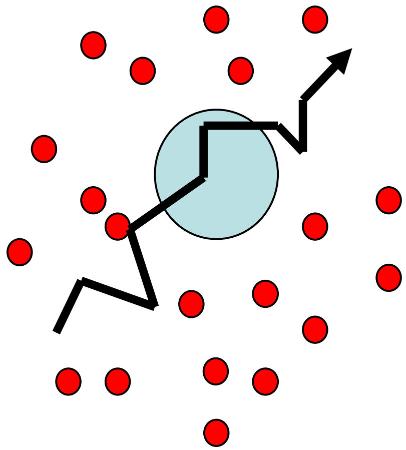
	Lectures	Exercises/Home work problems	
Ordinary differential equations	Linear dynamics	E1	
	Non-linear dynamics	E2	
	Molecular dynamics		H1a/H1b
Stochastic methods	Monte Carlo integration	E3	
	Metropolis algorithm		H2a/H2b
	Brownian dynamics	E4	
Partial differential equations	Quantum structure	E5	H3a
	Quantum dynamics		H3b

Brownian dynamics

The erratic motion of particles dispersed in a fluid.
Observed by Brown for minute particles ejected from pollen grains.



- observed by Brown, a botanist, 1827
- key theoretical contribution by Einstein 1905
- a basic model for noise
- a standard model for a whole class of similar models
- an example of how one can take different time-scales into account and formulate a ”coarse-grained” mode

Brownian dynamics

Content:

- Langevin's equation
- Fokker-Planck equation
- With an external force

Algorithm BD2

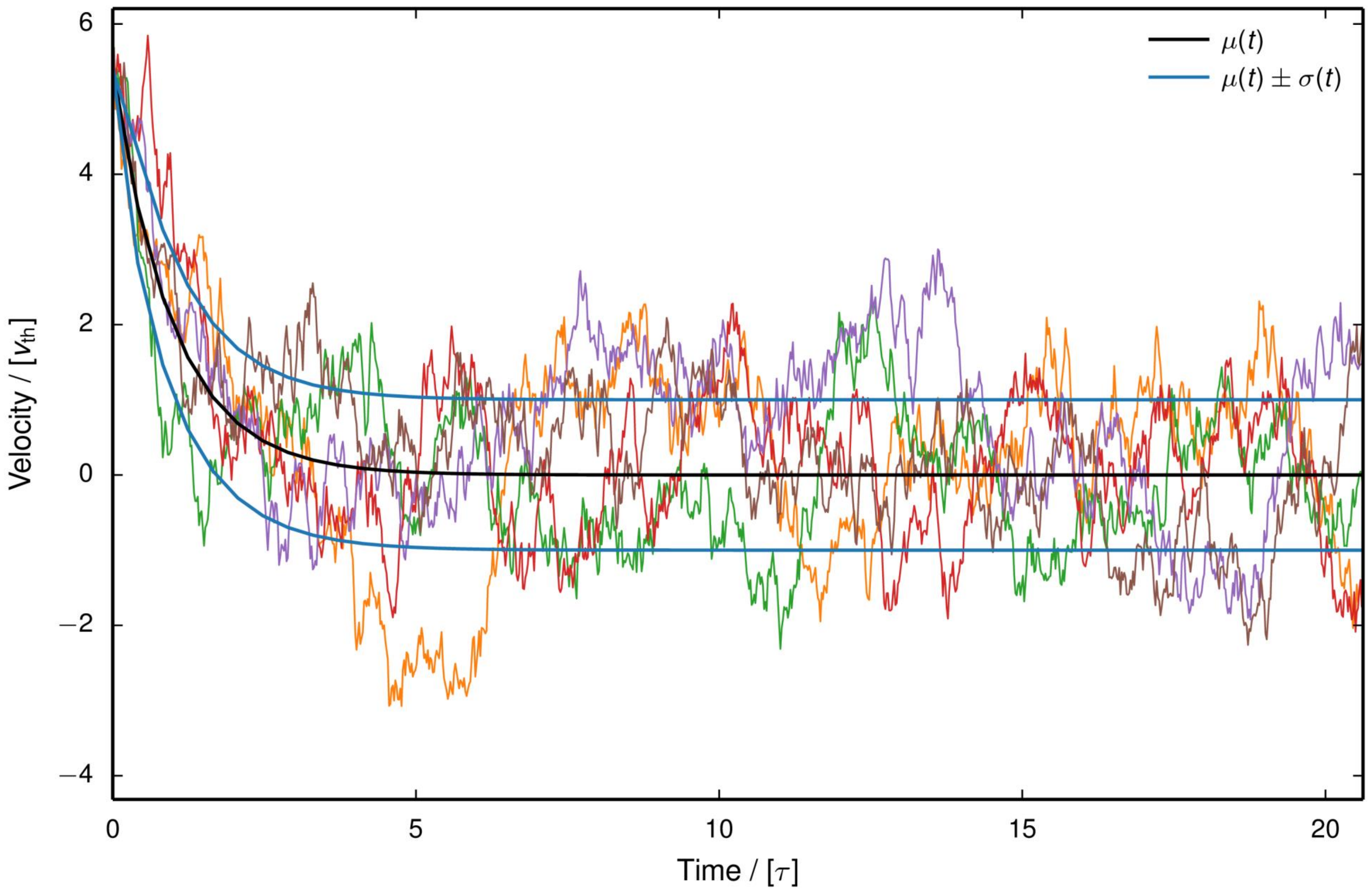
Algorithm BD2 The recommended algorithm for solving Langevin's equation is therefore

$$v_{n+1} = c_0 v_n + v_{th}\sqrt{1 - c_0^2}\, \mathcal{G}_n \qquad (15)$$

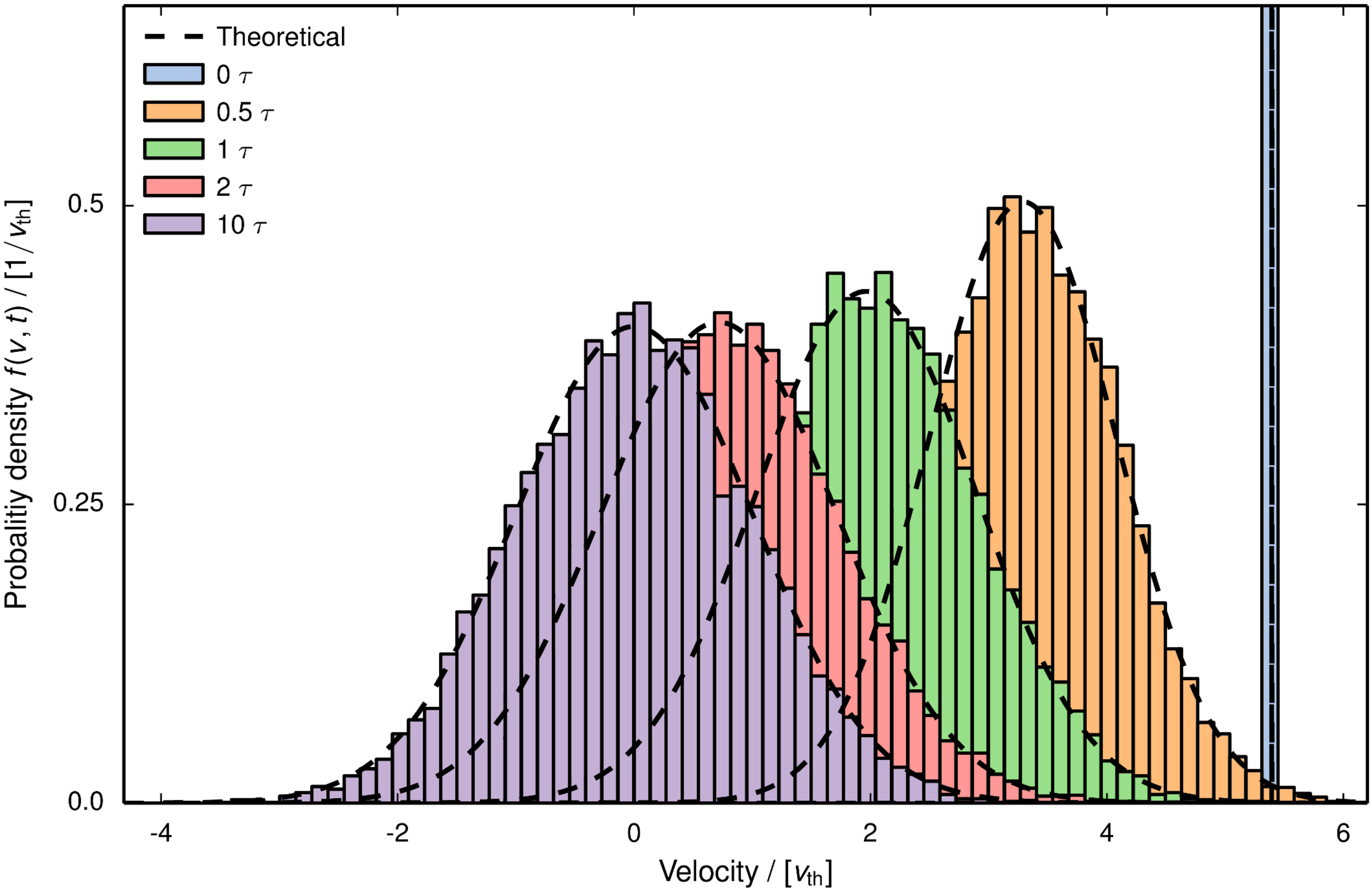
where

$$c_0 = e^{-\eta \Delta t} \quad \text{and} \quad v_{th} = \sqrt{k_B T/m}$$

and $\mathcal{G}_n$ is a Gaussian random number with zero mean, unit variance and uncorrelated in time $\langle \mathcal{G}_n \mathcal{G}_{n'} \rangle = \delta_{n,n'}$.



$\mu(t)$
$\mu(t) \pm \sigma(t)$
6
4
2
0
−2
−4
Velocity / [v_{th}]
0
5
10
15
20
Time / [τ]



Göran Wahnström, Department of Physics, Chalmers

Velocity Verlet algorithm

$$v(t + \Delta t/2) = v(t^+) + \frac{1}{2}a(t)\Delta t$$

$$x(t + \Delta t) = x(t) + v(t + \Delta t/2)\Delta t$$

`calculate new (external) accelerations/forces`

$$v(t^- + \Delta t) = v(t + \Delta t/2) + \frac{1}{2}a(t + \Delta t)\Delta t$$

Algorithm BD3

$$v(t^+) = \sqrt{c_0}v(t) + v_{th}\sqrt{1-c_0}\;\mathcal{G}_1$$

$$v(t+\Delta t/2) = v(t^+) + \frac{1}{2}a(t)\Delta t$$

$$x(t+\Delta t) = x(t) + v(t+\Delta t/2)\Delta t$$

`calculate new (external) accelerations/forces`

$$v(t^- + \Delta t) = v(t+\Delta t/2) + \frac{1}{2}a(t+\Delta t)\Delta t$$

$$v(t+\Delta t) = \sqrt{c_0}v(t^- + \Delta t) + v_{th}\sqrt{1-c_0}\;\mathcal{G}_2$$

Algorithm BD3

Algorithm BD3 The Langevin's equation with an external force (acceleration) that depends on the position can be numerically solved using the following algorithm (that reduces to the velocity Verlet in the limit $\eta \to 0$):

$$\tilde{v}_{n+1} = \frac{1}{2} a_n \Delta t + \sqrt{c_0} v_n + v_{th} \sqrt{1 - c_0}\, \mathcal{G}_{1,n}$$

$$x_{n+1} = x_n + \tilde{v}_{n+1} \Delta t$$

`calculate new external accelerations/forces`

$$v_{n+1} = \frac{1}{2} \sqrt{c_0} a_{n+1} \Delta t + \sqrt{c_0} \tilde{v}_{n+1} + v_{th} \sqrt{1 - c_0}\, \mathcal{G}_{2,n}$$

where

$$c_0 = e^{-\eta \Delta t} \quad \text{and} \quad v_{th} = \sqrt{k_B T / m}$$

and $\mathcal{G}_1$ and $\mathcal{G}_2$ are two independent Gaussian random numbers with zero mean, unit variance and uncorrelated in time $\left\langle \mathcal{G}_{1,n} \mathcal{G}_{1,n'} \right\rangle = \delta_{n,n'}$ and $\left\langle \mathcal{G}_{2,n} \mathcal{G}_{2,n'} \right\rangle = \delta_{n,n'}$.

Measurement of the Instantaneous Velocity of a Brownian Particle

Tongcang Li, Simon Kheifets, David Medellin, Mark G. Raizen*

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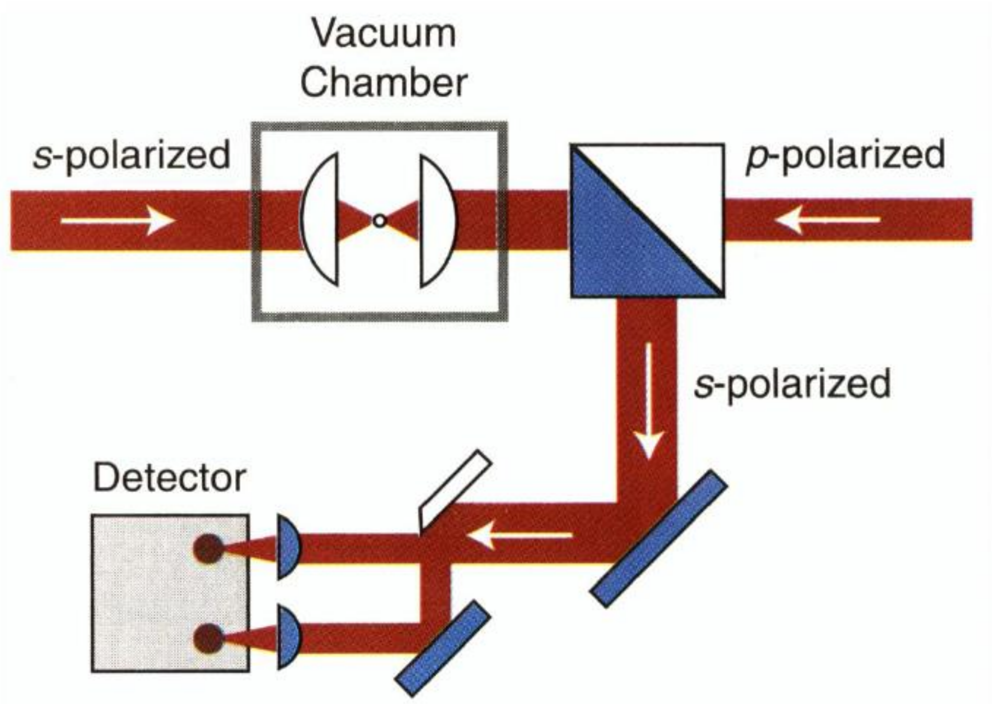

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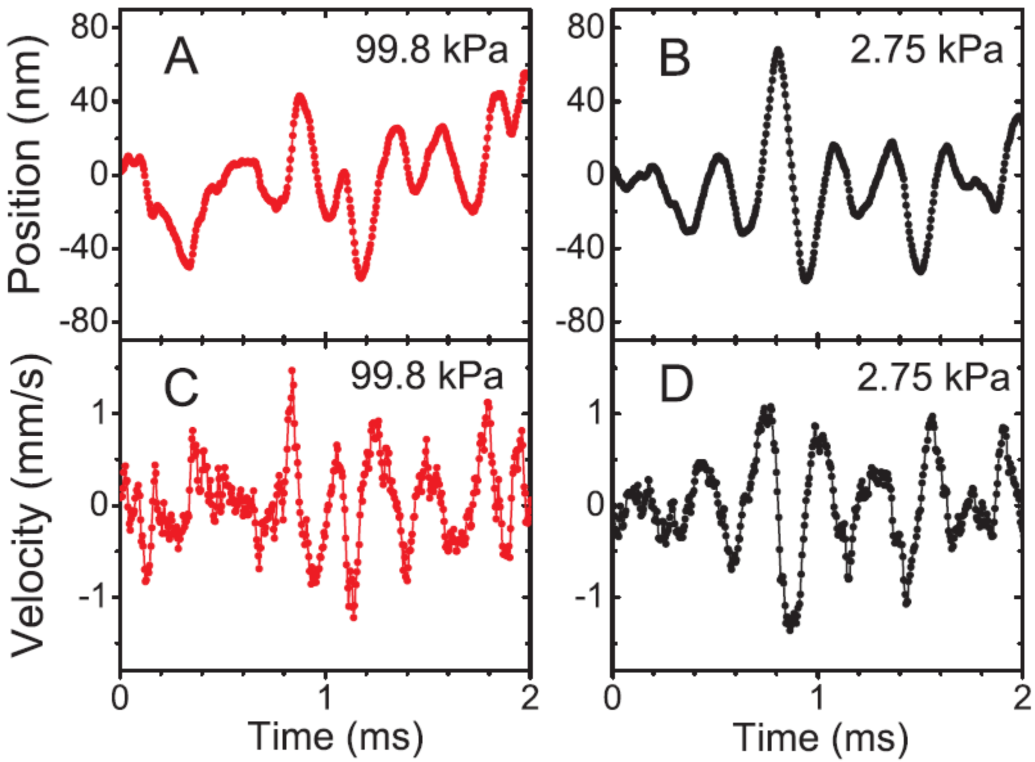

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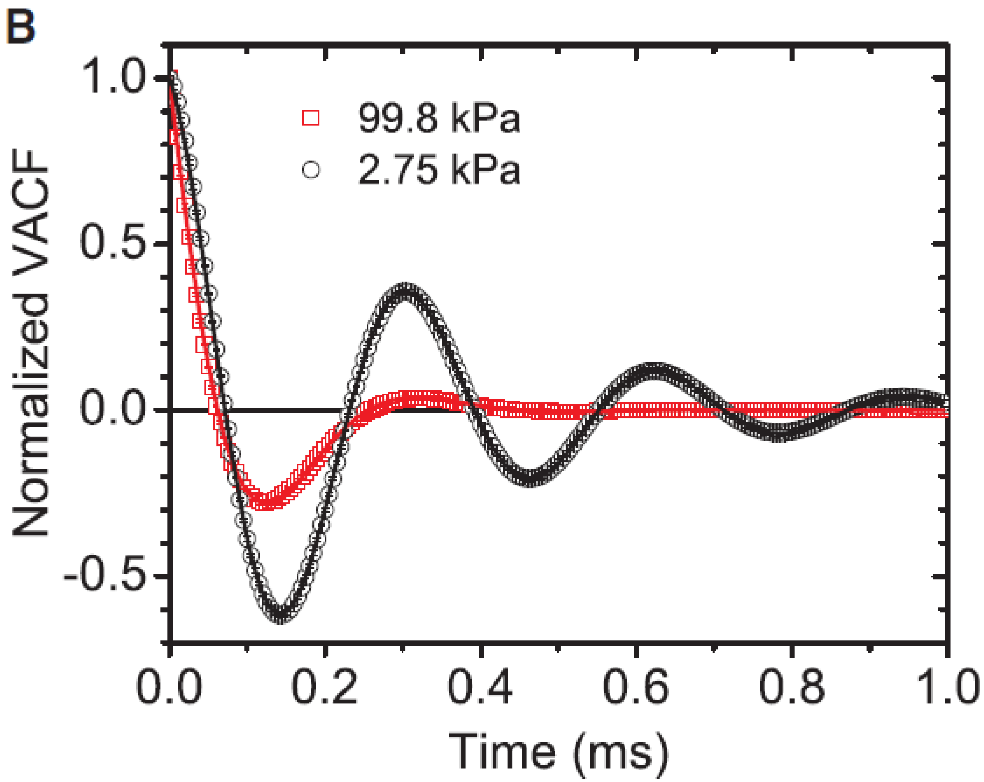

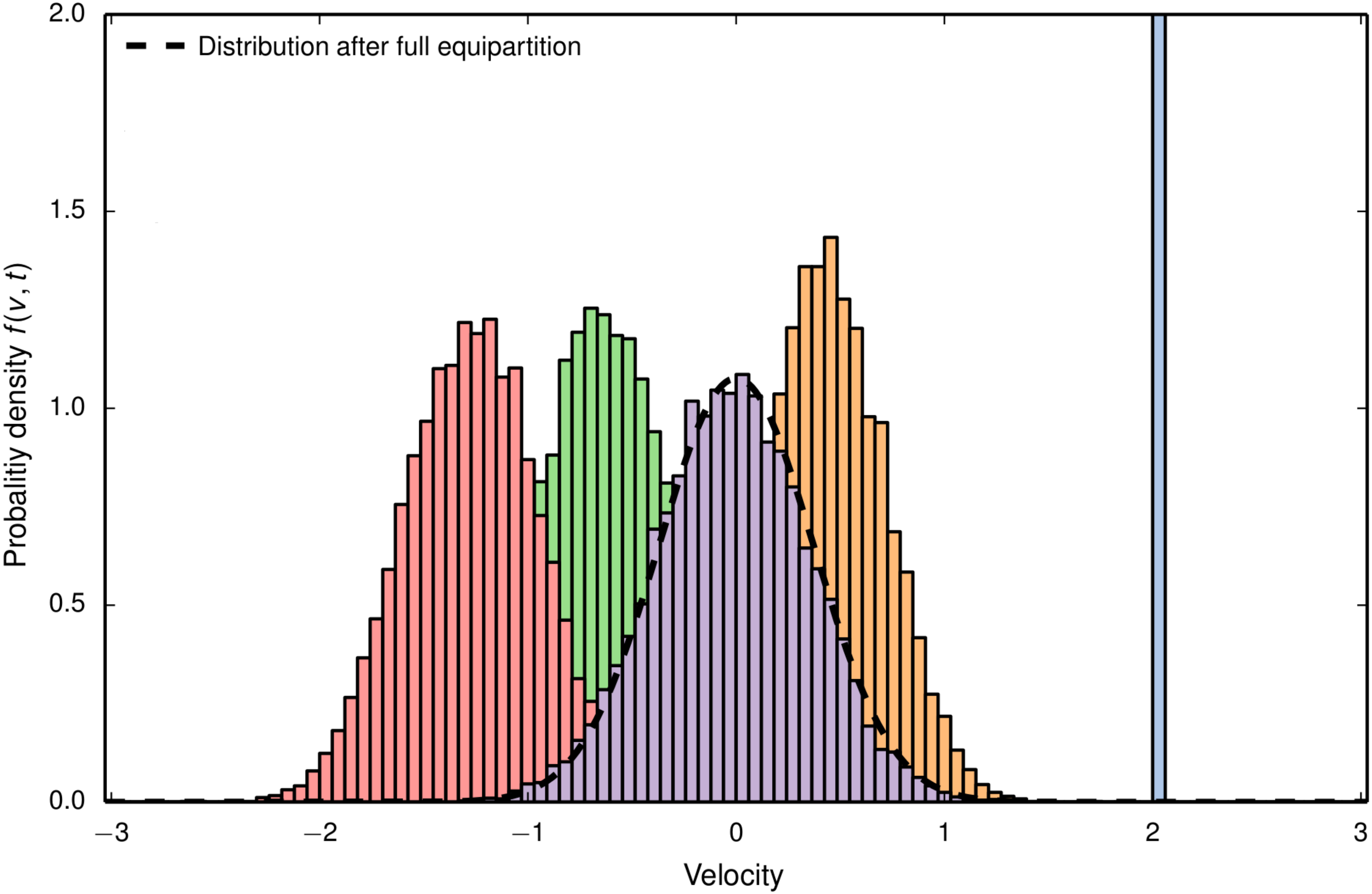
Distribution after full equipartition
2.0
1.5
1.0
0.5
0.0
Probalitiy density $f(v,t)$
−3
−2
−1
0
1
2
3
Velocity