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

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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

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

- Averaging
- 2 Approximations

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

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

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

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

- Averaging

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

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

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

$$\Big\Downarrow \text{ - 2 Approximations}$$

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

Part 1

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

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

$$\Big\downarrow \text{ - Averaging}$$

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

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

$$\mathbf{X}_i(\mathbf{r}_i) = -\nabla_{\mathbf{r}_i} V(\mathbf{r}^N, t) \qquad \text{sum of forces on particle } i$$
$$= -\nabla_{\mathbf{r}_i}\left(\sum_i V^{ext}(\mathbf{r}_i, t) + \frac{1}{2}\sum_{i,j} v_2(\mathbf{r}_i, \mathbf{r}_j) + \frac{1}{6}\sum_{i,j,k} v_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + ...\right)$$

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

$$LHS = \langle \frac{d}{dt}\psi^N \rangle := \int\int \frac{d}{dt}\psi^N f^N d\mathbf{r}^N d\mathbf{p}^N$$

$$RHS = \langle \frac{d}{dt}\mathcal{L}\psi^N \rangle := \int\int \frac{d}{dt}\mathcal{L}\psi^N f^N d\mathbf{r}^N d\mathbf{p}^N$$

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

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

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)

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

Reminder: the microscopic equations (1)

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

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

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

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

Part 2

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

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

$\Downarrow$ - 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 $\mathbf{r}^{N-1}$, $\mathbf{p}^{N-1}$

$$\int\int N\partial_t f^N d\mathbf{r}^{N-1} d\mathbf{p}^{N-1} = \int\int N\Big[-\frac{1}{m}\sum_{i=1}^{N}\mathbf{p}_i\cdot\nabla_{\mathbf{r}_i} f^N + \gamma\sum_{i=1}^{N}\nabla_{\mathbf{p}_i}\cdot\mathbf{p}_i f^N$$

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

Define reduced distribution functions (7):

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

$$\ldots$$

$$f^n(\mathbf{r}^n,\mathbf{p}^n,t) = \frac{N!}{(N-n)!}\int\int f^N d\mathbf{r}^{N-n} d\mathbf{p}^{N-n}$$

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

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

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

Define reduced distribution functions (7):

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

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

Example:

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

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

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

where (1):

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

We get (8):

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

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 $\mathbf{p}_1$:

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

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

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

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

we get (9):

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

where (10),(11):

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

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 $\mathbf{p}_1$

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

We get (12):

$$\partial_t \mathbf{j}(\mathbf{r}_1, t) = -\nabla \cdot \int \frac{\mathbf{p}_1 \otimes \mathbf{p}_1}{m^2} f^1 d\mathbf{p}_1 - \gamma \mathbf{j}(\mathbf{r}_1, t) - \frac{1}{m} \rho(\mathbf{r}_1, t) \nabla V^{ext}(\mathbf{r}_1, t)$$
$$- 0 - \frac{1}{m} \int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r_2}) d\mathbf{r_2} + \ldots$$

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)...

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

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

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

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

Summary of where we're at:

From (6):

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

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):

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

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)

$$\int \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t)\nabla v_2(\mathbf{r}_1 - \mathbf{r_2})d\mathbf{r_2} + ... \approxeq \rho(\mathbf{r}_1)\nabla\frac{\delta F_{ex}[\rho]}{\delta\rho}$$

Then Equation 2 becomes:

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

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):

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

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

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)

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

Then (23):

$$\mathbf{j} = \int \frac{\mathbf{p}_1}{m} f^1 d\mathbf{p}_1 \approxeq \rho(\mathbf{r}_1, t)\mathbf{v}(\mathbf{r_1}, t)$$

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

So, finally Equation 1 becomes (24):

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

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

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

$\Downarrow$ - 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

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

$$\Downarrow$$

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

$$\Downarrow$$

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

Part 3

Part 3: Simplifications - The Overdamped Limit

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

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

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

So we get (32):

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

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

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

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

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:

$$\rho^{(2)}(\mathbf{r}_1, \mathbf{r_2}, t) \approxeq \rho(\mathbf{r}_1, t)\rho(\mathbf{r_2}, t)$$

Then we get a mean-field equation:

$$\frac{\partial \rho}{\partial t} - \frac{1}{m\gamma} \nabla \cdot \left(\int \rho(\mathbf{r}_1, t)\rho(\mathbf{r_2}, t) \nabla v_2(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_2 \right) = 0$$