On the Kinetic Description of Objective Molecular Dynamics (OMD)

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Based on the joint work with Richard D. James (UMN) and Li Wang (UMN)

Outline

1. Introduction

Background and Motivation

"Scale": Newtonian Mechanics ⇒ **Kinetic Theory** ⇒ Continuum Mechanics

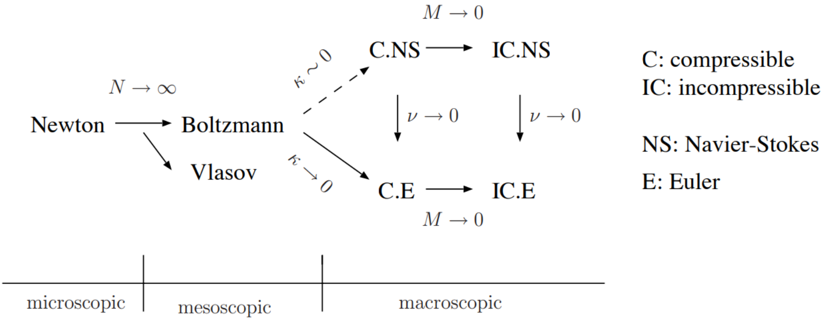

Figure: Role of kinetic theory in multiscale modeling hierarchy[1]

[1] S. Ukai and T. Yang, Mathematical Theory of Boltzmann Equation, '06

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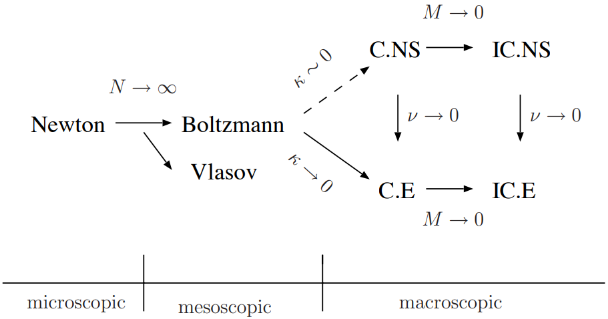

C: compressible
IC: incompressible

NS: Navier-Stokes

E: Euler

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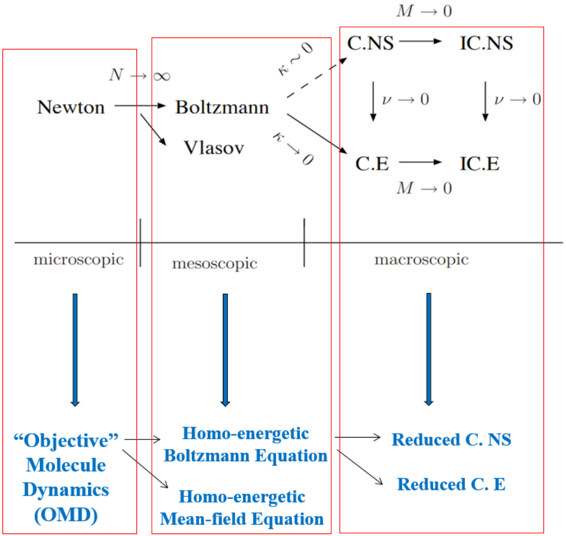

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"Objective Molecule Dynamics" (OMD)

"Objective Molecule Dynamics" (OMD) is a time-dependent invariant manifold of the equations of molecular dynamics.

Basic Set-up

- $\Longrightarrow$ **Simulated atoms**:

$$x_k(t), \quad k = 1, \ldots, M$$

"+" A discrete group of isometries [a]:

$$G = \{g_1, g_2, \ldots, g_N\}, \quad M \ll N$$

- $\Longrightarrow$ **Non-simulated atoms**:

$$x_{i,k}(t) = g_i(x_k(t))$$

$i = 1, \ldots, N, \; k = 1, \ldots, M.$

[a] $g_1 := Id$, so $x_{1,k}(t) = x_k(t)$

Objective Structure

1-OS: each atom "see the same environment"

A set of points in $\mathbb{R}^3$ is given, $\mathcal{S} = \{x_i \in \mathbb{R}^3, i = 1, ..., N\}$, $N \le \infty$. $\mathcal{S}$ is a 1-OS if there are orthogonal transformations $Q_1, ..., Q_N$ such that

$$\{x_i + Q_i(x_j - x_1) : j = 1, ..., N\} = \mathcal{S}, \text{ for } i = 1, ..., N$$

M-OS: $x_{i,k}$ "see the same environment" as $x_{1,k}$

Consider a structure consisting of N "molecules", each consisting of M atoms: $\mathcal{S} = \{x_{i,k} \in \mathbb{R}^3 : i = 1, ..., N, \ k = 1, ..., M\}$, $N \le \infty$, $M < \infty$.
$\mathcal{S}$ is an M-OS, if $x_{1,1}, ..., x_{1,M}$ are distinct and there are NM orthogonal transformations $Q_{i,k}$ such that

$$\{x_{i,k} + Q_{i,k}(x_{j,l} - x_{1,k}) : j = 1, ..., N, \ l = 1, ..., M\} = \mathcal{S}, \text{ for } i = 1, ..., N, \ k = 1, ..., M$$

Example of objective structure

Buckminsterfullerine (C_{60})

Let $G = \{R_1, ..., R_N\}$ be a finite subgroup of $O(3)$ with $N = 60$ and let $x_i = R_i x_1$

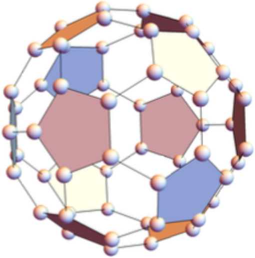

Figure: Buckminsterfullerine (C_{60})

Single-walled carbon nanotubes

Let $\vec{e}_1, \vec{e}_2, \vec{e}_3$ be an orthonormal basis and $R_\theta \in SO(3)$, the carbon nanotubes are given by

$$g_1^{\nu_1} g_2^{\nu_2} g_3^{\nu_3}, \quad \nu_1, \nu_2, \nu_3 \in \mathbb{Z}$$

with

$$g_1 = (R_{\theta_1}|t_1),\ g_2 = (R_{\theta_2}|t_2)$$
$$g_3 = (-I + 2e \otimes e|0)$$

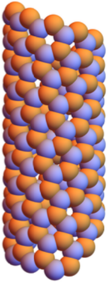

Figure: Carbon nanotube (1-OS) with chirality $n = 3, m = 8$

Symmetry and Invariance

Isometry Group

$$g = (Q|c), \quad Q \in O(3), \; c \in \mathbb{R}^3$$

$$g(x) = Qx + c, \quad x \in \mathbb{R}^3$$

- Closure: $g_1 = (R_1 \,|\, c_1), \; g_2 = (R_2 \,|\, c_2), \; g_1 g_2 = (R_1 R_2 \,|\, c_1 + R_1 c_2)$

  $\Rightarrow g_1 g_2(x) = g_1(g_2(x))$
- Identity: $Id = (I \,|\, 0)$
- Inverse: $(Q \,|\, c)^{-1} = (Q^\top \,|\, -Q^\top c)$

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- Identity: $Id = (I \,|\, 0)$
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Recall: For a typical dynamical system $(x_i(t), v_i(t))$: for $i = 1, \dots, N$,

$$\begin{cases} \dot{x}_i(t) = v_i(t), \\ \ddot{x}_i(t) = \dot{v}_i(t) = -\sum_{\substack{j=1 \\ j \neq i}}^{N} \nabla_{x_i} U\left(|x_i(t) - x_j(t)|\right). \end{cases}$$

Invariant requirement of the potential*

1. **Frame-indifference**: $Q \in O(3), \;\; c \in \mathbb{R}^3$

$$Q\frac{\partial U}{\partial x_{i,k}}(\dots, x_{i_1,1}, \dots, x_{i_1,M}, \dots, x_{i_2,1}, \dots, x_{i_2,M}) = \frac{\partial U}{\partial x_{i,k}}(\dots, Qx_{i_1,1} + c, \dots, Qx_{i_1,M} + c, \dots, Qx_{i_2,1} + c, \dots, Qx_{i_2,M} + c)$$

2. **Permutation invariance**:

$$\frac{\partial U}{\partial x_{\Pi(i,k)}}(\dots, x_{i_1,1}, \dots, x_{i_1,M}, \dots, x_{i_2,1}, \dots, x_{i_2,M}) = \frac{\partial U}{\partial x_{i,k}}(\dots, x_{\Pi(i_1,1)}, \dots, x_{\Pi(i_1,M)}, \dots, x_{\Pi(i_2,1)}, \dots, x_{\Pi(i_2,M)})$$

Requirement of isometry**

The isometries g_i can depend explicitly on $t > 0$, but this time dependence must be consistent with

$$\frac{\mathrm{d}^2 x_{j,k}(t)}{\mathrm{d}t^2} = \frac{\mathrm{d}^2}{\mathrm{d}t^2} g_i(x_k(t), t) = Q_i \frac{\mathrm{d}^2 x_k(t)}{\mathrm{d}t^2}$$

for $g_i = (Q_i | c_i) \in G, \;\; i = 1, \dots, N, \;\; k = 1, \dots, M$

Theorem ([James, ICM, '18])

Assumptions: **Invariant requirement of the potential*** + **Requirement of isometry****.

If $\mathbf{x_k(t)} = \mathbf{x_{1,k}(t)}$, $k = 1, \dots, N$ *satisfy the equation of molecular dynamics, i.e.,*

$$\begin{cases} m_k \ddot{x}_{1,k} = f_{1,k}(\dots, x_{j,1}, x_{j,2}, \dots, x_{j,M}, x_{j+1,1}, x_{j+1,2}, \dots, y_{j+1,M}, \dots) \\ \qquad\quad = f_{1,k}(\dots, g_j(y_{1,1}, t), \dots, g_j(y_{1,M}, t), g_{j+1}(y_{1,M}, t)), \dots, g_{j+1}(y_{1,M}, t) \\ x_{1,k}(0) = x_k^0, \quad \dot{x}_{1,k}(0) = v_k^0, \quad k = 1, \dots, M \end{cases}$$

Then, $\mathbf{x_{i,k}} = \mathbf{g(x_{1,k}(t), t)}$, $i = 1, \dots, N$, $k = 1, \dots, M$ *satisfy* **the same** *equations of molecular dynamics:*

$$m_k \ddot{x}_{i,k} = f_{1,k}(\dots, x_{j,1}, x_{j,2}, \dots, x_{j,M}, x_{j+1,1}, x_{j+1,2}, \dots, y_{j+1,M}, \dots)$$

Sketch of Proof

$$m_k \ddot{x}_{i,k} = m_k Q_i \ddot{x}_{1,k} \quad \textbf{[Requirement**]}$$

$$= Q_i f_{1,k}(\dots, x_{j,1}, \dots, x_{j,M}, x_{j+1,1}, x_{j+1,2}, \dots, y_{j+1,M}, \dots)$$

$$= Q_i f_{\Pi(i,k)}(\dots, x_{j,1}, \dots, x_{j,M}, x_{j+1,1}, x_{j+1,2}, \dots, y_{j+1,M}, \dots) \ \textbf{[Requirement* (2)]}$$

$$= Q_i f_{i,k}(\dots, x_{\Pi(j,1)}, \dots, x_{\Pi(j,M)}, x_{\Pi(j+1,1)}, x_{\Pi(j+1,2)}, \dots, y_{\Pi(j+1,M)}, \dots)$$

$$= Q_i f_{i,k}(\dots, g_i^{-1}(x_{j,1}), \dots, g_i^{-1}(x_{j,M}), g_i^{-1}(x_{j+1,1}), \dots, g_i^{-1}(x_{j+1,M}))$$

$$= Q_i f_{i,k}(\dots, Q_i^T(x_{j,1} - c_i), \dots, Q_i^T(x_{j,M} - c_i), Q_i^T(x_{j+1,1} - c_i), \dots, Q_i^T(x_{j+1,M} - c_i), \dots) \ \textbf{[Requirement* (1)]}$$

$$= f_{i,k}(\dots, x_{j,1}, x_{j,2}, \dots, x_{j,M}, x_{j+1,1}, x_{j+1,2}, \dots, y_{j+1,M}, \dots)$$

Requirement of isometry** $\Longrightarrow$ $Q_i = \text{const} \in O(3)$ and $c_i = a_i t + b_i$

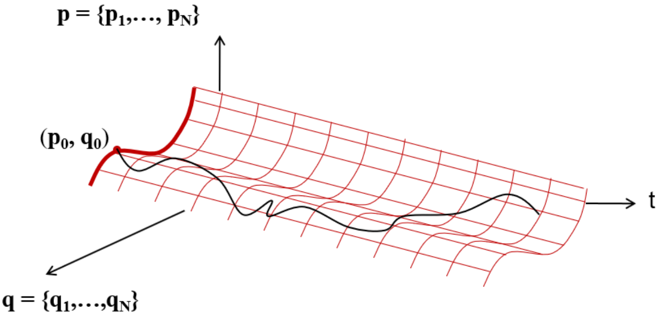


Figure: The invariant manifold of the equations of molecular dynamics.

$$\begin{cases} p = m_k \dot{x}_{i,k} = m_k \dfrac{\mathrm{d}}{\mathrm{d}t} g_i(x_{1,k}, t) = m_k Q_i \dot{x}_{1,k} + m_k a_i \\ q = x_{i,k} = g_i(x_{1,k}, t) = Q x_{1,k} + a_i t + b_i \end{cases}$$

The simplest example

Translation Group:

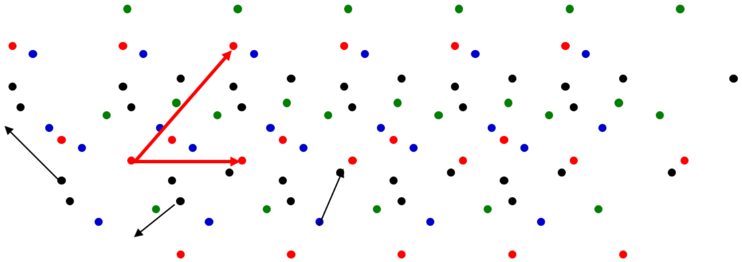
$$G_T = \{(\underbrace{I}_{:=Q} \mid \underbrace{\nu_1\vec{e}_1 + \nu_2\vec{e}_2 + \nu_3\vec{e}_3}_{:=c}) : \nu^1, \nu^2, \nu^3 \in \mathbb{Z}\}$$

then, Simulated atoms:

$$x_k(t) = x_{(0,0,0),k}(t), \quad k = 1, \dots, M$$

Non-simulated atoms:

$$x_{\nu,k}(t) = g_\nu(x_k(t), t) = x_k(t) + (I + tA)(\nu^i \vec{e}_i), \quad k = 1, \dots, M$$



Simple Shear

$$A = \begin{pmatrix} 0 & K & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

In Euerian Framework:

$$u(t,x) = A(I + tA)^{-1}x$$

http://www.aem.umn.edu/ james/research/people.html

By Pahlani-James

2. From Microscopic to Mesoscopic

From now, let us jump into the kinetic regime

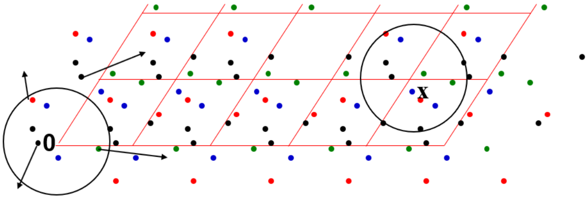


Figure: The invariant manifold of the equations of molecular dynamics in kinetic regime

What can be inherited from the invariant manifold?

- The velocities at $x_k = 0$ are $\dot{x}_k$, $k = 1, .., M$
- The velocities at $x = (I + tA)\nu$ are $\dot{x}_k + A\nu$, $k = 1, ..., M$
- Or, in the Eulerian form used in the kinetic theory, the velocities at x are $\dot{x}_k + A(I + tA)^{-1}x$, $k = 1, ..., M$

$$f(t,0,v) = f(t,x,v + A(I + tA)^{-1}x) \implies f(t,x,v) = g(t, \underbrace{v - A(I + tA)^{-1}x}_{=:w})$$

For Boltzmann equation

Classical Boltzmann equation

$$\frac{\partial}{\partial t} f(t,x,v) + v\cdot\nabla_x f(t,x,v) = Q(f,f)(t,x,v)$$

$$\Downarrow f(t,x,v) = g(t,w) \text{ with } w := v - A(I+tA)^{-1}x$$

$$\frac{\partial}{\partial t} g(t,w) + [A(I+tA)^{-1}w]\cdot\nabla_w g(t,w) = Q(g,g)(t,w)$$

Homo-energetic Boltzmann equation

$$Q(g,f) = \int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} \underbrace{\mathcal{B}(v-v_*,\sigma)}_{\text{collision kernel}}[\underbrace{g(v'_*)f(v')}_{\text{"gain"}} - \underbrace{g(v_*)f(v)}_{\text{"loss"}}]\,d\sigma\,dv_*$$

$$\begin{cases} v' = \dfrac{v+v_*}{2} + \dfrac{|v-v_*|}{2}\sigma \\ v'_* = \dfrac{v+v_*}{2} - \dfrac{|v-v_*|}{2}\sigma \end{cases}$$

where the parameter σ varies over the unit sphere $\mathbb{S}^{d-1}$.

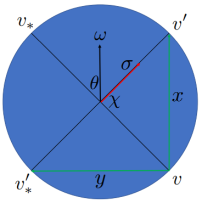


Figure: Velocities during a classical elastic collision

For Boltzmann equation

Classical Boltzmann equation

$$\frac{\partial}{\partial t} f(t,x,v) + v \cdot \nabla_x f(t,x,v) = Q(f,f)(t,x,v)$$

$$\Downarrow f(t,x,v) = g(t,w) \text{ with } w := v - A(I+tA)^{-1}x$$

$$\frac{\partial}{\partial t} g(t,w) + [A(I+tA)^{-1}w] \cdot \nabla_w g(t,w) = Q(g,g)(t,w)$$

Homo-energetic Boltzmann equation

$$Q(g,f) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \underbrace{\mathcal{B}(v-v_*,\sigma)}_{\text{collision kernel}} [\underbrace{g(v_*')f(v')}_{\text{"gain"}} - \underbrace{g(v_*)f(v)}_{\text{"loss"}}] \, \mathrm{d}\sigma \, \mathrm{d}v_*$$

$$\begin{cases} v' = \dfrac{v+v_*}{2} + \dfrac{|v-v_*|}{2}\sigma \\ v_*' = \dfrac{v+v_*}{2} - \dfrac{|v-v_*|}{2}\sigma \end{cases}$$

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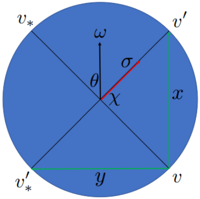


Figure: Velocities during a classical elastic collision

Remark I: Classification

$$f(t,x,v) = g(t,w) \quad \text{with} \quad w = v - \xi(t,x)$$

$$\xi(t,x) = L(t)x = A(I+At)^{-1}x$$

$$\begin{cases} \text{(i)} \ \dfrac{\partial \xi_k}{\partial x_j} \text{ independent on } x; \\ \text{(ii)} \ \partial_t \xi + \xi \cdot \nabla_x \xi = 0. \end{cases}$$

Simple shear:

$$L(t) = \begin{pmatrix} 0 & K & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad K \neq 0$$

Planar shear:

$$L(t) = \frac{1}{t}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & K \\ 0 & 0 & 1 \end{pmatrix} + O\left(\frac{1}{t^2}\right) \quad \text{as } t \to \infty.$$

Simple shear with decaying planar dilatation/shear.

$$L(t) = \begin{pmatrix} 0 & K_2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{t}\begin{pmatrix} 0 & K_1K_3 & K_1 \\ 0 & 0 & 0 \\ 0 & K_3 & 1 \end{pmatrix} + O\left(\frac{1}{t^2}\right), \quad K_2 \neq 0$$

Combined orthogonal shear:

$$L(t) = \begin{pmatrix} 0 & K_3 & K_2 - tK_1K_3 \\ 0 & 0 & K_1 \\ 0 & 0 & 0 \end{pmatrix}, \quad K_1K_3 \neq 0$$

Figure: The classification of deformation term.

Remark II: Collision kernel

The collision kernel $\mathcal{B}$ is a non-negative function that depends on its arguments only through $|v - v_*|$ and cosine of the deviation angle θ:

$$\mathcal{B}(v - v_*, \sigma) = B(|v - v_*|, \cos\theta), \quad \cos\theta = \frac{\sigma \cdot (v - v_*)}{|v - v_*|}.$$

For the inverse power law potential,

$$B(|v - v_*|, \cos\theta) = b(\cos\theta)\Phi(|v - v_*|)$$

- Kinetic part:

$$\Phi(|v-v_*|) = |v-v_*|^\gamma \Rightarrow \begin{cases} \gamma > 0, \text{ Hard potential} \Longrightarrow \textbf{Collision Dominated Case} \\ \gamma = 0, \text{ Maxwellian molecules} \Longrightarrow \textbf{Balanced Case} \\ \gamma < 0, \text{ Soft potential} \Longrightarrow \textbf{Hyperbolic Dominated Case} \end{cases}$$

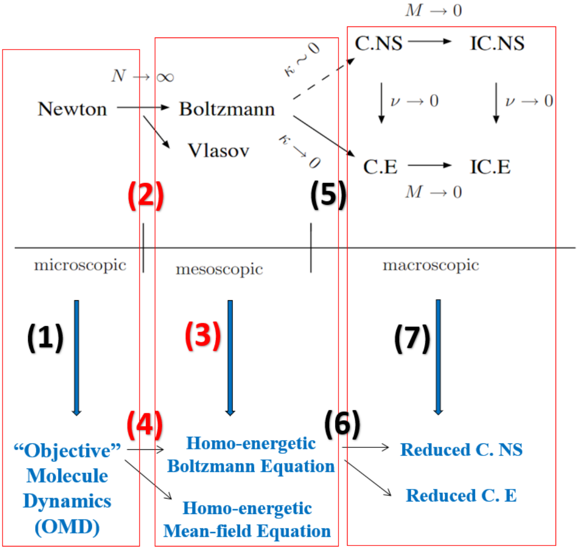
Consider the re-scaling $g(t,w) = \frac{1}{t}G(\tau,\xi)$ with $\tau = \log(t)$, $\xi_1 = \frac{w_1}{t}$ $\xi_j = w_j$, $j = 2,3$:

$$\frac{\partial G}{\partial \tau} - \text{div}_\xi[(\xi_1 + K\xi_2)\vec{e}_1 G] \approx e^{\gamma\tau} Q(G,G)$$

- Angular part:

$$\sin^{d-2}\theta b(\cos\theta)\Big|_{\theta\to 0} \sim K\theta^{-1-\nu}, \quad 0 < \nu < 2$$

Recall the Big Picture



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Previous work

Arrow (2): BBGKY hierarchy

- Mean-field Limit: $N \to \infty$.

$$\begin{cases} \dot{x}_i(t) = v_i(t), \\ \dot{v}_i(t) = -\frac{1}{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \nabla_{x_i} U\left(|x_i(t) - x_j(t)|\right). \end{cases}$$

[Braun-Hepp,'77], [Golse, '03], [Spohn, '12]

- Boltzmann-Grad Limit: $N\varepsilon^{d-1} \to O(1), \ N \to \infty, \ \varepsilon \to 0.$

$$\begin{cases} \dot{x}_i(t) = v_i(t), \\ \dot{v}_i(t) = -\frac{1}{\varepsilon} \sum_{\substack{j=1 \\ j \neq i}}^{N} \nabla_{x_i} U\left(\frac{|x_i(t) - x_j(t)|}{\varepsilon}\right). \end{cases}$$

[Grad,'49, '58], [Cercignani, '72], [Lanford, '75], [Gallagher-Raymond-Texier, '13]

Arrow (3): Homo-energetic Transformation $f(t,x,v) = g(t, \underbrace{v - A(I+tA)^{-1}x}_{=:w})$

[Dayal-James, '10], [James, '18], [James-Nota-Velazquez, '19]

Our first goal:

How to proceed with **Arrow (4)** ?

Previous work

Arrow (2): BBGKY hierarchy

- Mean-field Limit: $N \to \infty$.

$$\begin{cases} \dot{x}_i(t) = v_i(t), \\ \dot{v}_i(t) = -\frac{1}{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \nabla_{x_i} U\left(|x_i(t) - x_j(t)|\right). \end{cases}$$

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[Dayal-James, '10], [James, '18], [James-Nota-Velazquez, '19]

Our first goal:

How to proceed with **Arrow (4)** ?

Dynamical system of OMD

Simulated and Non-simulated atoms are indistinguishable in new variable

$$x_{i,k}(t) = x_k(t) + (I + tA)\nu_i$$

$$\Downarrow$$

$$\dot{x}_{i,k}(t) = \dot{x}_k(t) + A\nu_i \Rightarrow v_{i,k}(t) = v_k(t) + A\nu_i$$

$$\Downarrow$$

$$\underbrace{v_{i,k}(t) - A(I + tA)^{-1} x_{i,k}(t)}_{:= w_{i,k}(t)} = \underbrace{v_k(t) - A(I + tA)^{-1} x_k(t)}_{:= w_k(t)}$$

The dynamical system of OMD in new variables $(x_i(t), w_i(t))$: for $i = 1, \ldots, N$,

$$\begin{cases} \dot{x}_i(t) = w_i(t) + A(I + tA)^{-1} x_i(t), \\ \dot{w}_i(t) = -\sum_{\substack{j=1 \\ j \neq i}}^{N} \nabla_{x_i} U\left(|x_i(t) - x_j(t)|\right) - A(I + tA)^{-1} w_i(t). \end{cases}$$

Dynamical system of OMD

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Kinetic description

- **Mean-field type model**:

$$\textbf{(M)}\begin{cases}\dot{x}_i(t) = w_i(t) + A(I+tA)^{-1}x_i(t)\\ \dot{w}_i(t) = -\frac{1}{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\nabla_{x_i}U\left(|x_i(t)-x_j(t)|\right) - A(I+tA)^{-1}w_i(t)\end{cases}$$

$$\downarrow \quad N\to\infty$$

$$\frac{\partial g}{\partial t} + w\cdot\nabla_x g + [A(I+tA)^{-1}x]\cdot\nabla_x g - [A(I+tA)^{-1}w]\cdot\nabla_w g = [\nabla_x U * \rho_g](t,x)\cdot\nabla_w g$$

- **Boltzmann type model**:

$$\textbf{(B)}\begin{cases}\dot{x}_i(t) = w_i(t) + A(I+tA)^{-1}x_i(t)\\ \dot{w}_i(t) = -\frac{1}{\varepsilon}\sum_{\substack{j=1\\ j\neq i}}^{N}\nabla_{x_i}U\left(\frac{|x_i(t)-x_j(t)|}{\varepsilon}\right) - A(I+tA)^{-1}w_i(t)\end{cases}$$

$$\downarrow \quad N\varepsilon^{d-1}\to O(1),\ \text{as } N\to\infty,\ \varepsilon\to 0$$

$$\frac{\partial g}{\partial t} + w\cdot\nabla_x g + [A(I+tA)^{-1}x]\cdot\nabla_x g - [A(I+tA)^{-1}w]\cdot\nabla_w g = Q(g,g)$$

Kinetic description

- **Mean-field type model**:

$$\textbf{(M)}\begin{cases} \dot{x}_i(t) = w_i(t) + A(I+tA)^{-1}x_i(t) \\ \dot{w}_i(t) = -\frac{1}{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \nabla_{x_i} U\left(|x_i(t)-x_j(t)|\right) - A(I+tA)^{-1}w_i(t) \end{cases}$$

$$\downarrow \quad N\to\infty$$

$$\frac{\partial g}{\partial t} + w\cdot\nabla_x g + [A(I+tA)^{-1}x]\cdot\nabla_x g - [A(I+tA)^{-1}w]\cdot\nabla_w g = [\nabla_x U * \rho_g](t,x)\cdot\nabla_w g$$

- **Boltzmann type model**:

$$\textbf{(B)}\begin{cases} \dot{x}_i(t) = w_i(t) + A(I+tA)^{-1}x_i(t) \\ \dot{w}_i(t) = -\frac{1}{\varepsilon}\sum_{\substack{j=1\\ j\neq i}}^{N} \nabla_{x_i} U\left(\frac{|x_i(t)-x_j(t)|}{\varepsilon}\right) - A(I+tA)^{-1}w_i(t) \end{cases}$$

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$$\frac{\partial g}{\partial t} + w\cdot\nabla_x g + [A(I+tA)^{-1}x]\cdot\nabla_x g - [A(I+tA)^{-1}w]\cdot\nabla_w g = Q(g,g)$$

Derivation of mean-field limit

Denote

$$\Omega^N := \left\{(x_1, w_1, x_2, w_2 ..., x_N, w_N) \in \mathbb{R}^{6N} \;\middle|\; x_i \neq x_j,\; i \neq j\right\}$$

and let

$$P^{(N)}(t, x_1, w_1, x_2, w_2, ..., x_N, w_N)$$

be the N-particle distribution function.

Our goal: derive the mean-field equation $P^{(1)}(t, x_1, w_1)$

Starting with the Liouville equation satisfied by $P^{(N)}(t, x_1, w_1, ..., x_N, w_N)$

$$\frac{\partial P^{(N)}}{\partial t} + \sum_{i=1}^{N}\left[\dot{x}_i \cdot \nabla_{x_i} P^{(N)} + \dot{w}_i \cdot \nabla_{w_i} P^{(N)}\right] = 0\,,$$

and substituting system **(M)**, it leads to

$$\frac{\partial P^{(N)}}{\partial t} + \sum_{i=1}^{N} w_i \cdot \nabla_{x_i} P^{(N)} + \sum_{i=1}^{N}[A(I+tA)^{-1}x_i]\cdot\nabla_{x_i} P^{(N)}$$
$$-\frac{1}{N}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\nabla_{x_i}U\left(|x_i - x_j|\right)\cdot\nabla_{w_i}P^{(s)} - \sum_{i=1}^{N}[A(I+tA)^{-1}w_i]\cdot\nabla_{w_i}P^{(N)} = 0$$

Derivation of mean-field limit

Integrating over the domain $\{x_{s+1}, w_{s+1}, ..., x_N, w_N\}$, we obtain the corresponding kinetic equation of the s-marginal distribution $P^{(s)}$,

$$\frac{\partial P^{(s)}}{\partial t} + \underbrace{\int_{\mathbb{R}^{6(N-s)}} \left(\sum_{i=1}^{N} w_i \cdot \nabla_{x_i} P^{(N)} + \sum_{i=1}^{N} [A(I+tA)^{-1} x_i] \cdot \nabla_{x_i} P^{(N)} \right) \mathrm{d}x_{s+1} ... w_N}_{=:\textbf{(I)}}$$

$$\underbrace{- \int_{\mathbb{R}^{6(N-s)}} \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{s} \nabla_{x_i} U\left(|x_i - x_j|\right) - \sum_{i=1}^{N} [A(I+tA)^{-1} w_i] \right) \cdot \nabla_{w_i} P^{(N)} \, \mathrm{d}x_{s+1} ... w_N}_{=:\textbf{(II)}}$$

$$= \underbrace{\int_{\mathbb{R}^{6(N-s)}} \frac{1}{N} \sum_{i=1}^{N} \sum_{\substack{j=s+1 \\ j \neq i}}^{N} \nabla_{x_i} U\left(|x_i - x_j|\right) \cdot \nabla_{w_i} P^{(N)} \, \mathrm{d}x_{s+1} w_{s+1} ... x_N w_N}_{=:\textbf{(III)}}$$

Derivation of mean-field limit

For term (I),

$$(I) = \sum_{i=1}^{s} w_i \cdot \nabla_{x_i} P^{(s)} + \sum_{i=1}^{s} \left[A(I+tA)^{-1}x_i\right] \cdot \nabla_{x_i} P^{(s)} + \sum_{i=s+1}^{N} \int_{\mathbb{R}^{6(N-s)}} \left[A(I+tA)^{-1}x_i\right] \cdot \nabla_{x_i} P^{(N)} \, \mathrm{d}x_{s+1} \ldots w_N$$

$$= \sum_{i=1}^{s} w_i \cdot \nabla_{x_i} P^{(s)} + \sum_{i=1}^{s} [A(I+tA)^{-1}x_i] \cdot \nabla_{x_i} P^{(s)} - (N-s)\mathrm{Tr}[A(I+tA)^{-1}]P^{(s)}$$

For term (II),

$$(II) = -\frac{1}{N} \sum_{\substack{i,j=1 \\ i \neq j}}^{s} \nabla_{x_i} U(|x_i - x_j|) \cdot \nabla_{w_i} P^{(s)} - \sum_{i=1}^{s} [A(I+tA)^{-1}w_i] \cdot \nabla_{w_i} P^{(s)} + (N-s)\mathrm{Tr}[A(I+tA)^{-1}]P^{(s)}$$

For term (III), since particles are indistinguishable,

$$(III) = \frac{N-s}{N} \sum_{i=1}^{s} \int_{\mathbb{R}^6} \nabla_{x_i} U(|x_i - x_{s+1}|) \cdot \nabla_{w_i} P^{(s+1)}(t, X_s, W_s, x_{s+1} w_{s+1}) \, \mathrm{d}x_{s+1} w_{s+1}$$

$$= \frac{N-s}{N} \sum_{i=1}^{s} \nabla_{w_i} \cdot \int_{\mathbb{R}^6} \left[\nabla_{x_i} U(|x_i - x_{s+1}|) P^{(s+1)}(t, X_s, W_s, x_{s+1} w_{s+1})\right] \mathrm{d}x_{s+1} w_{s+1}$$

Derivation of mean-field limit

For term (I),

$$
\begin{aligned}
(I) = &\sum_{i=1}^{s} w_i \cdot \nabla_{x_i} P^{(s)} + \sum_{i=1}^{s} \left[A(I+tA)^{-1}x_i\right] \cdot \nabla_{x_i} P^{(s)} \\
&+ \sum_{i=s+1}^{N} \int_{\mathbb{R}^{6(N-s)}} \left[A(I+tA)^{-1}x_i\right] \cdot \nabla_{x_i} P^{(N)} \, \mathrm{d}x_{s+1} \ldots w_N \\
= &\sum_{i=1}^{s} w_i \cdot \nabla_{x_i} P^{(s)} + \sum_{i=1}^{s} \left[A(I+tA)^{-1}x_i\right] \cdot \nabla_{x_i} P^{(s)} - (N-s)\mathrm{Tr}\left[A(I+tA)^{-1}\right] P^{(s)}
\end{aligned}
$$

For term (II),

$$
\begin{aligned}
(II) = &-\frac{1}{N} \sum_{\substack{i,j=1 \\ i \neq j}}^{s} \nabla_{x_i} U\left(|x_i - x_j|\right) \cdot \nabla_{w_i} P^{(s)} - \sum_{i=1}^{s} \left[A(I+tA)^{-1}w_i\right] \cdot \nabla_{w_i} P^{(s)} \\
&+ (N-s)\mathrm{Tr}\left[A(I+tA)^{-1}\right] P^{(s)}
\end{aligned}
$$

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$$
\begin{aligned}
(III) = &\frac{N-s}{N} \sum_{i=1}^{s} \int_{\mathbb{R}^6} \nabla_{x_i} U\left(|x_i - x_{s+1}|\right) \cdot \nabla_{w_i} P^{(s+1)}(t, X_s, W_s, x_{s+1} w_{s+1}) \, \mathrm{d}x_{s+1} w_{s+1} \\
= &\frac{N-s}{N} \sum_{i=1}^{s} \nabla_{w_i} \cdot \int_{\mathbb{R}^6} \left[\nabla_{x_i} U\left(|x_i - x_{s+1}|\right) P^{(s+1)}(t, X_s, W_s, x_{s+1} w_{s+1})\right] \mathrm{d}x_{s+1} w_{s+1}
\end{aligned}
$$

Derivation of mean-field limit

For term (I),

$$
\begin{aligned}
(I) = &\sum_{i=1}^{s} w_i \cdot \nabla_{x_i} P^{(s)} + \sum_{i=1}^{s} \left[A(I+tA)^{-1}x_i\right] \cdot \nabla_{x_i} P^{(s)} \\
&+ \sum_{i=s+1}^{N} \int_{\mathbb{R}^{6(N-s)}} \left[A(I+tA)^{-1}x_i\right] \cdot \nabla_{x_i} P^{(N)} \, \mathrm{d}x_{s+1} \ldots w_N \\
= &\sum_{i=1}^{s} w_i \cdot \nabla_{x_i} P^{(s)} + \sum_{i=1}^{s} [A(I+tA)^{-1}x_i] \cdot \nabla_{x_i} P^{(s)} - (N-s)\mathrm{Tr}[A(I+tA)^{-1}]P^{(s)}
\end{aligned}
$$

For term (II),

$$
\begin{aligned}
(II) = &-\frac{1}{N} \sum_{\substack{i,j=1 \\ i \neq j}}^{s} \nabla_{x_i} U\left(|x_i - x_j|\right) \cdot \nabla_{w_i} P^{(s)} - \sum_{i=1}^{s} [A(I+tA)^{-1}w_i] \cdot \nabla_{w_i} P^{(s)} \\
&+ (N-s)\mathrm{Tr}[A(I+tA)^{-1}]P^{(s)}
\end{aligned}
$$

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$$
\begin{aligned}
(III) &= \frac{N-s}{N} \sum_{i=1}^{s} \int_{\mathbb{R}^6} \nabla_{x_i} U\left(|x_i - x_{s+1}|\right) \cdot \nabla_{w_i} P^{(s+1)}(t, X_s, W_s, x_{s+1} w_{s+1}) \, \mathrm{d}x_{s+1} w_{s+1} \\
&= \frac{N-s}{N} \sum_{i=1}^{s} \nabla_{w_i} \cdot \int_{\mathbb{R}^6} \left[\nabla_{x_i} U\left(|x_i - x_{s+1}|\right) P^{(s+1)}(t, X_s, W_s, x_{s+1} w_{s+1})\right] \mathrm{d}x_{s+1} w_{s+1}
\end{aligned}
$$

Derivation of mean-field limit

Combining the terms $(I)-(III)$ altogether,

$$\frac{\partial P^{(s)}}{\partial t}+\sum_{i=1}^{s} w_i\cdot\nabla_{x_i}P^{(s)}+\sum_{i=1}^{s}[A(I+tA)^{-1}x_i]\cdot\nabla_{x_i}P^{(s)}$$

$$-\sum_{i=1}^{s}[A(I+tA)^{-1}w_i]\cdot\nabla_{w_i}P^{(s)}-\frac{1}{N}\sum_{\substack{i,j=1\\ i\neq j}}^{s}\nabla_{x_i}U\left(|x_i-x_j|\right)\cdot\nabla_{w_i}P^{(s)}$$

$$=\frac{N-s}{N}\sum_{i=1}^{s}\nabla_{w_i}\cdot\int_{\mathbb{R}^6}\left[\nabla_{x_i}U\left(|x_i-x_{s+1}|\right)P^{(s+1)}(t,X_s,W_s,x_{s+1}w_{s+1})\right]\mathrm{d}x_{s+1}w_{s+1}$$

In particular, taking $s=1$ above, it reduces to the two-particle case:

$$\frac{\partial P^{(1)}}{\partial t}+w_1\cdot\nabla_{x_1}P^{(1)}+[A(I+tA)^{-1}x_1]\cdot\nabla_{x_1}P^{(1)}-[A(I+tA)^{-1}w_1]\cdot\nabla_{w_1}P^{(1)}$$

$$=\frac{N-s}{N}\nabla_{w_1}\cdot\int_{\mathbb{R}^6}\left[\nabla_{x_1}U\left(|x_1-x_2|\right)P^{(2)}(t,x_1w_1,x_2w_2)\right]\mathrm{d}x_2w_2$$

Derivation of mean-field limit

Combining the terms $(I)-(III)$ altogether,

$$\frac{\partial P^{(s)}}{\partial t}+\sum_{i=1}^{s} w_i\cdot\nabla_{x_i}P^{(s)}+\sum_{i=1}^{s}[A(I+tA)^{-1}x_i]\cdot\nabla_{x_i}P^{(s)}$$
$$-\sum_{i=1}^{s}[A(I+tA)^{-1}w_i]\cdot\nabla_{w_i}P^{(s)}-\frac{1}{N}\sum_{\substack{i,j=1\\ i\neq j}}^{s}\nabla_{x_i}U\left(|x_i-x_j|\right)\cdot\nabla_{w_i}P^{(s)}$$
$$=\frac{N-s}{N}\sum_{i=1}^{s}\nabla_{w_i}\cdot\int_{\mathbb{R}^6}\left[\nabla_{x_i}U\left(|x_i-x_{s+1}|\right)P^{(s+1)}(t,X_s,W_s,x_{s+1}w_{s+1})\right]\mathrm{d}x_{s+1}w_{s+1}$$

In particular, taking $s=1$ above, it reduces to the two-particle case:

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$$=\frac{N-s}{N}\nabla_{w_1}\cdot\int_{\mathbb{R}^6}\left[\nabla_{x_1}U\left(|x_1-x_2|\right)P^{(2)}(t,x_1w_1,x_2w_2)\right]\mathrm{d}x_2w_2$$

Derivation of mean-field limit

To close the hierarchy above, we consider the "propagation of chaos" assumption:

$$P^{(2)}(t, x_1 w_1, x_2 w_2) = P^{(1)}(t, x_1, w_1) P^{(1)}(t, x_2, w_2)$$

which says the two particles remain independent throughout the dynamics. Under this assumption, the right-hand side becomes

$$\begin{aligned}
&\frac{N-1}{N}\nabla_{w_1} \cdot \int_{\mathbb{R}^6} \left[\nabla_{x_1} U\left(|x_1 - x_2|\right) P^{(2)}(t, x_1, w_1, x_2, w_2)\right] \mathrm{d}x_2 \, \mathrm{d}w_2 \\
=&\frac{N-1}{N}\int_{\mathbb{R}^6} \left[\nabla_{x_1} U\left(|x_1 - x_2|\right) P^{(1)}(t, x_2, w_2) \nabla_{w_1} P^{(1)}(t, x_1, w_1)\right] \mathrm{d}x_2 \, \mathrm{d}w_2 \\
=&\frac{N-1}{N}\int_{\mathbb{R}^3} \left[\nabla_{x_1} U\left(|x_1 - x_2|\right) \int_{\mathbb{R}^3} P^{(1)}(t, x_2, w_2) \, \mathrm{d}w_2\right] \mathrm{d}x_2 \cdot \nabla_{w_1} P^{(1)}(t, x_1, w_1) \\
=&\frac{N-1}{N}\nabla_{x_1} U * \rho_{P^{(1)}}(t, x_1) \cdot \nabla_{w_1} P^{(1)}(t, x_1, w_1)
\end{aligned}$$

Finally, by re-naming $P^{(1)}(t, x_1, w_1)$ to $g(t, x, w)$

$$\frac{\partial g(t,x,w)}{\partial t} + w \cdot \nabla_x g + \left[A(I+tA)^{-1} x\right] \cdot \nabla_x g - \left[A(I+tA)^{-1} w\right] \cdot \nabla_w g$$

$$= \left[\nabla_x U * \rho_g\right](t, x) \cdot \nabla_w g$$

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$$\begin{aligned}
&\frac{N-1}{N} \nabla_{w_1} \cdot \int_{\mathbb{R}^6} \left[\nabla_{x_1} U\left(|x_1 - x_2|\right) P^{(2)}(t, x_1, w_1, x_2, w_2) \right] \mathrm{d}x_2 \, \mathrm{d}w_2 \\
=& \frac{N-1}{N} \int_{\mathbb{R}^6} \left[\nabla_{x_1} U\left(|x_1 - x_2|\right) P^{(1)}(t, x_2, w_2) \nabla_{w_1} P^{(1)}(t, x_1, w_1) \right] \mathrm{d}x_2 \, \mathrm{d}w_2 \\
=& \frac{N-1}{N} \int_{\mathbb{R}^3} \left[\nabla_{x_1} U\left(|x_1 - x_2|\right) \int_{\mathbb{R}^3} P^{(1)}(t, x_2, w_2) \, \mathrm{d}w_2 \right] \mathrm{d}x_2 \cdot \nabla_{w_1} P^{(1)}(t, x_1, w_1) \\
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Theorem (Existence, uniqueness and stability [James-Q.-Wang '23])

For any initial datum $g_0(x,w) \in \mathcal{P}_c(\mathbb{R}^3 \times \mathbb{R}^3)$*, there* *exists* *a measure-valued solution* $g_t(x,w) = g(t,x,w) \in C\big([0,+\infty), \mathcal{P}_c(\mathbb{R}^3 \times \mathbb{R}^3)\big)$ *to mean-field equation, and there is an increasing function* $R = R(T)$ *such that for all* $T > 0$,

$$\text{supp } g_t(\cdot,\cdot) \subset B_{R(T)} \subset \mathbb{R}^3 \times \mathbb{R}^3, \quad \forall\ t \in [0,T] \tag{1}$$

This solution is *unique* *among the family of solutions* $C\big([0,+\infty), \mathcal{P}_c(\mathbb{R}^3 \times \mathbb{R}^3)\big)$ *satisfying* (1).

Moreover, assume that $g_0, h_0 \in \mathcal{P}_c(\mathbb{R}^3 \times \mathbb{R}^3)$ *are two initial conditions, and* g_t, h_t *are the corresponding solutions to mean-field equation. Then,*

$$W_1(g_t(\cdot,\cdot), h_t(\cdot,\cdot)) \le e^{2tL} W_1(g_0(\cdot,\cdot), h_0(\cdot,\cdot)), \quad \forall t \ge 0$$

where L *is a constant depending on* A *and* U*, and* W_1 *is Monge-Kantorovich-Rubinstein distance defined as:*

$$W_1(\mu,\nu) := \sup\left\{\left|\int_{\mathbb{R}^3\times\mathbb{R}^3} \varphi(P)(\mu(P)-\nu(P))\,\mathrm{d}P\right|,\ \varphi \in \textit{Lip}(\mathbb{R}^3\times\mathbb{R}^3),\ \|\varphi\|_{\mathrm{Lip}} \le 1\right\}$$

Sketch of proof: Fix-point argument

Define a flow operator at time $t \in [0,T)$,

$$\mathcal{T}^t_{\xi,\mathcal{H}} : (X(0), W(0)) \mapsto (X(t), W(t)) \in \mathbb{R}^3 \times \mathbb{R}^3$$

For an initial probability measure $g_0(x,w)$, the function

$$g(t,x,w) : [0,T) \to \mathcal{P}_1(\mathbb{R}^3 \times \mathbb{R}^3), \quad t \mapsto g_t(x,w) := \mathcal{T}^t_{\xi,\mathcal{H}} \# g_0(x,w)$$

is a measure-valued solution in the distributional sense

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is a measure-valued solution in the distributional sense

Let $g_t^N(x,w) : [0,T] \mapsto \mathcal{P}_1(\mathbb{R}^3 \times \mathbb{R}^3)$ be a probability measure defined as

$$g_t^N(x,w) := \frac{1}{N}\sum_{i=1}^{N} \delta\big(x - x_i(t)\big)\delta\big(w - w_i(t)\big) \tag{2}$$

If $x_i, w_i : [0,T] \mapsto \mathbb{R}^3$, for $i = 1, ..., N$, is a solution to dynamics system, then $g_t^N(x,w)$ is the measure-valued solution to mean-field equation with the initial condition

$$g_0^N(x,w) := \frac{1}{N}\sum_{i=1}^{N} \delta\big(x - x_i(0)\big)\delta\big(w - w_i(0)\big) \tag{3}$$

Corollary (Convergence of the empirical measure)

Consider a sequence of g_0^N in the form of (3) such that

$$\lim_{N\to\infty} W_1\big(g_0^N(\cdot,\cdot), g_0(\cdot,\cdot)\big) = 0.$$

Let g_t^N be given by (2), where $(x_i(t), w_i(t))$ solves dynamics system with initial conditions $(x_i(0), w_i(0))$. Then we have

$$\lim_{N\to\infty} W_1\big(g_t^N(\cdot,\cdot), g_t(\cdot,\cdot)\big) = 0$$

for all $t \geq 0$, where $g_t(x,w)$ is the unique measure-valued solution to mean-field equation with initial data $g_0(x,w)$.

Let $g_t^N(x,w) : [0,T] \mapsto \mathcal{P}_1(\mathbb{R}^3 \times \mathbb{R}^3)$ be a probability measure defined as

$$g_t^N(x,w) := \frac{1}{N}\sum_{i=1}^{N} \delta\big(x - x_i(t)\big)\delta\big(w - w_i(t)\big) \tag{2}$$

If $x_i, w_i : [0,T] \mapsto \mathbb{R}^3$, for $i = 1, \dots, N$, is a solution to dynamics system, then $g_t^N(x,w)$ is the measure-valued solution to mean-field equation with the initial condition

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Consider a sequence of g_0^N in the form of (3) such that

$$\lim_{N\to\infty} W_1\big(g_0^N(\cdot,\cdot), g_0(\cdot,\cdot)\big) = 0.$$

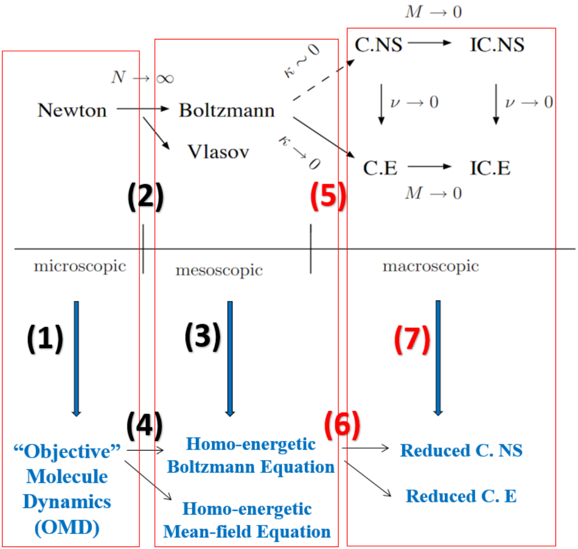
Let g_t^N be given by (2), where $(x_i(t), w_i(t))$ solves dynamics system with initial conditions $(x_i(0), w_i(0))$. Then we have

$$\lim_{N\to\infty} W_1\big(g_t^N(\cdot,\cdot), g_t(\cdot,\cdot)\big) = 0$$

for all $t \geq 0$, where $g_t(x,w)$ is the unique measure-valued solution to mean-field equation with initial data $g_0(x,w)$.

3. From Mesoscopic to Macroscopic

Recall the Big Picture



C: compressible
IC: incompressible

NS: Navier-Stokes

E: Euler

Previous work

Arrow (5): Hydrodynamic Limit

- Hilbert or Chapman-Enskoy Expansion :
  [Hilbert,'12], [Enskoy, '17], [Chapman-Cowling, '39]
- Asymptotic convergence:
  to C.E. [Caflish, '80], to IC.NS. [DeMasi-Esposito-Lebowitz, '89]
- Renormalized solution of Boltzmann to weak solution of E/NS:
  to IC. [Bardos-Golse-Levermore '93], [Lions-Masmoudi, '01], [Golse-Saint-Raymond, '04, '09], [Levermore-Masmoudi, '10], [Jiang-Masmoudi, '17]
- Strong solution near equilibrium:
  to C.E. [Nishida '78], to IC.NS [Bardos-Ukai '91], [Gallagher-Tristani '20]

Arrow (7): Homo-energetic Transformation for macroscopic quantities
[Pahlani-Schwartzentruber-James, '22, '23]

Our second goal:

How to proceed with **Arrow (6)** ?

Previous work

Arrow (5): Hydrodynamic Limit

- Hilbert or Chapman-Enskoy Expansion :
  [Hilbert,'12], [Enskoy, '17], [Chapman-Cowling, '39]
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Our second goal:

How to proceed with **Arrow (6)** ?

Macroscopic quantities of homo-energetic flow

- **Density** $\rho(t,x)$:

$$\rho(t,x) = \int_{\mathbb{R}^3} f(t,x,v)\ \mathrm{d}v = \int_{\mathbb{R}^3} g(t,w)\ \mathrm{d}w =: \rho(t)$$

- **Bulk velocity** $u(t,x)$:

$$\begin{aligned} u(t,x) = \frac{1}{\rho(t,x)} \int_{\mathbb{R}^3} f(t,x,v)v\ \mathrm{d}v =& \frac{1}{\rho(t)} \int_{\mathbb{R}^3} g(t,w)[w + L(t)x]\ \mathrm{d}w \\ =& \frac{1}{\rho} \int_{\mathbb{R}^3} gw\ \mathrm{d}w + [L(t)x]\frac{1}{\rho} \int_{\mathbb{R}^3} g\ \mathrm{d}w \\ =& L(t)x \end{aligned}$$

- **Internal energy** $e(t,x)$ and **temperature** $\theta(t,x)$:

$$\begin{aligned} \rho(t,x)e(t,x) =& \frac{1}{2} \int_{\mathbb{R}^3} f(t,x,v)|v - u(t,x)|^2\ \mathrm{d}v \\ =& \frac{1}{2} \int_{\mathbb{R}^3} g(t,w)|w|^2\ \mathrm{d}w =: \rho(t)e(t) \end{aligned}$$

  Consider the equation of state for perfect gas $e(t) = \frac{k_B\theta(t)}{\gamma_a - 1} = \frac{3}{2}\theta(t)$.

- **Stress tensor** $P_{ij}(t,x)$: for peculiar velocity c,

$$\begin{aligned} P_{ij}(t,x) =& \int_{\mathbb{R}^3} c_i(t,x)c_j(t,x)f(t,x,v)\ \mathrm{d}v \\ =& \int_{\mathbb{R}^3} w_i w_j g(t,w)\ \mathrm{d}w =: P_{ij}(t) \end{aligned}$$

  for $i,j = 1,2,3$.

By multiplying the collision invariants 1, w_j, and $\frac{1}{2}|w|^2$ to homo-energetic equations,

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\rho(t) + \mathrm{Tr}[L(t)]\rho(t) = 0 \\ \rho(t)\left(\dfrac{\mathrm{d}L(t)}{\mathrm{d}t} + L^2(t)\right) = 0 \\ \rho(t)\dfrac{\mathrm{d}e(t)}{\mathrm{d}t} + \sum_{i=1}^{3}\sum_{j=1}^{3} P_{ij}(t)L_{ij}(t) = 0 \end{cases}$$

Our Results:

- By applying the Hilbert expansion, we derive a reduced Euler system:

$$\begin{cases} \partial_t\rho(t) + \mathrm{Tr}[L(t)]\rho(t) = 0 \\ \partial_t\theta(t) + \dfrac{2}{3}\mathrm{Tr}[L(t)]\theta(t) = 0 \end{cases}$$

- By applying the Chapman-Enskog expansion, we obtain the corresponding reduced Navier-Stokes system with $O(\epsilon)$ correction terms:

$$\begin{cases} \partial_t\rho(t) + \mathrm{Tr}[L(t)]\rho(t) = 0 \\ \partial_t\theta(t) + \dfrac{2}{3}\mathrm{Tr}[L(t)]\theta(t) = \epsilon\mu(\theta)\dfrac{1}{2}\left(\mathrm{Tr}[L^2(t)] + L(t) : L(t) - \dfrac{2}{3}(\mathrm{Tr}[L(t)])^2\right) \end{cases}$$

where μ is the viscosity.

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where μ is the viscosity.

The compressible Euler limit via Hilbert expansion

Starting point:

$$\partial_t g(t,w) - [L(t)w]\cdot\nabla_w g(t,w) = \frac{1}{\epsilon}Q(g,g)(t,w)$$

where ϵ plays a role as Knudsen number.

Hilbert Expansion

Seek the solution in the form of a formal power series in ϵ:

$$g_\epsilon(t,w) = \sum_{n\geq 0}\epsilon^n g_n(t,w) = g_0(t,w) + \epsilon g_1(t,w) + \cdots.$$

For $O(\epsilon^{-1})$,

$$Q(g_0,g_0)(t,w) = 0$$

which implies that $g_0(t,w)$ is in the form of Maxwellian distribution, i.e.,

$$g_0(t,w) = \mathcal{M}_{[\rho(t),\theta(t)]} := \frac{\rho(t)}{[2\pi\theta(t)]^{\frac{3}{2}}}\,\mathrm{e}^{-\frac{|w|^2}{2\theta(t)}}, \quad \rho(t)>0, \quad \theta(t)>0$$

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For $O(\epsilon^0)$,

$$\Big(\partial_t - [L(t)w]\cdot\nabla_w\Big) g_0(t,w) = Q(g_0,g_1)(t,w) + Q(g_1,g_0)(t,w)\,.$$

Define the linearized Boltzmann collision operator

$$\mathcal{L}_{\mathcal{M}_{[\rho,\theta]}} g := -2\mathcal{M}_{[\rho,\theta]}^{-1} Q\Big(\mathcal{M}_{[\rho,\theta]}^{-1}, \mathcal{M}_{[\rho,\theta]}^{-1} g\Big)$$

which is an unbounded self-adjoint non-negative Fredholm operator.

$$\mathcal{L}_{g_0}\left(\frac{g_1}{g_0}\right) = -\Big(\partial_t - [L(t)w]\cdot\nabla_w\Big)\ln g_0(t,w)$$

We can rearrange the right-hand side, and express it as a linear combination of $1, w_i, |w|^2$,

$$-\mathcal{L}_{g_0}\left(\frac{g_0}{g_1}\right) = \frac{1}{\rho(t)}\Big(\partial_t\rho(t) + \mathrm{Tr}[L(t)]\rho(t)\Big) + \frac{1}{2}\left(\frac{|w|^2}{\theta(t)} - 3\right)\frac{1}{\theta(t)}\Big(\partial_t\theta(t) + \frac{2}{3}\mathrm{Tr}[L(t)]\theta(t)\Big) + A(W):D$$

where, for $W = \frac{w}{\sqrt{\theta(t)}}$, $A(W) \in (\mathrm{Ker}\,\mathcal{L}_{g_0})^{\perp}$ is

$$A(W) := W\otimes W - \frac{1}{3}|W|^2 I = \frac{1}{\theta(t)} w\otimes w - \frac{1}{3}\frac{|w|^2}{\theta(t)} I$$

and D is

$$D := \frac{1}{2}\Big(L(t) + [L(t)]^{\top} - \frac{2}{3}\mathrm{Tr}[L(t)] I\Big)$$

For $O(\epsilon^0)$,

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The compressible Navier-Stokes limit via Chapman-Enskoy expansion

Chapman-Enskoy Expansion

Seek the solution in the following form:

$$g_\epsilon(t,w) = \sum_{n\geq 0} \epsilon^n g_n[\vec{P}(t)](w) = g_0[\vec{P}(t)](w) + \epsilon g_1[\vec{P}(t)](w) + \cdots$$

Compared to the Hilbert expansion, we require that g_0 has the same first five moments as g_ϵ by construction:

$$\int_{\mathbb{R}^3} g_0[\vec{P}(t)](w) \begin{pmatrix} 1 \\ \frac{|w|^2}{2} \end{pmatrix} \mathrm{d}w = \vec{P}(t) = \begin{pmatrix} \rho(t) \\ \theta(t) \end{pmatrix}$$

where $\vec{P}$ is a vector of conserved quantities. hence,

$$\int_{\mathbb{R}^3} g_n[\vec{P}(t)](w) \begin{pmatrix} 1 \\ \frac{|w|^2}{2} \end{pmatrix} \mathrm{d}w = \vec{0}, \quad \text{for all} \quad n \geq 1$$

By taking the moments, the conserved quantities satisfy a system of conservation laws:

$$\partial_t \vec{P}(t) = \sum_{n\geq 0} \epsilon^n \Phi_n[\vec{P}](t) = \Phi_0(t) + \epsilon\Phi_1[\vec{P}](t) + \cdots$$

where the flux term $\Phi_n[\vec{P}](t)$ is denoted as

$$\Phi_n[\vec{P}](t) = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \frac{|w|^2}{2} \end{pmatrix} [L(t)w]\cdot\nabla_w g_n[\vec{P}(t)](w)\, \mathrm{d}w$$

for $n \geq 0$.

The compressible Navier-Stokes limit via Chapman-Enskoy expansion

Chapman-Enskoy Expansion

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for $n \geq 0$.

For $O(\epsilon^0)$,

$$0 = Q\left(g_0[\vec{P}(t)], g_0[\vec{P}(t)]\right)$$

For $O(\epsilon^1)$,

$$\Big(\partial_t - [L(t)w]\cdot\nabla_w\Big)g_0[\vec{P}(t)] = Q\left(g_0[\vec{P}(t)], g_1[\vec{P}(t)]\right)(w) + Q\left(g_1[\vec{P}(t)], g_0[\vec{P}(t)]\right)$$

The left-hand side is

$$\Big(\partial_t - [L(t)w]\cdot\nabla_w\Big)g_0[\vec{P}(t)]$$

$$= g_0[\vec{P}(t)]\Big[\frac{1}{\rho(t)}\Big(\partial_t\rho(t) + \mathrm{Tr}[L(t)]\rho(t)\Big) + \frac{1}{2}\left(\frac{|w|^2}{\theta(t)} - 3\right)\frac{1}{\theta(t)}\Big(\partial_t\theta(t) + \frac{2}{3}\mathrm{Tr}[L(t)]\theta(t)\Big)$$

$$+ [A(W):D]\Big]$$

$$= g_0[\vec{P}(t)](w)\,[A(W):D] + O(\epsilon)$$

$$\begin{cases} \mathcal{L}_{g_0[\vec{P}(t)]}\left(\dfrac{g_0[\vec{P}(t)]}{g_1[\vec{P}(t)]}\right) = -[A(W):D] \\ \displaystyle\int_{\mathbb{R}^3} g_1[\vec{P}(t)](w)\begin{pmatrix} 1 \\ \frac{|w|^2}{2}\end{pmatrix}\mathrm{d}w = \vec{0} \end{cases}$$

and therefore $g_1[\vec{P}(t)]$ can be solved:

$$g_1[\vec{P}(t)] = -g_0[\vec{P}(t)](w)\,[a(\theta, |W|)A(W):D]$$

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Hence, the first-order correction to the fluxes in the formal conservation law is

$$\Phi_1[\vec{P}(t)](w) = \int_{\mathbb{R}^3} [L(t)w]\cdot\nabla_w g_1[\vec{P}(t)](w) \begin{pmatrix} 1 \\ \frac{|w|^2}{2} \end{pmatrix} \mathrm{d}w$$

$$= \begin{pmatrix} 0 \\ \mu(\theta)\frac{1}{2}\Big(\mathrm{Tr}[L^2(t)] + L(t):L(t) - \frac{2}{3}(\mathrm{Tr}[L(t)])^2\Big) \end{pmatrix}$$

where the viscosity $\mu(\theta)$ can be computed as

$$\mu(\theta) = \frac{2}{15}\theta\int_0^\infty a(\theta,r)r^6\frac{1}{\sqrt{2\pi}}\mathrm{e}^{-r^2/2}\,\mathrm{d}r$$

Recall conservation law and keeps only the first two order terms

$$\partial_t\vec{P}(t) = \Phi_0[\vec{P}](t) + \epsilon\Phi_1[\vec{P}](t) \text{ mod } O(\epsilon^2)$$

Spelling out the flux terms, we have

$$\begin{cases} \partial_t\rho(t) + \mathrm{Tr}[L(t)]\rho(t) = 0, \\ \partial_t\theta(t) + \frac{2}{3}\mathrm{Tr}[L(t)]\theta(t) = \epsilon\mu(\theta)\frac{1}{2}\Big(\mathrm{Tr}[L^2(t)] + L(t):L(t) - \frac{2}{3}(\mathrm{Tr}[L(t)])^2\Big) \end{cases}$$

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$$= \begin{pmatrix} 0 \\ \mu(\theta)\frac{1}{2}\Big(\mathrm{Tr}[L^2(t)] + L(t):L(t) - \frac{2}{3}(\mathrm{Tr}[L(t)])^2\Big) \end{pmatrix}$$

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4. Related Numerical Simulation

Spectral Method for Boltzmann Equation

Let $q = v - v_*$ and $\hat{q}$ is the unit vector along q.

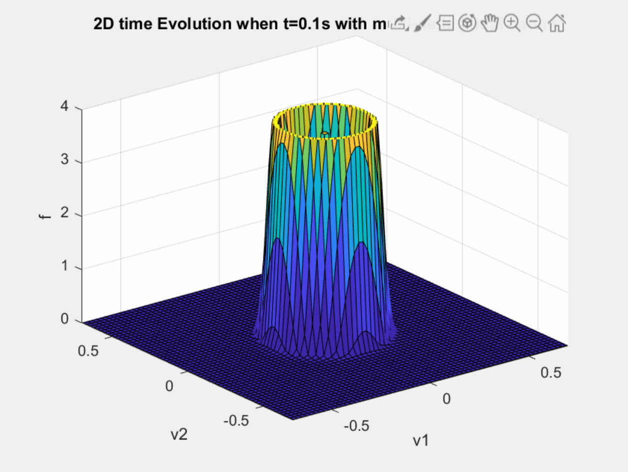
$$Q(f,f)(v) \approx Q_R(f,f)(v) = \int_{\mathcal{B}_{2R}} \int_{\mathbb{S}^{d-1}} B(|q|, \sigma \cdot \hat{q}) [f(v')f(v'_*) - f(v)f(v-q)] \, \mathrm{d}\sigma \, \mathrm{d}q$$

1. Truncate collision integral: in q to a ball $\mathcal{B}_R$ with $R \geq 2S$ with $\mathcal{B}_S \approx \mathrm{supp}_v(f)$.
2. Restrict probability density f into computed domain $\mathcal{D}_L = [-L, L]^d$: expand it periodically to the whole space.
3. Approximate density function f: by a truncated Fourier series, $k \in \mathbb{Z}^d : -\frac{N}{2} \leq k_1, \ldots, k_d \leq \frac{N}{2} - 1$,
$$f(v) \approx f_N(v) = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{f}_k \, \mathrm{e}^{\mathrm{i}\frac{\pi}{L} k \cdot v} \text{ with } \hat{f}_k = \frac{1}{(2L)^d} \int_{\mathcal{D}_L} f(v) \, \mathrm{e}^{-\mathrm{i}\frac{\pi}{L} k \cdot v} \, \mathrm{d}v.$$
4. Substitute and apply of Galerkin projection:
$$\hat{Q}_k = \frac{1}{(2L)^d} \int_{D_L} Q(f_N, f_N) \, \mathrm{e}^{-\mathrm{i}\frac{\pi}{L} k \cdot v} \, \mathrm{d}v.$$

Numerical Simulation (I): Multi-bumps initial condition [Hu-Q., JCP '20]

Apply our fast spectral solver, coupled with RK4 scheme for time discretization, to solve $\partial_t f = Q(f,f)$ with initial datum $F_0(v)$:

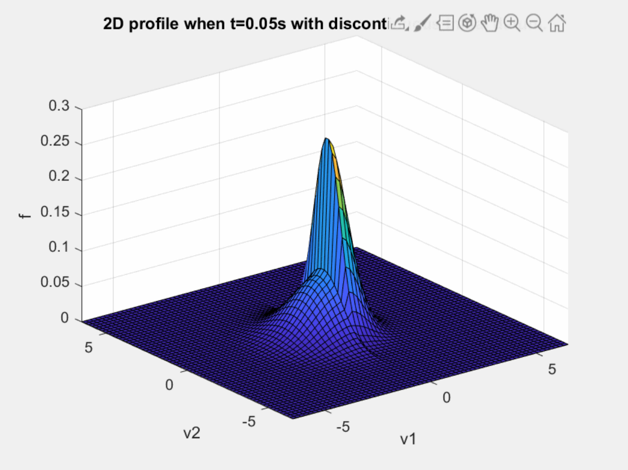
$$F_0(v) = \frac{1}{3}\left(\delta_w(v) + \delta_w(|v| - 0.2)\right)$$



Numerical Simulation (II): Discontinuous initial condition [Hu-Q., JCP '20]

For a typical discontinuous initial datum:

$$F^0(v) = \begin{cases} \frac{\rho_1}{2\pi T_1}\exp\left(-\frac{|v|^2}{2T_1}\right), & \text{for} \quad v_1 > 0 \\ \frac{\rho_2}{2\pi T_2}\exp\left(-\frac{|v|^2}{2T_2}\right), & \text{for} \quad v_1 < 0 \end{cases}$$

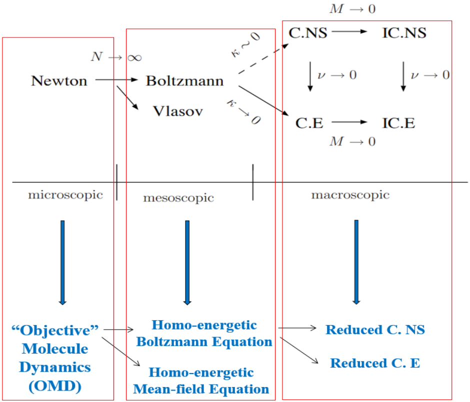


5. Summary and Outlook

Summary

"Take-home" messages

- Micro: A special class of dynamics system – **OMD**
- Micro → Meso: **Mean-field** and **Boltzmann-Grad** Limit
- Meso: A simplified kinetic equation – **Homo-energetic Mean-field** and **Boltzmann**
- Meso → Macro: **Hilbert** and **Chapman-Enskoy** expansion



C: compressible
IC: incompressible

NS: Navier-Stokes
E: Euler

Outlook

Ongoing work:

Well-posedness:

- Finite energy: General deformation [James-Nota-Velazquez '19], [Bobylev-Nota-Velazquez '20], Shear flow [Duan-Liu '21]
- **Infinite energy**: ?

Long-time Behavior:

- Balance between collision and hyperbolic effect: [James-Nota-Velazquez '19]
- Collision dominated: [James-Nota-Velazquez '19], [Duan-Liu '22], [Kepka '22]
- **Hyperbolic dominated**: ?

Future work:

1. Theoretical perspective: rigorous justification of multiscale hierarchy.
2. Numerical perspective: dimension reduction or high-order scheme.
3. Other Boltzmann-related models: apply the kinetic ideas to Physical, Biology, Quantum systems...

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Thanks for your attention!

Papers and preprints can be found at my homepage
https://kunlun-qi.github.io/