Mesoscopic Modeling, Concurrent Coupling and Multiscale Framework

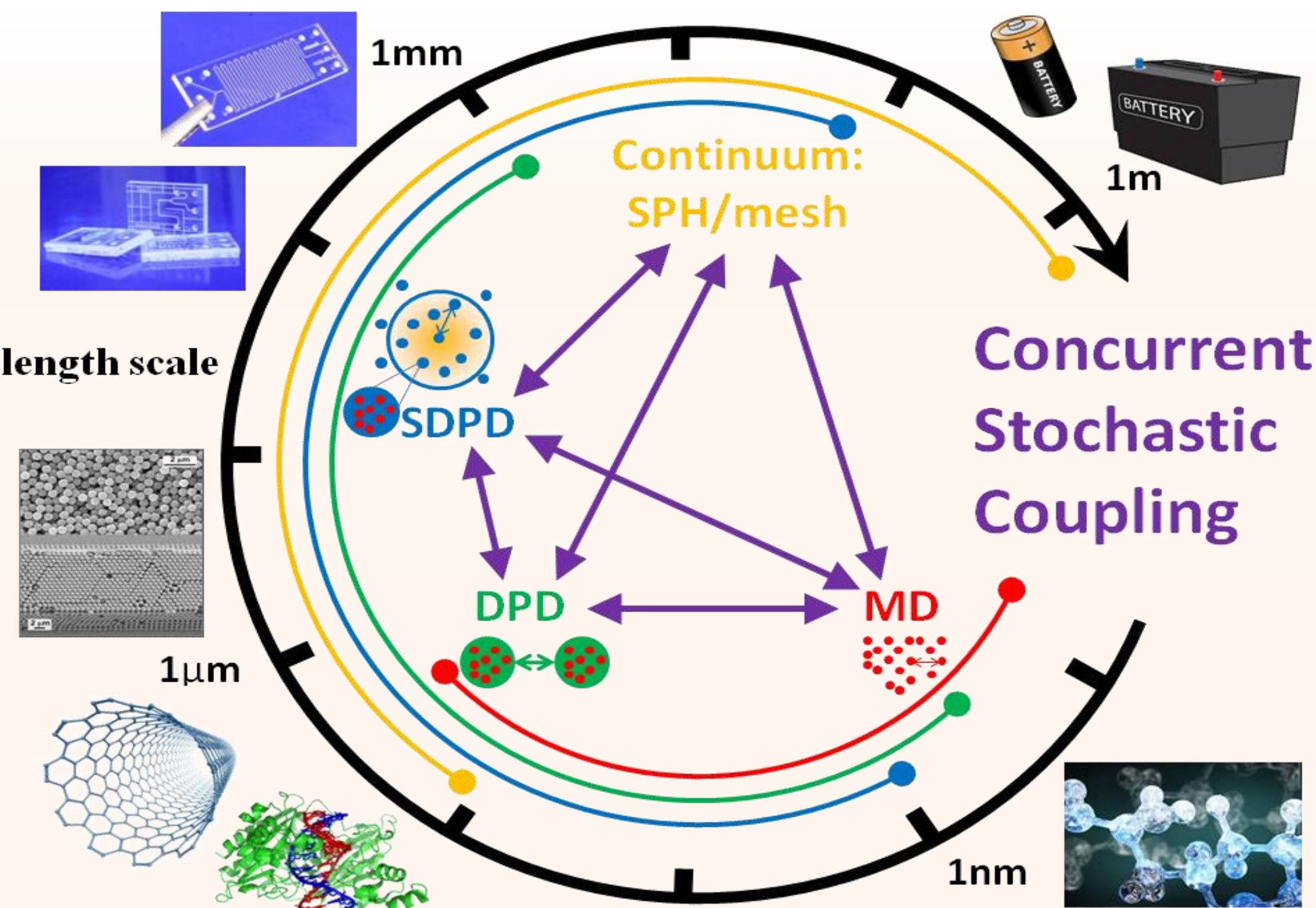**Zhen Li[1], Xin Bian[2], Yu-Hang Tang[1], George Em Karniadakis[1]**

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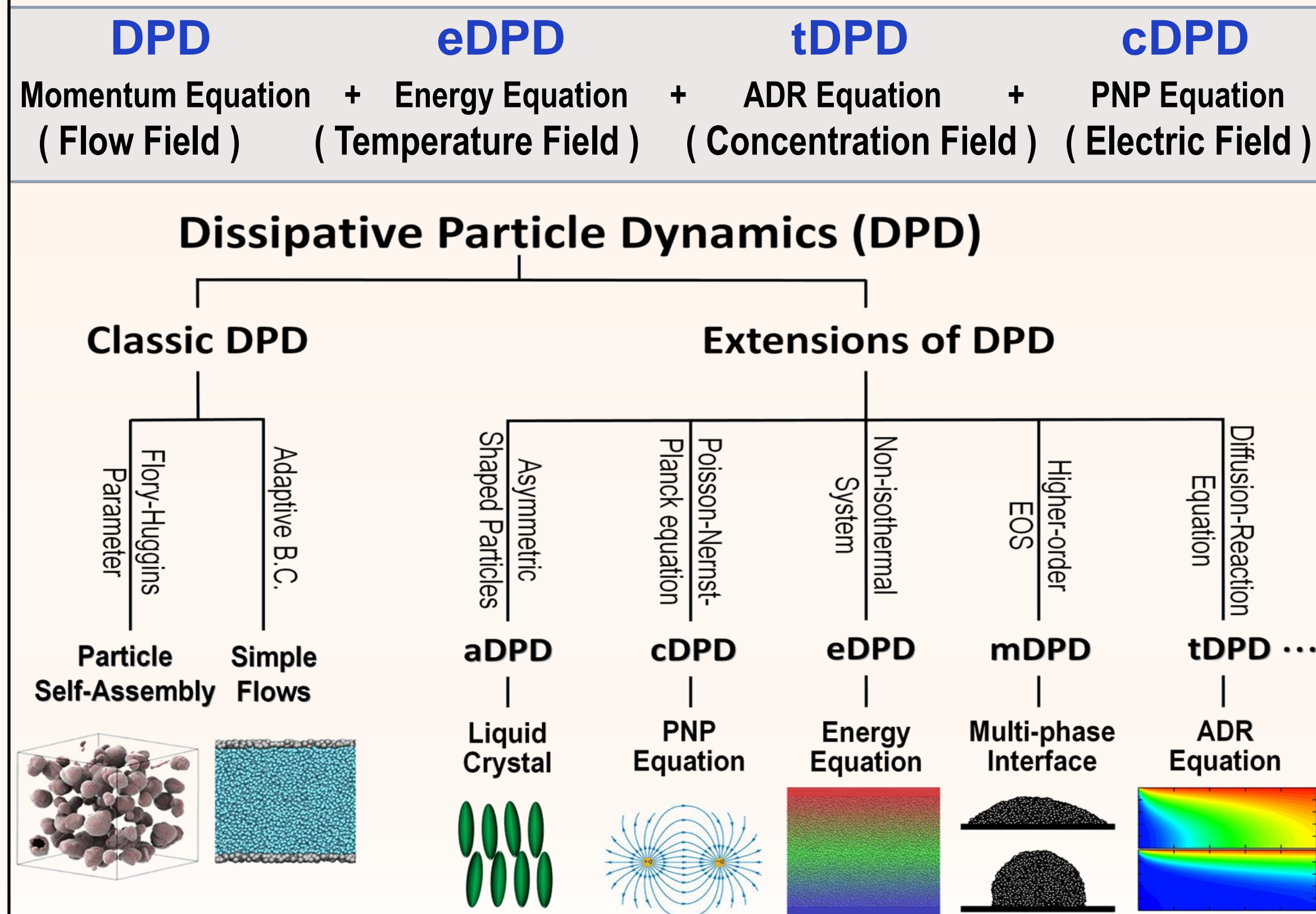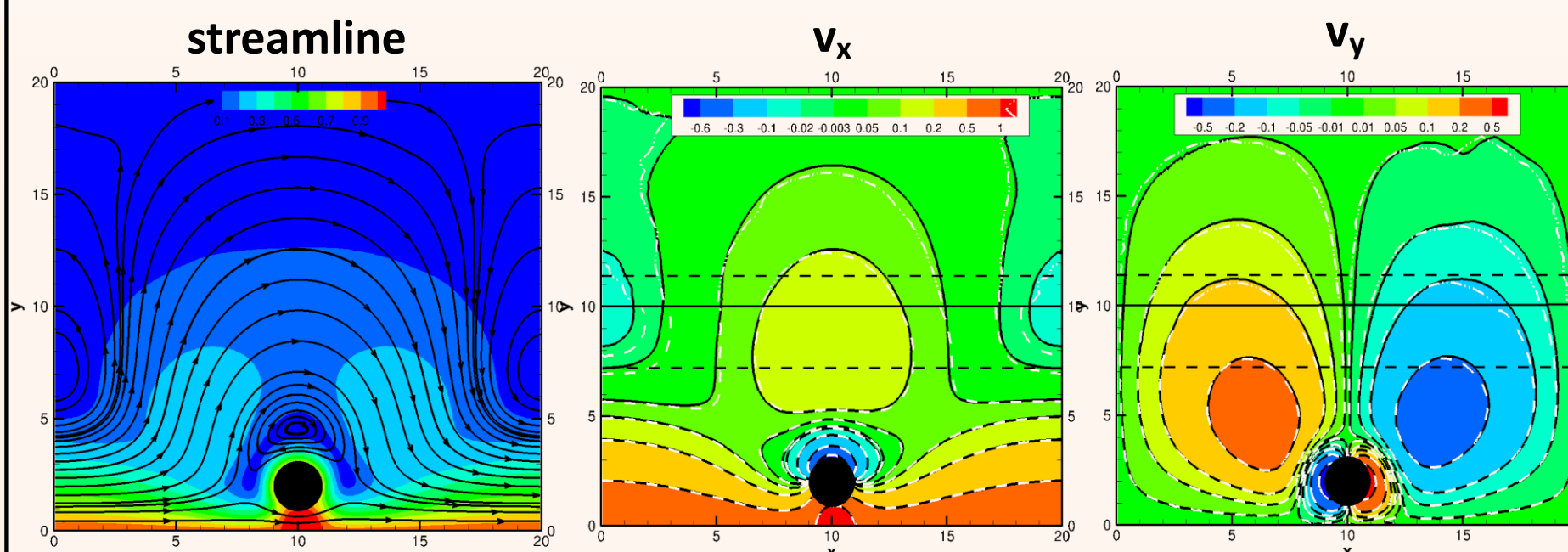[2]*Chair of Aerodynamics and Fluid Mechanics, Technical University of Munich, Germany*

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General Goals

1mm
1m
length scale
1μm
1nm

Continuum: SPH/mesh
SDPD
DPD
MD

Concurrent Stochastic Coupling

Mesoscopic Modeling

DPD	eDPD	tDPD	cDPD
Momentum Equation	+ Energy Equation	+ ADR Equation	+ PNP Equation
(Flow Field)	(Temperature Field)	(Concentration Field)	(Electric Field)

Dissipative Particle Dynamics (DPD)

Classic DPD

- Flory-Huggins Parameter
- Adaptive B.C.

Particle Self-Assembly — Simple Flows

Extensions of DPD

- Asymmetric Shaped Particles
- Poisson-Nernst-Planck equation
- Non-isothermal System
- Higher-order EOS
- Diffusion-Reaction Equation

aDPD — Liquid Crystal
cDPD — PNP Equation
eDPD — Energy Equation
mDPD — Multi-phase Interface
tDPD ··· — ADR Equation

Concurrent Coupling

1. Domain Decomposition
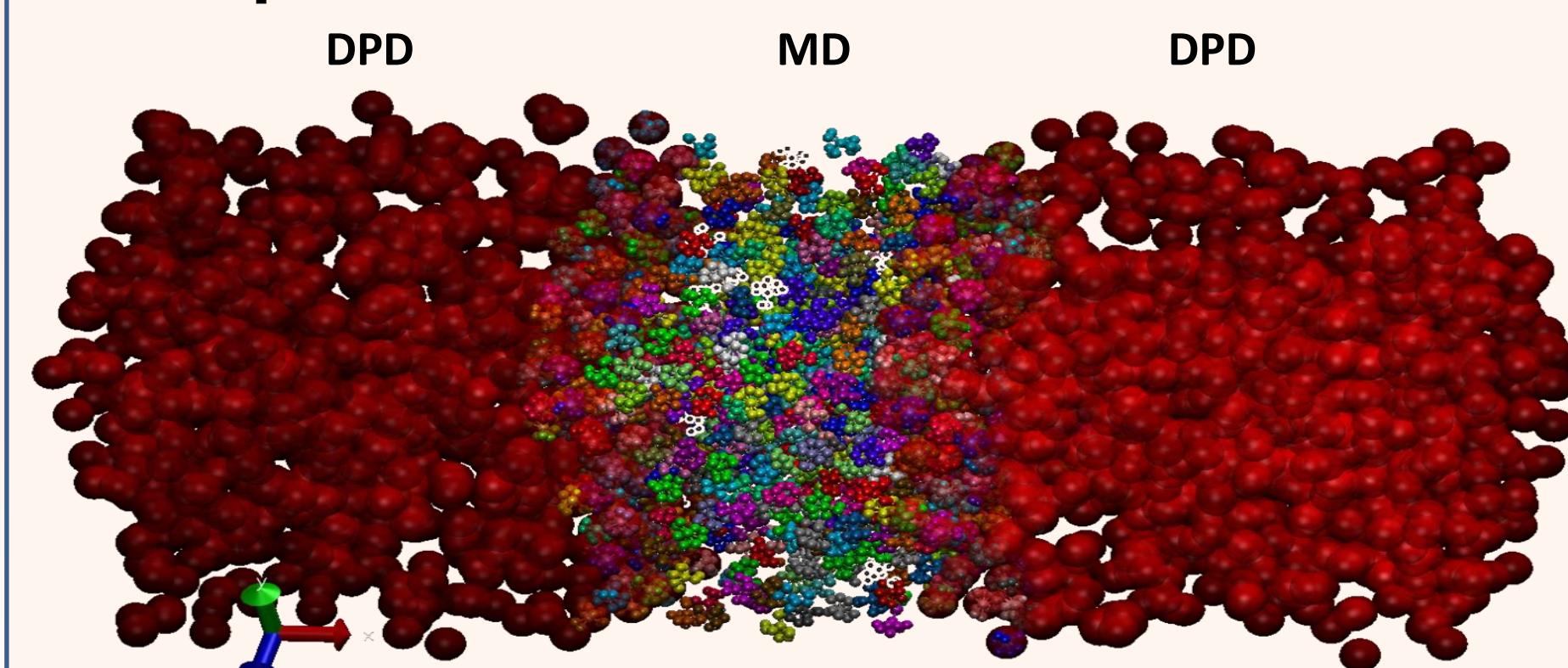
(a) Multi-resolution SPH–SPH for Wannier flow

streamline v_x v_y

(b) Multi-scale SPH–DPD for flow over polymeric surface

Analytical, DPD, SPH
t = 10000, t = 2000, t = 1000, t = 500, t = 200, t = 100
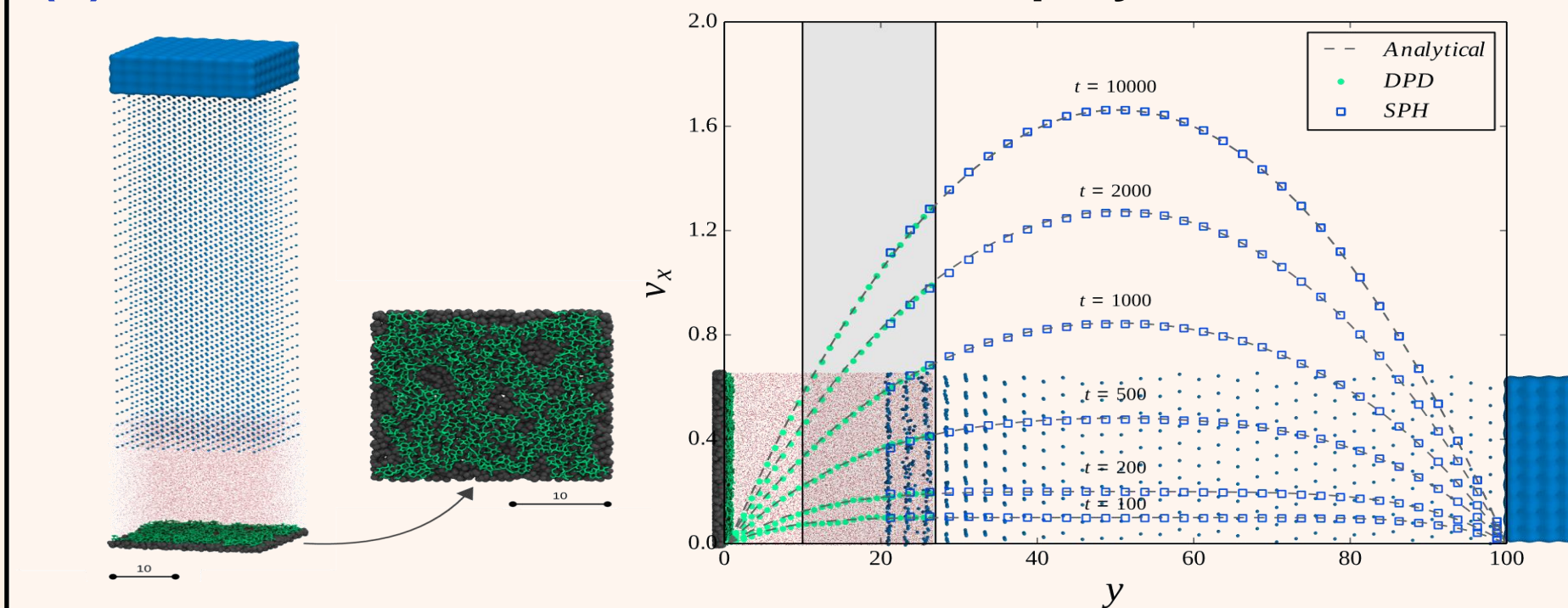
(c) Multi-physics FEM–eDPD for conjugate heat transfer

$T(K)$
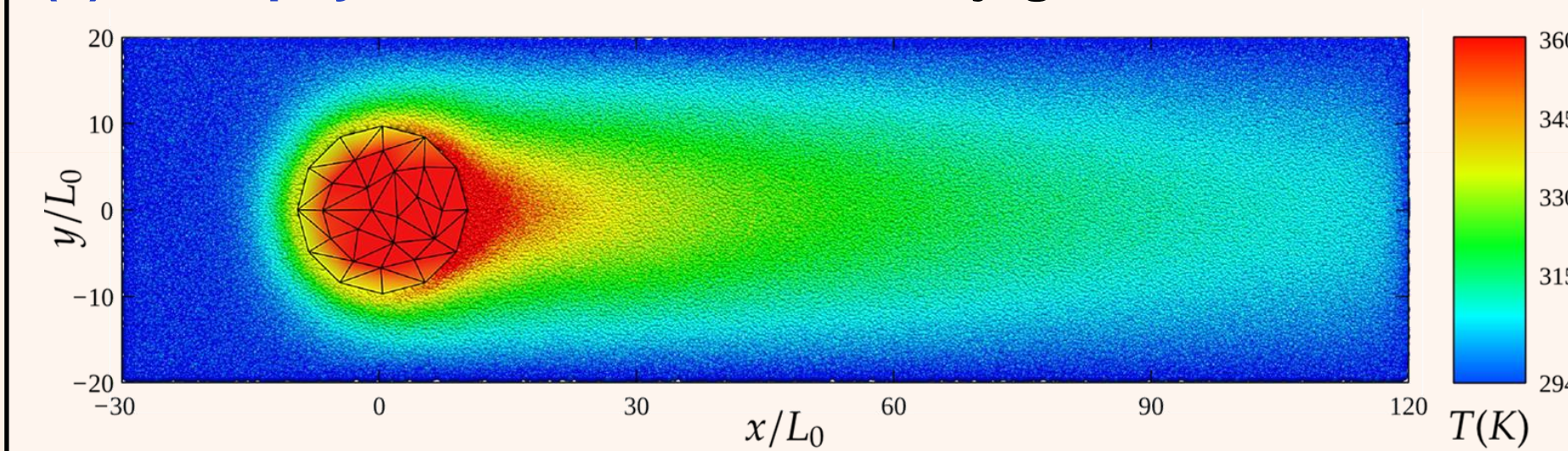
2. Adaptive Resolution Scheme
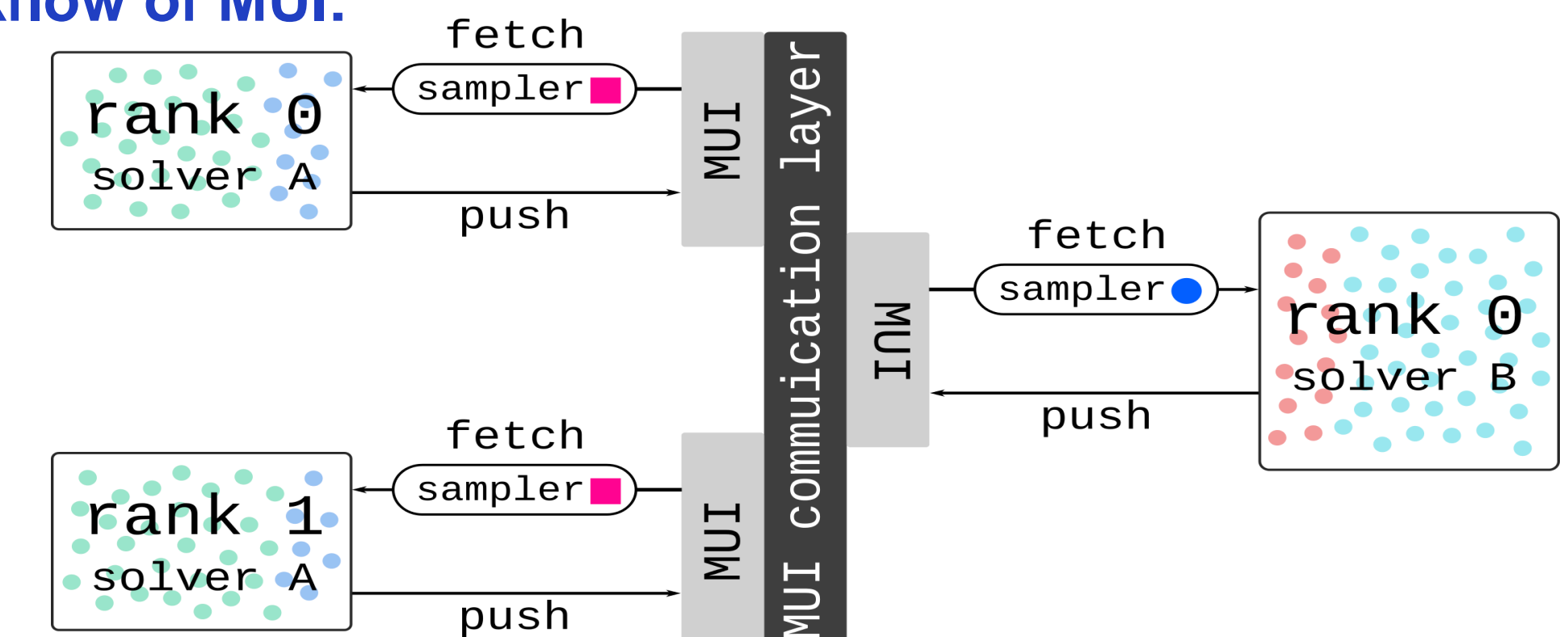
DPD   MD   DPD

Multiscale Framework

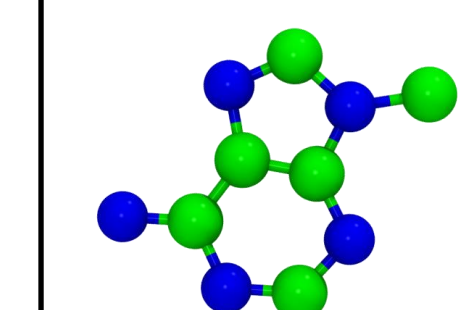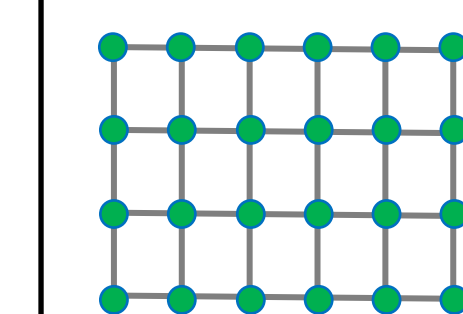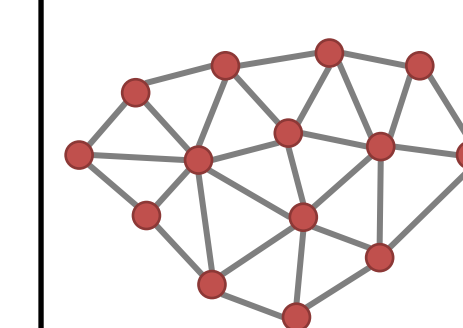### Software: Multiscale Universal Interface (MUI)

- ❖ **A plug-and-play platform** for testing ideas on multiscale coupling.
- ❖ **A communication layer** for multi-solver information exchange.
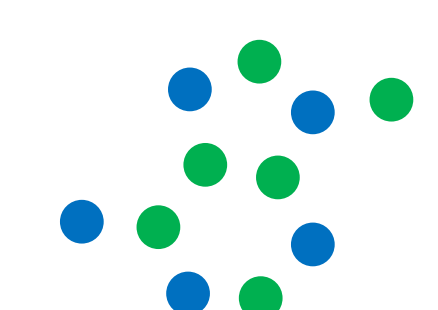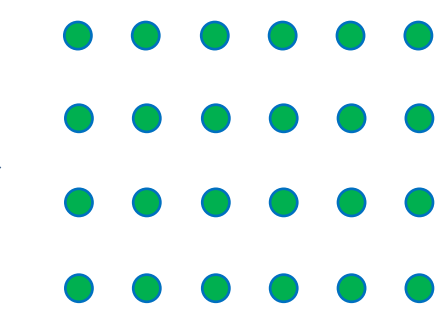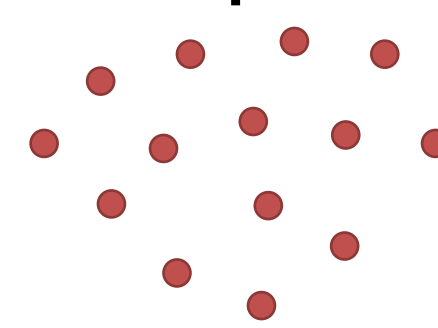- ❖ **A header-only C++ library** that can be dropped into existing codes easily.
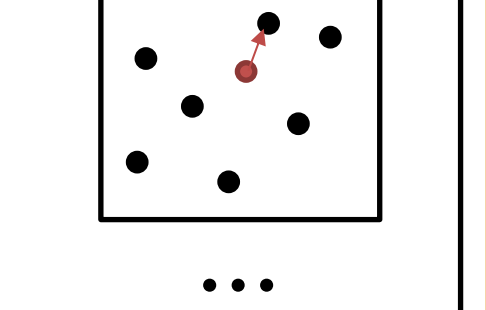
Workflow of MUI:

rank 0 solver A — fetch / sampler / push
rank 1 solver A — fetch / sampler / push
MUI communication layer
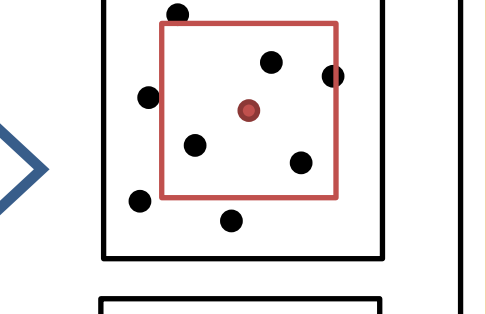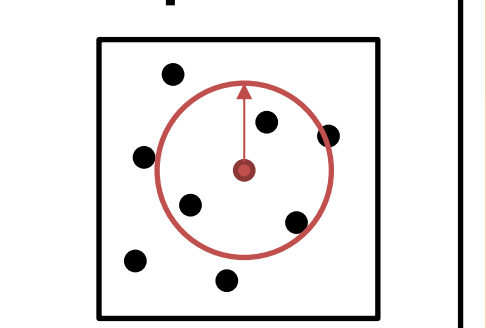rank 0 solver B — fetch / sampler / push

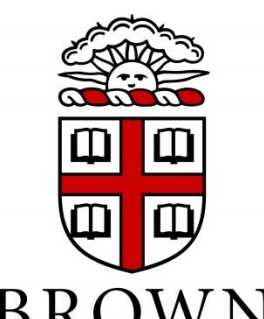Data with structure — abstraction — Data points — sampling — Interpolation

Summary

- New developed mesoscopic models (DPD-alphabet) enable accurate modeling of mesoscopic phenomena involving multiple physics and multiple fields.
- The numerical algorithms of concurrent coupling give the possibility to solve equations at different scales in heterogeneous adjacent multiple domains.
- The toolbox of multiscale universal interface (MUI) provides an efficient framework for handshakes between heterogeneous solvers for modeling multiscale phenomena.
- The integration of these models and numerical algorithms using the MUI framework paves the way for investigation of important multiscale modeling problems related to mesoscopic transport processes in complex materials.

References:
- M. Deng, Z. Li, O. Borodin and G. Karniadakis. J. Chem. Phys., 2016, **145**: 144109.
- Z. Li, A. Yazdani, A. Tartakovsky and G.E. Karniadakis. J. Chem. Phys., 2015, **143**: 014101.
- Y. Tang, S. Kudo, X. Bian, Z. Li and G. Karniadakis. J. Comput. Phys., 2015, **297**: 13-31.
- X. Bian, Z. Li and G. Karniadakis. J. Comput. Phys., 2015, **297**:132-155.

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