Incompressible and compressible Fluids Concerning With Lagrangian

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Abstract - **This paper covers that an as of late proposed variational rule with a spasmodic Lagrangian for thick stream is reinterpreted against the foundation of stochastic variational portrayals of dissipative frameworks, supporting its physical premise from an alternate perspective. It is appeared extra non-traditional commitments to the rubbing power happening in the energy equalization disappear by time averaging. In like manner, the spasmodic Lagrangian can on the other hand be comprehended from the outlook of a comparable to deterministic model for irreversible procedures of stochastic character. An examination is made with set up stochastic variational portrayals and an option deterministic methodology dependent on a first fundamental of Navier–Stokes conditions is embraced. The materialness of the broken Lagrangian approach for various Reynolds number routines is examined considering the Kolmogorov time scale. A speculation for compressible stream is explained and its utilization exhibited for damped sound waves.**

keywords - **variational calculus, Navier–Stokes equations, field description, stochastic variational description, compressible fluid, incompressible fluid**

Introduction:

Discovering variational details for physical frameworks is useful concerning a more profound comprehension of the framework and for setting up new arrangement techniques, both investigative and numerical. As is outstanding, this deliberate idea is in a perfect world fit to, for instance, the field of moderate Newtonian mechanics. As opposed to this, in continuum hypotheses many open issues stay unsolved, ordinarily in the field of thick stream; since there are, when all is said in done, no required development rules for building up variational standards, for specific issues an assortment of proposals have showed up from various creators dependent on various methodologies. One needs to recognize two noteworthy classes, in particular between variational plans dependent on a field portrayal (Eulerian depiction), and stochastic variational portrayal dependent on a material portrayal (Lagrangian portrayal) and averaging molecule movement.

Clebsch transformation

Early attempts by Millikan[1] showed the non-existence of a Lagrangian in terms of the velocity *u*, the pressure *p* and their first-order derivatives that delivers the Navier–Stokes equations as Euler–Lagrange equations. A different approach based on the representation of the velocity *u* by three potentials, i.e. by auxiliary fields, has been established by Clebsch[2], Lamb[3], Panton[4], but in its original form his approach is restricted to inviscid flows. Later modified forms of the Clebsch transformation have been applied successfully to magnetohydrodynamics (MHD)[5] and plasma dynamics[6]. A generalized Clebsch transformation for viscous flow has been suggested by Scholle & Marner[7], but the field equations resulting from it are not self-adjoint.

Since in viscous flow dissipation[1] leads to an irreversible transfer of mechanical energy to heat, thermal degrees of freedom have to be considered in order to remain consistent with Noether's theorem which implies conservation of energy for every Lagrangian being invariant with respect to time-translations. Seliger & Whitham[8] made a first decisive step by establishing a Lagrangian that can be interpreted as a generalized form of Clebsch's Lagrangian, supplemented by two additional fields: the specific entropy *s* and an additional field ϑ, introduced three decades previously by Van Dantzig[9] as the material integral of the temperature *T*, i.e. $D_t\vartheta = T$, and termed *thermasy*, where $D_t = \partial/\partial t + u \cdot \nabla$.

Despite including thermal degrees of freedom, Seliger and Whitham's approach remains restricted to adiabatic and therefore reversible processes. As a continuation of their work, Zuckerwar & Ash[10] suggested an extended Lagrangian considering only volume viscosity, leading to equations of motion containing qualitatively the effect of volume viscosity but differing quantitatively from the compressible Navier–Stokes equations, also known as the *Navier–Stokes–Duhem equations*[11,12] without shear viscosity. They interpret their result as a generalization of the theory of viscous flow towards thermodynamic non-equilibrium. Based on a rigorous analysis of the fundamental symmetries the Lagrangian has to fulfil, with particular regard to Galilean invariance[13], Scholle & Marner[14] suggested a Lagrangian for viscous flow considering both shear viscosity η and volume viscosity η' reproducing Zuckerwar and Ash's Lagrangian for the case $\eta = 0$. Again, the resulting equations of motion differ from the Navier–Stokes–Duhem equations. Considering six simple flow examples, two of them (steady shear flows) gave exact reproductions of the classical solutions, two other (transient flows) show the impact of viscosity on the flow at least in a qualitatively correct manner, whereas no physically reasonable solutions could be constructed for two pressure-driven flows.

In order to resolve the above issue, Scholle & Marner[14] made use of an analogy between quantum mechanics and fluid mechanics discovered by Madelung[15] to formulate a new Lagrangian by relating the specific entropy *s* and the thermasy ϑ to a complex field χ, termed the *field of thermal excitation* by Anthony[16], ending up with a discontinuous Lagrangian containing an additional parameter ω_0. By a careful analysis it is proven that the dynamics resulting from Hamilton's principle can consistently

be interpreted as a generalization of the theory of viscous flow towards thermodynamic non-equilibrium, with the parameter ω_0 being the relaxation rate, giving rise to recovery of the well-known Navier–Stokes equations and the balance of inner energy when applying the limit $\omega_0 \to \infty$ to the resulting equations of motion.

The behavior of fluids in small spaces, with one of the characteristic dimensions of the order of few fluid particle diameters, can be significantly different from the bulk. Some of the well-studied features of such confined fluids are the formation of layering structure normal to the confining walls,[1] inhomogenous pressure equation of state,[1] appearance of surface induced phase transitions,[2,3] and shift in the glass transition temperature.[4,5] The scientific progress on some of the issues related to the behavior of confined fluids has been biased towards understanding the structural changes and associated thermodynamic properties due to confinement. In fact, now we have theories at our disposal which can predict the implications of confinement on the thermodynamic properties quantitatively over a wide range of conditions.[6] On the contrary, the situation is not so satisfactory for predicting the dynamic behavior (such as the average self-diffusivity) of confined fluids.[7–9] One of the reasons for this slow advancement on understanding fluid dynamics under confinement is the lack of tractable kinetic theories even for the bulk fluid behavior over the whole equilibrium fluid range.

Recent studies have utilized a different strategy to predict the transport properties of fluids under confinement; their aim is to find empirical correlations between thermodynamic and dynamic quantities which remain approximately unchanged due to confinement.[10–12] The thermodynamic quantity used to find such correlations can be as simple as the average fluid density,[10] although significantly better results are obtained by using quantities such as the excess entropy[10,11,13,14] of the fluid with respect to the ideal gas state and the available volume.[12,15] The idea is to utilize these correlations obtained from the bulk fluid behavior along with the information about the thermodynamic property of confined fluids (which can be easily obtained via theory, molecular simulation, or laboratory experiment) to calculate the dynamic quantity with quantitative accuracy. This line of enquiry seems rather promising from the studies so far on equilibrium fluids as one can predict the effect of confinement on the self-diffusivity (or alternatively shear viscosity which follows trivially from the Stokes-Einstein relationship for equilibrium fluids) for a wide range of fluid models such as hard-sphere, Lennard-Jones (LJ), square well and others by utilizing "excess entropy-diffusivity"[10,11] and "available volume-diffusivity"[12] bulk relationships.

The possible explanation for the observed correlations between these quantities of seemingly different origin (thermodynamic versus dynamic) even in the bulk has mostly been qualitative and there is no first principle based justification available. It has been argued that excess entropy should naturally be a quantity which will track the fluid dynamics as it characterizes the reduced number of states due to interparticle correlations.[16] But it is not clear what the functional relationship should be[17,18] and if there is a universal connection or something more like a parameteric fit with fitting coefficients dependent on the state of the fluid (density, temperature) and the type of fluid (strong versus fragile). Whether these correlations persist in the supercooled state is also somewhat an open question[19] with previous work pointing towards the need for an additional adjustable parameter (as a function of density in case of binary Lennard-Jones[20] and SPC/E water[21]).

In this regard, recent results from the single particle barrier hopping theory of Schweizer and co-workers[22] may be an important step towards bridging the gap between observations and fundamental understanding. One specific result out of many predictions made by this theory is that the relaxation time (or inverse diffusivity D) for the bulk hard-sphere fluid should scale with the compressibility factor $Z = \beta P/\rho$ as,[23]

$$\frac{D}{D_0} \propto exp\left(a\varphi^{-1}(Z-1)^2\right), \quad (1)$$

where $\beta = [k_B T]^{-1}$, k_B is the Boltzmann constant, T is temperature, P is pressure, ρ is the fluid density, D_0 is an elementary diffusion scale, a is a numerical prefactor, $\varphi = \pi\rho\sigma^3/6$ is the fluid packing fraction, and σ is the fluid diameter. A qualitative agreement with the predictions of eq 1 was already found in a previous work on the dynamics of polydisperse hard-sphere fluid which showed that the relaxation time as a function of Z for several different polydispersity values can be approximately collapsed onto a single curve.[24] A quantitative comparison of eq 1 with the actual diffusion data will provide a useful starting point for understanding some of the outstanding issues related to the dynamics of supercooled fluids. As the focus of this paper is the equilibrium fluid dynamics under confinement, we will only touch upon this issue very briefly in the beginning of results and discussion section. Detailed results and the discussion on the supercooled fluid behavior from the perspective of eq 1 will be provided in a future publication.

Here, instead we focus on the possiblity of D–Z relationship as observed in the bulk for an equilibrium hard-sphere fluid as a predictor of diffusion under confinement by utilizing the knowledge about its Z. For confined systems, pressure is a tensorial quantity (and therefore Z) and for a slit-pore system (fluid confined between walls in one direction) pressure has two components, parallel and normal to the walls. For average diffusion parallel to the walls (which will be the main dynamic quantity of interest in this work), we expect that the compressibility factor based on the average pressure component in the parallel direction will be relevant. As our fluid models, we consider both a single-component and a binary mixture of hard-sphere particles. For confinement models, we consider slit-pore geometry with hard walls and attractive square-well walls and rectangular channels with hard walls. We find that the bulk D–Z relationship remains essentially unchanged due to these different types of confinement and can be successfully used to predict the diffusivity of confined fluids with quantitative accuracy for most of the state points. We further notice that any expected deviations from the exact diffusion values are generally negative (under-prediction) for low to intermediate density states and positive (overprediction) for high density states. Data from previous studies show that qualitatively similar deviations are expected from the excess entropy - diffusivity and available volume - diffusivity correlations.[12] An attractive aspect of our observed correlation between the compressibility factor and diffusivity, as compared to previous work on other thermodynamic measures, is that one can calculate Z fairly easily using colloidal hard sphere

experiments in bulk (and possibly under confinement with appropriate modifications in the analysis)[25] and in molecular simulations.

Simulation

We have used discontinuous molecular dynamics (DMD) simulations[26] to track various thermodynamic and dynamic properties of the hard-sphere (HS) fluid model. The DMD simulations each involved $N = 10000$ HS particles contained within a simulation cell of volume $V = H_x \times H_y \times H_z$, where H_i is the box length in a given direction ($i = x,y,z$). Periodic boundary conditions were applied in all three directions for bulk and in two directions (x and y) for the slit-pore, and in one direction (x) for the rectangular channel. The non-periodic directions in case of confined fluids can be either smooth "hard" walls which are perfectly reflecting or "attractive" walls with a square-well potential between the fluid particles and the confining walls,

$$
\begin{aligned}
u(z) &= \infty && z < \sigma/2 \\
&= -\varepsilon\mathbf{w} && \sigma/2 \leq z < \sigma \quad (2)\\
&= 0 && z \geq \sigma,
\end{aligned}
$$

where z represents the shortest distance between a given particle center and the wall of interest, and ε_w is the strength of the effective particle-wall interaction. We only consider hard walls in case of rectangular channels.

The diffusivity D of the fluid was obtained by fitting the long-time behavior of the average mean-squared displacement of the particles to the Einstein relation $\langle \Delta r_{2d} \rangle = 2dDt$, where $\langle \Delta r_{2d} \rangle$ corresponds to the mean-square displacement per particle in the d periodic directions after time t. To calculate the compressibility factor Z, we use the following form of the virial theorem,[27,28]

$$
Z = 1 + \frac{m \sum_{collisions} (\mathbf{r}_{ij} \cdot \Delta \mathbf{v}_i)}{dNk_BTt_e}, \quad (3)
$$

where $\mathbf{r}_{ij}$ is the position vector between particles i and j, $\mathbf{v}_i$ is the change in velocity of particle i after the collision, N is the number of particles, and the summation is over all the collisions during the elapsed time t_e. In case of confined systems, the vector product includes only the periodic components of $\mathbf{r}_{ij}$ and $\mathbf{v}_i$ for Zparallel to the walls and non-periodic components for Z normal to the walls. We test our Z calculations against the GC-TMMC simulation results[29,30] and find favorable comparison for both bulk and confined systems (less than 0.5%) difference.[13,14] To simplify the notation in this paper, we have implicitly non-dimensionalized all quantities by appropriate combinations of a characteristic length scale (which we take to be the HS particle diameter σ) and time scale (which we choose to be $\sigma\sqrt{m\beta}$, where m is particle mass). As a result, all quantities with dimensions of energy are understood to be "per k_BT", the only energy scale in the problem.

Result

Bulk hard-sphere fluid

First we check the predictions of eq 1 for the bulk HS fluid. Although the barrier hopping theory in its ultralocal limit is expected to be valid for strongly supercooled liquids,[23] we want to see if this can also provide some reasonable predictions for weakly supercooled and equilibrium fluid states. As we are using a monatomic fluid which is hard to supercool and will crystallize readily, it is not possible to access strongly supercooled regime. Figure 1 shows the D data plotted against φ (top panel) as well as $(Z-1)_2/\varphi$ (bottom panel) as expected from eq 1 for $\varphi \leq 0.53$. We are able to fit the data for most of the dense fluid range ($D < 0.1$ and $\varphi > 0.40$) to eq 1. Equation 1 is only valid for fluid states above the ideal glass transition packing fraction ($\varphi_i = 0.432$) at which the activated barrier hopping dynamics becomes important[22] and the deviations seen in Figure 1 at low density are therefore expected. We also show the inverse viscosity $1/\eta$ on the same plot and the expected fit from the Stokes-Einstein relationship, i.e., $D\eta = 1/2\pi$ in the bottom panel. To verify that the fluid systems between $\varphi = 0.49$ to $\varphi = 0.53$ are not phase separated (as coexistence between the fluid-solid phase for the HS model is between $\varphi = 0.494-0.545$),we check the time evolution of Z as well as several other order parameters, e.g., bond-orientationl order Q_6, pair-correlation function $g(r)$, translational order parameter s_2 and do not find any evidence of phase separation at the time scale of the simulations. Of course, if we run the simulations for long enough, these state points will show fluid and solid phases in coexistence. We use a similar approach to identify stable and metastable (at the simulation timescales) state points for the confined HS system for which the location of the fluid-solid phase boundary may not be known apriori. In future we will investigate whether the trends observed here also hold in the deeply supercooled state by utilizing a polydisperse HS fluid to avoid crystallization.
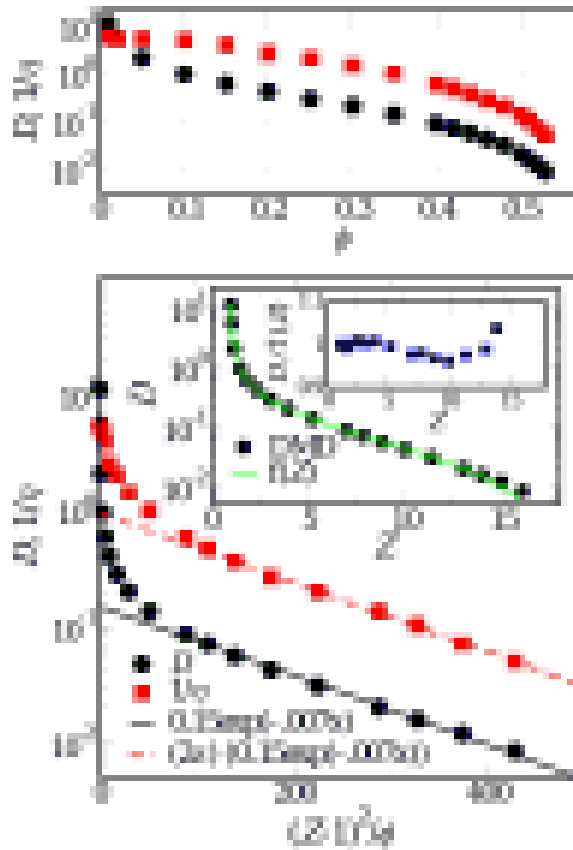
Figure 1

Bulk data. (Top panel) Diffusivity D and inverse viscosity $1/\eta$ data are plotted as a function of φ. (Bottom panel) Diffusivity D and inverse viscosity $1/\eta$ data are plotted as a function of $(Z-1)_2/\varphi$ along with a **...**

Next, we want to examine if the correspondence between D and Z observed in the bulk is unchanged due to confinement and can therefore be used as a predictive tool for confined fluid diffusivity. To facilitate this process, we fit our bulk data to an analytic functional form[34] $D = f(Z)$ as shown in the inset of Figure 1. To simplify the analysis we have used D–Z relationship but $D-(Z-1)_2/\varphi$ can also be used for rest of the analysis in this paper. Further, we plot the ratio of the actual DMD data and $f(Z)$ to assess the reliability of our fit, and find overall good agreement with less than 5% error for $Z > 5$. From now onwards we will use $f(Z)$ as a functional representation of our bulk D data.

Hard-sphere fluid confined between hard walls

First, we test the effect of hard-wall confinement on the D–Z relationship. Figure 2 shows the data for bulk HS (solid line), HS confined between slit-pores of size $H = H_z$, and rectangular channels with dimensions $H_y \times H_z$. Overall, the collapse of confined fluid data on the bulk curve is good suggesting that $f(Z)$ can be used as a predictor of diffusivity if Z for the confined fluid is known. For more restrictive confinements, e.g., in rectangular channels and for a slit-pore of size $H = 4$, D–Z curves have a different slope from the bulk curve which gives rise to underprediction in D from $f(Z)$ at intermediate Z and overprediction in D at high Z as shown in the inset of Figure 2. The Z-range (or alternatively φ-range) considered here covers most of the equilibrium state points as known from the exact fluid-solid phase diagram.
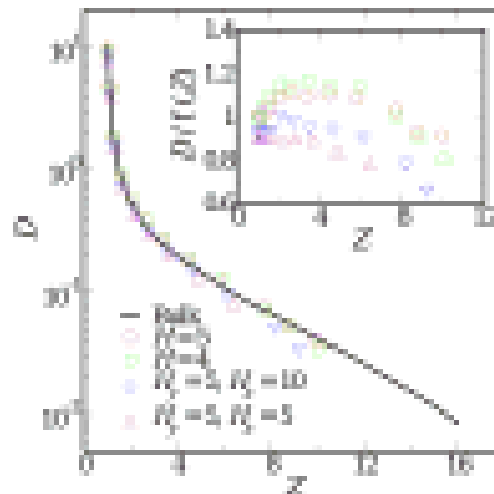

Figure 2

Hard wall confinement. Diffusivity D versus compressibility factor Z for hard-sphere fluid in bulk (line) and confined between hard-walls (symbols). The ratio $D/f(Z)$ as a function of Z is also shown in the inset.

Hard-sphere fluid confined between attractive walls

To test if D–Z correspondence is still valid when we introduce fluid-wall interactions, we calculate these quantities for systems with varying attraction strength ε_w (eq 2). Figure 3 shows the bulk HS data (line) along with the confined fluid data (symbols) which demonstrates that indeed the D–Z relationship remains unchanged. To assess quantitative differences, we plot $D/f(Z)$ in the inset of Figure 3 which shows that difference between the bulk and confined diffusivity based on Z is less than 10% for 75% of the state points and always less than 15%.
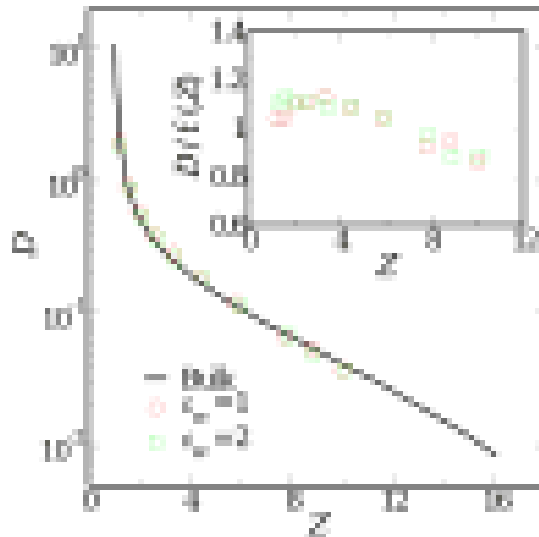

Figure 3

Attractive wall confinement. Diffusivity D versus compressibility factor Z for hard-sphere fluid in bulk (line) and confined between attractive walls represented by a square-well potential eq. 2(symbols). The ratio $D/f(Z)$ as a function of Z is also **...**

Conclusion

We have shown that the relationship between a thermodynamic and a dynamic quantity, i.e., between "diffusivity and compressibility factor" can be used to predict the effect of confinement on fluid diffusivity. Along with the knowledge of bulk D–Z relationship, the information about the confined fluid's compressiblity factor is needed which can be easily estimated from experiments or approximated using existing theoretical approaches such as the density functional theory. This provides an indirect but quantitative route to predict confined fluid diffusivity based on its thermodynamics. One of the interesting features about the observed D–Z correlations is that the barrier hopping theory for supercooled fluid dynamics in its ultralocal limit predicts such an expectation for a bulk hard-sphere fluid and a precise functional form for these correlations. We find that this expected functional dependency is satisfied for a single-component hard-sphere fluid in a weakly supercooled state and even in the equilibrium fluid state. In future work, we will focus on understanding the D–Z correlations for supercooled fluids in bulk and under confinement by utilizing polydisperse fluids to thwart crystallization and size segregation. We are currently also investigating if D–Z correlations can be used to predict the effect of confinement on dynamics for attractive fluids with square-well or Lennard-Jones interactions.

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