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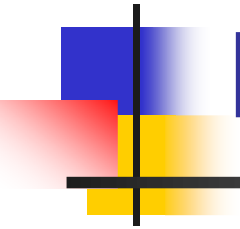

Modeling of CO-LIF

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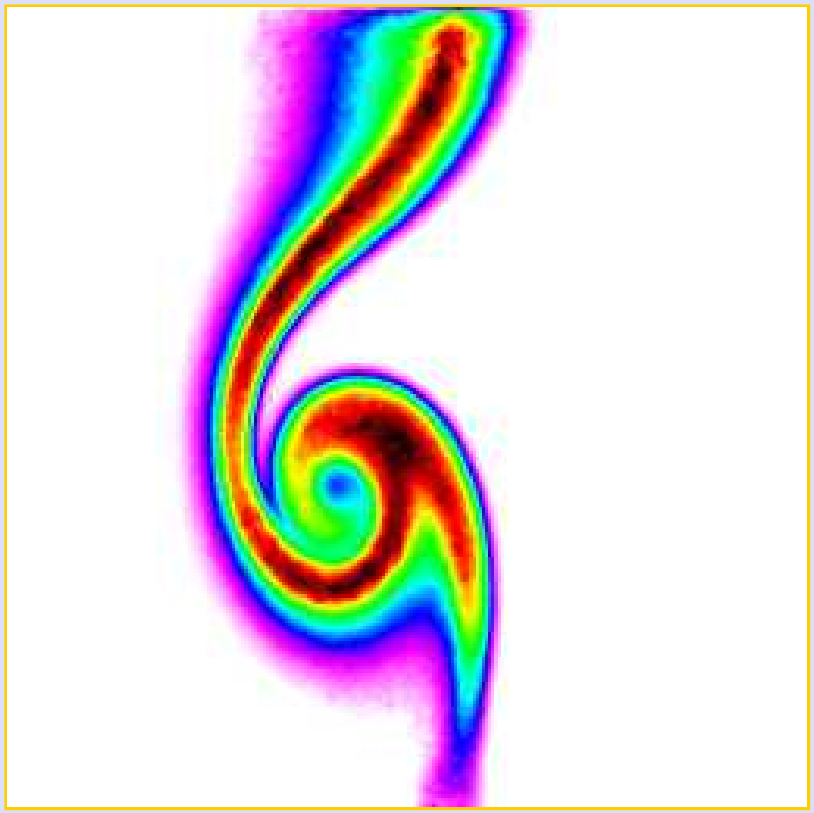
Motivation

- CO LIF is a sensitive technique that can be used to measure concentrations of CO.
- CO is an important intermediate species and a pollutant in combustion.
- Quantitative measurements of CO concentrations are essential for understanding of flame chemistry and to reduce emissions.

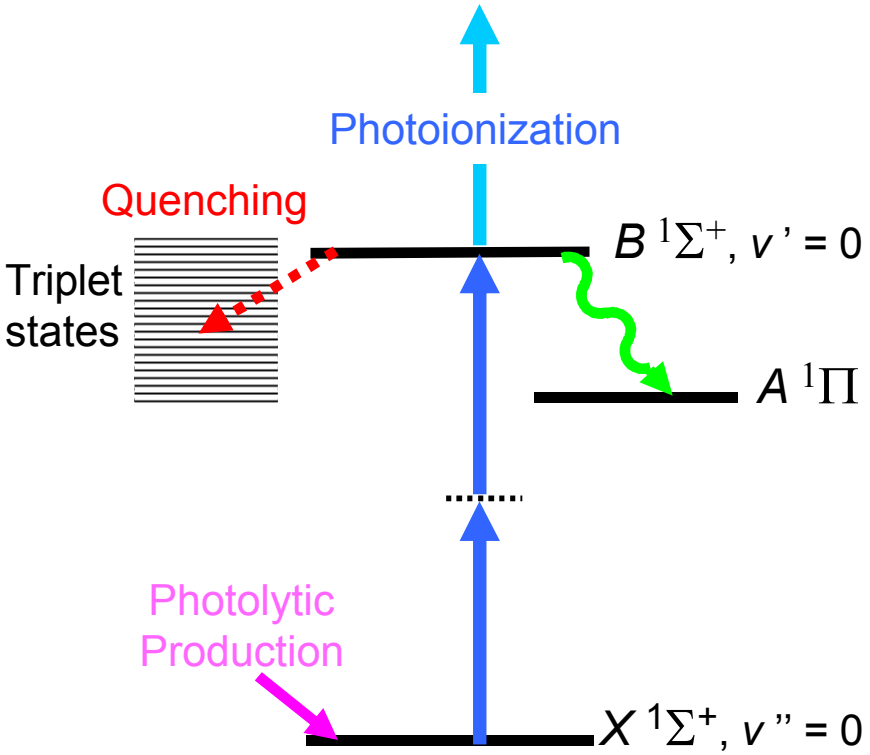
Background



Planar LIF image of CO in flame
(CRF Advanced Imaging Laboratory)

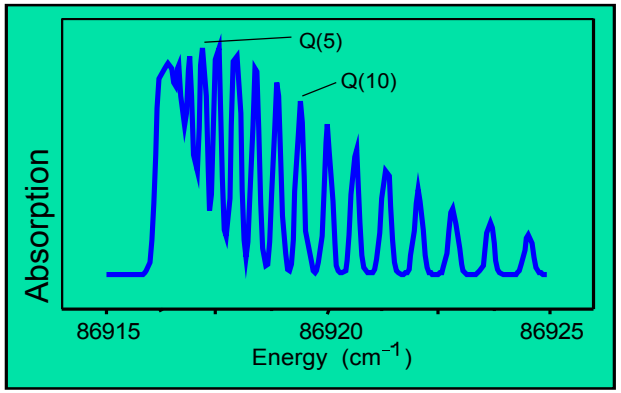
- Two-Photon LIF is a potentially powerful CO diagnostic
  - "point" measurement
  - imaging
  - 100's of ppm sensitivity
- Implementations at the CRF
  - single-point: TDF (Barlow)
  - line image: TCL (Barlow)
  - PLIF: AIL (Frank)

Background



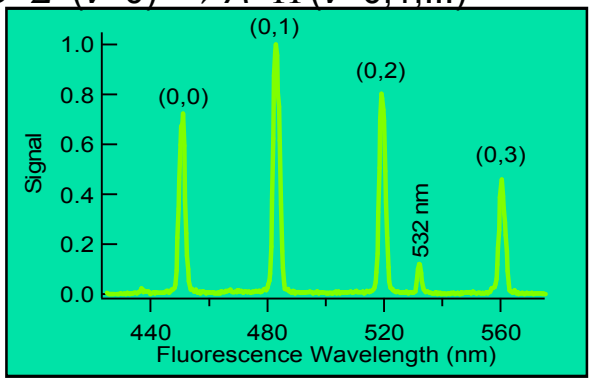
TP Excitation via the Hopfield-Birge system

$B\ ^1\Sigma^+ \leftarrow\leftarrow X\ ^1\Sigma^+\ (0,0)$



Fluorescence detection of the Angström bands

$B\ ^1\Sigma^+(v=0) \rightarrow A\ ^1\Pi\ (v=0,1,...)$



Predictive Modeling

- Develop computational simulations
- Considerations:
  - Photoionization
  - Quenching
  - Photolytic Production

Predictive Modeling

- Use Density Matrix Formalism to model the excitation and relaxation dynamics
- The population densities for rotational levels J in $X\,^1\Sigma^+(v{=}0)$ and J′ in $B\,^1\Sigma^+(v'{=}0)$ are given by the diagonal density matrix elements ρ_J and $\rho_{J'}$
- Assume that coherences between levels such that J ≠J′ are zero.

Differential Equations

$$
\begin{aligned}
\dot{\rho}_J &= -\Omega_J \beta_J - \rho_J \Gamma_J + \sum_i \rho_{J_i} R_{J_i J} \\
\dot{\rho}_{J'} &= +\Omega_J \beta_J - \rho_{J'} \Gamma_{J'} + \sum_i \rho_{J'_i} R_{J'_i J'} \\
\dot{\alpha}_J &= -\Delta \beta_J - (\gamma_J + \gamma_L)\, \alpha_J \\
\dot{\beta}_J &= +\Delta \alpha_J - (\gamma_J + \gamma_L)\, \beta_J \\
&\quad +\Omega_J (\rho_J - \rho_{J'})/2
\end{aligned}
$$

- α_j, β_j are the real and imaginary parts of the coherence.
- Ω_J is the time dependent Rabi frequency. It is a function of laser intensity.
- Δ is the two-photon laser detuning.
- Γ_J is the total collisional population loss rate.
- $\Gamma_{J'}$ is the total collisional population loss rate in addition to spontaneous emission, quenching and photoionization.
- γ_J is the coherence dephasing rate.
- R_{JJ} is the rotational energy transfer rate.

Differential Equations

$$\dot{\rho}_{\rm ion} = \left(\rho_B + \sum_i \rho_{J_i}\right)\sigma_{\rm ion}\frac{I(t)}{\hbar\omega_{\rm L}} ,$$

$$\dot{\rho}_{\rm lost} = \left(\rho_B + \sum_i \rho_{J_i}\right)(Q + A) ,$$

$$\dot{\rho}_X = -\rho_X\Gamma_X + \sum_i \rho_{J_i} R_{J_i X} ,$$

$$\dot{\rho}_B = -\rho_B\Gamma_B + \sum_i \rho_{J'_i} R_{J'_i B} .$$

$$\dot{\rho}_1 = -W_{\rm ph}\rho_1$$

$$\dot{S}_{\rm LIF} = \left(\rho_B + \sum_i \rho_{J'}\right)A$$

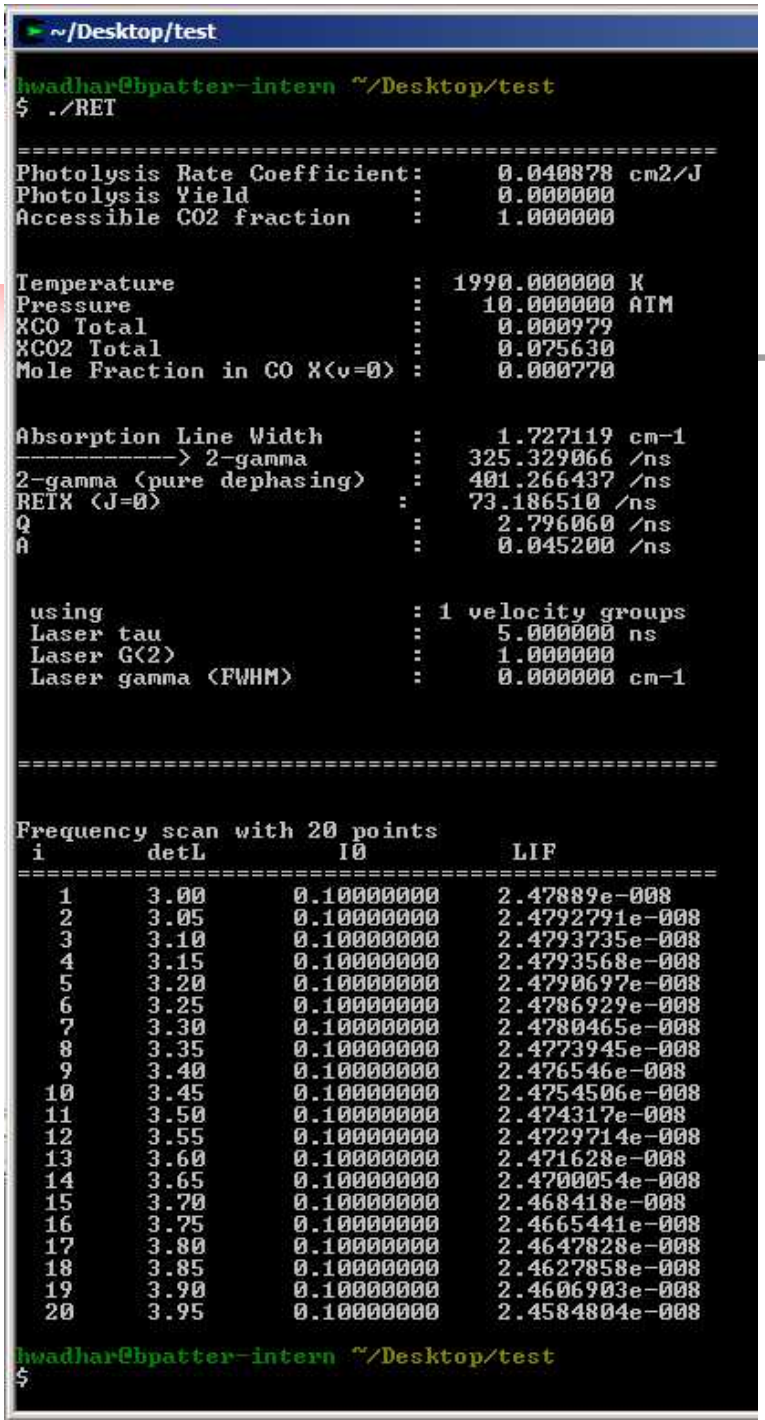
- In addition we have to track the
  - CO- ion population
  - Population lost
  - "Bath" levels for X and B states.
- We also have CO2 molecules photolytically creating CO (in the ground state)
- Finally S is the LIF signal generated by all of these equations.

Numerical Considerations

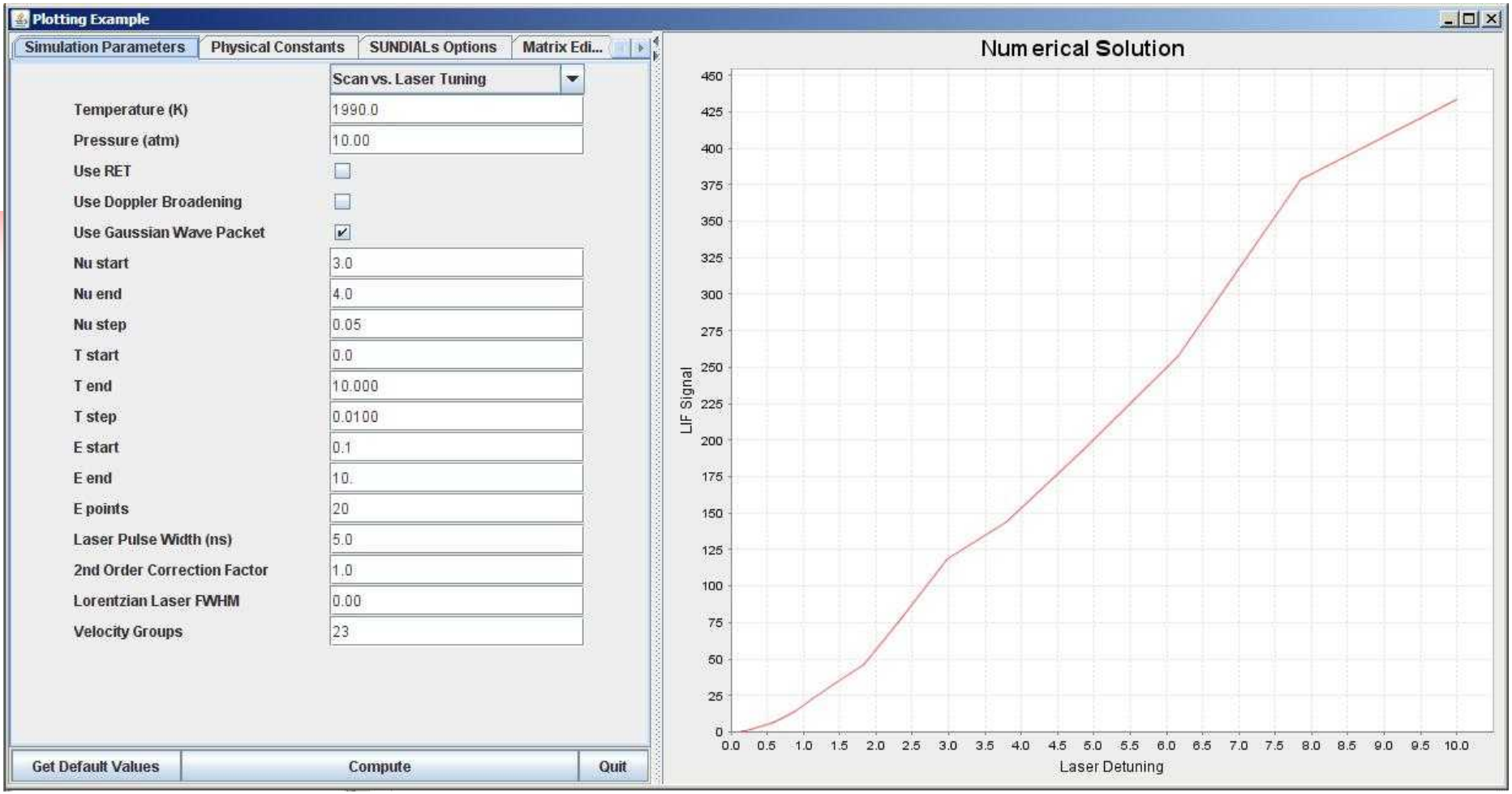
- In total we have
  - #Equations = 4(#Levels) + 7
  - Our system size can become large
- We use the Adams-Bashforth Method implemented by SUNDIALS

$$y_{n+1} = y_n + h \sum_{j=0}^{s} b_j f(t_{n-j}, y_{n-j}), \quad 0 \le r \le n$$

$$b_j = \frac{(-1)^j}{j!(s-j)!} \int_0^1 \prod_{i=0, i \neq j}^{s} (u+i)\, du, \quad j = 0, \ldots, s.$$



- Terminal Window Program
  - Programmed in C
  - Runs very fast



- JAVA GUI and Plotting Routines
- Platform Independent and portable
- Uses the Java native interface (JNI) to link with the C program to produce data