PME5429 – MÉTODOS NUMÉRICOS PARA ESCOAMENTOS EM NANO E MICROESCALAS

MD + CONTINUUM – AULA 01

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OUTLINE

- PRESENTATION AND CLASSES WORFLOW
- INTRODUCTION AND MOTIVATION TO MICRO- AND MACRO- MODELLING
  - WHERE/WHEN/HOW IS IT IMPORTANT?
- BASE GROUNDS FOR DISCUSSION
- GENERAL ISSUES AND CHALLENGES IN COUPLING MULTIPLE SCALES
- SIMPLE COUPLING
- ADVANCED COUPLIS

BRIEF OVERVIEW ON FOLLOWING LECTURES

Briefly Presenting Myself
Rafael Gioria

- Brief Background
  - 2003 Graduation in Mechanical Eng. Specialty in Aeronautics @ EESC-USP
  - 2010 PhD in Mechanical Eng. @ POLI-USP
    - Incompressible flow stability and transition
    - Spectral Element Method
    - Floquet Theory
  - 2010-2012 Post-Doc @ POLI-USP
    - Finite Element Methods for Fluids and numerical analysis
    - Reduced Order Modelling from fundamental equations (still open and ongoing work)
  - Since 2013, Prof. In Petroleum Eng. Course – Santos – POLI-USP

Classes Workflow

- LECTURES
  - Open for discussions
  - If possible one hands-on FEM using FreeFEM or Fenics with immiscible fluids – simple coupling of scales
- PAPER READING FOR DISCUSSION
  - One short essay on a paper of choice
- FINAL PROJECT
  - Prof. Caetano proposed it in initial lectures

INTRODUCTION AND MOTIVATION

Why coupling two “distant” approaches I

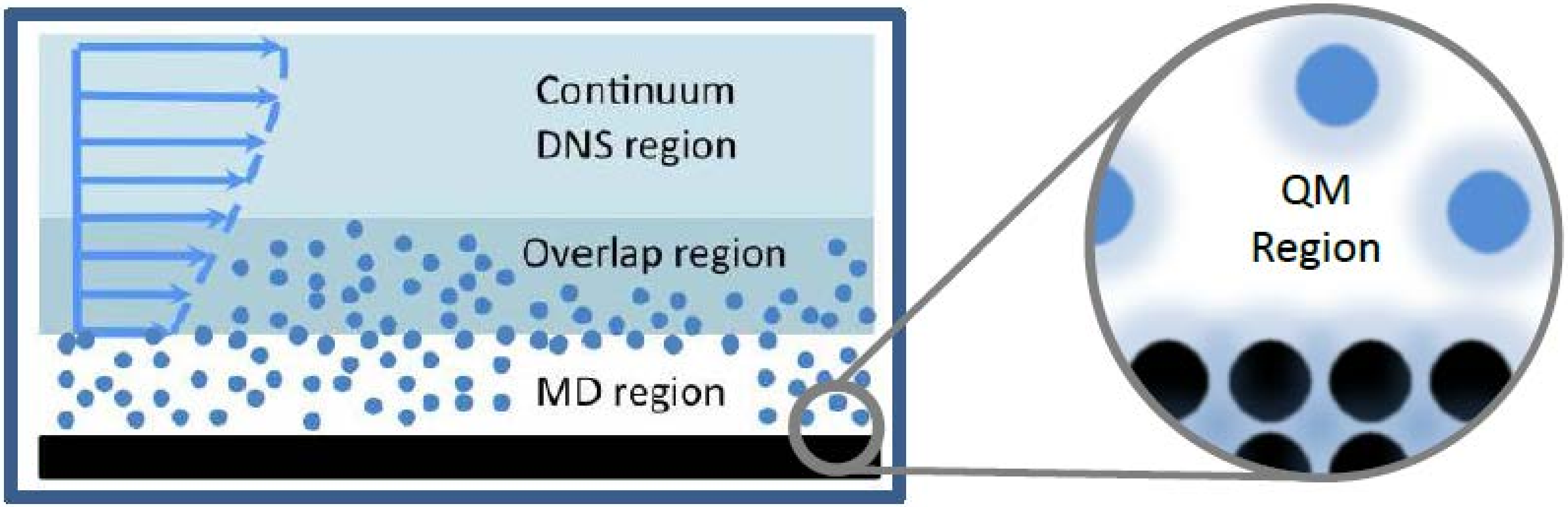
- Both scales may represent the same phenomenon
- Engineering modeling is pointing to issues concerning both scales
- Multiscale models: predicted as a scientific milestone in near future by the 2020 Science Group. [Nature (2006)]
- Engineering problems need sub-continuum modelling (including some in RCGI)
  - Complex fluids near interfaces: microfluidics, slip of liquid flow past surfaces, roughness.
  - Fluid-fluid or soft interfaces (membranes)
  - Phase changing and reacting flows
  - Wetting phenomena: microscopic treatment of the wetting front
  - Constant chemical potential simulations for confined systems: osmosis driven flows through membranes, thin films, water in clays, emulsions

Why coupling two "distant" approaches II

- Cons of each scale (Smith, 2014)
  - Molecular dynamics is still prohibitively expensive for an engineering problem
  - Continuum modeling (CFD) needs closure relations (diffusion and slip for example)
- Hence, why not taking best of both worlds?
  - Multi-scale coupling overcomes these limitations
    - by linking to cheaper method (link MD to CFD)
    - Closure relations are needed (enriching CFD with MD, interfaces for example)
- Coupling MD and CFD is recent
  - O'Connell & Thompson 1995, Flekkøy et al 2000, Nie, Chen, E & Robbins 2004, Delgado-Buscalioni & Coveney, 2004

Multiphysics and multiscale model

- Objectives
  - Multiphysics and multiscale approach of engineering problem ensuring the dynamics agree in both scales in a physically meaningful manner
- Example: boundary layer with fluid-solid interface

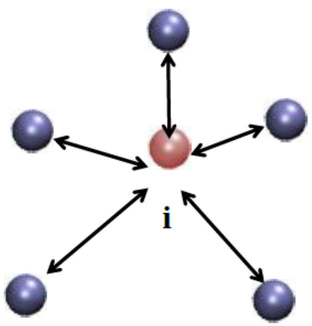


Source: Smith (2014) DNS – Direct Numerical Simulations; MD – Molecular Dynamics; QM – Quantum Mechanics

COMMON GROUNDS FOR DISCUSSION

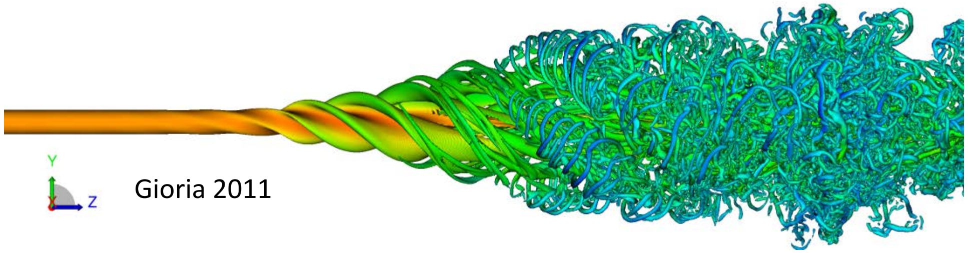
Common Grounds: MD x Continuum Mechanics Approaches

- MD
  - Positions of particles evolve continuously in time: position and velocity from acceleration
  - Acceleration by Newton's Law
  - Particle-wise force interactions



Source: Smith (2014)

- CFD
  - Continuum everywhere in space
  - Mass balance (and species)
    $$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$
  - Momentum Balance
    $$\frac{\partial}{\partial t}\rho \boldsymbol{u} + \boldsymbol{\nabla} \cdot \rho \boldsymbol{u}\boldsymbol{u} = \boldsymbol{\nabla} \cdot \boldsymbol{\Pi}$$
  - Energy Conservation
    $$\frac{\partial}{\partial t}\rho \mathcal{E} = -\boldsymbol{\nabla} \cdot [\rho \mathcal{E} \boldsymbol{u} + \boldsymbol{\Pi} \cdot \boldsymbol{u} + \boldsymbol{q}]$$



Gioria 2011

MAIN ISSUES AND CHALLENGES IN MULTISCALE MODELLING

Issues and Challenges I

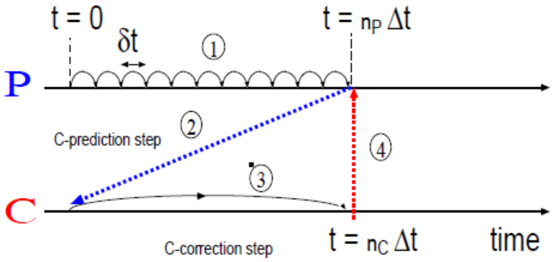
Source: Smith (2014)

- From Molecular Dynamics Point-of-View
  - MD is planned for Thermodynamic problem: steady state and periodic boundaries have clear solutions and well definade averages for ensembles
  - Non-equilibrium: non-trivial averages, thermodynamic noise
  - Non simple geometry: forces modelled and heat unbalance
- From CFD point-of-view
  - Time scale and numerical stability
  - Dealing with discontinuous fields
  - Noise from MD

Issues and Challenges II

Source: Smith (2014)

- General and coupling points of view
  - Time scales

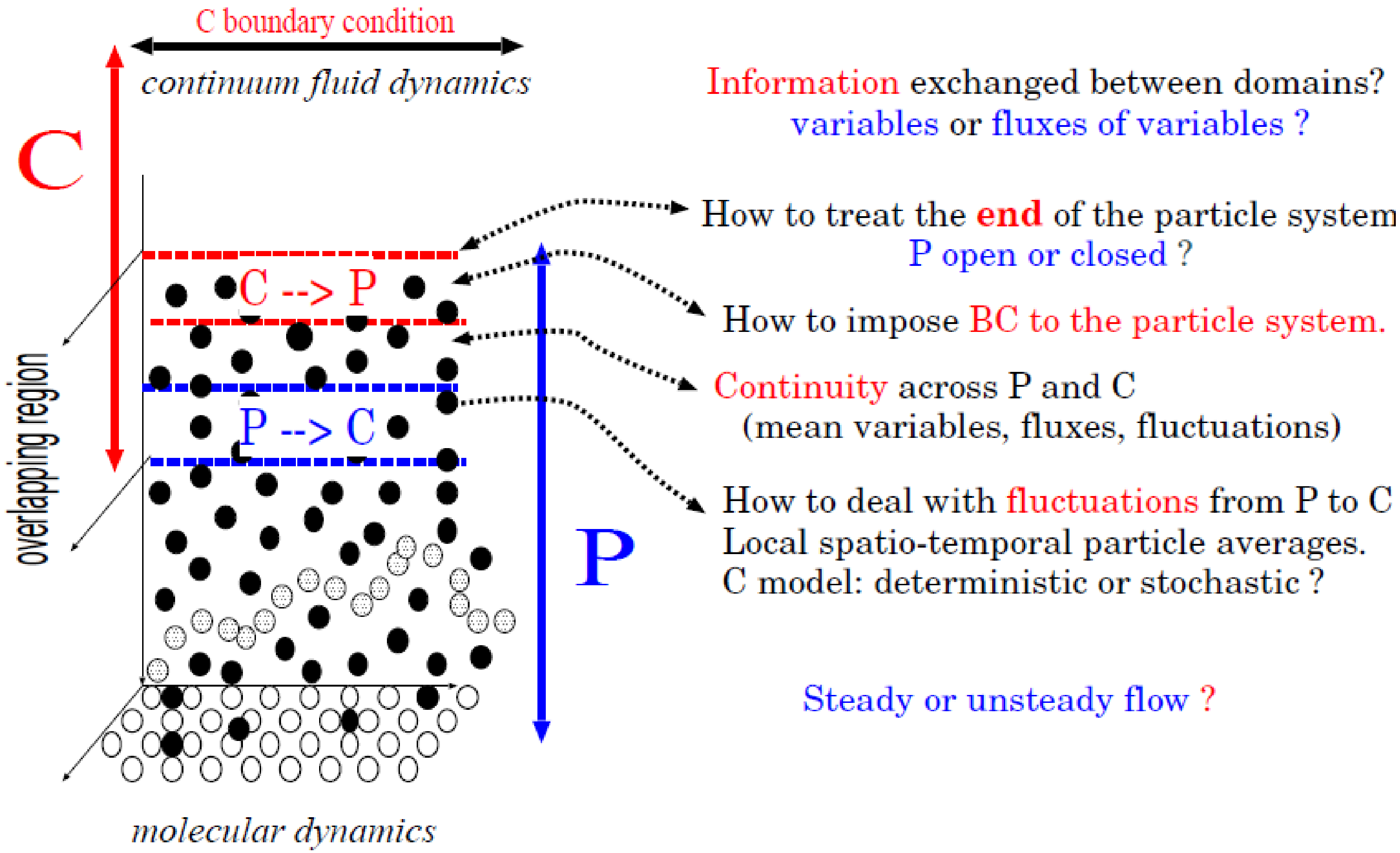


Source: Delgado-Buscalioni (website)

  - Noise from MD to CFD
  - Communicating/transferring different kind of data used in each scale, specially from CFD to MD
    - Statistical ensemble to macroscopic is defined, but the other way round has non-unique solutions
  - **VALIDATION?**

Issues and Challenges Coupling

Source: Delgado-Buscalioni (website)



HOW TO: MD AND CONTINUUM

How to couple MD and Continuum
Simple coupling

- Weak one-way coupling
  - MD for closing relations in Continuum description
    - Transport Properties: Viscosity, Diffusion (Interesting for Maxwell-Steffan diffusion, or non-binary diffusion)
    - Rheology
    - Simple Slip Condition (non-dynamic slip length)
    - Interfacial tension
    - Equilibrium/static wettability – contact angle
  - MD for estimating in thermodynamic conditions not attainable in laboratory

Some works on Hybrid Atomistic Continuum modelling (HAC) – strong coupling

Source: Delgado-Buscalioni (website)

SOLIDS	QM-MD MD-FD QM-MD-FD	PRL **93**, 175503 (2004) PRL **87**(8),086104 (2001) Abraham
GASES	DSMC-CFD MC-CFD	AMAR [A. Garcia] Depostion (crystal growth from vapour phase) PRB, **64** 035401.(2001)
MEMBRANES	MD-MPM	Ayton et al. J.CHem.Phys **122**, 244716(2005)
LIQUIDS	Domain decomposition: MD-CFD, MD-FH Eulerian-Lagrangian: MD-LB, MD-FH Velocity-Stress coupling: MD-SMFD, MD-FD Particle-particle: MD-SRD; new method: JChemPhys, **123** 224106 (2005)	

Acronyms

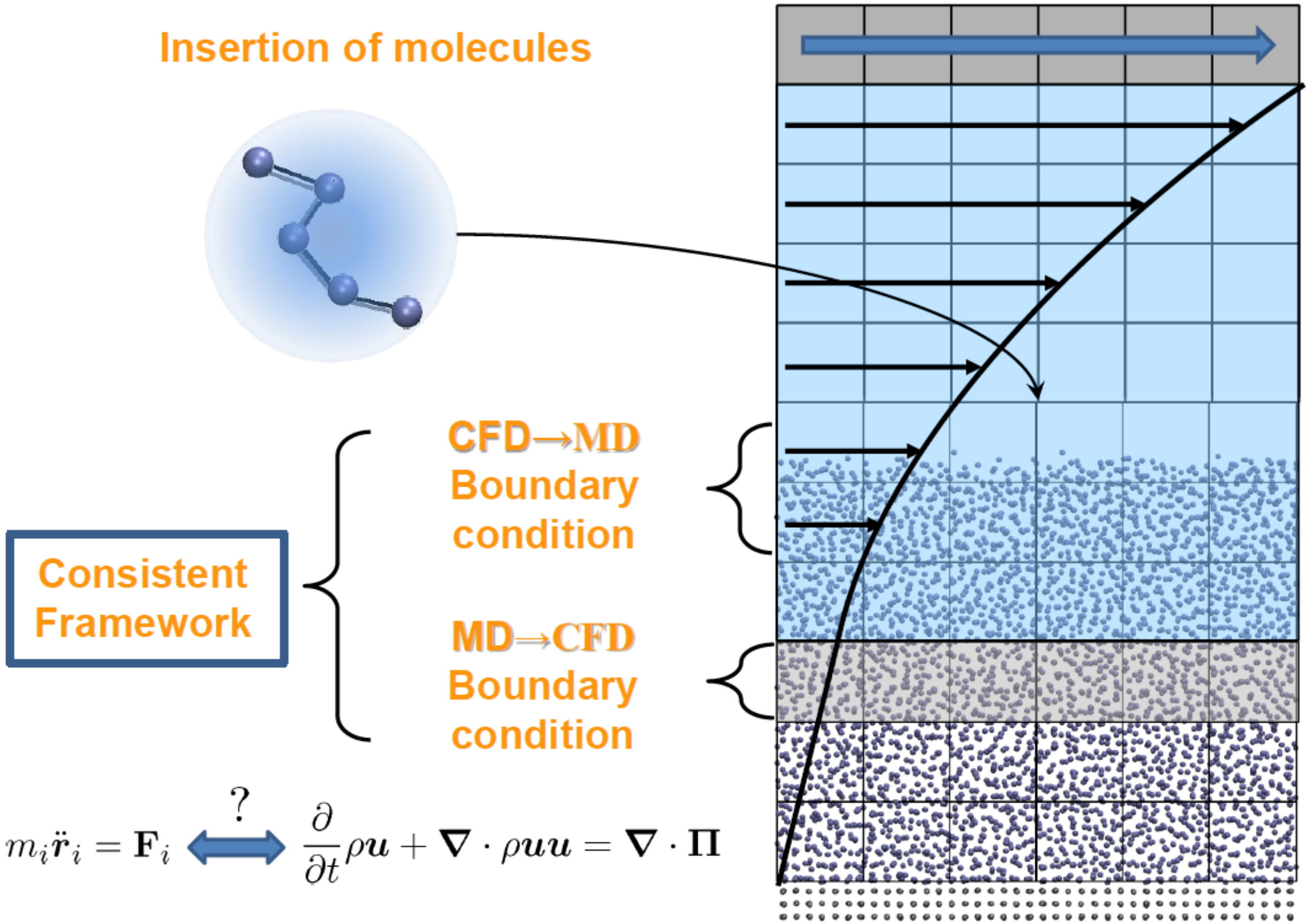
Particle methods	Continuum methods
QM= Quantum mechanics MD= Molecular dynamics MC= Monte Carlo DSMC= Direct simulation Monte Carlo	FD= finite difference CFD=Computational fluid dynamics SMFD=Spectral methods for fluid dynamics LB=Lattice Boltzmann FH=Fluctuating hydrodynamics SRD=Stochastic Rotation Dynamics MPM=Mass point method

Hybrid Atomistic Continuum modelling (HAC) General Challenges

- Key Challenges
  - Determine spatial relationship between MD and Continuum
    - Embedded
    - Different Regions with or without overlap
  - Termination of MD simulation domain
    - Molecules escape the region – uses buffer region, or forces
  - Averaging MD to communicate info to CFD
    - Turn this into B.C., Averaging and noise issues
  - Constraint to MD region from CFD
    - Non-unique, comply to mass flux and Energy conservation

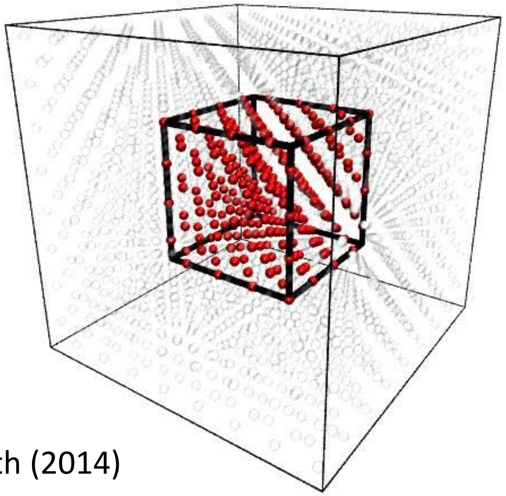
Hybrid Atomistic Continuum modelling (HAC) Fundamentals I

Source: Smith (2014)



Hybrid Atomistic Continuum modelling (HAC) Fundamentals II

- Smith et al (2012) argue that there must be a consistent framework to HAC
  - Based on transport analysis in Irving and Kirkwood (1950)
  - Reynolds transport Theorem (applicable to any conserved quantity)
    - Applied to Molecular scale
    - Applied to Continuum scale
    - Brings up a Control Volume approach



Source: Smith (2014)

Hybrid Atomistic Continuum modelling (HAC) Fundamentals III

Source: Smith (2014)

MD on left

Continuum on right

- Mass Conservation

$$\frac{d}{dt}\sum_{i=1}^{N} m_i\vartheta_i = -\sum_{i=1}^{N} m_i\mathbf{v}_i\cdot d\boldsymbol{S}_i$$

$$\frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho\boldsymbol{u}\cdot d\mathbf{S}$$

- Momentum Balance

$$\frac{d}{dt}\sum_{i=1}^{N} m_i\mathbf{v}_i\vartheta_i = -\sum_{i=1}^{N} m_i\mathbf{v}_i\mathbf{v}_i\cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i,j}^{N}\boldsymbol{f}_{ij}\vartheta_{ij}$$

$$\frac{\partial}{\partial t}\int_V \rho\boldsymbol{u}dV = -\oint_S \rho\boldsymbol{u}\boldsymbol{u}\cdot d\mathbf{S} + \mathbf{F}_{\text{surface}}$$

- Energy Conservation

$$\frac{d}{dt}\sum_{i=1}^{N} e_i\vartheta_i = -\sum_{i=1}^{N} e_i\mathbf{v}_i\cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j}^{N}\frac{\mathbf{p}_i}{m_i}\cdot\boldsymbol{f}_{ij}\vartheta_{ij}$$

$$\frac{\partial}{\partial t}\int_V \rho\mathcal{E}dV = -\oint_S \rho\mathcal{E}\boldsymbol{u}\cdot d\mathbf{S} - \oint_S \mathbf{\Pi}\cdot\boldsymbol{u}\cdot d\mathbf{S} + \mathbf{q}\cdot d\mathbf{S}$$

2:

Hybrid Atomistic Continuum modelling (HAC) Fundamentals IV

- Pressure is the tensor resposible for the forces
  - **Continuum Control Volume equations in terms of the pressure tensor**

Source: Smith (2014)

$$\frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\oint_S \rho \boldsymbol{u}\boldsymbol{u}\cdot d\mathbf{S} \quad + \mathbf{F}_{\text{surface}}$$

$$\mathbf{F}_{\text{surface}} \rightarrow -\frac{\partial}{\partial \boldsymbol{r}}\cdot\int_V \boldsymbol{\Pi} dV$$

$$\mathbf{F}_{\text{surface}} \rightarrow -\oint_S \boldsymbol{\Pi}\cdot d\boldsymbol{S}$$

  - **Molecular Control Volume equations in terms of the pressure tensor**

Volume Average
(Lutsko 1988 & Cormier et al 2001)

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\vartheta_{ij}$$

$$\frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\vartheta_{ij} \rightarrow -\frac{\partial}{\partial \boldsymbol{r}}\cdot \frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\boldsymbol{r}_{ij}\int_0^1 \vartheta_s ds$$

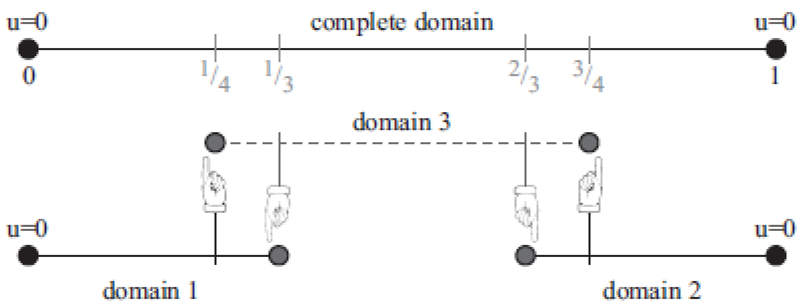
$$\frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\vartheta_{ij} \rightarrow -\frac{1}{4}\sum_{i,j}^{N} \varsigma_{ij}\cdot d\mathbf{S}_{ij}$$

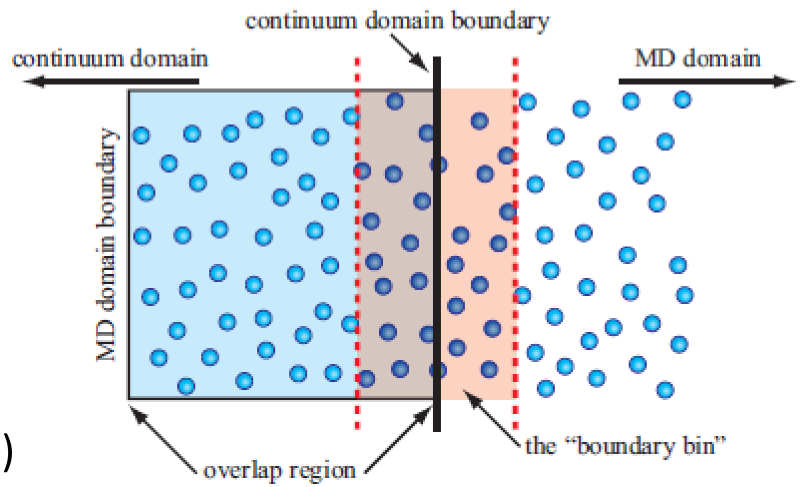
Hybrid Atomistic Continuum modelling (HAC) Approaches

- Note that there are two ways to write the pressure effect
  - Through control surface interaction integral
    - Flux Coupling
      - Flekkøy et al (2000)
      - Delgado-Buscalioni & Coveney, (2004)
  - Through control volume integral
    - State Variables Coupling:
      - O'Connell & Thompson (1995)
      - Nie, Chen, E & Robbins (2004)

Hybrid Atomistic Continuum modelling (HAC) Approaches

- Some techniques for coupling B.C. between MD and CFD
  - Overlapping – Schwarz overlap turn single BVP into several composed BVP





Source: Markesteijn (2011)

  - Interface (Flux based approach)

NEXT LECTURE

Readings

- General review on HAC
    - WINJESINGHE, HADJICONSTANTINOU, “*Discussion of Hybrid Atomistic-Continuum Methods for Multiscale Hydrodynamics*”, **International Journal for Multiscale Computational Engineering,** v.2(2), 2004.
- HAC for fluid and wall interaction
    - Slip Condition
    - Some new approach:
        - SMITH, HEYES, DINI, ZAKI, “*Control-volume representation of molecular dynamics*”, **Phys. Rev. E**, v.85, 2012.
- Contact line of 2 fluid interface
    - HADJICONSTANTINOU, “*Hybrid Atomistic–Continuum Formulations and the Moving Contact-Line Problem*”, **International Journal for Multiscale Computational Engineering,** v.2(2), 2004

SOME REFERENCES

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THANK YOU