Accelerating a multiscale continuum-particle fluid dynamics model with on-the-fly machine learning

(Part 1)

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Marcos Rojas-Cárdenas, Irina Graur, Pierre Perrier, J. Gilbert Méolans
and
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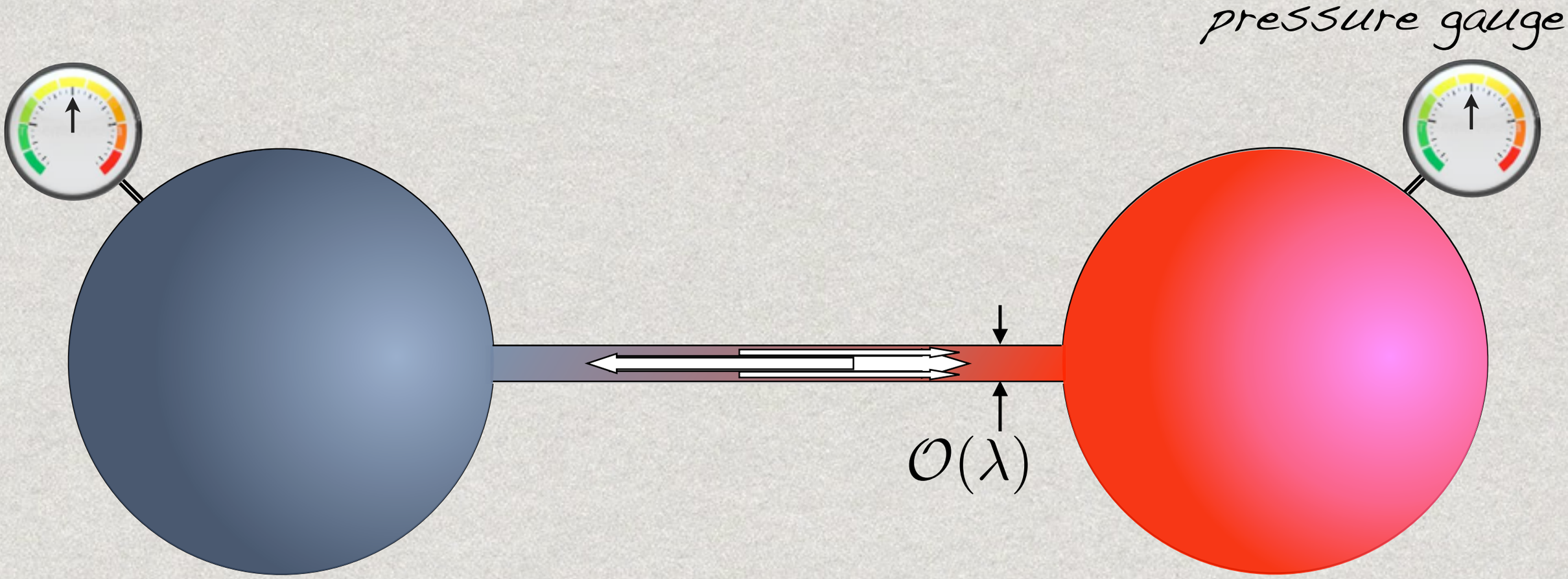
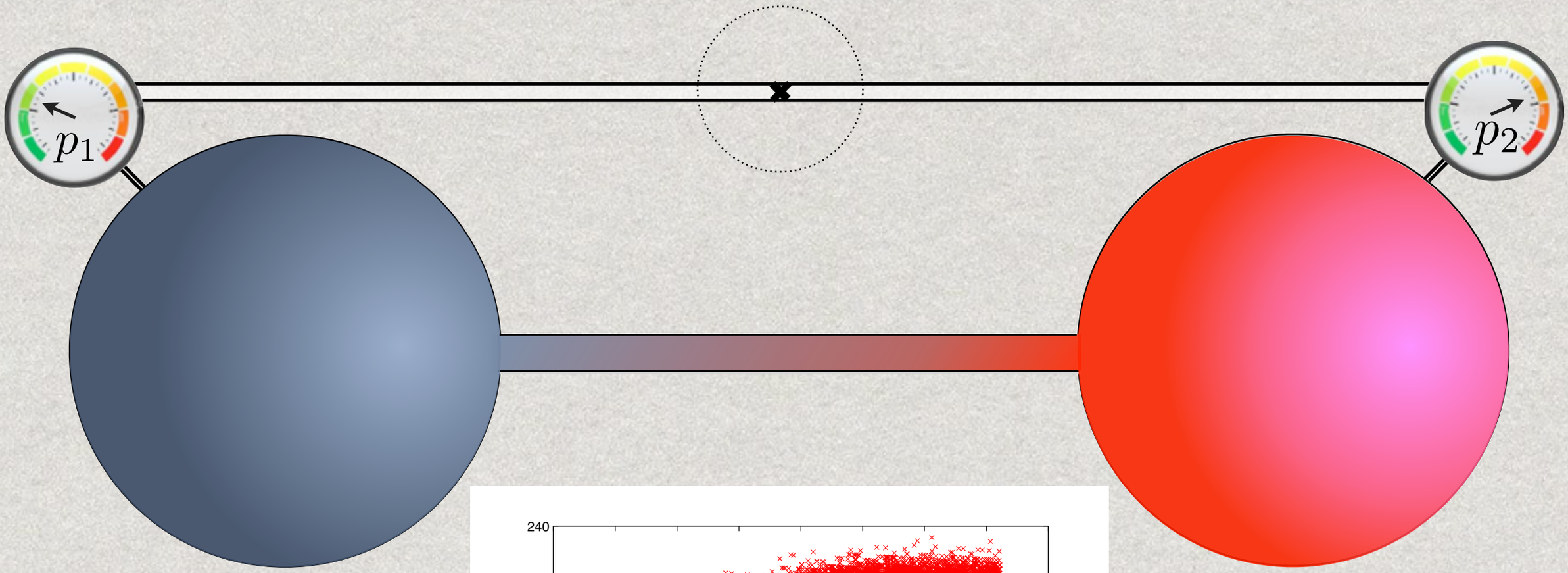
The Knudsen Pump

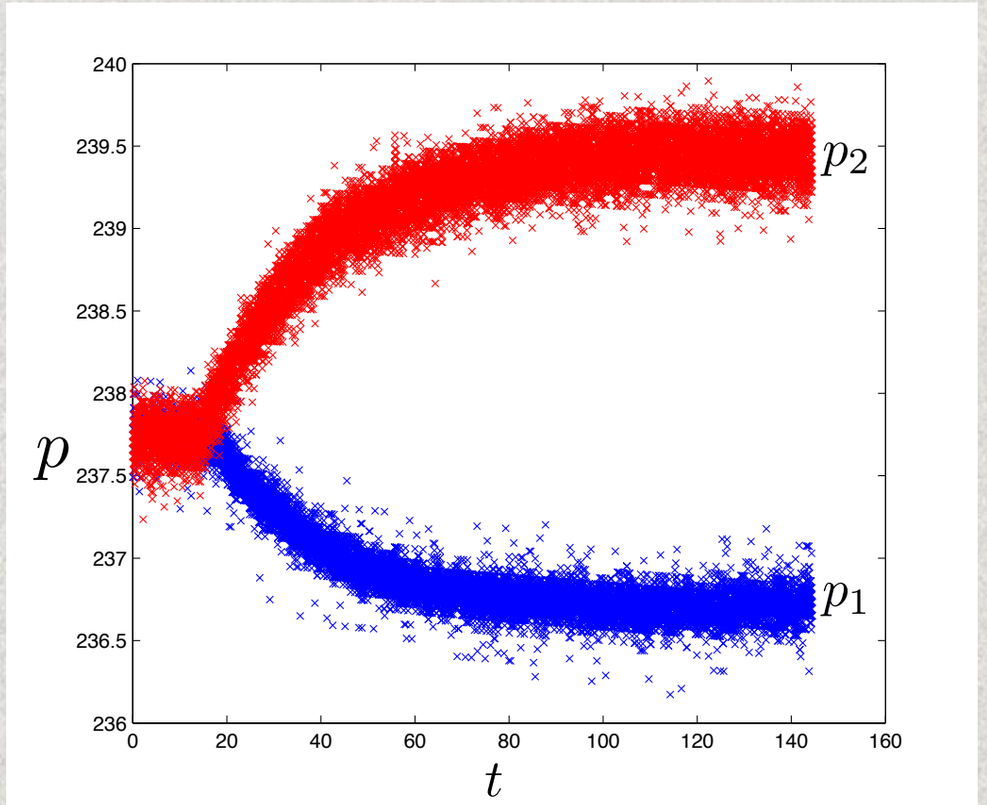


- Rarefied flow in channel driven by *thermal transpiration*
- What is the transient response?

M. Rojas-Cárdenas, I. Graur, P. Perrier, J. G. Méolans, Time-dependent experimental analysis of a thermal transpiration rarefied gas flow, Physics of Fluids 25 (2013).

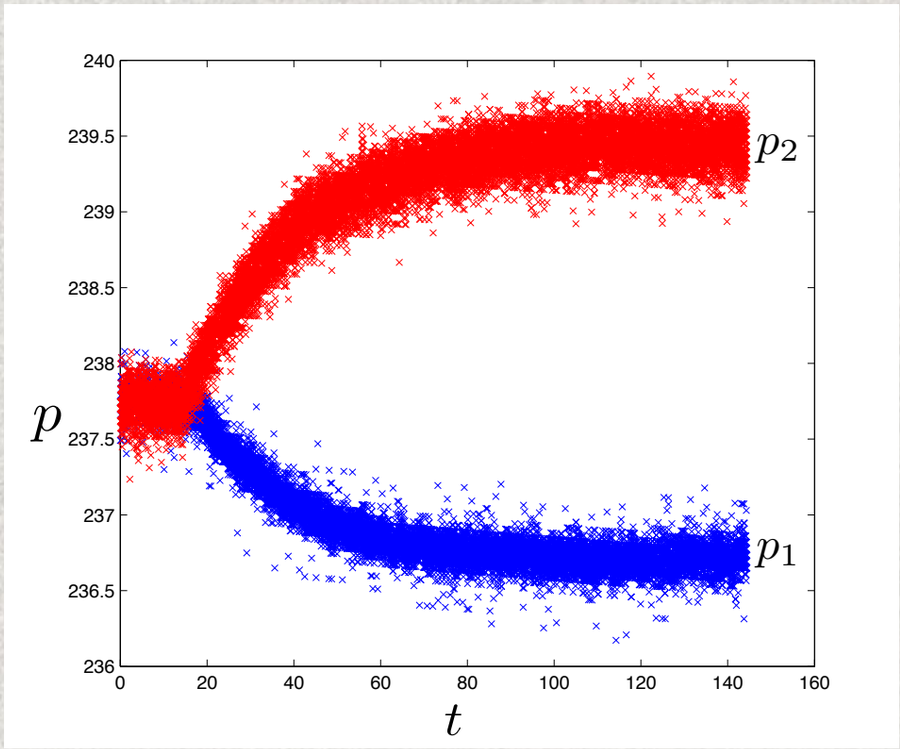
The Knudsen Pump





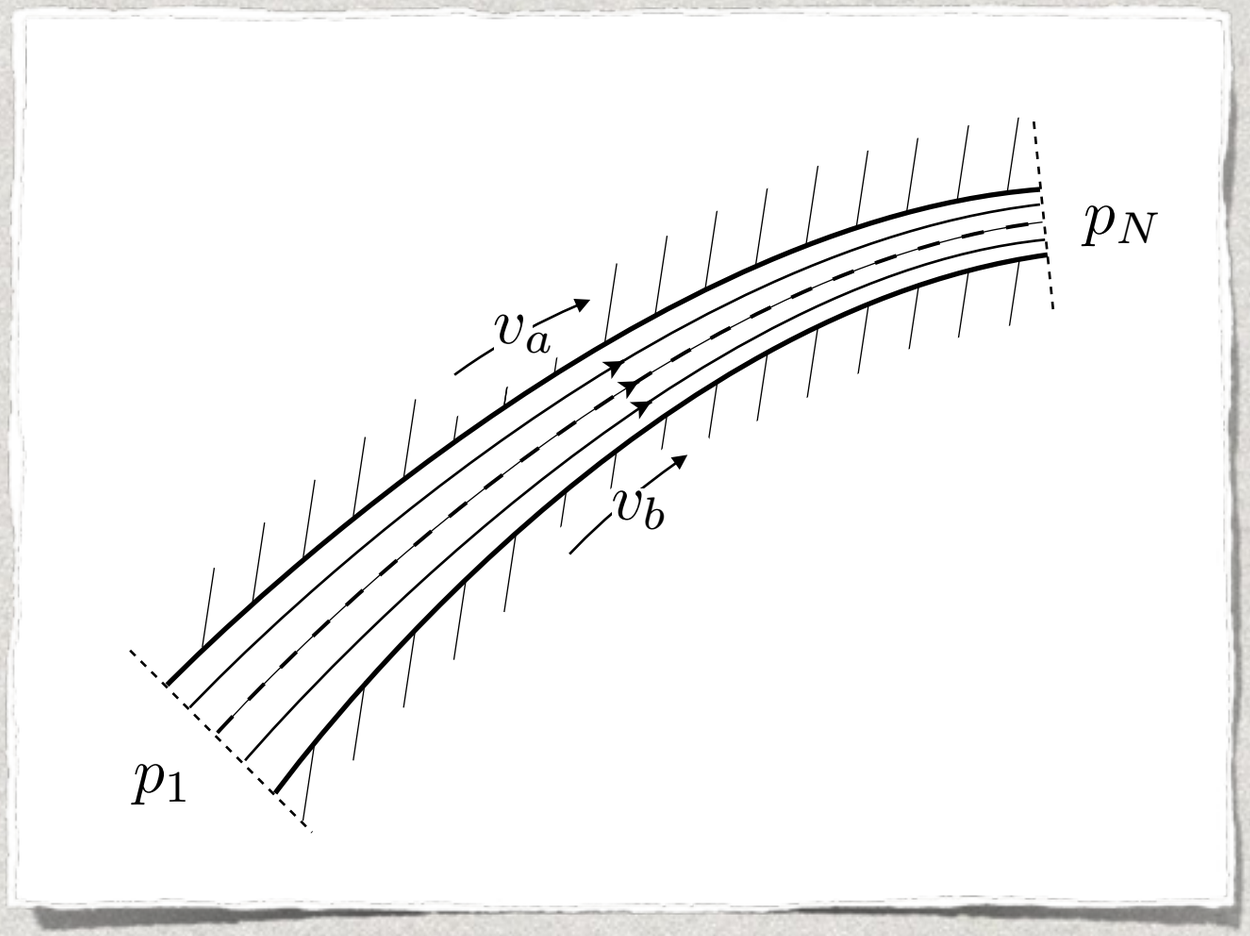
The Modelling Challenge

- Beyond physical model of conventional CFD …
- but a full DSMC (molecular-based) solution is too expensive
- A multiscale problem: high Kn number *and* high aspect ratio



Internal-flow Multiscale Method (IMM)

a variant of HMM (Ren & E (2005) *J. Comp. Phys.* **204,** 1-26)



Borg, Lockerby & Reese (2015) J. Fluid. Mech. 768: 388-414
Patronis & Lockerby (2014) J. Comp. Phys. 270: 532-543

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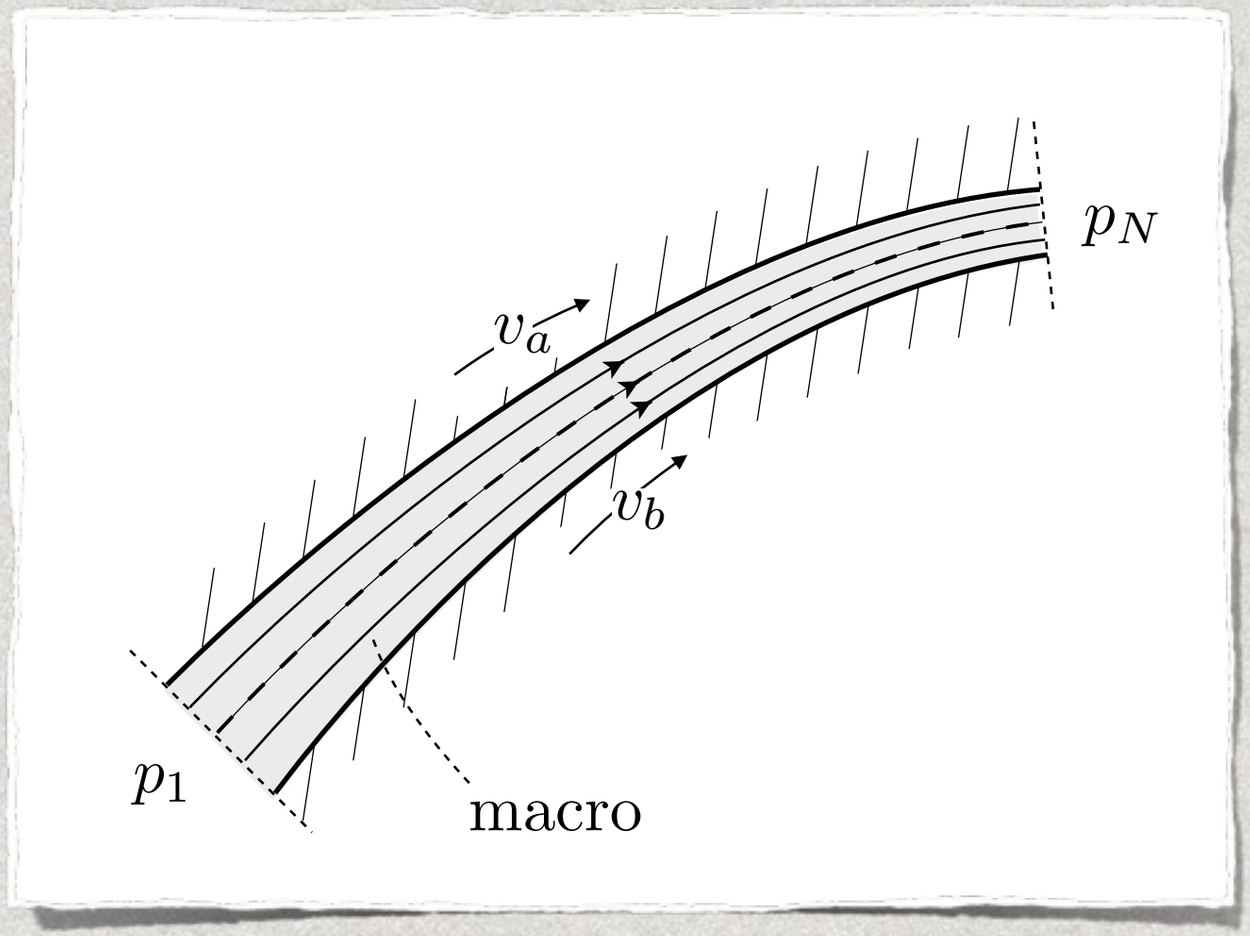

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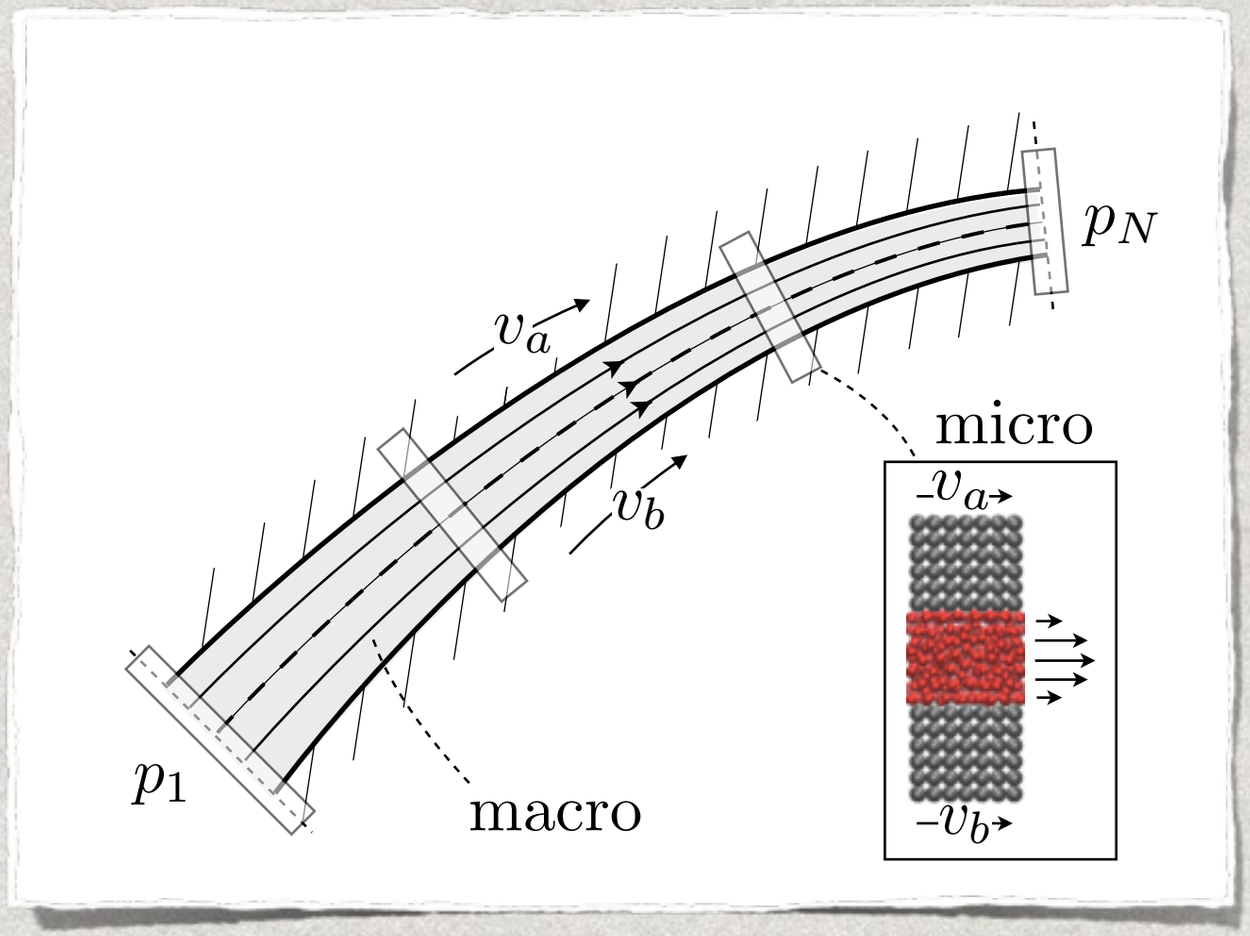

- Scale separation allows *local parallel-flow* assumption
- How are the macro and micro descriptions coupled?

Borg, Lockerby & Reese (2015) J. Fluid. Mech. 768: 388-414
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The Macro Model

- The continuity equation:

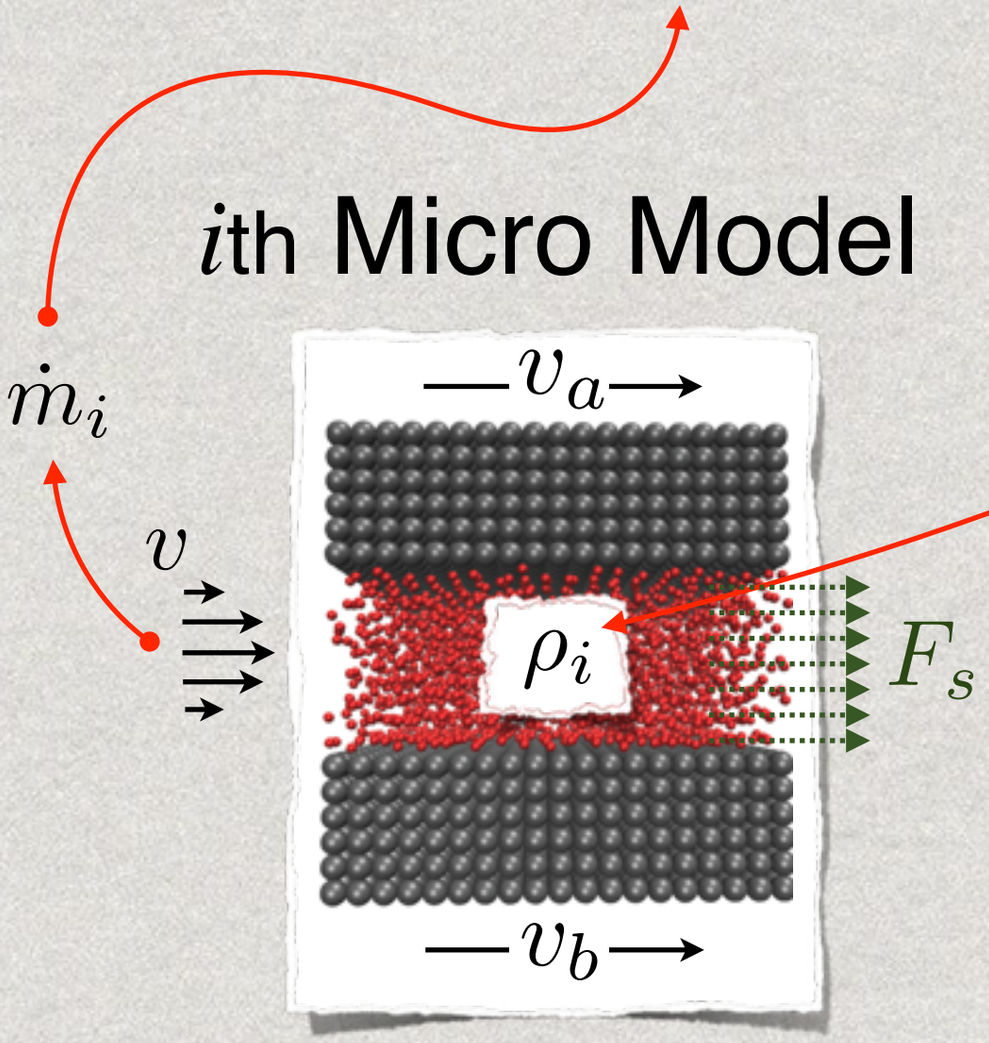
$$\frac{\partial \rho_i}{\partial t} + \frac{1}{A_i}\frac{\partial \dot{m}}{\partial s}\bigg|_i = 0$$

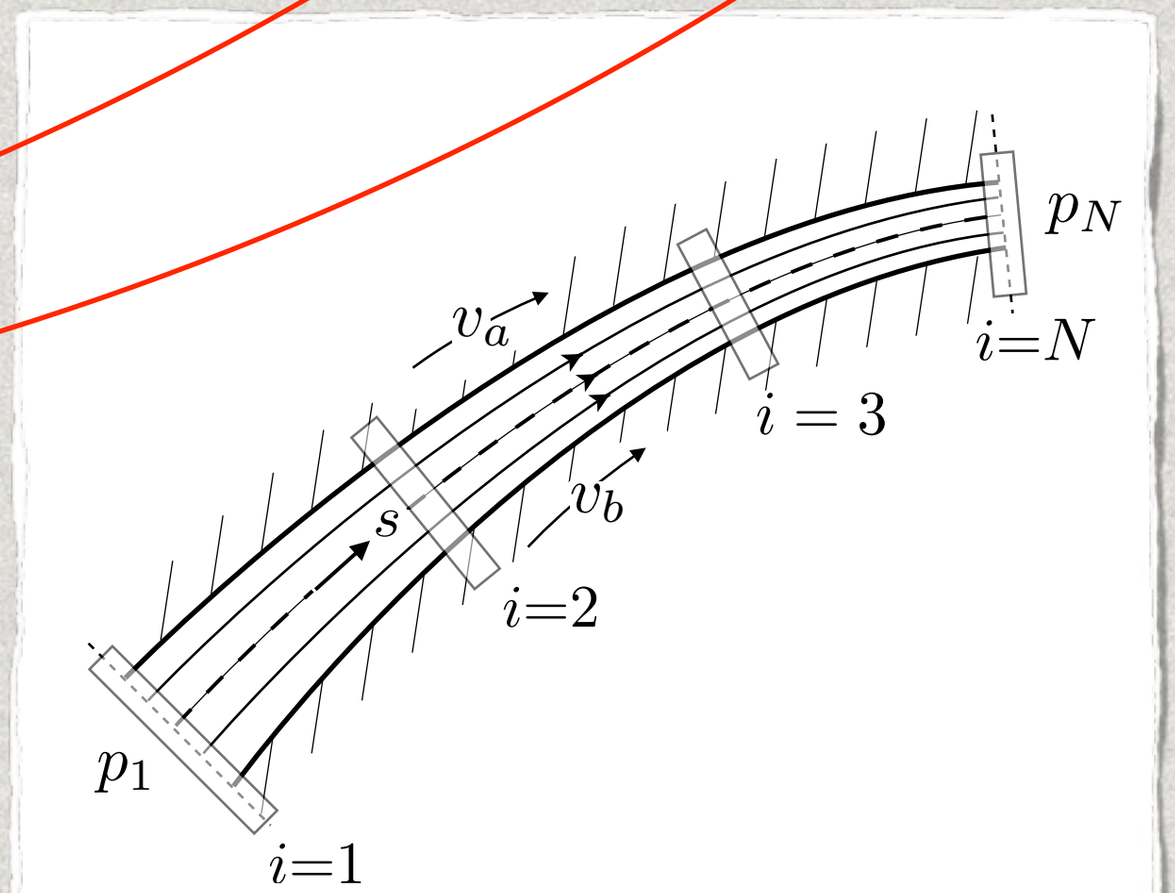
- An equation of state:

$$p_i = f(\rho_i)$$

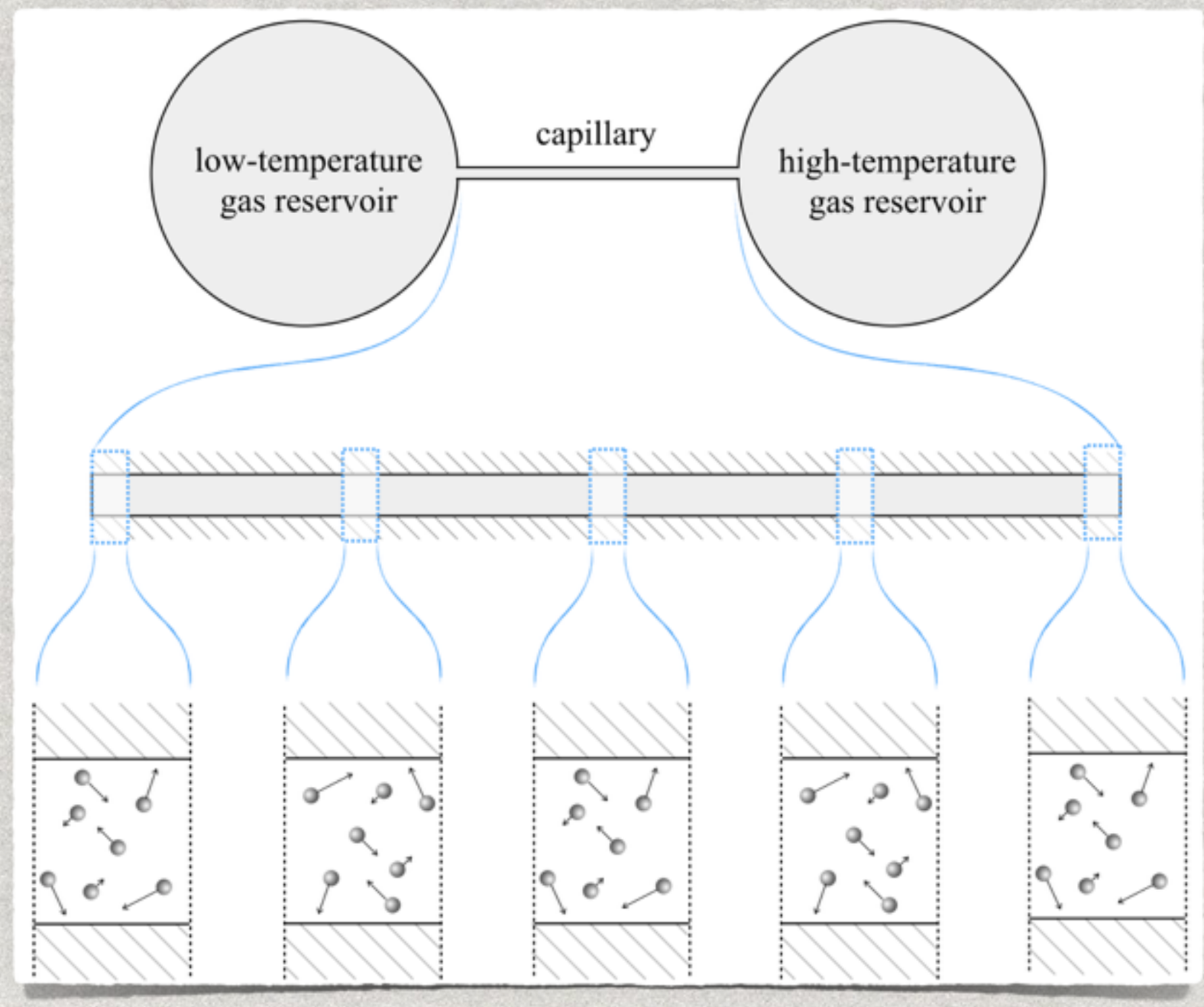
- Outputs: ρ_i and $\dfrac{\mathrm{d}p}{\mathrm{d}s}\bigg|_i$

ith Micro Model



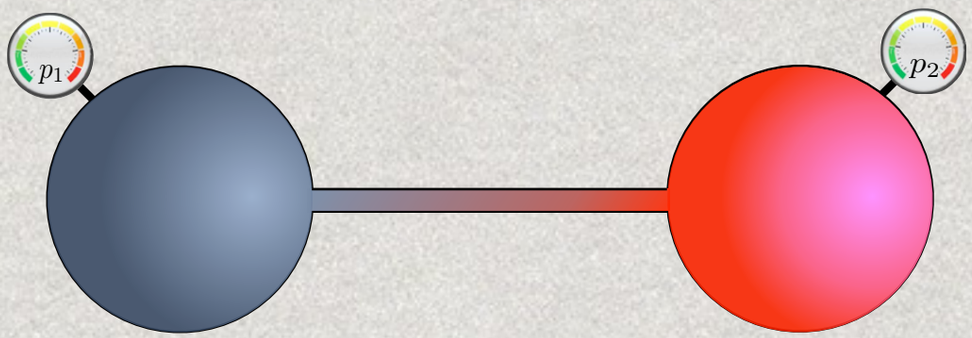


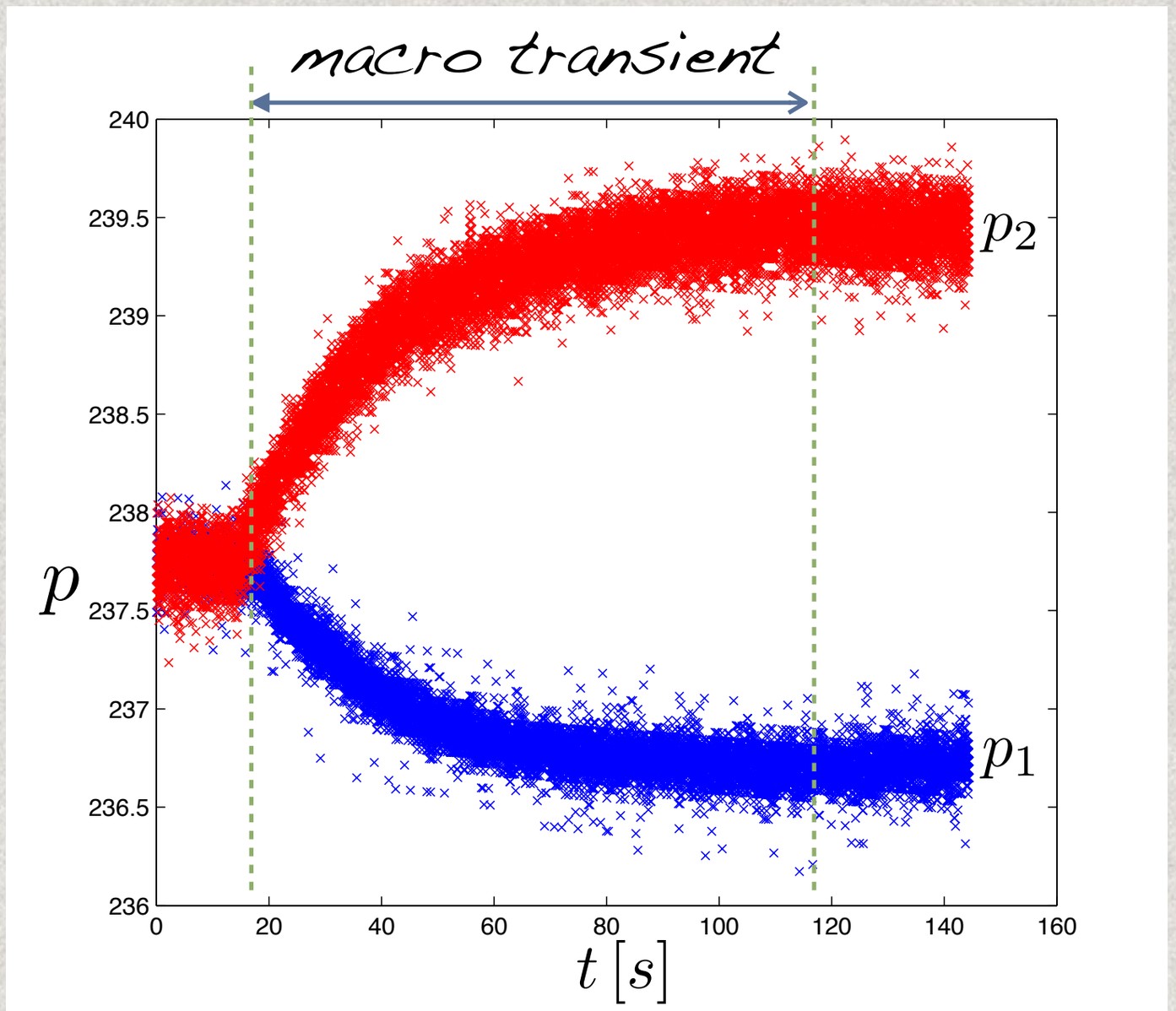
Application to the Knudsen pump



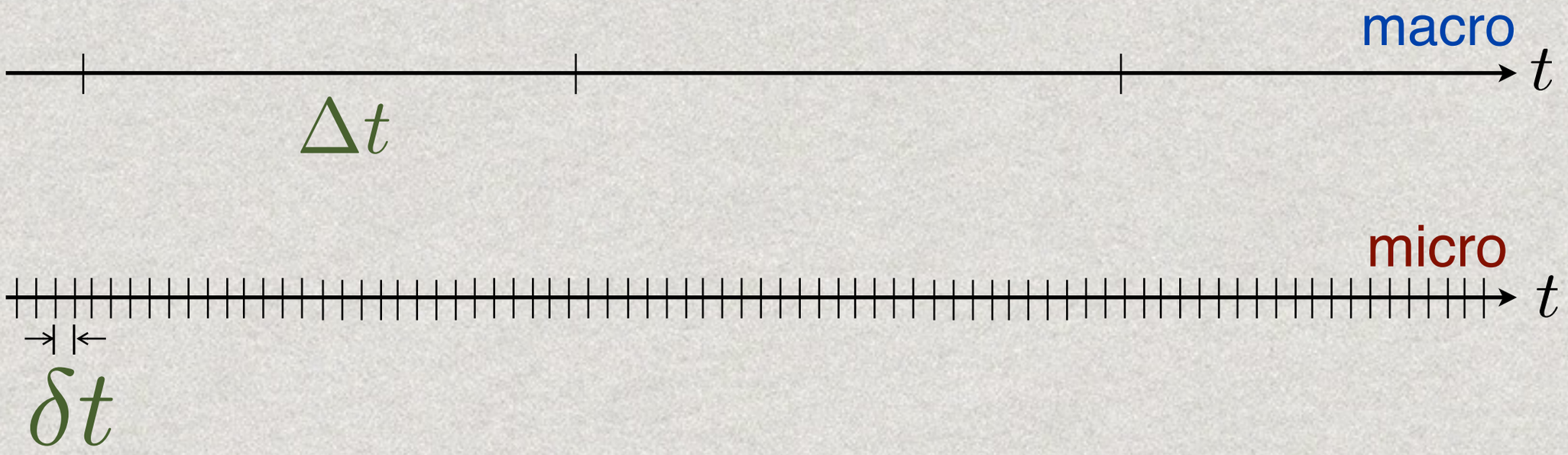
The modelling challenge (Part II)

- mean molecular collision period: $\approx 100\,\mathrm{ns}$
- macro transient: $\approx 100\,\mathrm{s}$





Multiscaling in time



E, Ren, Vanden-Eijnden (2009) J. Comp. Phys. 228, 5437-5453
Lockerby, Duque-Daza, Borg, Reese (2013) J. Comp. Phys. 237, 344-365

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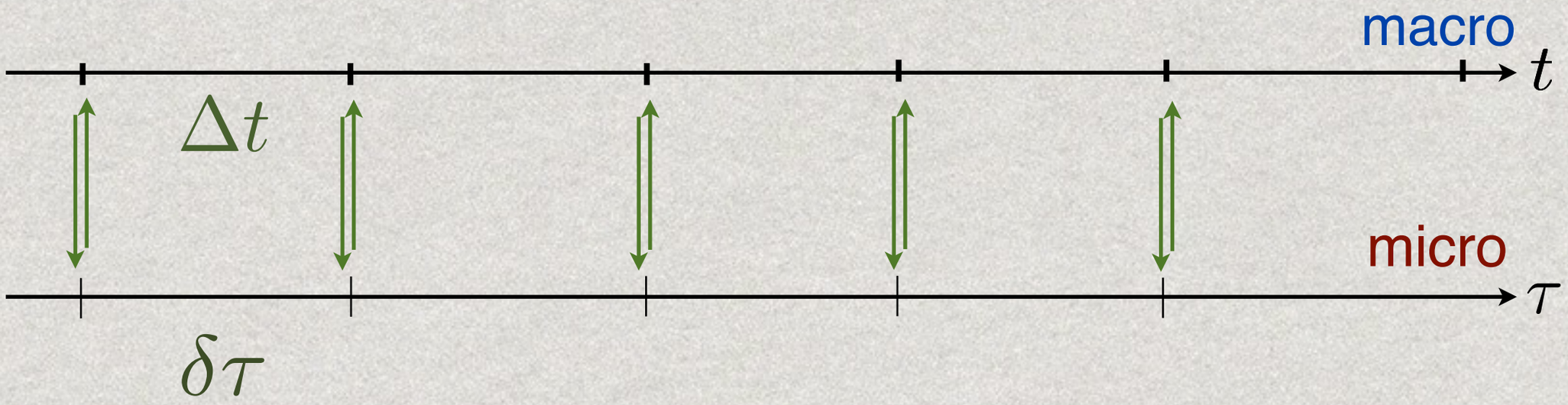

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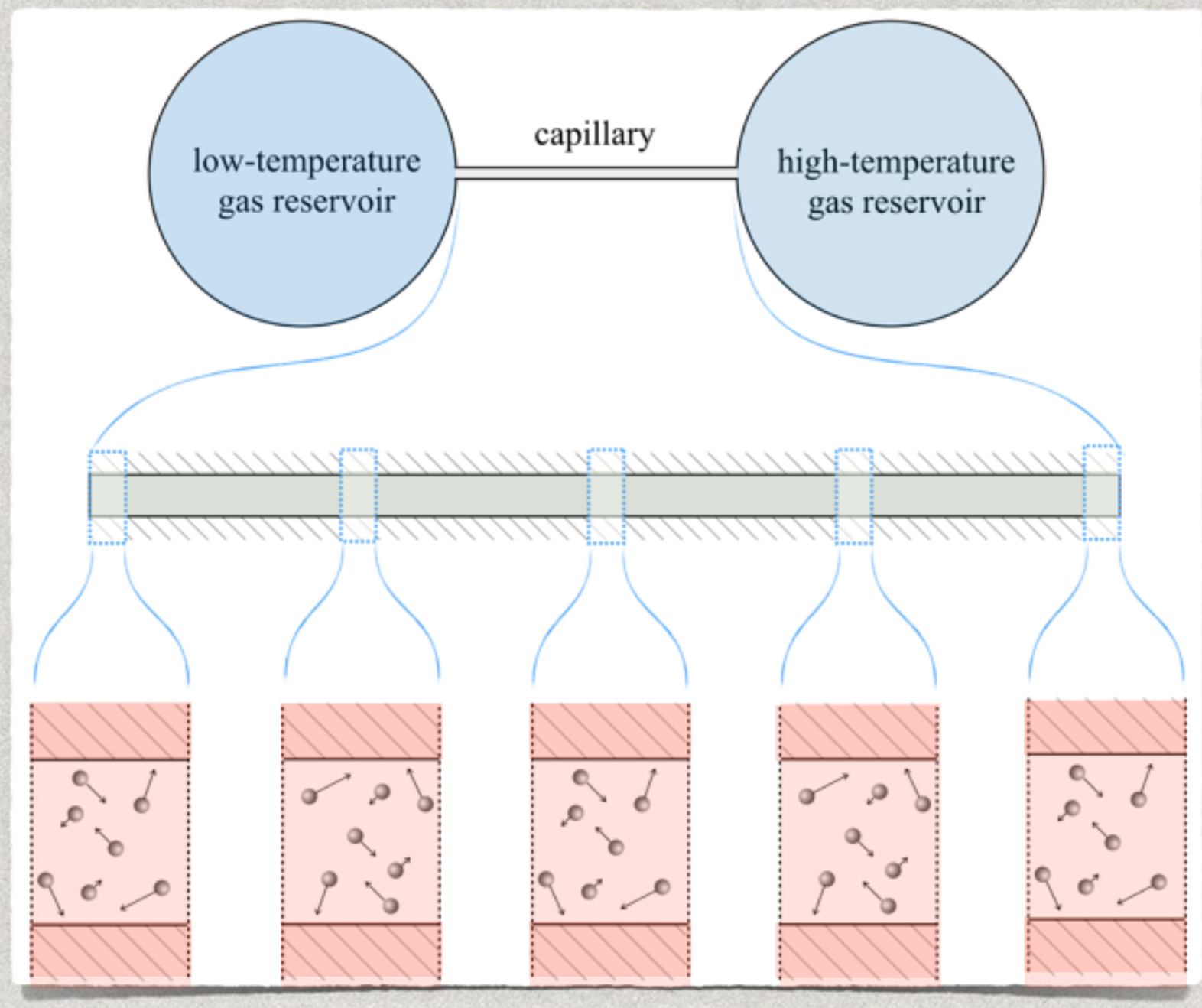
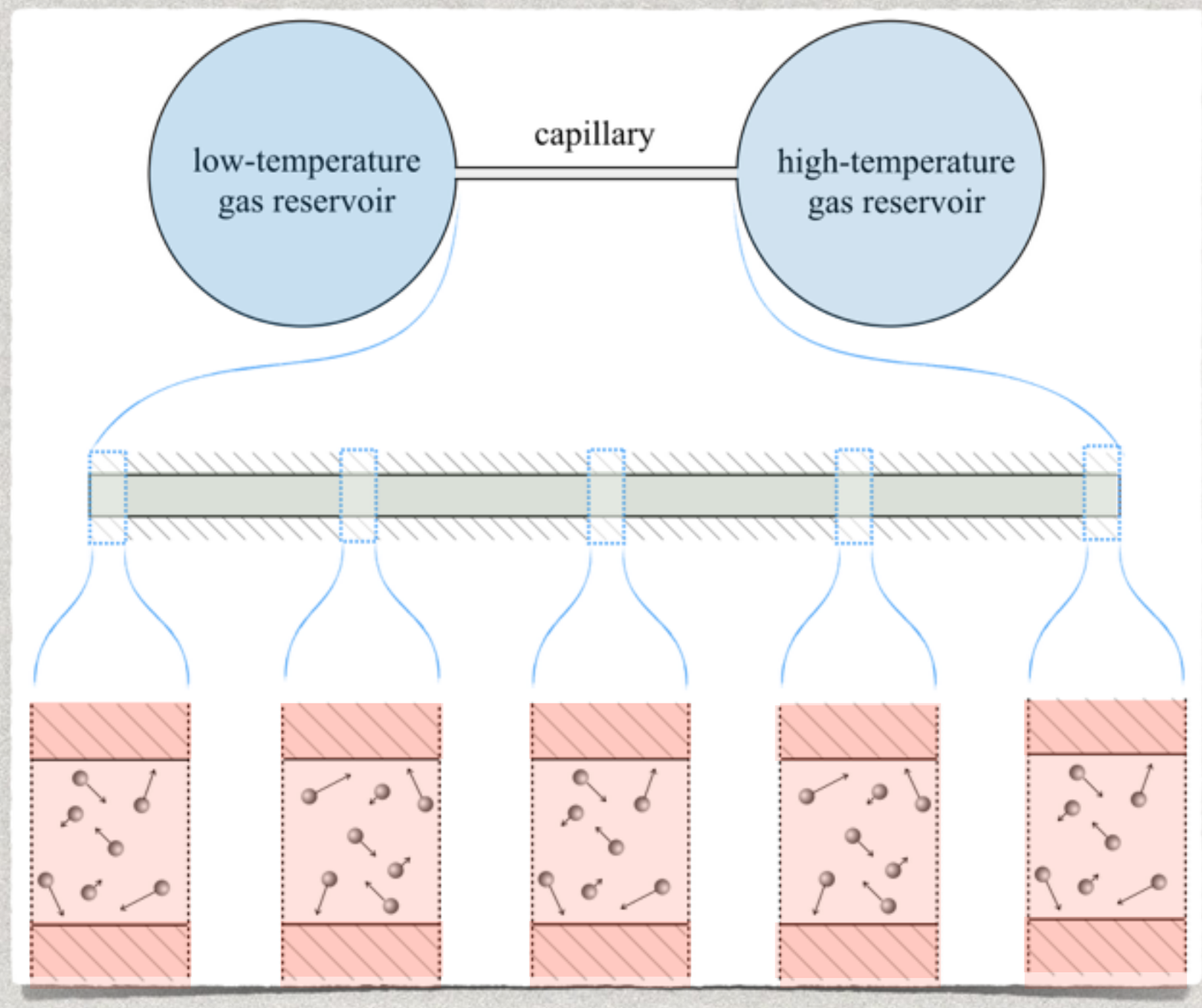


Mass conservation

Continuity Equation

LVDSMC

Application to the Knudsen pump

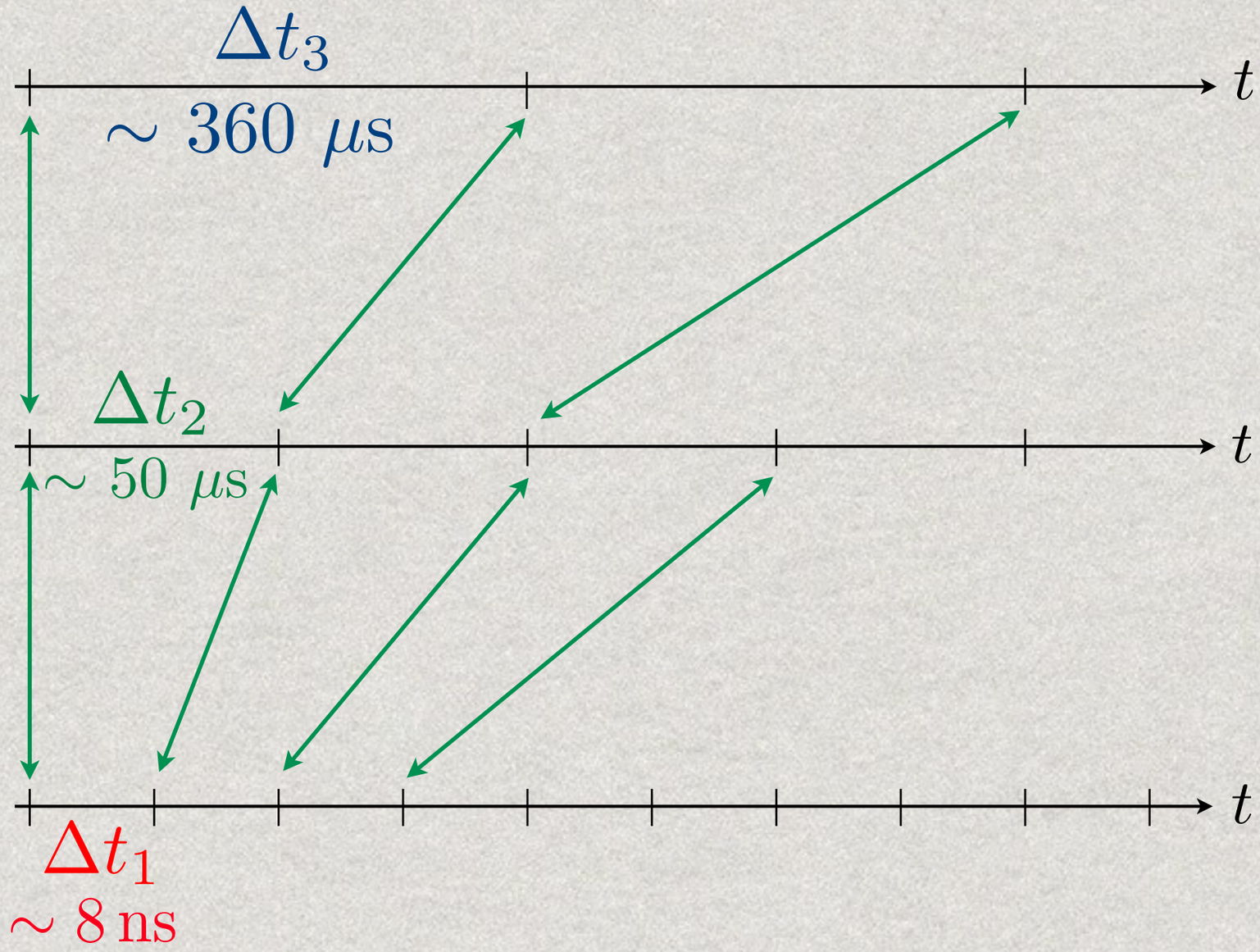


$T_{\mathrm{macro}}=100\ \mathrm{s}$

$T_{\mathrm{meso}}=5\ \mathrm{ms}$

$T_{\mathrm{micro}}=10\ \mu\mathrm{s}$

Multiple Time Scales



Mass conservation

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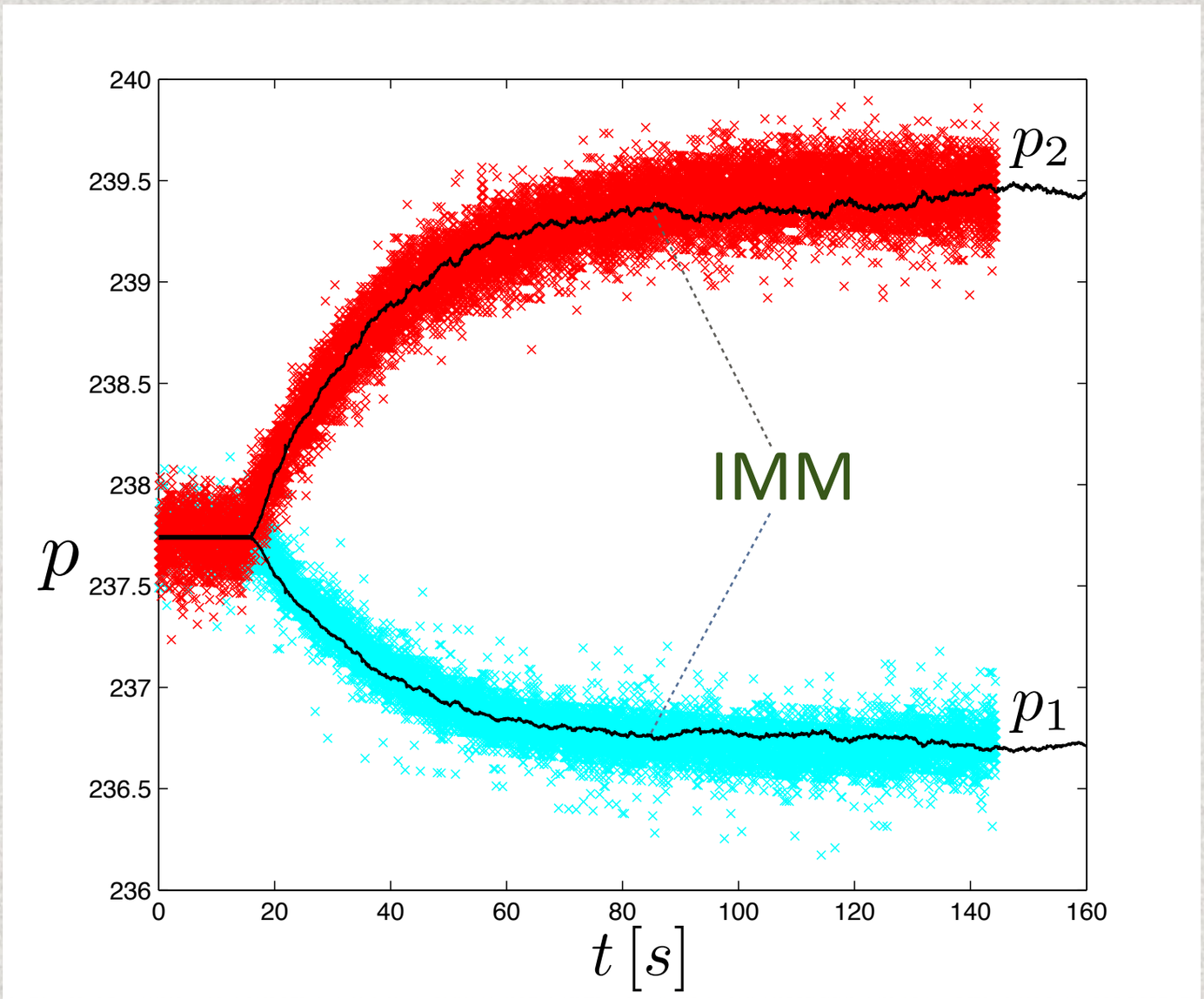
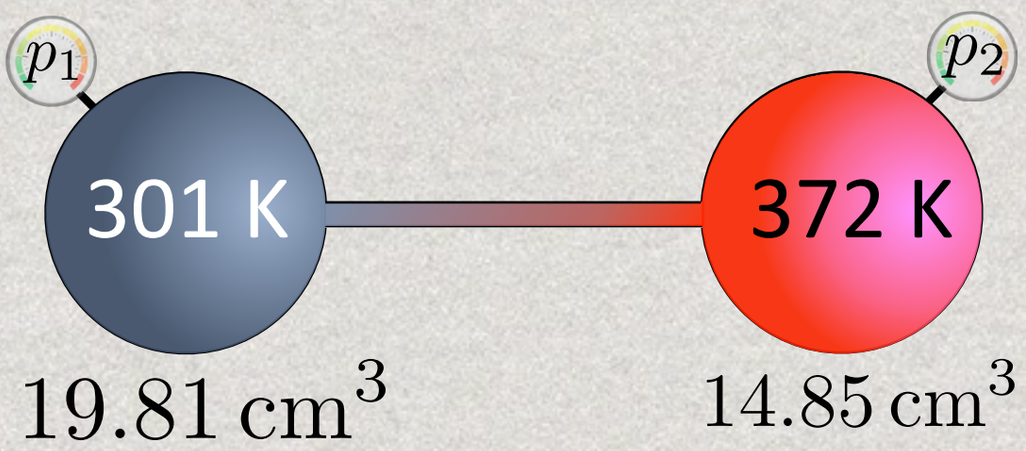
Lockerby, Patronis, Borg, Reese (2015) J. Comp. Phys. 284, 261-272

Comparison with Experiment



- Argon gas
- Channel length: 52.7 mm
- Channel radius: 0.242 mm
- Initial pressure: 238 Pa



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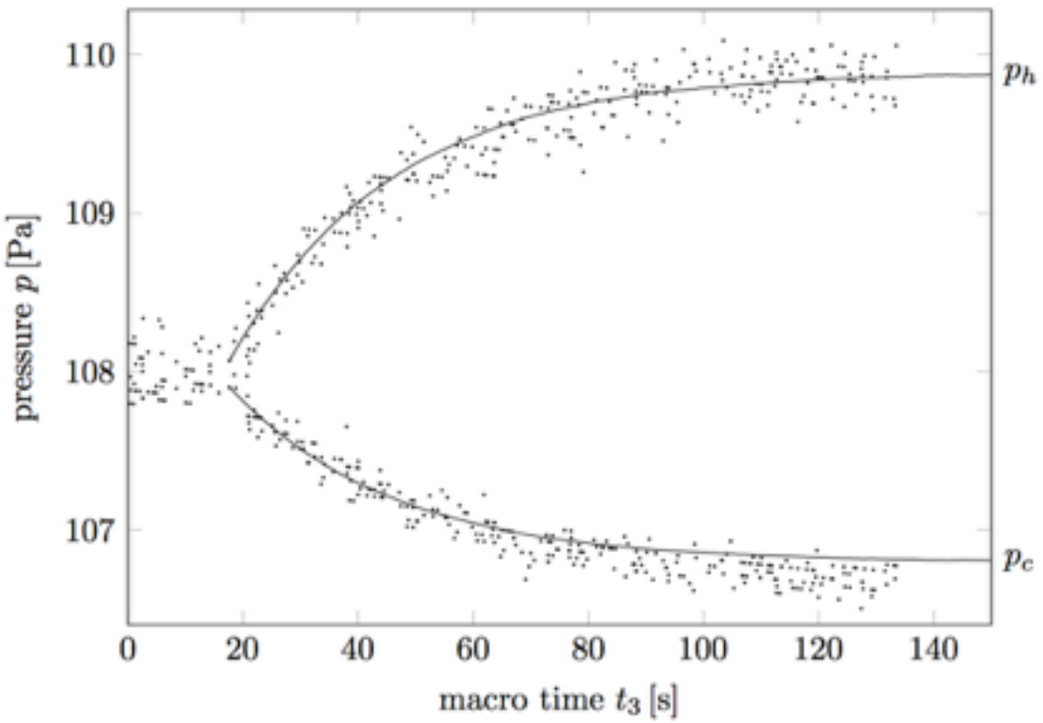
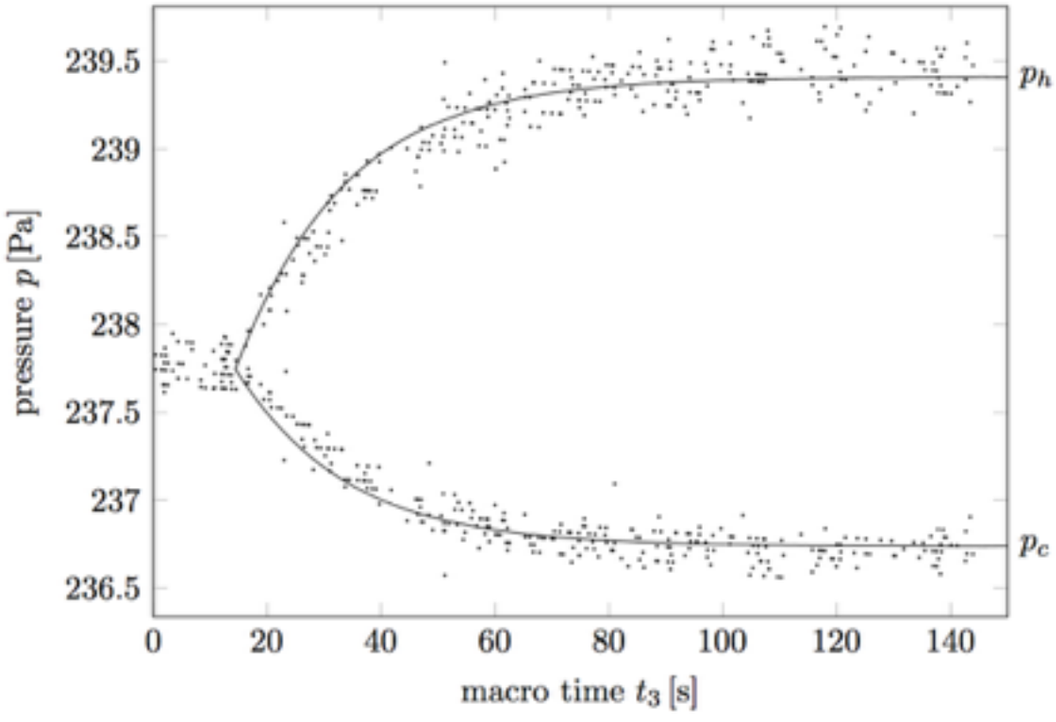
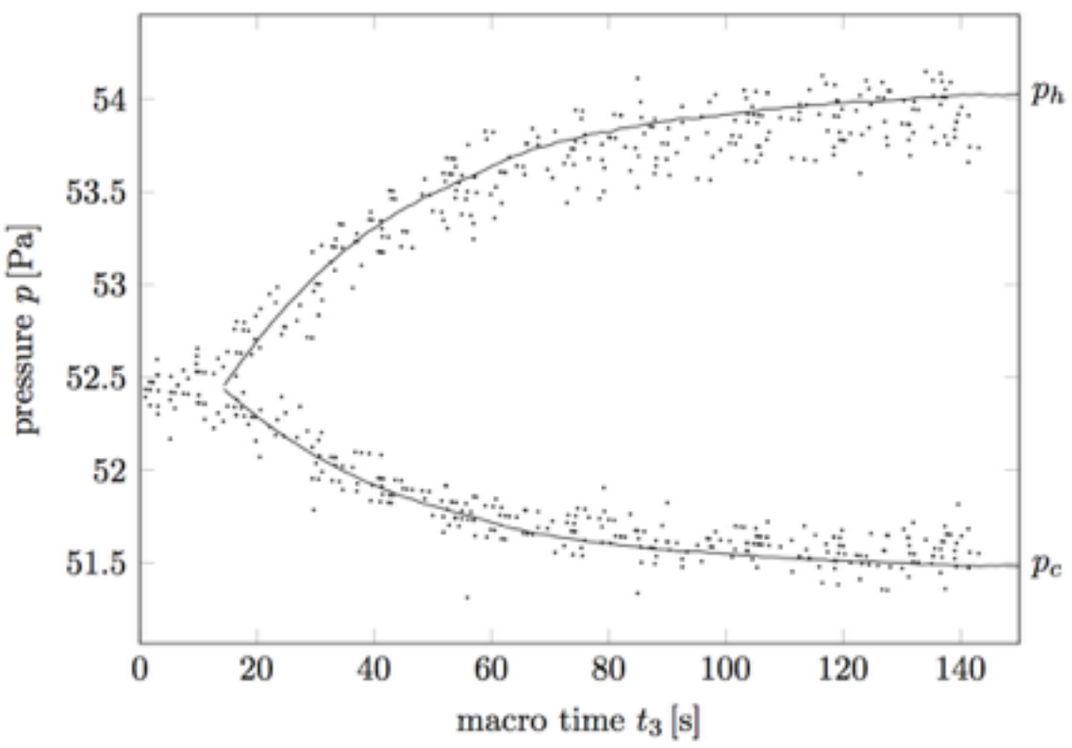
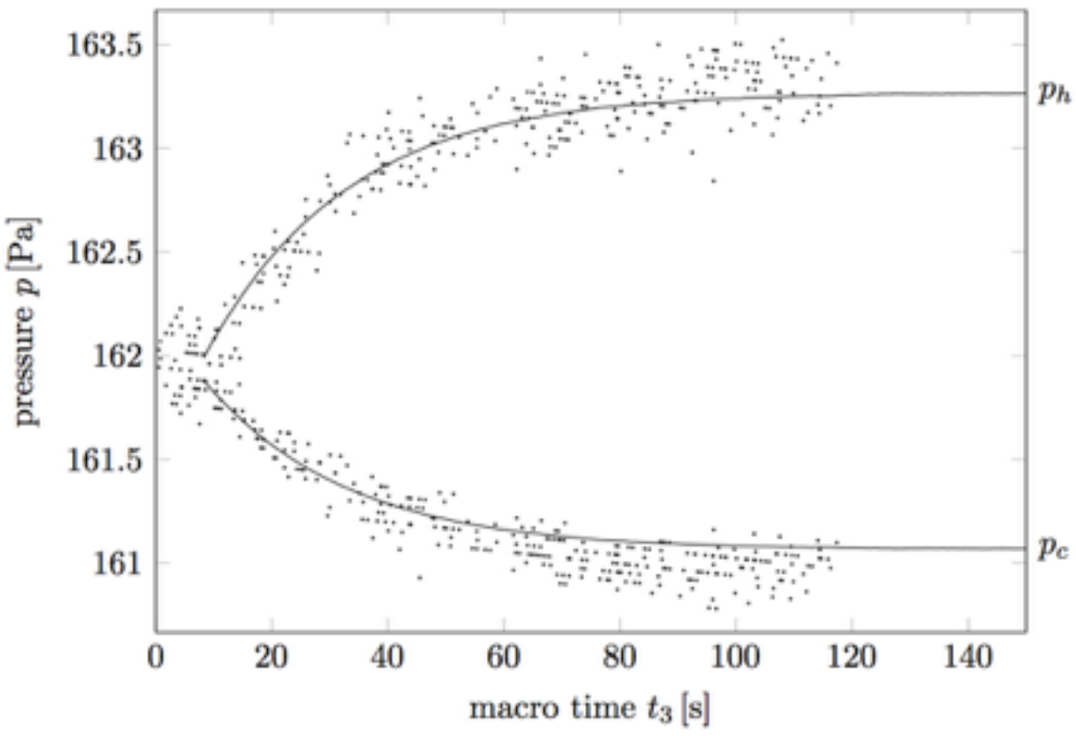


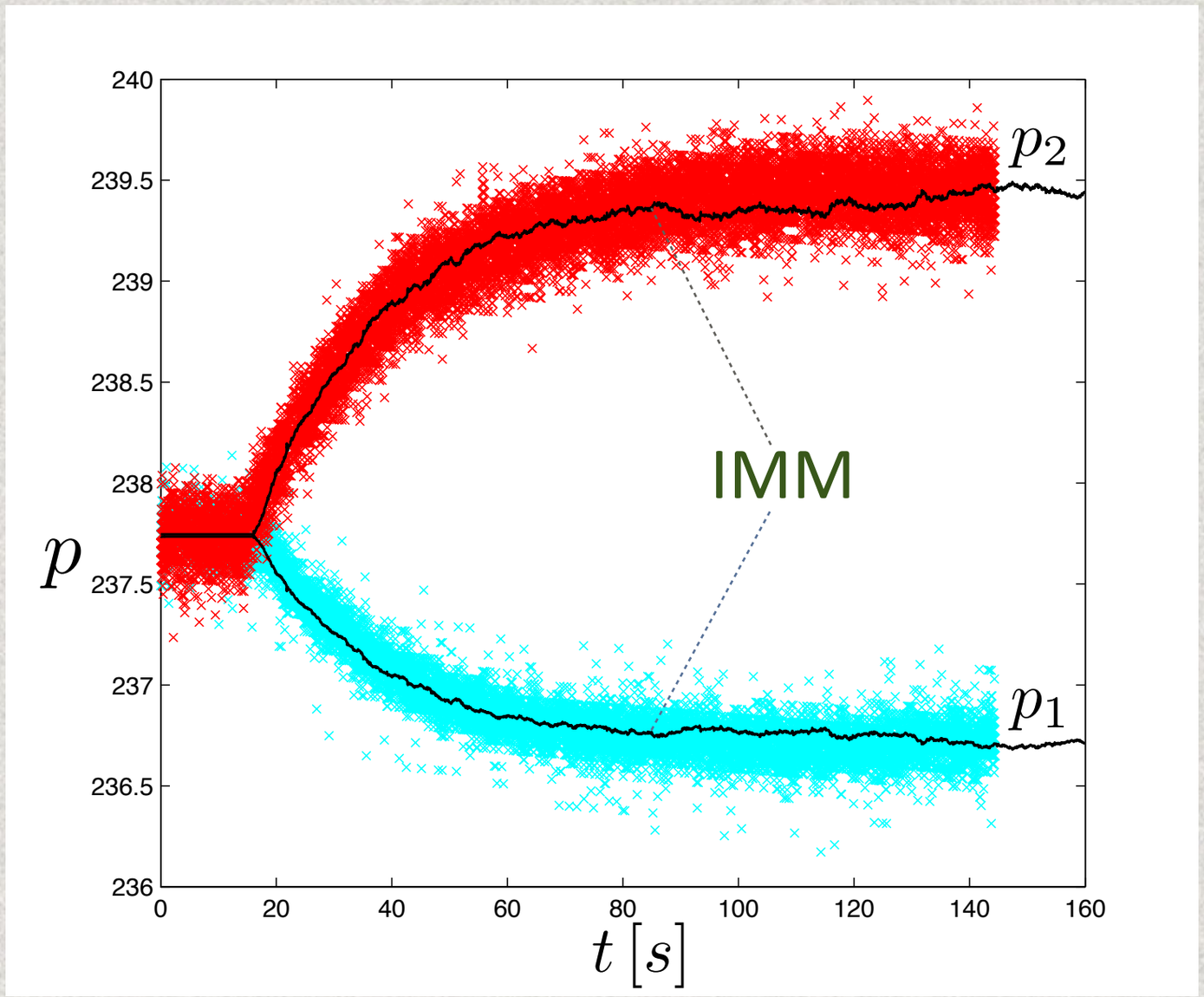






Comparison with Experiment

- IMM allows ~300x fewer (deviational) particles
- Asynchronous coupling allows ~40,000 times fewer timesteps
- Overall ~10 million times faster than a full particle simulation



Hybrid model classification

molecular pre-simulations

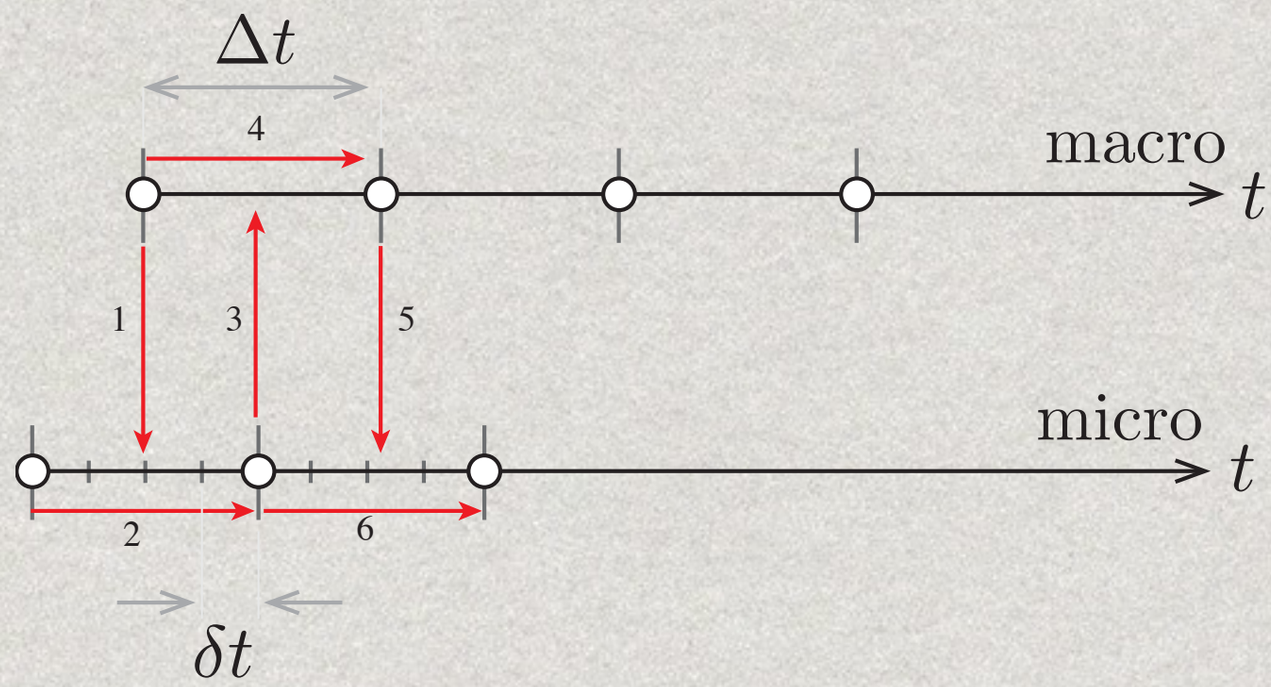
LIBRARY

DATA

- constitutive
- boundary
- state

CFD simulations

Type A. Sequential
(molecular-*then*-continuum)



Type B. Concurrent
(molecular-*with*-continuum)

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