MATERIALS AND MANUFACTURING ACADEMY

SIMULATING PHYSICAL VAPOUR DEPOSITION ON STEEL SUBSTRATE USING THE DIRECT SIMULATION MONTE CARLO (DSMC) METHOD

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Objectives

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- Simulate flow of particles under vacuum conditions
- Benchmark existing research of Copper vapour
- Identify wall interaction behaviour
- Expand upon current boundary patches
- Realistic modelling of metallic vapour

Physical Vapour Deposition

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- Physical Vapour Deposition (PVD) is under development for galvanising steel strip
- Metallic coating with ZnMg vapour
- Thin coating with great surface appearance
- Excellent corrosion resistance
- Reduction of Zinc consumption
- Vacuum conditions have to be sustained continuously

Rarefied Gas

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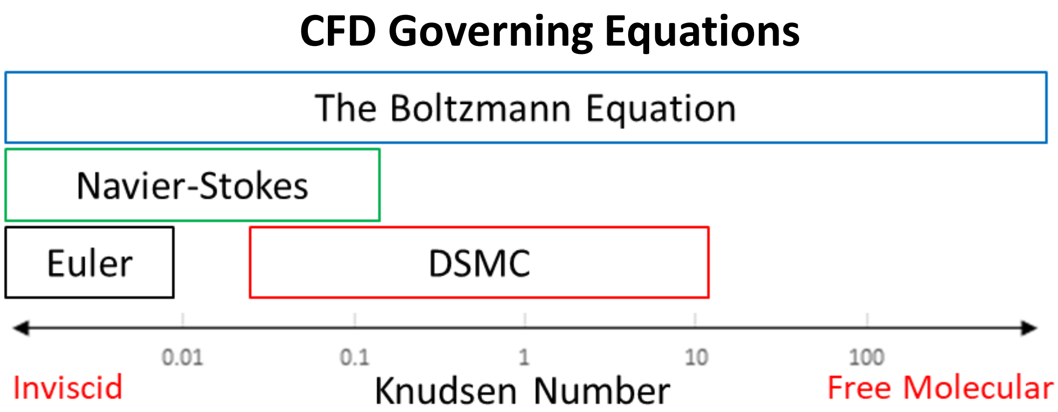

- Low pressure conditions for coating equates to higher Knudsen numbers, $K_n = \frac{\lambda}{L}$
- Traditional CFD solving flow using the N-S equations becomes inadequate for rarefied gas
- DSMC Direct Simulation Monte Carlo Method

Direct Simulation Monte Carlo Method (DSMC)

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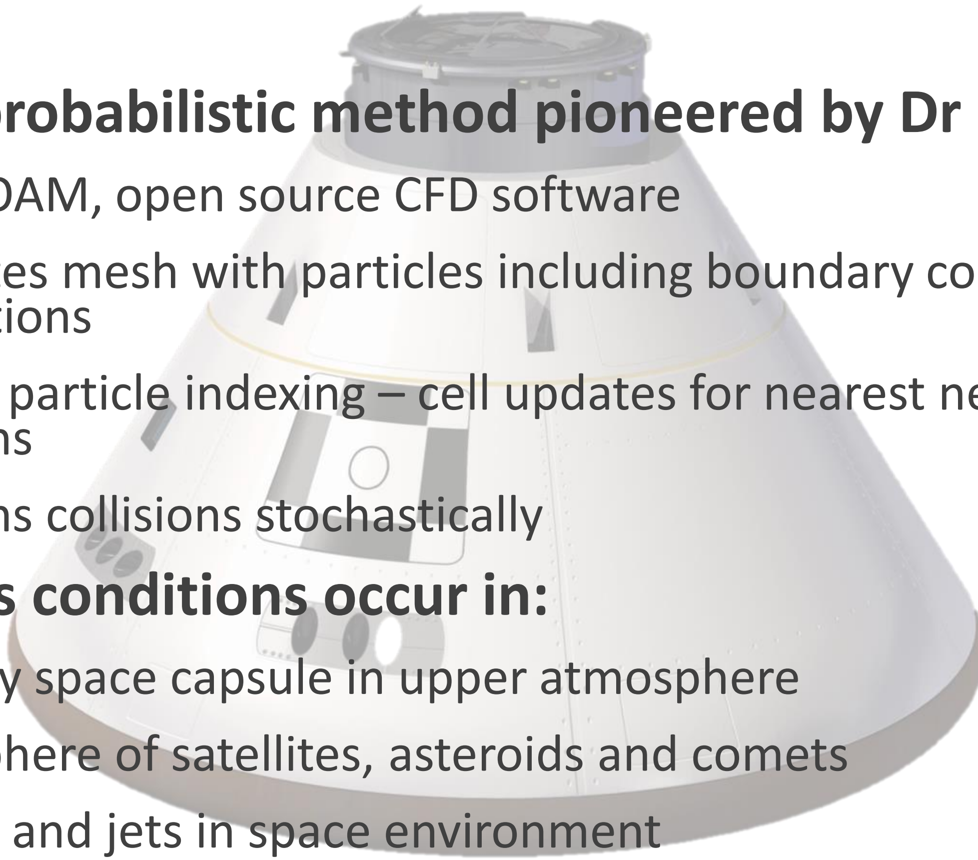


DSMC is a probabilistic method pioneered by Dr Graeme Bird

- OpenFOAM, open source CFD software
- Populates mesh with particles including boundary condition interactions
- Update particle indexing – cell updates for nearest neighbour collisions
- Performs collisions stochastically

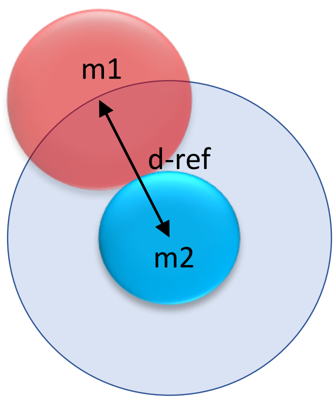
Rarefied gas conditions occur in:

- Re-entry space capsule in upper atmosphere
- Atmosphere of satellites, asteroids and comets
- Nozzles and jets in space environment
- Thin film deposition

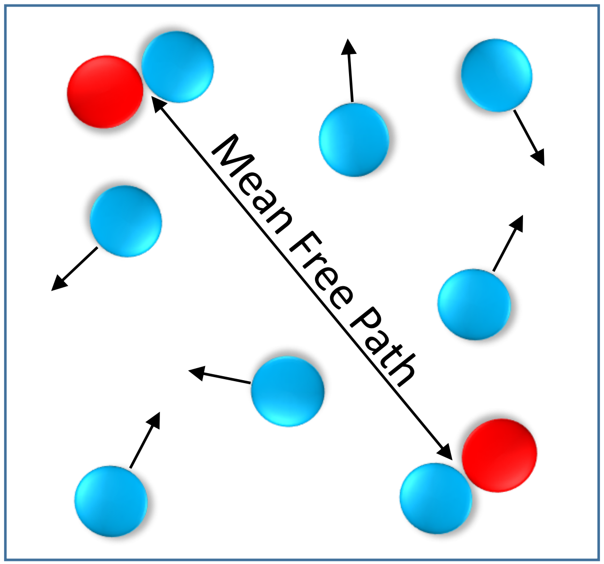
Image Source: https://www.nasa.gov/mission_pages/constellation/multimedia/orion_contract_images.html

Variable Hard Sphere (VHS)

Quantum scale



Kinetic scale



$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n}$$

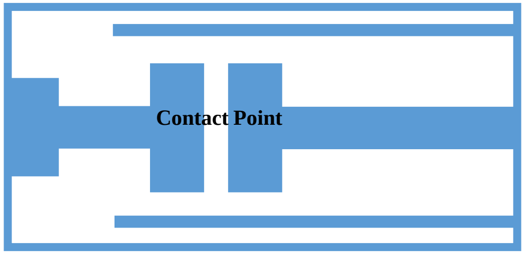
- Essential to simulate particle collisions in (DSMC)
- Cross-section collisions (dref) derived from coefficients of viscosity (μref)
- Angular scattering
- Theoretically determined from the variable hard sphere (VHS)method

Vacuum Interrupter

Vacuum Interrupter Image

K. Hencken, "Investigation of Metallic Vapor Condensation in a Vacuum Interrupter using dsmcFOAM DSMC Introduction," 9th OpenFOAM® Work., 2014

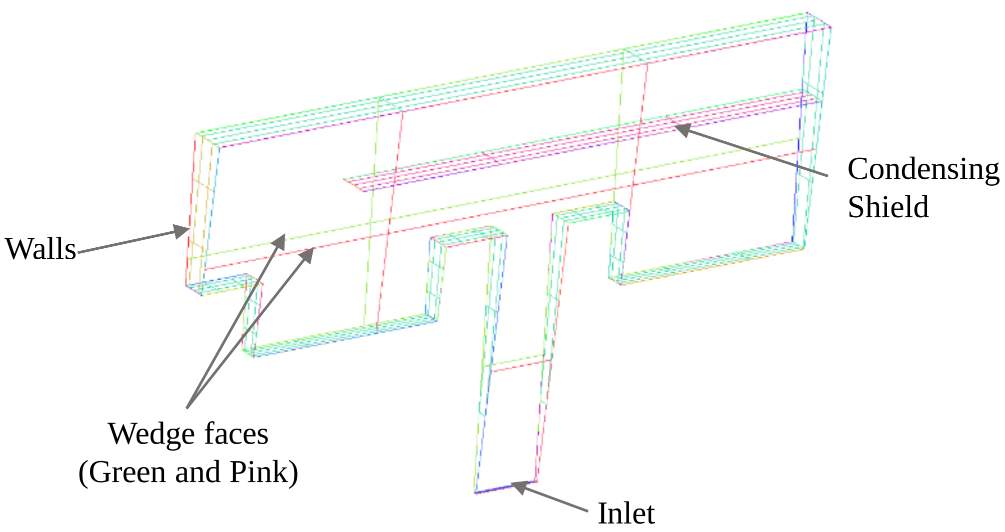
Vacuum Interrupter simplified



- Used as circuit breaker switch in high voltage networks
- Vacuum sealed chamber
- Metal arc forms between open contacts
- Copper vapour deposited anywhere within the chamber
- Deposited vapour causes component failure

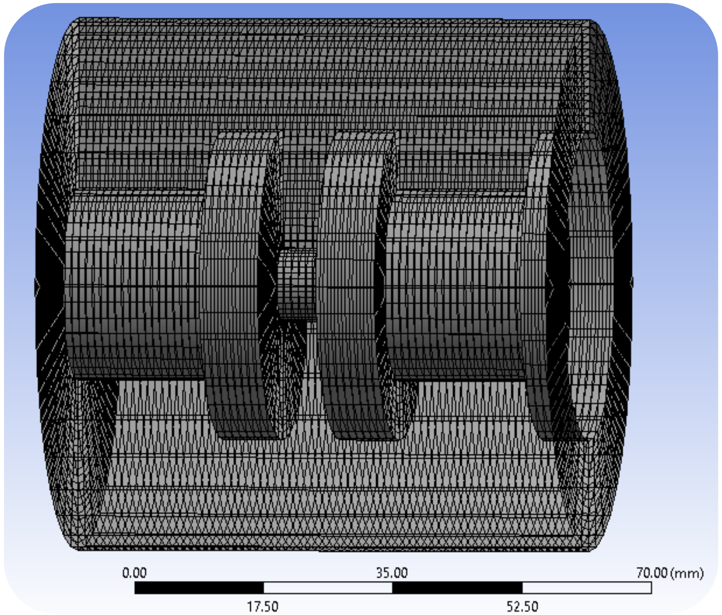
Benchmarking

5° revolved axisymmetric image



- 5 degree axisymmetric model
- Approximate dimensions
- FluentMeshToFoam ASCII mesh

360° revolved axisymmetric image



- 3D image of Vacuum Interrupter

Metallic Vapour

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Copper properties: *Sourced from; Venkattraman and A. A. Alexeenko, "Direct simulation Monte Carlo modeling of metal vapor flows in application to thin film deposition," Vacuum, vol. 86, no. 11, pp. 1748–1758, 2012.*

- Reference Diameter (VHS) = 0.450 (nm)
- Reference Temperature 300 K
- Temperature dependence, $\omega = 0.920$
- Angular scattering parameter, $\alpha = 0.420$

Calculated Copper properties:

- Mass flow rate, 20 grams of Copper per second
- Number density Copper 1.9e23

Direct Simulation Monte Carlo (DSMC) Simulations

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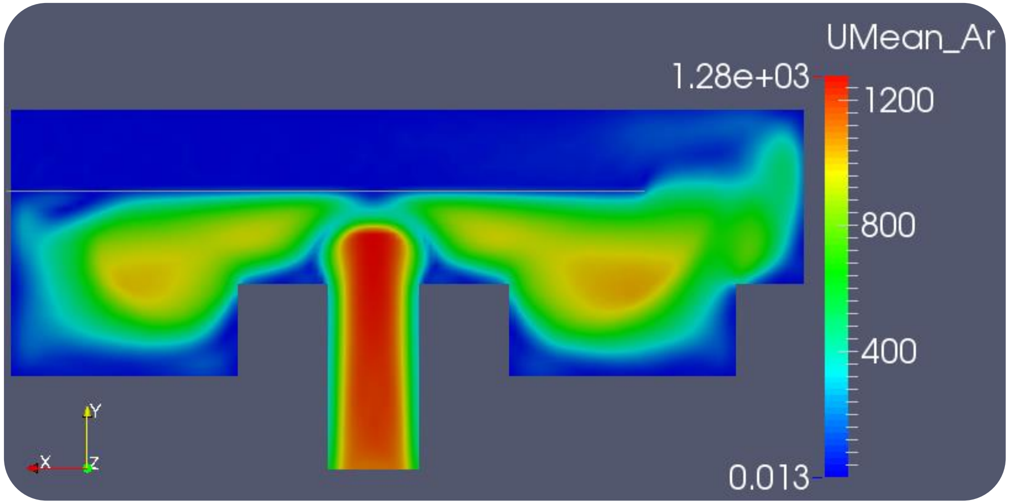
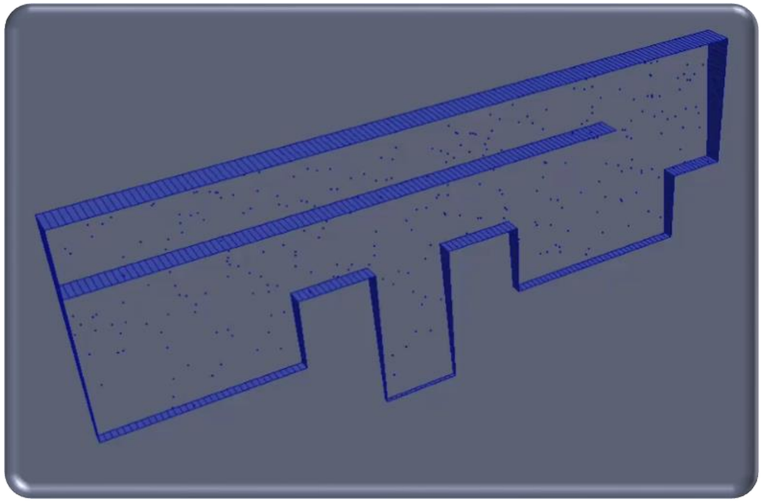
Argon gas flow



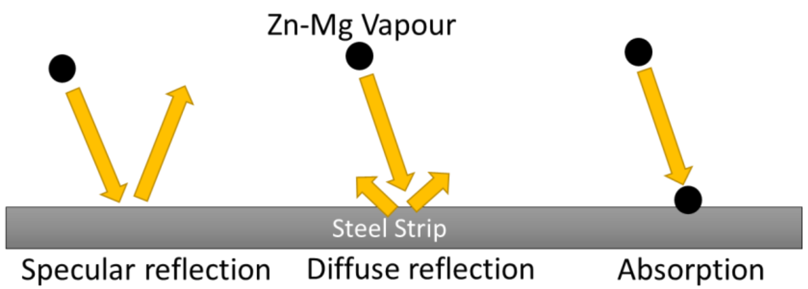
Collisions of Copper particles



- Argon particle flow mean velocity
- Copper particle flow wall interactions (Number density field)

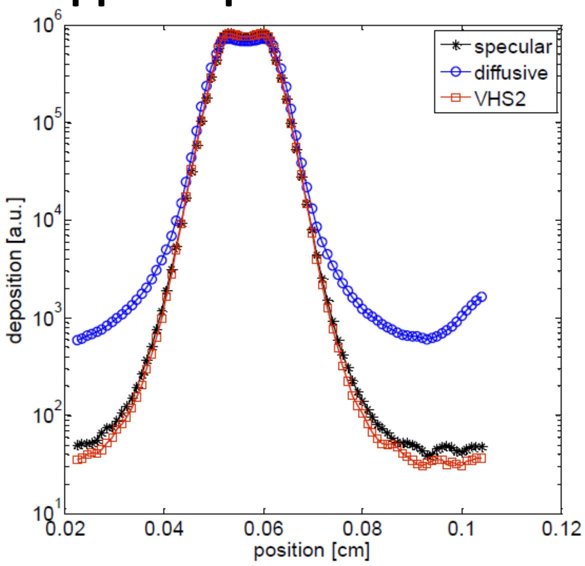
Absorbing Wall Patch

Wall interaction



- Adaption of MixedSpecularDiffuse wall interaction model
- Tracking particles that interact with wall surfaces
- Deleting the particles upon wall collisions
- Three possible simulated wall interactions

Copper deposited on surface



K. Hencken, "Investigation of Metallic Vapor Condensation in a Vacuum Interrupter using dsmcFOAM DSMC Introduction," 9th OpenFOAM® Work., 2014

Vapour Distribution Box (VDB)

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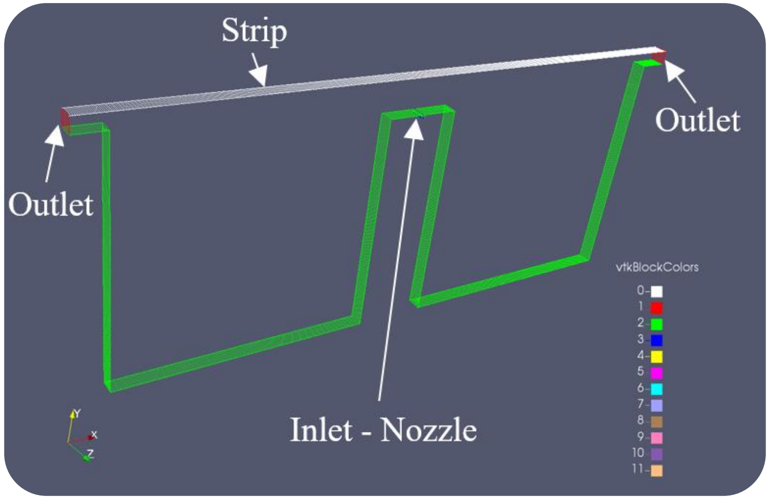
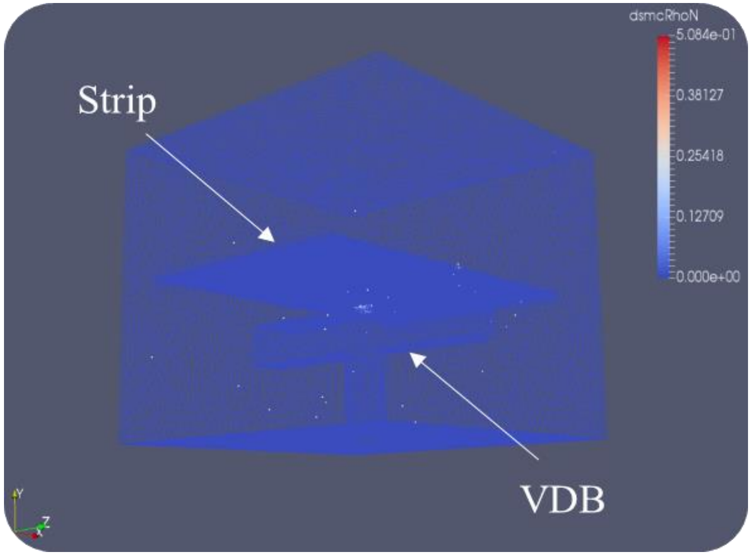
VDB and Strip – 2D



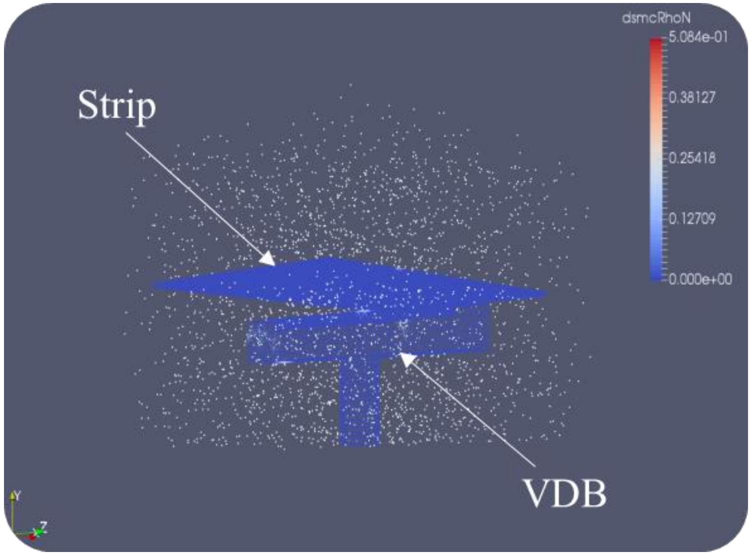
- Electro-magnetic Levitation (EML) PVD
- Benchmarked geometry enabled the creation of strip surface
- Boundary conditions determined from benchmark analysis

Vapour Distribution Box (VDB)

Coating Chamber – 3D



VDB and Strip – 3D



- Particles interacted with surfaces
- 3D simulation very computationally expensive
- Vacuum chamber will not be completely evacuated

Next Steps

- Development of the absorbing wall function
- Comparison of results with the benchmark
- Zinc vapour simulation within the VDB

Future work:

- Optimisation of vacuum lock design
- Pumping requirements of system

Summary

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- Simulated particle flow using the DSMC Method
- Applied simplified benchmark to PVD application
- Metallic Vapour simulated for Copper
- Absorbing wall boundary patch in initial stage
- Further investigation required to model Zinc vapour

Questions

M2A
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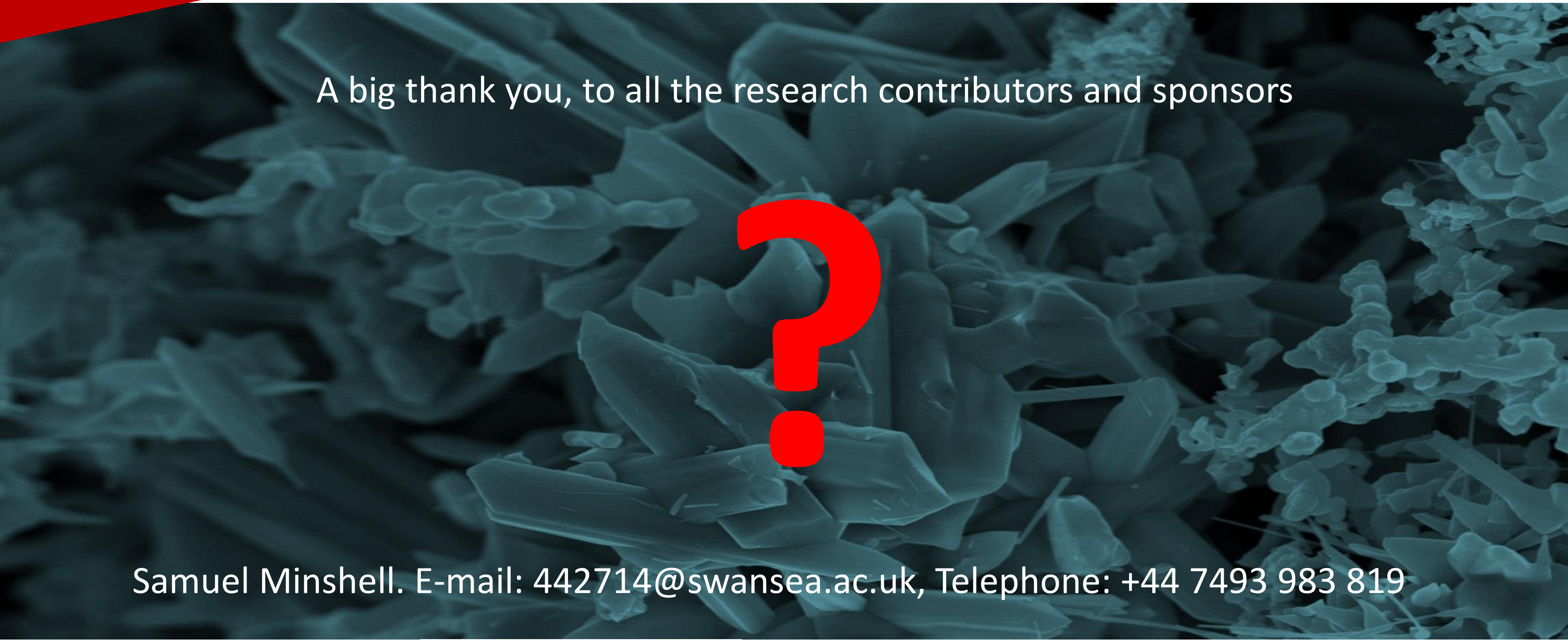

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