



**CATAPULT**  
High Value Manufacturing



**HTFS-III (High Throughput Formulation Screening)**  
**National Formulation Centre, Sedgefield, County Durham, UK**  
**Wednesday 26th April 2017**

**Developing 21st Century Formulated Products & Manufacturing Processes**  
**Challenges & Opportunities**

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**John Carroll**

Technical Strategy Director, Formulation; CPI

**CATAPULT**  
High Value Manufacturing



# High Value Manufacturing Catapult

**£460 million** invested to date

Over **£240 million** for the next 5 years

Over **2300** industry clients

A combined **1300** staff and growing

A light grey map of the United Kingdom is shown on the right side of the slide. Several logos of partner organizations are overlaid on the map, each pointing to a specific geographical location. The logos include AFRC, cpi, MTC, WMG, and the National Composites Centre.

**AFRC**

The cpi logo, consisting of a stylized circular sunburst icon and the lowercase letters 'cpi'.The logo for the Manufacturing Technology Centre (MTC), featuring a stylized circular icon with a blue and purple gradient.The logo for WMG (Worcester Manufacturing Group), featuring a stylized circular icon with a blue and purple gradient.The logo for WMG (Worcester Manufacturing Group), featuring a stylized circular icon with a blue and purple gradient.The logo for the Manufacturing Technology Centre (MTC), featuring a stylized circular icon with a blue and purple gradient.The logo for the National Composites Centre, featuring a stylized circular icon with a blue and purple gradient.

# Who are CPI?



CPI is a UK technology **innovation** centre and the process element of the Government's **High Value Manufacturing Catapult**.



**National Printable  
Electronics Centre**



**National Industrial  
Biotechnology Facility**



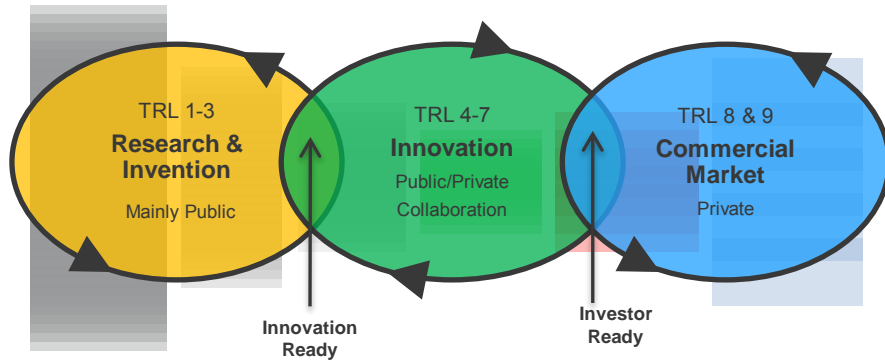
**National Biologics  
Manufacturing Centre**



**National  
Formulation Centre**

We use applied knowledge in science and engineering combined with state of the art facilities to enable our clients to **develop, prove, prototype** and **scale-up** the next generation of products and processes.

# De-risking Translation from Invention to Invoices



**WE SUPPORT COMPANIES CROSSING THE GAP BETWEEN RESEARCH AND COMMERCIALISATION**

# Formulation (Integrate to Deliver Surprising Benefits)



Formulation, the creation of multi-component, multi-phase products, is an **enabling capability**

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Creating value through intricate **microstructures** and powerful **ingredient synergies**

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Underpins many **sectors** in our economy and **high-value manufacturing** industries globally.

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The formulated products market in the UK is worth around **£180 billion per annum** with a potential for companies in emerging overseas markets of around **£1,000 billion per annum**



# The National Formulation Centre - Overview



Create value for UK-based companies through formulation science by enabling bigger, cheaper or faster innovation

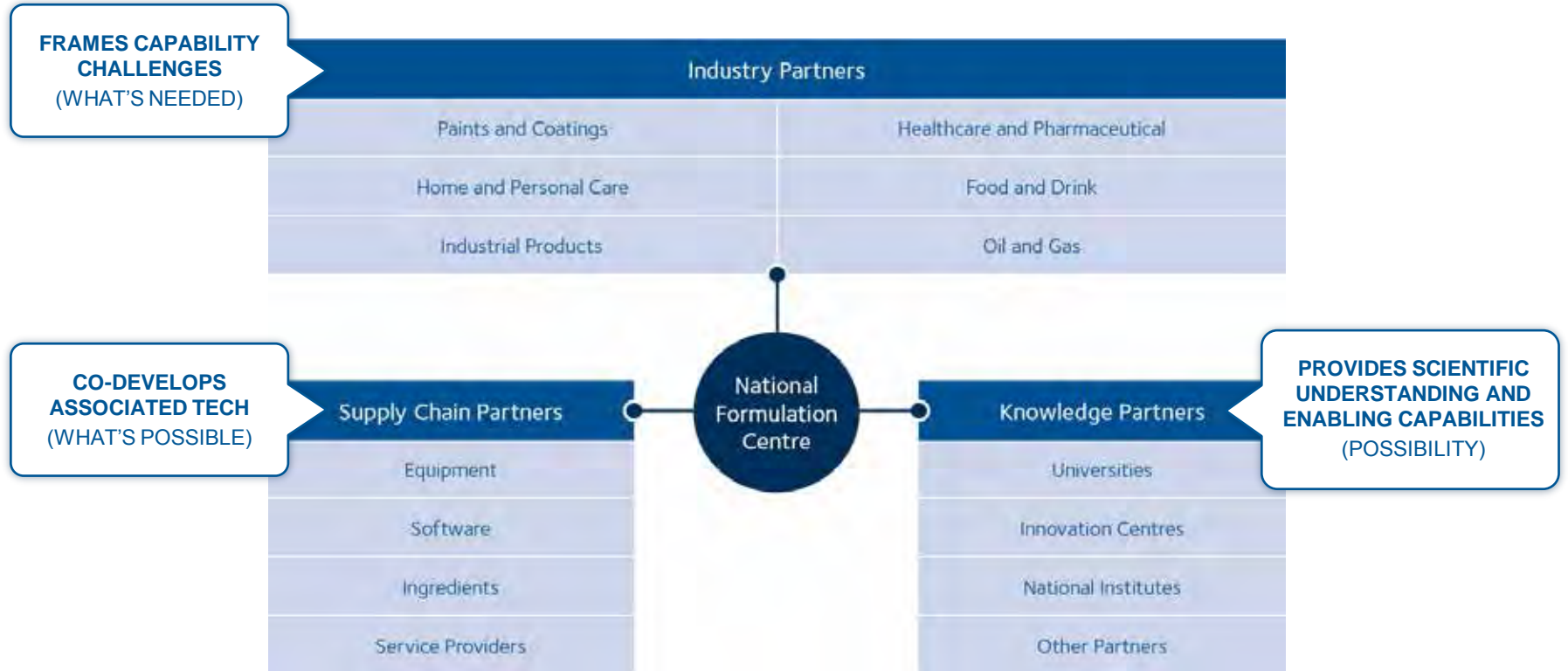
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**Productivity from value-creating strategic alliances** with industry and the wider UK formulation eco-system (inc SME/supply chain and Knowledge Base (Academic) partners)

Create and use an **industry-led portfolio of advanced capabilities**. **Sweat the UK assets** by best harnessing current capabilities and then plugging any critical gaps identified

**Sustainability from enduring access and application of advanced capabilities**

# Structure – Activating the Innovation Eco-system





# Potential for UK Leadership in a Global Capability Race



Past	2014	2017	2020	2025	2030	
Empirical	Semi-empirical	Predictive (Sub-systems)		Predictive (System)		Formulation Maturity
Data-poor	Data-rich	Information-rich		Knowledge-rich		Knowledge Intensity
“Experts”	Fragmented Systems	Connected Systems / Data Standards		Closed-loop Design		Knowledge Capture

**CPI National Formulation Centre**  
Transforming formulation from art to science, faster

- Transformation potential through advances in enabling technologies such as informatics, modelling, measurement and sensors (Telemetry), and automation - robotics
- Faster progress through integration model

# Capability Themes to Work Against

Revalidated by Industry Steering Group (ISG)



## Predictive Designs

### Faster Innovation

Faster, more reliable approaches to get to ideal formulation design

## Radical Effects

### Bigger Innovation

Unexpected synergistic effects to deliver bigger/disruptive benefits

## Manufacturability

### Process Innovation

Optimised, reliable system to guarantee ideal formulated product delivery

**4IR Capable**

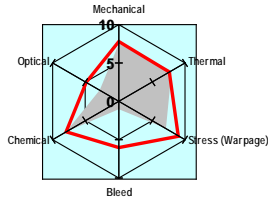
### Innovation Enabler

Critical foundational component for knowledge management and connectivity

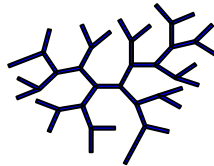
# Formulations operate at different length & time scales to deliver required functional effects



# High Throughput Formulation and Product Development



**Functional Properties**  
Mechanical, Surface,  
Electrical, Optical, Thermal  
Chemical, Biological, Sensory



Final Form

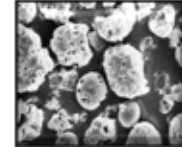
Material in End-Use

Secondary Structure

Functional Materials or Formulations

Primary Structure

Raw Material(s)



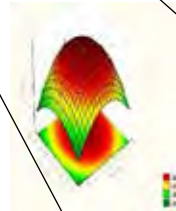
# The Spectrum of Knowledge

**Empirically  
Driven**



**Complete  
understanding**

- Very little is really known.
- Progress is made mostly by leveraging previous experience /guesswork and trial and error



- Pockets of knowledge
- Little or no transferability
- No real learning or understanding generated

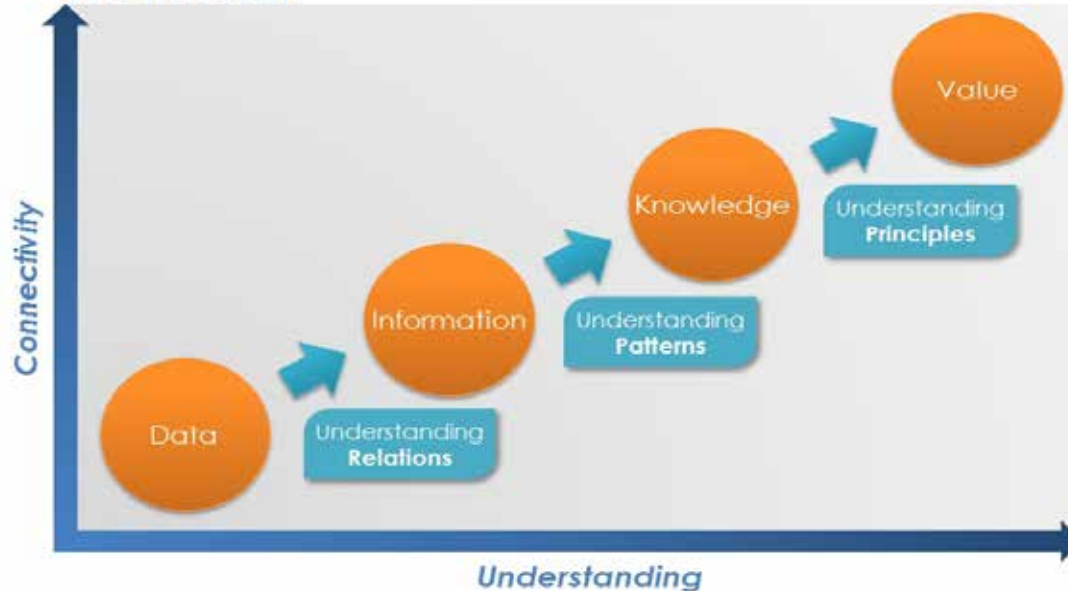
- Can write equations to describe every aspect of the problem

# The difference between data and knowledge

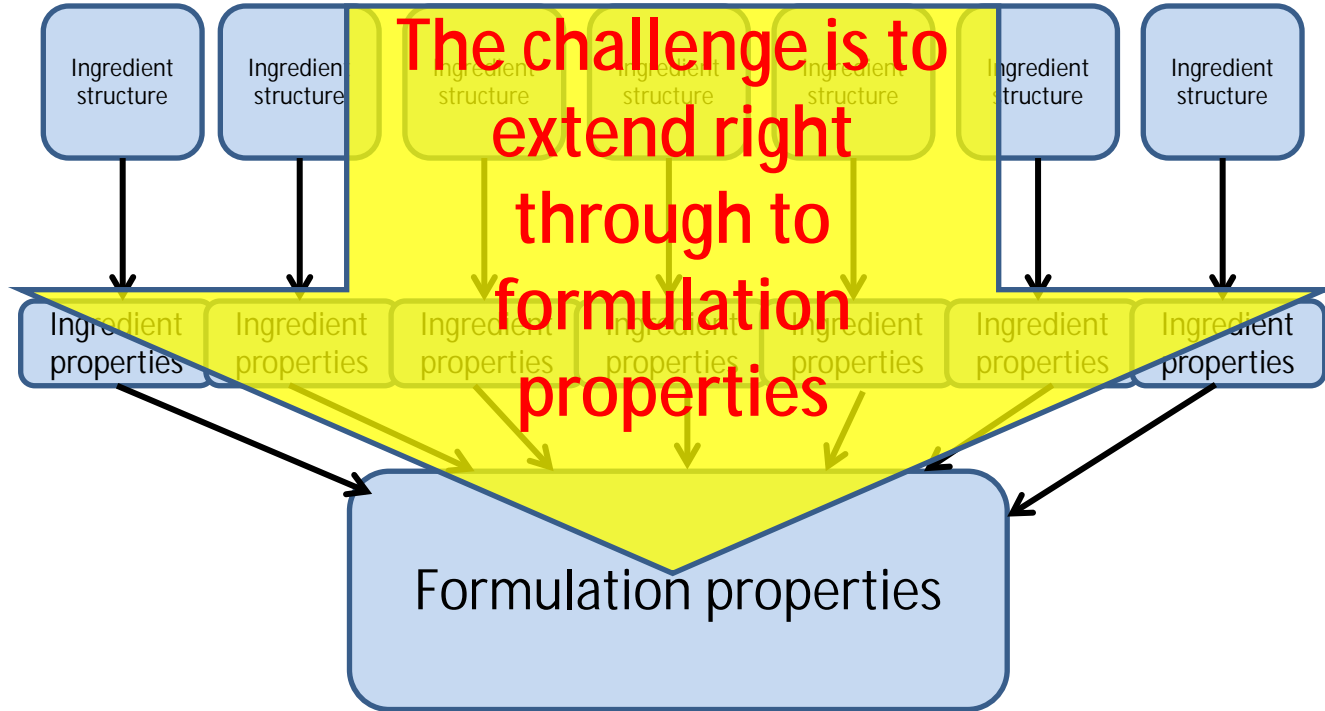
- We have a huge amount of formulation data
  - But what do these data teach us about achieving the required functional properties that add commercial value to products

**Data  $\neq$  knowledge**

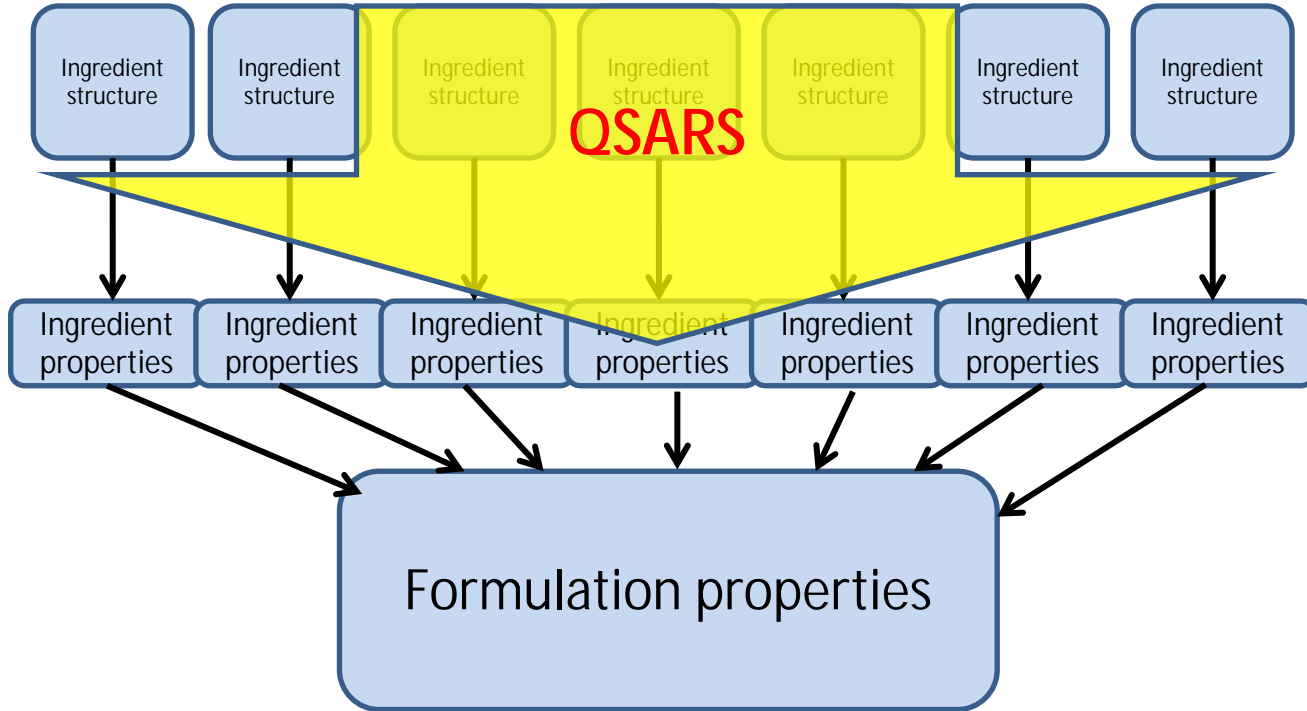
*Data in itself is valueless: value is created via connectivity and understanding.*



# Can we change this?



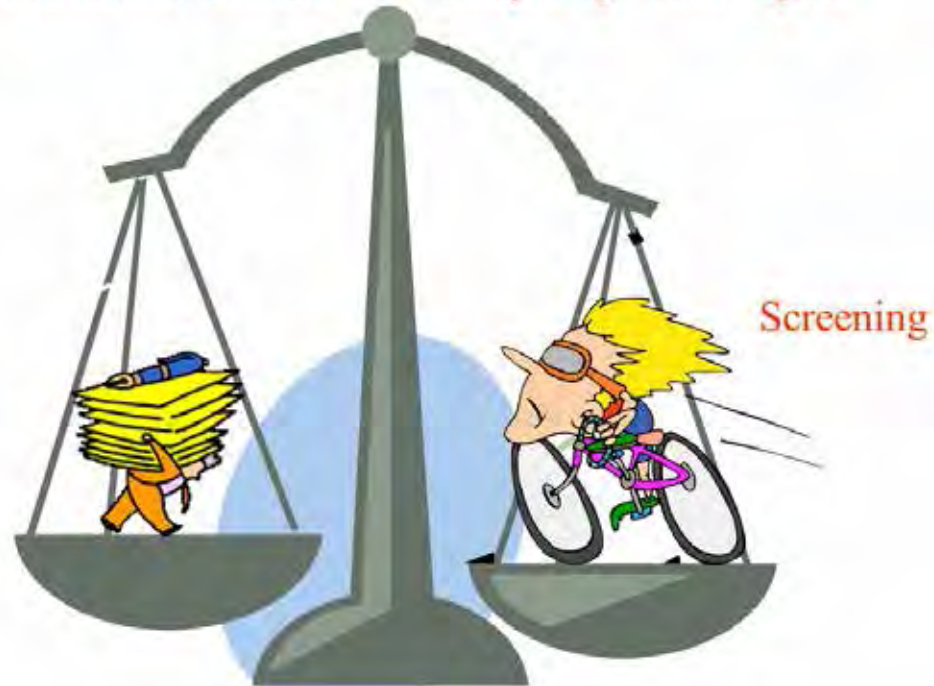
# Can we change this?





# To screen or not to screen

Information Content vs. Simplicity \ Time \ Speed



# Functional Requirements – Coatings

## Appearance

Colour, texture, opacity

## Stay Clean

Antibiofouling, antibacterial, appearance

## Thermal Management

Heat protection, efficient energy coupling

## Structural / Mechanical

Anti scratch, non cracking etc.

## Protective

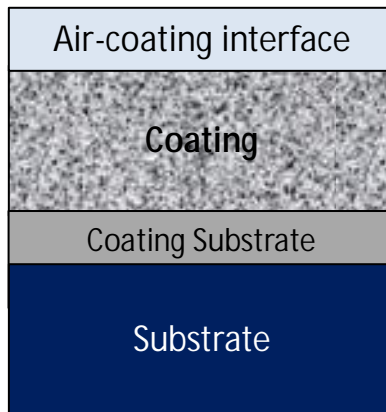
Anti corrosion, packaging, chemical resistance

## Electrical / Magnetic

EM, shielding, transmission

## Extended Durability

Light Stability, weatherability



## Uncured Coating Properties

Rheology  
Wetting behaviour, surface tension  
Shelf life, colloidal stability  
Thermal stability  
Appearance  
Reactivity, cure behaviour

## Surface Properties

Light reflection  
Hardness  
Scratch resistance  
Friction/surface roughness  
Repellent properties  
Erosion resistance

## Bulk Coating Properties

Opacity  
Colour  
Flexibility  
Barrier  
Chemical resistance  
Environmental resistance

## Coating Substrate Interface

Adhesion  
Durability  
Anti corrosion

# Functional Requirements – Inks

## Appearance

Colour, opacity

## Hiding Power

Colour, opacity, particle size?

## Compatibility with Print head

Evaporation, chemical compatibility

## Dispensability

Flow properties, droplet formation

## Surface Coverage

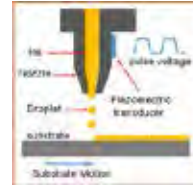
Flow properties, substrate wetting

## Electrical / Magnetic

Conductivity, magnetism

## Extended Durability

Light stability, environmental resistance



Air-Ink Interface

**Bulk Ink Properties**

Ink Substrate Interface

Substrate

## Properties of Dispensed Ink

Surface tension (droplet formation)

Flow properties

Colour

Opacity

Chemical Compatibility

## Surface Properties

Light reflection

## Bulk Ink Properties (on substrate)

Opacity

Colour

Flexibility

Conductivity

Environmental resistance

## Ink Substrate Interface

Adhesion and spreading

Durability



# Functional Requirements – Composites

## Structural / Mechanical Properties

Anti crack, scratch resistance, toughness, lightweight

## Environmental Resistance

Extended durability, chemical resistance

## Thermal Management

Thermal stability, heat dissipation

## Electrical Properties

Conductivity

## Adhesive Properties

Fibre-resin interaction



Resin-Air Interface

Resin Matrix

Resin-Fibre Interface

Woven Fibre Matrix

## Resin – Air Interface

Hardness  
Scratch resistance  
Friction/surface roughness  
Repellent properties  
Environmental resistance  
Chemical resistance  
Light reflection

## Resin Matrix

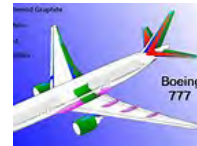
Tensile strength of resin and composite  
Impact resistance  
Cure, flexibility, morphology

## Resin – Fibre Interface

Interfacial bonding  
Durability  
Fibre volume fraction

## Woven Fibre Network

Tensile strength of individual fibres  
Interconnectivity (weave, shape, orientation)



# The Real Challenge for Formulation Product Development & Manufacturing

- Data Space is vast not tractable even with HTE
- Need Predictive Models that allow rapid selection of candidate systems
- Information about ingredients and their relevant chemistry/material properties is linked to formulation data
- Experiments are designed to reveal fundamental science and inform models
- Informatics is used to recognize clues hidden in the data that contain real learning
- Discovery properties are scalable into flexible manufacturing processes
- We make a conscious effort to move the state of the art forward in a way that adds real value to companies and the way they approach formulation

# Integrating Existing and Developing Capabilities



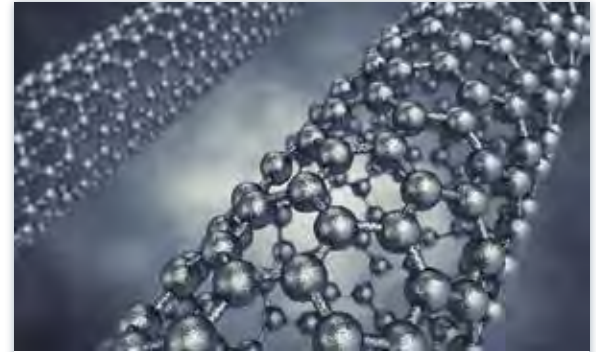
## CENTRE FOR INNOVATIVE FORMULATION

Power of serving NE innovators



## NATIONAL FORMULATION CENTRE

Power of UK innovation ecosystem



## GRAPHENE APPLICATIONS CENTRE

Power of nano-expertise to application

SHARED CAPABILITIES THAT SPAN GENERAL FORMULATION TO SPECIFICS IN NANO-MATERIALS

## OVERARCHING CAPABILITY TO ENABLE OUTSTANDING R&D

- i. Digital Infrastructure- Informatics and Modelling
- ii. Experimental Design
- iii. Data Analytics



## COMPLEX SOLIDS HANDLING AND PREPARATION

- i. SHEQ Enabled for powders and Nano-materials
- ii. Milling
- iii. Plasma functionalisation
- iv. Mixing (high shear, low shear, turbine)
- v. Atomic layer Deposition/ Chemical vapour deposition



## COMPLEX LIQUIDS HANDLING AND PREPARATION

- i. Flow reactors
- ii. OBR
- iii. Microfluidics



## FORMULATION PREPARATION

- i. High Throughput Experimentation
- ii. Draw downs (coatings)
- iii. Plaques (composites)
- iv. Injection Moulding



## FORMULATION APPLICATION TESTING

- i. Electrical
- ii. Thermal
- iii. Abrasion
- iv. Lubricity



## PROCESS SCALE-UP AND METROLOGY

- i. Metrology
- ii. Modelling



# Real Physical Facilities in Place at NETPark

Temporary solution to enable accelerated company support





# Capability Themes to Work Against

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**4IR Capable**

### Innovation Enabler

Critical foundational component for knowledge management and connectivity

# Microstar: Microfluidic Platform for prediction of stability and rheology of complex fluids



## INTEGRATED LIQUID STABILITY AND RHEOLOGY PREDICTION TOOLKIT

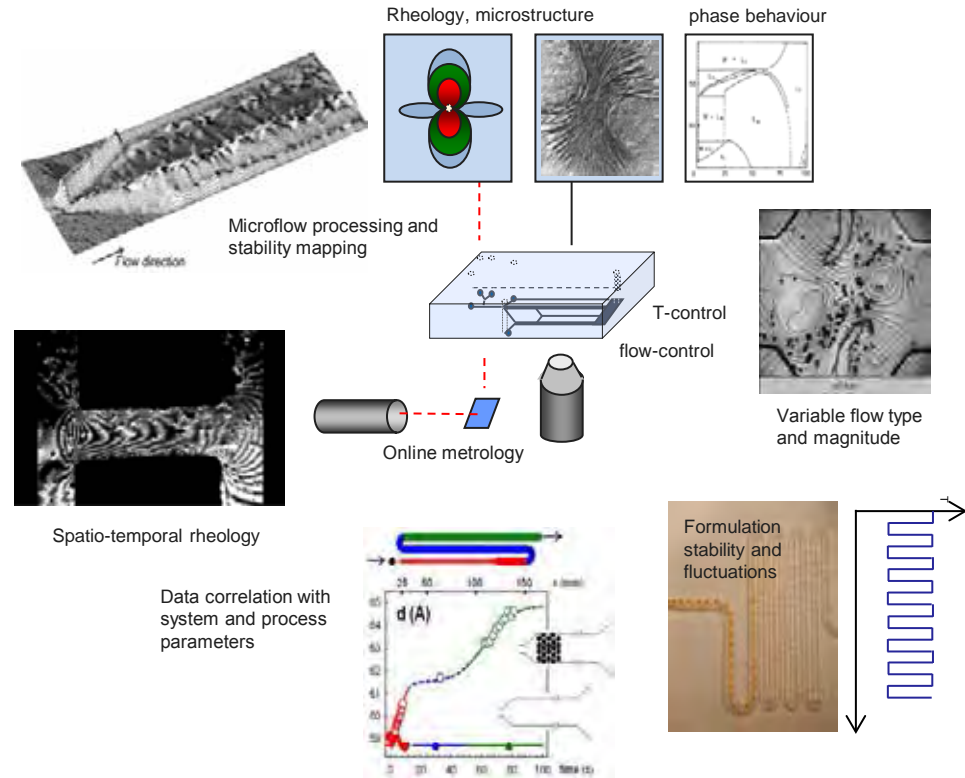
- Novel micro-flow methods for rapid screening of phase and metastability with relevant process variables
- Accelerated ageing tests; structural/dynamic metrology
- Cross-sector open-access test rig (Research Infrastructure)

## PHASE BEHAVIOUR/STABILITY MAPS OF COMPLEX MODELS AND REAL-WORLD SYSTEMS

- Generic open-learning
- Company-specific private-learning

## PARTNERS:

P&G, BP, Imperial, Durham



# PROSPECT: Proving of Real-wOrld Scalable PrEdiCtive Tools / Technologies



## LIQUID SCALE-UP LEARNING LOOP

Simple, flexible, multi-scaled rig to screen/trial sensor and control scheme technologies

## ASSOCIATED MODEL LIQUID FORMULATION

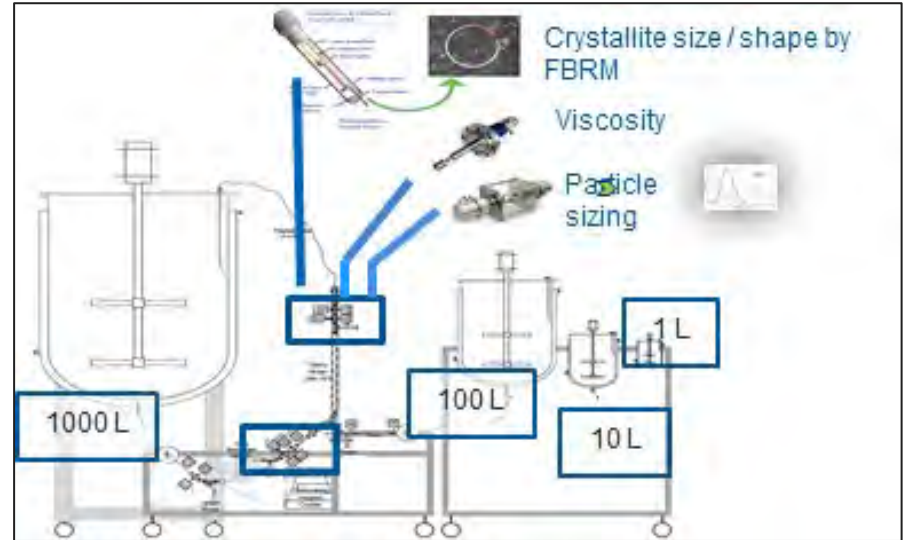
Enables closer to real-world studies - complex material structures and properties.

## PLATFORM TO IDENTIFY PROXY MEASURES

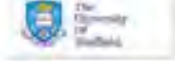
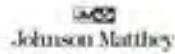
To enable cost efficient and operator friendly process sensing upgrade – cheap, 24/7, widely adopted, info-rich sensing.

## PARTNERS:

Birmingham, Leeds, Edinburgh



# Implementation of Particle Models for Industry



Currently major capability gap to transfer models from Academia to Industry.

## METHODOLOGY AND FRAMEWORK FOR TRANSLATING MODELS TO INDUSTRY

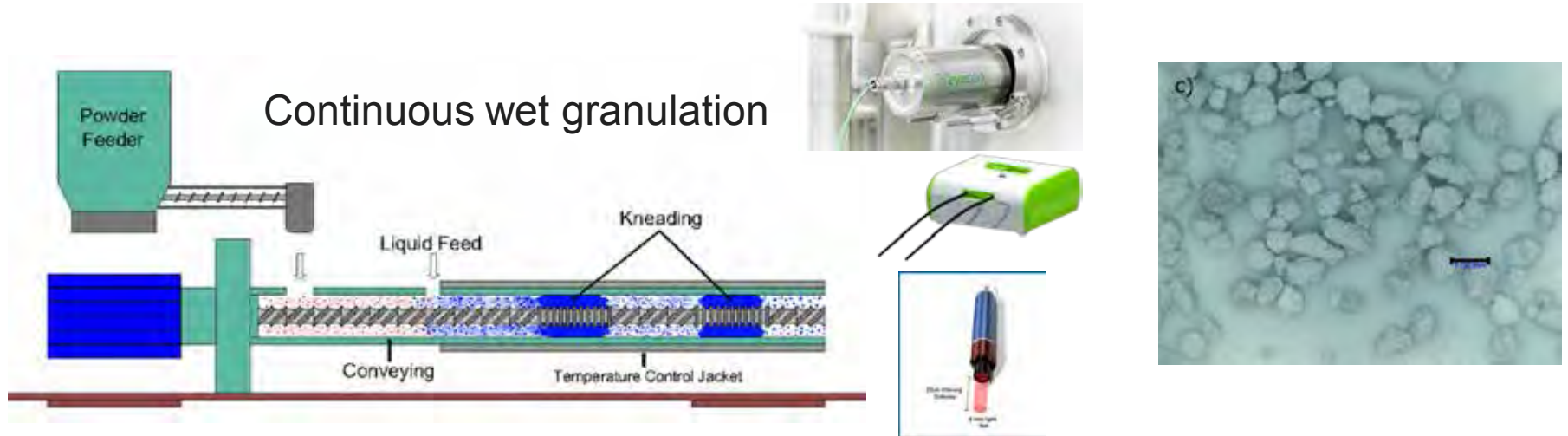
- Wet granulation case study which will fit as a tool within CPI- Chariot granules facility

## METHODOLOGY /BEST PRACTICE GUIDE AND SUPPORT NETWORK CAN BE APPLIED TO OTHER MANUFACTURING PROCESSES

- Driving step-change modelling adoption
- Complement commercial vendors
- Creating UK hub for model commercialisation and in-silico development



# Supporting Pharmaceutical Product Development

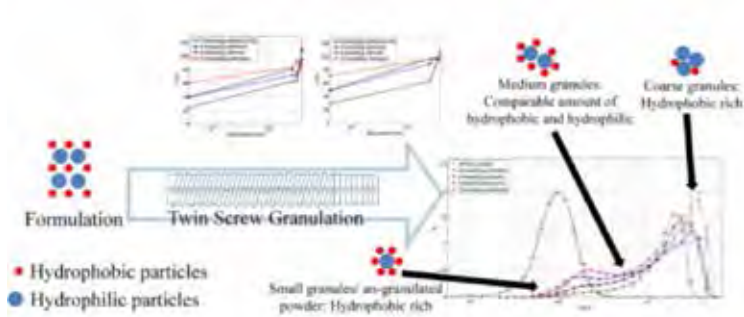


Creating and validating a national open-access contract development facility to support the development and registration of new products and processes

- **PAT enabled process understanding to support ‘development for launch’**
- **Marrying data from multiple sensors to finished product attributes**
- **Facilitating the industrial implementation of innovative process analytics**
- **Data to inform commercial control strategies – real products, real-life situations**

# Innovation Knowledge Flow

Mechanistic insight, modelling, analytical and process innovation



Yu et al; Int. J. Pharm. Sci. 475(1-2) (2014) 82-96

Academia  
Discovery & Understanding

Commercial process understanding



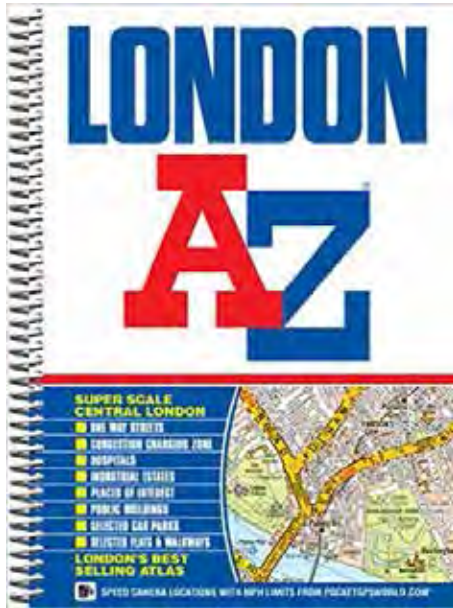
CPI Test Bed  
Commercial Process Development

Commercial control strategy



Pharma & CMO  
Commercial Manufacture

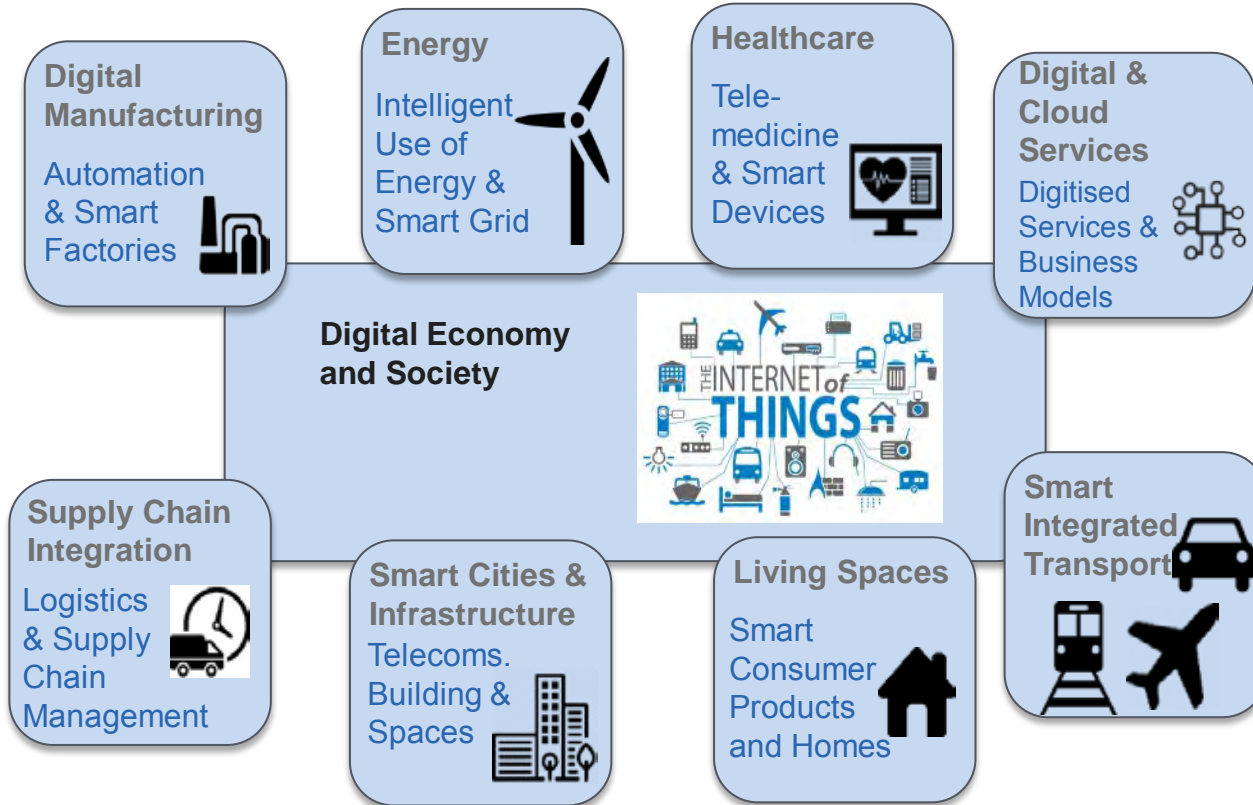
# Dynamic Information Availability and Interaction has changed the way we Live



**Static Look up**

**Real time update**

# Strategic Drivers



**Embedded electronics** seamlessly connects products, equipment and structures to digital and big data services and user interfaces



It's a critical capability to the future of manufacturing and new product innovation.



Critical to UK Manufacturing.





**Innovation Enabler**  
 Critical foundational component for knowledge management and problem solving  
**Industry 4IR Capable**

**IOT**

Connected → Interactive → Responsive

**Industry 4IR**

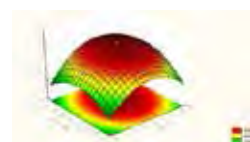
Formulation Design → Formulation Optimisation → Formulation Manufacturability



**Predictive Designs**

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**Faster Innovation**  
Faster, more reliable approaches to get to ideal formulation design



**Radical Effects**

---


**Bigger Innovation**  
Unexpected synergistic effects to deliver bigger/disruptive benefits



**Manufacturability**

---

**Process Innovation**  
Optimised, reliable system to guarantee ideal formulated product delivery



Real Time Data Capture & Interrogation



Connected & Secure Data

# Formulation Lighthouse Vision 2030



**Productivity** and **Simplification** in Innovation  
by Predictive Design

Ultimately created **autonomously**, from self-learning, IoT connected systems

**MORE ROBUST  
UNDERSTANDING OF  
COMPLEX SYSTEMS  
TO ENABLE MODEL  
DEVELOPMENT**

- SOLIDS
- LIQUIDS

**PREDICTIVE DESIGN  
FROM MODELS OF  
EVOLVING SYSTEMS**

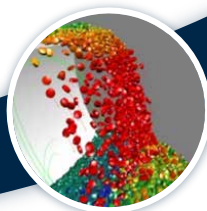
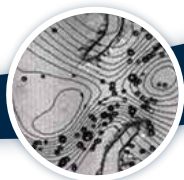
- INNOVATION EFFICIENCY
  - PRODUCTIVITY
  - R&D SIMPLIFICATION

**DEVELOP TRULY  
DELIGHTFUL PRODUCTS IN  
FUNCTION AND DESIGN**

(STEM TO STEAM)

**AUTONOMOUS LEARNING WITH  
SYSTEMS IOT ENABLED TO  
FORMULATE AGAINST REAL  
NEED/CONDITIONS**

**CURRENT ART OF  
FORMULATED  
PRODUCTS**



# Dynamic Adaptive Product Design : Formula design to real world performance: Automotive Lubricants

IOT



Product Model



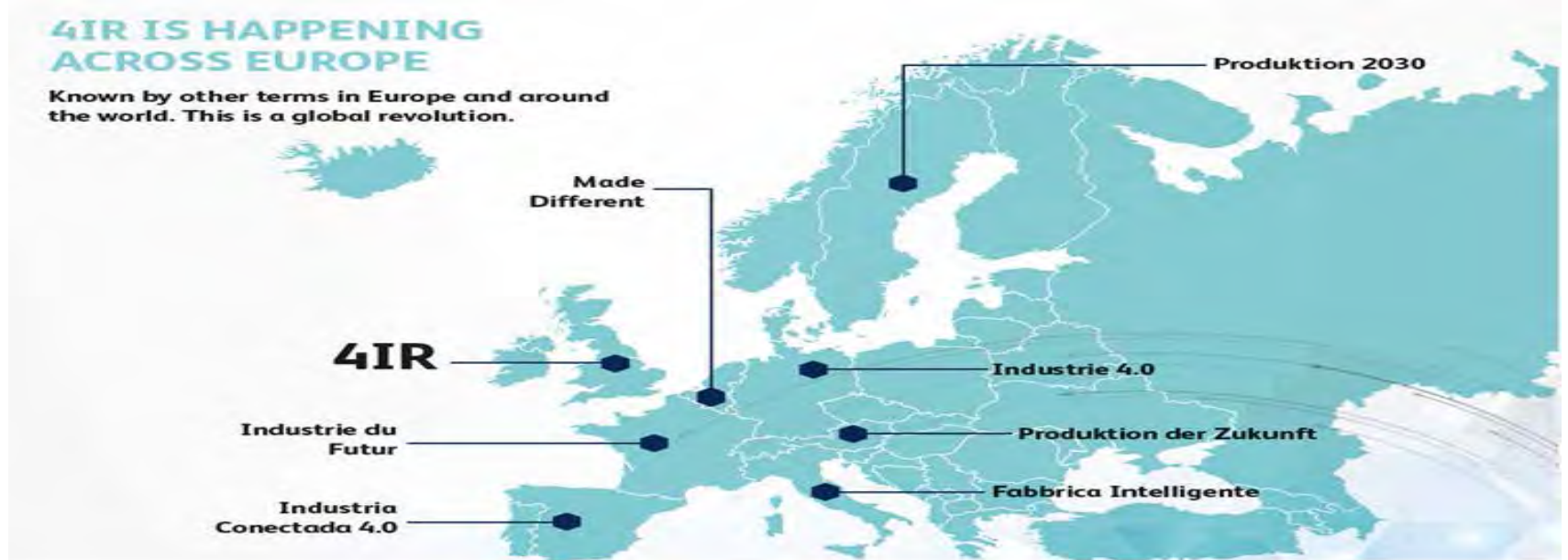
Real time  
Monitoring -  
learning real  
conditions

Ideal Product  
development for  
the real  
conditions -  
Enable  
Superiority  
Claims grow  
business

New car- first fill



# Digital Evolution or Revolution?

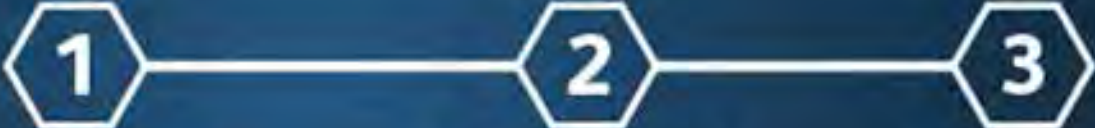


# Connecting Digital Product Design To Digital Manufacturing



## 4IR IS ABOUT CONNECTIVITY

It's about linking physical networks with cyber networks as one system, to allow real time information flow. This will allow insights to be discovered and acted upon quickly, boosting the value add to customers.



The three core components:

1 The Industrial Internet of Things - machines and other technologies that collect, share and act on data between themselves

2 Big Data (the capture of data on everything) and real time analysis of that data by machines and systems

3 Secure and reliable digital infrastructure to connect it all up



# Digital Engineering and Manufacturing Leadership Group

1 December 2016



# The project

7 centres:



4 partners



Supported by:



Innovate UK



# The Industry Leadership and Collaborators:

**CATAPULT**  
High Value Manufacturing





# The Working Groups



Business  
models

Implementation



Research

Skills, Work  
and Society



Cyber-Security and  
Legal Aspects

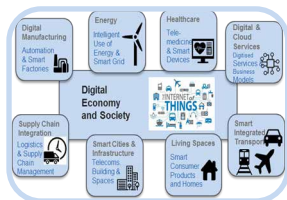


Standards  
and Regulation

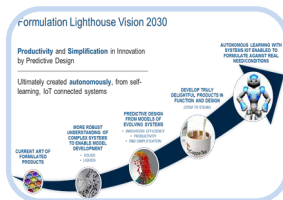
# Formulation - What next?

By 2020, 7.7 billion people will be online, 6.1 billion will have smartphones, 200 billion things will be connected to the Internet, and everyone on earth will have one thing in common.

## Drivers



Increasingly Digitally enabled world



Reatime Feedback on Product Performance



Increased Personalisation

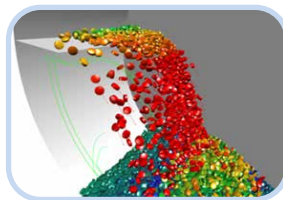


Sustainability/regulatory

## Requirements



Computer Designed molecules & materials



Need for Predictive Models to rapidly get to best formulated candidate systems



Integration of Characterisation and HTE formulation for verification of candidate formulation performance



Digitally enabled flexible manufacturing

# Thank you...

For more information visit [www.uk-cpi.com](http://www.uk-cpi.com)

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**Twitter:** [@ukCPI](https://twitter.com/ukCPI)

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[www.uk-cpi.com](http://www.uk-cpi.com)

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