Particulate Matter: lifecycle and mitigation
University of Leicester
March 11th, 2024

Simulating the aerodynamics of soot particles

Duncan Lockerby (University of Warwick)

Thanks to: Jos Jordan, Anirudh Rana, Rory Claydon, Abhay Shrestha, Ben Collyer and James Sprittles

This work is financially supported in the UK by the EPSRC

PART 1

MODELLING CHALLENGE: NON-SPHERICITY

PART 2

MODELLING CHALLENGE: NON-CONTINUUM

PART 3

APPLICATION: SOOT PARTICLES

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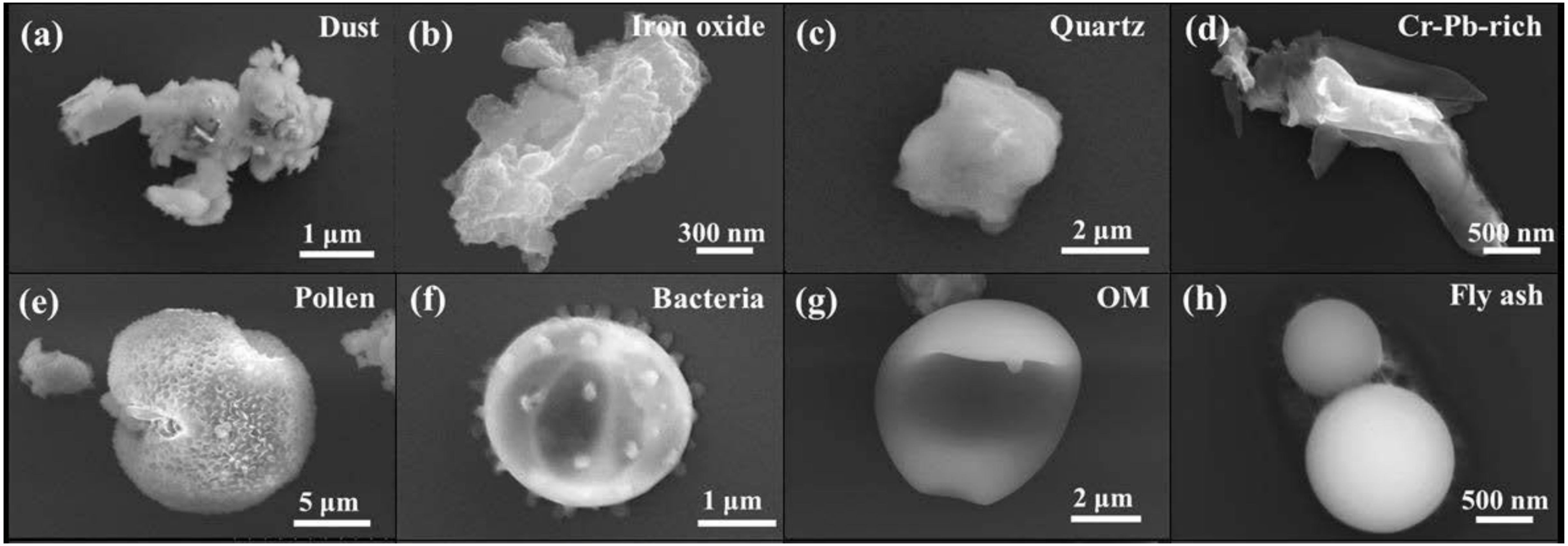
The 1st Challenge

- Particulate have complex geometries, requiring complex meshing



Li *et al*. (2016) Portrait and Classification of Individual Haze Particulates. Journal of Environmental Protection, 7, 1355-1379.

- Slow-moving particles have a long-range influence, and require very large domains.
- Finite-volume method not very efficient for single particulate, and not tractable for large numbers of interacting particles.

Method of Fundamental Solutions (MFS)

- What is the flow response to a point forcing?

$$\nabla \cdot \boldsymbol{v} = 0$$

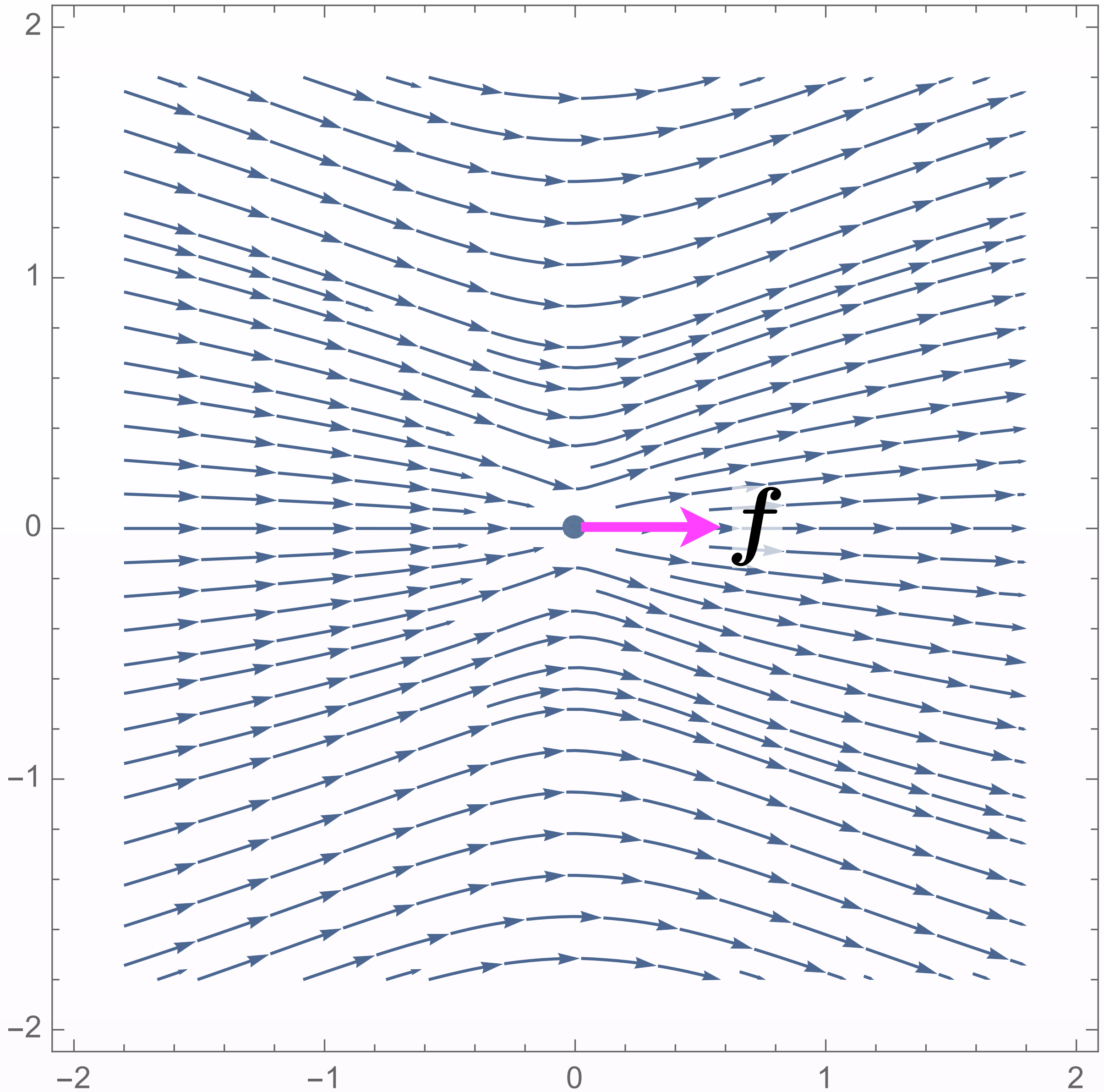
$$\nabla p - \mu \nabla^2 \boldsymbol{v} = \boldsymbol{f} \delta(\boldsymbol{r})$$

Method of Fundamental Solutions (MFS)

- What is the flow response to a point forcing?

$$\boldsymbol{v} = \frac{\boldsymbol{f}}{8\pi\mu} \cdot \left[\frac{\mathbb{I}}{\|\boldsymbol{r}\|} + \frac{\boldsymbol{r}\boldsymbol{r}}{\|\boldsymbol{r}\|^3} \right]$$

the Stokeslet



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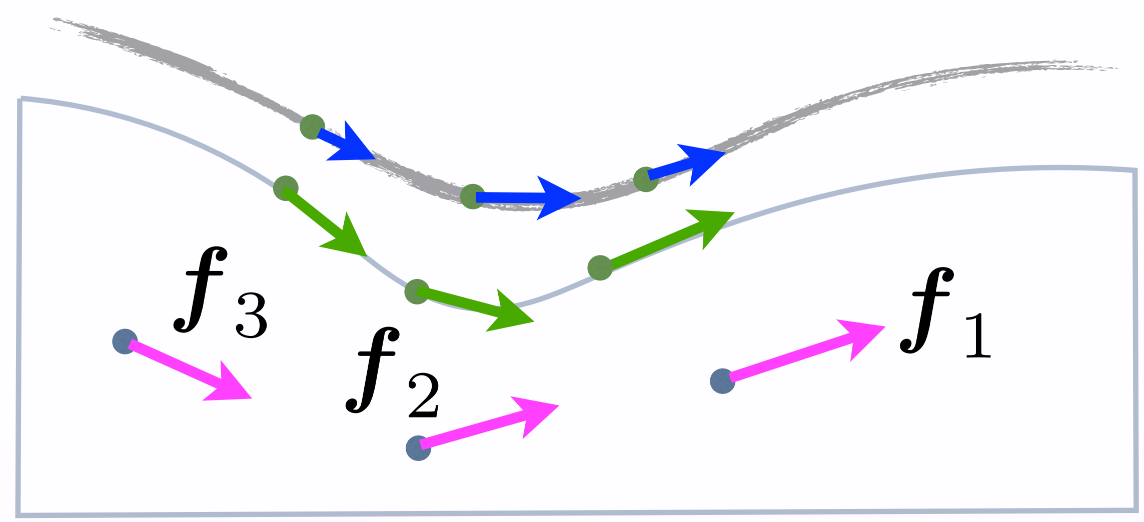
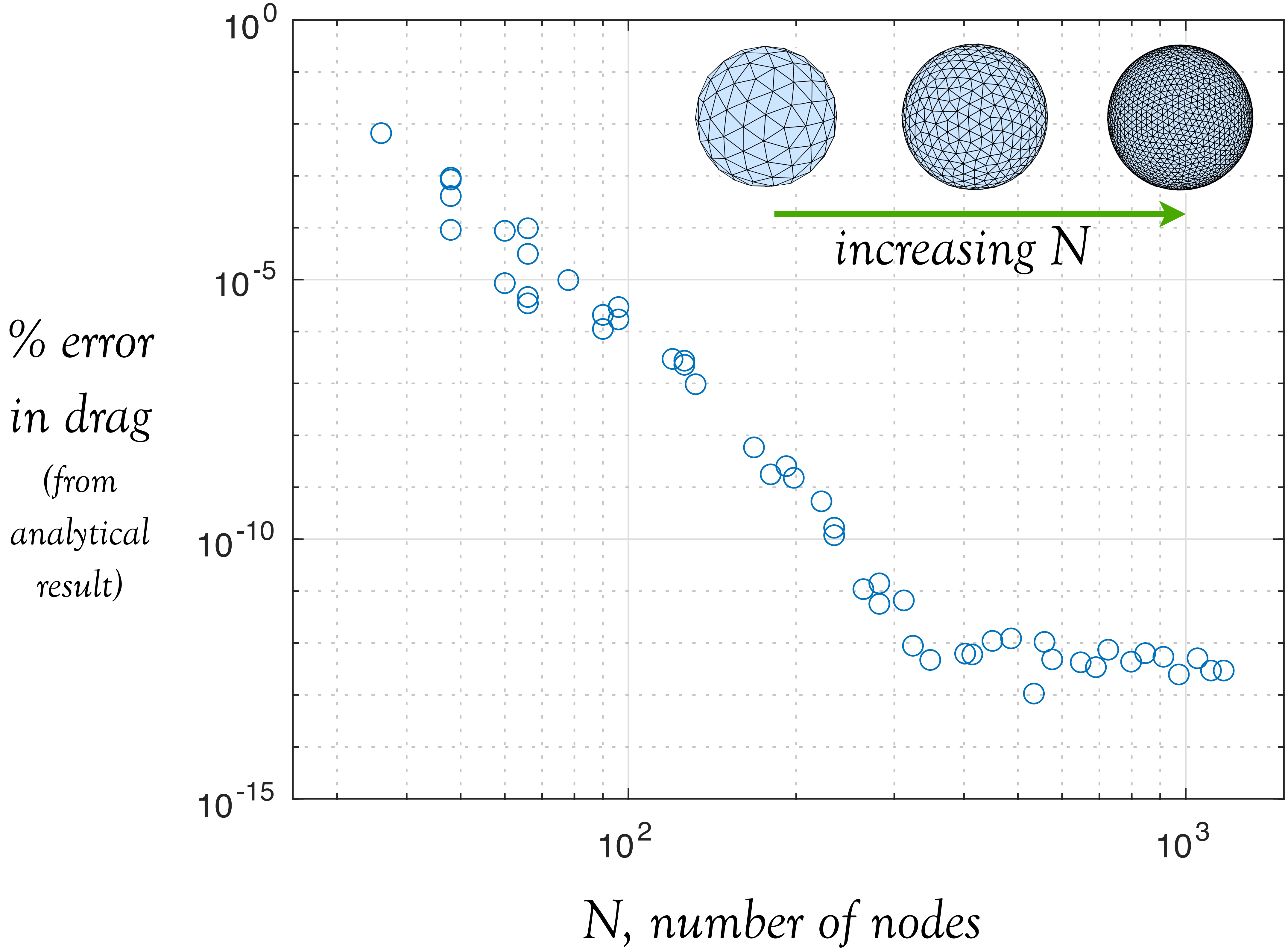
Method of Fundamental Solutions (MFS)

$$\boldsymbol{v} = \frac{\boldsymbol{f}}{8\pi\mu} \cdot \left[\frac{\mathbb{I}}{\|\boldsymbol{r}\|} + \frac{\boldsymbol{r}\boldsymbol{r}}{\|\boldsymbol{r}\|^3} \right]$$

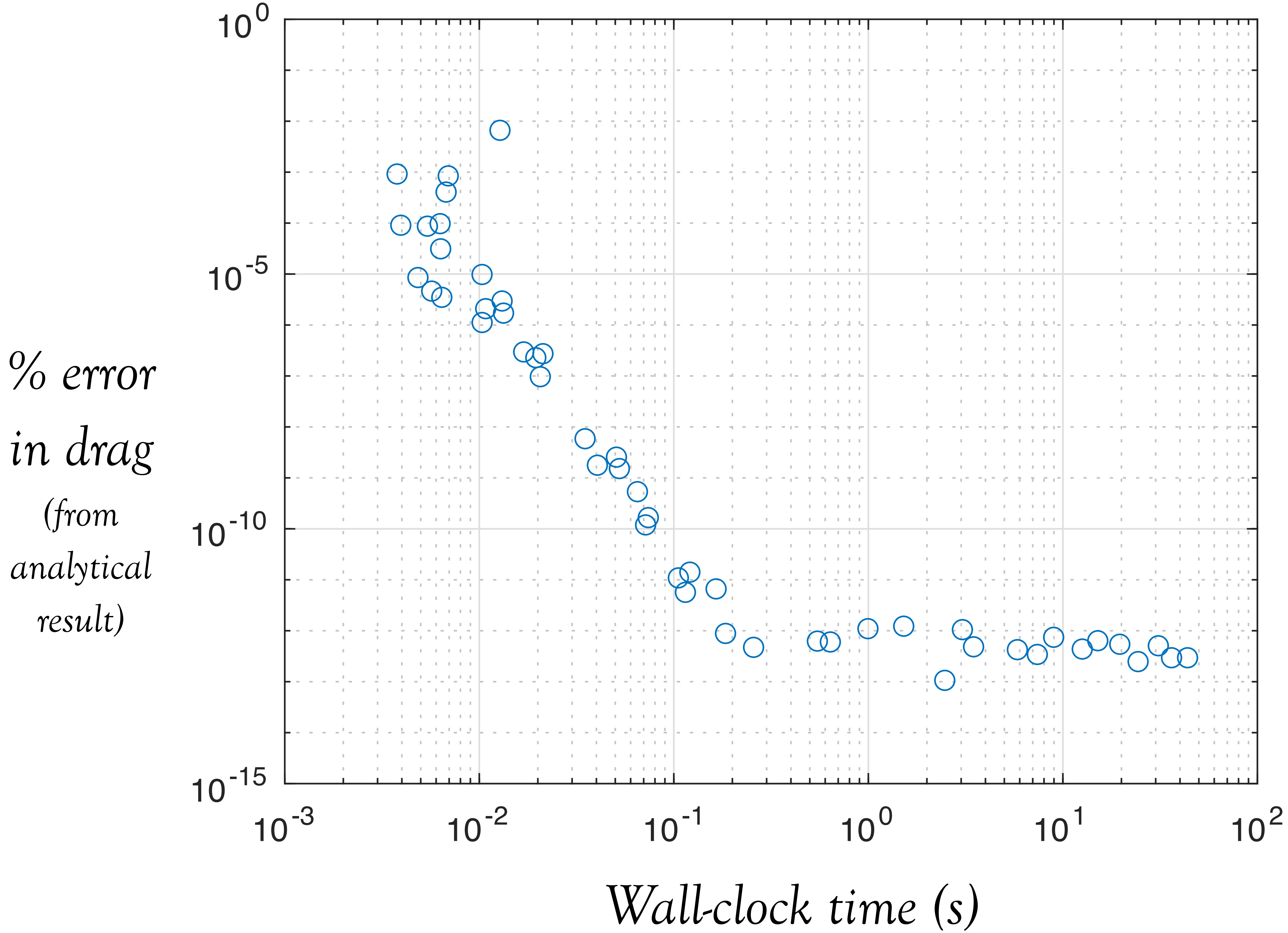


Drag on a sphere



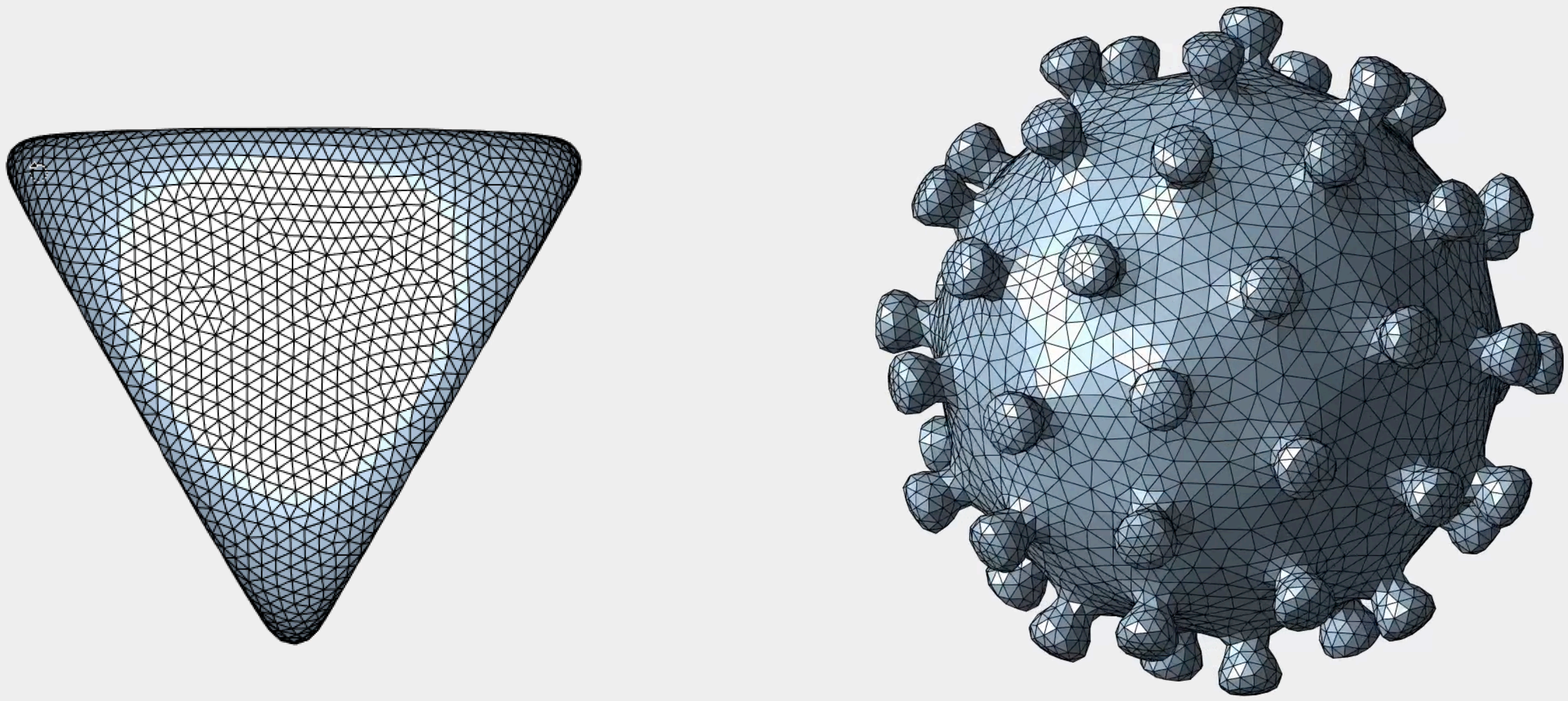
MFS_static/figNE.m

Drag on a sphere



(calculations performed on an early 2019 MacBook pro)

MFS_static/figNE2.m



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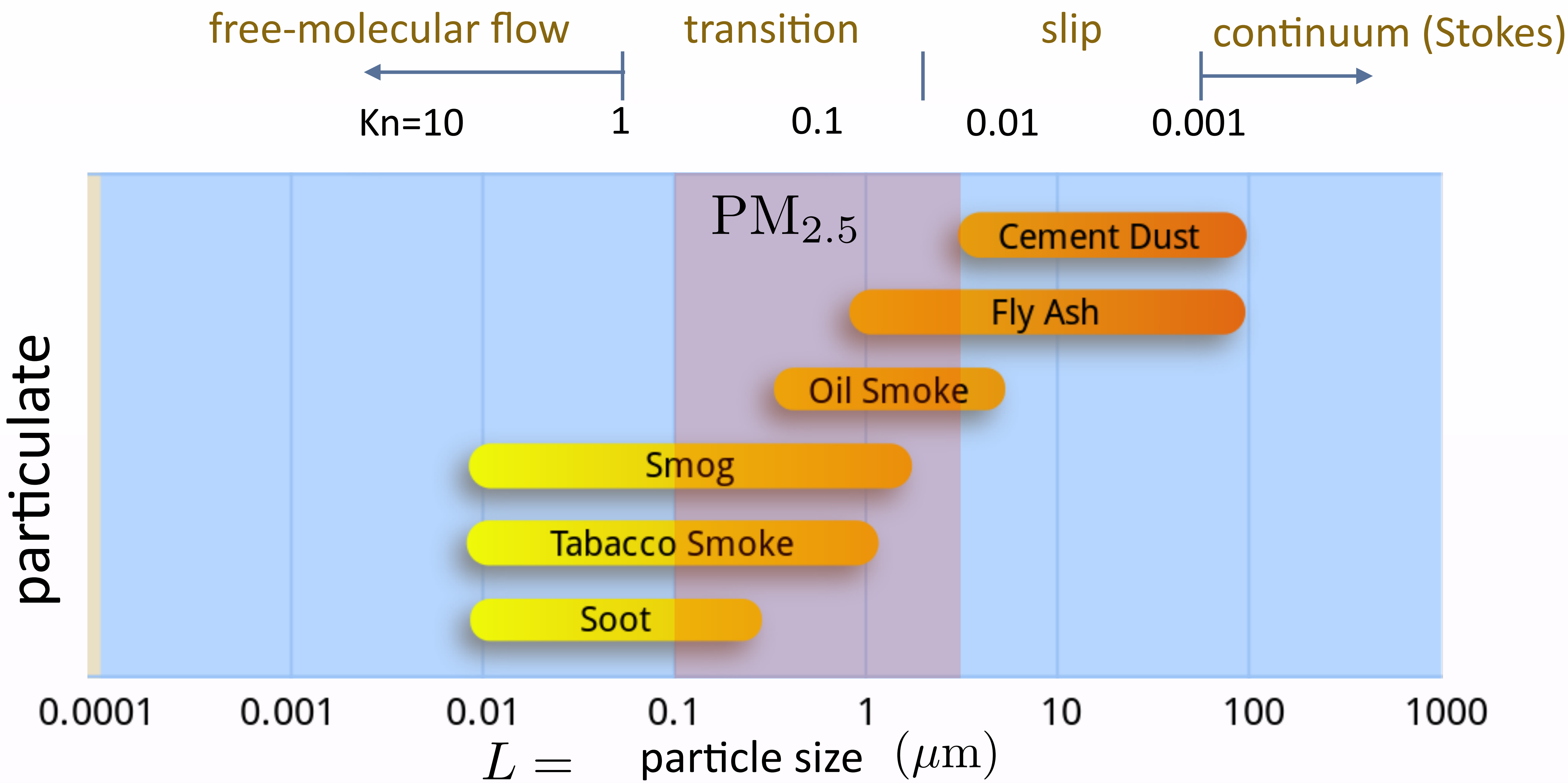
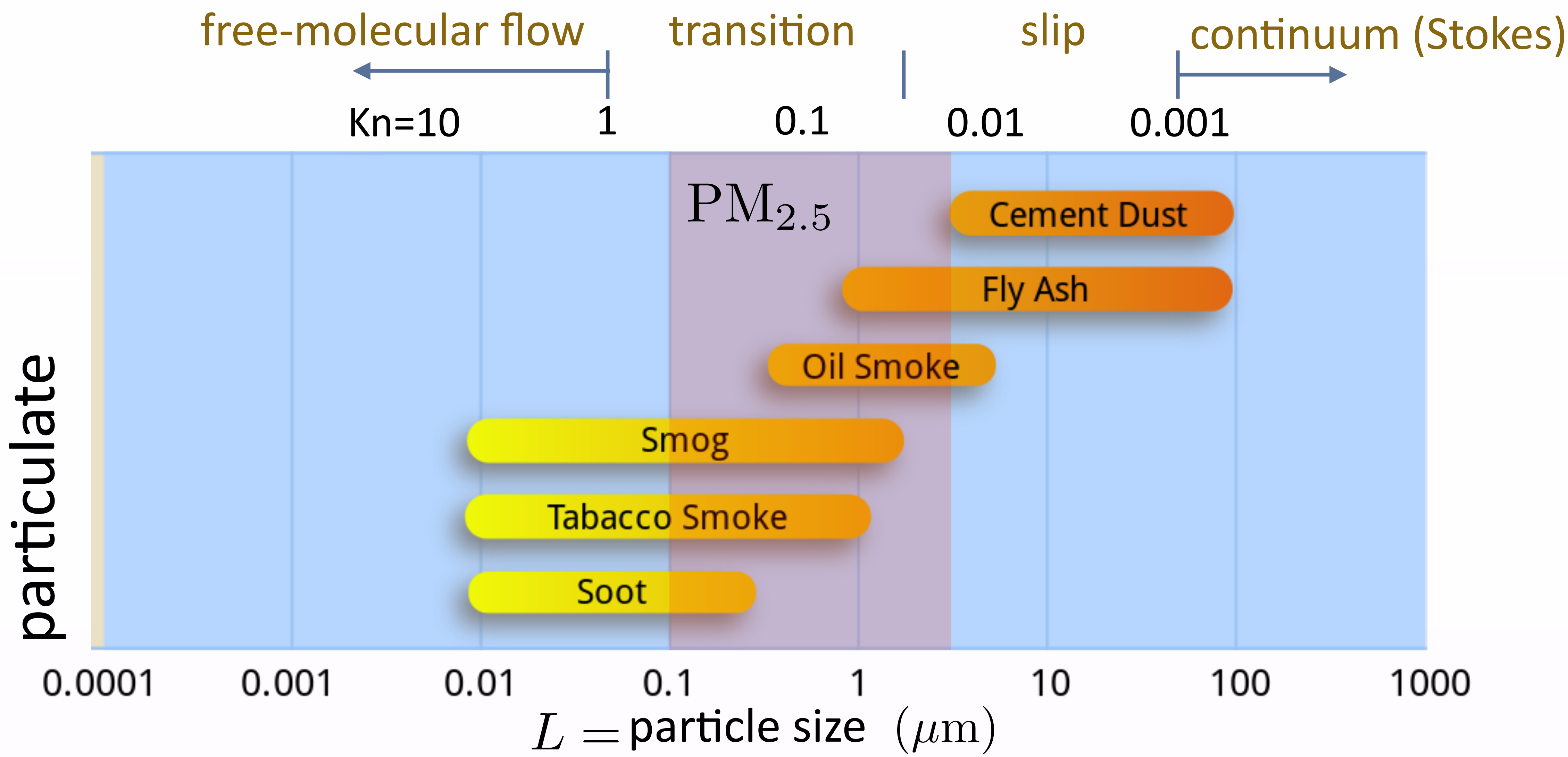
The 2nd Challenge

Knudsen number, $$\mathrm{Kn} = \frac{\lambda}{L}$$



Going beyond the Stokes equations



- Boltzmann equation too expensive; Navier-Stokes too inaccurate.
- Extended continuum equations offer a best-of-both-worlds solution

The linearised G13 equations

- Continuum equations derived from the Boltzmann equation
- Grad's 13-moment equations (and Regularised set, R13) obtained from Hermite polynomial expansion of the velocity distribution function about a local equilibrium state
- Linearised steady form of Grad's 13 moment equations:

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0$$

$$\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \mathbb{S} = 0$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{q} = 0$$

$$\mathbb{S} = -2Kn' \overline{\boldsymbol{\nabla} \boldsymbol{v}} - \boxed{\frac{4}{5} Kn' \overline{\boldsymbol{\nabla} \boldsymbol{q}}} \, ,$$

$$\boldsymbol{q} = -\frac{15}{4} Kn' \boldsymbol{\nabla} \theta - \boxed{\frac{3}{2} Kn' \boldsymbol{\nabla} \cdot \mathbb{S}}$$

G13

Fundamental solutions to G13 equations

- Continuum equations derived from the Boltzmann equation
- Grad's 13-moment equations (and Regularised set, R13) obtained from Hermite polynomial expansion of the velocity distribution function about a local equilibrium state
- Linearised steady form of Grad's 13 moment equations:

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0$$

$$\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \mathbb{S} = \boldsymbol{f}\, \delta(\boldsymbol{r})$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{q} = g\, \delta(\boldsymbol{r})$$

$$\mathbb{S} = -2Kn' \overline{\boldsymbol{\nabla} \boldsymbol{v}} - \frac{4}{5} Kn' \overline{\boldsymbol{\nabla} \boldsymbol{q}}\,,$$

$$\boldsymbol{q} = -\frac{15}{4} Kn' \boldsymbol{\nabla} \theta - \frac{3}{2} Kn' \boldsymbol{\nabla} \cdot \mathbb{S}$$

G13

G13 boundary conditions

- The velocity boundary condition:

$$\boldsymbol{v}_j = \boldsymbol{v}_{\mathrm{w},j} - \underbrace{\sqrt{\frac{\pi}{2}}\boldsymbol{n}_j \cdot \boldsymbol{S}_j \cdot (\boldsymbol{I} - \boldsymbol{n}_j\boldsymbol{n}_j)}_{\text{slip}} - \underbrace{\frac{1}{5}\boldsymbol{q}_j \cdot (\boldsymbol{I} - \boldsymbol{n}_j\boldsymbol{n}_j)}_{\text{thermal creep}},$$

- The temperature boundary condition:

$$\theta_j = \theta_{\mathrm{w},j} - \underbrace{\frac{1}{2}\sqrt{\frac{\pi}{2}}\boldsymbol{n}_j \cdot \boldsymbol{q}_j}_{\text{jump}} - \underbrace{\frac{1}{4}\boldsymbol{n}_j \cdot \boldsymbol{S}_j \cdot \boldsymbol{n}_j}_{\dots},$$

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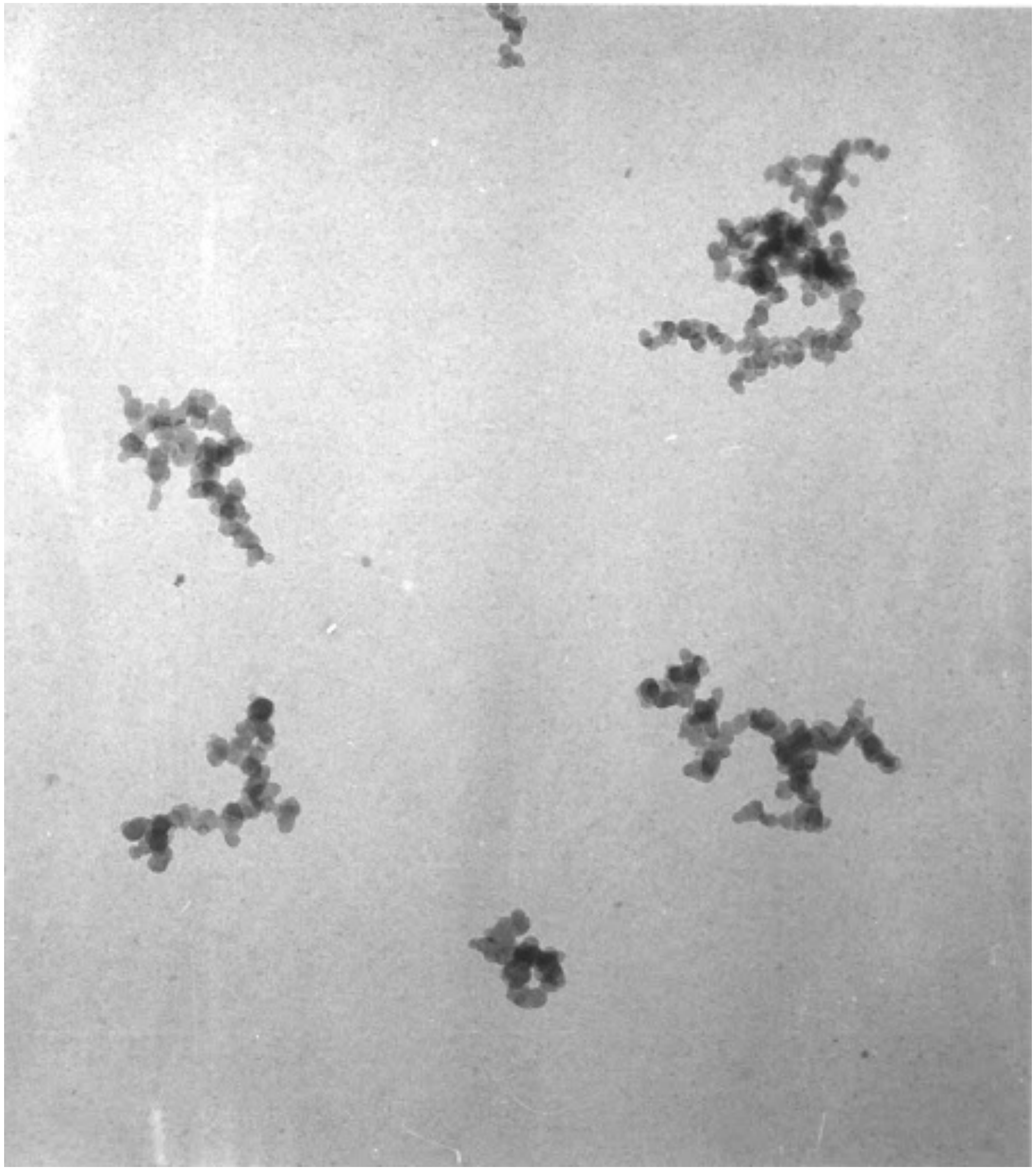
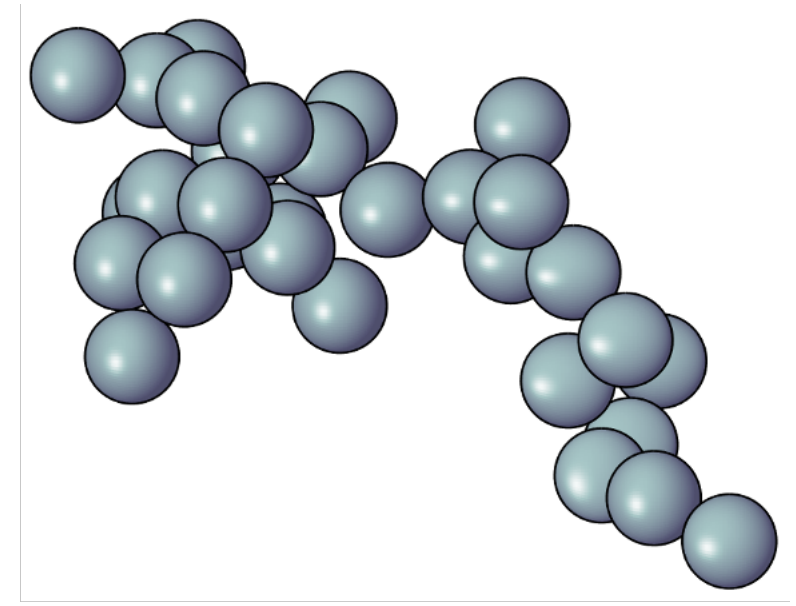
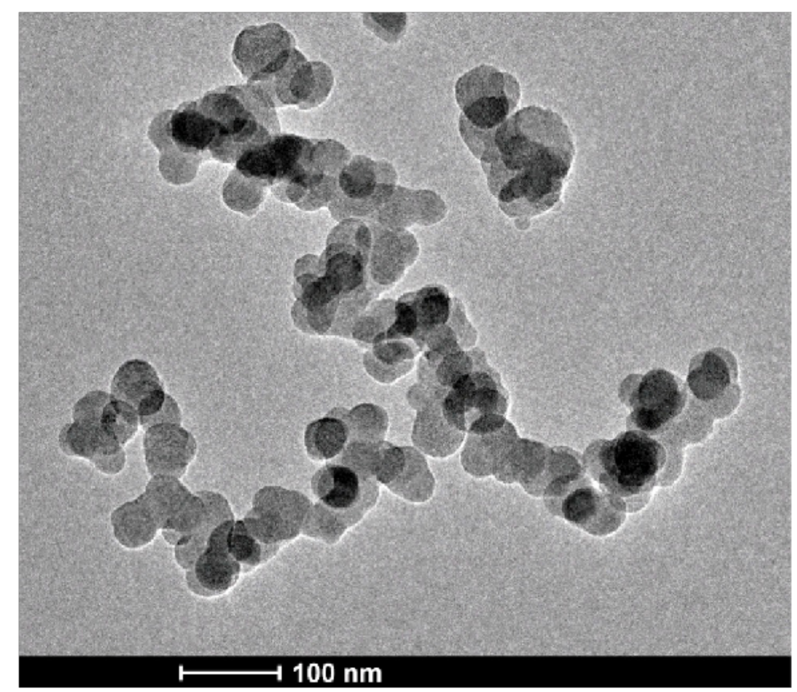
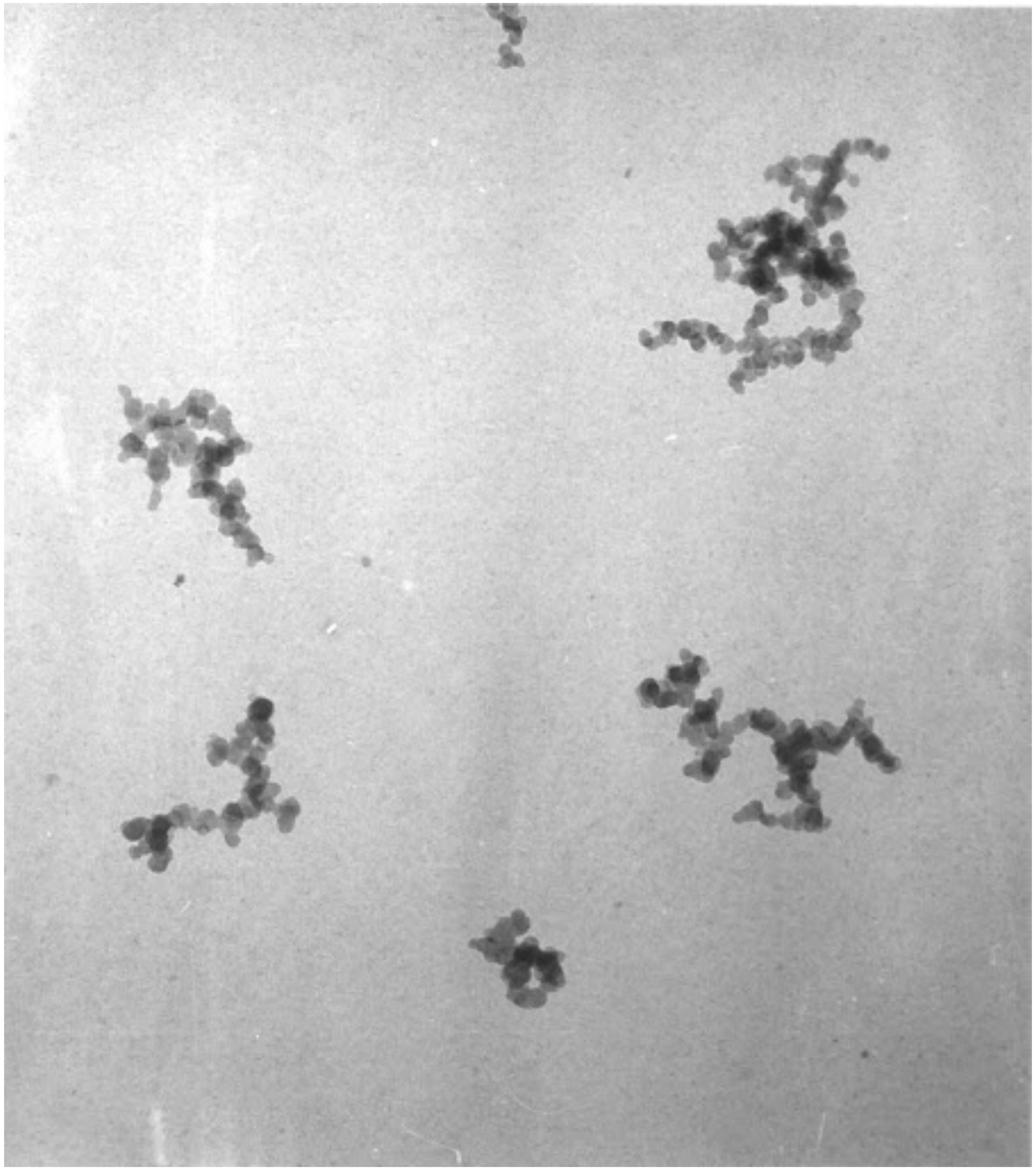


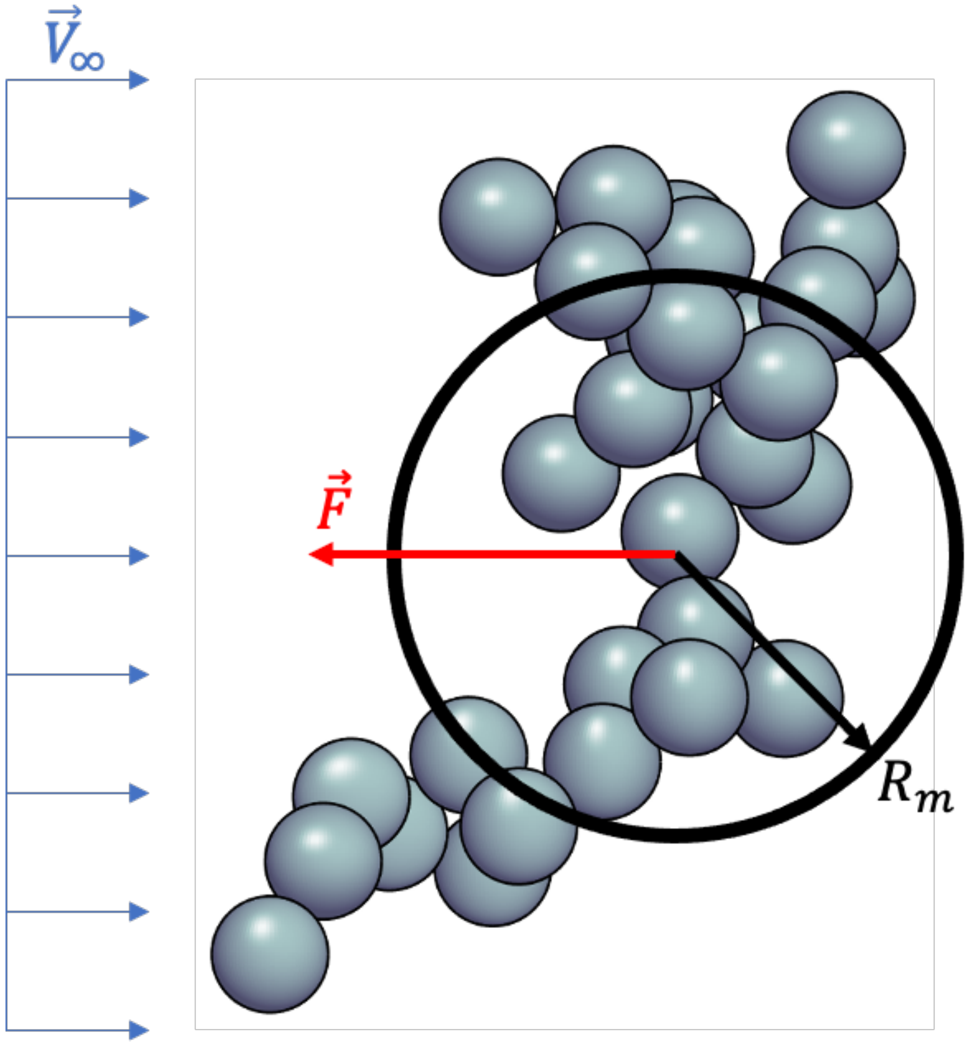


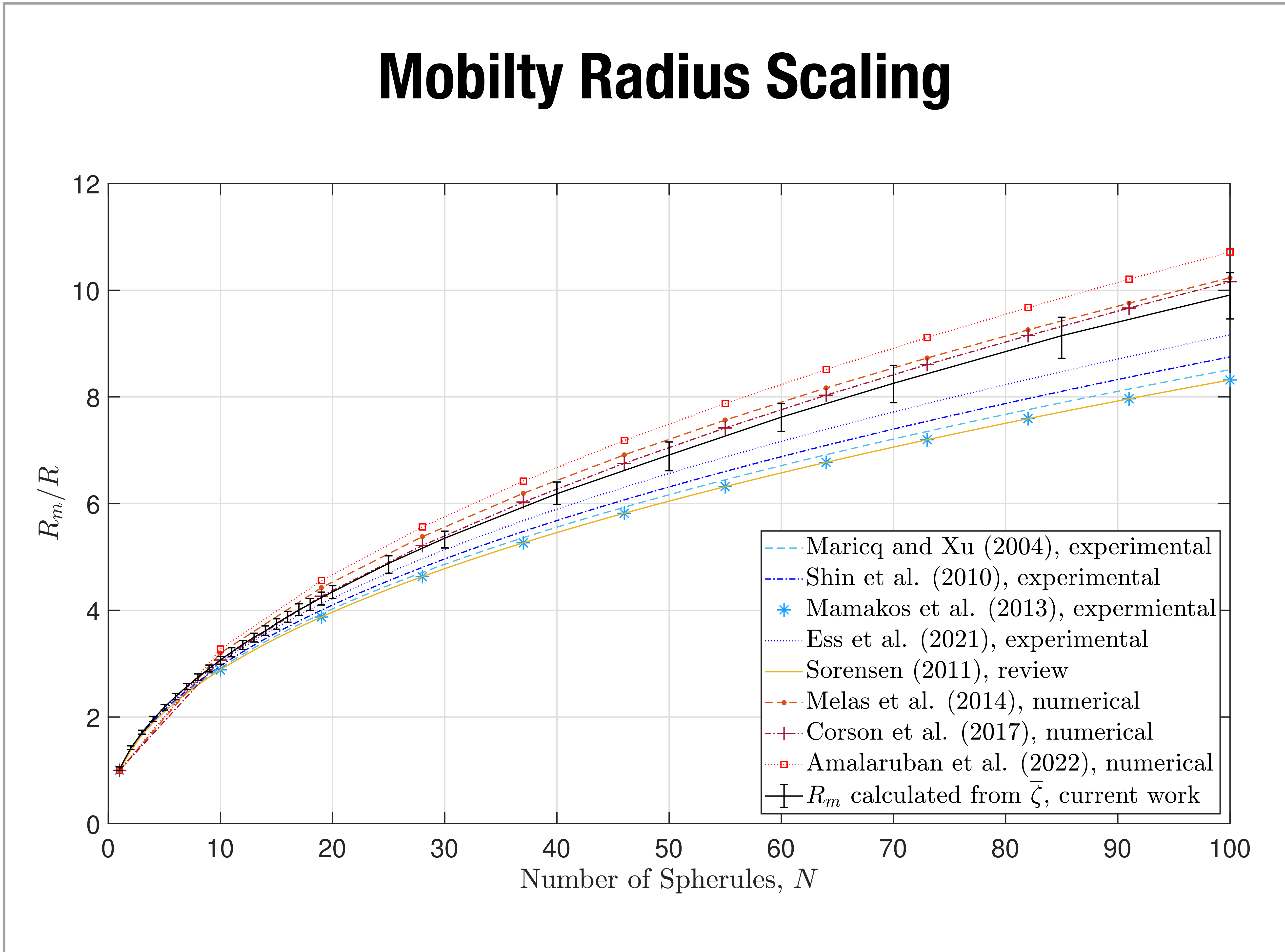


Kempema and Long, 2016

Simulating Soot



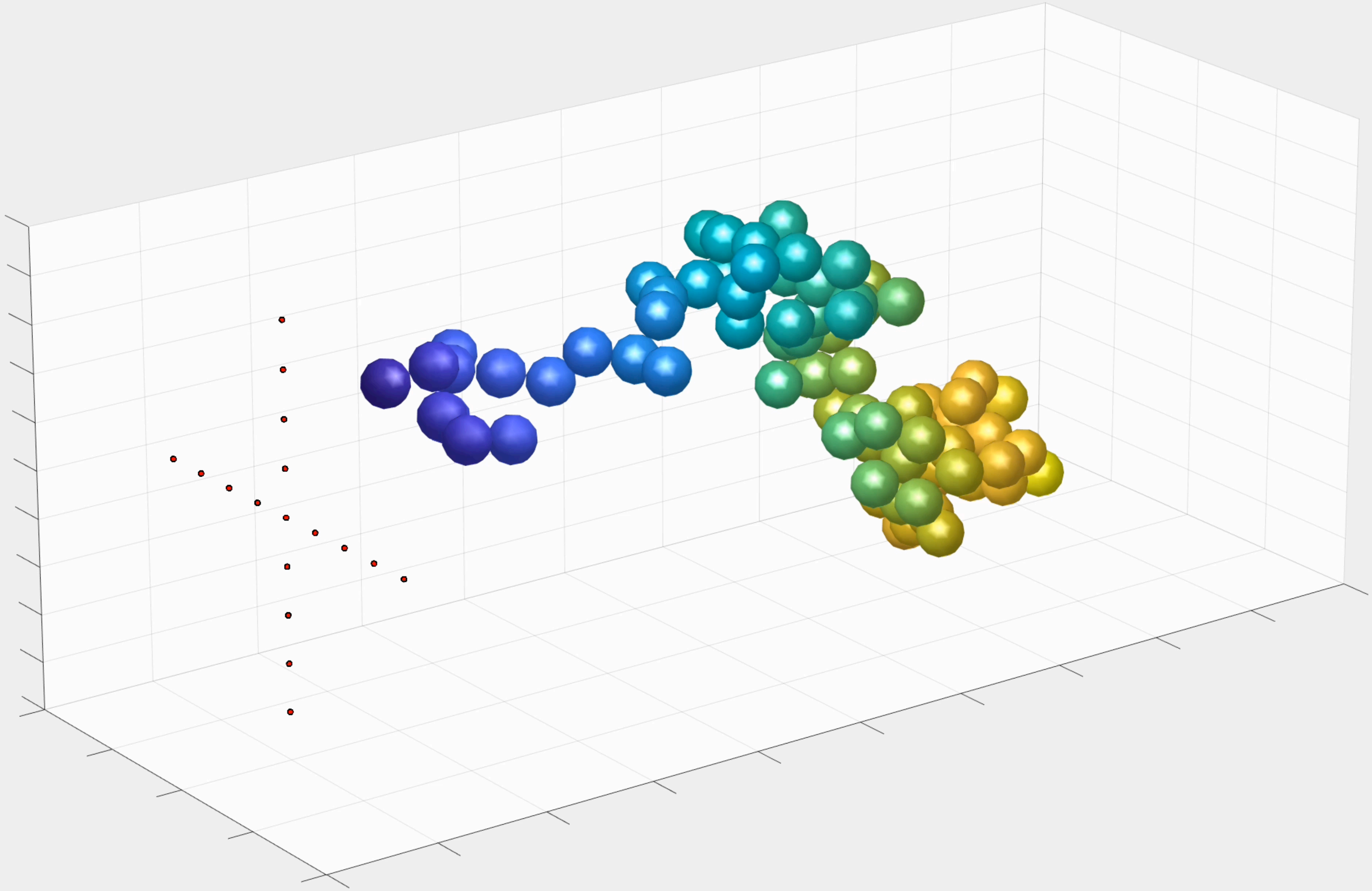




Mobilty Radius Scaling
R_m/R
Number of Spherules, N
0
2
4
6
8
10
12
0
10
20
30
40
50
60
70
80
90
100
Maricq and Xu (2004), experimental
Shin et al. (2010), experimental
Mamakos et al. (2013), expermiental
Ess et al. (2021), experimental
Sorensen (2011), review
Melas et al. (2014), numerical
Corson et al. (2017), numerical
Amalaruban et al. (2022), numerical
R_m calculated from $\overline{\zeta}$, current work

Simulating Soot

thermophoresis



aggloDemo.m; aggloVid.m;

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