Big Idea Title (maximum 10 words):

Mathematical modelling for next generation formulated products.

Summary Pitch (maximum 30 words):

The drive towards rapid, smarter, greener and personalised formulation requires the insight provided by new predictive mathematical approaches. In particular, understanding linkage between microstructure, complex processes, and perception will unlock productivity gains across the formulation sector.

W**hat is the Big Idea? (maximum 300 words)**

- *Give a description of the proposed opportunity, why it is exciting to researchers, government and the public, in non-technical language*
- *Highlight the transformational aspirations of the idea*
- *Explain how this idea is beyond the scale of an individual research project or proposal such as a programme grant*

The Formulated Products Sector contributed in excess of £ 149 bn to UK GVA in 2016 which is far more than aerospace and automotive [1]. The UK relies on this sector to provide food, pharmaceuticals, cosmetics, coatings and many other chemical products vital for everyday life. The business ecosystem is diverse containing many small, medium and large companies. There is a growing shift in the formulated product sector towards **rapid** development of **smarter, greener** and **personalised** formulations. Specific opportunities include:

- the removal of salt and fat and the increasing use of vegetable products to enable the UK to lead the world in the development of safe, high quality, inexpensive food that could shift population behaviour to a more nutritious, sustainable diet.
- the rapid formulation of medicines, therapeutics, and foods to provide cost effective, and personalised products to help different age / health groups, e.g. personalised nutrition for diabetics.
- reformulation to adapt to new ingredients due to regulatory changes, shortages arising from trade disruption, or supply chain failures as seen during the pandemic.

This shift requires new, predictive methods which use multiscale modelling to understand multiphase behaviour and ultimately provide links and insight into how products will perform, for example how taste and texture are perceived. Providing an **end-to-end predictive capability between the microscale of formulated products and the consumer** will allow manufacturers to address key challenges in unlocking manufacturing productivity, sustainability and Net Zero,

[1] https://admin.ktn-uk.co.uk/app/uploads/2018/07/Formulated-Products-Sector-Strategic-Priorities-2018-Final.pdf

and healthy ageing. The formulated product sector underpins almost everything we do each day.

The science required to address this shift is under-developed, complex and multi-disciplinary and it is often tackled in silos which are not shared across applications. Despite the importance of the formulated products sector, securing funding has historically been focussed on isolated aspects of the challenge with inadequate investment in comparison with other sectors [1]. The problems in these sectors are extremely complex and need many different skills, so it is a perfect candidate for the Big Ideas type of funding.

The scale of the challenge requires input from chemical engineers, statisticians, neurologists, biologists, physicists, data scientists and others. It is proposed here that predictive design for the formulated product sector can be **transformed by using the mathematical sciences to provide a naturally overarching framework** to advance the multidisciplinary research. This proposal will be transformative by enabling a cross-sector ecosystem for predictive design built firmly upon cutting-edge mathematical science.

IMPACT - WHAT impact would it have if successful? (maximum 300 words)

- *What knowledge, people, societal and economic impact will there be? Please describe the benefits of this.*
- *What would the 'big win' be for the UK if the idea is realised (both scientifically and non-scientifically)?*

The knowledge generated by this proposal will be accessible to multiple UK organisations in a pre-competitive manner which cuts across multiple societal challenges. It will also stimulate basic scientific research across many disciplines led by mathematics and data science. The proposal highlights the importance of multidisciplinary research, as well as software & tools development, ensuring that the fundamental knowledge is embedded into the formulated product sector. Implementation of the knowledge through research, people and tools will enable the formulated product sector to accelerate its ability to innovate, and ultimately:

- Reduce expensive development cycles in industry through better predictive modelling. Reducing expensive development cycles will have a knock-on effect on productivity in this, the largest UK manufacturing sector. This sector represents a **diverse ecosystem of SMEs, and multinationals** meaning the benefits would be felt across many UK businesses. Cheaper and more rapidly developed products could include vaccines, therapeutics, and healthier food for the consumer. On a national level, a comprehensive understanding through modelling of formulated products will help the UK be internationally competitive and agile at high-quality manufacturing.
- Reduce waste, and resource consumption through efficient process design. Cutting waste from the design and manufacturing cycles will be an enabler to the Government's Net Zero

strategy in its biggest manufacturing sector. For example, models which better predict ingredient shelf life will reduce waste and minimise the amount of virgin resource exploited.

- Provide a step change in the ability to create innovative products by fully exploring a wider spectrum of formulation designs. Formulated products need to be rapidly adaptable and resilient to new ingredient substitution in response to regulatory change, supply chain disruptions, and uptake of plant-based raw materials introduced to increase biodiversity. **Complementing conventional experience-based approaches with modern predictive modelling** will ensure the product quality is not compromised in such radically new formulations. A modelling capability which is agile and adaptable, whilst capturing the intrinsic uncertainty in these novel ingredients is required to handle these challenges.

WHY is it timely now? (maximum 200 words)

- *Why is it important to do now?*
- *What has changed (in the development of the science, in the research landscape, and/or the political landscape) to make the realisation of this idea more likely or possible now?*
- *What are the risks for the UK of not supporting this opportunity now?*

It is timely to support the formulated product sector transition to a more rapid, green, sustainable and personalised formulation, which is reflected in detail in sector specific strategy documents [2,3,4]. These strategy documents identify the following pre-competitive innovation needs: **predictive modelling, "right-first-time" manufacturing, product structure design and digital manufacturing, improved models of existing formulations across length scales, advanced process analytics and modelling to reduce the number of trials.** These are key enablers for a productive formulated product sector.

In recent months we have seen the importance of the formulation sector in tackling the Covid-19 crisis. Alcoholic gels were reformulated for hand sanitising, and pharmaceutical products have been rapidly developed at great cost. Anecdotal evidence hints that this reaction relied on experience knowledge rather than a thorough understanding of underpinning mechanisms. Looking forward, personalised nutrition and diets are enablers to tackling long-term health challenges in the UK, for example a shift to vegetable-based low-fat low-salt diets. Formulators need to understand how new ingredients behave in such products and use to achieve these goals. The manufacturing sector needs to innovate to meet climate change commitments and a step change in understanding of product knowledge is needed before processes can be optimised. The risks of not developing this capability are that this vast manufacturing sector will not be adaptable enough to innovate quickly to the opportunities outlined earlier in the impact section. Moreover, a lack of coordination and support for high quality, highly multidisciplinary

2 https://www.fdf.org.uk/events/Pre-Comp-Food-Booklet-Final.pdf
3 https://admin.ktn-uk.co.uk/app/uploads/2018/02/Food-Sector-Precompetitive-Needs-and-Alignment-with-the-Industrial-Strategy-V7.1.pdf
4 https://www.nationalfoodstrategy.org

science risks the pre-competitive insights gained by such research not being shared for the benefit of UK Plc.

According to [1], there is only sporadic funding into the fundamental science vital to address the inherent complexity of future formulation challenges. In addition, the multidisciplinary nature of the challenge requires coordination across research areas. It is proposed here that, with a coordinated and mathematically-inspired research endeavour, the landscape can be equipped with pre-competitive methods and tools for use by UK companies. In some of the research themes we have identified, **the global infancy of reliable predictive modelling represents a significant opportunity for the UK to become the world leader**, for example in relation to perception modelling.

WHAT is the current investment landscape, both in the UK and globally? HOW does the idea relate to other priorities in the UK landscape (maximum 200 words)

- *Does the UK currently have the capacity and infrastructure needed to address this opportunity?*
- *Describe how this idea fits in the international context and the UK's position in relation to this opportunity*
- *How does the idea fit with other current UK strategic priorities?*
- *How will this idea galvanise the research communities to work together to realise the opportunity?*

The UK Formulated Products Sector is vital to the UK economy and plays a key role in tackling the societal challenges that we now face. The UK has a strong competitive advantage in formulation and is poised to take a global competitive lead to drive and take advantage of future market growth. Sales of formulated products by UK companies currently total around £180 billion per year and there is a rapidly developing overseas market. The UK has commercialisation expertise in the form the National Formulation Centre (NFC, part of the High Value Manufacturing Catapult) and is a vital resource for connecting the landscape and thereby the effectiveness of this proposal.

The UK is home to many relevant R&D active organisations (see some of the Letters of Support for an indication of the scale of this UK effort) with strong links to universities, albeit often limited to one or two departments. There is also a strong academic base that can be leveraged using, for example RTO investment, and there are a number of Centres for Doctoral Training that underpin the skills base in the sector [1,5].

Innovation in this manufacturing sector is key to addressing some of the UK future priorities; Net Zero (through optimising manufacturing processes and loss of valuable virgin resource), Healthy Ageing (through personalised nutrition, medication and low-cost medicines), increased productivity (through quicker developments of product to market), and transforming our diets (through nutritious, yet tasty food products).

5 https://epsrc.ukri.org/newsevents/news/formmfrres/

To better coordinate the accelerated innovation required across the identified research topics for reliable predictive design, an engaged mathematical science community is essential. Fortunately, the UK currently boasts a diverse mathematical and data science base which has strong links with many industry sectors. Although links into the formulated product sector and materials modelling are relatively weak, there are academic links between mathematics and biological and physical sciences, such as chemical engineering, neurology, and psychology, and other research areas required for this challenge. **These links will be strengthened by this proposal, which will enable the scientific community to grasp the huge opportunity for multidisciplinary research driven by this sector.**

DELIVERY - WHAT will it take to deliver this Big Idea? (maximum 450 words; 420 actual)

- Comment on the achievability of the idea. And on what timescales. Please give an initial indication of the expected time to delivery (in years) and scale of investment required to deliver this idea
- Highlight the underpinning research challenges that are required to support the realisation of this opportunity
- If multidisciplinary: what are the relevant disciplines? Is it multidisciplinary just across the EPS disciplines or across other Research Council or Innovate UK remits too?
- Who/which research communities/industry sectors etc will need to be involved to realise the idea?
- How much effort and resource is needed to deliver this idea? (Skills; People: groups, universities, industry)?

This proposal will be structured into three funding streams:

- multidisciplinary research studies,
- usable tools, and
- knowledge dissemination.

These streams will be delivered in parallel over five years. The underlying research areas have been co-created with industry input so that multiple sectors and organisations may benefit from the research outputs in a pre-competitive fashion. Given the breadth and interaction between the themes**, special attention will be given to knowledge-sharing and commercial software development to enable seamless transition** into implementation. A breakdown is detailed below:

- **Multidisciplinary Research Studies (Years 1 - 5) – Total £ 14.0 m**
- **PhD Students (Years 1 – 3) Total £ 4.0 m;**
- **Call for multi-disciplinary proposals (Years 1 – 5) Total £ 10.0 m:** These calls will be in the areas suggested below and each will involve at least one interdisciplinary mathematical scientist.

These areas were identified at a workshop at the Isaac Newton Institute in February 2020 [6].

- Scalable methods for heat & mass transfer and reactions in multiphase systems: Developing scalable and predictive methods which model complex, multiphase systems over differing timescales; applications could include powder flow, emulsion stability, complex rheology and processing.
- Transforming Microstructure: Systematising the understanding of commercially important systems in which the microstructure transforms during processing. Developing quantitative links between inputs such as materials and process parameters and outputs in the form of final microstructure and macroscopic properties. Developing novel mathematical and numerical homogenisation for multiscale processes.
- Mathematics of Feel (Quantification of Sensory Perception): Developing mathematical models that can quantify and simulate taste, feel and dissolution / breakdown processes - matching sensory perceptions to user groups' preferences.

- **Usable Tools (Years 3 – 5) – Total £ 3.0 m**
    - **Innovate UK CR&D:** To engage with commercial software vendors, software engineering departments, and NFC to develop the next generation of formulated product tools based on the emerging science developed in the Multidisciplinary Research Studies.

- **Knowledge Dissemination & Coordination (Years 2 - 5) – Total £ 1.2 m**
    - **Formulation Internships (£ 0.8 m):** Short-term placements to support the translation of knowledge from the Multidisciplinary Research Studies in situations where sector or companies specific input is required.
    - **Formulation Study Groups (£ 0.3 m)** Yearly Study Groups will stimulate future projects and provide fertile ground for the multiple research areas to work together.
    - **Yearly Formulation KE Conference (£ 0.1 m)** Given the focus on multi-disciplinarity around a mathematical science framework, these conferences will involve all project participants, sharing research findings and providing guidance on future priorities.

The mathematical science researchers involved will have expertise in areas including: continuum mechanics, scientific computing, statistics, data science, mathematical biology, asymptotics, soft matter.

This proposal cuts across UKRI. While it aims to engage the entire mathematical science community including data scientists and statisticians, it will require close collaboration with chemical engineers, biologists, psychologists, neurologists, and others. As such, a multi-council

6 https://www.newton.ac.uk/event/ooew01

approach would be beneficial in order to engage those in BBSRC and MRC communities. In addition, developing useable tools could be achieved through interaction with Innovate UK.

The beneficiaries will be the collaborating companies in the industrial sectors which will include health & pharma, food & drink, home & personal care, paints & coatings, speciality chemical & agri-chemicals and fuels & lubricants.

WHICH of the following does this idea fit with

- Fundamental research
- Multidisciplinary (mathematicians, chemical engineers, data scientists, food scientists, physicists, and engineers)

WHO has been involved in the development in this Big Idea? (Maximum 100 words).

*** indicates individuals from organizations providing letters of support)**

Abrahams	David	University of Cambridge
Addison	Tim	National Formulation Centre*
Aitken	Mungo	University of Cambridge
Alberini	Federico	University of Birmingham*
Allwright	David	University of Oxford
Amador	Carlos	Proctor & Gamble
Andrews	James	University of Birmingham*
Ang	Caroline	University of Bath
Babasola	Oluwatosin	University of Bath
Bayly	Andrew	University of Leeds*
Benham	Graham	University of Cambridge
Beverly	David	Diageo*
Booth	Jonathan	Croda
Bows	John	PepsiCo
Breward	Chris	University of Oxford
Budd	Chris	University of Bath
Bugg	Dean	Scott Bader
Butchers	Matt	KTN
Cates FRS	Mike	University of Cambridge
Chahal.	Surinder.	Croda*
Chapman	Jon	University of Oxford
Charalambides	Maria	Imperial College London
Chen	Tao	University of Surrey
Cowley	Stephen	University of Cambridge
Cruickshank.	Graeme.	CPI*
Cupples	Gemma	University of Birmingham*

Dalwadi	Mohit	University of Oxford
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Donaldson	Joe	Unilever
Dougill	Andrew	University of Leeds*
Drakopoulos	Alexis	Intellegens
Drap	Oliver	Pfizer
Dyson	Rosemary	University of Birmingham*
Engmann	Jan	Nestlé Research*
Field	Jamie	Britvic
Findlay	Rachel	CPI*
Finney	Karen	UKRI MRC
Fryer.	Peter.	University of Birmingham*
Gibbon	Simon	AkzoNobel
Gill	Josh	EPSRC
Goddard	Ben	University of Edinburgh
Good.	Chris.	University of Birmingham*
Griffiths	Ian	University of Oxford
Hall	Cameron	University of Bristol
Hardalupas	Yannis	Imperial College London
Harris	Lawrence	Mondelez International*
Hinch FRS	John	University of Cambridge
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Holland	Sonia	Diageo*
Icardi	Matteo	University of Nottingham
Ilg	Patrick	University of Reading
Ingmire	Tim	Quorn Foods
Ioannou	Phivos	The MTC
Kalogirou	Anna	University of Nottingham
King	John	University of Nottingham
Kinninmonth	Malcolm	Walgreens Boots Alliance
Koumakis	Nick	University of Edinburgh
Kowalski	Adam	Unilever
Kusumaatmaja	Halim	Durham University
Kyprianou	Andreas	University of Bath
Lacey	Andrew	Heriot-Watt University
Lee	William	University of Huddersfield
Lillford	Peter	University of Birmingham
Linter	Bruce	PepsiCo
Lopez Quiroga	Estefania	University of Birmingham*

Mottram	Nigel	University of Glasgow
Murray	Brent	University of Leeds*
Noble	Ian	Mondelez International*
O Conchuir	Breanndan	IBM Research*
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Ockendon FRS	John	University of Oxford
Owen	Jade	Johnson Matthey
Parker	Ritchie	Nestlé*
Parr	Andrea	CPI*
Pelan	Eddie	University of Birmingham*
Perry	Richard	Sterling
Piette	Bernard	Durham University
Please	Colin	University of Oxford
Poulos	Andreas	Unilever
Powell	Hugh	Nestec York Ltd *
Reynolds	Gavin	AstraZeneca
Rodriguez Garcia	Julia	University of Reading
Shah	Nilay	Imperial College London
Shendruk	Tyler	University of Edinburgh
Singleton	Colin	CountingLab Limited
Sutton	Mike	Lubrizol
Tayeb	Tariq	CPI*
Thijssen	Job	University of Edinburgh
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Tibos	Stacie	PepsiCo
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Whitehead	Tom	Intellegens
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Lead contact details

[redacted]

PepsiCo International

[redacted]

Is there any additional information that is relevant to your application that EPSRC staff and those who are part of the decision making process should be made aware of, such as a conflict of interest or related submissions. (maximum 100 words)

None