UK Consortium on Mesoscale Engineering Sciences (UKCOMES)

ARCHER2
Advancing Science and Technology at Mesoscales

Kai Luo (UCL, PI)

ARCHER2 Celebration of Science, 7-8 March 2024, The University of Edinburgh

UKCOMES Membership

- 29 UK institutions
- Over 20 international partner institutions in 4 continents

Main LBM codes

- DL_MESO
- HemeLB
- UCLBM
- LB3D

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Consortium on Mesoscale Engineering Sciences

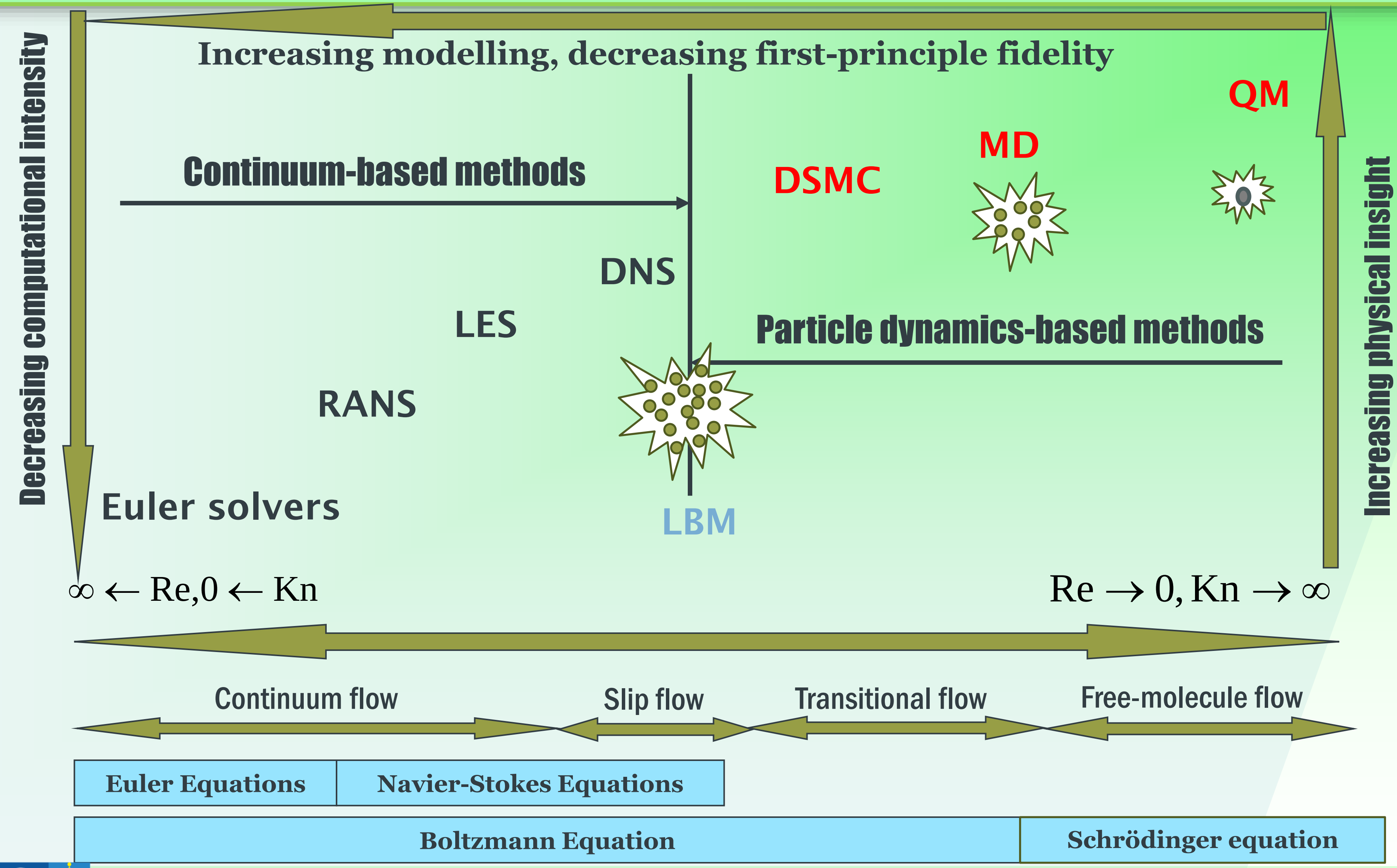
UKCOMES Objectives

- To advance the emerging mesoscale science and engineering through exploitation of national high-end computing (HEC) and tier-2 resources
- To bring together world-leading and multidisciplinary expertise to make critical theoretical discoveries and model developments, and translate them into software codes that are able to exploit current and emerging computing architectures
- To improve and maintain open-source community codes of mesoscale modelling and simulation for both the research and end-user communities
- To enable cutting-edge simulations on national HEC and tier-2 services in strategically important areas ranging from net zero energy technologies to healthcare
- To act as the focal point for the mesoscale research and application communities in the UK and the world through leadership and active engagement
- To provide a stimulating, collaborative and interdisciplinary environment to train research students and early career researchers as well as future leaders in the field

UKCOMES Work Packages

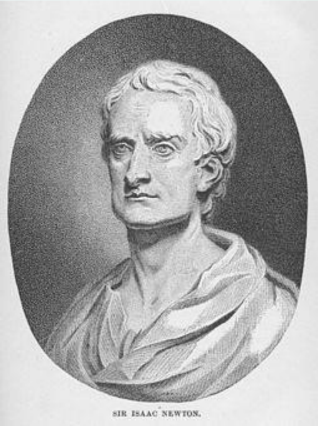
- **WP1: Community Codes Development, Optimisation & Dissemination**
  (Leader: David Emerson)
- **WP2: Simulation & Optimisation of Net Zero Energy Systems**
  (Leader: Qiong Cai)
- **WP3: Mesoscale Simulation & Design in Advanced Manufacturing**
  (Leader: Rongshan Qin)
- **WP4: Simulation & Application of Multiphase & Interfacial Flows**
  (Leader: Halim Kusumaatmaja)
- **WP5: Hemodynamics Simulation & Application in Healthcare**
  (Leader: Miguel Bernabeu)
- **WP6: VVUQ, Machine Learning & Data Analytics**
  (Leader: Peter Coveney)
- **WP7: Engagement, Outreach, Dissemination and Impact Delivery**
  (Leader: Kai Luo)

A Hierarchy of Modelling and Simulation Approaches



Luo et al., J. Multiscale Modelling, 1 (2009); Li et al., Progress in Energy and Combustion Science, 52 (2016)

The Hierarchy of Governing Equations



Sir Issac Newton PRS
(1642–1726)

Newton's Law

$$\vec{F} = m\frac{d\vec{v}}{dt}$$

Schrödinger equation

$$i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle$$

Ewin Schrödinger
(1886–1961)

The Boltzmann equation

$$\frac{\partial f}{\partial t} + \xi_i\frac{\partial f}{\partial x_i} + F_i\frac{\partial f}{\partial \xi_i} = \Omega\left(f, f_*\right)$$

Ludwig Boltzmann
(1844 – 1906)

Claude-Louis Navier
(1785–1836)

Navier-Stokes equation
&
Macroscopic Properties

Sir George Gabriel Stokes FRS
(1819–1903)

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Lattice Boltzmann Method – A Mesoscale Approach

Kinetic-based particle distribution functions (PDFs):

$$\mathbf{f}(t+\Delta t, \mathbf{x}+\mathbf{e}_\alpha \Delta t) - \mathbf{f}(t,\mathbf{x}) = \mathbf{\Lambda}(\mathbf{f}^{eq} - \mathbf{f}) + \mathrm{F} \qquad \mathbf{\Lambda} = \frac{\Delta t}{\tau}\mathbf{I}$$

Equilibrium PDF:

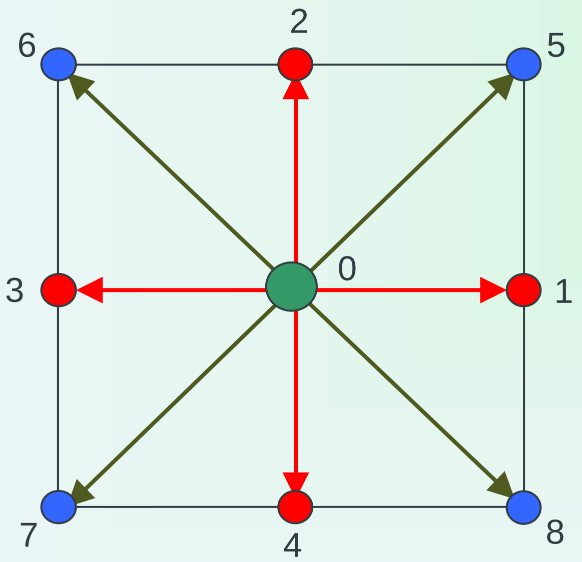
$$f_\alpha^{eq} = w_\alpha \rho \left\{ 1 + \frac{\mathbf{e}_\alpha \mathbf{u}}{c_s^2} + \frac{\mathbf{u}\mathbf{u}}{c_s^2}\left(\frac{\mathbf{e}_\alpha \mathbf{e}_\alpha}{c_s^2} - \delta_\alpha \right) \right\}$$

Recovering macroscopic quantities:

$$\rho = m \sum_\alpha f_\alpha$$

$$\rho u_i = m \sum_\alpha e_{\alpha,i} f_\alpha$$

$$\tau_{ij} = m \sum_\alpha e_{\alpha,i} e_{\alpha,j} (f_\alpha^{eq} - f_\alpha)$$



D2Q9

Recovering NS equations with:

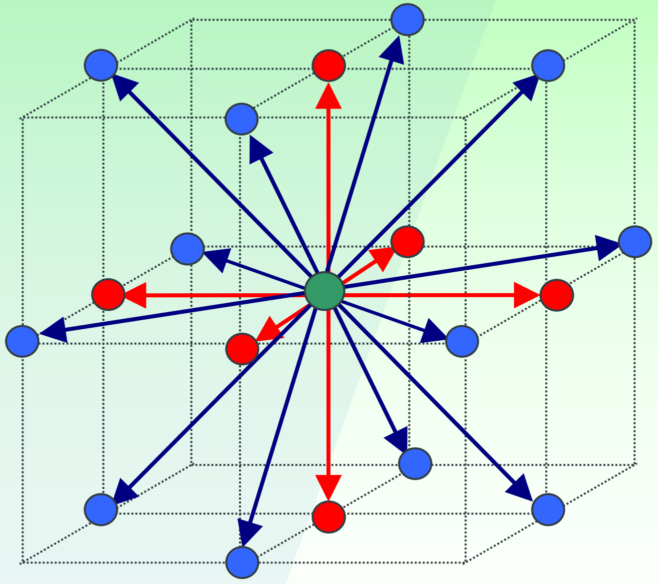
$$p = c_s^2 \rho$$

$$\nu = c_s^2 \left(\tau - \tfrac{1}{2}\right)\Delta t$$

$$\mathrm{D}d\mathrm{Q}n$$

Spatial dimension

Lattice velocity number



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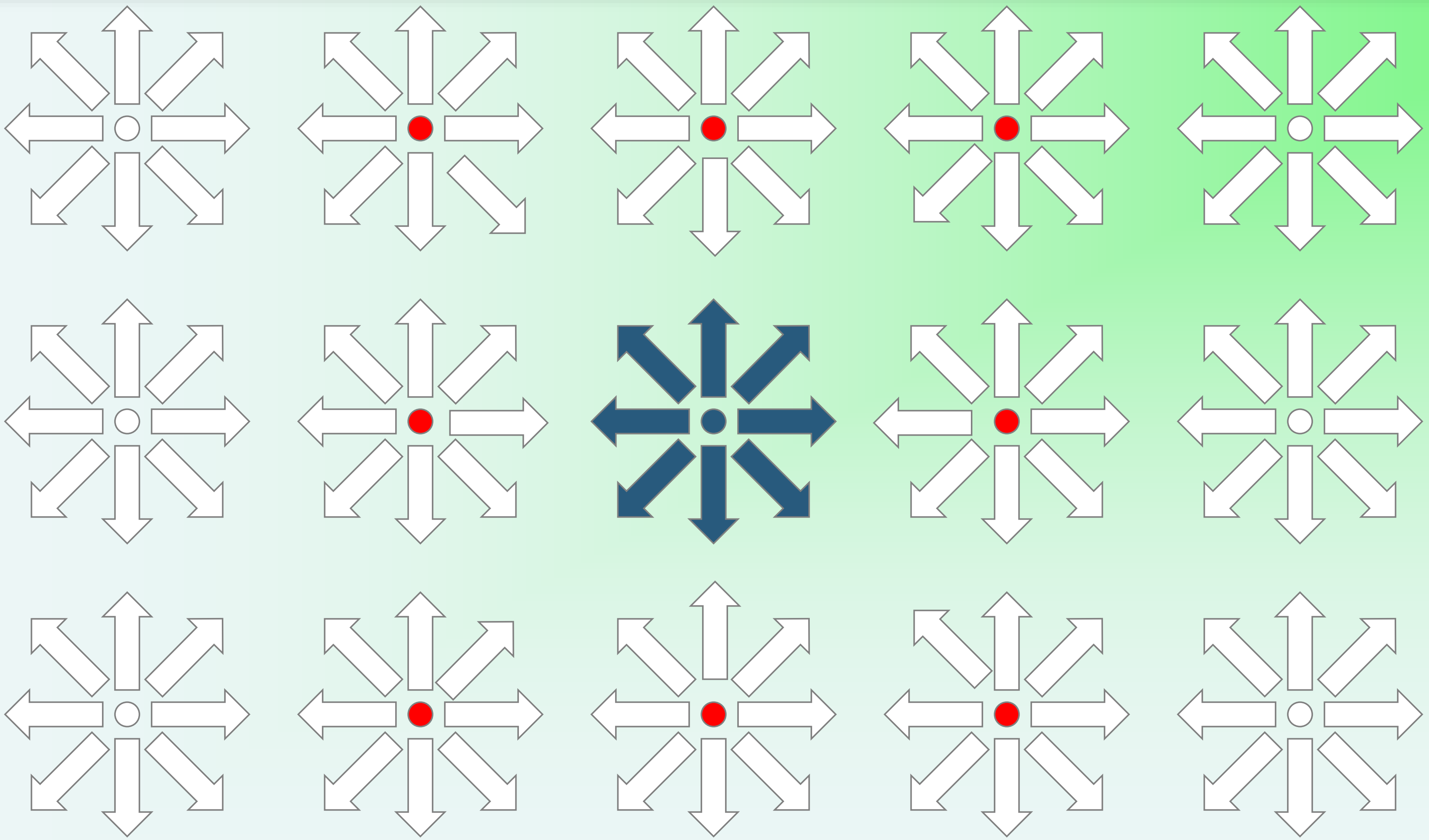
LBM Algorithm: Interactions between Lattice Sites



Local collision:

$$f_\alpha^*(x_i,t) = f_\alpha(x_i,t) + \frac{1}{\tau}(f_\alpha^{eq} - f_\alpha)$$

Streaming:

$$f_\alpha(x_i + e_{\alpha,i}\Delta t, t+\Delta t) = f_\alpha^*(x_i,t)$$

“Embarrassingly” efficient on parallel computers!

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The Unified Lattice Boltzmann Model (ULBM) Framework

Distribution function

Raw moment space

Single-relaxation- time model: ULBM (SRT)

$$f_i^* = (\mathbf{1} - 1/\tau) f_i(\boldsymbol{x}, t) + 1/\tau f_i^{eq}$$

When:

$\mathbf{S} = (1/\tau)\mathbf{I}$

$$\mathbf{S} = diag(0,1,1,1,s_v,s_v,s_v,s_b,s_v,s_v,s_3,s_3,s_3,s_3,s_3,s_3,s_{3b},s_4,s_4,s_4,s_{4b},s_{4b},s_{4b},s_5,s_5,s_5,s_6).$$

Multiple relaxation time model: ULBM (MRT)

$$f_i^* = \boldsymbol{M}^{-1}(1 - \mathbf{S})\boldsymbol{M} f_i + \boldsymbol{M}^{-1}\boldsymbol{S}\boldsymbol{M} f_i^{eq}$$

When:

$\mathbf{N} = \mathbf{I}$

- **Unified Lattice Boltzmann Method (ULBM):**

$$f_i(\boldsymbol{x} + \boldsymbol{e}_i \Delta t, t + \Delta t) \equiv f_i^*(\boldsymbol{x}, t) =$$

$$\boldsymbol{M}^{-1}\boldsymbol{N}^{-1}(\mathbf{I} - \mathbf{S})\boldsymbol{N}\boldsymbol{M} f_i(\boldsymbol{x}, t) + \boldsymbol{M}^{-1}\boldsymbol{N}^{-1}\boldsymbol{S}\boldsymbol{N}\boldsymbol{M} f_i^{eq}(\boldsymbol{x}, t)$$

f - distribution functions $\mathbf{S}$ - relaxation matrix

$\mathbf{M}$ - transformation matrix, transfer the distribution function to raw moments

$\boldsymbol{N}$ - shift matrix, shift the raw moments into the central moments

In central moment space:

$$\left|\tilde{T}_i\right\rangle = \mathbf{N}\left|T_i\right\rangle = \mathbf{MN}\left|f_i\right\rangle.$$

$$\mathbf{S} = diag(0,1,1,1,s_v,s_v,s_v,s_v\gamma,s_v,s_v,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma,s_v\gamma).$$

When introduce entropic stabilizer in **S**

Central moment space

Cascaded lattice Boltzmann model: ULBM (CLBM)

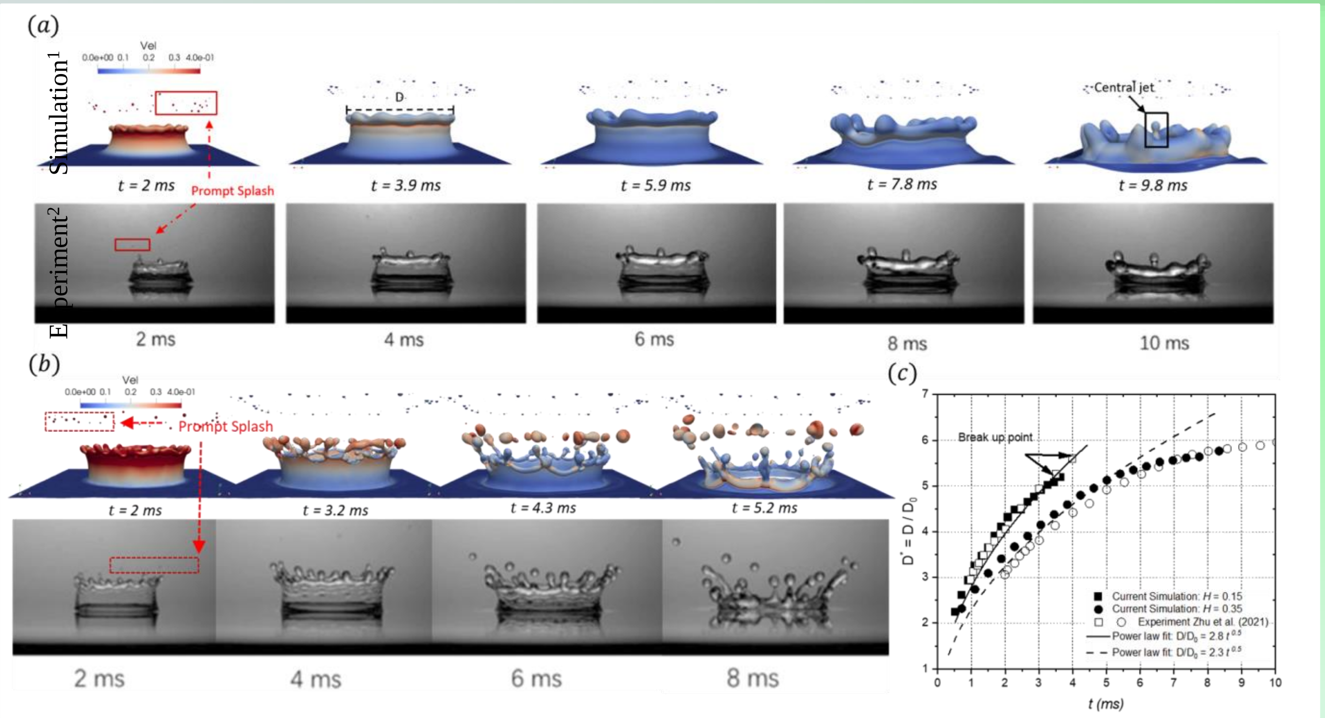
$$f_i^* = \boldsymbol{M}^{-1}\boldsymbol{N}^{-1}(\mathbf{I} - \mathbf{S})\left|\tilde{T}_i\right\rangle + \boldsymbol{M}^{-1}\boldsymbol{N}^{-1}\boldsymbol{S}\left|\tilde{\mathrm{T}}^{eq}\right\rangle$$

Entropic lattice Boltzmann model: ULBM (KBC)

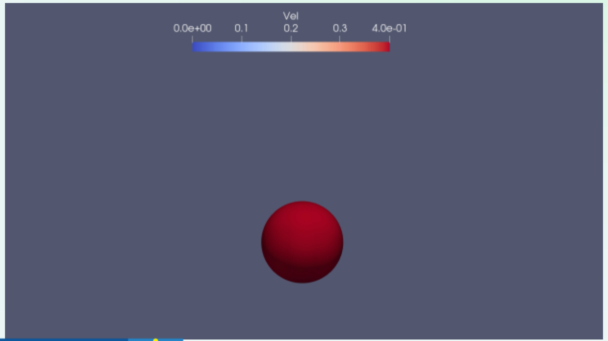
$$f_i^* = \boldsymbol{M}^{-1}\boldsymbol{N}^{-1}(\mathbf{I} - \mathbf{S})\left|\tilde{T}_i\right\rangle + \boldsymbol{M}^{-1}\boldsymbol{N}^{-1}\boldsymbol{S}\left|\tilde{\mathrm{T}}^{eq}\right\rangle$$

UCL: Luo, Fei and Wang, Phil. Trans. Royal Society, A 379 (2021)

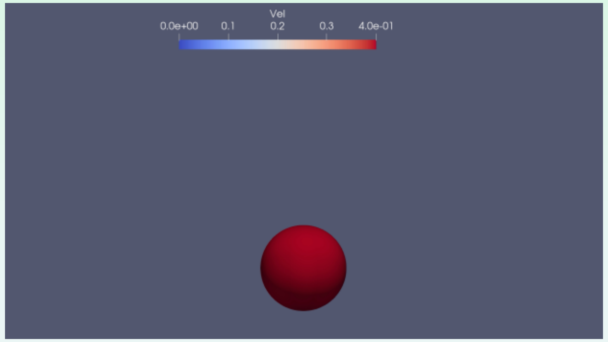
LB Simulation of Splashing of Droplet Impingement on a Liquid Film



- Case (a): h* = 0.16



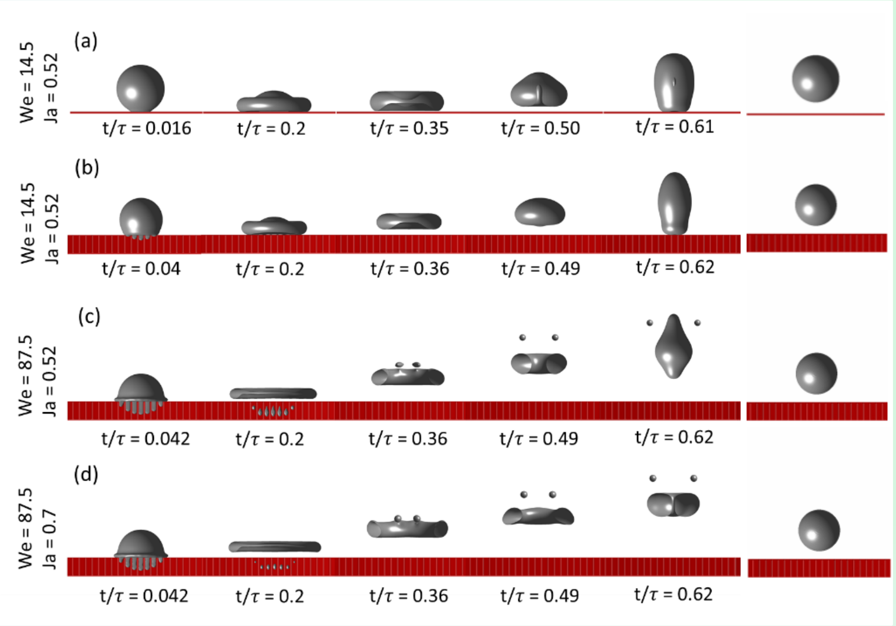
- Case (b): h* = 0.07

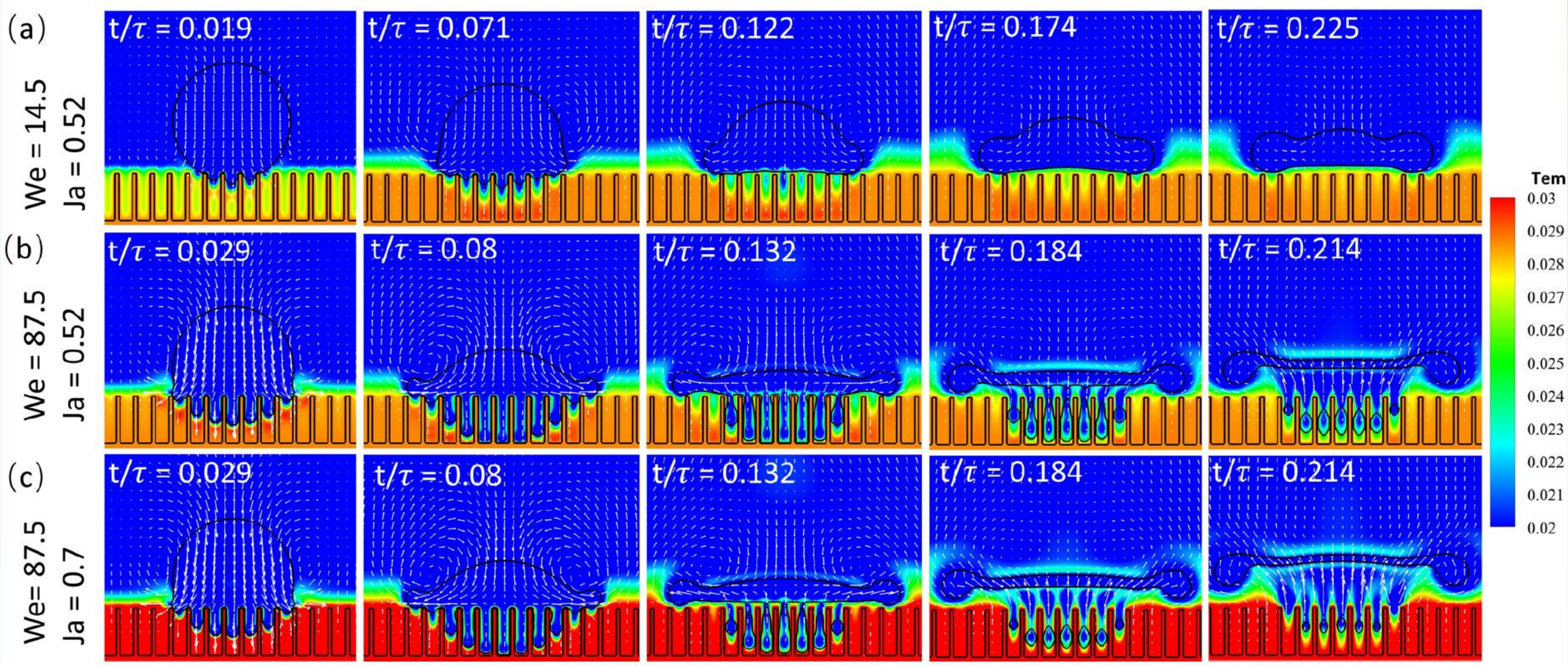


- Water droplet splashing on liquid film with different film thickness (We = 380, Re = 6000)
- The simulations are conducted on ARCHER2, typically with 2048 cores running over 10 hours.
- Realistic water – air density ratio is achieved
- Excellent quantitative and qualitative agreement with experimental data
- Applications: printing, cooling, etc.

Experiment - Zhu, J., et . Experiments in Fluids, 62, 1-13. (2021) LBM – UCL: Luo, Wang et al., Int. J. Multiphase Flow 168, 104582 (2023)

LB Simulation of Droplet Impingement on a Heated Porous Hydrophilic Substrate (T > Leidenfrost point)





- **Influence of Weber number:** contact time, bouncing height, droplet shape, etc. are affected
- **Influence of evaporation:** The vapour formed by the evaporation of the penetrated liquid provides additional lift force and promotes droplet rebound

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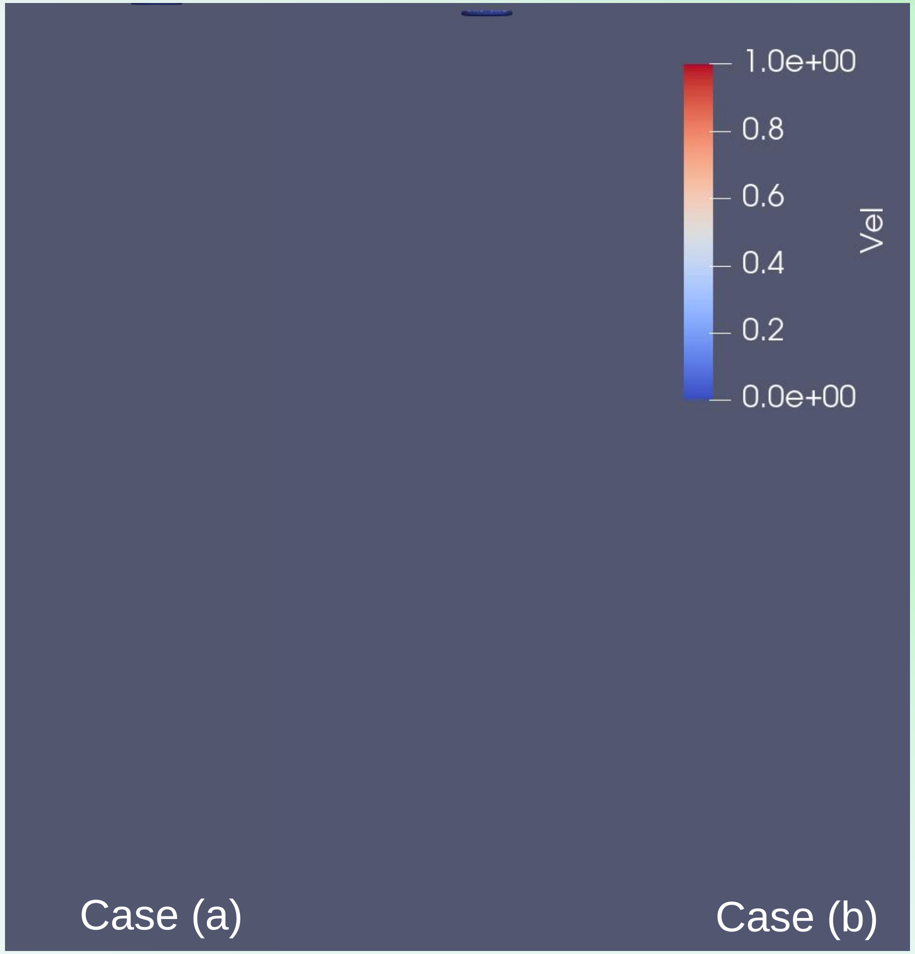
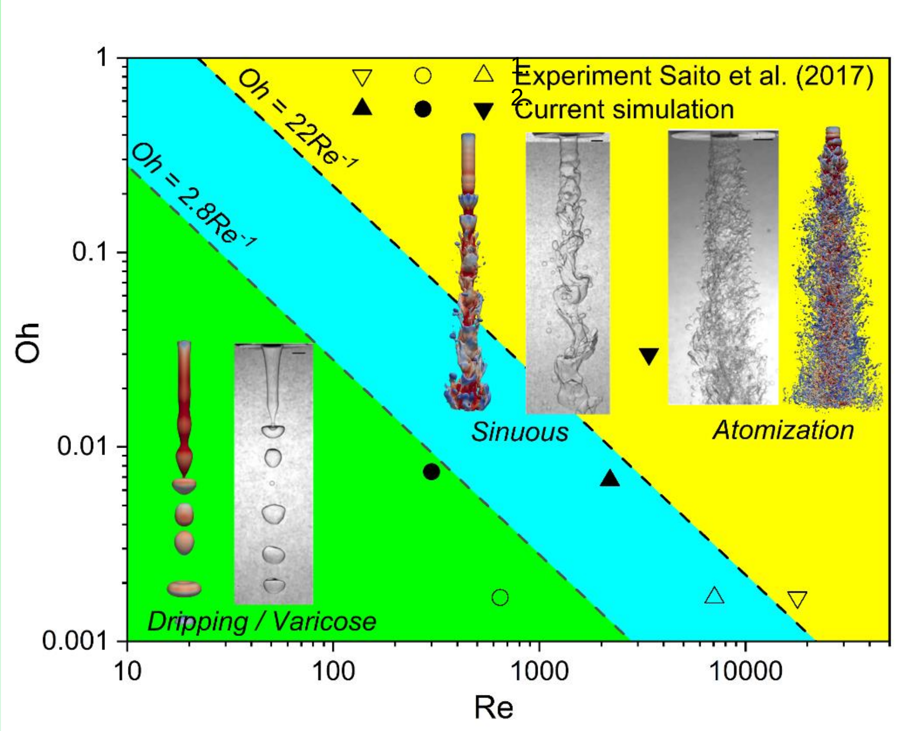
UCL: Luo, Wang et al., Phys. Fluids, 5.0118079 (2022)

Lattice Boltzmann Simulation of Liquid Jet Spray



(a) Sinuous case:
Re = 2200
Oh = 0.0075

(b) Atomization case:
Re = 3400
Oh = 0.03



- The number of lattice sites exceeds 500 million
- The LB simulations are conducted on ARCHER2, with 2048 cores running over 22 hours
- Various Instabilities in liquid jet spray are naturally captured
- Effects of Reynolds number and Ohnesorge number revealed

Experiment - Saito et al., Phys. Rev. E 96, 013317 (2017) UCL: Simulation – Luo, Wang et al., Int. J. Multiphase Flow 168, 104582 (2023)

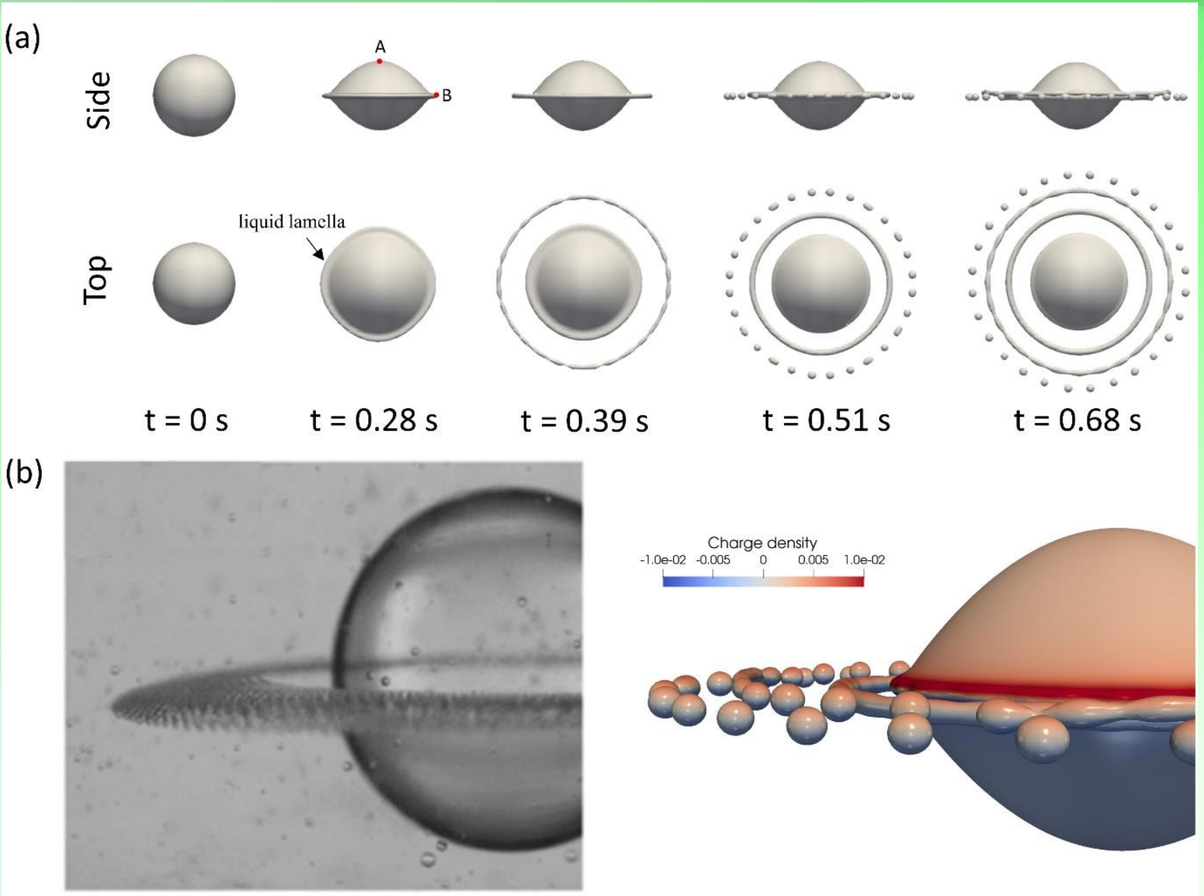
Lattice Boltzmann Simulation of Droplet Equatorial Streaming in Electric Field

- Droplet equatorial streaming

  The droplet forms a lens shape, and liquid rings continuously detach from its equatorial plane and subsequently break up into satellite droplets

- Application
  - electrospray mass spectrometry
  - Electrospray Ionization
  - Electrospinning

- Simulation requirements
  - in a strong electric field,
  - a weakly conductive, low-viscosity droplet
  - immersed in a highly conductive, high-viscosity medium

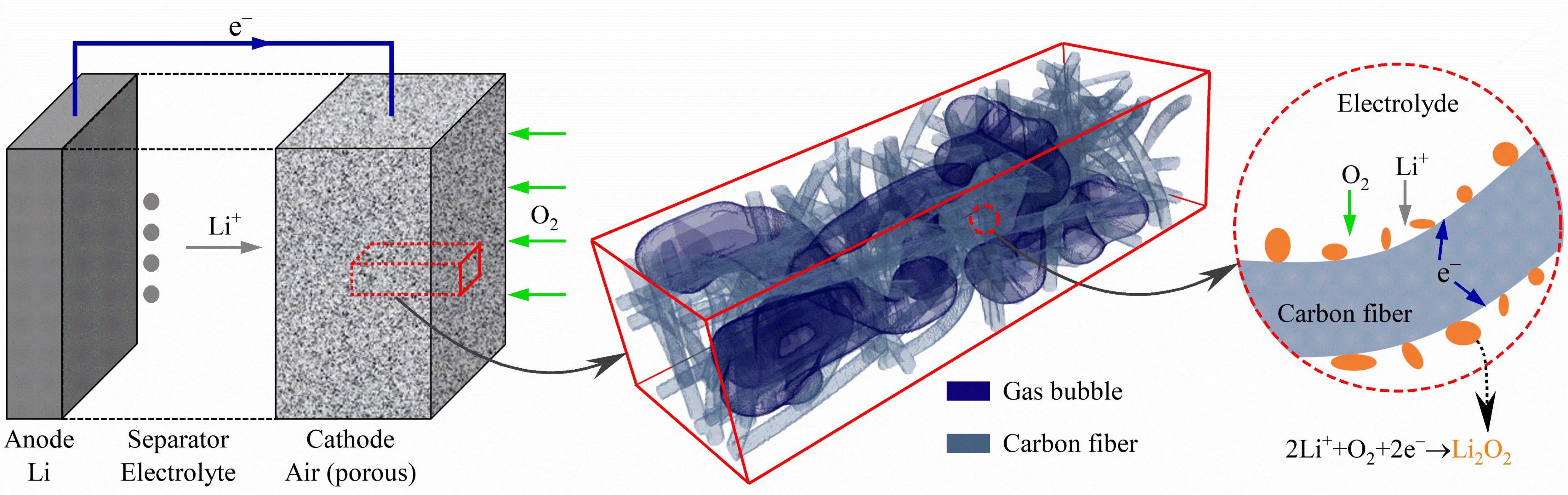


(a) evolution process of droplet equatorial streaming (b) comparison of experiment[1] result and simulation[2] result.

- The LB simulation reproduces, for the first time, the complete process of droplet equatorial streaming, including the continuous ejection and breakup of liquid rings on the equatorial plane.

Experiment - Brosseau & Vlahovska, Physical review letters 119(3), 034501 (2017) Simulation – UCL: Luo, Wang et al. (2024)

Battery Research & Design:
LB Simulation of Discharge of Li-Air Battery



(a) Li-Air battery (b) Computational domain (c) Electrochemical reaction

- **Domain size**: 0.64 um * 1.92 um * 0.5 um (Grid: 128*384*100, 5.0 nm/grid); **Fiber diameter**: 50 nm (10 grids);
- **Maximum thickness of Li_2O_2** on cathode: 10 nm (2 grids); Cathode **porosity**: ϕ = 0.8; **Current density**: I_0 = 2.5 A/m^2;
- **Parallel simulations on Archer2**: 3-hour computation of 3840 cores for 100% DoD

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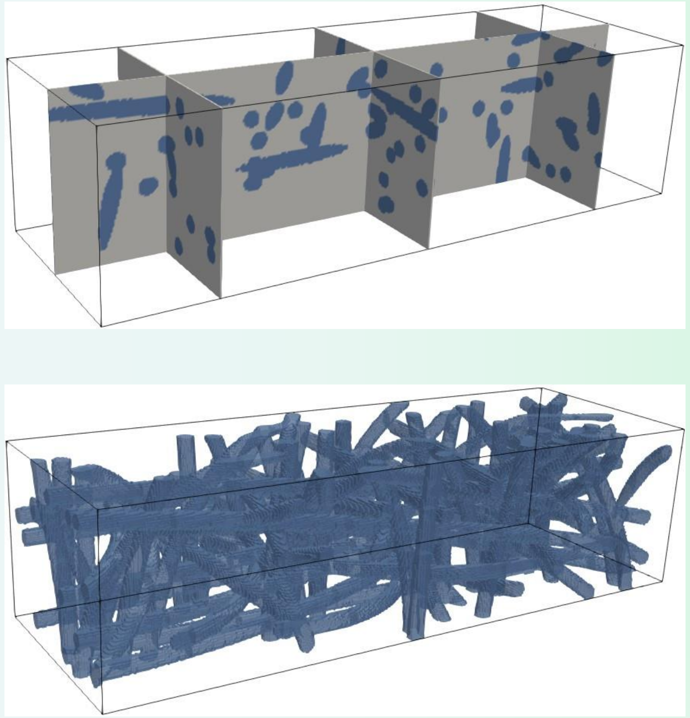
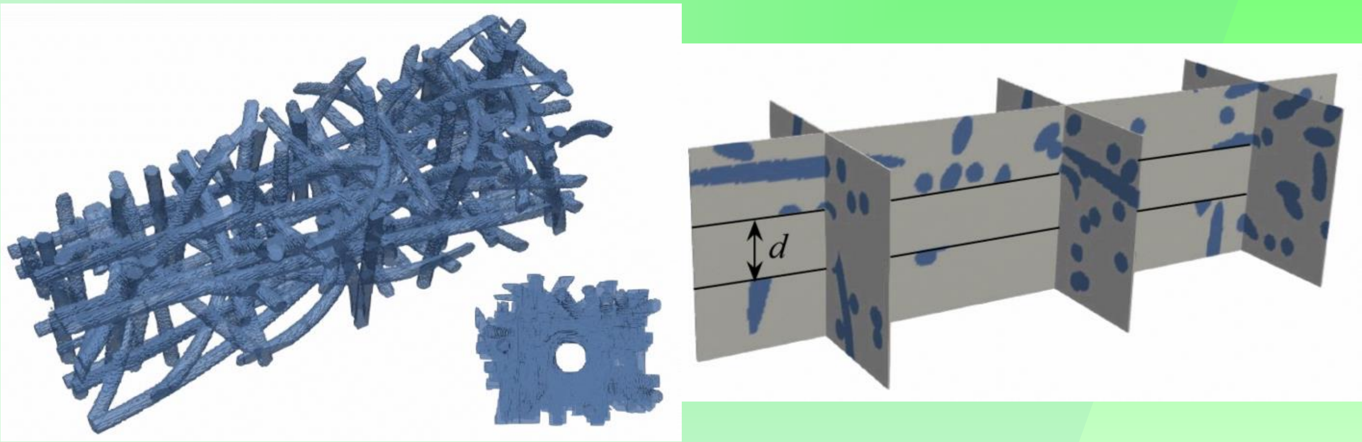
UCL: Luo, Lei et al. (2024)

Battery Research & Design:
LB Simulation of Discharge of Li-Air Battery

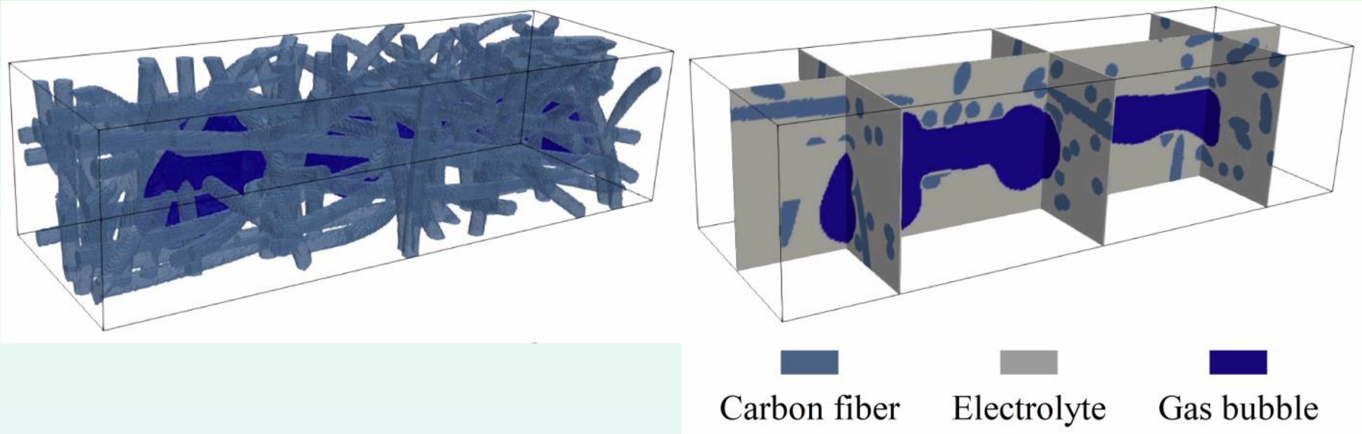


Base case

Rational design



Step 1: Perforated middle hole (MH)



Step 2: Filling middle hole with gas bubble (**MHG**)

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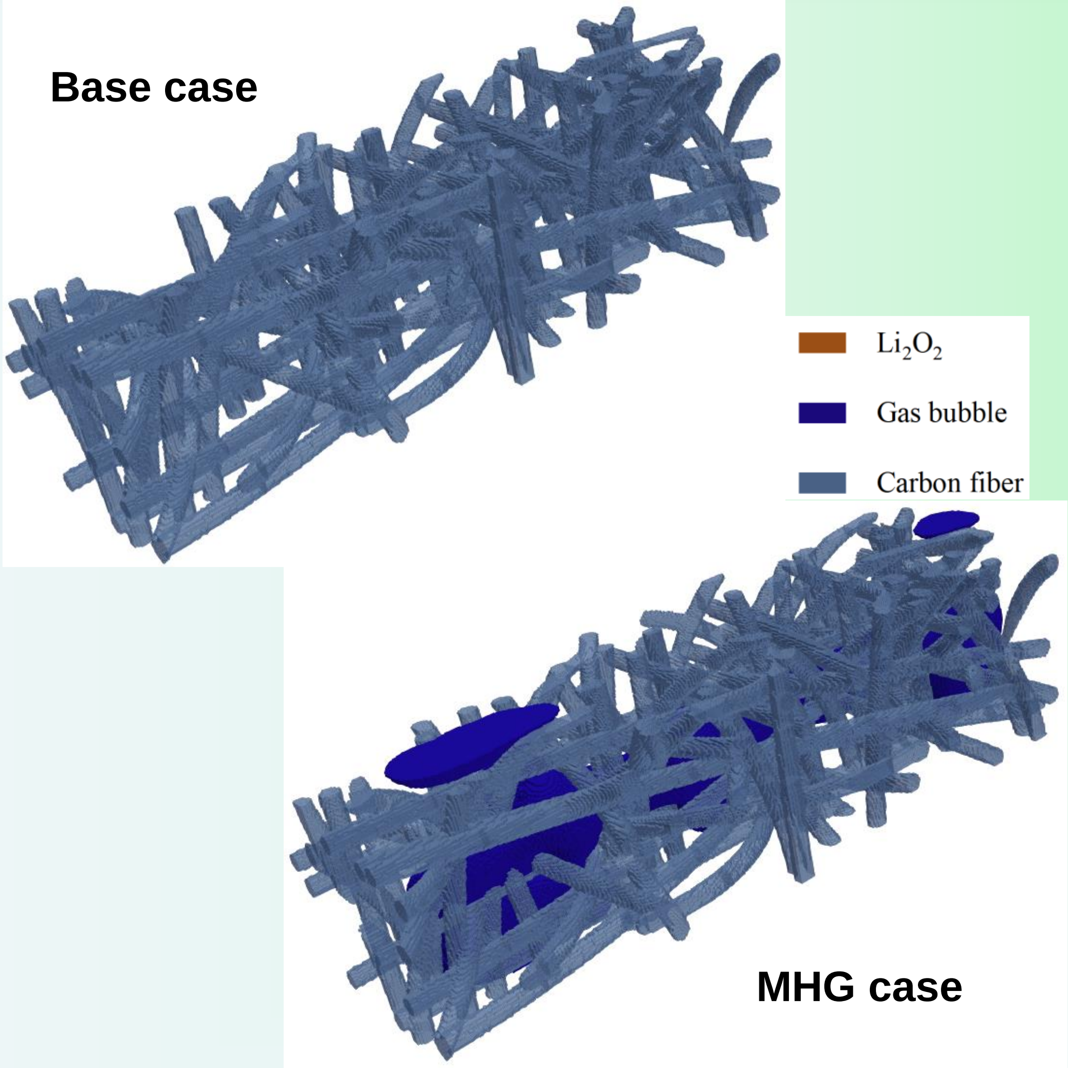
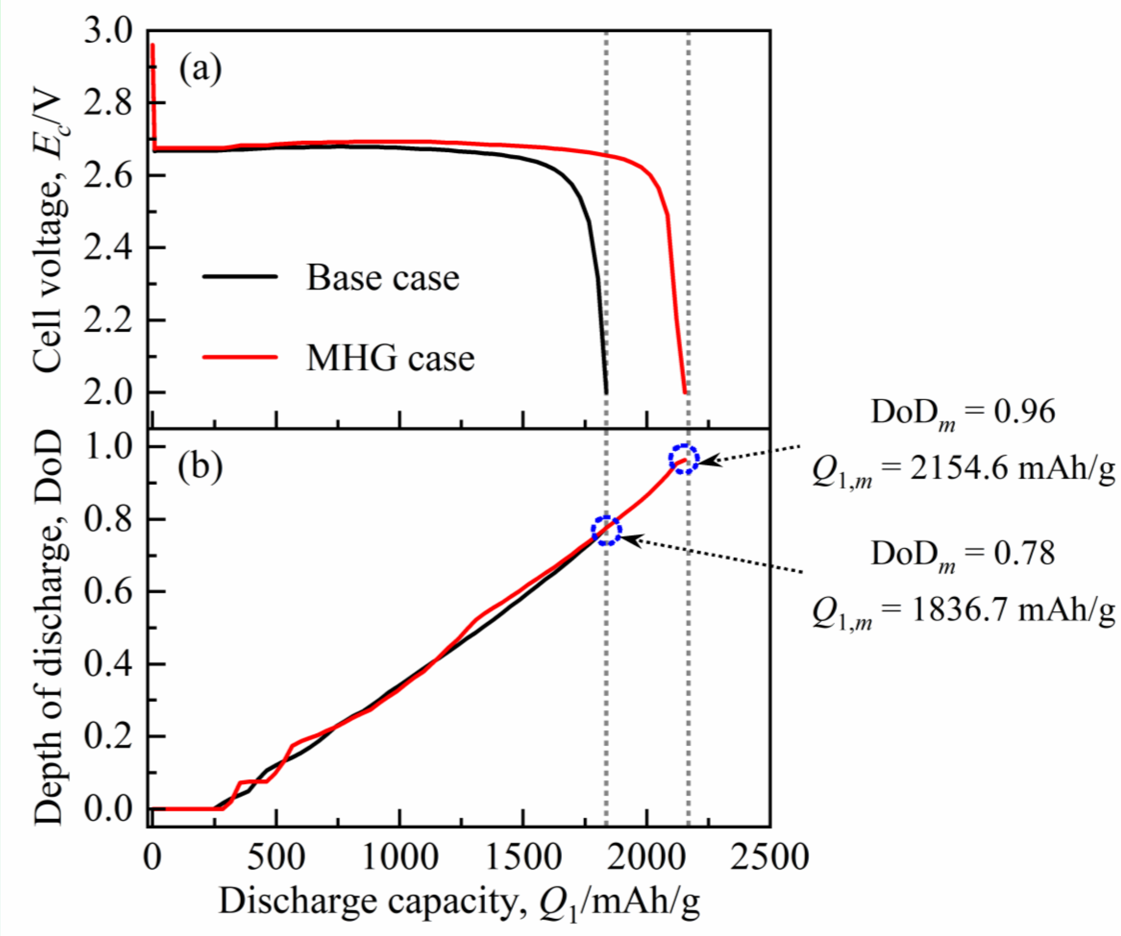
UCL: Luo, Lei et al. (2024)

Battery Research & Design:
LB Simulation of Discharge of Li-Air Battery





- Rational design **MHG** can reach **DoD_m=0.96**
- Battery **capacity is improved**

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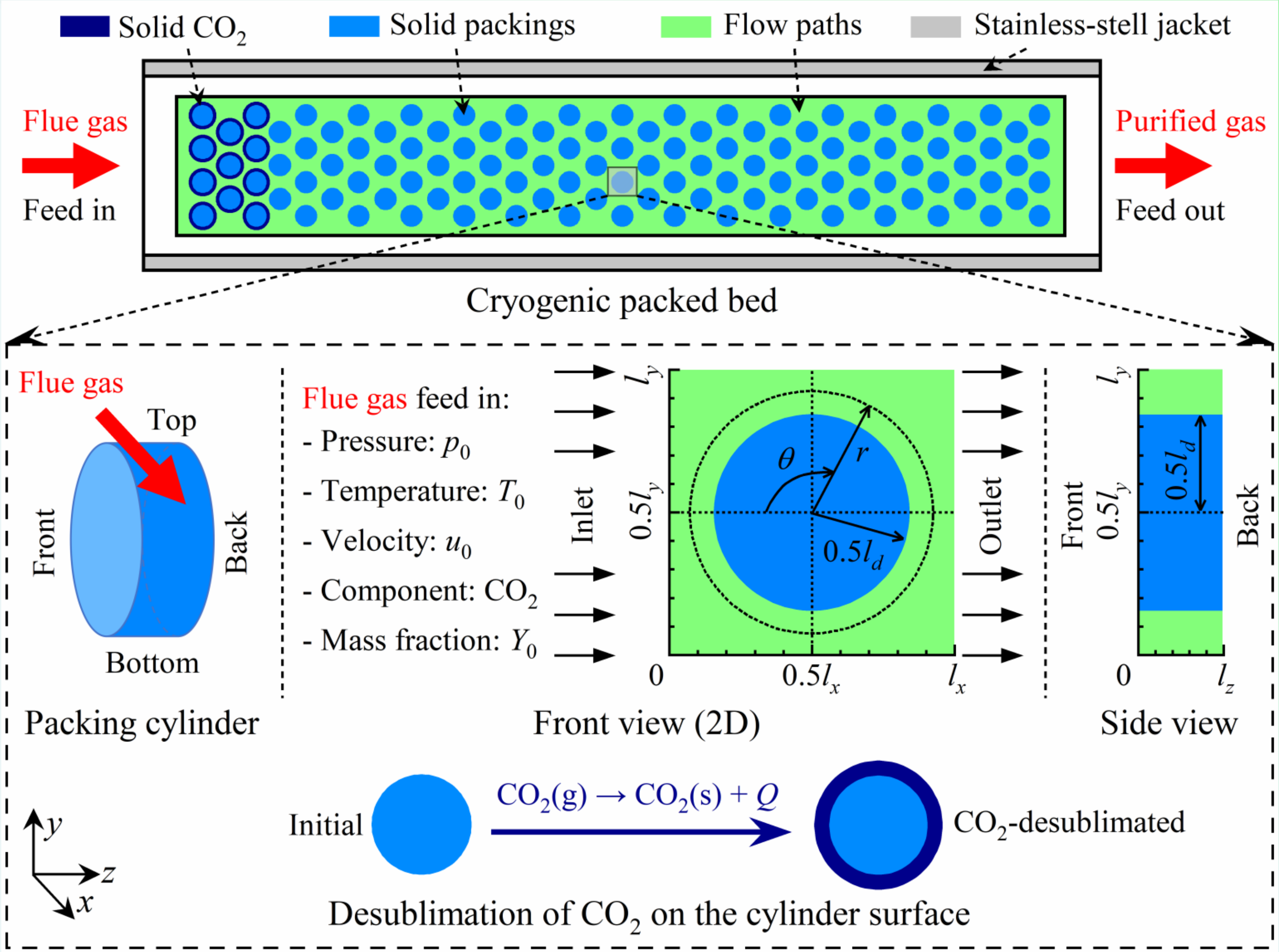
UCL: Luo, Lei et al. (2024)

Cryogenic Carbon Capture (CCC): LB Simulation of CO_2 Desublimation & Sublimation



- **Domain size**
  - Single: 14.7 mm * 14.7 mm * 0.7 um
  - Bed: 124.8 mm * 20.8 mm * 0.7 mm
- **Grid size**
  - Single: 640 * 640 * 30
  - Bed: 5400 * 900 * 30
- **CO_2 desublimation & sublimation**
  - CO_2 (g) → CO_2 (s) + **heat**
  - CO_2 (s) + heat → CO_2 (s)
- **Parallel simulations on Archer2**
  - Single: 2-hour computation of 384 cores
  - Bed: 14-hour computation of 7040 cores

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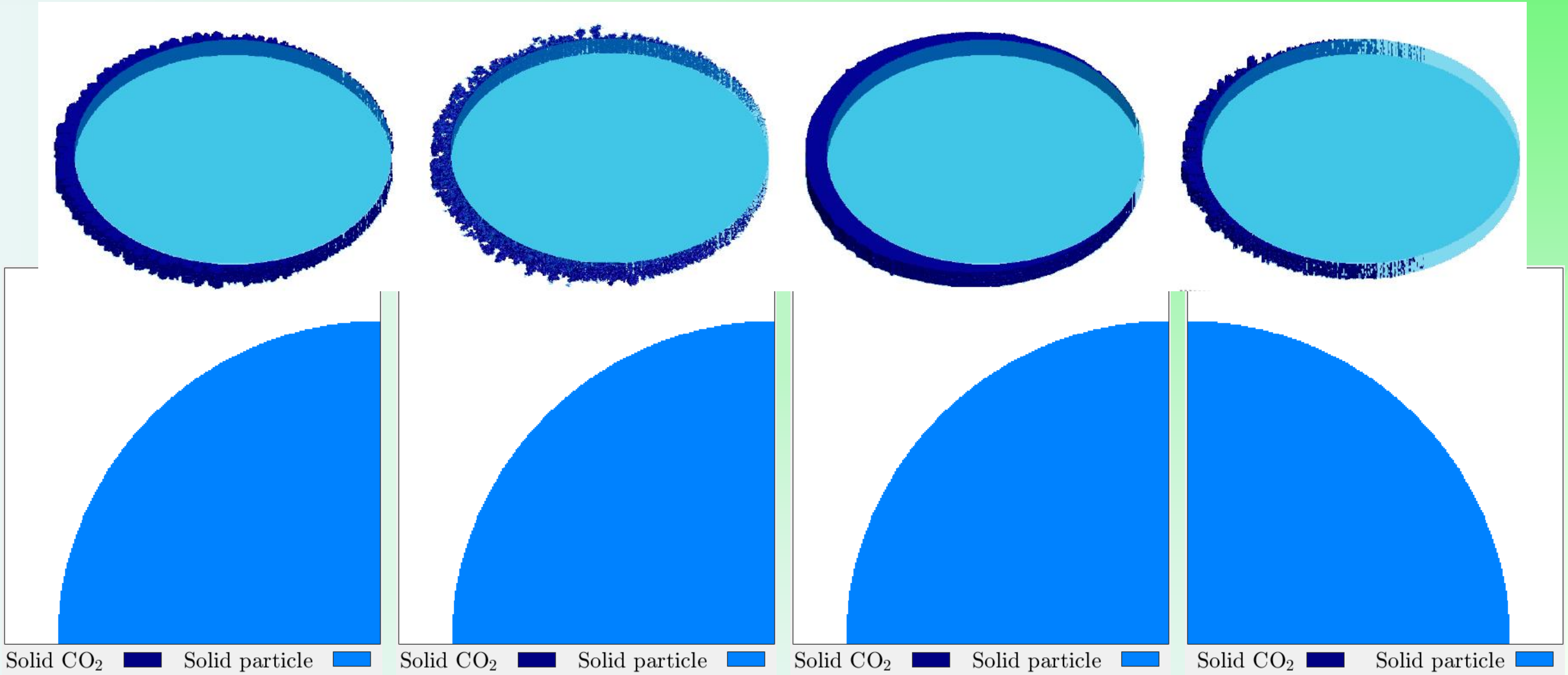
UCL: Luo, Lei *et al*, Journal of Fluid Mechanics 964:A1 (2023)

Cryogenic Carbon Capture (CCC): LB Simulation of CO_2 Desublimation & Sublimation



I: Dendritic structure; Joint-controlled regime

II: Cluster structure; Diffusion-controlled regime

III: Dense structure; Desublimation-controlled

IV: Incomplete-coated structure; Convection-controlled regime

- ✓ **4 microscale structures** of solid CO_2 are identified, corresponding to **4 desublimation regimes**

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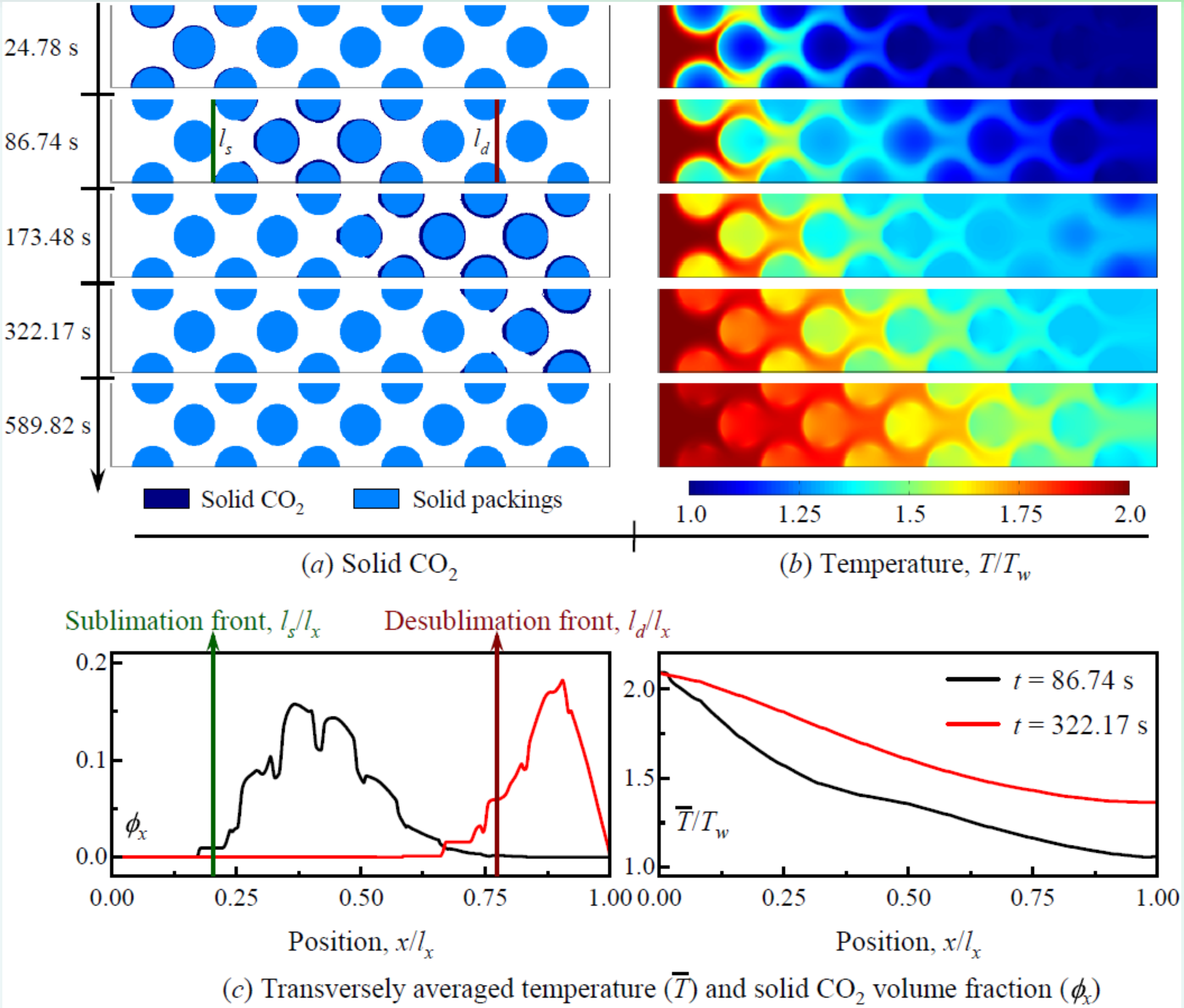
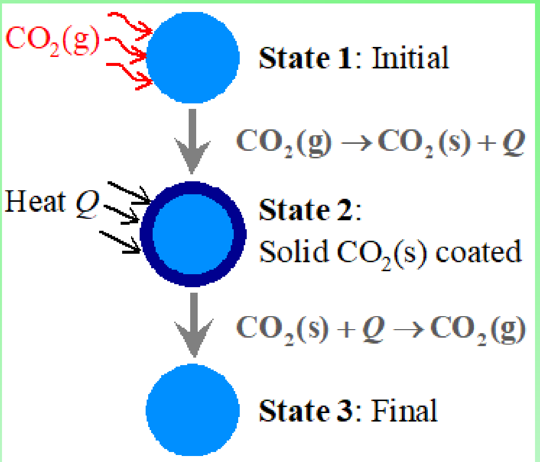
UCL: Luo, Lei *et al*, Journal of Fluid Mechanics 964:A1 (2023)

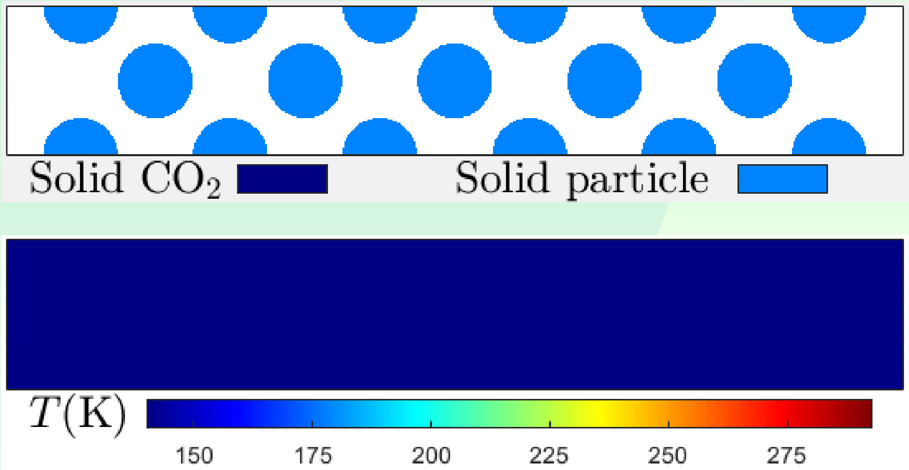
Cryogenic Carbon Capture (CCC):
LB Simulation of CO_2 Desublimation & Sublimation





Capture

Recovery



✓ The **capture** and **recovery** steps of CCC are successfully modelled

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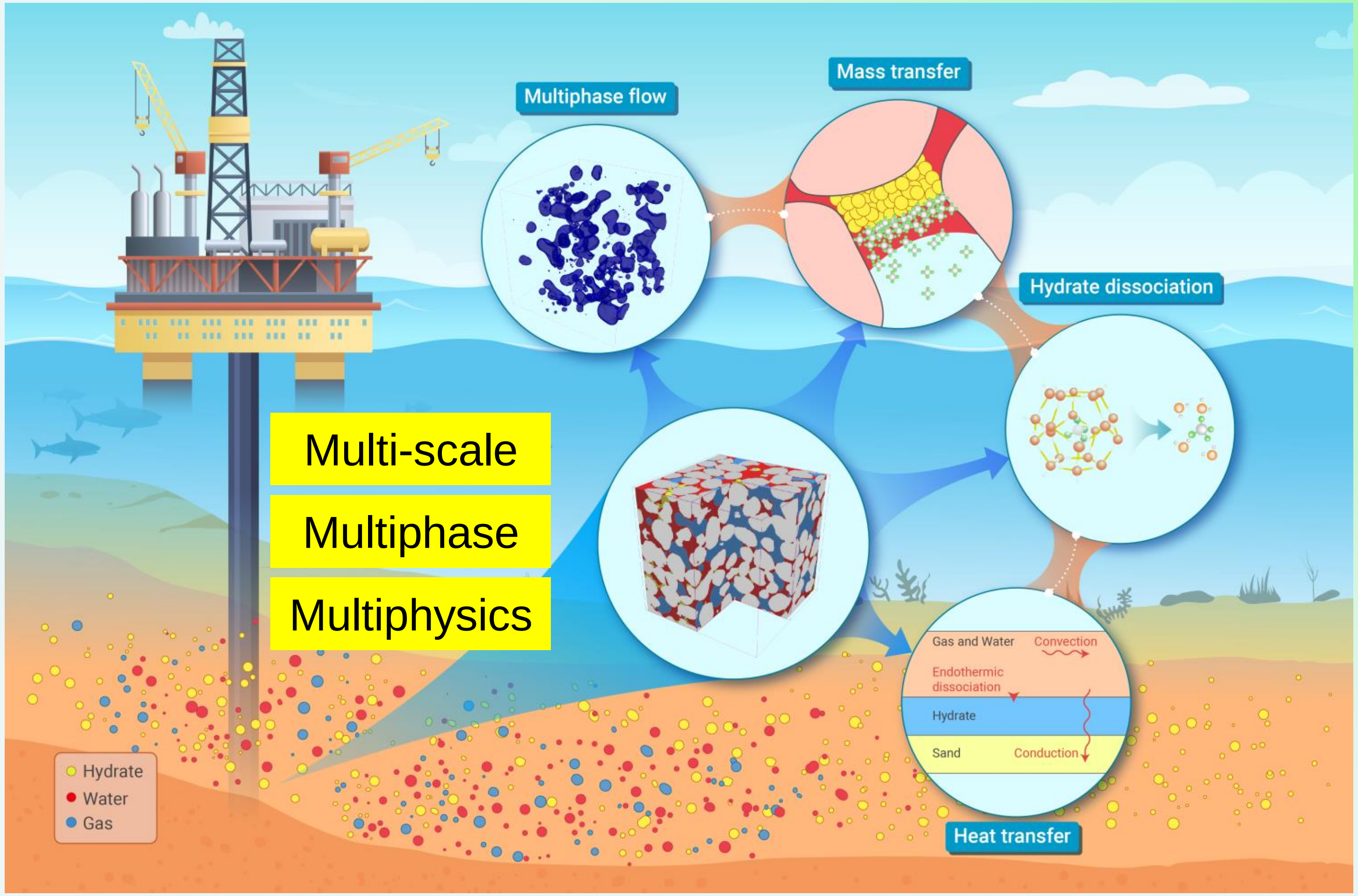
UCL: Luo, Lei *et al*, Journal of Fluid Mechanics 964:A1 (2023)

Multiscale Multiphysics Undersurface Engineering: LBM of Geological CO_2 Storage & Fuel Extraction

☐ Pore-scale understanding of multiphysics mechanisms is significant in the subsurface engineering



Multiphysics process during methane hydrate exploitation

➢ Multiphysics mechanisms

- Transport in porous media
- Multiphase flow
- Conjugate heat transfer
- Interfacial mass transfer
- Heterogenous reaction

➢ Complex pore structures

- Micrometer-sized pores
- Various phase distribution

➢ Tough numerical challenges

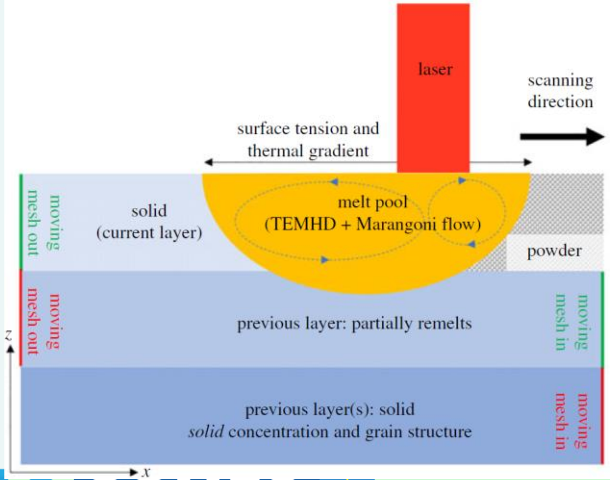
- Hundreds of millions of grids
- Multiple governing equations coupled
- Complicated boundary treatment

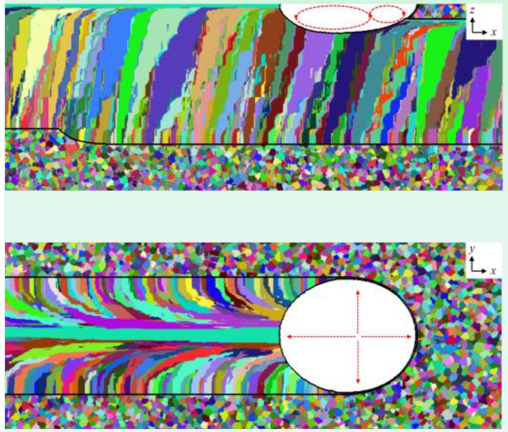
High-performance numerical simulation!

UCL: Luo, Yang *et al*, The Innovation Energy 1, 100015 (2024)

Advanced Manufacturing:
Multi-physics Modelling and Simulation of Solidification

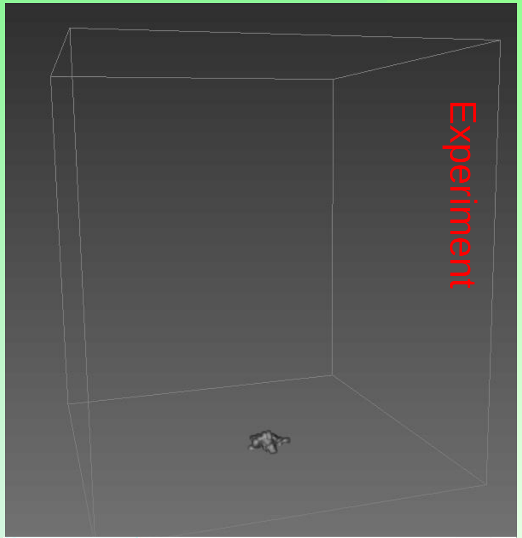
Additive Manufacturing (AM):
Thermoelectric magnetohydrodynamic control of melt pool dynamics & microstructure evolution



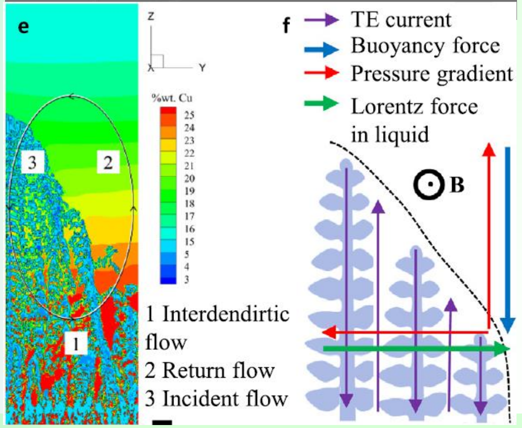


Control of Solidification Microstructures:
Thermoelectric magnetohydrodynamic control of microstructure evolution

Simulation



Experiment



Heat & mass transfer
Phase change
Lorentz forces
Marangoni flow
Splattering
Denudation

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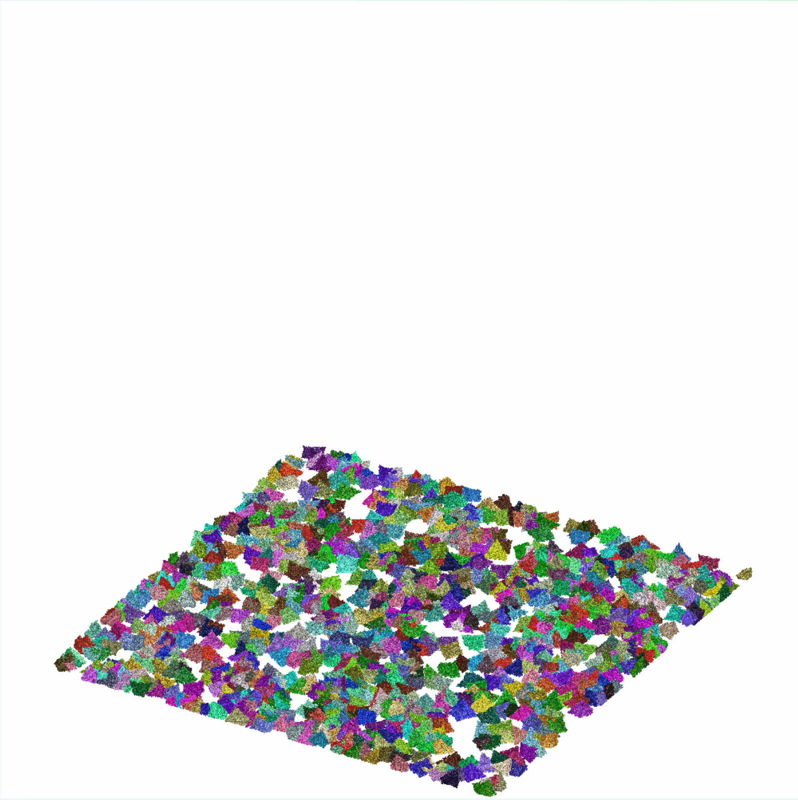
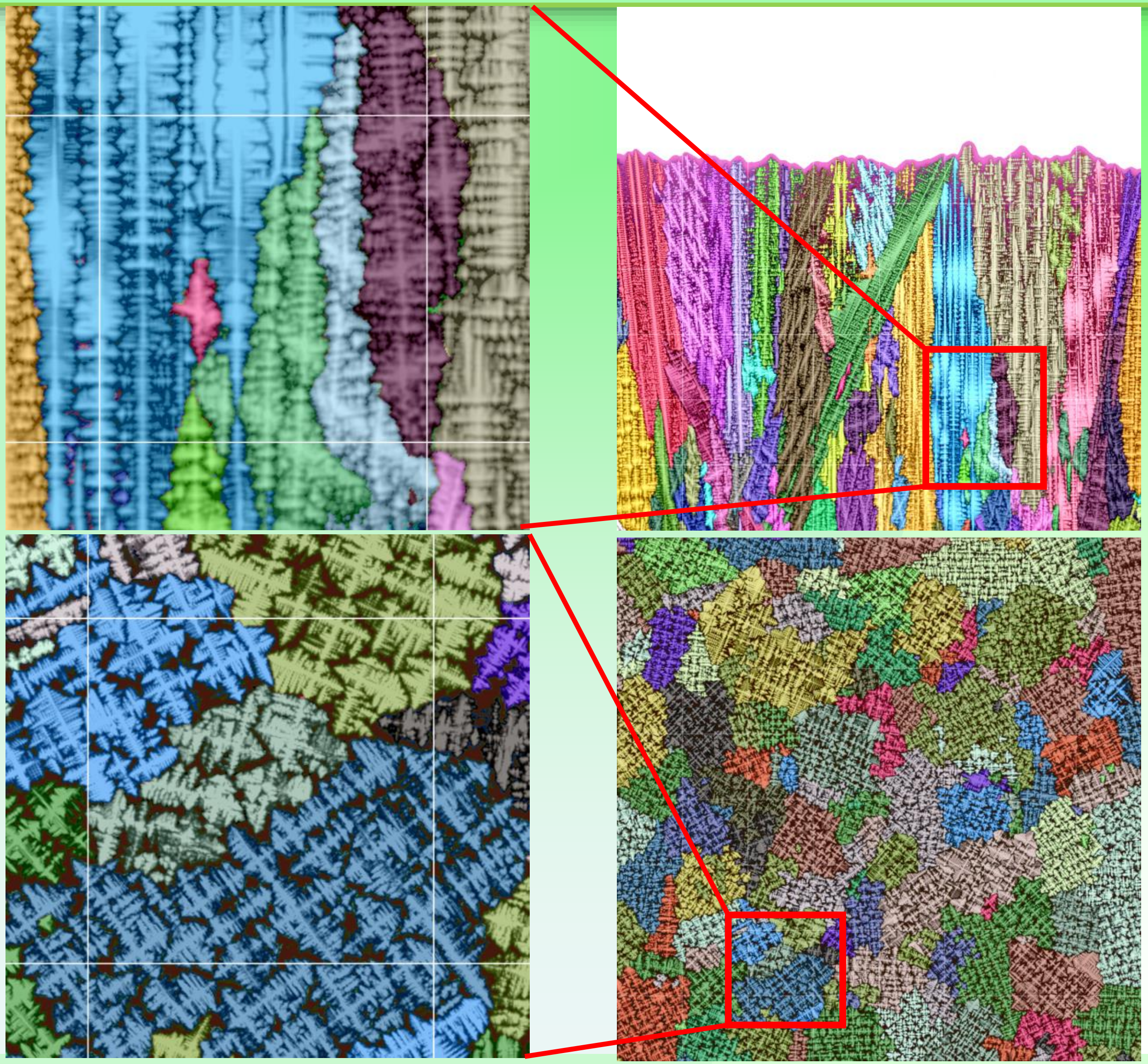
University of Greenwich: Kao et al.

Advanced Manufacturing:
Single Crystal Superalloy Casting

Polycrystalline Solidification Modelling:

- 8 billion cell calculation representing a 40 mm cube
- Component, grain and dendritic scales, all captured from a microscale perspective over realistic solidification times (500 s)





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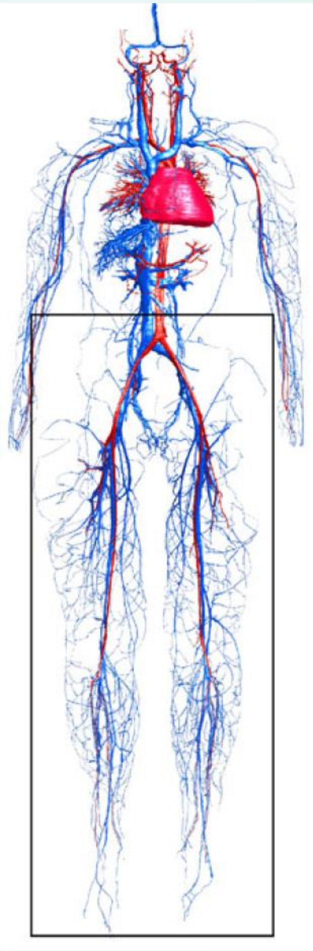
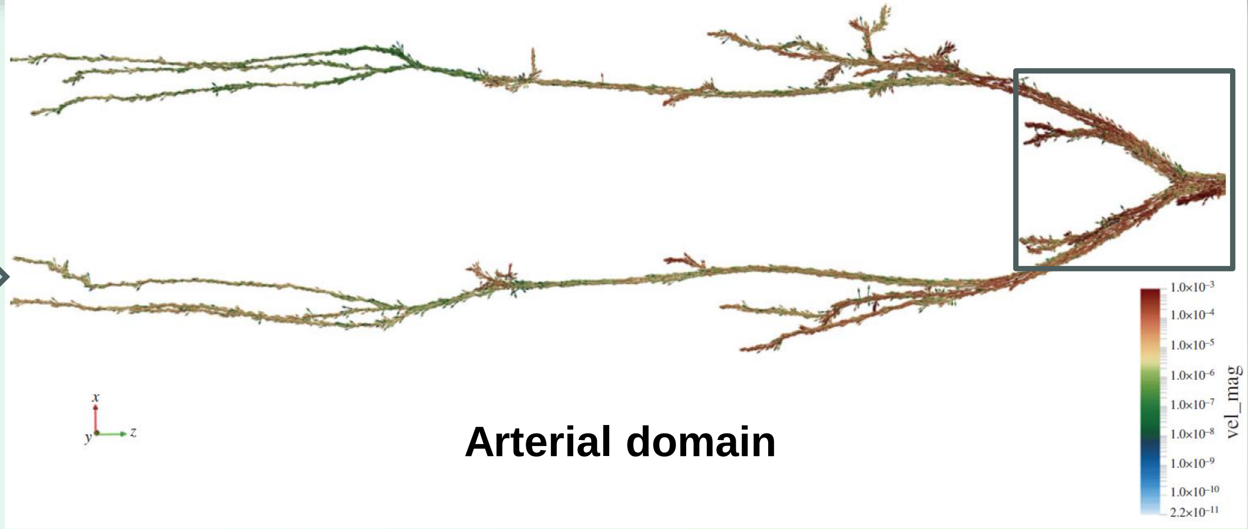
University of Greenwich: Kao et al.

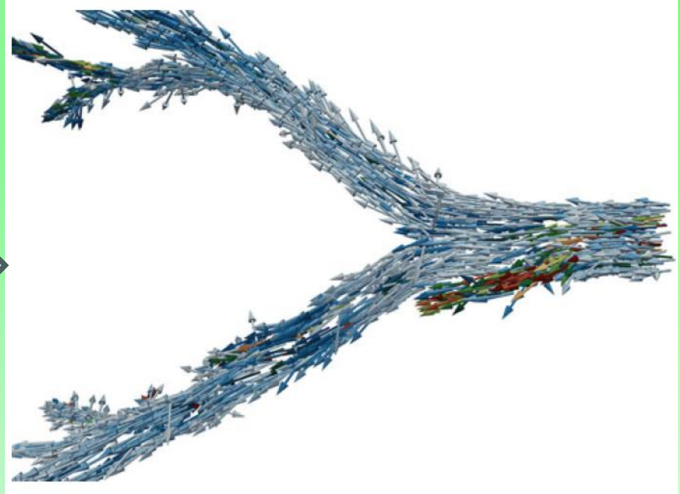
Blood Flow in Virtual Human:
Towards a digital replica of an individual and its physiological processes



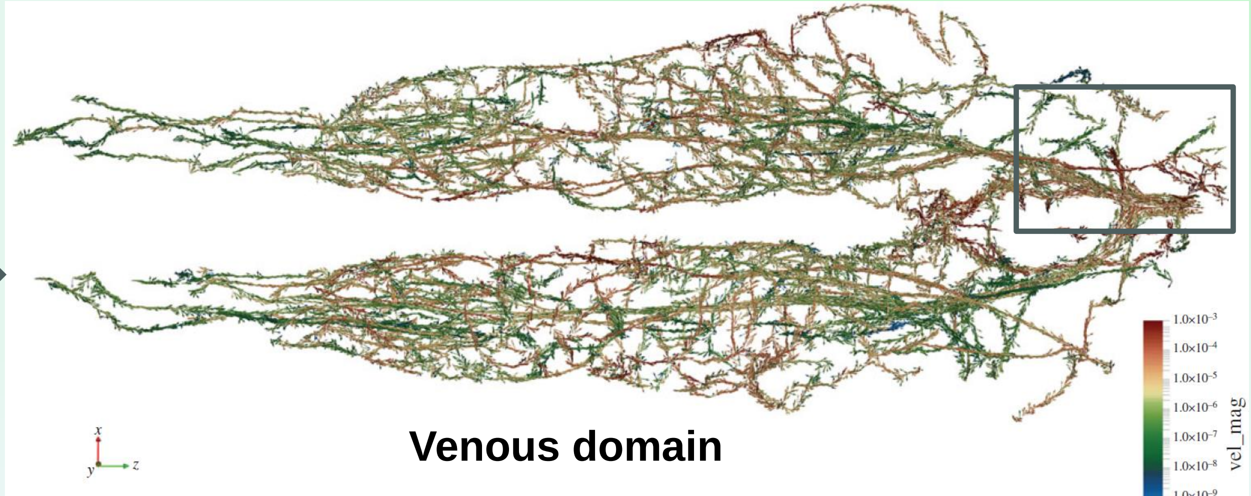
Human vasculature



Arterial domain

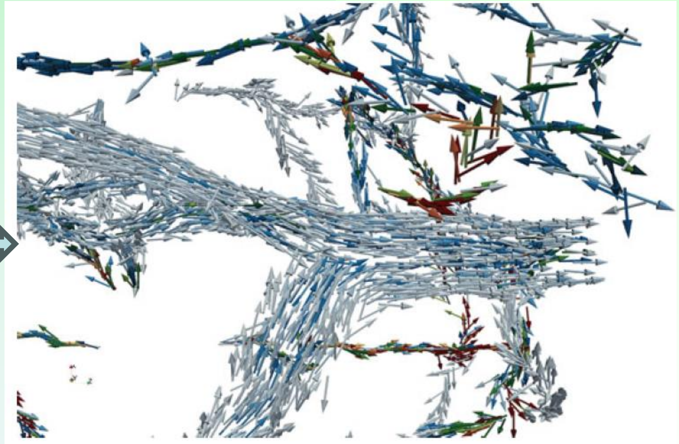


Velocity vectors



Venous domain

(450 million lattice sites, 75 micron resolution, 10,080 cores)



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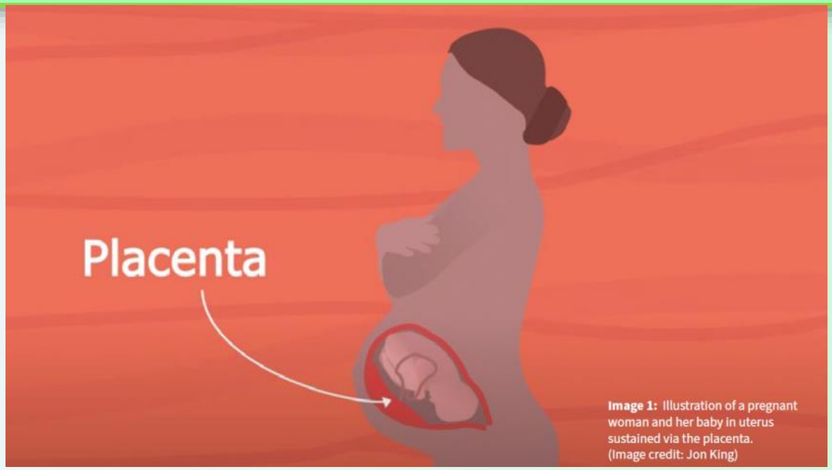
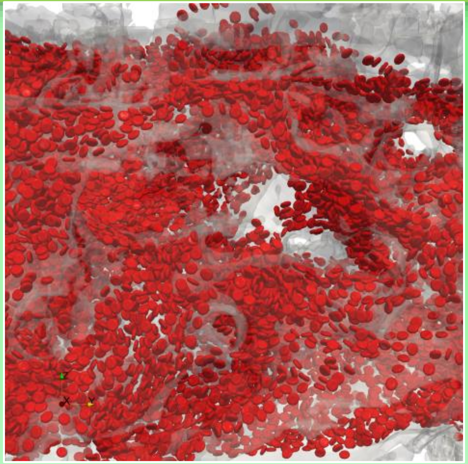
UCL: Coveney et al.

Placental Haemodynamics and Artificial Placentas
Towards a digital replica of an individual and its physiological processes

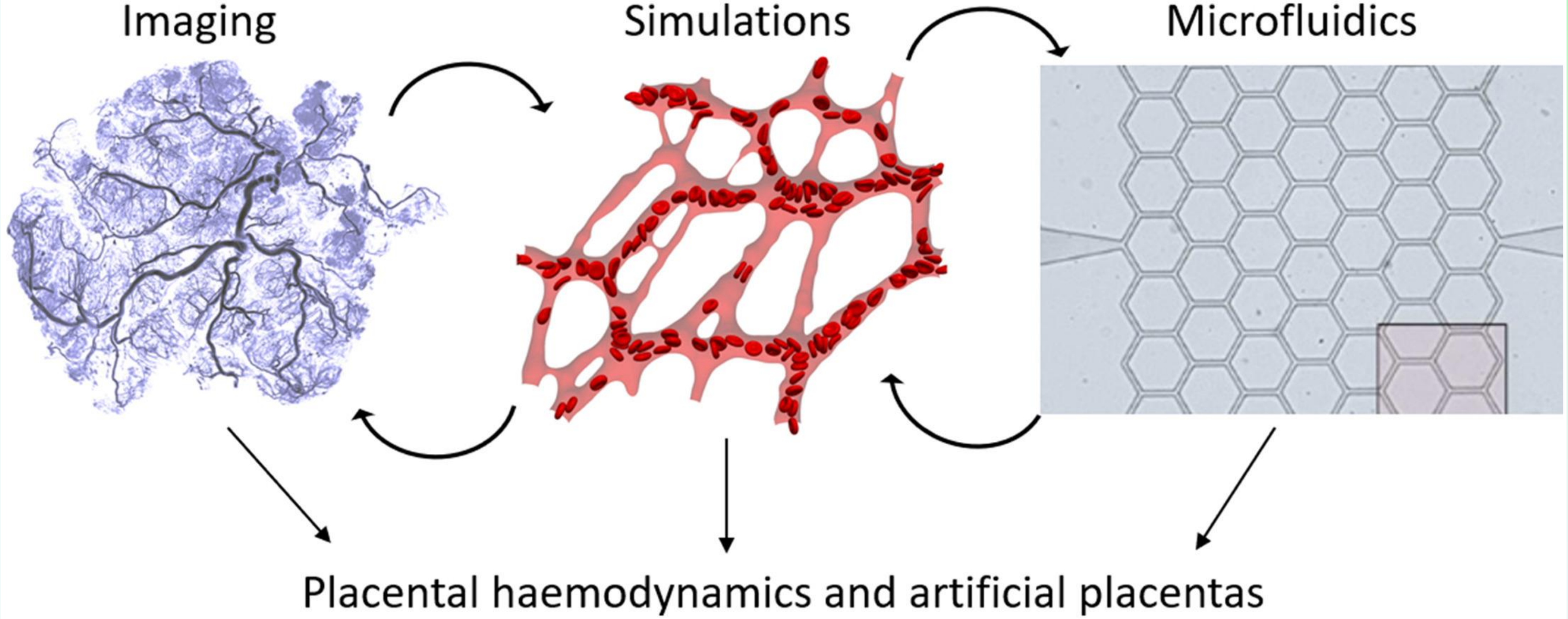


Red blood cell transport in materno-placental tissues

LB simulation with 30 million lattice sites, 6,000 cores



2023



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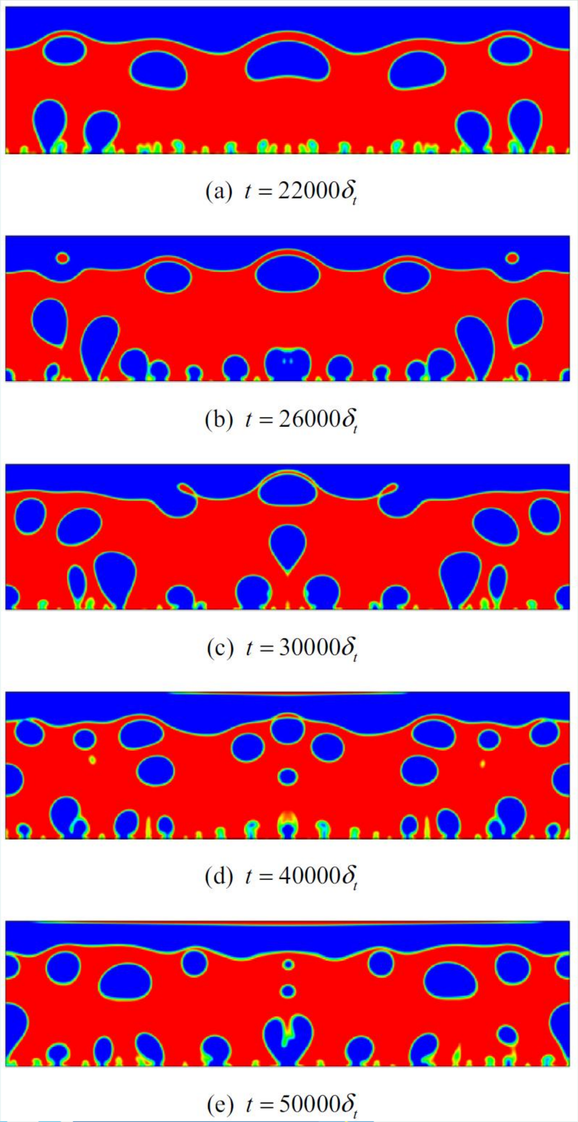
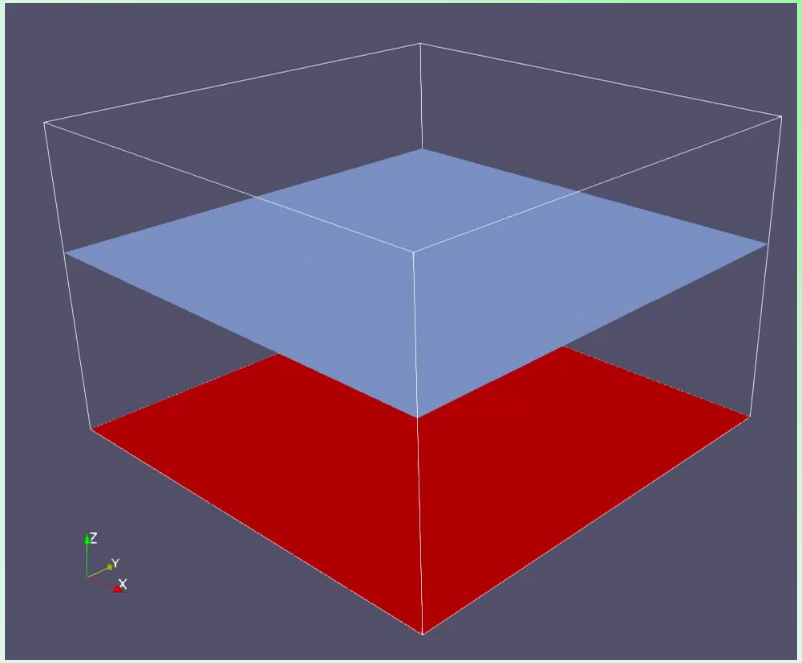
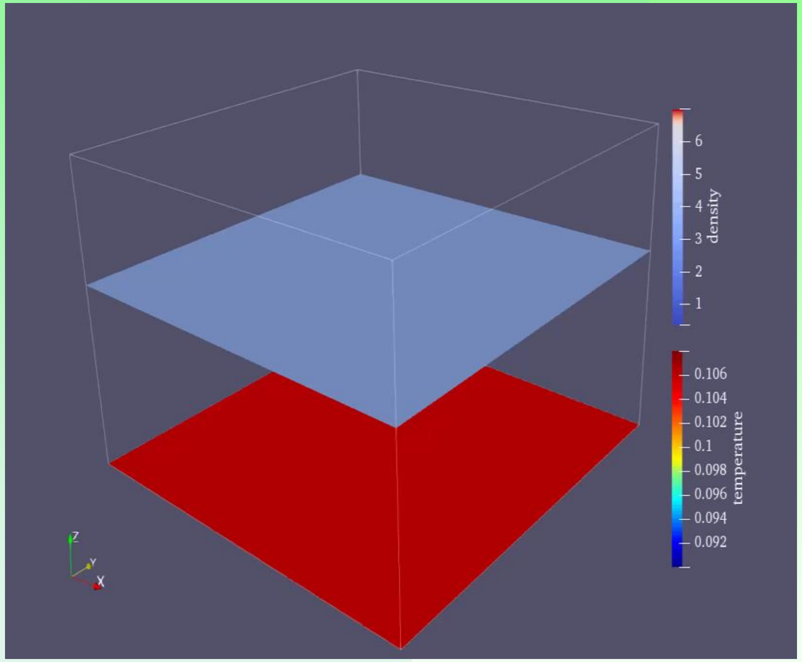
University of Edinburgh: Zhou, Krüger and Bernabeu et al.

2D and 3D LBM Simulations of Pool Boiling over a Heated Surface





$\Delta T = 0.0135$



$\Delta T = 0.015$

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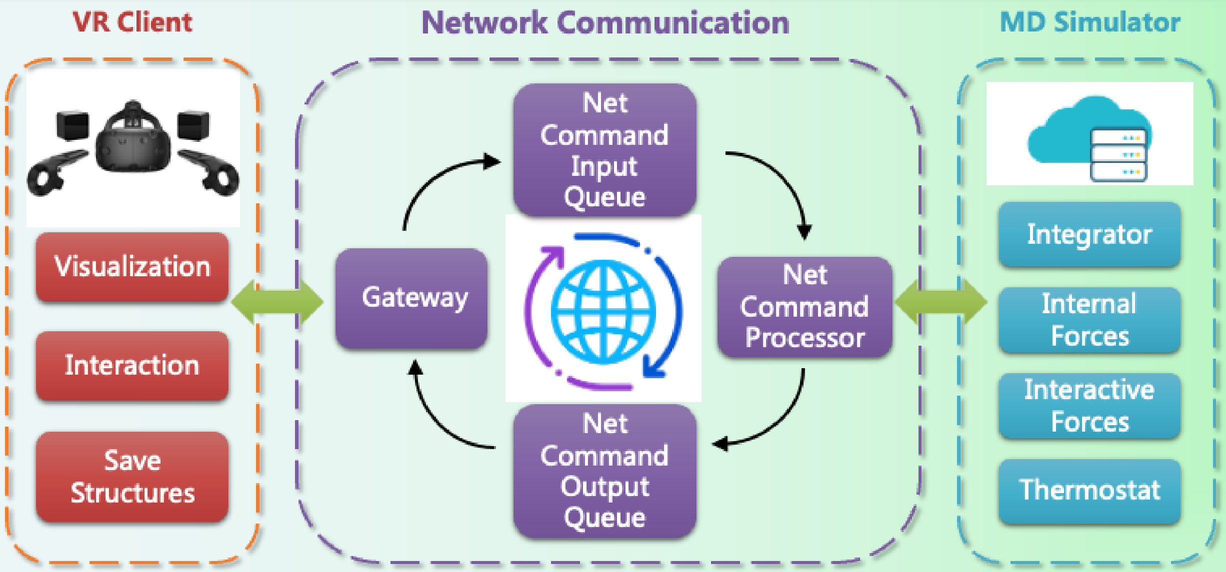
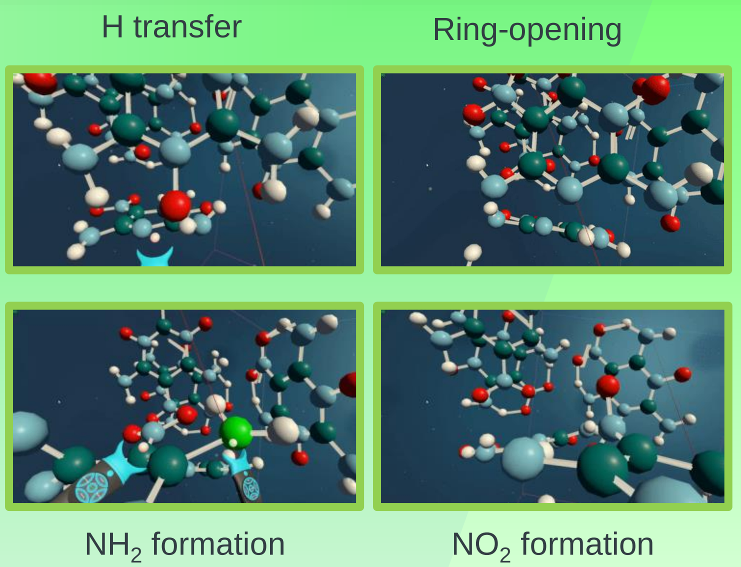
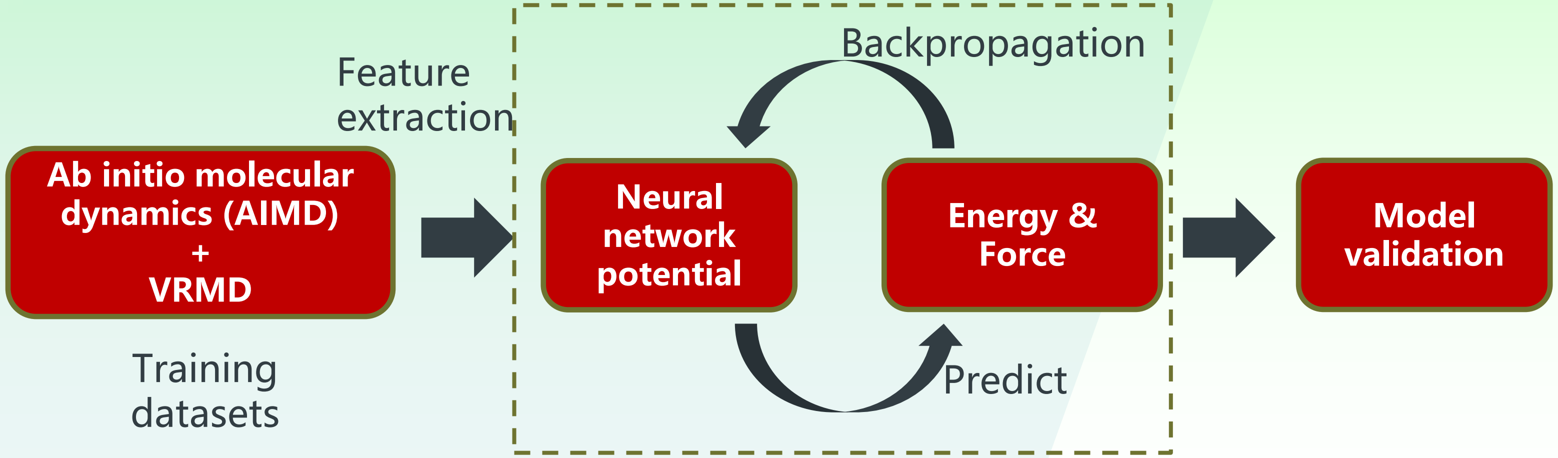
UCL: Luo, Fei and Wang, Phil. Trans. Royal Society, A 379 (2021)

Interactive MD Simulations in Virtual Reality (VRMD)



The VRMD allows flexible manipulation of molecular structures and VR forces to accelerate the reaction processes.





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UCL: Luo, Chu et al., The Journal of Physical Chemistry Letters, 13 (2022)

Summary

- **UKCOMES is a large and enlarging community advancing the emerging mesoscale science and engineering**

- **Using ARCHER2, cutting-edge simulations have been performed, providing unprecedented insights into and guidance for energy, healthcare, advanced manufacturing, multiphase, and multiphysics processses**

- **UKCOMES is uniquely positioned, in a global context, to exploit emerging science and technology at the interfaces of traditional disciplines, including data-driven modelling and AI**

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