Cybernetics, School of Systems Engineering

Feedback Applications in Measurement Systems

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My Background

• 2 degrees in Biological Sciences from the University of Leeds
• PhD in Instrumentation and Measurement from the department of Cybernetics in 1996/collaborations with the Optoelectronics centre in Strathclyde.
• 2 years Post-doctoral experience as a EC TMR Fellow working on THz technology in UK and Germany (RWTH Aachen and DLR Berlin).
• Member of staff in the School of Systems Engineering since 2000.
• My research interests are in developing novel instrumentation and new measurement solutions in the microwave, terahertz, infrared and optical parts of the electromagnetic spectrum.
• I am also involved in the development of new signal processing routines developed by the Systems Identification community to analyze spectroscopic data.
SOFIA Stratospheric Observatory for Infrared Astronomy
The central topic of this talk is the Application of Feedback Principles in a variety of Measurement Systems

- I will first discuss simple optoelectronics measurement schemes based on feedback principles and explain how you can build cheap sensors in a school classroom and perform experiments using fibre-optics transducers.

- I will then extend these concepts and discuss how to build optical force-feedback microphones and how these can be used to build an ultrasensitive absolute photoacoustic power meter for terahertz radiation.

- I will then discuss the relevance of null-balance bridge techniques to further calibrate this power meter.

- I will introduce the concept of electrical feedback substitution and explain how this can be used to study biological systems.

- Finally I will introduce you to the fascinating world of femtosecond pulse systems and explain how evolutionary feedback techniques may one day be used to control our genome.
Optical Fibre sensing schemes for Feedback Applications

- Description of novel single cut and double cut emitter-detector probes for improved responsivity
- Using these fibre-optic configurations we can build: displacement/velocity/acceleration/force/pressure transducers and a dew point sensor
- An amplitude modulation intensity referencing scheme is also necessary to ensure measurements are precise (shot noise limited detection).

The PMMA fibres have a critical angle $\theta_c$ of 71.8 degrees and a refractive index $n_{\text{fibre}}=1.49$

Optimal cutting requires $n_{\text{air}} \sin 90 = n_{\text{fibre}} \sin [(90- \theta_c) + \alpha]$ so $\alpha=23.8$ degrees
Response curves for the three configurations

- The responses are for (a) uncut, (b) single cut and (c) double cut configurations.
- A complete radiometric analysis of the three probes can be found in: Review of Scientific Instruments, vol. 71 (number 8), August 2000, pp. 3007-3009.
There is a variety of sensor configurations that can be explored.
The amplitude modulation intensity referencing scheme

- Local feedback for thermal stabilisation of the emitter and optimal optical coupling so that the standing noise in the two photodetectors is equal

\[
Q = \frac{\text{OUTPUT}}{\text{REF1}} = \frac{A}{1 + AB} R B \approx R
\]

\[
\therefore \text{OUTPUT} = R \text{REF1}
\]
Photodiode

I-V LPF

Unity gain inv./noninv. Op-amp

Active compensator filter

Stabilised Reference Voltage

Lock-in reference

Multiplexer switch

High gain (4000)

LED

V-I

Square wave modulator

Measurement Science and Technology, 7, 1611-1618 (1996)
Description of a feedback dew point sensor

- Typical dew point sensors comprise of a Peltier cooled mirror surface and an optical probe that detects dew formation.

*Measurement Science and Technology, 11, 1-10 (2000)*
The ambient temperature and the mirror temperature are sensed using rapid response time thermocouples connected to monolithic op-amps having cold junction compensation.

Closed loop operation is achieved by reversing the current on the Peltier.

The onset of dew is observed using the optical sensor.

The reference voltage corresponds to a reference reflectance setting on the mirror with which the sensor output is compared.

The difference between the two temperatures (ambient-mirror) is related to the vapour pressure in the air.

The system produces an output that is proportional to the reference voltage and the reflectance function only.
Results related to the feedback dew point sensor

Figure 9. Typical operation of the sensor with derivative control around the point of dew formation at a frequency of 2.5 Hz. The switching action of the Peltier and the input signal supplied to the comparators is also shown.
Results related to the feedback dew point sensor

- Closed loop operation of the dew point sensor using uncut (left) and double cut (right) fibres showing mirror reflectance and mirror temperature variation
Other possible applications using optical fibres

- Measurements of pressure (such as inside a pressure chamber or as sensing element in a microphone capsule)
- Measurements of force (amount of force that produces an observed change in displacement)
- Measurements of changes in concentration (Beer’s law) of osmotic solutions.
- Measurements of changes in refractive index of solutions.
- Can be used to monitor localised light induced fluorescence.
- Measurements of displacement in seismometry where capacitive transducers are used instead.
Feedback Seismometers (Guralp Instruments) Spin-off from our lab

- Capacitive transducers measure displacement in 3 axes.
- Optical fibres (amplitude modulating probes) can be used instead to observe the movement of the inertial mass with similar resolution.
- Interferometry would be the next logical phase (modulation of phase of a laser).

**Output sensitivity**

- $2 \times 750 \text{ V/m/s}^2$ (1500 V/m/s$^2$) standard
- The CMG-3T is available with any user-specified sensitivity in the range $2 \times 500 \text{ V/m/s}^2$ to $2 \times 10,000 \text{ V/m/s}^2$

**Peak output**
- $\pm 10 \text{ V differential}$

**Lowest spurious resonance**
- $> 140 \text{ Hz (vertical)}$
- $> 111 \text{ dB (USGS figures)}$

**Linearity, vertical**
- $> 107 \text{ dB (USGS figures)}$

**Linearity, horizontal**
- $> 65 \text{ dB}$
Optical Microphones

• A more sensitive measurement of displacement can be made using laser interferometry.

• In this measurement modality instead of modulating the amplitude of the source we modulate instead the phase of the sinusoidal electromagnetic field.

• One can use free space optics or fibre-optics for this implementation.

• A low phase noise (long coherence length) laser must be chosen for all interferometric applications.

• Gas lasers (He-Ne) are ideal but nowadays, some semiconductor lasers with such characteristics have been developed (e.g. Redfern diodes) for such applications.
**Fabry-Perot Interferometer**

- Assume a plane wave $E = A_0 e^{i(\omega t - kx)}$ incident at an angle $\alpha$ on a plane transparent plate with two parallel partially reflecting surfaces. At each surface the amplitude $A_i$ is split into a reflected component $A_r = A_i \sqrt{T}$ and a refracted component $A_t = A_i \sqrt{1-R}$ (neglecting absorption and assuming $T+R=1$). The reflectivity depends on the angle of incidence, $\alpha$ and on the polarization of the incident wave. Provided the refractive index $n$ is known $R$ can be calculated from Fresnel's formula.

- With reference to the diagram below we can write the following formulas:

\[
\begin{align*}
|A_1| &= \sqrt{R} |A_0| ; \\
|B_1| &= \sqrt{1-R} |A_0| ; \\
|C_1| &= \sqrt{R(1-R)} |A_0| ; \\
|D_1| &= (1-R) |A_0| ; \\
|A_2| &= \sqrt{1-R} |C_1| = (1-R) \sqrt{R} |A_0| ; \\
|C_2| &= R \sqrt{R(1-R)} |A_0| ; \\
|D_2| &= R (1-R) |A_0| ; \\
|A_3| &= \sqrt{1-R} |C_2| = R^{3/2} (1-R) |A_0| ; ... .
\end{align*}
\]
Optical Force-Feedback Microphone

Laser Feedback System

Laser Loop

PBS

Laser Diode

Laser Control Photosensor

(OP)

Output Photosensor

Microphone Loop

/4 Plate

Fixed Mirror

Fabry-Perot cavity

Diaphragm

Electrodes (+,-)

Microphone Feedback System
Reflected intensity (normalised)

\[ r_2^2 = 0.9 \text{ (chosen curve)} \quad r_2^2 = 0.1 \]
Block diagram of a force-feedback optical microphone

Electrostatics for the feedback loop:

\[ F = \frac{\varepsilon_o \cdot a \cdot V^2}{2 \cdot s^2} \]

\[ F = \frac{a \cdot \varepsilon_o \cdot (V_p + V_s)^2}{2 \cdot s^2} - \frac{a \cdot \varepsilon_o \cdot (V_p - V_s)^2}{2 \cdot s^2} \]

\[ F = \frac{2 \cdot a \cdot \varepsilon_o \cdot V_p \cdot V_s}{s^2} \]
Advantages of the proposed scheme

• Extremely sensitive (more sensitive than capacitive transducers).
• A completely distortionless microphone (the membrane does not move)!
• Exceptional long term stability across all frequencies (no need for re-calibration due to humidity absorbed by the membrane).
• Absolute measurements traceable to NPL’s national standards (membrane not moving so no dead-volume in pressure measurements), can be used to define pressure in terms of voltage from a Josephson junction function generator!
• Very sensitive at high frequencies (low-mass thin diaphragm can be used).
• Very sensitive at low frequencies (smaller self noise as the membrane can be attached loosely at the rim since the electrostatic force holds the membrane always in place).
• Can advance Audio technology (and in particular, speaker design), can be used in all applications of non-destructive testing as the FFT signal is absolute (e.g. crack detection in composite panels for aviation, Ultrasonic Biomedical applications, environmental sensing eg echolocation following earthquakes, scientific instruments: photoacoustics, etc)
• The Future: Multiple probes integrated on a sensing head using fibre-optic multiplexing schemes. Also, a transition from MEMS to NEMS.
Feedback Photoacoustics at the THz part of the EM spectrum

<table>
<thead>
<tr>
<th>Microwave</th>
<th>mm wave</th>
<th>Terahertz</th>
<th>Far infrared</th>
<th>Infrared</th>
<th>VIS</th>
<th>UV</th>
<th>X-UV</th>
<th>X Rays</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 GHz</td>
<td>100 GHz</td>
<td>1 THz</td>
<td>10 THz</td>
<td>100 THz</td>
<td>1 PHz</td>
<td>10 PHz</td>
<td>100 PHz</td>
<td></td>
</tr>
</tbody>
</table>

- **A**: Frequency
- **B**: Wavelength (mm)
- **C**: Wave number (cm⁻¹)
- **D**: Energy (eV)
- **E**: Energy (J)
- **F**: Molar energy (kJ mol⁻¹)
- **G**: Molar energy (kcal mol⁻¹)
- **H**: Temperature (K)

- **C-C bond**: (348 kJ mol⁻¹)
- **H-O-H bond**: (463 kJ mol⁻¹)
- **C=O bond**: (498 kJ mol⁻¹)
ACBAR, the Arcminute Cosmology Bolometer Array Receiver, is a 16 element, 300 mK bolometer array designed specifically for observations of CMB anisotropy. It operates in atmospheric windows spanning millimeter to submillimeter wavelengths. Extending the spectral range over which observations of CMB anisotropies are made is necessary to separate CMB signals from foreground contamination. Multifrequency observations will make it possible to measure CMB anisotropies and determine galaxy cluster velocities. ACBAR was deployed on the Viper telescope in early 2002.
Atmospheric Sciences

- Atmospheric measurements from satellites
  - oxygen, ozone, water vapour, pollution greenhouse gases
  - use mountain sites/balloon/aircraft/satellite platforms
  - medium to large scale meteorological observations (atmospheric dynamics)

Emission spectrum of Earths atmosphere measured with balloon-borne Martin-Puplett spectrometer

B. Carli, *IRMMW 2001*, 1-2 – 1-6, 2001
Security Applications (ceramic blades)

Terahertz image of a knife placed in a shoe (centre)
94 GHz Passive Imaging

View from Malvern Hills, 94 GHz (top), visible (bottom)

Communications

- large bandwidth (WDM) and hence suitable for mobile multimedia services (satellite navigation in cars/traffic information, electronic maps for yachts, dynamic information update on buses/trains)
- cellular telephony currently at 900 MHz, cheap electronics but spectrum very difficult to obtain
- future plans for above 60 GHz at data rates up to 155 Mb/s but will require line-of-sight (above 3GHz)
- 60 and 120 GHz oxygen absorption, 180 and 325 GHz water vapour absorption
- Choose for 0.01 dB/km attenuation at 10 GHz or 0.1 dB/Km at 40 GHz
- trends are towards higher frequencies and shorter range to increase capacity

Military-civil uses / surveillance

- increased range and angular resolution radar
- reduced radar clutter
- superior penetration through fog/rain/wood/paper from IR
- collision avoidance
- cohort communications / line-of-sight wireless communications
Studies of radar reflection signatures using scale models of aircraft
Drug polymorphism and patent rights protection for the Pharma industry

**Quality Assurance**

- count items in packages
- control quality of pharmaceuticals
- help airline pilots navigate through fog
- detect dangerous flaws in space shuttle components
Fingerprinting of explosives and illicit drug detection

- HMX, RDX, C-4 and TNT reflect radiation in the 10 GHz-450 GHz range.

Measurements at Prof. Ito’s and K. Kawase’s group at Riken Japan: Two lines may be distinguished in the absorption spectrum of cocaine HCl placed in an enveloped (2nd picture the empty envelope spectrum).

Typical problem of such measurements is the thickness of the packaging and diffuse reflection has been suggested as an alternative to recording transmittance spectra.
Biomedical Imaging

Basal cell carcinoma

Melanoma

Signal (a.u.)

2 mm
3.5 mm
4 mm
5.6 mm

Signal (a.u.)

index $n = 1.5$

0 5 10 15 20 25 ps

Plant Water Content

Attenuation

Time delay

Pulse dispersion

Index $n = 1.5$
Commercially available power meters have an NEP of $10^{-6}$ W Hz$^{-1/2}$. Golay cells can reach NEP values of $10^{-10}$ W Hz$^{-1/2}$ but are not absolute detectors. We should be able to develop *electrical feedback substitution* (absolute) radiometers using force feedback microphones for sensing the null signal.
- The signal beam passes through a thin metallic film absorber mounted in a closed gas cell which has a side-arm containing a microphone.

- The power absorbed heats the surrounding gas and this produces a periodic pressure change which is detected by the microphone and recorded by the PSD (phase sensitive detector) system (otherwise known as a lock-in amplifier).

- To make the power meter absolute, current passes through the thin film absorber in anti-phase with the signal beam to give zero output from the PSD.

- Dissipated power is measured by measuring the current required to null the signal at the microphone.

- Sinusoidal modulation of the THz beam is also possible using a rotating grid.
Other considerations

- Radiation pressure noise from the laser to the diaphragm can be eliminated using two identical microphones and a correlation technique.
- It is possible to compensate for pressure and temperature fluctuations using two mm-wave cells.
- The absorbance of a mm-wave cell can be calculated after measuring its transmittance and reflectance using quasi-optical null-balance bridge techniques.

Summary

- Limitations to receiver sensitivity arising from fluctuations in background thermal radiation are of the order of $5 \times 10^{-11}$ W Hz$^{-1/2}$.
- Limitations to receiver sensitivity due to Brownian noise are of the order of $9 \times 10^{-12}$ W Hz$^{-1/2}$.
- Limitations to receiver sensitivity due to shot noise in photodiode are of the order of $2 \times 10^{-8}$ W Hz$^{-1/2}$ assuming a 3 mW laser diode is used.
**Photoacoustic cell window calibration**

**Null-balance quasi-optical bridge reflectometer / transmissometer**


\[ S = T e^{-j\phi} \]

\[ R(\theta) = \begin{bmatrix} -\cos^2 \theta & -\cos \theta \sin \theta \\ \cos \theta \sin \theta & \sin^2 \theta \end{bmatrix} \]

\[ M = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \]

\[ T(\theta) = \begin{bmatrix} -\cos \theta \sin \theta & \sin \theta \cos \theta \\ \cos \theta \sin \theta & \cos \theta \cos \theta \end{bmatrix} \]

\[ C_1 = R(-45^\circ) M e^{-jkd} M M T(\theta) M R(45^\circ) T(0^\circ) \]

\[ C_2 = T(45^\circ) M S M T(45^\circ) T(0^\circ) \]

\[ D = T(90^\circ)(C_1 + C_2) \]
\[
P = \left| \frac{1 - \sin 2\theta}{4} \right| e^{-jkd} e^{-j\phi} \left( \frac{T}{2} e^{-j\phi} \right)^2 P_0.
\]
Null balance transmissometer (Continued)

- A train of lenses are used, each converging the beam to a narrowest point or beam-waist from which it will diverge as it propagates to be picked up and re-converged by the next lens.

- Each pair of lenses is separated by the sum of the individual focal lengths, giving frequency independent beam-waist locations and consequent multi-octave operation.

- Wire grid polarising beam splitters made of parallel arrays of 10 \( \mu \text{m} \) diameter tungsten wires on a 25 \( \mu \text{m} \) centre-to-centre spacing are other important components.

- The linearly polarised component of an incident beam with E-vector parallel to the grid wires is reflected, while the orthogonal component is transmitted.

- Such grids give good performance over the whole frequency range.

- Both instruments used in this work are based on a hybrid Mach-Zehnder/Martin-Puplett interferometer.
null balance transmissometer (Continued)

- Jones matrices may be used to relate the angle between the orientations of the reference beam grid that result in nulls to the amplitude transmission coefficient of the sample

\[ |t| = \cos^2 \gamma \]

- where \( \gamma \) is half the angle between adjacent null orientations measured about the reference beam grid orientation that transmits all of the incident polarisation.

- The use of a null-balancing technique means that the measurement precision depends on the precision with which the null angles can be measured and is independent of source and detector fluctuations (which affect both the sample and reference beams in equal proportion).

- The IMPATT oscillator was square-wave modulated at 1.5 kHz and the output from the detector, a Flann Microwave point-contact crystal detector fitted with a corrugated feed horn was fed into a lock-in amplifier.

- The beam at the sample location has a Gaussian transverse amplitude distribution with a 1/e amplitude half-width of 10 mm.
Quasi-optical Reflectometer

\[ C_1 = R(\theta)MR(0^\circ)T(0^\circ)[0 \ 1]^T \]
\[ C_2 = T(-45^\circ)MST(45^\circ)T(0^\circ)[0 \ 1]^T \]
\[ D = R(0^\circ)(C_1 + C_2) \]
In conventional control systems, the goal is to attain the highest possible gain–bandwidth product and ensure that the output of the controller is a direct measurement of the effect of an external influence on the plant, i.e.:

\[ W_f(s) = -\left(\frac{G(s)K(s)}{1+G(s)K(s)}\right)W_e(s) + \left(\frac{K(s)}{1+G(s)K(s)}\right)V_n(s) \]

This is different in FCESM, where the controller is designed to maintain the plant in a constant state, i.e.

\[ G(s)\{W_f(s) + W_e(s)\} = 0 \]

We want:

\[ G(s)K(s)(1+G(s)K(s))^{-1}W_e(s) = -1 \]
\[ G(s)(1+G(s)K(s))^{-1}V_n(s) = 0 \]

across all frequencies. A controller design strategy is required that takes into consideration these two conflicting requirements.
Feedback substitution schemes

CHARACTERISTICS

- Self referenced
- Absolute measurements
- No need for calibrations
Analytical approach

First order detector \( G(s) = \frac{\mathcal{R}}{1 + \tau s} \) where \( \mathcal{R} \) is the responsivity (V/W), PSD is modelled as a first order filter \( F(s) = \frac{1}{1 + \tau_f s} \), PI controller and overall gain \( \mu \).

The time domain response is given by

\[
\frac{w_h(t)}{L^{-1}} = \left\{ P(s) w_r(s) + Q(s) \left[ \frac{u_d(s)}{\mathcal{R}} \right] \right\}
\]

where \( P(s) \) is the transfer function of the external radiation

\[
P(s) = \frac{1 + \tau_i s}{(1 + \tau_i s) + \left( \frac{\tau_i}{\mu} \right) s(1 + \tau_f s)(1 + \tau)}
\]

and \( Q(s) \) is the noise transfer function

\[
Q(s) = \frac{(1 + \tau_i s)(1 + \tau)}{(1 + \tau_i s) + \left( \frac{\tau_i}{\mu} \right) s(1 + \tau_f s)(1 + \tau)}
\]

(White, J. F. and Clare D. R., Appl. Optics, 1989)
The objective of the design is to optimize the response time and the noise power gain at the same time.

To define the response time, a small tolerance value $\varepsilon = 0.001$ is introduced, the system is designed to have an overshoot of and the response time is defined as the time to reach a value of $1 - \varepsilon$ in the output.

The noise power gain is given by

$$ G^2 = \frac{1}{\tau} \left( \frac{u_d}{\mathcal{R}} \right)^2 \frac{\tau}{4 \pi j} \int_{-\infty}^{\infty} |Q(s)|^2 \, ds \bigg|_{s=j\omega} = \frac{1}{\tau} \left( \frac{u_d}{\mathcal{R}} \right)^2 G^2 $$

for a third order system an expression is derived in (Pickup 1981)

$$ G^2 = \left[ \frac{c_2^2 b_1 + b_3 (c_1^2 - 2c_2) + b_2 b_3}{4b_3 (b_1 b_2 - b_3)} \right] $$

where $c$ and $b$ are the coefficients of the noise transfer function rearranged as

$$ f(s) = \frac{1 + c_1 s + c_2 s^2}{1 + b_1 s + b_2 s^2 + b_3 s^3} $$
Optimal systems

To find the optimal solution the time constants are normalized to the detector time constant \( \tau_f = x \tau \) and \( \tau_i = y \tau \), then the three design parameters of the system are \( \mu, x \) and \( y \). For every combination of \( \mu \) and \( x \), a value of \( y \) that meets the overshoot constraint is found.

a) Contours of \( y \) in the plane \( x, \mu \).
b) Contours of response time in the plane \( x, \mu \).
c) Contours of noise power gain in the plane \( x, \mu \).
d) Contours of response time and noise power gain on the plane \( x, \mu \).
• Pareto front representation of the optimisation results.
\[ V_d = G(W_r + W_h) \]

\[ W_h = gKFe \]

\[ e = V_a - n - V_d \]

\[ V_d = \frac{GW_r + GgKFV_a - GgKFn}{1 + GgKF} \]

The designed controller \( K \) must provide good tracking of input \( \langle W_h \rangle = -\langle W_r \rangle \), good disturbance \( n \) attenuation as well as to limit the control signal energy \( KS \)

\[ S = \frac{1}{1 + GgKF} \]

\[ T = \frac{GgKF}{1 + GgKF} \]

\( S \) is the transfer function between disturbance and output, \( T \) the complementary sensitivity. \( S = (I + L)^{-1} \), \( S + T = 1 \)

\( KS \) is the transfer function between disturbance and controller signals

\( KS \) is shaped for limiting the size and bandwidth of the controller and hence the controller energy used. Also it is used for robust stability with respect to uncertainty modeled as additive plant perturbation.

High \( S \) ensures good tracking and disturbance attenuation, high \( T \) ensures robustness & minimizes plant sensitivity to noise, high \( KS \) penalizes large inputs.
Re-casting the problem as an $H$-infinity controller design problem

Objective: find a controller $K$ that minimizes the $H$-infinity norm from $w$ to $z$. i.e., to minimize the output $z$ in the sense of energy over all inputs $w$ with energy less than or equal to 1.

The analysis above is sufficiently generic that it can provide a design methodology for optimizing the controller performance in the force-feedback microphone (the only difference being that it is a 2$^{nd}$ order plant).
Loop Shaping Design Procedure with $H^\infty$ synthesis (taking robustness into consideration)

The original plant is augmented with pre and post compensators that act as shaping functions used to satisfy the design requirements. The resulting shaped plant is $G_s$.

A co-prime factorization of the shaped plant $G_s$ is used to introduce uncertainty, the result is a perturbed plant $G_{\Delta}$.

A $H^\infty$ controller is synthesized to robustly stabilize the plant.
System objectives as inequalities

System specifications in the time and frequency domain are expressed as inequalities of the form \( \varphi_i(p_j) \leq \varepsilon_i \)

Where \( \phi \) is an objective function of the parameters \( p \) with a desired value less or equal to \( \varepsilon \)

\[
\varphi_1 = \left| W_h \left[ t, W_r (t) \right] - \frac{\varepsilon_T}{500} \right| \leq W_r (t) + \varepsilon_T, \quad t > 0 \\
\varphi_2 = \left| W_h \left[ t, W_r (t) \right] - \frac{\varepsilon_T}{500} \right| \leq W_r (t) - \varepsilon_T, \quad t > t_r \\
\varphi_3 = \min \left[ \frac{\tau}{4 \pi j} \int_{-\infty}^{\infty} \left| Q(s) \right|^2 ds \right]_{s=j\omega} \\
\varphi_4 = \left\| \begin{bmatrix} K (1 - KG)^{-1} M^{-1} \\ (1 - KG)^{-1} M^{-1} \end{bmatrix} \right\|_\infty \leq \frac{1}{0.25}
\]

Overshoot = \( \varepsilon_T \pm \varepsilon_T / 500 \)

Undershoot < \( \varepsilon_T - \varepsilon_T / 500 \)

Minimize noise power gain

Maximize the robust stability margin
Multi-objective Optimisation Genetic Algorithm (MOGA)

Auxiliary vector to transform inequalities into minimization problem

\[ \lambda_i(p_j, \varepsilon_i) = \begin{cases} 0 & \text{if } \varphi_i(p_j) \leq \varepsilon_i \\ \varphi_i(p_j) - \varepsilon_i & \text{if } \varphi_i(p_j) > \varepsilon_i \end{cases} \]

Weighting functions parameterization

\[ W_1 = p_9 \frac{(s + p_5)(s + p_6)(s^2 + p_7 s + p_8)}{(s + \nu)(s + p_1)(s + p_2)(s^2 + p_3 s + p_4)} \]
\[ W_2 = p_{10} \]

Two part chromosomes

Coefficient parameters

Activation parameters
MOGA solution convergence

• Population is randomly initialized
• Objective functions evaluated
• Best individuals selected for recombination
• Mating and mutation
• Repeat until objectives are met
Performance of $F_{SH}^\infty$ with MOGA

With systems of order 4\textsuperscript{th} to 16\textsuperscript{th} it was possible to reduce the noise power gain whilst maintaining the same measurement time.

The minimum response time achievable while maintaining good robustness for the $F_{SH}^\infty$ with MOGA is limited by the time needed by the nominal plant to settle.
Future prospects for Kinetic inductance THz detectors for single cell calorimetry for Biology, yocto-calorimetry in Chemistry and time of flight mass spectrometry (ToF-MS).

The enthalpy (denoted as $H$) is a quotient or description of thermodynamic potential of a system, which can be used to calculate the "useful" work obtainable from a closed thermodynamic system under constant pressure and entropy.

The enthalpy of solution (or enthalpy of dissolution) is the enthalpy change associated with the dissolution of a substance in a solvent at constant pressure.

Enthalpimetry can be used to gain information on the chemical potential of a solution composed of many species because the enthalpy is

$$dH = TdS + Vdp + \sum_{i} \mu_i dn_i$$

where $T$ and $S$ relate to the temperature and entropy of the system.

Enthalpimetric measurements (e.g., enthalpimetric titration or immobilized enzyme flow injection enthalpimetry) are normally performed using calorimetric techniques.

A very sensitive calorimeter is therefore very often installed in many well equipped labs.
There is scope to perform measurements within single cells (to gain information on metabolic activity) as well as tissue.

The requirement for the presence of a thermometer cannot always be fulfilled because of accessibility limitations; furthermore it can induce a detrimental effect to the measurements as it has its own heat capacity.

A very sensitive thermal detector that could be placed next to the area of interest would be useful.

One of the most exciting emerging technologies within the THz community is the development of kinetic inductance detectors (KIDs).

Each KID comprises a thin-film superconducting microwave resonator whose resonant frequency, typically around 4 GHz, and transmission phase, change when a photon is absorbed.

By using slightly different resonant frequencies for the elements of an array, devices can be read out individually.

The KID detection mechanism is manifested by a temporal change in the surface kinetic inductance of a superconductor when a photon of energy $h\nu \geq 2\Delta T$ (where $\Delta T$ is the superconducting gap parameter) disturbs the lattice structure transferring momentum.

High energy photons break Cooper pairs, creating a non-equilibrium population of quasi-particles.
These recombine in a characteristic time, producing pulse-like changes in the surface impedance.

As the impedance of a superconductor is mostly inductive, especially for \( T \leq T_c \) the superconductor can be engineered as the inductive element in a RLC-like resonant circuit.

The quality factor of the resonant circuit determines both the sensitivity and speed of the device. Such devices are remarkably sensitive to the arrival of photons and therefore are useful for radiometric and hence calorimetric applications.

Furthermore, there is a current interest in using kinetic inductance arrays to observe at high spatial resolution the photo-ionization fragments obtained in mass spectrometry.

Mass spectrometry is a well established tool used to analyze the levels of individual amico-acids and proteins expressed.

Microchannel plates suffer from a considerable decrease in sensitivity for ion masses above a few tens of kDa and large masses (say greater than 50 kDa) are difficult to detect.

The impact of an accelerated molecule fragment on a superconductor surface transfers the kinetic energy of the fragment into the material \( E = 0.5m_{ion}v^2 = eV \).
where it generates a number of excess quasi-particles (QP) and phonons (PH), by means of a Cooper pair breaking process.

These excess QP and PH are measured by the detector as a temperature rise or as a tunnelling current thus providing a signal that sets the arrival time.

This signal strength is proportional to the kinetic energy of the molecule fragment.

Detectors based on the transient change of the kinetic inductance in a superconductive strip (KIDs), are capable of picosecond time resolution and single photon detection.

In a ToF-MS system, the very fast time response translates into a very good mass resolution.

A further advantage of KIDs compared to other superconductive detectors is that it could operate at higher temperature (in the 2–4 K range), depending on the specific material choice and configuration, thus allowing the use of simpler and less expensive cryogenic systems.
Proposed detector for macromolecules impact and interrogation scheme

Additional note: THz technology is also at the core of Josephson junction technology e.g. ADC converters with a 100 GHz bandwidth and absolute function generators!
Description of a time-domain THz-transient spectrometer

- Assuming a time bandwidth relation $\Delta \nu \Delta t = 0.32$, using the shortest visible pulses (around 4-5 fs) usable power from 0-160 THz ($\lambda = 1.8$ mm) could be achieved.

- Measurements with bandwidths up to 37 THz have been achieved (X.C. Zhang’s group, Physics Department Rensselaer Polytechnic Institute NY) but the signal-to-noise ratio is relatively poor.
Osmometry

• A dual-beam optical arrangement incorporating a reference vapour cell may be used accordingly to provide an active calibration for the measurement.

• It is proposed that a THz-transient spectrometer may be used to perform the above task.

• Advantages of the proposed technique are the inherent phase stability of the measurements which enable us to measure absorption as well as refraction independently without requiring the use of the Kramers-Kronig relations, as well as the fact that the THz pulses are inherently broadband and can thus provide simultaneous measurements integrated over the whole absorption line or across several absorption lines simultaneously (Fellgett advantage), thus increasing the measurement accuracy for a fixed integration time.

• This should permit us to observe very small pressure changes thus improving instrument resolution.
(a) Water vibrational modes spectrum from (a) 0 to 400 cm\(^{-1}\) and (b) 0 to 2000 cm\(^{-1}\) (from HITRAN 2004), indicating the difference in line absorption strength when performing these water vapor concentration measurements in the THz part of the spectrum (lines B, C and D) instead of the infrared (line A).
When the freely available water of a salt solution is allowed to equilibrate under isothermal conditions inside a TPX cuvette, a THz transmittance measurement of the water vapour component within the cuvette is performed with

\[ T = T_{\text{air}} \rightarrow \text{TPX} T_{\text{TPX}} \rightarrow \text{vapour} T_{\text{vapour}} \rightarrow \text{TPX} T_{\text{TPX}} \rightarrow \text{air} \]

This is compared ratiometrically to the transmittance after evacuating the cuvette. Assuming the refractive index of air within the path length from the source to the detector excluding the cuvette path length as \( n_{\text{air}} = n_{\text{vacuum}} = 1 \) we have the following expressions as a function of angular THz frequency:

\[
T(\omega)_{\text{sample}} = \frac{16n_{\text{TPX}}^2(\omega)n_{\text{vapour}}(\omega)}{[1+n_{\text{TPX}}(\omega)]^2 \left[ n_{\text{TPX}}(\omega) + n_{\text{vapour}}(\omega) \right]^2}
\]

\[
T(\omega)_{\text{reference}} = \frac{16n_{\text{TPX}}^2(\omega)}{[1+n_{\text{TPX}}(\omega)]^4}
\]

\[
\frac{T(\omega)_{\text{sample}}}{T(\omega)_{\text{reference}}} = \frac{\left[1+n_{\text{TPX}}(\omega)\right]^2 n_{\text{vapour}}}{\left[ n_{\text{TPX}}(\omega) + n_{\text{vapour}}(\omega) \right]^2}
\]
The observed equilibration times within an osmometer cuvette are due to processes obeying first order dynamics, which are driven by water potential differences between the water potential in the tissue under study and the water vapor in the cuvette atmosphere.

\[ \Psi_{wv} = RT \ln \left( \frac{P_{wv}}{P_{wv}^*} \right) / \bar{V}_w \]

Under non-equilibrium conditions, water stored in a sample tissue of hydraulic capacitance \( C_h \) diffuses out, crossing the entire tissue area \( A \) at an average volume flux density \( J_V \). Thus, the tissue looses water at a rate \( J_V A = \Delta \Psi / R_h \) where \( R_h \) is the tissue hydraulic conductance. The time constant \( \tau = R_h C_h \) dictates the time required for the tissue water potential to change to within \( 1/e \) or 37% of its initial value.
Pump-Probe spectrometry

Semiconductor Physics

Pump-Probe spectrometry for time-resolved studies

e.g. charge transport
Solar energy research with focus on transient photoconductivity in colloidal sintered TiO$_2$

- Colloidal sintered TiO$_2$ forms the heart of the so-called “Gratzel cell”, a dye-sensitized solar cell that has attracted attention since 1991.

- The general idea is that even though the photon energy may not be great enough to excite an electron from the valence to conduction band in the bulk, carriers can still be generated by photoexciting a dye molecule on the surface which then injects an electron into the semiconductor.

- Most of the ultrafast spectroscopy done on this system has focused on the dye molecule. That is, a sharp reduction in fluorescence quantum yield and lifetime is observed when the molecule is adsorbed to TiO$_2$ compared to when it is in solution, and this is attributed to rapid electron injection upon photoexcitation.

- The aim of the studies would be to characterize the photo-injected electron dynamics following excitation by monitoring the transient THz absorption.
Background

Basic concepts from photochemistry and photobiology: In photochemistry and photobiology, instead of energy per photon, we are usually interested in the energy per Avogadro's number \( N (6\times10^{23}) \) of photons.

So the energy per photon on a mole basis is \( E_i=\frac{Nh\epsilon}{I_{\text{vacuum}}} \) (where \( h \) is \( 6.023\times10^{-34} \text{ J s} \)).

Our femtosecond pulse system will generate energies between 598.5 kJ mol\(^{-1}\) (200 nm) to 11.9 kJ mol\(^{-1}\) (10 \( \mu \)m) whereas our THz pulse system will cover the range between 3.99 kJ mol\(^{-1}\) (10 THz or 30 \( \mu \)m) and 0.041 kJ mol\(^{-1}\) (100 GHz or 3 mm).

The hydrolysis of ATP, the main currency for chemical energy in biology, generally yields about 40 – 50 kJ mol\(^{-1}\) under physiological conditions.

The carbon-carbon bond energy is 348 kJ mol\(^{-1}\), the oxygen-hydrogen bond energy is 463 kJ mol\(^{-1}\) and the energy of an isolated carbon-carbon double bond is near 647 kJ mol\(^{-1}\) (185 nm).

Furthermore, the effectiveness in absorbing electromagnetic radiation and the wavelengths involved are affected by the number of double bonds in conjugation (alteration between single and double bonds).
Facilities at Reading

Catalysis Centre Facilities

Transcriptomomics Facilities

Ultrafast Laser Laboratory previously at Reading
Now at Imperial

Biocentre Facilities
The concept of using the repetition rate of one frequency comb to interrogate the other frequency comb is similar to the electronic sampling technique used in storage oscilloscopes which provides them the capability to resolve transients beyond the bandwidth of the analog to digital converter used, provided the input waveform is repetitive.

Since the signal from a frequency comb is a repetitive one, the technique works very efficiently, and the fast transient waveform can be built up very quickly if a high repetition rate can be provided by the triggering circuit.

Under the ASOPS mode of operation, a fixed difference in the repetition rate between the two lasers is ensured using a phase locked loop which locks the rep rate of one laser (the slave) to the rep rate of the other laser (master).

The phase of one frequency comb, therefore slides at a fixed speed relative to the phase of the other.

The phase lock loop which adjusts the slave ring resonator length by means of a low mass mirror mounted on a piezoelectric transducer, ensures that there is negligible jitter between the two frequency comb phases in the process. An immediate advantage of the adopted approach is that the requirement for the traditional scanning delay line used in conventional time-domain spectrometry is obviated.

A further advantage of eliminating the translation stage from the spectrometer is that the spot size of the optical beam propagating through the reference path of the interferometer is no longer of variable spot size (due to diffractive spreading of the optical beam) for different path lengths imposed by the translation stage as is the case for a conventional THz transient spectrometer.
ASOPS spectrometer

- Locking one comb to the other will also be possible (we are aiming for sub-femtosecond jitter but some feedback electronics need still to be developed and coupled to the pulse diagnostics equipment).

- The Ti:sapphire lasers must be pumped by two separate 5 Watt sources (only one currently available at the ULL).

- Using a 10 W source and a beam splitter is inappropriate due to thermal lensing problems.

- There currently no more than 5 such systems worldwide.

I suggested the development of the Gigajet twin prototype for GigaOptics GmbH (two feedback controlled resonators)

(Data courtesy of GigaOptics GmbH)
Schematic of the developed ASOPS THz set-up showing the control loop for the synchronization of the repetition rate of the two femtosecond ring resonators in the ULL at Reading University.

\[
V_{out} = \frac{A}{1 + AB} V_{REF} = \frac{A}{AB} V_{REF} = \frac{V_{REF}}{B}
\]
Frequency spectrum produced by the two beating frequency combs and b) the down-converted radio frequency spectrum produced by heterodyning the longer wavelength component with its in-phase shorter frequency component which is co-propagating through the GaSe non-linear crystal. The observation of four individual frequency bins using dedicated lock-in amplifiers is also shown (diagrams re-drawn and modified from original ones by Keilsmann).
F-comb spectrometer (Infrared)

• We have a harmonic series of evenly spaced frequencies $nf_r$ where $n = 1...N$ and we superimpose a second coherent frequency comb with slightly different frequency spacing $f_r = f_r' - \Delta$ where $\Delta < f_r / 2N$ and we get via interference power modulation at

$$nf_r - n(f_r' - \Delta) = n\Delta$$

• Each modulation element $n\Delta$ can be viewed as a heterodyne signal that uniquely measures one comb component.

• All modulations together may be viewed as a time-domain interferogram that when Fourier transformed in the frequency domain results in a harmonic radio frequency comb spectrum $n\Delta$ that is an exact replica of the dual beam’s spectrum.

• The mid-infrared radiation from the two outputs is focused onto 0.5 and 1 mm GaSe crystals and through second order non-linearity we get 2 pulses whose overlapping bandwidth is centered at different frequencies.

• A ZnSe combiner directs the two beams to the detector and the down-converted signal may be captured by a fast detector.

• Chemometric information of the down-converted signals is obtained using a bank of lock-in amplifiers.
Pump-Probe femtochemistry

- Pump-probe experiments are well established in the optical/infrared part of the spectrum since 1987 (A. Zewail).

- Originally, they were used for probing of ‘transition states’ in chemical reactions. Attention was given to unimolecular and bimolecular reactions, the evolution of resonance states in molecules, photofragmentation and dissociation processes.

- In femtochemistry, one monitors the reaction using two laser pulses of different colours. The first pulse initiates the reaction and sets the zero of time (clocking). The second pulse probes the fragments as they separate from each other. The high temporal resolution implies that the separation can be observed with sub-Angstrom resolution.

- Initially, the absorption of the probe pulse is negligible but becomes substantial when the fragments achieve large internuclear distance and are non-interacting. The delay at which the probe absorption turns on is a direct measurement of the time required for complete internuclear separation. The time required to break a bond is a fundamental measurement.
• An alternative way of seeing such experiments is in relation to potential energy surfaces.

• There is now considerable interest in using such schemes to control reactions.

• These advances are paving the way for the generation of programmable waveforms whose overall strength, bandwidth and repetition rate can exceed those used in most current experiments.

• This justifies the placement of measurements performed with time-domain spectrometers in a system identification framework that may be formulated in the time, frequency or wavelet domain.

• A persistent excitation of the sample implies that all the possible system states are sufficiently excited to become observable. This is important if one’s goal is to perform mapping of intramolecular potential surfaces in an accurate manner.

• More recently, more elaborate coherent control schemes have been developed, aimed at enhancing desirable intramolecular dynamical events through constructive interference, while the undesirable states are attenuated through destructive interference.
• Such coherent control schemes using adaptive learning algorithms have been remarkably successful in accomplishing their task, although the approach is ‘blind’ in the sense that it is performed without requiring a knowledge of the Hamiltonian for their implementation.

• An alternative approach is to use system identification to provide an inversion of the Hamiltonian. There are several applications where a complete inversion of the Hamiltonian is required such as quantum computing, the study of wavefunction decoherence, phenomena in mesoscopic devices, the study of entangled states in quantum metrology and information processing, or for systematically performing massive numbers of high-throughput pump-probe experiments in combinatorial laser chemistry.

• The development of optimal pulse shaping techniques using more rigorous models for optical and THz excitation of samples is, therefore, required.
Pulse shaping and applications

Optical pulse shaping is of interest for new pulse compression schemes, the control of molecules as well as the control of quantum wave function of atoms.

- This may be accomplished by placing in a 4f optical system a 128 pixel liquid crystal modulator (LCM) or an acousto-optic modulator (AOM) excited by an ultrasonic transducer coupled to an RF arbitrary waveform generator. These schemes enable us to implement both amplitude and phase modulation to the femtosecond transient.

4f optical setup at Warren’s lab at Princeton and high resolution pulse shaping using a 43 bit pulse sequence encoded in the time domain of an RF sinusoidal signal and frequency domain of an optical femtosecond pulse. The contrast ratio achieved is 12 dB.
Adaptive Pulse Shaping for molecular control

Passive and active control

Algorithm

Learning loop

Pulse shaper

Experiment

Initial guess

E-field

time [fs]

Cell

probe

control

Startup Phase

Reference Algorithm

Less Greedy, More Robust

More Greedy, Less Robust

Fitness

0.1

0.2

0.3

0.4

0.5

0.6

0.7

0.8

0.9

1.0

Log of Generations

0

2

4

6

8

10

Rapid Descent Phase

Asymptotic Phase

Credit = \frac{\text{Bestfit} - \text{Childfit}}{\text{Avgfit} - \text{Bestfit}}
As a starting point for our evolutionary algorithm, we adopted procedures extracted from the literature (Bucksbaum’ group, Ann Arbor Michigan, US).

The operators that were used are: two-point frequency crossover, average crossover, mutation, polynomial phase mutation, creep, smoothing, time-domain crossover assuming a random number \( r_i \) in \([0,1]\), \( P=\text{parent}, \ C=\text{child}, \ \Phi=\text{phase} \) and \( A=\text{amplitude} \):

\[
\text{e.g. Two-point crossover:} \quad P_1 = [\Phi_{P_1}(\omega_i), A_{P_1}(\omega_i)] \quad P_2 = [\Phi_{P_2}(\omega_i), A_{P_2}(\omega_i)]
\]

\[
C_1 = \begin{cases} 
[\Phi_{P_2}(\omega_i), A_{P_2}(\omega_i)] & \text{if } j < i < k \\
[\Phi_{P_1}(\omega_i), A_{P_1}(\omega_i)] & \text{all other } i 
\end{cases}
\]

\[
C_2 = \begin{cases} 
[\Phi_{P_1}(\omega_i), A_{P_1}(\omega_i)] & \text{if } j < i < k \\
[\Phi_{P_2}(\omega_i), A_{P_2}(\omega_i)] & \text{all other } i 
\end{cases}
\]

- At this stage it is worth noting that optimal control of molecular states in a learning loop has already been performed with a parametrisation in both frequency and time domain to speed-up the convergence rate of the evolutionary algorithm (Max-Planck Institute of Quantum Optics, Garching, Germany).

  We have introduced some new operators
  We also plan to use state-space control algorithms
**1. Chemical Catalysis**

**Time resolved experiments**
- Fluorescence lifetime imaging and non-linear microscopy with ASOPS
- Diffuse pulse spectroscopy to characterise enzyme immobilisation on magnetic nanoparticles (biosensor development)
- New insights on enzymatic mechanisms and reaction rates in allosteric proteins (with state space analysis & Sys. Id. tools)
- Studies of product formation with voltammetric, thermographymetric, calorimetric, TOF MS sensing

**Novelty**
- Formation of new chemical products through combinatorial chemistry
- Develop totally new enzymatic processes using optical activation
- Life defined as autocatalytic steps
- In-silico genomics & artificial life

**Use optical activation processes to couple with enzymatic steps**
\[ \Delta G^* = G_{\text{transition state}} - G_{\text{substrate}} \]

- Vibrational ladder climbing experiments
- Preferential production of specific isomers
- Control of phosphorylation reactions
- Interfere with cell mitotic cycle

The cyclins bind to the CDK molecules, thereby regulating the CDK activity and selecting the proteins to be phosphorylated.
2. Proteomics / Transcriptomics

Use tailored fs pulses for *in vitro* studies of biochemical control

- Use tailored fs pulses to fragment macro-molecules studied with TOF-MS

Replace enzyme digestion (e.g. trypsin) with tailored fs pulses to fragment macro-molecules studied with TOF-MS

Use tailored fs pulses for *in vivo* studies of biochemical control

Novelty

- Use light pulses to replace the function of hydrolases, kinases, esterases, aldol-condensation reactions
- Remote control of cellular metabolome
- Complement the 2-D electrophoresis step in MALDI, increasing specificity in TOF–MS for proteomic sequencing
- Optical control of energy budgets in cells and gene expression in prokaryotic and eukaryotic organisms (quantified by Q-RT PCR)
3. Microfluidics

- Polaritonic integrated optical pump THz probe spectroscopy chip prototype at MIT

- Specifications for mass-produced application-specific integrated devices
- Suppression of cancerous processes in erythrocytes, optical activation of cryo-protection processes in cells

We propose:

- Integrated fibre-optic ASOPs source/detectors
- Microfluidic technology
- Integrated fs dressed state excitation for optical pump THz probe spectroscopy

- On-line measurement and control of certain cellular functions
- Verification of microfluidic chip function using TOF-MS/proteomics
- Suppression of cancerous processes in erythrocytes, optical activation of cryo-protection processes in cells
- Specifications for mass-produced application-specific integrated devices

In a genomics, transcriptomics and metabolomics era, economics will once again be the deciding factor in our attempt to optically control the fate of our genome
Vision: establish a multidisciplinary centre pioneering the new field of **Ultrafast Biomolecular Control**

### Exploitable Targets
- Explore the use of microfluidic devices in conjunction with medical applications.
- Commercial exploitation of purpose-built microfluidic devices.

### Gene Control in cells
- *in vitro* control of cellular metabolome with adaptively shaped femtosecond excitation.
- Coupling fs pulses into cells (using dispersion pre-compensation) for *in vivo* control of gene expression (by studying the proteome with MS).

### Adaptive Ultrafast Pulse Shaping
Set-up time-resolved experiments
- Develop a range of evolutionary algorithms
- Develop a coherent control methodology
- Develop novel algorithms for signal processing of spectra

### Microfluidic Devices
- Tailor-made non-dispersive micro-fluidic devices which will provide simultaneous measurement (FLIM) and control of cellular processes within individual cells (with RAL).

### Chemical Catalysis
- Mapping of PE surfaces by pump-probe spectroscopy
- Optically drive families of chemical and biochemical reactions with adaptively shaped femtosecond pulses.
- Study charge transport processes, isomerisation reactions, enzyme inhibition reactions, kinetic studies

### Exploitable Targets
- Novel bioreactor technologies
- Can we patent particular pulse shapes that act as catalysts in certain environments?
Instrumentation and Measurement are at the heart of all natural sciences extending our senses. Good engineering practice implies extensive use of feedback at the instrument design process. Solutions cut across several disciplines.
Conclusions

• We have discussed simple optoelectronics measurement schemes based on feedback principles for sensing humidity, displacement and acceleration and contrasted with capacitive transducers (force-feedback seismometers).

• Discussed the concept of force-feedback optical microphones and how these can be used to built an ultrasensitive absolute photoacoustic power meter for terahertz radiation.

• I explained the principles of null-balance bridge techniques and the concept of electrical feedback substitution, a concept that can be used beyond metrology to study biological systems.

• I introduced you to the fascinating world of femto-second pulse systems and explained how evolutionary feedback techniques may one day be used to control our genome.

• An in-depth knowledge of feedback principles can lead to important advances in Instrumentation for Physicists, Biologists and Chemists.

• **Studying Systems Engineering at Reading will enable students to acquire a multidisciplinary background so they can further pursue a research career in the Natural Sciences.**

Thank you!