

DDFT for Molecular and Colloidal Fluids: A microscopic approach to fluid mechanics

A. J. Archer

Loughborough University

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What we'll do today

- ▶ Part 1: From the microscopic equations to the N-body PDE
 - ▶ The microscopic dynamics
 - ▶ Hand-wavy derivation of the N-dimensional Fokker-Planck Equation
- ▶ Part2: From the N-body PDE to the one-body equations
 - ▶ Limiting cases, modelling assumptions and limitations of the model
 - ▶ The derivation of the one-body equations
- ▶ Part 3: Connections to simpler equations (time permitting)

What we're actually doing today

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}$$

$$\frac{d\mathbf{p}_i}{dt} = -\gamma\mathbf{p}_i + \mathbf{X}_i(\mathbf{r}_i) + \mathbf{G}_i(t)$$



- Averaging
- 2 Approximations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot (\nabla \mathbf{v}) + \gamma \mathbf{v} = -\frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}$$

Part 1: From the microscopic equations to the N-body PDE

$$\begin{aligned}\frac{d\mathbf{r}_i}{dt} &= \frac{\mathbf{p}_i}{m} \\ \frac{d\mathbf{p}_i}{dt} &= -\gamma\mathbf{p}_i + \mathbf{X}_i(\mathbf{r}_i) + \mathbf{G}_i(t)\end{aligned}$$



- Averaging

$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{X}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$

Part 2: From the N-body PDE to the one-body equations

$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{x}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$



- 2 Approximations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot (\nabla \mathbf{v}) + \gamma \mathbf{v} = -\frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}$$

Part 1

Part 1: From the microscopic equations to the N-body PDE

$$\begin{aligned}\frac{d\mathbf{r}_i}{dt} &= \frac{\mathbf{p}_i}{m} \\ \frac{d\mathbf{p}_i}{dt} &= -\gamma\mathbf{p}_i + \mathbf{X}_i(\mathbf{r}_i) + \mathbf{G}_i(t)\end{aligned}$$



- Averaging

$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{X}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$

Part 1: From the microscopic equations to the N-body PDE

The microscopic equations (1)

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}$$

$$\frac{d\mathbf{p}_i}{dt} = -\gamma\mathbf{p}_i + \mathbf{X}_i(\mathbf{r}_i) + \mathbf{G}_i(t)$$

$\mathbf{G}_i(t)$ stochastic white noise term

$\mathbf{X}_i(\mathbf{r}_i) = -\nabla_{\mathbf{r}_i} V(\mathbf{r}^N, t)$ sum of forces on particle i

$$= -\nabla_{\mathbf{r}_i} \left(\sum_i V^{\text{ext}}(\mathbf{r}_i, t) + \frac{1}{2} \sum_{i,j} v_2(\mathbf{r}_i, \mathbf{r}_j) + \frac{1}{6} \sum_{i,j,k} v_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \dots \right)$$

Part 1: From the microscopic equations to the N-body PDE

The hand-wavy derivation

(see MAC-MIGs modelling course, Lecture 3)

1. Define $\psi^N(\mathbf{r}^N, \mathbf{p}^N, t)$, where $\mathbf{r}^N = \{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\}$ and $\mathbf{p}^N = \{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_N\}$
2. Apply Itô's Lemma to ψ^N
 \Rightarrow get process $d\psi^N(\mathbf{r}^N, \mathbf{p}^N, t) = \dots$
3. Define average $\langle \psi^N \rangle$ and apply to the process $d\psi^N$:
 $\langle d\psi^N \rangle = \langle d[\dots] \rangle$
 \Rightarrow deterministic, since noise averages to zero
4. Average is integral against the probability distribution $f^N(\mathbf{r}^N, \mathbf{p}^N, t)$

$$\begin{aligned} LHS &= \left\langle \frac{d}{dt} \psi^N \right\rangle := \int \int \frac{d}{dt} \psi^N f^N d\mathbf{r}^N d\mathbf{p}^N \\ RHS &= \left\langle \frac{d}{dt} \mathcal{L} \psi^N \right\rangle := \int \int \frac{d}{dt} \mathcal{L} \psi^N f^N d\mathbf{r}^N d\mathbf{p}^N \end{aligned}$$

Part 1: From the microscopic equations to the N-body PDE

The hand-wavy derivation, continued

5. Integrate by parts to get derivatives in terms of f^N instead of ψ^N

$$\begin{aligned} LHS &= \int \int \frac{d}{dt} \psi^N f^N d\mathbf{r}^N d\mathbf{p}^N = \int \int \psi^N \partial_t f^N d\mathbf{r}^N d\mathbf{p}^N \\ RHS &= \int \int \frac{d}{dt} \mathcal{L} \psi^N f^N d\mathbf{r}^N d\mathbf{p}^N = \int \int \psi^N \mathcal{L}^* f^N d\mathbf{r}^N d\mathbf{p}^N \end{aligned}$$

6. Since this holds for all ψ^N

$$\Rightarrow \partial_t f^N = \mathcal{L}^* f^N$$

Part 1: From the microscopic equations to the N-body PDE

The N-body PDE for the distribution $f^N(\mathbf{r}^N, \mathbf{p}^N, t)$ (6)

$$\begin{aligned} \partial_t f^N = \mathcal{L}^* f^N = & -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N \\ & + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{X}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N \end{aligned}$$

Reminder: the microscopic equations (1)

$$\begin{aligned} \frac{d\mathbf{r}_i}{dt} &= \frac{\mathbf{p}_i}{m} \\ \frac{d\mathbf{p}_i}{dt} &= -\gamma \mathbf{p}_i + \mathbf{X}_i(\mathbf{r}_i) + \mathbf{G}_i(t) \end{aligned}$$

Part 1: From the microscopic equations to the N-body PDE

$$\begin{aligned}\frac{d\mathbf{r}_i}{dt} &= \frac{\mathbf{p}_i}{m} \\ \frac{d\mathbf{p}_i}{dt} &= -\gamma\mathbf{p}_i + \mathbf{X}_i(\mathbf{r}_i) + \mathbf{G}_i(t)\end{aligned}$$



- Averaging

$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{X}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$

Part 2

Part 2: From the N-body PDE to the one-body equations

$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{x}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$



- 2 Approximations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot (\nabla \mathbf{v}) + \gamma \mathbf{v} = -\frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}$$

Part 2: From the N-body PDE to the one-body equations

1. Multiply (6) by N and integrate over $\mathbf{r}^{N-1}, \mathbf{p}^{N-1}$

$$\int \int N \partial_t f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} = \int \int N \left[-\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{x}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N \right] d\mathbf{r}^{N-1} d\mathbf{p}^{N-1}$$

Define reduced distribution functions (7):

$$\begin{aligned} f^1(\mathbf{r}_1, \mathbf{p}_1, t) &= N \int \int f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} \\ &\dots \\ f^n(\mathbf{r}^n, \mathbf{p}^n, t) &= \frac{N!}{(N-n)!} \int \int f^N d\mathbf{r}^{N-n} d\mathbf{p}^{N-n} \end{aligned}$$

Part 2: From the N-body PDE to the one-body equations

1. Multiply (6) by N and integrate over $\mathbf{r}^{N-1}, \mathbf{p}^{N-1}$

$$\begin{aligned} \int \int N \partial_t f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} = \int \int N \left[-\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N \right. \\ \left. - \sum_{i=1}^N \mathbf{x}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N \right] d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} \end{aligned}$$

Define reduced distribution functions (7):

$$\begin{aligned} f^1(\mathbf{r}_1, \mathbf{p}_1, t) &= N \int \int f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} \\ &\dots \\ f^n(\mathbf{r}^n, \mathbf{p}^n, t) &= \frac{N!}{(N-n)!} \int \int f^N d\mathbf{r}^{N-n} d\mathbf{p}^{N-n} \end{aligned}$$

Part 2: From the N-body PDE to the one-body equations

Example:

$$\begin{aligned}\int \int N \partial_t f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} &= \partial_t N \int \int f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} \\ &= \partial_t f^1(\mathbf{r}_1, \mathbf{p}_1, t)\end{aligned}$$

where

$$f^1(\mathbf{r}_1, \mathbf{p}_1, t) = N \int \int f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1}$$

Part 2: From the N-body PDE to the one-body equations

$$\int \int N \partial_t f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} = \int \int N \left[-\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{x}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N \right] d\mathbf{r}^{N-1} d\mathbf{p}^{N-1}$$

where (1):

$$\mathbf{x}_i(\mathbf{r}_i) = -\nabla_{\mathbf{r}_i} \left(\sum_i V^{\text{ext}}(\mathbf{r}_i, t) + \frac{1}{2} \sum_{i,j} v_2(\mathbf{r}_i, \mathbf{r}_j) + \dots \right)$$

We get (8):

$$\partial_t f^1 = -\frac{\mathbf{p}_1}{m} \cdot \nabla_{\mathbf{r}_1} f^1 + \gamma \nabla_{\mathbf{p}_1} \cdot (\mathbf{p}_1 f^1) + \nabla_{\mathbf{r}_1} V^{\text{ext}}(\mathbf{r}_1) \cdot \nabla_{\mathbf{p}_1} f^1 + \gamma m k_B T \nabla_{\mathbf{p}_1}^2 f^1 + \int \int \nabla_{\mathbf{r}_1} v_2(\mathbf{r}_1 - \mathbf{r}_2) \cdot \nabla_{\mathbf{p}_1} f^2 d\mathbf{r}_2 d\mathbf{p}_2 + \dots$$

Part 2: From the N-body PDE to the one-body equations

Taking two momentum moments to give 2 equations:

2. First momentum moment: Integrate with respect to \mathbf{p}_1
3. Second momentum moment: Multiply by $\frac{\mathbf{p}_1}{m}$, then integrate with respect to \mathbf{p}_1

2. First momentum moment: Integrate with respect to \mathbf{p}_1 :

$$\int \partial_t f^1 d\mathbf{p}_1 = \int \left[-\frac{\mathbf{p}_1}{m} \cdot \nabla_{\mathbf{r}_1} f^1 + \gamma \nabla_{\mathbf{p}_1} \cdot (\mathbf{p}_1 f^1) + \nabla_{\mathbf{r}_1} V^{\text{ext}}(\mathbf{r}_1) \cdot \nabla_{\mathbf{p}_1} f^1 \right. \\ \left. + \gamma m k_b T \nabla_{\mathbf{p}_1}^2 f^1 + \int \int \nabla_{\mathbf{r}_1} v_2(\mathbf{r}_1 - \mathbf{r}_2) \cdot \nabla_{\mathbf{p}_1} f^2 d\mathbf{r}_2 d\mathbf{p}_2 + \dots \right] d\mathbf{p}_1$$

Part 2: From the N-body PDE to the one-body equations

2. First momentum moment: Integrate with respect to \mathbf{p}_1

$$\int \partial_t f^1 d\mathbf{p}_1 = \int \left[-\frac{\mathbf{p}_1}{m} \cdot \nabla_{\mathbf{r}_1} f^1 + \gamma \nabla_{\mathbf{p}_1} \cdot (\mathbf{p}_1 f^1) + \nabla_{\mathbf{r}_1} V^{\text{ext}}(\mathbf{r}_1) \cdot \nabla_{\mathbf{p}_1} f^1 \right. \\ \left. + \gamma m k_b T \nabla_{\mathbf{p}_1}^2 f^1 + \int \int \nabla_{\mathbf{r}_1} v_2(\mathbf{r}_1 - \mathbf{r}_2) \cdot \nabla_{\mathbf{p}_1} f^2 d\mathbf{r}_2 d\mathbf{p}_2 + \dots \right] d\mathbf{p}_1$$

we get (9):

$$\partial_t \rho(\mathbf{r}_1, t) + \nabla_{\mathbf{r}_1} \cdot \mathbf{j} = 0$$

where (10),(11):

$$\partial_t \rho(\mathbf{r}_1, t) := \partial_t \int f^1 d\mathbf{p}_1, \quad \nabla_{\mathbf{r}_1} \cdot \mathbf{j}(\mathbf{r}_1, t) := \nabla_{\mathbf{r}_1} \cdot \int \frac{\mathbf{p}_1}{m} f^1 d\mathbf{p}_1$$

Part 2: From the N-body PDE to the one-body equations

3. Second momentum moment: Multiply by $\frac{\mathbf{p}_1}{m}$, then integrate with respect to \mathbf{p}_1

$$\int \frac{\mathbf{p}_1}{m} \partial_t f^1 d\mathbf{p}_1 = \int \frac{\mathbf{p}_1}{m} \left[-\frac{\mathbf{p}_1}{m} \cdot \nabla_{\mathbf{r}_1} f^1 + \gamma \nabla_{\mathbf{p}_1} \cdot (\mathbf{p}_1 f^1) + \nabla_{\mathbf{r}_1} V^{\text{ext}}(\mathbf{r}_1) \cdot \nabla_{\mathbf{p}_1} f^1 \right. \\ \left. + \gamma m k_b T \nabla_{\mathbf{p}_1}^2 f^1 + \int \int \nabla_{\mathbf{r}_1} v_2(\mathbf{r}_1 - \mathbf{r}_2) \cdot \nabla_{\mathbf{p}_1} f^2 d\mathbf{r}_2 d\mathbf{p}_2 + \dots \right] d\mathbf{p}_1$$

We get (12):

$$\partial_t \mathbf{j}(\mathbf{r}_1, t) = -\nabla \cdot \int \frac{\mathbf{p}_1 \otimes \mathbf{p}_1}{m^2} f^1 d\mathbf{p}_1 - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{\text{ext}}(\mathbf{r}_1, t) \\ - 0 - \frac{1}{m} \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 + \dots$$

where (13):

$$\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) = \int \int f^2 d\mathbf{p}_1 d\mathbf{p}_2$$

Part 2: From the N-body PDE to the one-body equations

Rewriting some terms (15)-(17)...

$$\begin{aligned}\partial_t \mathbf{j}(\mathbf{r}_1, t) = & -\nabla \cdot \int \frac{\mathbf{p}_1 \otimes \mathbf{p}_1}{m^2} f^1 d\mathbf{p}_1 + \frac{k_b T}{m} \nabla \cdot \int \mathbf{1} f^1 d\mathbf{p}_1 - \frac{k_b T}{m} \nabla \rho(\mathbf{r}_1, t) \\ & - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{\text{ext}}(\mathbf{r}_1, t) - \frac{1}{m} \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 + \dots\end{aligned}$$

$$\begin{aligned}\partial_t \mathbf{j}(\mathbf{r}_1, t) = & -\nabla \cdot \int \frac{\mathbf{p}_1 \otimes \mathbf{p}_1}{m^2} f^1 d\mathbf{p}_1 + \frac{k_b T}{m} \nabla \cdot \int \mathbf{1} f^1 d\mathbf{p}_1 - \frac{k_b T}{m} \nabla \rho(\mathbf{r}_1, t) \\ & - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{\text{ext}}(\mathbf{r}_1, t) - \frac{1}{m} \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 + \dots\end{aligned}$$

$$\begin{aligned}\partial_t \mathbf{j}(\mathbf{r}_1, t) = & -\mathbf{A}(\mathbf{r}_1, t) - \frac{k_b T}{m} \nabla \rho(\mathbf{r}_1, t) \\ & - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{\text{ext}}(\mathbf{r}_1, t) - \frac{1}{m} \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 + \dots\end{aligned}$$

Part 2: From the N-body PDE to the one-body equations

Summary of where we're at:

From (6):

$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{x}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$

1. Multiply by N and integrate over \mathbf{r}^{N-1} , \mathbf{p}^{N-1}
2. First momentum moment gives Equation 1 (9):

$$\partial_t \rho(\mathbf{r}_1, t) + \nabla_{\mathbf{r}_1} \cdot \mathbf{j} = 0$$

3. Second momentum moment gives Equation 2 (16):

$$\begin{aligned} \partial_t \mathbf{j}(\mathbf{r}_1, t) = & -\mathbf{A}(\mathbf{r}_1, t) - \frac{k_b T}{m} \nabla \rho(\mathbf{r}_1, t) \\ & - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{\text{ext}}(\mathbf{r}_1, t) - \frac{1}{m} \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 + \dots \end{aligned}$$

Part 2: From the N-body PDE to the one-body equations

The first approximation The interactions in the nonequilibrium fluid can be approximated by the interactions in the equilibrium fluid (18)-(19)

$$\int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 + \dots \cong \rho(\mathbf{r}_1) \nabla \frac{\delta F_{ex}[\rho]}{\delta \rho}$$

Then Equation 2 becomes:

$$\begin{aligned} \partial_t \mathbf{j}(\mathbf{r}_1, t) = & -\mathbf{A}(\mathbf{r}_1, t) - \frac{k_b T}{m} \nabla \rho(\mathbf{r}_1, t) - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{\text{ext}}(\mathbf{r}_1, t) \\ & - \frac{1}{m} \rho(\mathbf{r}_1) \nabla \frac{\delta F_{ex}[\rho]}{\delta \rho} \end{aligned}$$

Part 2: From the N-body PDE to the one-body equations

Note: $\nabla \rho(\mathbf{r}_1, t) = \rho(\mathbf{r}_1, t) \ln(\rho(\mathbf{r}_1, t))$

Then Equation 2 is (20):

$$\begin{aligned}\partial_t \mathbf{j}(\mathbf{r}_1, t) &= -\mathbf{A}(\mathbf{r}_1, t) - \frac{k_b T}{m} \rho(\mathbf{r}_1, t) \ln(\rho(\mathbf{r}_1, t)) - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{\text{ext}}(\mathbf{r}_1, t) \\ &\quad - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla \frac{\delta F_{\text{ex}}[\rho]}{\delta \rho} \\ \partial_t \mathbf{j}(\mathbf{r}_1, t) &= -\mathbf{A}(\mathbf{r}_1, t) - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla \frac{\delta F[\rho]}{\delta \rho}\end{aligned}$$

Part 2: From the N-body PDE to the one-body equations

The second approximation We can make a "local-equilibrium" approximation for f^1 (22)

$$f_{l.e.}^1(\mathbf{r}_1, \mathbf{p}_1, t) = c_1 \rho(\mathbf{r}_1, t) \exp \left\{ -c_2 (\mathbf{p} - m\mathbf{v})^2 \right\}$$

Then (23):

$$\mathbf{j} = \int \frac{\mathbf{p}_1}{m} f^1 d\mathbf{p}_1 \cong \rho(\mathbf{r}_1, t) \mathbf{v}(\mathbf{r}_1, t)$$

Part 2: From the N-body PDE to the one-body equations

So, finally Equation 1 becomes (24):

$$\begin{aligned}\partial_t \rho(\mathbf{r}_1, t) + \nabla_{\mathbf{r}_1} \cdot \mathbf{j} &= 0 \\ \partial_t \rho(\mathbf{r}_1, t) + \nabla_{\mathbf{r}_1} \cdot (\rho(\mathbf{r}_1, t) \mathbf{v}(\mathbf{r}_1, t)) &= 0\end{aligned}$$

Part 2: From the N-body PDE to the one-body equations

And since (17):

$$\mathbf{A}(\mathbf{r}_1, t) := -\nabla \cdot \int \frac{\mathbf{p}_1 \otimes \mathbf{p}_1}{m^2} f^1 d\mathbf{p}_1 + \frac{k_b T}{m} \nabla \cdot \int \mathbf{1} f^1 d\mathbf{p}_1$$

we have that Equation 2 (20):

$$\partial_t \mathbf{j}(\mathbf{r}_1, t) = -\mathbf{A}(\mathbf{r}_1, t) - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla \frac{\delta F[\rho]}{\delta \rho}$$

becomes (26):

$$\partial_t (\rho \mathbf{v}) = -\nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) - \gamma \rho \mathbf{v} - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla \frac{\delta F[\rho]}{\delta \rho}$$

Part 2: From the N-body PDE to the one-body equations

Then Equation 2 (26):

$$\partial_t (\rho \mathbf{v}) = -\nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) - \gamma \rho \mathbf{v} - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla \frac{\delta F[\rho]}{\delta \rho}$$

becomes (30)-(31):

$$\partial_t \mathbf{v} = -\mathbf{v} \cdot (\nabla \mathbf{v}) - \gamma \mathbf{v} - \frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}$$

by rewriting $\nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v})$ and $\partial_t (\rho \mathbf{v})$ and cancelling a factor of ρ .

Part 2: From the N-body PDE to the one-body equations

Therefore, the one-body equations (Equation 1 and Equation 2) are (24) and (30):

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\partial_t \mathbf{v} = -\mathbf{v} \cdot (\nabla \mathbf{v}) - \gamma \mathbf{v} - \frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}$$

Part 2: From the N-body PDE to the one-body equations

$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{x}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$



- 2 Approximations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot (\nabla \mathbf{v}) + \gamma \mathbf{v} = -\frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}$$

Summary

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}$$

$$\frac{d\mathbf{p}_i}{dt} = -\gamma\mathbf{p}_i + \mathbf{X}_i(\mathbf{r}_i) + \mathbf{G}_i(t)$$



$$\partial_t f^N = -\frac{1}{m} \sum_{i=1}^N \mathbf{p}_i \cdot \nabla_{\mathbf{r}_i} f^N + \gamma \sum_{i=1}^N \nabla_{\mathbf{p}_i} \cdot \mathbf{p}_i f^N - \sum_{i=1}^N \mathbf{X}_i \cdot \nabla_{\mathbf{p}_i} f^N + \gamma m k_B T \sum_{i=1}^N \nabla_{\mathbf{p}_i}^2 f^N$$



$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot (\nabla \mathbf{v}) + \gamma \mathbf{v} = -\frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}$$

Part 3

Part 3: Simplifications - The Overdamped Limit

We can take the overdamped limit when γ is large. Then $\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot (\nabla \mathbf{v}) = 0$

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot (\nabla \mathbf{v}) + \gamma \mathbf{v} &= -\frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho}\end{aligned}$$

So we get (32):

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \mathbf{v} &= -\frac{1}{m\gamma} \nabla \frac{\delta F[\rho]}{\delta \rho}\end{aligned}$$

and finally get an overdamped equation in ρ only (5):

$$\frac{\partial \rho}{\partial t} - \frac{1}{m\gamma} \nabla \cdot \left(\rho \nabla \frac{\delta F[\rho]}{\delta \rho} \right) = 0$$

Part 3: Simplifications - The Diffusion Equation

From this overdamped equation:

$$\frac{\partial \rho}{\partial t} - \frac{1}{m\gamma} \nabla \cdot \left(\rho \nabla \frac{\delta F[\rho]}{\delta \rho} \right) = 0$$

we can recover the diffusion equation! Choose

$$F[\rho] = \int \rho(\mathbf{r})(\log \rho(\mathbf{r}) - 1) d\mathbf{r}$$

then

$$\frac{\delta F[\rho]}{\delta \rho} = \log \rho(\mathbf{r}), \quad \nabla \frac{\delta F[\rho]}{\delta \rho} = \nabla \log \rho(\mathbf{r}) = \frac{\nabla \rho}{\rho}, \quad \rho \nabla \frac{\delta F[\rho]}{\delta \rho} = \nabla \rho.$$

and

$$\frac{\partial \rho}{\partial t} - \frac{1}{m\gamma} \nabla \cdot (\nabla \rho) = 0 \quad \Rightarrow \quad \frac{\partial \rho}{\partial t} = D_0 \nabla \cdot (\nabla \rho) = D_0 \Delta \rho$$

Part 3: Simplifications - A Mean-Field Equation

From this overdamped equation:

$$\frac{\partial \rho}{\partial t} - \frac{1}{m\gamma} \nabla \cdot \left(\rho \nabla \frac{\delta F[\rho]}{\delta \rho} \right) = 0$$

we can get a Mean Field Equation! Choose

$$\rho(\mathbf{r}_1, t) \frac{\delta F[\rho]}{\delta \rho} = \rho(\mathbf{r}_1, t) \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2$$

then

$$\frac{\partial \rho(\mathbf{r}_1, t)}{\partial t} - \frac{1}{m\gamma} \nabla \cdot \left(\rho(\mathbf{r}_1, t) \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 \right) = 0$$

Part 3: Simplifications - A Mean-Field Equation

From this equation:

$$\frac{\partial \rho}{\partial t} - \frac{1}{m\gamma} \nabla \cdot \left(\int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 \right) = 0$$

We make the mean field approximation:

$$\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \cong \rho(\mathbf{r}_1, t) \rho(\mathbf{r}_2, t)$$

Then we get a mean-field equation:

$$\frac{\partial \rho}{\partial t} - \frac{1}{m\gamma} \nabla \cdot \left(\int \rho(\mathbf{r}_1, t) \rho(\mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 \right) = 0$$