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Title: Optimal Control Methods for Explosives Detection

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Optimal Control Methods for Explosives Detection

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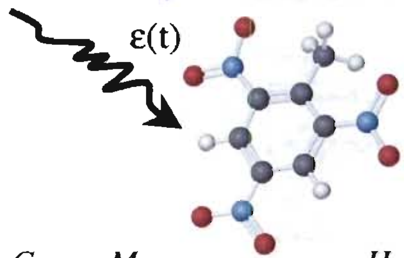
Shock and Detonation Physics Group, WX-9

We are exploring the capabilities of optimal control methods to significantly enhance the standoff detection of explosives. In collaboration with Princeton University, we take advantage of the best capabilities of recent laser technology and recent discoveries in optimal shaping of laser pulses for the optimal dynamic detection of explosives (ODD-Ex). ODD-Ex is a methodology wherein laser pulses are optimally shaped to simultaneously enhance the sensitivity and selectivity of any of a wide variety of spectroscopic methods for explosives signatures while reducing the influence of noise and environmental perturbations. Recent results from ODD-Ex enhanced selectivity of signatures of target analytes in mixtures will be presented. In collaborations with Purdue University and the University of Missouri-Columbia, we are exploring control of remote stimulation of enhanced signatures via energy localization in bulk explosives. We will also present results from a preliminary study of enhanced signatures from remote stimulation using ultrasonic and mm-wave sources.

Optimal Control Methods for Explosives Detection



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Participants and Outline

- **Princeton:**
  - Herschel Rabitz; Jon Roslund
- **Los Alamos:**
  - David Moore; Shawn McGrane; Jason Scharff; Margo Greenfield, Robert Chalmers; Dallas Smith

Outline

- Background
- Optimal Control
- Bandwidth broadening / vibronic control
- Multiplex CARS / mixtures
- Other applications
- Summary

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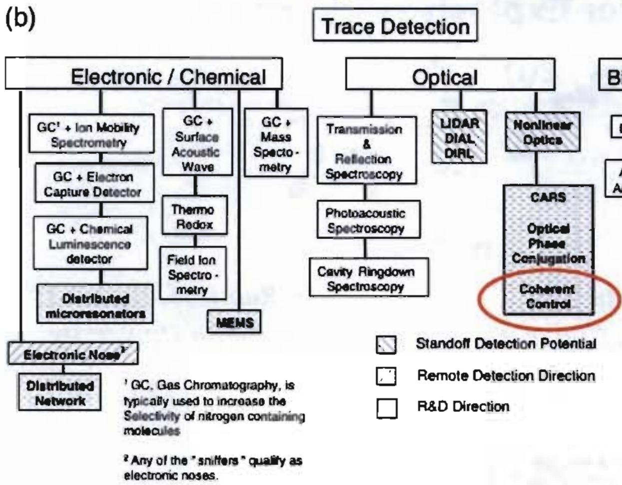
NRC Review

Existing and Potential Standoff Explosives Detection Techniques (2004)

(b)



"Using a new research technique called coherent control could further enhance molecular selectivity…one could choose to selectively ionize or dissociate particular explosive molecules…"

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DHS Workshop

Transformational Breakthroughs - Physics Approaches (LLNL - 2005)

Laser Spectroscopy Topic Area - Recommendations

- Tailored desorption methods to increase vapor phase concentration and suppress substrate lift-off
  - "spatial and temporal laser pulse shaping"
- Expand detected emission spectral range, especially for LIBS
  - LIBS is destructive of both the explosive molecule and the surface
  - Pulse shaping (quantum control) should allow use of much lower laser energies as well as lead to expanded emission spectral range
- Non-linear optical methods
  - Pulse shaping can enhance molecular resonances allowing long distance stand-off detection (i.e., force target molecules to spill out their signatures, or be strong emitters with a unique signature)

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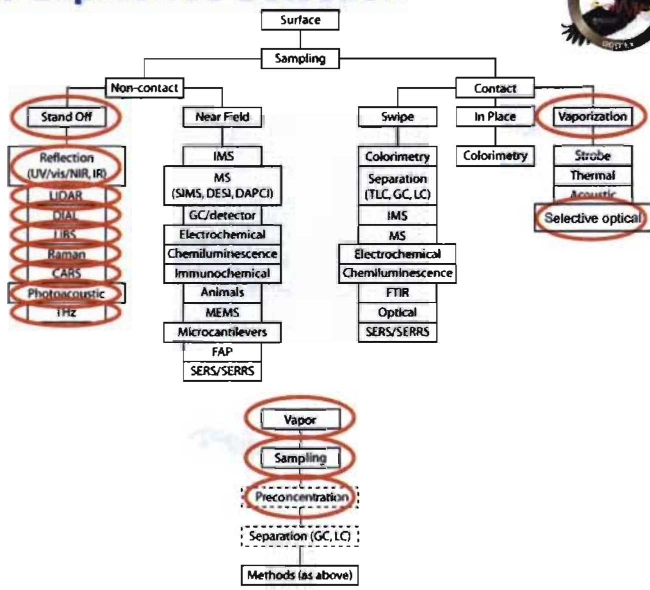
Application to Explosives Detection

- We foresee a large number of applicable areas for ODD
  - Circled in red
  - One can imagine a large number of spectroscopies with vastly improved characteristics



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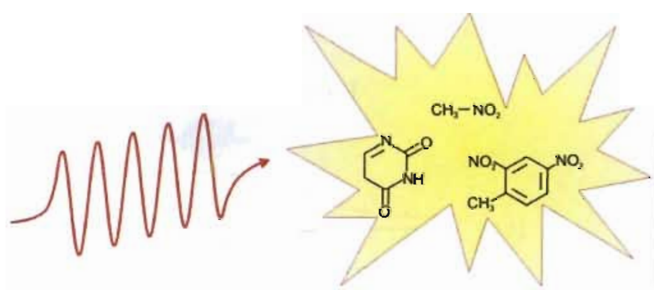
Linear spectroscopy - unshaped pulses

- Conventional steady-state or linear spectroscopy using unshaped pulses
  - Poor molecular discrimination



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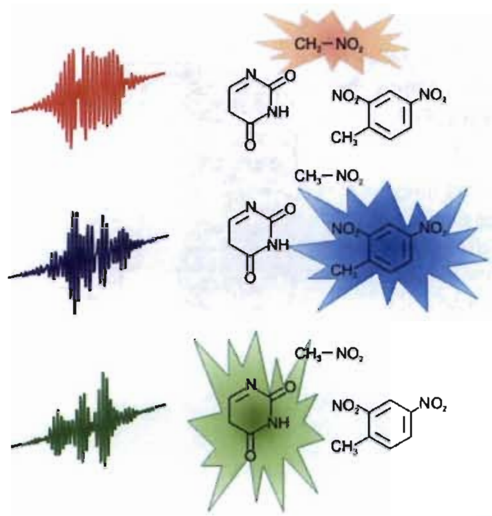
Quantum Optimal Dynamic Discrimination (ODD)

- **Concept**: Optimally tailored laser pulses (photonic reagents)
  - Enables selective addressing of different species



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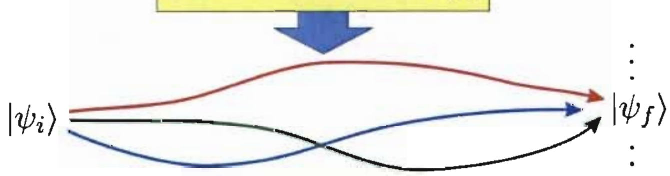
Control of Quantum Systems

- **Customization** of molecular Hamiltonian by optimally shaped field

$$H(t) = H_0 - \mu\epsilon(t)$$

- **Optimally drive** quantum system towards desired final state

Laser Control Field $\epsilon(t)$



- Constructive interference for $|\psi_f\rangle$
- Destructive interference for $|\psi_{f'}\rangle \neq |\psi_f\rangle$

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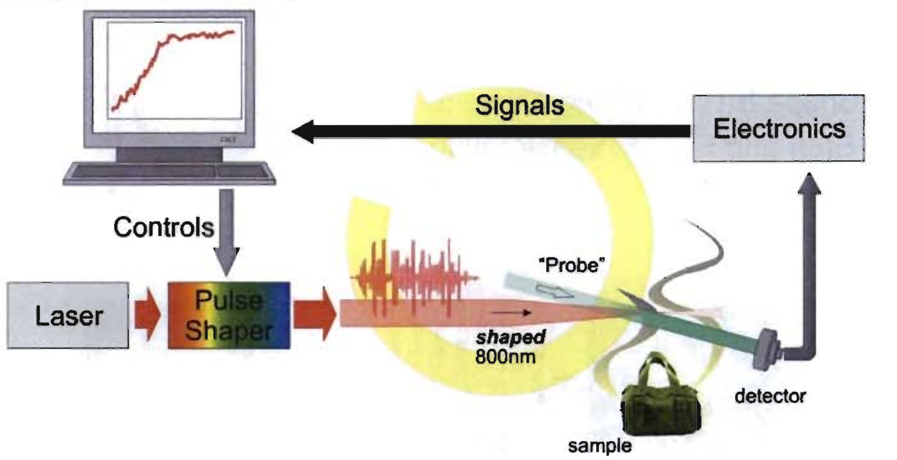
Discovery of Optimal Photonic Reagents

- **Fully automated** high duty cycle closed-loop operation



- **High finesse control** of system without *a priori* model of the physical sample

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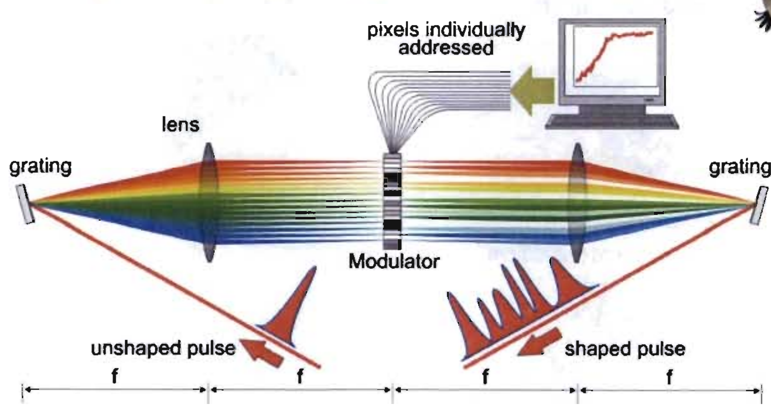
Creating Photonic Reagents on Demand



- Start with raw, featureless, ultrafast laser pulse (30-100 fs)
- Filter spectral amplitude and phase (SLM or AOM)
- Fully automated computer generation of photonic reagents

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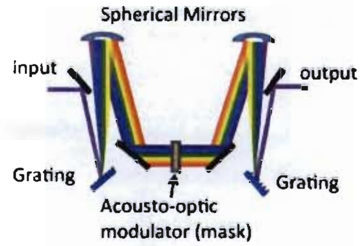
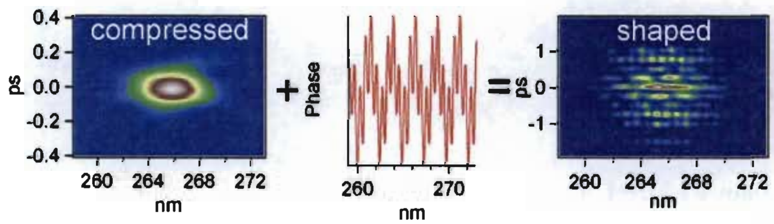
Pulse Shaping : Time Dependent Electric Field

- **Femtosecond optical pulse shaping**
  - Shape E(t) by adding phase to E(ω) and Fourier transforming
  - $E(t) = a(t)e^{i\varphi(t)}$





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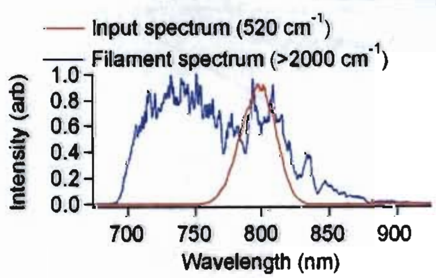
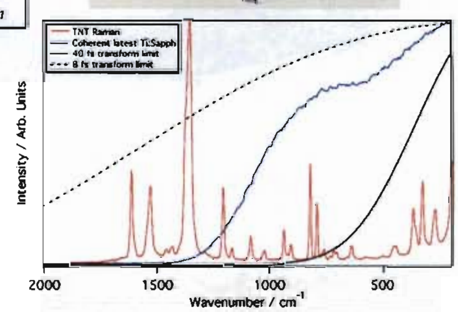
Increasing the Control Bandwidth

Filamentation



New Laser Technology



~2000 cm^{-1} bandwidth is comparable to vibrational fingerprint region

- Allows coherent Raman spectroscopies
  - and vibronic control of emission

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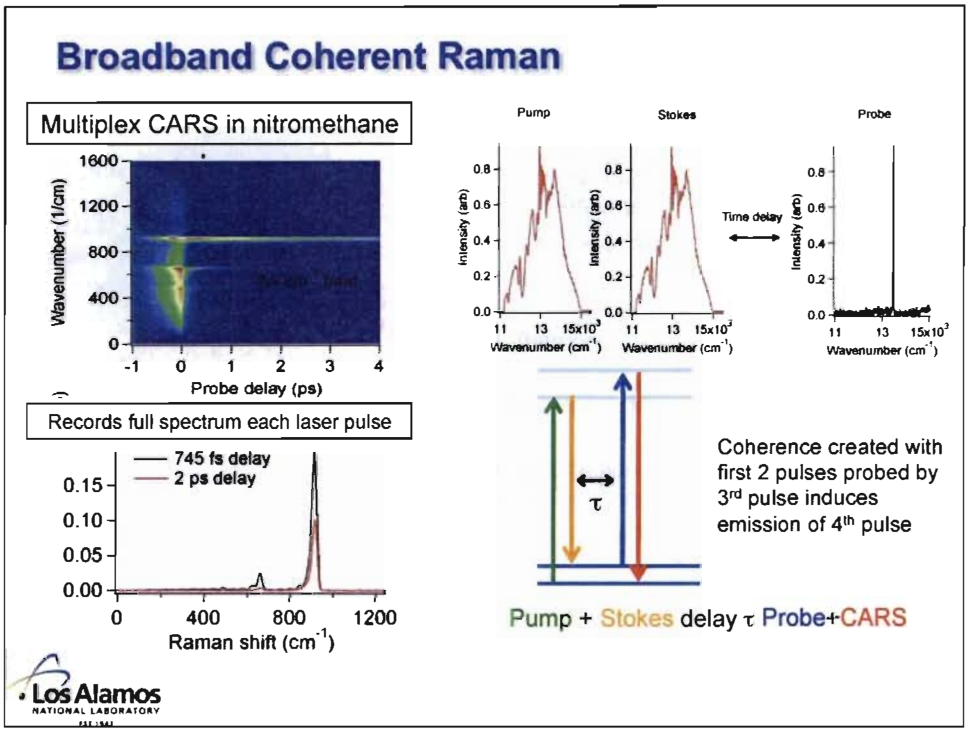
Broadband Coherent Raman
Multiplex CARS in nitromethane
Wavenumber (1/cm)
Probe delay (ps)
Records full spectrum each laser pulse
745 fs delay
2 ps delay
Raman shift (cm-1)
Pump
Stokes
Probe
Time delay
Intensity (arb)
Wavenumber (cm-1)
τ
Coherence created with first 2 pulses probed by 3rd pulse induces emission of 4th pulse
Pump + Stokes delay τ Probe+CARS
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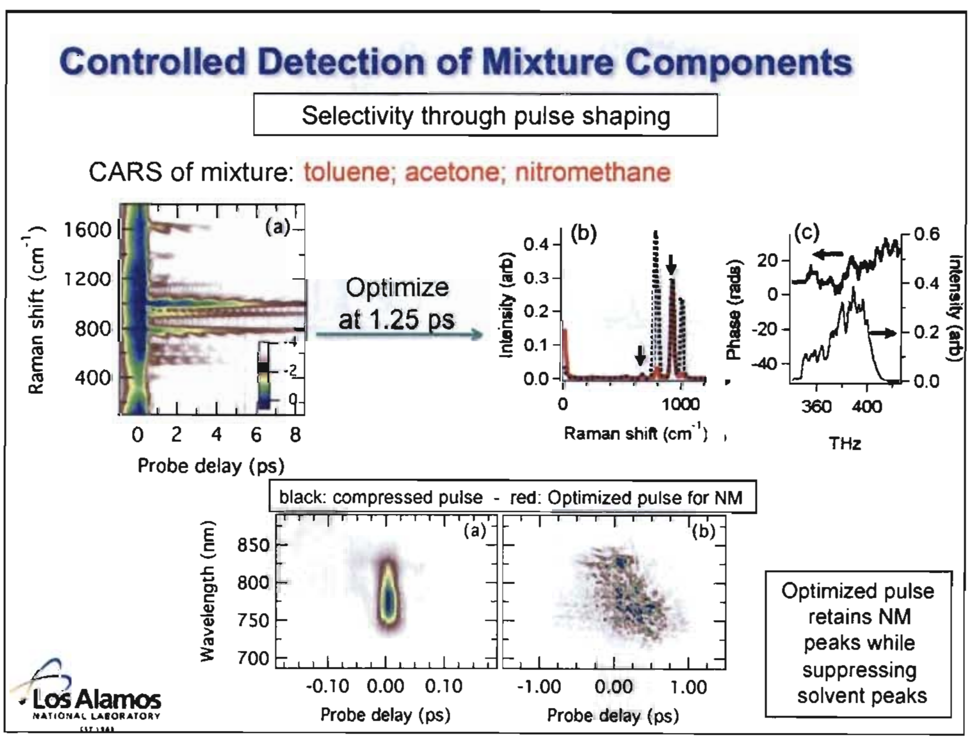
Controlled Detection of Mixture Components
Selectivity through pulse shaping
CARS of mixture: toluene; acetone; nitromethane
Raman shift (cm-1)
Probe delay (ps)
Optimize at 1.25 ps
Intensity (arb)
Raman shift (cm-1)
Phase (rads)
Intensity (arb)
THz
black: compressed pulse - red: Optimized pulse for NM
Wavelength (nm)
Probe delay (ps)
Optimized pulse retains NM peaks while suppressing solvent peaks
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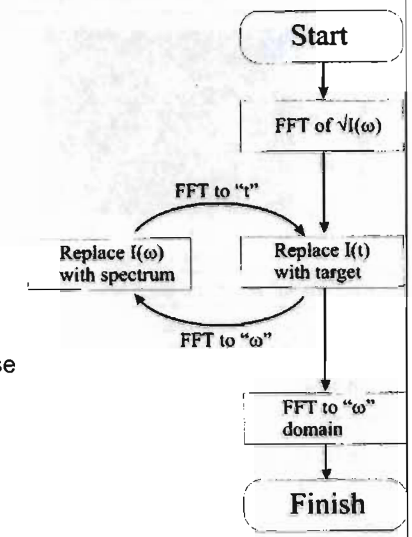
Faster Optimization

Use of Gerchberg-Saxton Algorithm

- GS is independent of target complexity, pulse shaper resolution; no cost functions, weight factors or optimization parameters.
- Only requires known target spectrum and the raw laser spectrum
- Algorithm steps:
  - FFT of the laser pulse (spectrum), starting with random phase
  - Replace amplitude with target spectrum, retain phase
  - IFFT back to spectral domain, replace amplitude with laser spectrum, retain phase
  - Iterate until minimal changes



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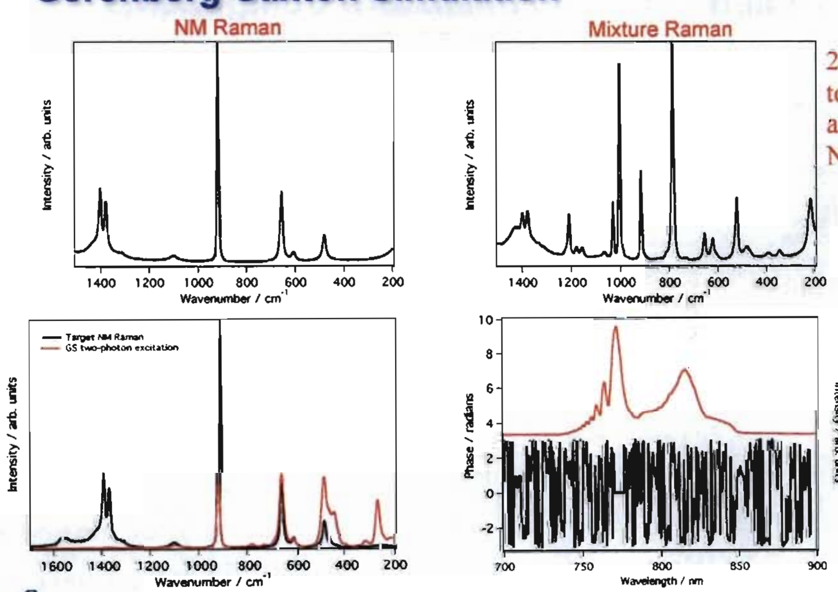
Gerchberg-Saxton Simulation



2:2:1 toluene: acetone: NM

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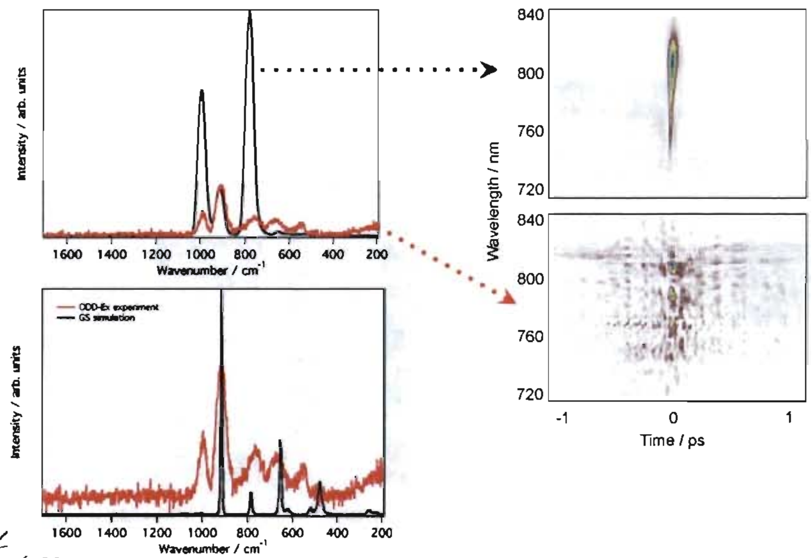
ODD-Ex with Gerchberg-Saxton Phase



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Building Blocks for ODD-Ex

- A compact, engineered ODD apparatus is envisioned

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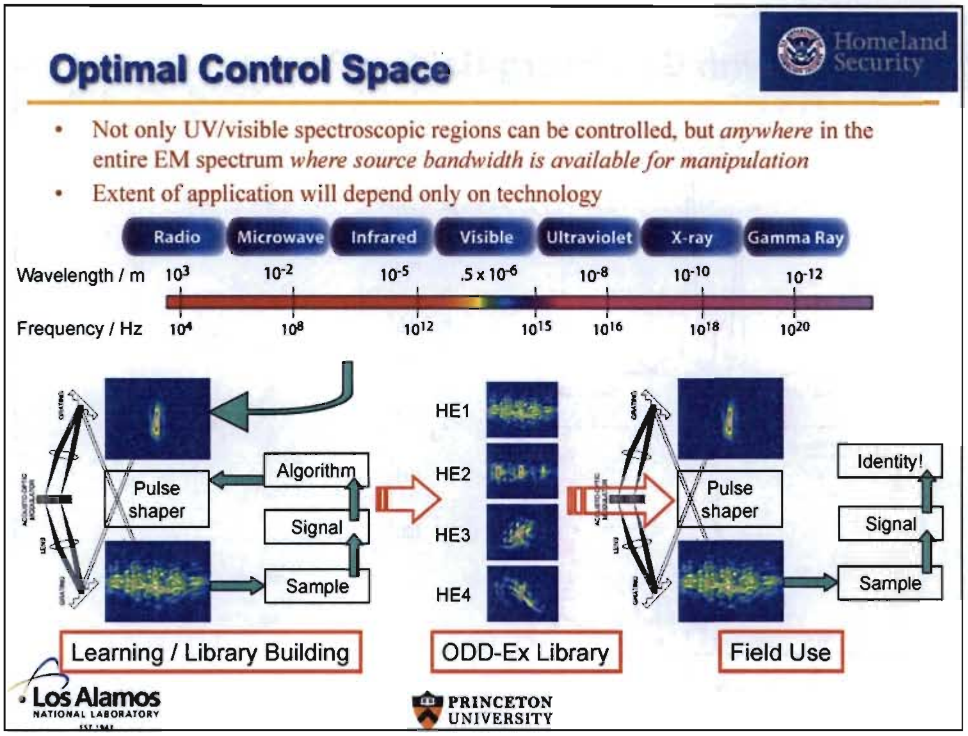
Optimal Control Space
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• Not only UV/visible spectroscopic regions can be controlled, but *anywhere* in the entire EM spectrum *where source bandwidth is available for manipulation*
• Extent of application will depend only on technology
Radio
Microwave
Infrared
Visible
Ultraviolet
X-ray
Gamma Ray
Wavelength / m 10^{3} 10^{-2} 10^{-5} $.5 \times 10^{-6}$ 10^{-8} 10^{-10} 10^{-12}
Frequency / Hz 10^{4} 10^{8} 10^{12} 10^{15} 10^{16} 10^{18} 10^{20}
Pulse shaper
Algorithm
Signal
Sample
HE1
HE2
HE3
HE4
Pulse shaper
Identity!
Signal
Sample
Learning / Library Building
ODD-Ex Library
Field Use
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Stand-off stimulation of alternate signatures
Remote Stimulation
Why?
• Increases HE detectable signatures
– Thermal
– Vapor phase
– RF emission
High Power Array
mmW Sensor
THz Sensor
Ultrasonic Array
IR Sensor
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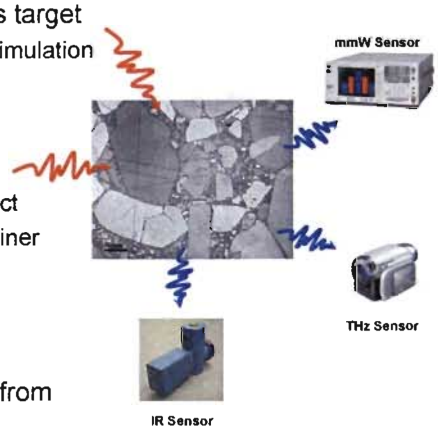
Raytheon
Space and Airborne Systems

Shaping Acoustic Stimulation

- Smart acoustic pulse stimulates target
  - Creates a unique controllable stimulation
- Alternate acoustic generation
  - RF conversion via piezoelectric effect
  - EM to acoustic conversion on container



- Feedback for optimization from
  - Thermal signal
  - RF/THz/microwave emission
  - Vapor or other chemical emission

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Summary

- **Optimal Dynamic Detection** offers a viable path to significant improvements in selectivity and sensitivity
- **Photonic reagents** are optimally tailored electromagnetic pulses that enable selective addressing of different species
- **Single pulse** photonic reagent can be designed to create a tailored wavepacket in the analyte excited state and interrogate the system by a stimulated signal
  - The optimally controlled multispectral stimulated signal is sensitive to detailed sample vibronic structure and dynamics
- **Large bandwidth sources** allow coherent Raman spectroscopies and vibronic control of emission
- **Multiobjective optimization** to balance selectivity and sensitivity
- Optimal control of **alternate signature methods**

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