Measurement traceability and new measurement modalities

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CCIMI
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Metrology primer

- Standard units of measurement: metre, kilogram, second, ampere, kelvin, mole, candela
- Primary realisations of the units: e.g., laser interferometry, artefact, atomic clock, triple point of water
- 2018: Planck’s constant, Boltzmann constant

- Traceability chains: unbroken documented series of calibrations, each with a stated uncertainty
- Knowledge specified in terms of probability distributions
  - Estimate: mean of the distribution
  - Standard uncertainty: standard deviation of the distribution
- Typical assumptions: normality, independence, unbiased, linearity

Confidence in Measurement

The NMIs ensure confidence in measurement through:

- An organisational structure for reaching consensus and making decisions: BIPM, Consultative Committees, JCGM
- An agreed set of standard units: SI
- Standardised experimental procedures
- An agreed vocabulary: VIM
- An agreed methodology for uncertainty evaluation and establishing traceability: GUM
- Investment in validation exercises: Key Comparisons

Achieving a high level of **reproducibility**, **inter-operability** and **trust**.

- Spatially: global manufacturing, efficient international trade
- Temporally: measurements now can be compared directly with measurements made 100 years ago
    - Climate change, etc.

Addressing societal challenges
Sensor networks
Imaging

Laboratory	Real world
Single instrument	Networks of sensors
Single measurand	Multiple measurands, fields
Static	Dynamic
Controlled environmental conditions	Uncontrolled environment
Modest number of degrees of freedom	Possibly very large number of degrees of freedom
Validated, simple models	Partially known models
Modest amount of data	Big data? Data efficiency
Optimisation, model fitting	Data assimilation, statistical/machine learning
Uncertainty propagation	Uncertainty quantification

Uncertainty quantification

- *Specification uncertainty,* standard units, documented methodologies
- *Experimental uncertainty*, random effects, repeatability and reproducibility
- *Parameter uncertainty*, systematic effects
- *Structural uncertainty*, model inadequacy, model bias, or model discrepancy
    - Approximate models
    - Surrogate models
    - Model selection
    - Model averaging
    - Model augmentation and model calibration
    - Model validation
- *Algorithmic uncertainty*, numerical uncertainty
    - Formalised computational aims, ontologies
- *Computational uncertainty*
    - Generation of reference data and results

Ambient air networks I PAHs

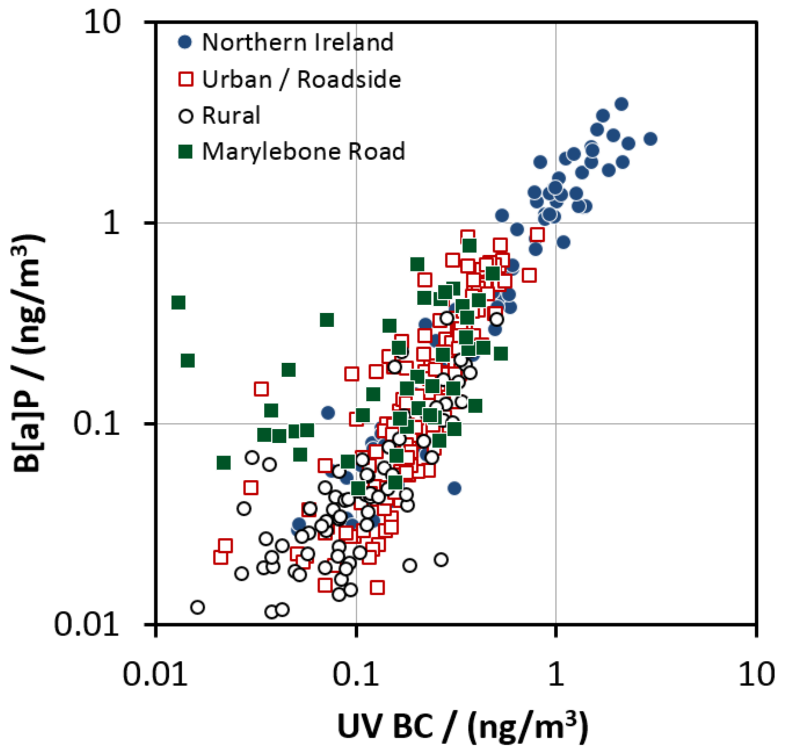
- UK Polycyclic Aromatic Hydrocarbon Network (PAHs)
- These are analysed for some toxic PAHs required by European Directives 2008/50/EC:
    - SO2, NOx, PM10, PM2.5, lead, benzene, CO
    - Data Quality Objectives
    - Requirement for traceability

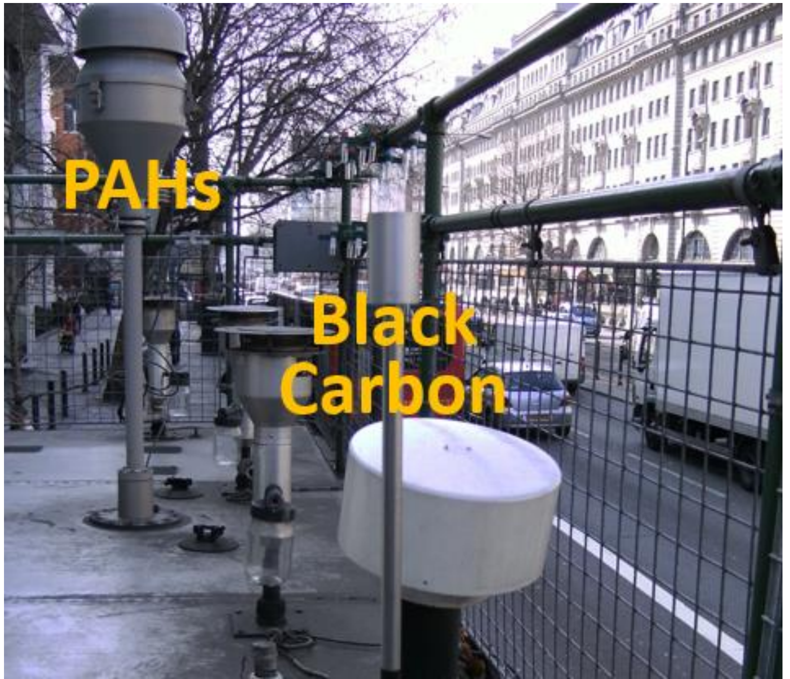
Ambient air networks II
Diffusive Samplers

- Collect UK wide data on NO_2 supplied from local authorities, and NPL field intercomparison exercise
- Monthly co-location studies of three diffusive samplers and automatic reference method
  - Sensor characterization again reference sensors

Ambient air networks III
Black carbon

- Additional measurements of black carbon (BC) produced at a number of PAH locations
- Analysis of correlation between PAHs and BC
  - Use of surrogate measurements





Noise

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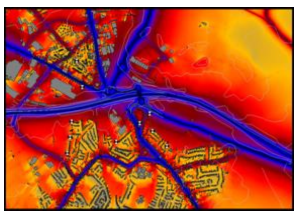
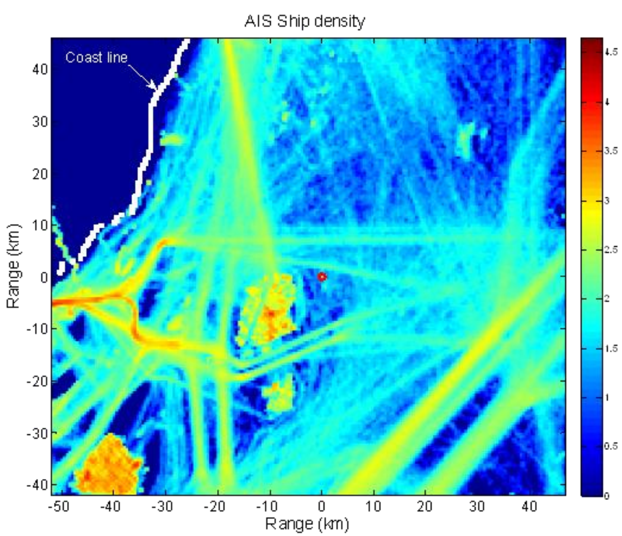
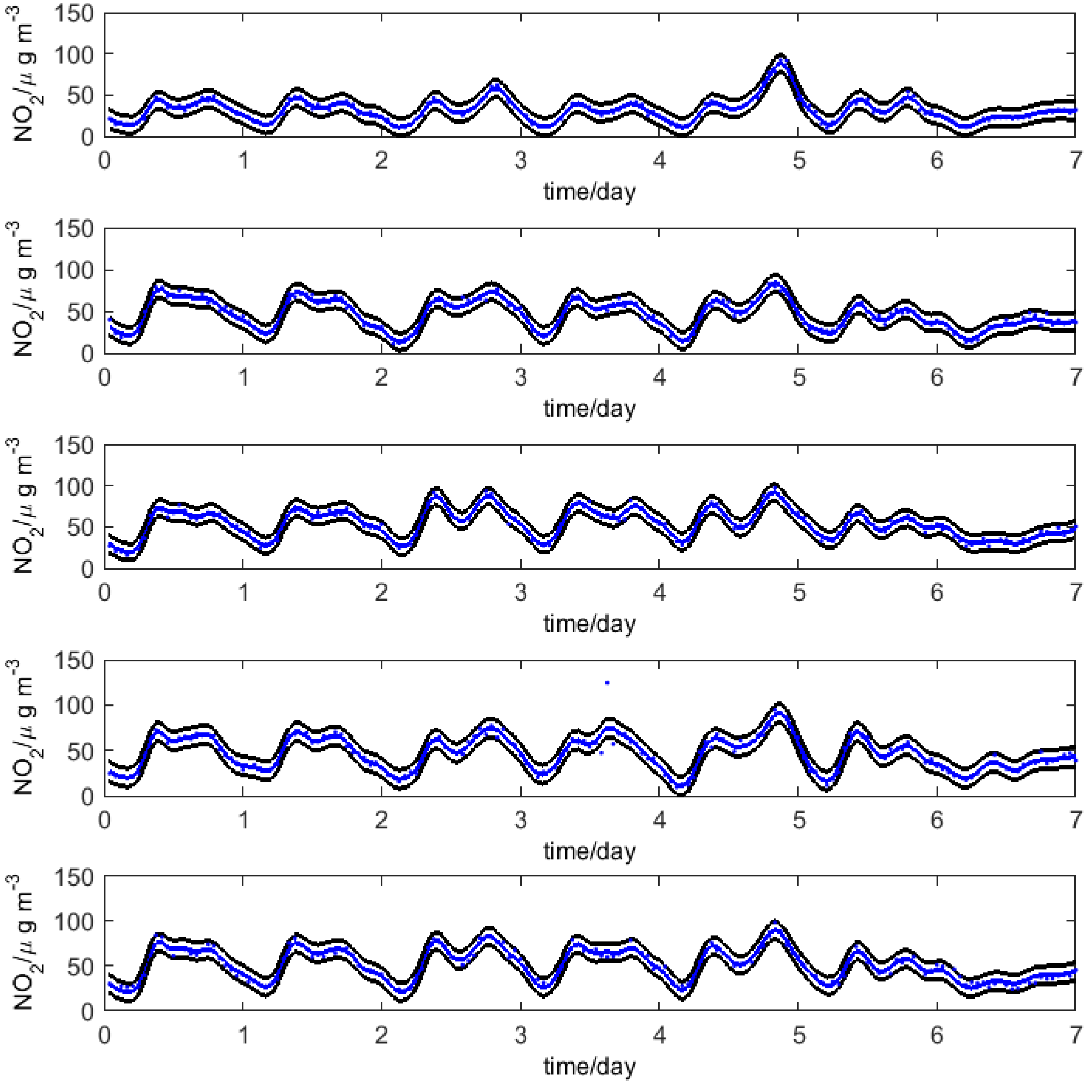




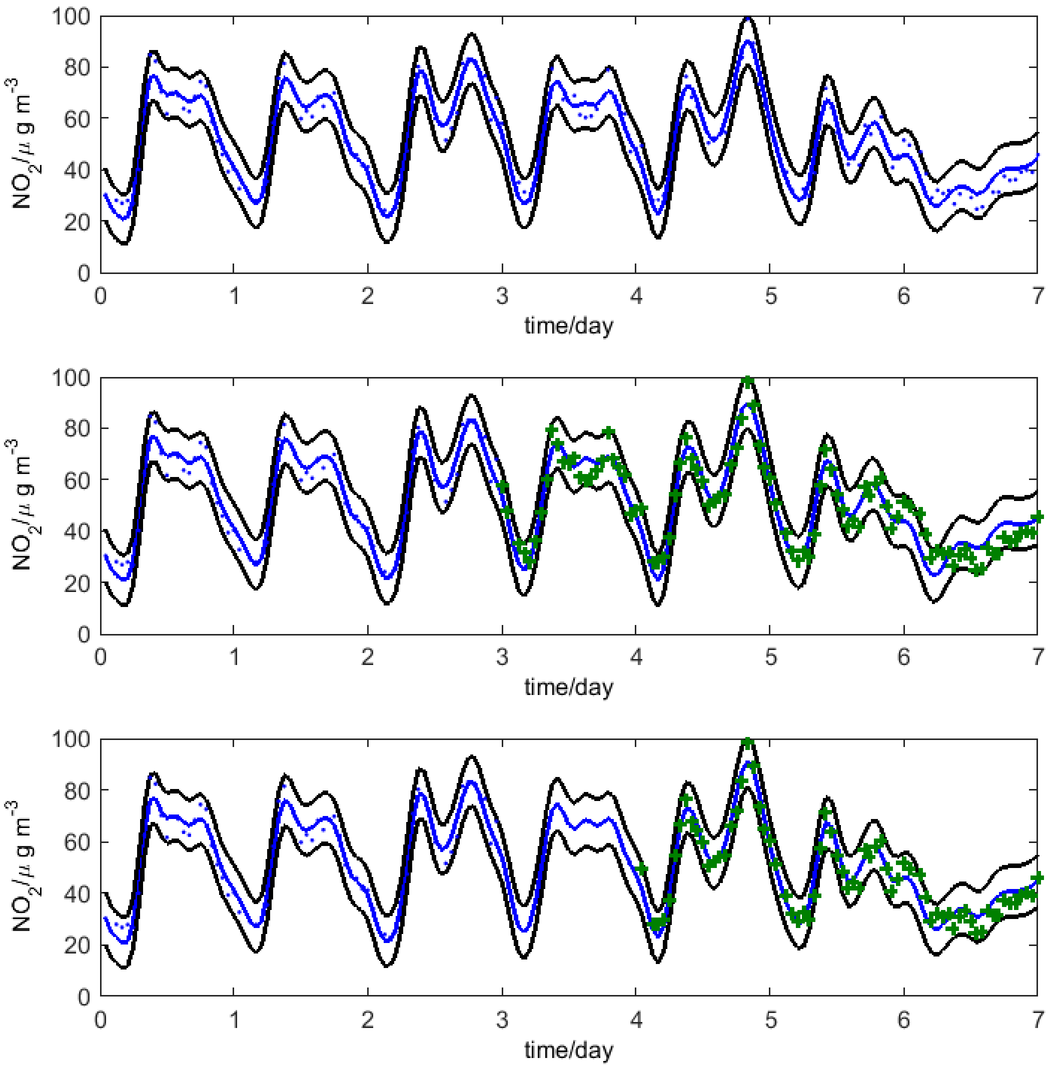
Confidence in SN measurement

- Sensor characterisation and calibration
  - In the laboratory
  - in situ
- Sampling points
  - Macroscale issues: representativeness
  - Microscale issues: atypical micro-environments
- Reference networks
  - few, designed locations, calibrated
- Low cost networks:
  - many, opportunistic locations, calibration status doubtful
- Modelling and inference
  - Extrapolation from discrete samples to a continuous field
  - Multi-modal sensing and surrogate measurements

London Air Quality Network



In situ calibration



Imaging

- Used across all sectors
- Different modalities (specification uncertainty)
- Example: XCT for industrial inspection
  - X-ray source: beam homogeneity (spatially, temporally)
  - Detector array: sensitivity, geometric alignment, drift
  - Spindle system: geometric alignment, drift
  - Reconstruction algorithms
  - Thesholding applied to absorption voxel map
  - Feature extraction, classification algorithms

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UQ for reconstruction algorithms

- Ill-posed inverse problem
- Regularisation approach
- Prior distributions for Bayesian approaches
- Model uncertainty or information gain

UQ for machine learning

- Accuracy of the training data
- Correctness of the labelling of training data
- Representativeness of training data
- Loss of information due to dimension reduction
- Uncertainty associated with classifications
- Sensitivity analysis: what training data is driving the algorithm
- Reproducibility of results
- Explainability of decisions

NPL investment in UQ

Institution	Activity
Cambridge (CCIMI)	Joint appointment in quantitative imaging
Cambridge	PhD studentship in ML for spectral imaging
Cambridge	PhD studentship in SN for smart infrastructure
Cambridge	PhD studentship in analytics for air quality
Imperial	PhD studentship in computational Bayesian inference for environmental monitoring
Surrey	PhD studentship in UQ for earth observation
Manchester	PhD studentship in UQ for inverse problems
Strathclyde	PhD studentship in trust architectures for SN
Nottingham	PhD studentship in software validation
Oxford	PhD studentship in reconstruction algorithms for SN
Bath	PhD studentship in UQ for machine learning

Challenges ahead

- National Metrology Institutes
  - More accuracy, seeing further, finding more
  - Reproducibility of scientific research
  - Addressing societal challenges
- Balance of uncertainty contributions
- Networks of sensors
  - Environmental monitoring
  - Factory of the Future, Industry 4.0
- Quantitative Imaging
- UQ for machine learning
- Quality assurance indicators for data

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Thank you

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