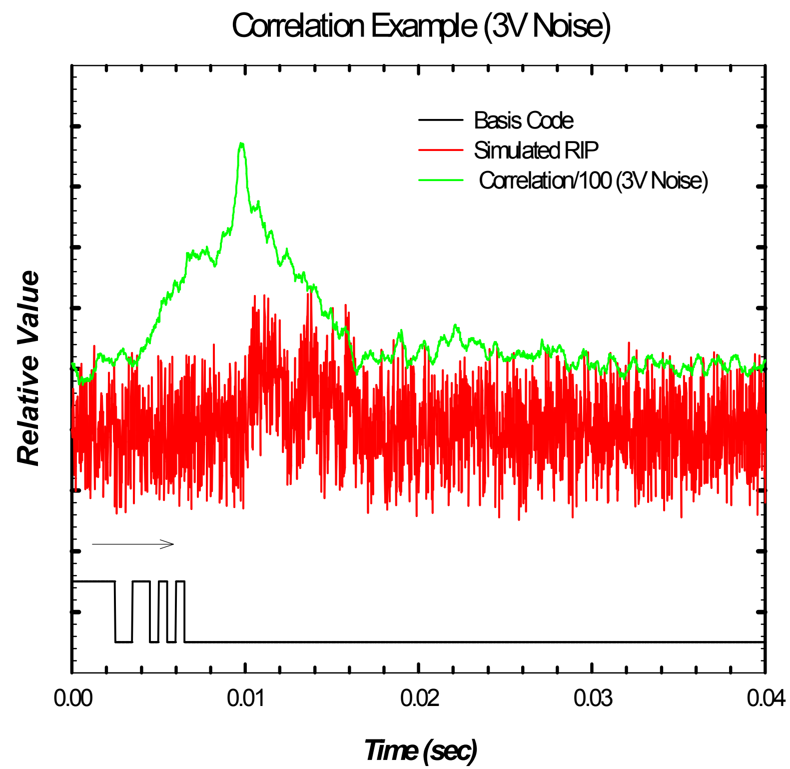
$$g(t) = (+ + + + + - - + + - + - +) \qquad \begin{cases} "+" = 1 \\ "-" = -1 \end{cases}$$





CIMS Illustrated





CIMS Processing "Simply" Stated

1) $$i(t) = \int_{-\infty}^{\infty} g(\tau)\, h(t - t_d - \tau)\, d\tau.$$

2) $$g(t) = \tfrac{1}{2} \sum_{m=-\infty}^{\infty} A_m e^{j\omega_m t}\,, \quad \omega_m = \frac{2\pi m}{T}$$

3) $$i(t) = \tfrac{1}{2} \int_{-\infty}^{\infty} \sum_{m=-\infty}^{\infty} A_m\, e^{j\omega_m \tau}\, h(t - t_d - \tau)\, d\tau =$$

$$\tfrac{1}{2} \sum_{m=-\infty}^{\infty} A_m \int_{-\infty}^{\infty} e^{j\omega_m \tau}\, h(t - t_d - \tau)\, d\tau$$

4) $$i(t) = \tfrac{1}{2} \sum_{m=-\infty}^{\infty} A_m\, H(\omega_m)\, e^{j\omega_m (t - t_d)}$$

5) $$C(t) = \int_{0}^{T} g^*(\tau)\, i(t + \tau)\, d\tau =$$

$$\tfrac{1}{4} \int_{0}^{T} \sum_{m=-\infty}^{\infty} A_m^*\, e^{-j\omega_m \tau} \sum_{n=-\infty}^{\infty} A_n\, H(\omega_n)\, e^{j\omega_n (t - t_d + \tau)}\, d\tau$$

6) $$C(t) = \tfrac{1}{4} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} A_m^*\, A_n\, H(\omega_n)\, e^{j\omega_n (t - t_d)} \int_{0}^{T} e^{j(\omega_n - \omega_m)\tau}\, d\tau$$

$$\delta_{n,m} = \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases}$$

7) $$C(t) = \tfrac{1}{4} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} A_m^*\, A_n\, H(\omega_n)\, e^{j\omega_n (t - t_d)}\, \delta_{n,m} = \tfrac{1}{4} \sum_{k=-\infty}^{\infty} A_k^*\, A_k\, H(\omega_k)\, e^{j\omega_k (t - t_d)}$$

$$= \tfrac{1}{4} \sum_{k=-\infty}^{\infty} \left|A_k\right|^2 H(\omega_k)\, e^{j\omega_k (t - t_d)}$$

CIMS Processing Simply Stated

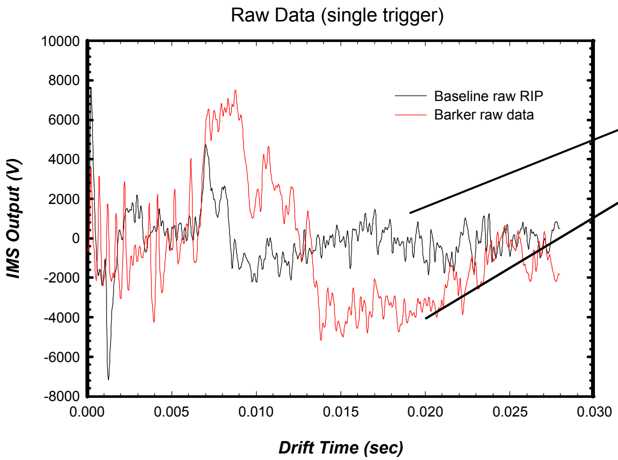
Mass transport of ions in temporally dispersive system does not affect the location of the correlation peak!! Therefore the ion peak position is identified in CIMS. Area under the correlation peak is proportional to amplitude of ion peak! All data is retained.

$$\mathrm{Re}\left[\frac{dC(t)}{dt}\right] = \mathrm{Re}\left[\tfrac{j}{4}\sum_{k=-\infty}^{\infty} \omega_k \left|A_k\right|^2 H(\omega_k)\, e^{j\omega_k (t-t_d)}\right]$$

$$= \tfrac{1}{4}\sum_{k=-\infty}^{\infty} \mathrm{Re}\left[\left|A_k\right|^2 H(\omega_k)\right]\omega_k \sin\left(\omega_k (t-t_d)\right) = 0$$

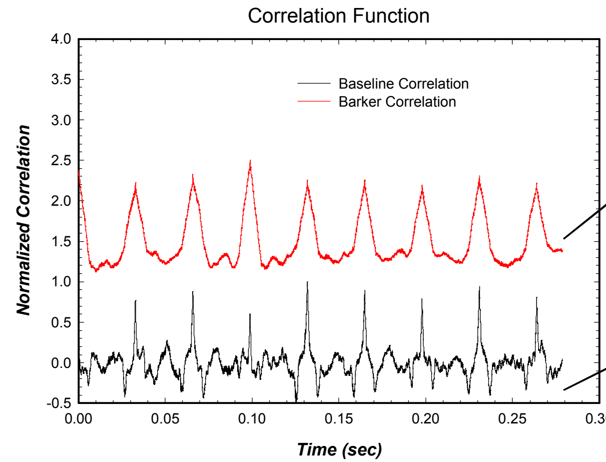
$$\text{when} \quad t = t_d$$

Signal-to-Noise Enhancement



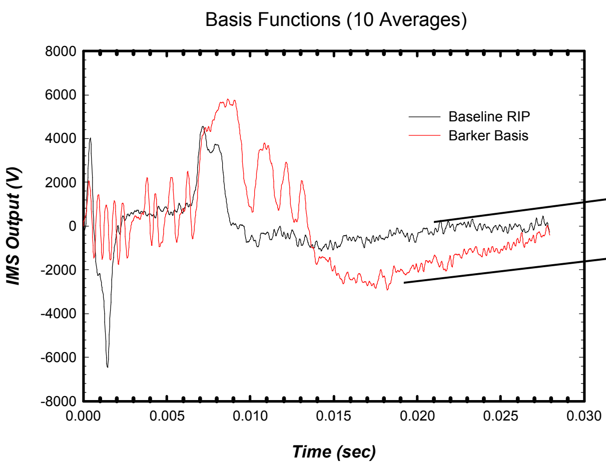
SNR_{Base}=1.84

SNR_{Barker}=2.4



SNR_{Barker}=30.0

SNR_{Base}=12.4



SNR_{Base}=5.0

SNR_{Barker}=7.3

$$SNR_{ave} = \sqrt{10}SNR_1$$

SNR Enhancement using CIMS is a factor of

12.5

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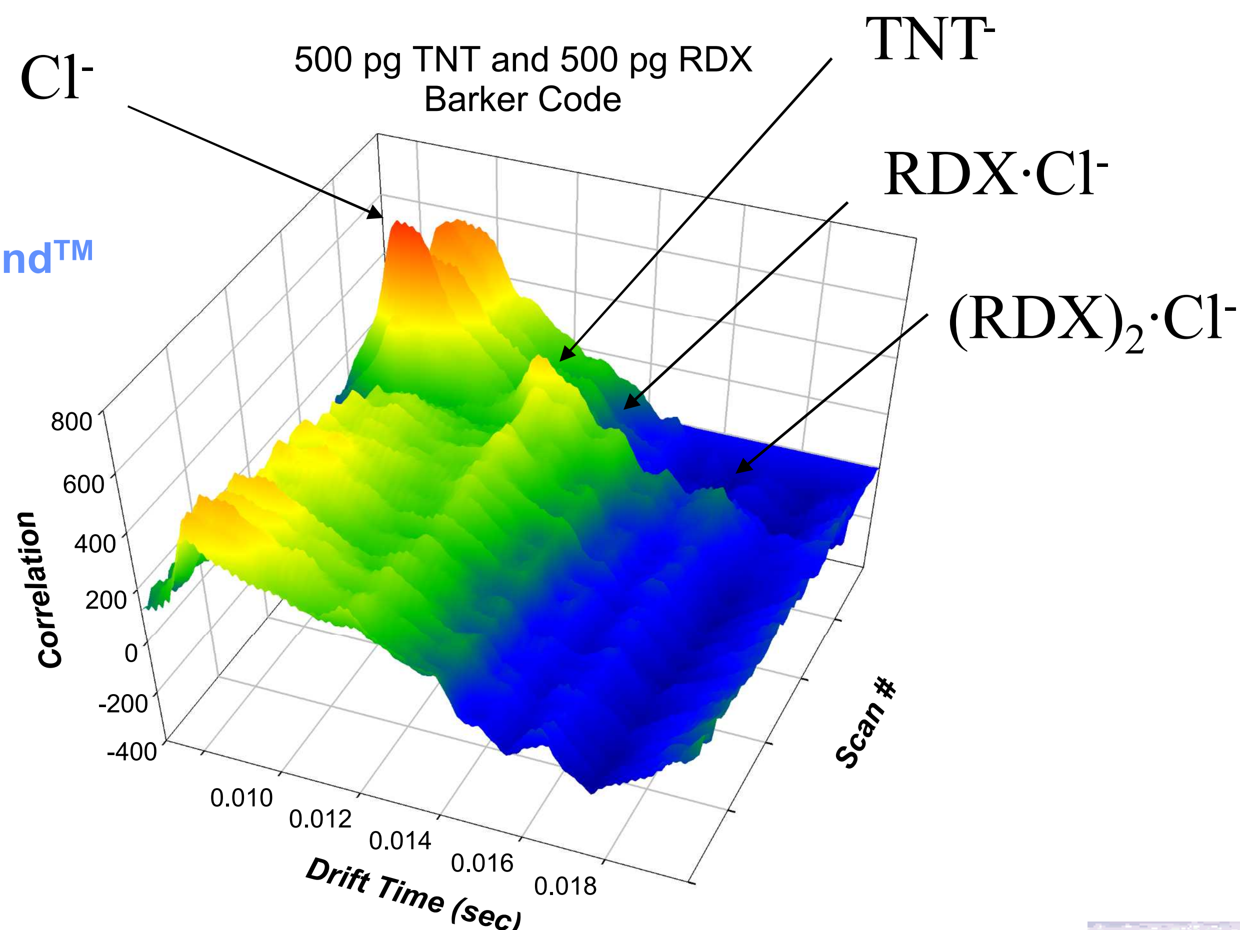
ISIMS 2006
Honolulu, HI
July 23-28, 2006

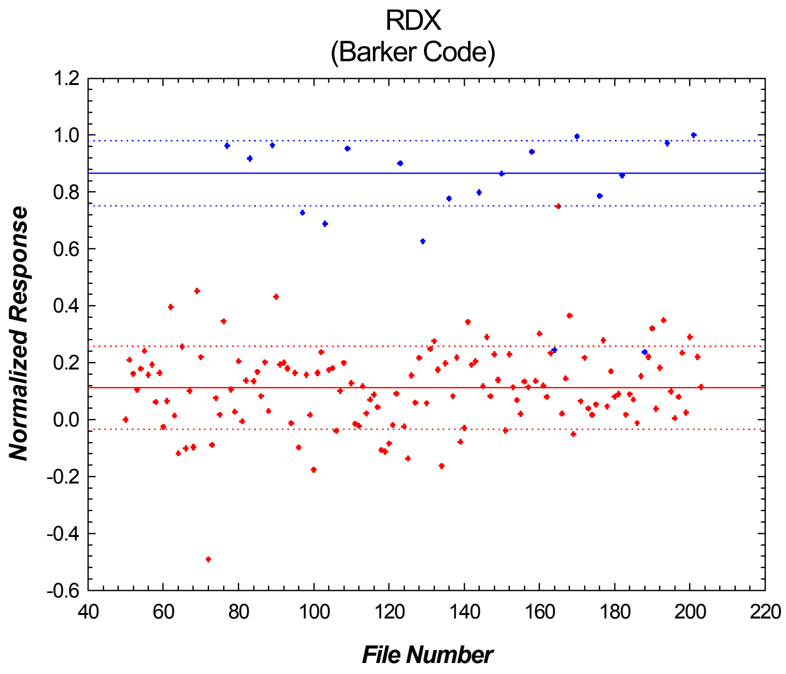
Sandia National Laboratories

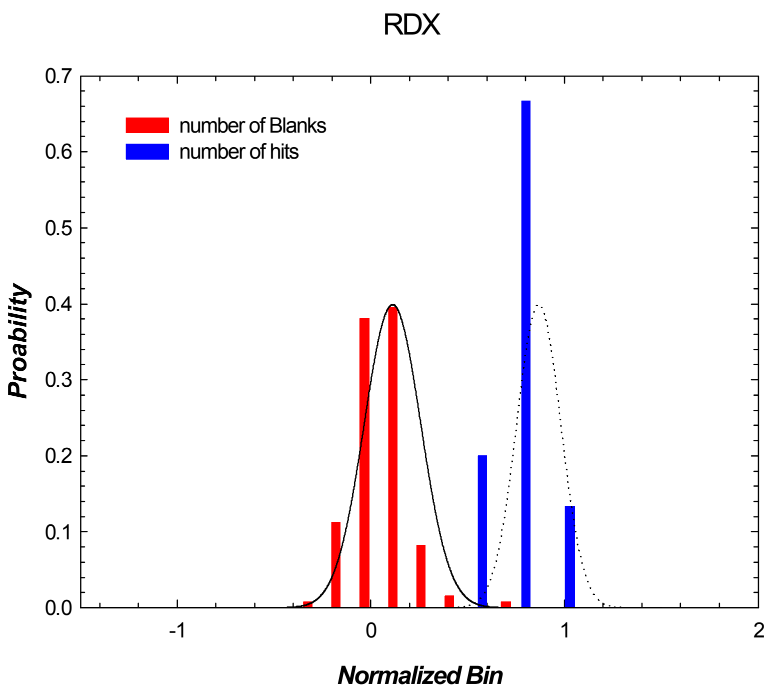
500pg TNT and 500 pg RDX

Thermal desorption experiment in μ-Hound™ system.



RDX Statistics





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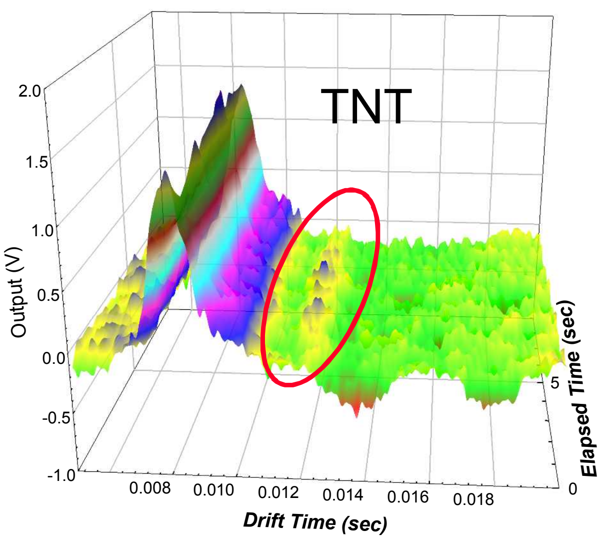
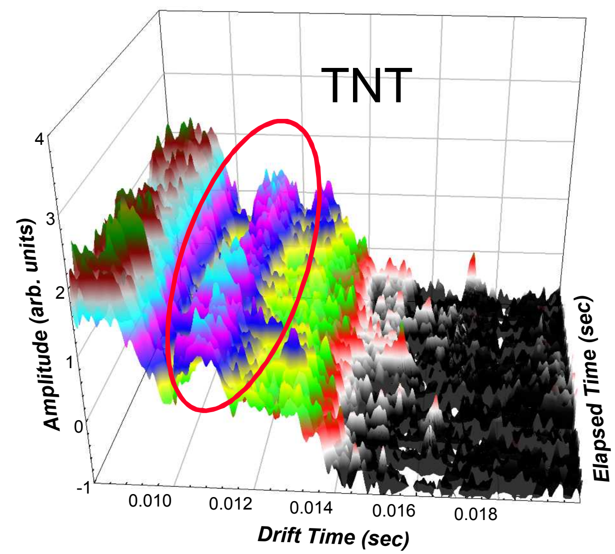
10 ng TNT Comparison

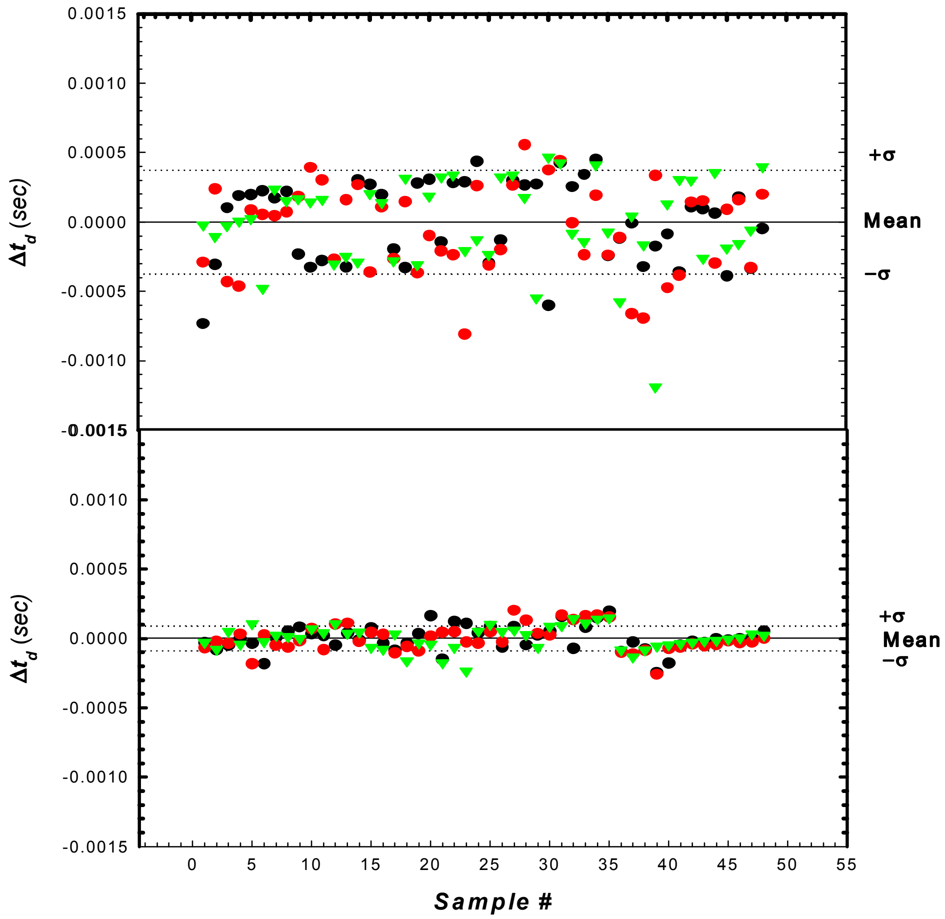
10 ng (Normal Mode)



10 ng TNT Correlated



"Jitter"



Uncorrelated peak has uncertainty of ±400 μsec

Correlated peak has uncertainty of ±80 μsec

Peak location is enhanced by factor of ~5 in this example.

System and Processing

"Ain't nothin' free but the air you breathe" - D. M. Pfeifer 1923-1996

Processing Requirements for CIMS

$$C(t) = \int_{-\infty}^{\infty} y_{signal}(\lambda)\, y_{Code}(t_0 - t - \lambda)\, d\lambda$$

$$C(t) = \sum_{i=1}^{n} y_{signal}(\lambda_i)\, y_{Code}(t - t_0 - \lambda_i)$$

Hardware Requirements for CIMS

1. None required!
2. Dedicated hardware trigger control (optional)
3. Dedicated hardware matched filter to perform correlation (optional)
4. Matched filter in software or hardware (required)

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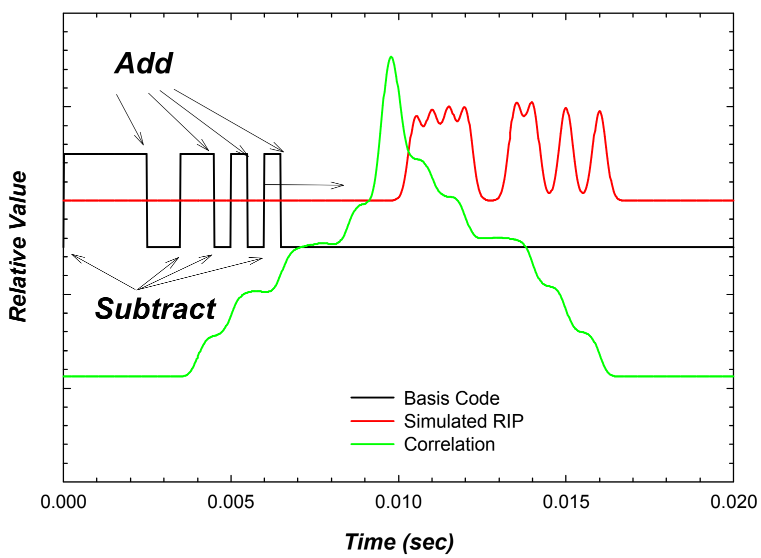
Processing Efficiency



- Barker codes (digital) can be implemented using ***no*** floating point multiplications.
- All digital code correlations can be implemented using simple addition and subtraction algorithms requiring minimal processing overhead to implement.

Conclusions

- SNR improvement equivalent to 169 averages of data observed using conventional mode.

  169*20 msec = 3.4 sec integration time (conventional).

  20 msec integration time (CIMS).

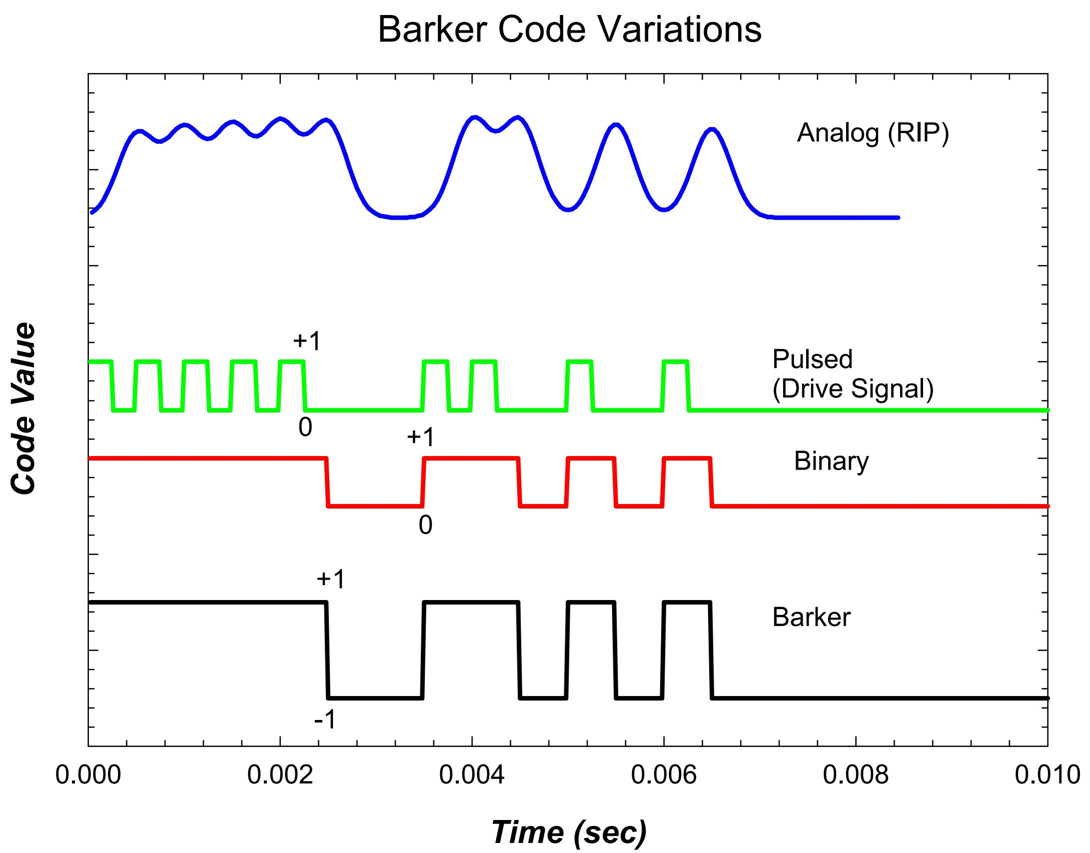
<u>Allows Measurement of Fast Transient Concentrations!!!</u>

- Significant Improvement in LOD (*13x SNR Enhancement*)
- Peak Location Improvement 5x.
- Excellent peak location and sensitivity observed for binary mixtures.

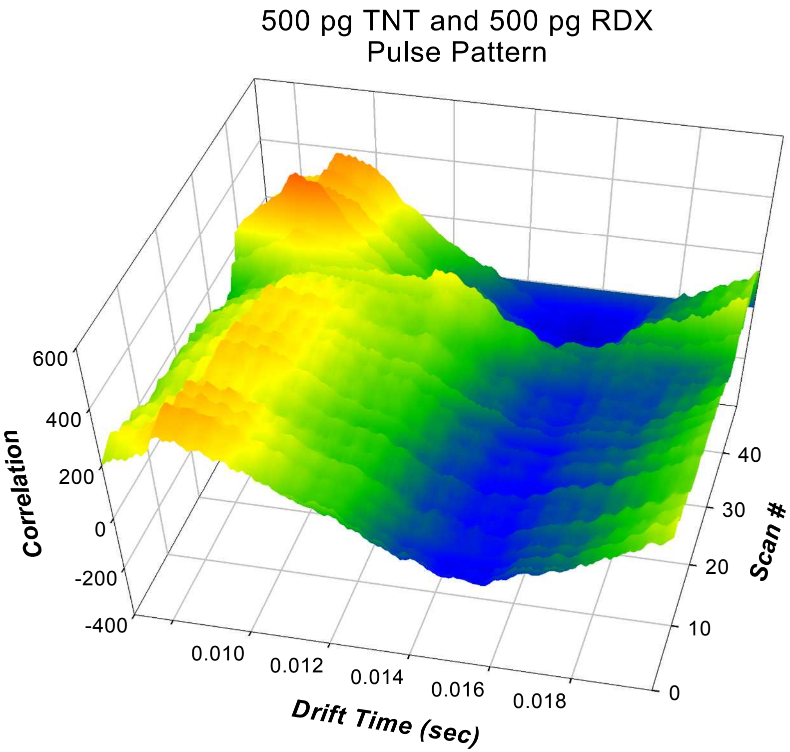
Questions

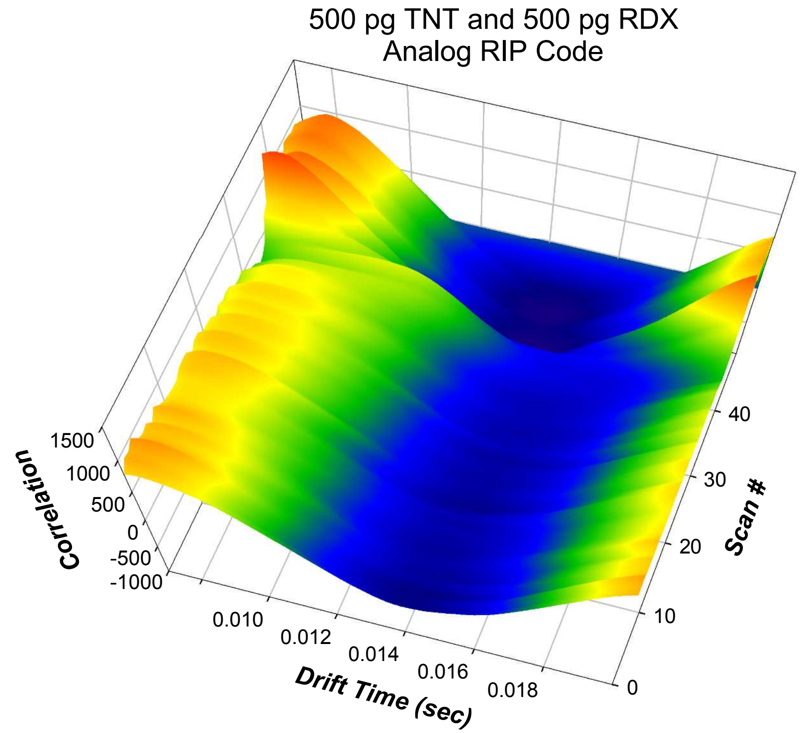
??

Codes Explored



Code Comparison
500pg TNT and 500 pg RDX





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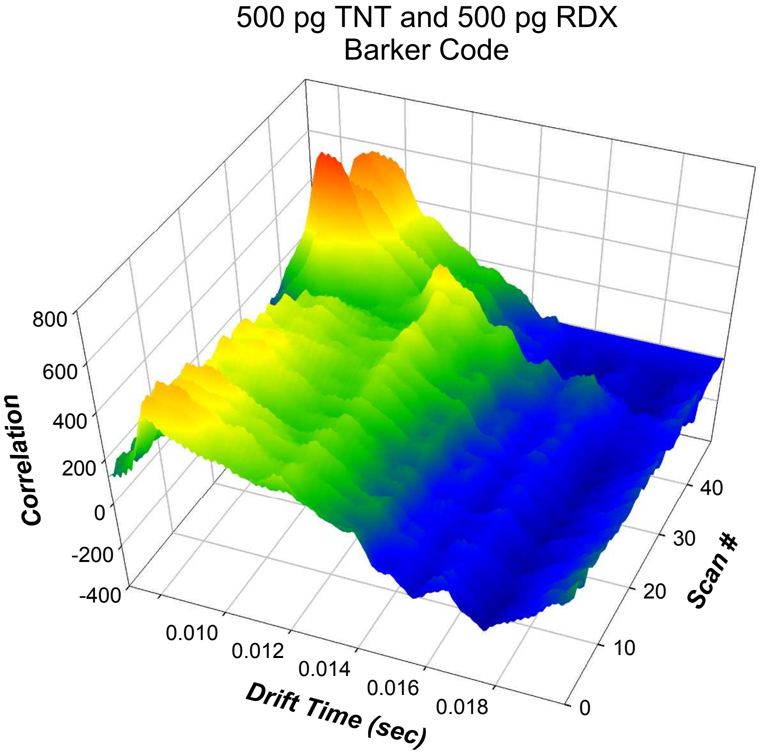
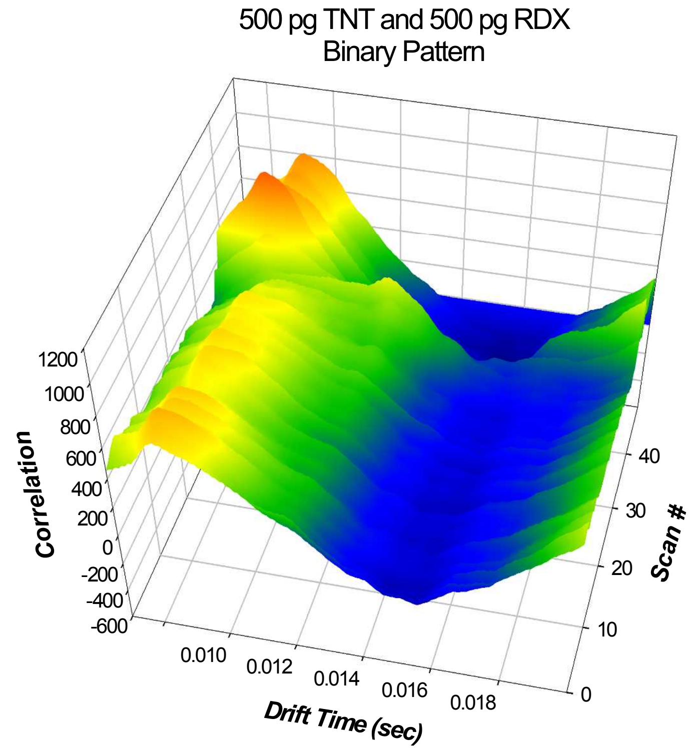
500pg TNT and 500 pg RDX





CIMS Processing Simply Stated

"Someone told me that each equation I included in the book would halve the sales."

Stephen Hawking