

Paper Reading Notes --- Polymer Simulation

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05/03/20

额外的任务：看 **Dissipative particle dynamics, Lattice Boltzmann** 的 YouTube 视频以及维基百科

3) “Ginzburg–Landau free energy”

3.1 看 YouTube 笔记 (iPad 上)

05/05/20

任务：(i) “critical phase transition” --> “critical exponents” (or the so-called “mean field critical exponents”); (看一下 polymer 的那本 textbook 看看有没有介绍 mean field critical exponents 的)

(1) “Magnetic susceptibility”

https://en.wikipedia.org/wiki/Magnetic_susceptibility

Magnetic susceptibility

From Wikipedia, the free encyclopedia

In electromagnetism, the **magnetic susceptibility** (*Latin*: *susceptibilis*, "receptive"; denoted χ) is a measure of how much a material will become magnetized in an applied magnetic field. Mathematically, it is the ratio of **magnetization M** (magnetic moment per unit volume) to the applied magnetizing field **intensity H** . This allows a simple classification of most materials' response to an applied magnetic field into two categories: an alignment with the magnetic field, $\chi > 0$, called **paramagnetism**, or an alignment against the field, $\chi < 0$, called **diamagnetism**.

(2) “Phase Transition”

https://en.wikipedia.org/wiki/Phase_transition#Characteristic_properties

“The term phase transition (or phase change) is most commonly used to describe transitions between solid, liquid, and gaseous states of matter, as well as plasma in rare cases. A phase of a thermodynamic system and the states of matter have uniform physical properties. During a phase transition of a given medium, certain properties of the medium change, often discontinuously, as a result of the change of external conditions, such as temperature, pressure, or others. For example, a liquid may become gas upon heating to the boiling point, resulting in an abrupt change in volume. The measurement of the external conditions at which the transformation occurs is termed the phase transition. Phase transitions commonly occur in nature and are used today in many technologies.

I. Classifications

(A) Ehrenfest classification (似乎比下面的 modern classification 更重要一些)

Paul Ehrenfest classified phase transitions based on the behavior of the thermodynamic free energy as a function of other thermodynamic variables. Under this scheme, phase transitions were labeled by the lowest derivative of the free energy that is discontinuous at the transition. **First-order phase transitions exhibit a discontinuity in the first derivative of the free energy with respect to some thermodynamic variable.** The various solid/liquid/gas transitions are classified as first-order transitions because they involve a discontinuous change in density, which is the (inverse of the) first derivative of the free energy with respect

to pressure. **Second-order phase transitions** are continuous in the first derivative (**the order parameter, which is the first derivative of the free energy with respect to the external field, is continuous across the transition**) **but exhibit discontinuity in a second derivative of the free energy**. These include the ferromagnetic phase transition in materials such as iron, where the magnetization, which is the first derivative of the free energy with respect to the applied magnetic field strength, increases continuously from zero as the temperature is lowered below the Curie temperature. The magnetic susceptibility, the second derivative of the free energy with the field, changes discontinuously. Under the Ehrenfest classification scheme, there could in principle be third, fourth, and higher-order phase transitions.

The Ehrenfest classification implicitly allows for continuous phase transformations, where the bonding character of a material changes, but there is no discontinuity in any free energy derivative. An example of this occurs at the supercritical liquid–gas boundaries.

(B) Modern classifications

In the modern classification scheme, phase transitions are divided into two broad categories, named similarly to the Ehrenfest classes:

(i) **First-order phase transitions** are those that involve a latent heat. During such a transition, a system either absorbs or releases a fixed (and typically large) amount of energy per volume. During this process, the temperature of the system will stay constant as heat is added: the system is in a "mixed-phase regime" in which some parts of the system have completed the transition and others have not. Familiar examples are the melting of ice or the boiling of water (the water does not instantly turn into vapor, but forms a turbulent mixture of liquid water and vapor bubbles). Imry and Wortis showed that quenched disorder can broaden a first-order transition. That is, the transformation is completed over a finite range of temperatures, but phenomena like supercooling and superheating survive and hysteresis is observed on thermal cycling.

(Note: “latent heat” https://en.wikipedia.org/wiki/Latent_heat

Latent heat (also known as latent energy, or as Heat of Transformation) is energy released or absorbed, by a body or a thermodynamic system, during a constant-temperature process — usually a first-order phase transition.)

(ii) **Second-order phase transitions** are also called "continuous phase transitions". They are characterized by a **divergent susceptibility, an infinite correlation length, and a power law decay of correlations near criticality**. Examples of second-order phase transitions are the ferromagnetic transition, superconducting transition (for a Type-I superconductor the phase transition is second-order at zero external field and for a Type-II superconductor the phase transition is second-order for both normal-state—mixed-state and mixed-state—superconducting-state transitions) and the superfluid transition. In contrast to viscosity, thermal expansion and heat capacity of amorphous materials show a relatively sudden change at the glass transition temperature which enables accurate detection using differential scanning calorimetry measurements. Lev **Landau** gave a phenomenological theory of second-order phase transitions.

(II) Characteristic properties

(i) Phase coexistence

A disorder-broadened first-order transition occurs over a finite range of temperatures where the fraction of the low-temperature equilibrium phase grows from zero to one (100%) as the temperature is lowered. This continuous variation of the coexisting fractions with temperature raised interesting possibilities. On cooling, some liquids vitrify (玻璃化) into a glass rather than transform to the equilibrium crystal phase. This happens if the cooling rate is faster than a critical cooling rate, and is attributed to the molecular motions becoming so slow that the molecules cannot rearrange into the crystal positions. This slowing down happens below a glass-formation temperature T_g , which may depend on the applied pressure. If the first-order freezing transition occurs over a range of temperatures, and T_g falls within this range, then there is an

interesting possibility that the transition is arrested when it is partial and incomplete. Extending these ideas to first-order magnetic transitions being arrested at low temperatures, resulted in the observation of incomplete magnetic transitions, with two magnetic phases coexisting, down to the lowest temperature. First reported in the case of a ferromagnetic to anti-ferromagnetic transition, such persistent phase coexistence has now been reported across a variety of first-order magnetic transitions. The interesting feature of these observations of T_g falling within the temperature range over which the transition occurs is that the first-order magnetic transition is influenced by magnetic field, just like the structural transition is influenced by pressure. The relative ease with which magnetic fields can be controlled, in contrast to pressure, raises the possibility that one can study the interplay between T_g and T_c in a detailed way. Phase coexistence across first-order magnetic transitions will then enable the resolution of outstanding issues in understanding glasses.

(ii) Critical points

In any system containing liquid and gaseous phases, there exists a special combination of pressure and temperature, known as the critical point, **at which the transition between liquid and gas becomes a second-order transition**. Near the critical point, the fluid is sufficiently hot and compressed that the distinction between the liquid and gaseous phases is almost non-existent.

(iii) Symmetry

Phase transitions often involve a symmetry breaking process. For instance, **the cooling of a fluid into a crystalline solid breaks continuous translation symmetry: each point in the fluid has the same properties, but each point in a crystal does not have the same properties (unless the points are chosen from the lattice points of the crystal lattice)**. Typically, **the high-temperature phase contains more symmetries than the low-temperature phase due to spontaneous symmetry breaking**, with the exception of certain accidental symmetries (e.g. the formation of heavy virtual particles, which only occurs at low temperatures).

(iv) Order parameters (See more details in “Qi Group’s Paper Notes”)

An order parameter is a measure of the degree of order across the boundaries in a phase transition system; it normally ranges **between zero** in one phase (usually above the critical point) **and nonzero** in the other. At the critical point, the order parameter susceptibility will usually diverge.

An example of an order parameter is the net magnetization in a ferromagnetic system undergoing a phase transition. For liquid/gas transitions, the order parameter is the difference of the densities.

From a theoretical perspective, order parameters arise from symmetry breaking. When this happens, one needs to introduce one or more extra variables to describe the state of the system. For example, in the ferromagnetic phase, one must provide the net magnetization, whose direction was spontaneously chosen when the system cooled below the Curie point. However, note that order parameters can also be defined for non-symmetry-breaking transitions.

Some phase transitions, such as superconducting and ferromagnetic, **can have order parameters for more than one degree of freedom**. In such phases, the order parameter may take the form of a complex number, a vector, or even a tensor, the magnitude of which goes to zero at the phase transition.

(v) Critical exponents and universality classes

Continuous phase transitions are easier to study than first-order transitions due to the absence of latent heat, and they have been discovered to have many interesting properties. **The phenomena associated with continuous phase transitions are called critical phenomena, due to their association with critical points.**

It turns out that continuous phase transitions can be characterized by parameters known as critical exponents. The most important one is perhaps the exponent describing the divergence of the thermal correlation length by approaching the transition.

(Note: “**divergence**” (Google Translate) --- the inner product of the operator del and a given vector $(\nabla \cdot \vec{v})$, which gives **a measure of the quantity of flux** emanating (发出) from any point of the vector field **or the rate of loss of mass, heat, etc., from it**.

For instance, let us examine the behavior of the heat capacity near such a transition. We vary the temperature T of the system while keeping all the other thermodynamic variables fixed, and find that the transition occurs at some critical temperature T_c . When T is near T_c , the heat capacity C typically has a power law behavior,

$$C \propto |T_c - T|^{-\alpha}.$$

The heat capacity of amorphous materials has such a behaviour near the glass transition temperature where the universal critical exponent $\alpha = 0.59$ ^[24] A similar behavior, but with the exponent ν instead of α , applies for the correlation length.

The exponent ν is positive. This is different with α . Its actual value depends on the type of phase transition we are considering.

It is widely believed that the critical exponents are the same above and below the critical temperature. It has now been shown that this is not necessarily true: When a continuous symmetry is explicitly broken down to a discrete symmetry by irrelevant (in the renormalization group sense) anisotropies, then some exponents (such as γ , the exponent of the susceptibility) are not identical.^[25]

△ ↘ 结

For $-1 < \alpha < 0$, the heat capacity has a "kink" at the transition temperature. This is the behavior of liquid helium at the lambda transition from a normal state to the superfluid state, for which experiments have found $\alpha = -0.013 \pm 0.003$. At least one experiment was performed in the zero-gravity conditions of an orbiting satellite to minimize pressure differences in the sample.^[26] This experimental value of α agrees with theoretical predictions based on variational perturbation theory.^[27]

For $0 < \alpha < 1$, the heat capacity diverges at the transition temperature (though, since $\alpha < 1$, the enthalpy stays finite). An example of such behavior is the 3D ferromagnetic phase transition. In the three-dimensional Ising model for uniaxial magnets, detailed theoretical studies have yielded the exponent $\alpha \sim +0.110$.

Some model systems do not obey a power-law behavior. For example, mean field theory predicts a finite discontinuity of the heat capacity at the transition temperature, and the two-dimensional Ising model has a logarithmic divergence. However, these systems are limiting cases and an exception to the rule. Real phase transitions exhibit power-law behavior.

Several other critical exponents, β , γ , δ , ν , and η , are defined, examining the power law behavior of a measurable physical quantity near the phase transition. Exponents are related by scaling relations, such as

$$\beta = \gamma / (\delta - 1), \quad \nu = \gamma / (2 - \eta).$$

It can be shown that there are only two independent exponents, e.g. ν and η .

It is a remarkable fact that phase transitions arising in different systems often possess the same set of critical exponents. This phenomenon is known as universality. For example, the critical exponents at the liquid–gas critical point have been found to be independent of the chemical composition of the fluid.

More impressively, but understandably from above, they are an exact match for the critical exponents of the ferromagnetic phase transition in uniaxial magnets. Such systems are said to be in the same universality class. Universality is a prediction of the renormalization group theory of phase transitions, which states that the thermodynamic properties of a system near a phase transition depend only on a small number of features, such as dimensionality and symmetry, and are insensitive to the underlying microscopic properties of the system. Again, the divergence of the correlation length is the essential point.

(vi) Critical slowing down and other phenomena

There are also other critical phenomena; e.g., besides static functions there is also critical dynamics. As a consequence, at a phase transition one may observe critical slowing down or speeding up. The large static universality classes of a continuous phase transition split into smaller dynamic universality classes. In addition to the critical exponents, there are also universal relations for certain static or dynamic functions of the magnetic fields and temperature differences from the critical value.

(3) “Critical exponent” https://en.wikipedia.org/wiki/Critical_exponent

“Critical exponents describe the behavior of physical quantities near continuous phase transitions. It is believed, though not proven, that they are universal, i.e. they do not depend on the details of the physical system, but only on some of its general features. For instance, for ferromagnetic systems, the critical exponents depend only on:

- the dimension of the system
- the range of the interaction
- the spin dimension

These properties of critical exponents are supported by experimental data. Analytical results can be theoretically achieved in mean field theory in high dimensions or when exact solutions are known such as the two-dimensional Ising model. The theoretical treatment in generic dimensions requires the renormalization group approach or the conformal bootstrap techniques. Phase transitions and critical exponents appear in many physical systems such as water at the liquid-vapor transition, in magnetic systems, in superconductivity, in percolation and in turbulent fluids. The critical dimension above which mean field exponents are valid varies with the systems and can even be infinite. It is 4 for the liquid-vapor transition, 6 for percolation and probably infinite for turbulence. Mean field critical exponents are also valid for random graphs, such as Erdős–Rényi graphs, which can be regarded as infinite dimensional systems.

Definition:

The control parameter that drives phase transitions is often temperature but can also be other macroscopic variables like pressure or an external magnetic field. For simplicity, the following discussion works in terms of temperature; the translation to another control parameter is straightforward. The temperature at which the transition occurs is called the critical temperature T_c . We want to describe the behavior of a physical quantity f in terms of a power law around the critical temperature, we introduce the reduced temperature:

$$\tau := \frac{T - T_c}{T_c}$$

which is zero at the phase transition, and define the critical exponent k :

$$k \stackrel{\text{def}}{=} \lim_{\tau \rightarrow 0} \frac{\log |f(\tau)|}{\log |\tau|} \quad M = G_0 \left(1 - \frac{T}{T_c}\right)^k \Rightarrow \log M = \log G_0 + \beta \log \left(\frac{T_c - T}{T_c}\right)$$

This results in the power law we were looking for:

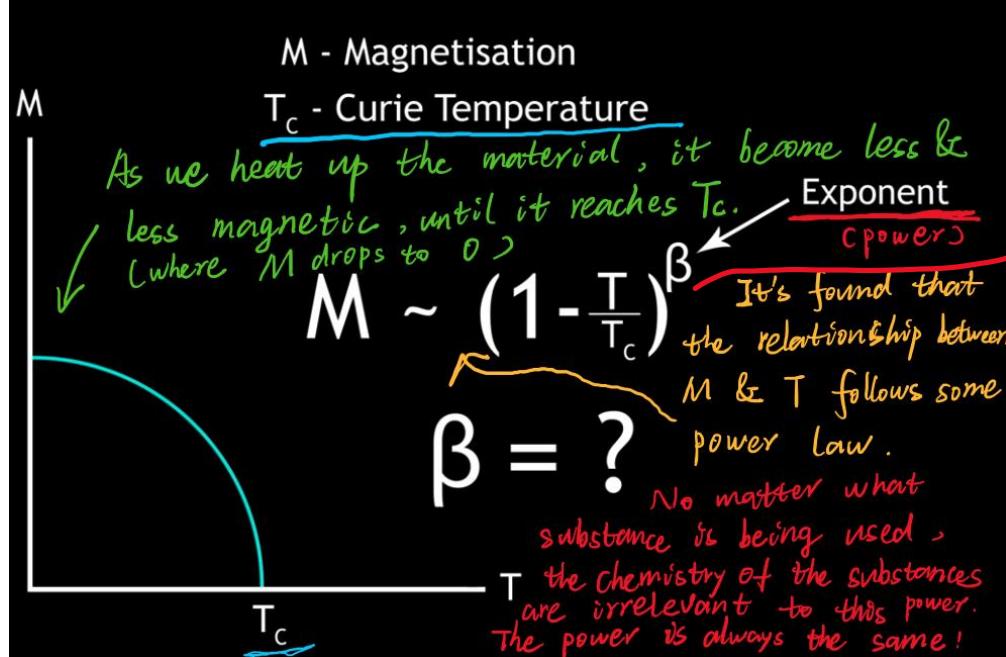
$$f(\tau) \propto \tau^k, \quad \tau \approx 0$$

It is important to remember that this represents the asymptotic behavior of the function $f(\tau)$ as $\tau \rightarrow 0$.

More generally one might expect

$$f(\tau) = A\tau^k (1 + b\tau^{k_1} + \dots)$$

(See Notes:



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The most important critical exponents [edit]

Let us assume that the system has two different phases characterized by an order parameter Ψ , which vanishes at and above T_c .

Consider the disordered phase ($\tau > 0$), ordered phase ($\tau < 0$) and critical temperature ($\tau = 0$) phases separately.

Following the standard convention, the critical exponents related to the ordered phase are primed. It is also another standard convention to use superscript/subscript + (-) for the disordered (ordered) state. In general spontaneous symmetry breaking occurs in the ordered phase.

Definitions

Ψ	order parameter (e.g. $\frac{\rho - \rho_c}{\rho_c}$ for the liquid–gas critical point, magnetization for the Curie point, etc.)
τ	$\frac{T - T_c}{T_c}$
f	specific free energy
C	specific heat; $-T \frac{\partial^2 f}{\partial T^2}$
J	source field (e.g. $\frac{P - P_c}{P_c}$ where P is the pressure and P_c the critical pressure for the liquid–gas critical point, reduced chemical potential, the magnetic field H for the Curie point)
χ	the susceptibility, compressibility, etc.; $\frac{\partial \Psi}{\partial J}$
ξ	correlation length
d	the number of spatial dimensions
$\langle \psi(\vec{x}) \psi(\vec{y}) \rangle$	the correlation function
r	spatial distance

The following entries are evaluated at $J = 0$ (except for the δ entry)

Critical exponents for $\tau > 0$ (disordered phase)

Greek letter	relation
α	$C \propto \tau^{-\alpha}$
γ	$\chi \propto \tau^{-\gamma}$
ν	$\xi \propto \tau^{-\nu}$

Critical exponents for $\tau < 0$ (ordered phase)

Greek letter	relation
α'	$C \propto (-\tau)^{-\alpha'}$
β	$\Psi \propto (-\tau)^\beta$
γ'	$\chi \propto (-\tau)^{-\gamma'}$
ν'	$\xi \propto (-\tau)^{-\nu'}$

Critical exponents for $\tau = 0$

Greek letter	relation
δ	$J \propto \Psi^\delta$
η	$\langle \psi(0) \psi(r) \rangle \propto r^{-d+2-\eta}$

with symmetry

lose some symmetry

The critical exponents can be derived from the specific free energy $f(J, T)$ as a function of the source and temperature. The correlation length can be derived from the functional $F[J; T]$.

These relations are accurate close to the critical point in two- and three-dimensional systems. In four dimensions, however, the power laws are modified by logarithmic factors. These do not appear in dimensions arbitrarily close to but not exactly four, which can be used as a way around this problem.^[3]

Mean field critical exponents of Ising-like systems [edit]

The classical [Landau theory](#) (also known as [mean field theory](#)) values of the critical exponents for a scalar field (of which the Ising model is the prototypical example) are given by

$$\alpha = \alpha' = 0, \quad \beta = \frac{1}{2}, \quad \gamma = \gamma' = 1, \quad \delta = 3$$

If we add derivative terms turning it into a mean field [Ginzburg–Landau theory](#), we get

$$\eta = 0, \quad \nu = \frac{1}{2}$$

One of the major discoveries in the study of critical phenomena is that [mean field theory of critical points is only correct when the space dimension of the system is higher than a certain dimension called the upper critical dimension](#) which excludes the physical dimensions 1, 2 or 3 in most cases. [The problem with mean field theory is that the critical exponents do not depend on the space dimension](#). This leads to a quantitative discrepancy below the critical dimensions, where the true critical exponents differ from the mean field values. It can even lead to a qualitative discrepancy at low space dimension, where a critical point in fact can no longer exist, even though mean field theory still predicts there is one. This is the case for the Ising model in dimension 1 where there is no phase transition. The space dimension where mean field theory becomes qualitatively incorrect is called the lower critical dimension.

Experimental values [edit]

The most accurately measured value of α is $-0.0127(3)$ for the phase transition of [superfluid helium](#) (the so-called [lambda transition](#)). The value was measured on a space shuttle to minimize pressure differences in the sample.^[4] This value is in a significant disagreement with the most precise theoretical determinations^{[5][6][7]} coming from high temperature expansion techniques, [Monte Carlo](#) methods and the [conformal bootstrap](#).^[8]

Theoretical predictions [edit]

Critical exponents can be evaluated via [Monte Carlo](#) simulations of lattice models. The accuracy of this first principle method depends on the available computational resources, which determine the ability to go to the infinite volume limit and to reduce statistical errors. Other techniques rely on theoretical understanding of critical fluctuations. The most widely applicable technique is the [renormalization group](#). The [conformal bootstrap](#) is a more recently developed technique, which has achieved unsurpassed accuracy for the [Ising critical exponents](#).

Unsolved problem in physics:

Explain the discrepancy between the experimental and theoretical determinations of the heat capacity critical exponent α for the superfluid transition in Helium-4.^[8]

(more unsolved problems in physics)

unsurpassed (未曾超过的)

Scaling functions [edit]

In light of the critical scalings, we can reexpress all thermodynamic quantities in terms of dimensionless quantities. Close enough to the critical point, everything can be reexpressed in terms of certain ratios of the powers of the reduced quantities. These are the scaling functions.

The origin of scaling functions can be seen from the renormalization group. The critical point is an infrared fixed point. In a sufficiently small neighborhood of the critical point, we may linearize the action of the renormalization group. This basically means that rescaling the system by a factor of a will be equivalent to rescaling operators and source fields by a factor of a^{Δ} for some Δ . So, we may reparameterize all quantities in terms of rescaled scale independent quantities.

Scaling relations [edit]

It was believed for a long time that the critical exponents were the same above and below the critical temperature, e.g. $\alpha \equiv \alpha'$ or $\gamma \equiv \gamma'$. It has now been shown that this is not necessarily true: When a continuous symmetry is explicitly broken down to a discrete symmetry by irrelevant (in the renormalization group sense) anisotropies, then the exponents γ and γ' are not identical.^[9]

Critical exponents are denoted by Greek letters. They fall into universality classes and obey the scaling relations

$$\nu d = 2 - \alpha = 2\beta + \gamma = \beta(\delta + 1) = \gamma \frac{\delta + 1}{\delta - 1}$$

$$2 - \eta = \frac{\gamma}{\nu} = d \frac{\delta - 1}{\delta + 1}$$

These equations imply that there are only two independent exponents, e.g., ν and η . All this follows from the theory of the renormalization group.

Anisotropy [edit]

There are some anisotropic systems where the correlation length is direction dependent. For percolation see Dayan et al.^[10]

Directed percolation can be also regarded as anisotropic percolation. In this case the critical exponents are different and the upper critical dimension is 5.^[11]

Multicritical points [edit]

More complex behavior may occur at multicritical points, at the border or on intersections of critical manifolds. They can be reached by tuning the value of two or more parameters, such as temperature and pressure.

Static versus dynamic properties [edit]

The above examples exclusively refer to the static properties of a critical system. However dynamic properties of the system may become critical, too. Especially, the characteristic time, τ_{char} , of a system diverges as $\tau_{\text{char}} \propto \xi^z$, with a *dynamical exponent* z . Moreover, the large *static universality classes* of equivalent models with identical static critical exponents decompose into smaller *dynamical universality classes*, if one demands that also the dynamical exponents are identical.

The critical exponents can be computed from [conformal field theory](#).

See also [anomalous scaling dimension](#).

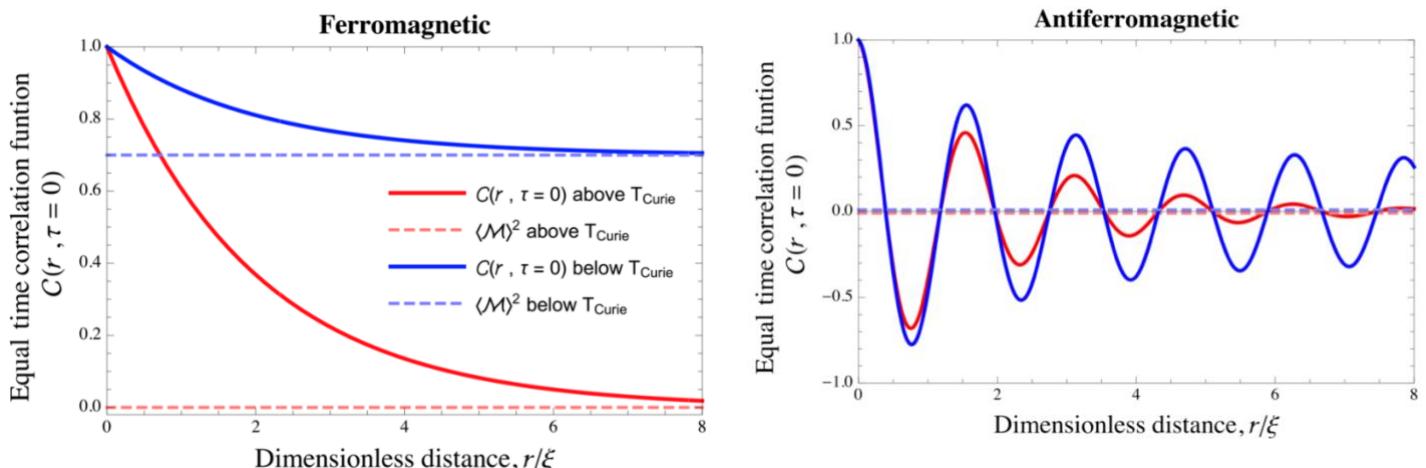
Transport properties [edit]

Critical exponents also exist for transport quantities like [viscosity](#) and [heat conductivity](#). A recent study suggests that critical exponents of percolation play an important role in city traffic.^[12]

(4) Correlation function (statistical mechanics)

[https://en.wikipedia.org/wiki/Correlation_function_\(statistical_mechanics\)](https://en.wikipedia.org/wiki/Correlation_function_(statistical_mechanics))

In statistical mechanics, **the correlation function is a measure of the order in a system**, as characterized by a mathematical correlation function. Correlation functions describe how **microscopic variables**, such as **spin and density**, at different positions are related. More specifically, correlation functions quantify how microscopic variables co-vary with one another on average across space and time. A classic example of such spatial correlations is in ferro- and antiferromagnetic materials, where the spins prefer to align parallel and antiparallel with their nearest neighbors, respectively. The spatial correlation between spins in such materials is shown in the figure below.



“Schematic equal-time spin correlation functions for ferromagnetic and antiferromagnetic materials both above and below T_{Curie} versus the distance normalized by the correlation length, ξ . In all cases, correlations are strongest nearest to the origin, indicating that a spin has the strongest influence on its nearest neighbors. All correlations gradually decay as the distance from the spin at the origin increases. Above the Curie temperature, the correlation between spins tends to zero as the distance between the spins gets very large. In contrast, below T_{Curie} , the correlation between the spins does not tend toward zero at large distances, but instead decays to a level consistent with the long-range order of the system. The difference in these decay behaviors, where correlations between microscopic random variables become zero versus non-zero at large distances, is one way of defining short- versus long-range order.”

(i) Definitions

The most common definition of a correlation function is the canonical ensemble (thermal) average of the scalar product of two random variables, s_1 and s_2 , at positions R and $R + r$ and times t and $t + \tau$:

$$C(r, \tau) = \langle s_1(R, t) \cdot s_2(R + r, t + \tau) \rangle - \langle s_1(R, t) \rangle \langle s_2(R + r, t + \tau) \rangle.$$

Here the brackets, $\langle \dots \rangle$, indicate the above-mentioned thermal average. It is a matter of convention whether one subtracts the uncorrelated average product of s_1 and s_2 , $\langle s_1(R, t) \rangle \langle s_2(R + r, t + \tau) \rangle$ from the correlated product, $\langle s_1(R, t) \cdot s_2(R + r, t + \tau) \rangle$, with the convention differing among fields. The most common uses of correlation functions are when s_1 and s_2 describe the same variable, such as a spin-spin correlation function, or a particle position-position correlation function in an elemental liquid or a solid (often called a **Radial distribution function** or a pair correlation function). Correlation functions between the same random variable are **autocorrelation functions**. However, in statistical mechanics, not all correlation functions are autocorrelation functions. For example, in multicomponent condensed phases, the pair correlation function between different elements is often of interest. Such mixed-element pair correlation functions are an example of **cross-correlation functions**, as the random variables s_1 and s_2 represent the average variations in density as a function position for two distinct elements.

Equilibrium equal-time (spatial) correlation functions [edit]

Often, one is interested in solely the *spatial* influence of a given random variable, say the direction of a spin, on its local environment, without considering later times, τ . In this case, we neglect the time evolution of the system, so the above definition is re-written with $\tau = 0$. This defines the **equal-time correlation function**, $C(r, 0)$. It is written as:

$$C(r, 0) = \langle s_1(R, t) \cdot s_2(R + r, t) \rangle - \langle s_1(R, t) \rangle \langle s_2(R + r, t) \rangle.$$

Often, one omits the reference time, t , and reference radius, R , by assuming equilibrium (and thus time invariance of the ensemble) and averaging over all sample positions, yielding:

$$C(r) = \langle s_1(0) \cdot s_2(r) \rangle - \langle s_1(0) \rangle \langle s_2(r) \rangle.$$

where, again, the choice of whether to subtract the uncorrelated variables differs among fields. The **Radial distribution function** is an example of an equal-time correlation function where the uncorrelated reference is generally not subtracted. Other equal-time spin-spin correlation functions are shown on this page for a variety of materials and conditions.

Equilibrium equal-position (temporal) correlation functions [edit]

One might also be interested in the *temporal* evolution of microscopic variables. In other words, how the value of a microscopic variable at a given position and time, R and t , influences the value of the same microscopic variable at a later time, $t + \tau$ (and usually at the same position). Such temporal correlations are quantified via **equal-position correlation functions**, $C(0, \tau)$. They are defined analogously to above equal-time correlation functions, but we now neglect spatial dependencies by setting $r = 0$, yielding:

$$C(0, \tau) = \langle \mathbf{s}_1(R, t) \cdot \mathbf{s}_2(R, t + \tau) \rangle - \langle \mathbf{s}_1(R, t) \rangle \langle \mathbf{s}_2(R, t + \tau) \rangle.$$

Assuming equilibrium (and thus time invariance of the ensemble) and averaging over all sites in the sample gives a simpler expression for the equal-position correlation function as for the equal-time correlation function:

$$C(\tau) = \langle \mathbf{s}_1(0) \cdot \mathbf{s}_2(\tau) \rangle - \langle \mathbf{s}_1(0) \rangle \langle \mathbf{s}_2(\tau) \rangle.$$

The above assumption may seem non-intuitive at first: how can an ensemble which is time-invariant have a non-uniform temporal correlation function? Temporal correlations remain relevant to talk about in equilibrium systems because a time-invariant, macroscopic ensemble can still have non-trivial temporal dynamics microscopically. One example is in diffusion. A single-phase system at equilibrium has a homogeneous composition macroscopically. However, if one watches the microscopic movement of each atom, fluctuations in composition are constantly occurring due to the quasi-random walks taken by the individual atoms. Statistical mechanics allows one to make insightful statements about the temporal behavior of such fluctuations of equilibrium systems. This is discussed below in the section on the temporal evolution of correlation functions and Onsager's regression hypothesis.

Generalization beyond equilibrium correlation functions [edit]

All of the above correlation functions have been defined in the context of equilibrium statistical mechanics. However, it is possible to define correlation functions for systems away from equilibrium. Examining the general definition of $C(r, \tau)$, it is clear that one can define the random variables used in these correlation functions, such as atomic positions and spins, away from equilibrium. As such, their scalar product is well-defined away from equilibrium. The operation which is no longer well-defined away from equilibrium is the average over the equilibrium ensemble. This averaging process for non-equilibrium system is typically replaced by averaging the scalar product across the entire sample. This is typical in scattering experiments and computer simulations, and is often used to measure the radial distribution functions of glasses.

One can also define averages over states for systems perturbed slightly from equilibrium. See, for example, <http://xbeams.chem.yale.edu/~batista/vaa/node56.html>

(ii) Measuring correlation functions

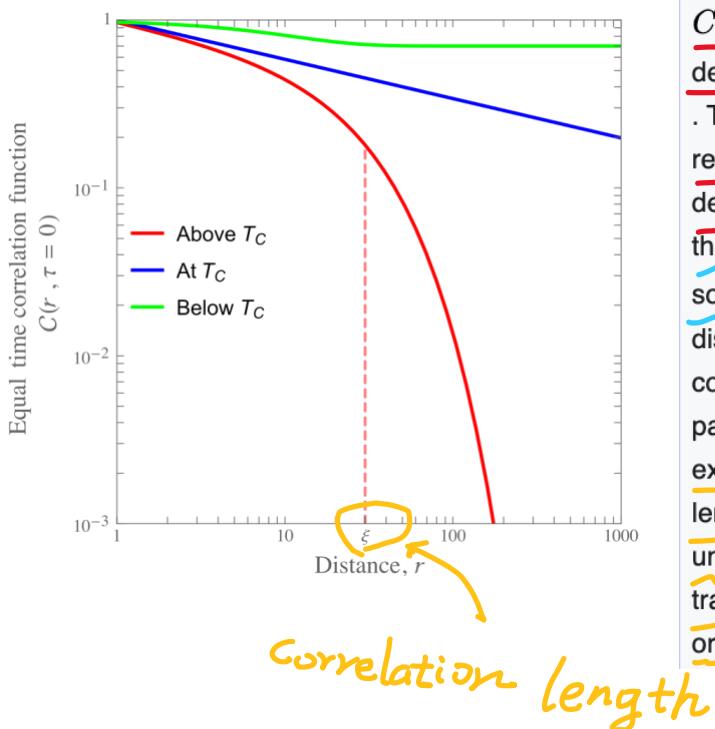
Correlation functions are typically measured with scattering experiments. For example, x-ray scattering experiments directly measure electron-electron equal-time correlations. From knowledge of elemental structure factors, one can also measure elemental pair correlation functions. See Radial distribution function for further information. Equal-time spin–spin correlation functions are measured with neutron scattering as opposed to x-ray scattering. Neutron scattering can also yield information on pair correlations as well. For systems composed of particles larger than about one micrometer, optical microscopy can be used to measure both equal-time and equal-position correlation functions. Optical microscopy is thus common for colloidal suspensions, especially in two dimensions.

(iii) Time evolution of correlation functions

In 1931, Lars Onsager proposed that the regression (回归) of microscopic thermal fluctuations at equilibrium follows the macroscopic law of relaxation of small non-equilibrium disturbances. This is known as the **Onsager regression hypothesis**. As the values of microscopic variables separated by large timescales, τ , should be uncorrelated beyond what we would expect from thermodynamic equilibrium, the evolution in time of a correlation function can be viewed from a physical standpoint as the system gradually 'forgetting' the initial conditions placed upon it via the specification of some microscopic variable. There is actually an intuitive connection between the time evolution of correlation functions and the time evolution of macroscopic systems: on average, the correlation function evolves in time in the same manner as if a system was prepared in the conditions specified by the correlation function's initial value and allowed to evolve. Equilibrium fluctuations of the system can be related to its response to external perturbations via the Fluctuation-dissipation theorem.

(iv) The connection between phase transitions and correlation functions

Continuous phase transitions, such as order-disorder transitions in metallic alloys and ferromagnetic-paramagnetic transitions, involve a transition from an ordered to a disordered state. In terms of correlation functions, the equal-time correlation function is non-zero for all lattice points below the critical temperature, and is non-negligible for only a fairly small radius above the critical temperature. As the phase transition is continuous, the length over which the microscopic variables are correlated, ξ , must transition continuously from being infinite to finite when the material is heated through its critical temperature. This gives rise to a power-law dependence of the correlation function as a function of distance at the critical point. This is shown in the figure below for the case of a ferromagnetic material, with the quantitative details listed in the section on magnetism.



Equal-time correlation functions, $C(r, \tau = 0)$, as a function of radius for a ferromagnetic spin system above, at, and below at its critical temperature, T_C . Above T_C , $C(r, \tau = 0)$ exhibits a combined exponential and power-law dependence on distance: $C(r, \tau = 0) \propto r^{-(d-2+\eta)} e^{-r/\xi(T)}$. The power-law dependence dominates at distances short relative to the correlation length, ξ , while the exponential dependence dominates at distances large relative to ξ . At T_C , the correlation length diverges, $\xi(T_C) = \infty$, resulting in solely power-law behavior: $C(r, \tau = 0) \propto r^{-(d-2+\eta)}$. T_C is distinguished by the extreme non-locality of the spatial correlations between microscopic values of the relevant order parameter without long-range order. Below T_C , the spins exhibit spontaneous ordering and thus infinite correlation length. Continuous order-disorder transitions can be understood as the process of the correlation length, ξ , transitioning from being infinite in the low-temperature, ordered state, to finite in a high-temperature, disordered state.

(v) Applications

Magnetism [edit]

In a **spin** system, the equal-time correlation function is especially well-studied. It describes the canonical ensemble (thermal) average of the scalar product of the spins at two lattice points over all possible orderings: $C(r) = \langle \mathbf{s}(R) \cdot \mathbf{s}(R+r) \rangle - \langle \mathbf{s}(R) \rangle \langle \mathbf{s}(R+r) \rangle$. Here the brackets mean the above-mentioned thermal average. Schematic plots of this function are shown for a ferromagnetic material below, at, and above its Curie temperature *above*.

Even in a magnetically disordered phase, spins at different positions are correlated, i.e., if the distance r is very small (compared to some length scale ξ), the interaction between the spins will cause them to be correlated. The alignment that would naturally arise as a result of the interaction between spins is destroyed by thermal effects. At high temperatures exponentially-decaying correlations are observed with increasing distance, with the correlation function being given asymptotically by

$$C(r) \approx \frac{1}{r^\vartheta} \exp\left(-\frac{r}{\xi}\right),$$

At high T
 $\xi \rightarrow 0$
 $r/\xi \rightarrow \infty$

where r is the distance between spins, and d is the dimension of the system, and ϑ is an exponent, whose value depends on whether the system is in the disordered phase (i.e. above the critical point), or in the ordered phase (i.e. below the critical point). At high temperatures, the correlation decays to zero exponentially with the distance between the spins. The same exponential decay as a function of radial distance is also observed below T_c , but with the limit at large distances being the mean magnetization $\langle M^2 \rangle$. Precisely at the critical point, an algebraic behavior is seen

$$C(r) \approx \frac{1}{r^{(d-2+\eta)}},$$

where η is a critical exponent, which does not have any simple relation with the non-critical exponent ϑ introduced above. For example, the exact solution of the two-dimensional Ising model (with short-ranged ferromagnetic interactions) gives precisely at criticality $\eta = \frac{1}{4}$, but above criticality $\vartheta = \frac{1}{2}$ and below criticality $\vartheta = 2$. [3][4]

As the temperature is lowered, thermal disordering is lowered, and in a continuous phase transition the correlation length diverges, as the correlation length must transition continuously from a finite value above the phase transition, to infinite below the phase transition:

$$\xi \propto |T - T_c|^{-\nu},$$

with another critical exponent ν .

means $\xi \rightarrow \infty$

This **power law** correlation is responsible for the **scaling**, seen in these transitions. All exponents mentioned are independent of temperature. They are in fact **universal**, i.e. found to be the same in a wide variety of systems.

Radial distribution functions [edit]

One common correlation function is the [radial distribution function](#) which is seen often in [statistical mechanics](#) and [fluid mechanics](#). The correlation function can be calculated in exactly solvable models (one-dimensional Bose gas, spin chains, Hubbard model) by means of [Quantum inverse scattering method](#) and [Bethe ansatz](#). In an isotropic XY model, time and temperature correlations were evaluated by Its, Korepin, Izergin & Slavnov.^[5]

Higher order correlation functions [edit]

Higher-order correlation functions involve multiple reference points, and are defined through a generalization of the above correlation function by taking the expected value of the product of more than two random variables:

$$C_{i_1 i_2 \dots i_n}(s_1, s_2, \dots, s_n) = \langle X_{i_1}(s_1) X_{i_2}(s_2) \cdots X_{i_n}(s_n) \rangle.$$

However, such higher order correlation functions are relatively difficult to interpret and measure. For example, in order to measure the higher-order analogues of pair distribution functions, coherent x-ray sources are needed. Both the theory of such analysis^{[6][7]} and the experimental measurement of the needed X-ray cross-correlation functions^[8] are areas of active research.

(5) “Critical phenomena” https://en.wikipedia.org/wiki/Critical_phenomena

In physics, [critical phenomena](#) is the collective name associated with the physics of critical points. Most of them stem from the divergence of the correlation length, but also the dynamics slows down. Critical phenomena include scaling relations among different quantities, power-law divergences of some quantities (such as the magnetic susceptibility in the ferromagnetic phase transition) described by critical exponents, universality, fractal behaviour, and ergodicity breaking.. Critical phenomena take place in second order phase transitions, although not exclusively.

The critical behavior is usually different from the mean-field approximation which is valid away from the phase transition, since the latter neglects correlations, which become increasingly important as the system approaches the critical point where the correlation length diverges. Many properties of the critical behavior of a system can be derived in the framework of the renormalization group.

In order to explain the physical origin of these phenomena, we shall use the Ising model as a pedagogical example.

(i) The critical point of the 2D Ising model

Consider a $2D$ square array of classical spins which may only take two positions: $+1$ and -1 , at a certain temperature T , interacting through the [Ising](#) classical [Hamiltonian](#):

$$H = -J \sum_{[i,j]} S_i \cdot S_j$$

where the sum is extended over the pairs of nearest neighbours and J is a coupling constant, which we will consider to be fixed. There is a certain temperature, called the [Curie temperature](#) or [critical temperature](#), T_c below which the system presents [ferromagnetic](#) long range order. Above it, it is [paramagnetic](#) and is apparently disordered.

At temperature zero, the system may only take one global sign, either +1 or -1. At higher temperatures, but below T_c , the state is still globally magnetized, but clusters of the opposite sign appear. As the temperature increases, these clusters start to contain smaller clusters themselves, in a typical Russian dolls picture. Their typical size, called the correlation length, ξ grows with temperature until it diverges at T_c . This means that the whole system is such a cluster, and there is no global magnetization. Above that temperature, the system is globally disordered, but with ordered clusters within it, whose size is again called correlation length, but it is now decreasing with temperature. At infinite temperature, it is again zero, with the system fully disordered.

(ii) Divergences at the critical point

The correlation length diverges at the critical point: as $T \rightarrow T_c$, $\xi \rightarrow \infty$. This divergence poses no physical problem. Other physical observables diverge at this point, leading to some confusion at the beginning.

The most important is susceptibility. Let us apply a very small magnetic field to the system in the critical point. A very small magnetic field is not able to magnetize a large coherent cluster, but with these fractal clusters the picture changes. It affects easily the smallest size clusters, since they have a nearly paramagnetic behaviour. But this change, in its turn, affects the next-scale clusters, and the perturbation climbs the ladder until the whole system changes radically. Thus, critical systems are very sensitive to small changes in the environment.

Other observables, such as the specific heat, may also diverge at this point. All these divergences stem from that of the correlation length.

(iii) Critical exponents and universality

As we approach the critical point, these diverging observables behave as $A(T) \propto (T - T_c)^\alpha$ for some exponent α , where, typically, the value of the exponent α is the same above and below T_c . These exponents are called critical exponents and are robust observables. Even more, they take the same values for very different physical systems. This intriguing phenomenon, called universality, is explained, qualitatively and also quantitatively, by the renormalization group.

(iv) Critical dynamics

Critical phenomena may also appear for dynamic quantities, not only for static ones. In fact, the divergence of the characteristic time τ of a system is directly related to the divergence of the thermal correlation length ξ by the introduction of a dynamical exponent z and the relation $\tau = \xi^z$. [1] The voluminous static universality class of a system splits into different, less voluminous dynamic universality classes with different values of z but a common static critical behaviour, and by approaching the critical point one may observe all kinds of slowing-down phenomena.

(v) Ergodicity (遍历性) breaking

大量的

Ergodicity is the assumption that a system, at a given temperature, explores the full phase space, just each state takes different probabilities. In an Ising ferromagnet below T_c this does not happen. If $T < T_c$, never mind how close they are, the system has chosen a global magnetization, and the phase space is divided into two regions. From one of them it is impossible to reach the other, unless a magnetic field is applied, or temperature is raised above T_c .

(vi) Mathematical tools

The main mathematical tools to study critical points are renormalization group, which takes advantage of the Russian dolls picture or the self-similarity to explain universality and predict numerically the critical exponents, and variational perturbation theory, which converts divergent perturbation expansions into convergent strong-coupling expansions relevant to critical phenomena. In two-dimensional systems, conformal field theory is a powerful tool which has discovered many new properties of 2D critical systems, employing the fact that scale invariance, along with a few other requisites, leads to an infinite symmetry group.

(vii) Critical point in renormalization group theory

The critical point is described by a conformal field theory. According to the renormalization group theory, the defining property of criticality is that the characteristic length scale of the structure of the physical system, also known as the correlation length ξ , becomes infinite. This can happen along critical lines in phase space. This effect is the cause of the critical opalescence that can be observed as a binary fluid mixture approaches its liquid–liquid critical point.

临界乱光

In systems in equilibrium, the critical point is reached only by precisely tuning a control parameter. However, in some non-equilibrium systems, the critical point is an attractor of the dynamics in a manner that is robust with respect to system parameters, a phenomenon referred to as self-organized criticality.^[2]

05/13/2020

(I) 任务：流体动力学 (Hydrodynamics) 以及 Navier-Stokes Equation

1) YouTube Title: A Brief History of the Navier-Stokes Equations

是从 Euler equations (fluid dynamics) 发展出来的 ==> Navier-Stokes Equation (N-S Equation)

<https://www.youtube.com/watch?v=g-5bi7dxHP4>

现在还没有 N-S Equation 的解析解，只能求出数值解。(Numerical solution). 而求解数值解的这个学科叫做 Computational Fluid Mechanics (CFD). (---> Remember COMSOL 软件)

2) Bilibili Title: 【图灵鸡】什么是计算流体力学 CFD?

<https://www.bilibili.com/video/BV1yt411g7iU?from=search&seid=6152445066686356695>

什么是 N-S Equation? --> 它是通过分析流体委员的受力情况，及牛顿第二定律来得出的一个描述不可压缩流体动量守恒的基本方程，即流体力学的一个基本控制方程，描述了流体的流动。是一个二阶偏微分方程。



$$\rho \left[\frac{\partial V}{\partial t} + (V \cdot \nabla) V \right] = -\nabla P + \rho g + \mu \nabla^2 V$$

Annotations pointing to terms:

- $\frac{\partial V}{\partial t}$: change of velocity with time
- $(V \cdot \nabla) V$: Convective term
- $-\nabla P$: Pressure term: Fluid flows in the direction of largest change in pressure
- ρg : Body force term: external forces that act on the fluid (such as gravity, electromagnetic, etc.)
- $\mu \nabla^2 V$: viscosity controlled velocity diffusion term

对于 N-S Equation 来说，经过不断的发展，有了许多不同的形式，如：守恒型的，非守恒型的，有适用于不同的流动条件的。。。

N-S Equation 的解即为流动情况。要求出数值解，我们必须要知道 the initial condition & boundary condition. 之后，通过有限元法(FEM, Finite Element Method)，有限差分法(Finite Difference)，有限体积法(Finite Volume Method)等数值方法不断迭代，并且缩小计算与原偏微分方程的精确解析解的误差，来得到近似的流场解。在数值方法中，通过将整个流场划分网格，然后通过使用一个物理量的有限差分去代替掉偏微分。, 近似的求解出方程在各个网格上的近似解（就是通过有限差分法进行的偏微分方程的离散化，将解析解近似为了有限个网格点（即离散点）的近似解，进而

近似出原偏微分方程的解，得出流场的流动情况。当流场中的划分的网格无线密集时，也就是有限差分变为偏微分时，这样有限差分所求出的解就是原来 N-S Equation 的解析解了。)

在 CFD (Computational Fluid Mechanics)中，网格划分是一个非常重要的问题，如笛卡尔网格回归技术，自适应网格，Thompson 椭圆网格等。现在有很多 CFD 软件网格划分工具可以不用编程自动划分出计算网格了，如 OpenFOAM 或者 ANSYS 的 ICEM, GAMBIT 等。

偏微分方程的特性/分类：双曲线型，抛物型，椭圆形，共三种。事实上，偏微分方程的分类可以通过克莱默法则和特征值法进行区分（暂时不用太了解）。这一基本的分类，对于 CFD 的数值求解算法的选择是一个至关重要的事情。（CFD 数值求解算法有显示算法及隐式算法两个大的类别--- 不用太了解）

考虑拟线性方程组

$$a_1 \frac{\partial u}{\partial x} + b_1 \frac{\partial u}{\partial y} + c_1 \frac{\partial v}{\partial x} + d_1 \frac{\partial v}{\partial y} = f_1$$
$$a_2 \frac{\partial u}{\partial x} + b_2 \frac{\partial u}{\partial y} + c_2 \frac{\partial v}{\partial x} + d_2 \frac{\partial v}{\partial y} = f_2$$

分类方法一：克莱姆法则

$$a = (a_1c_2 - a_2c_1)$$
$$b = -(a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)$$
$$c = (b_1d_2 - b_2d_1)$$

$b^2 - 4ac > 0$ 方程组是双曲型

$b^2 - 4ac = 0$ 方程组是抛物型

事实上，偏微分方程的分类可以通过克莱默法则和特征值法进行区分

分类方法二：特征值法

$$N = \begin{bmatrix} a_1 & c_1 \\ a_2 & c_2 \end{bmatrix}^{-1} \begin{bmatrix} b_1 & d_1 \\ b_2 & d_2 \end{bmatrix}$$

N 的特征值是实数，方程是双曲型
N 的特征值是虚数，方程是椭圆型
N 的特征值是实数和虚数的混合，方程组是混合特性

二阶偏微分方程
 $AU_{xx} + BU_{xy} + CU_{yy} + \dots = 0$
 $\Delta = B^2 - 4AC$
 $\Delta > 0$: 双曲型
 $\Delta = 0$: 抛物型

事实上，偏微分方程的分类可以通过克莱默法则和特征值法进行区分

N-S Equation 可以用来描述湍流流动的诸多细节。

湍流 (Turbulent Motion) , 是与层流 (Laminar Motion) 相对的一种流动, 又称为乱流, 絮流。当流场中流体的流速快过某一数值时, 流体最小的基本单位 --- 流体微元, 所流经的路径开始变得混乱, 直到流线不能再清晰可辨, 流体中出现了许多的漩涡, 层流被破坏, 这样的流动便是湍流。

湍流运动

[编辑](#) [讨论](#)

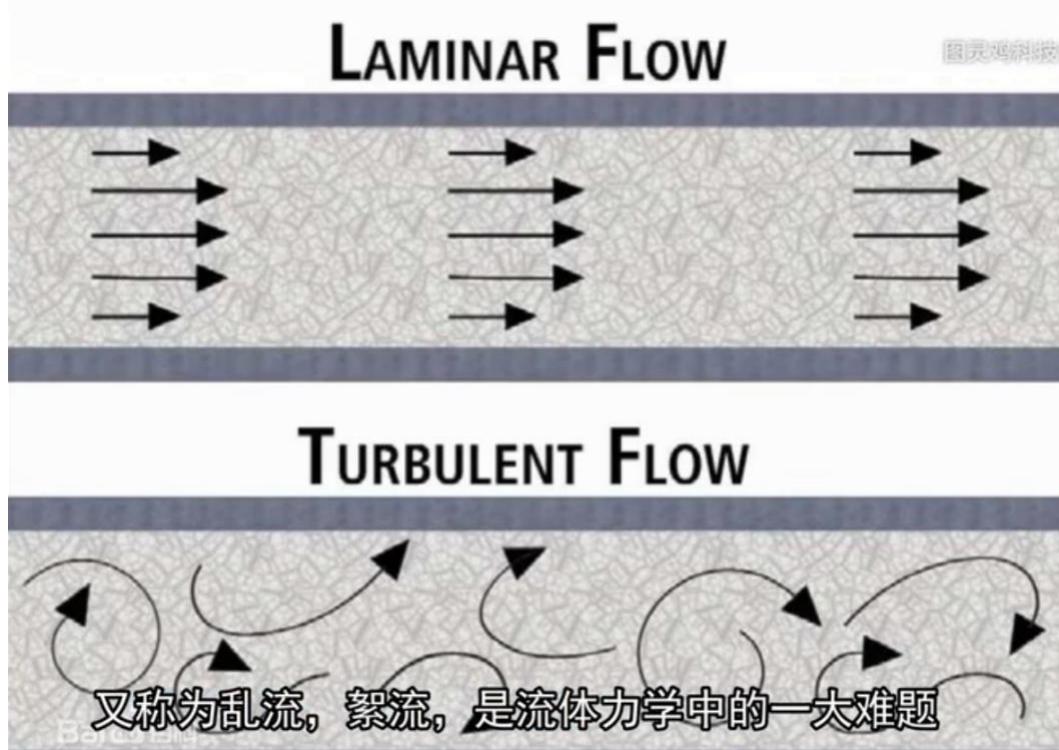
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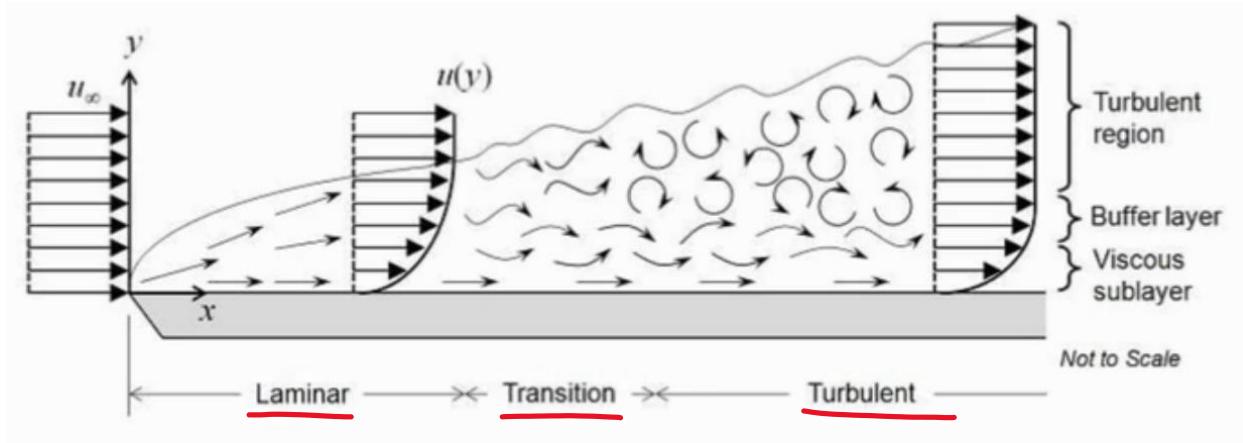
本词条由“科普中国”科学百科词条编写与应用工作项目 审核。

湍流是流体的一种流动状态。当流速增加到很大时, 流线不再清楚可辨, 流场中有许多小漩涡, 层流被破坏, 相邻流层间不但有滑动, 还有混合, 形成湍流, 又称为乱流、扰流或紊流。

在自然界中, 我们常遇到流体作湍流, 如江河急流、空气流动、烟囱排烟等都是湍流。

中文名	湍流运动	产生原因	流体系统的不稳定性
外文名	turbulent motion	特征	流体微团运动的随机性
		判断依据	雷诺数Re





2) See notes in the “Notability” App for a YouTube video.

3) Wikipedia 中文 (纳维-斯托克斯方程)

纳维尔 – 斯托克斯方程 (Navier-Stokes equations, N-S equations)，是一组描述像液体和空气这样的流体物质的方程。这些方程建立了流体的粒子动量的改变率 (力) 和作用在液体内部的压力的变化和耗散粘滞力 (类似于摩擦力) 以及重力(或者电场力等外力)之间的关系。这些粘滞力产生于分子的相互作用，能告诉我们液体有多粘。这样，纳维-斯托克斯方程描述作用于液体任意给定区域的力的动态平衡。纳维尔 – 斯托克斯方程可用于描述大量在学术研究和经济生活中的重要现象之物理过程，因此有很重要的研究价值。它们可以用于模拟天气，洋流，管道中的水流，星系中恒星的运动，翼型周围的气流。它们也可以用于飞行器和车辆的设计，血液循环的研究，电站的设计，污染效应的分析，等等。

纳维-斯托克斯方程依赖微分方程来描述流体的运动。不同于代数方程，这些方程不寻求建立所研究的变量 (譬如速度和压力) 的关系，而寻求建立这些量的变化率或通量之间的关系。用数学术语来讲，这些变化率对应于变量的导数。其中，最简单情况的 0 粘滞度的理想流体的纳维-斯托克斯方程表明，加速度 (速度的导数，或者说变化率) 是和内部压力的导数成正比的。这表示对于给定的物理问题，至少要用微积分才可以求得其纳维-斯托克斯方程的解。实用上，也只有最简单的情况才能用这种方法获得已知解。这些情况通常涉及稳定态 (流场不随时间变化) 的非紊流，其中流体的粘滞系数很大或者其速度很小 (低雷诺数)。对于更复杂的情形，例如厄尔尼诺这样的全球性气象系统或机翼的升力，纳维-斯托克斯方程的解必须借助计算机才能求得。这个科学领域称为计算流体力学。虽然紊流是日常经验中就可以遇到的，但这类非线性问题极难求解。

(i) N-S equations 的性质

(a) 非线性

纳维 – 斯托克斯方程在大多数实际情况下是非线性的偏微分方程。在某些情况下，一维流和斯托克斯流 (或蠕动流) 方程可以简化为线性方程组。非线性使得很多的问题很难或者没法解决，但是它却是动荡方程组模型的重要影响因素。**非线性是由于对流加速 (与点速度变化相关联的加速度) ，因此，任何对流无论湍流与否都会涉及非线性。**

(b) 湍流 (紊流)

湍流是时变的无序行为，这种行为常见于许多流体流动中。人们普遍认为，这是由于惯性流体被看作为一个整体而产生的：时间依赖性和对流加速度；因此惯性的影响很小的流体往往是层流（雷诺数量化了流所受惯性的大小）。虽然不完全确定，但一般相信纳维－斯托克斯方程能够合理地描述湍流。纳维－斯托克斯方程关于湍流的数值解是非常难得到的，而且由于湍流的显著不同的混合长度的尺度，需要精细分辨率的稳定解的计算时间变得不可行（见直接数值模拟）。尝试使用层流来解决湍流问题的方法通常会导致时间不稳定的解，它不能够适当收敛。为了解决这个问题，时间平均方程，如雷诺平均纳维-斯托克斯方程（RANS），再辅以湍流模型，被用作实际的计算流体动力学模拟湍流时（CFD）的应用程序。例如 Spalart-Allmaras 湍流，K- ω 湍流，k- ϵ 湍流和 SST 模型。另一种方法解决数值的纳维－斯托克斯方程是大涡模拟（LES）。这种方法在计算上是比 RANS 方法更昂贵（在时间和计算机存储器上），但因为较大的湍流尺度被明确地解决所以会产生更好的结果。

(c) 适用性

补充方程（例如，质量守恒定律）和良好的边界条件，使纳维－斯托克斯方程似乎可以进行流体运动的精确建模；甚至湍流（平均而言）也符合实际观察结果。纳维－斯托克斯方程假定所研究的流体是连续（它是无限可分的，而不是由粒子组成），并且是相对静止的。在非常小的尺度或极端条件下，由离散分子组成的真实流体将产生与由纳维－斯托克斯方程建模的连续流体不同的结果。根据 Knudsen 数的问题，统计力学甚至分子动力学可能是一个更合适的方法。另一个限制是方程的复杂性。对于普遍流体家族的公式是存在的，但纳维－斯托克斯方程对不常见流系的应用，往往会导致非常复杂的构成，而且该配方是目前研究的一个领域。出于这个原因，这些方程通常用于描述牛顿流体。研究这种液体是“简单”的，因为粘度模型最终被线性化；真正描述其他类型流体（如血液）的普遍的模型截至 2012 年还不存在。

(ii) 基本假设

在解释纳维-斯托克斯方程的细节之前，我们必须首先对流体的性质作几个假设。第一个假设是流体是连续的。这强调它不包含形成内部的空隙，例如，溶解的气体的气泡，而且它不包含雾状粒子的聚合。另一个必要的假设是所有涉及到的场，全部是可微的，例如压强，速度，密度，温度，等等。该方程从质量，动量，和能量的守恒的基本原理导出。对此，有时必须考虑一个有限的任意体积，称为控制体积，在其上这些原理很容易应用。该有限体积记为 Ω ，而其表面记为 $\partial\Omega$ 。该控制体积可以在空间中固定，也可能随着流体运动。这会导致一些特殊的结果，我们将在下节看到。

(a) 随质导数

运动流体的属性的变化，譬如大气中的风速的变化，可以有两种不同的方法来测量。可以用气象站或者气象气球上的风速仪来测量。显然，第一种情况下风速仪测量的速度是所有运动的粒子经过一个固定点的速度，而第二种情况下，仪器在测量它随着流体运动时速度的变化。同样的论证对于密度、温度、等等的测量也是成立的。因此，当作微分时必须区分两种情况。第一种情况称为空间导数或者欧拉导数。第二种情况称为实质或拉格朗日导数。

随质导数定义为算子（operator）：

$$\frac{D}{Dt}(\star) = \frac{\partial(\star)}{\partial t} + (\mathbf{v} \cdot \nabla)(\star)$$

其中 \mathbf{v} 是流体的速度。方程右边的第一项是普通的欧拉导数（也就是在静止参照系中的导数）而第二项表示由于流体的运动带来的变化。这个效应称为移流（advection）。

\mathbf{L} 的守恒定律在一个控制体积上的积分形式是：

$$\frac{d}{dt} \int_{\Omega} \mathbf{L} d\Omega = 0$$

因为 Ω 是共动的，它随着时间而改变，所以我们不能将时间导数和积分简单的交换。

$$\frac{d}{dt} \int_{\Omega} \mathbf{L} d\Omega = \int_{\Omega} \frac{\partial}{\partial t} \mathbf{L} d\Omega + \int_{\partial\Omega} \mathbf{L} (\mathbf{v} \cdot \mathbf{n} d\partial\Omega) = \int_{\Omega} \left[\frac{\partial}{\partial t} \mathbf{L} + \nabla \cdot (\mathbf{L}\mathbf{v}) \right] d\Omega = 0$$

因为这个表达式对于所有 Ω 成立，它可以简化为：

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

对于不是密度的量（因而它不必在空间中积分）， $\frac{D}{Dt}$ 给出了正确的共动时间导数。

(b) 守恒定律

NS方程可以从守恒定律通过上述变换导出，并且需要用状态定律来闭合。

在控制体积上，使用上述变换，下列的量视为守恒：

- 质量
- 能量
- 动量
- 角动量

连续性方程 [编辑]

质量的守恒写作：

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

其中

ρ 是流体的密度。

在不可压缩流体的情况 ρ 不是时间或空间的函数。方程简化为：

$$\underline{\nabla \cdot \mathbf{v} = 0}$$

动量守恒 [编辑]

动量守恒写作：

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla (\rho \mathbf{v} \otimes \mathbf{v}) = \sum \rho \mathbf{f}$$

注意 $\mathbf{v} \otimes \mathbf{v}$ 是一个张量， \otimes 代表张量积。

我们可以进一步简化，利用连续性方程，这成为：

$$\rho \frac{D\mathbf{v}}{Dt} = \sum \rho \mathbf{f}$$

我们可以认出这就是通常的 $F=ma$ 。

(iii) 方程组

一般形式

(a) 方程组的形式

纳维-斯托克斯方程的一般形式是：

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \mathbb{P} + \rho \mathbf{f}$$

关于动量守恒。 张量 \mathbb{P} 代表施加在一个流体粒子上的表面力（应力张量）。 除非流体是由象旋涡这样的旋转自由度组成， \mathbb{P} 是一个对称张量。一般来讲，我们有如下形式：

$$\mathbb{P} = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{pmatrix} = - \begin{pmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{pmatrix} + \begin{pmatrix} \sigma_{xx} + p & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} + p & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} + p \end{pmatrix}$$

其中 σ 是法向约束，而 τ 是切向约束。

迹 $\sigma_{xx} + \sigma_{yy} + \sigma_{zz}$ 在流体处于平衡态时为 0。这等价于流体粒子上的法向力的积分为 0。

我们再加上连续性方程：

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0$$

对于处于平衡的液体， \mathbb{P} 的迹是 $3p$ 。

其中

p 是压强

最后，我们得到：

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \mathbb{T} + \rho \mathbf{f}$$

其中 \mathbb{T} 是 \mathbb{P} 的非对角线部分。

(b) 闭合问题

这些方程是不完整的。要对它们进行完备化，必须对 \mathbb{P} 的形式作一些假设。例如在理想流体的情况 τ 分量为 0。用于完备方程组的方程是状态方程。

再如，压强 可以主要是密度和温度的函数。

要求解的变量是速度的各个分量，流体密度，静压力，和温度。 流场假定为可微并连续，使得这些平衡得以用偏微分方程表达。这些方程可以转化为涡度和流函数这些次变量的威尔金森方程组。解依赖于流体的性质（例如粘滞度、比热、和热导率），并且依赖于所研究的区域的边界条件。

\mathbb{P} 的分量是流体的一个无穷小元上面的约束。它们代表垂直和剪切约束。 \mathbb{P} 是对称的，除非存在非零的自旋密度。

所谓非牛顿流体就是其中该张量没有特殊性质使得方程的特殊解出现的流体

(iv) 特殊形式

这些是问题的特定的常见简化，有时解是已知的。

(a) 牛顿流体

在牛顿流体中，如下假设成立：

$$\tau_{ij} = \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{v} \right)$$

其中

μ 是液体的粘滞度。

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot \mathbf{v} \right) = \rho \mathbf{f} - \nabla p + \mu \left(\Delta \mathbf{v} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{v}) \right)$$

$$\rho \left(\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} \right) = \rho f_i - \frac{\partial p}{\partial x_i} + \mu \left(\frac{\partial^2 v_i}{\partial x_j \partial x_j} + \frac{1}{3} \frac{\partial^2 v_i}{\partial x_i \partial x_j} \right)$$

其中为简化书写，对脚标使用了爱因斯坦求和约定。

不采用简化书写的完整形式非常繁琐，分别为：

动量守恒：

$$\begin{aligned} \rho \cdot \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) &= k_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[\mu \cdot \left(2 \cdot \frac{\partial u}{\partial x} - \frac{2}{3} \cdot (\nabla \cdot \vec{v}) \right) \right] + \frac{\partial}{\partial y} \left[\mu \cdot \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[\mu \cdot \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] \\ \rho \cdot \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) &= k_y - \frac{\partial p}{\partial y} + \frac{\partial}{\partial y} \left[\mu \cdot \left(2 \cdot \frac{\partial v}{\partial y} - \frac{2}{3} \cdot (\nabla \cdot \vec{v}) \right) \right] + \frac{\partial}{\partial z} \left[\mu \cdot \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] + \frac{\partial}{\partial x} \left[\mu \cdot \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \\ \rho \cdot \left(\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) &= k_z - \frac{\partial p}{\partial z} + \frac{\partial}{\partial z} \left[\mu \cdot \left(2 \cdot \frac{\partial w}{\partial z} - \frac{2}{3} \cdot (\nabla \cdot \vec{v}) \right) \right] + \frac{\partial}{\partial x} \left[\mu \cdot \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[\mu \cdot \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] \end{aligned}$$

质量守恒：

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho \cdot u)}{\partial x} + \frac{\partial(\rho \cdot v)}{\partial y} + \frac{\partial(\rho \cdot w)}{\partial z} = 0$$

因为密度是一个未知数，我们需要另一个方程。

能量守恒：

$$\rho \left(\frac{\partial e}{\partial t} + u \frac{\partial e}{\partial x} + v \frac{\partial e}{\partial y} + w \frac{\partial e}{\partial z} \right) = \left(\frac{\partial}{\partial x} \left(\lambda \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \cdot \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda \cdot \frac{\partial T}{\partial z} \right) \right) - p \cdot (\nabla \cdot \vec{v}) + \vec{k} \cdot \vec{v} + \rho \cdot \dot{q}_s + \mu \cdot \Phi$$

其中：

$$\Phi = 2 \cdot \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 - \frac{2}{3} \cdot \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2$$

假设一个理想气体：

$$e = c_p \cdot T - \frac{p}{\rho}$$

上面是一共6个方程6个未知数的系统。 (u, v, w, T, e) 以及 ρ 。

(b) 宾汉 (Bingham) 流体

在宾汉流体中，我们有稍微不同的假设：

$$\tau_{ij} = \tau_0 + \mu \frac{\partial v_i}{\partial x_j}, \quad \frac{\partial v_i}{\partial x_j} > 0$$

那些流体在开始流动之前能够承受一定的剪切。牙膏是一个例子。

(c) 幂律流体

这是一种理想化的流体，其剪切应力， τ ，由下式给出

$$\tau = K \left(\frac{\partial u}{\partial y} \right)^n$$

该形式对于模拟各种一般流体有用。

小的 summary:

看来对于前三种不同类型的流体，他们之间最主要的区别在于张量 P 的形式的不同。（特别是 τ_{ij} 的不同）

(d) 不可压缩流体

其纳维－斯托克斯方程 (Navier-Stokes equation) 分为动量守恒公式

$$\underbrace{\rho \left(\underbrace{\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v}}_{\text{Unsteady acceleration}} \right)}_{\text{Inertia}} = \underbrace{-\nabla p}_{\text{Pressure gradient}} + \underbrace{\mu \nabla^2 \mathbf{v}}_{\text{Viscosity}} + \underbrace{\mathbf{f}}_{\text{Other forces}}$$

和质量守恒公式

$$\nabla \cdot \mathbf{v} = 0.$$



其中，对不可压缩牛顿流体来说，只有对流项 (convective terms) 为非线性形式。对流加速度 (convective acceleration) 来自于流体流动随空间之变化所产生的速度改变，例如：当流体通过一个渐缩喷嘴 (convergent nozzle) 时，流体产生加速之情况。由于此项的存在，对于暂态运动中的流体来说，其流场速度变化不再单是时间的函数，亦与空间有关。

另外一个重要的观察重点，在于黏滞力 (viscosity) 在流场中的以流体速度作拉普拉斯运算来表现。这暗示了在牛顿流体中，黏滞力为动量扩散 (diffusion of momentum)，与热扩散方程式非常类似。

$$e_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right);$$

$\Delta = e_{ii}$ 是散度，

δ_{ij} 是克罗内克记号。

若 μ 在整个流体上均匀，动量方程简化为

$$\rho \frac{D u_i}{D t} = \rho f_i - \frac{\partial p}{\partial x_i} + \mu \left(\frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{1}{3} \frac{\partial \Delta}{\partial x_i} \right)$$

(若 $\mu = 0$ 这个方程称为欧拉方程；那里的重点是可压缩流和冲击波)。

如果现在再有 ρ 为常数，我们得到如下系统：

$$\begin{aligned}\rho \left(\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right) &= \mu \left[\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right] - \frac{\partial p}{\partial x} + \rho g_x \\ \rho \left(\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right) &= \mu \left[\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right] - \frac{\partial p}{\partial y} + \rho g_y \\ \rho \left(\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right) &= \mu \left[\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right] - \frac{\partial p}{\partial z} + \rho g_z\end{aligned}$$

连续性方程（假设不可压缩性）：

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0$$

N-S方程的简化版本。采用《不可压缩流》，Ronald Panton所著第二版

注意纳维—斯托克斯方程仅可近似描述液体流，而且在非常小的尺度或极端条件下，由离散的分子和其他物质（例如悬浮粒子和溶解的气体）的混合体组成的真实流体，会产生和纳维—斯托克斯方程所描述的连续并且齐性的液体不同的结果。依赖于问题的纳森数，统计力学可能是一个更合适的方法。但是，纳维—斯托克斯方程对于很大范围的实际问题是有效的，只要记住他们的缺陷是天生的就可以了。

4) Wikipedia 英文 https://en.wikipedia.org/wiki/Navier%20-%20Stokes_equations

In physics, the Navier–Stokes equations (N-S Equations), describe the motion of viscous fluid substances. These balance equations arise from applying Isaac Newton's second law to fluid motion, together with the assumption that the stress in the fluid is the sum of a diffusing viscous term (proportional to the gradient of velocity) and a pressure term—hence describing viscous flow.

The main difference between them and the simpler Euler equations for inviscid flow (无粘性流) is that Navier–Stokes equations also factor in the Froude limit (no external field) and are not conservation equations, but rather a dissipative system, in the sense that they cannot be put into the quasilinear homogeneous form:

$$\mathbf{y}_t + \mathbf{A}(\mathbf{y})\mathbf{y}_x = 0$$

The Navier–Stokes equations are useful because they describe the physics of many phenomena of scientific and engineering interest. They may be used to model the weather, ocean currents, water flow in a pipe and air flow around a wing. The Navier–Stokes equations, in their full and simplified forms, help with the design of aircraft and cars, the study of blood flow, the design of power stations, the analysis of pollution, and many other things. Coupled with Maxwell's equations, they can be used to model and study magnetohydrodynamics. The Navier–Stokes equations are also of great interest in a purely mathematical sense. Despite their wide range of practical uses, it has not yet been proven whether solutions always exist in three dimensions and, if they do exist, whether they are smooth – i.e. they are infinitely differentiable at all points in the domain. These are called the Navier–Stokes existence and smoothness problems. The Clay Mathematics Institute has called this one of the seven most important open problems in mathematics and has offered a US\$1 million prize for a solution or a counterexample.

(i) Flow velocity

The solution of the equations is a flow velocity. It is a vector field - to every point in a fluid, at any moment in a time interval, it gives a vector whose direction and magnitude are those of the velocity of the fluid at that point in space and at that moment in time. It is usually studied in three spatial dimensions and one time dimension, although the two (spatial) dimensional case is often useful as a model, and higher-dimensional analogues are of both pure and applied mathematical interest. Once the velocity field is calculated, other quantities of interest such as pressure or temperature may be found using dynamical equations and relations. This is different from what one normally sees in classical mechanics, where solutions are typically trajectories of position of a particle or deflection of a continuum. Studying velocity instead of position makes more sense for a fluid; however for visualization purposes one can compute various trajectories. In particular, the streamlines of a vector field, interpreted as flow velocity, are the paths along which a massless fluid particle would travel. These paths are the integral curves whose derivative at each point is equal to the vector field, and they can represent visually the behavior of the vector field at a point in time.

(ii) General continuum equations

The Navier–Stokes momentum equation can be derived as a particular form of the Cauchy momentum equation, whose general convective form is

$$\frac{D\mathbf{u}}{Dt} = \frac{1}{\rho} \nabla \cdot \boldsymbol{\sigma} + \mathbf{g}$$

By setting the Cauchy stress tensor $\boldsymbol{\sigma}$ to be the sum of a viscosity term $\boldsymbol{\tau}$ (the deviatoric stress) and a pressure term $-p\mathbf{I}$ (volumetric stress) we arrive at

Cauchy momentum equation(convective form)

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

where

- $\frac{D}{Dt}$ is the material derivative, defined as $\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$,
- ρ is the density,
- \mathbf{u} is the flow velocity,
- $\nabla \cdot$ is the divergence,
- p is the pressure,
- t is time,
- $\boldsymbol{\tau}$ is the deviatoric stress tensor, which has order two,
- \mathbf{g} represents body accelerations acting on the continuum, for example gravity, inertial accelerations, electrostatic accelerations, and so on,

In this form, it is apparent that in the assumption of an inviscid fluid -no deviatoric stress- Cauchy equations reduce to the [Euler equations](#).

Assuming [conservation of mass](#) we can use the mass continuity equation (or simply continuity equation),

$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$ to arrive to the conservation form of the equations of motion. This is often written:^[3]

Cauchy momentum equation (conservation form)

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

where \otimes is the [outer product](#):

$$\mathbf{u} \otimes \mathbf{v} = \mathbf{u}\mathbf{v}^T.$$

The left side of the equation describes acceleration, and may be composed of time-dependent and convective components (also the effects of non-inertial coordinates if present). The right side of the equation is in effect a summation of hydrostatic effects, the divergence of deviatoric stress and body forces (such as gravity).

All non-relativistic balance equations, such as the [Navier–Stokes equations](#), can be derived by beginning with the Cauchy equations and specifying the stress tensor through a [constitutive relation](#). By expressing the deviatoric (shear) stress tensor in terms of [viscosity](#) and the fluid [velocity](#) gradient, and assuming constant viscosity, the above Cauchy equations will lead to the Navier–Stokes equations below.

Convective acceleration

A significant feature of the Cauchy equation and consequently all other continuum equations (including Euler and Navier–Stokes) is the presence of convective acceleration: the effect of acceleration of a flow with respect to space. While individual fluid particles indeed experience time-dependent acceleration, the convective acceleration of the flow field is a spatial effect, one example being fluid speeding up in a nozzle.

(iii) Compressible flow

Remark: here, the Cauchy stress tensor is denoted as σ (instead of τ) as it was in the general continuum equations and in the incompressible flow section). The compressible momentum Navier–Stokes equation results from the following assumptions on the Cauchy stress tensor:

- the stress is **Galileian invariant**: it does not depend directly on the flow velocity, but only on spatial derivatives of the flow velocity. So the stress variable is the tensor gradient $\nabla \mathbf{u}$.
- the stress is **linear** in this variable: $\sigma(\nabla \mathbf{u}) = \mathbf{C} : (\nabla \mathbf{u})$, where \mathbf{C} is the fourth-order tensor representing the constant of proportionality, called the viscosity or **elasticity tensor**, and $:$ is the **double-dot product**.
- the fluid is assumed to be **isotropic**, as with gases and simple liquids, and consequently \mathbf{V} is an isotropic tensor; furthermore, since the stress tensor is symmetric, by **Helmholtz decomposition** it can be expressed in terms of two scalar **Lamé parameters**, the **bulk viscosity** λ and the **dynamic viscosity** μ , as it is usual in **linear elasticity**:

Linear stress constitutive equation (*expression used for elastic solid*)

$$\sigma = \lambda(\nabla \cdot \mathbf{u})\mathbf{I} + 2\mu\epsilon$$

where \mathbf{I} is the identity tensor, $\epsilon(\nabla \mathbf{u}) \equiv \frac{1}{2}\nabla \mathbf{u} + \frac{1}{2}(\nabla \mathbf{u})^T$ is the **rate-of-strain tensor** and $\nabla \cdot \mathbf{u}$ is the rate of expansion of the flow. So this decomposition can be explicated as:

$$\sigma = \lambda(\nabla \cdot \mathbf{u})\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T).$$

Since the **trace** of the rate-of-strain tensor in three dimensions is:

$$\text{tr}(\epsilon) = \nabla \cdot \mathbf{u}.$$

The trace of the stress tensor in three dimensions becomes:

$$\text{tr}(\sigma) = (3\lambda + 2\mu)\nabla \cdot \mathbf{u}.$$

So by alternatively decomposing the stress tensor into **isotropic** and **deviatoric** parts, as usual in fluid dynamics:^[5]

$$\sigma = \left(\lambda + \frac{2}{3}\mu\right)(\nabla \cdot \mathbf{u})\mathbf{I} + \mu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I}\right)$$

Introducing the **second viscosity** ζ ,

$$\zeta \equiv \lambda + \frac{2}{3}\mu,$$

we arrive to the **linear constitutive equation** in the form usually employed in **thermal hydraulics**:^[4]

Linear stress constitutive equation (*expression used for fluids*)

$$\sigma = \zeta(\nabla \cdot \mathbf{u})\mathbf{I} + \mu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I}\right)$$

Both second viscosity ζ and dynamic viscosity μ need not be constant – in general, they depend on density, on each other (the viscosity is expressed in pressure), and in compressible flows also on temperature. Any equation expliciting one of these **transport coefficient** in the **conservation variables** is called an **equation of state**.^[6]

By computing the divergence of the stress tensor, since the divergence of tensor $\nabla \mathbf{u}$ is $\nabla^2 \mathbf{u}$ and the divergence of tensor $(\nabla \mathbf{u})^T$ is $\nabla(\nabla \cdot \mathbf{u})$, one finally arrives to the compressible (most general) Navier–Stokes momentum equation:^[7]

Navier–Stokes momentum equation (convective form)

$$\rho \frac{D\mathbf{u}}{Dt} = \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla \bar{p} + \mu \nabla^2 \mathbf{u} + \frac{1}{3} \mu \nabla(\nabla \cdot \mathbf{u}) + \rho \mathbf{g}.$$

where D/Dt is the [material derivative](#). The left hand side changes in the conservation form of the Navier–Stokes momentum equation:

Navier–Stokes momentum equation (conservation form)

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla \bar{p} + \mu \nabla^2 \mathbf{u} + \frac{1}{3} \mu \nabla(\nabla \cdot \mathbf{u}) + \rho \mathbf{g}.$$

Bulk viscosity is assumed to be constant, otherwise it should not be taken out of the last derivative. The effect of the volume viscosity ζ is that the mechanical pressure is not equivalent to the thermodynamic [pressure](#):^[8]

$$\bar{p} \equiv p - \zeta \nabla \cdot \mathbf{u},$$

This difference is usually neglected, sometimes by explicitly assuming $\zeta = 0$, but it could have an impact in sound absorption and attenuation and shock waves.^[9] The convective acceleration term can also be written as

$$\mathbf{u} \cdot \nabla \mathbf{u} = (\nabla \times \mathbf{u}) \times \mathbf{u} + \frac{1}{2} \nabla \mathbf{u}^2,$$

where the vector $(\nabla \times \mathbf{u}) \times \mathbf{u}$ is known as the [Lamb vector](#).

For the special case of an [incompressible flow](#), the pressure constrains the flow so that the volume of [fluid elements](#) is constant: [isochoric flow](#) resulting in a [solenoidal](#) velocity field with $\nabla \cdot \mathbf{u} = 0$.^[10]

(iv) Incompressible flow

The incompressible momentum Navier–Stokes equation results from the following assumptions on the Cauchy stress tensor:^[4]

- the stress is [Galilean invariant](#): it does not depend directly on the flow velocity, but only on spatial derivatives of the flow velocity. So the stress variable is the tensor gradient $\nabla \mathbf{u}$.
- the fluid is assumed to be [isotropic](#), as with gases and simple liquids, and consequently τ is an isotropic tensor; furthermore, since the deviatoric stress tensor can be expressed in terms of the [dynamic viscosity](#) μ :

Stokes' stress constitutive equation (*expression used for incompressible elastic solids*)

$$\tau = 2\mu \epsilon$$

where

$$\epsilon = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

is the [rate-of-strain tensor](#). So this decomposition can be explicitated as:^[4]

Stokes's stress constitutive equation (*expression used for incompressible viscous fluids*)

$$\boldsymbol{\tau} = \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

Dynamic viscosity μ need not be constant – in incompressible flows it can depend on density and on pressure. Any equation expliciting one of these **transport coefficient** in the **conservative variables** is called an **equation of state**.^[6]

The divergence of the deviatoric stress is given by:

$$\nabla \cdot \boldsymbol{\tau} = 2\mu \nabla \cdot \boldsymbol{\varepsilon} = \mu \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) = \mu \nabla^2 \mathbf{u}$$

because $\nabla \cdot \mathbf{u} = 0$ for an incompressible fluid. Incompressibility rules out density and pressure waves like sound or **shock waves**, so this simplification is not useful if these phenomena are of interest. The incompressible flow assumption typically holds well with all fluids at low **Mach numbers** (say up to about Mach 0.3), such as for modelling air winds at normal temperatures.^[11] For incompressible (uniform density ρ_0) flows the following identity holds:

$$\frac{1}{\rho_0} \nabla p = \nabla \left(\frac{p}{\rho_0} \right) \equiv \nabla w$$

where w is the specific (with the sense of *per unit mass*) **thermodynamic work**, the internal source term. Then the incompressible Navier–Stokes equations are best visualised by dividing for the density:

Incompressible Navier–Stokes equations (*convective form*)

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nu \nabla^2 \mathbf{u} = -\nabla w + \mathbf{g}.$$

where $\nu = \frac{\mu}{\rho_0}$ is called the **kinematic viscosity**.

It is well worth observing the meaning of each term (compare to the **Cauchy momentum equation**):

$$\underbrace{\frac{\partial \mathbf{u}}{\partial t} + \underbrace{(\mathbf{u} \cdot \nabla) \mathbf{u}}_{\text{Convection}}}_{\substack{\text{Inertia (per volume)} \\ \text{Variation}}} - \underbrace{\nu \nabla^2 \mathbf{u}}_{\substack{\text{Divergence of stress} \\ \text{Diffusion}}} = \underbrace{-\nabla w}_{\substack{\text{Internal} \\ \text{source}}} + \underbrace{\mathbf{g}}_{\substack{\text{External} \\ \text{source}}}.$$

The higher-order term, namely the **shear stress** divergence $\nabla \cdot \boldsymbol{\tau}$, has simply reduced to the **vector Laplacian** term $\mu \nabla^2 \mathbf{u}$.^[12] This Laplacian term can be interpreted as the difference between the velocity at a point and the mean velocity in a small surrounding volume. This implies that – for a Newtonian fluid – viscosity operates as a *diffusion of momentum*, in much the same way as the **heat conduction**. In fact neglecting the convection term, incompressible Navier–Stokes equations lead to a vector **diffusion equation** (namely **Stokes equations**), but in general the convection term is present, so incompressible Navier–Stokes equations belong to the class of **convection–diffusion equations**.

In the usual case of an external field being a [conservative field](#):

$$\mathbf{g} = -\nabla\varphi$$

by defining the [hydraulic head](#):

$$h \equiv w + \varphi$$

one can finally condense the whole source in one term, arriving to the incompressible Navier–Stokes equation with conservative external field:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nu \nabla^2 \mathbf{u} = -\nabla h.$$

The incompressible Navier–Stokes equations with conservative external field is the [fundamental equation of hydraulics](#). The domain for these equations is commonly a 3 or less [Euclidean space](#), for which an [orthogonal coordinate](#) reference frame is usually set to explicit the system of scalar partial differential equations to be solved. In 3D orthogonal coordinate systems are 3: [Cartesian](#), [cylindrical](#), and [spherical](#). Expressing the Navier–Stokes vector equation in Cartesian coordinates is quite straightforward and not much influenced by the number of dimensions of the Euclidean space employed, and this is the case also for the first-order terms (like the variation and convection ones) also in non-Cartesian orthogonal coordinate systems. But for the higher order terms (the two coming from the divergence of the deviatoric stress that distinguish Navier–Stokes equations from Euler equations) some [tensor calculus](#) is required for deducing an expression in non-Cartesian orthogonal coordinate systems.

The incompressible Navier–Stokes equation is composite, the sum of two orthogonal equations,

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} &= \Pi^S (-(\mathbf{u} \cdot \nabla) \mathbf{u} + \nu \nabla^2 \mathbf{u}) + \mathbf{f}^S \\ \rho^{-1} \nabla p &= \Pi^I (-(\mathbf{u} \cdot \nabla) \mathbf{u} + \nu \nabla^2 \mathbf{u}) + \mathbf{f}^I\end{aligned}$$

where Π^S and Π^I are solenoidal and [irrotational](#) projection operators satisfying $\Pi^S + \Pi^I = 1$ and \mathbf{f}^S and \mathbf{f}^I are the non-conservative and conservative parts of the body force. This result follows from the [Helmholtz theorem](#) (also known as the fundamental theorem of vector calculus). The first equation is a pressureless governing equation for the velocity, while the second equation for the pressure is a functional of the velocity and is related to the pressure Poisson equation.

The explicit functional form of the projection operator in 3D is found from the Helmholtz Theorem:

$$\Pi^S \mathbf{F}(\mathbf{r}) = \frac{1}{4\pi} \nabla \times \int \frac{\nabla' \times \mathbf{F}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV', \quad \Pi^I = 1 - \Pi^S$$

with a similar structure in 2D. Thus the governing equation is an [integro-differential equation](#) similar to [Coulomb](#) and [Biot–Savart law](#), not convenient for numerical computation.

An equivalent weak or variational form of the equation, proved to produce the same velocity solution as the Navier–Stokes equation,^[13] is given by,

$$\left(\mathbf{w}, \frac{\partial \mathbf{u}}{\partial t} \right) = - (\mathbf{w}, (\mathbf{u} \cdot \nabla) \mathbf{u}) - \nu (\nabla \mathbf{w} : \nabla \mathbf{u}) + (\mathbf{w}, \mathbf{f}^S)$$

for divergence-free test functions \mathbf{w} satisfying appropriate boundary conditions. Here, the projections are accomplished by the orthogonality of the solenoidal and irrotational function spaces. The discrete form of this is eminently suited to finite element computation of divergence-free flow, as we shall see in the next section. There one will be able to address the question "How does one specify pressure-driven (Poiseuille) problems with a pressureless governing equation?".

The absence of pressure forces from the governing velocity equation demonstrates that the equation is not a dynamic one, but rather a kinematic equation where the divergence-free condition serves the role of a conservation equation. This all would seem to refute the frequent statements that the incompressible pressure enforces the divergence-free condition.

因为不太能看懂省略一部分。。。

(v) Properties

(a) Nonlinearity

The Navier–Stokes equations are nonlinear partial differential equations in the general case and so remain in almost every real situation. In some cases, such as one-dimensional flow and Stokes flow (or creeping flow), the equations can be simplified to linear equations. The nonlinearity makes most problems difficult or impossible to solve and is the main contributor to the turbulence that the equations model. **The nonlinearity is due to convective acceleration, which is an acceleration associated with the change in velocity over position.** Hence, any convective flow, whether turbulent or not, will involve nonlinearity. An example of convective but laminar (nonturbulent) flow would be the passage of a viscous fluid (for example, oil) through a small converging nozzle. Such flows, whether exactly solvable or not, can often be thoroughly studied and understood.

(b) Turbulence

Turbulence is the time-dependent chaotic behavior seen in many fluid flows. It is generally believed that it is due to the inertia (惯性) of the fluid as a whole: the culmination (高潮) of time-dependent and convective acceleration; hence flows where inertial effects are small tend to be laminar (**the Reynolds number quantifies how much the flow is affected by inertia**). It is believed, though not known with certainty, that the Navier–Stokes equations describe turbulence properly.

The numerical solution of the Navier–Stokes equations for turbulent flow is extremely difficult, and due to the significantly different mixing-length scales that are involved in turbulent flow, the stable solution of this requires such a fine mesh resolution that the computational time becomes significantly infeasible for calculation or direct numerical simulation. Attempts to solve turbulent flow using a laminar solver typically result in a time-unsteady solution, which fails to converge appropriately. To counter this, time-averaged equations such as the **Reynolds-averaged Navier–Stokes equations (RANS)**, **supplemented with turbulence models, are used in practical computational fluid dynamics (CFD) applications when modeling turbulent flows.** Some models include the Spalart–Allmaras, $k-\omega$, $k-\epsilon$, and SST models, which add a variety of additional equations to bring closure to the RANS equations. Large eddy (涡流) simulation (LES) can also be used to solve these equations numerically. This approach is computationally more expensive—in time and in computer memory—than RANS, but produces better results because it explicitly resolves the larger turbulent scales.

(c) Applicability

Together with supplemental equations (for example, conservation of mass) and well formulated boundary conditions, the Navier–Stokes equations seem to model fluid motion accurately; even turbulent flows seem (on average) to agree with real world observations. The Navier–Stokes equations assume that the fluid being studied is a continuum (it is infinitely divisible and not composed of particles such as atoms or molecules), and is not moving at relativistic velocities. At very small scales or under extreme conditions, real fluids made out of discrete molecules will produce results different from the continuous fluids modeled by the Navier–Stokes equations. For example, capillarity of internal layers in fluids appears for flow with high gradients. For large Knudsen number of the problem, the Boltzmann equation may be a suitable replacement. Failing that, one may have to resort to molecular dynamics or various hybrid methods. Another limitation is simply the complicated nature of the equations. Time-tested formulations exist for common fluid families, but the application of the Navier–Stokes equations to less common families tends to result in very complicated formulations and often to open research problems. For this reason, these equations are usually written for Newtonian fluids where the viscosity model is linear; truly general models for the flow of other kinds of fluids (such as blood) do not exist.

5) <https://cn.comsol.com/multiphysics/navier-stokes-equations>

什么是纳维-斯托克斯方程？

纳维-斯托克斯方程是用于描述流体运动的方程，可以看作是流体运动的牛顿第二定律。对于可压缩的牛顿流体，可以得到

$$\underbrace{\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right)}_1 = \underbrace{-\nabla p}_2 + \underbrace{\nabla \cdot (\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I})}_3 + \underbrace{\mathbf{F}}_4$$

其中， \mathbf{u} 是流体速度， p 是流体压力， ρ 是流体密度， μ 是流体动力黏度。

式中各项分别对应于惯性力（1）、压力（2）、黏性力（3），以及作用在流体上的外力（4）。纳维-斯托克斯方程是由纳维、泊松、圣维南和斯托克斯于 1827 年到 1845 年之间推导出来的。

这些方程总是要与连续性方程同时进行求解：

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

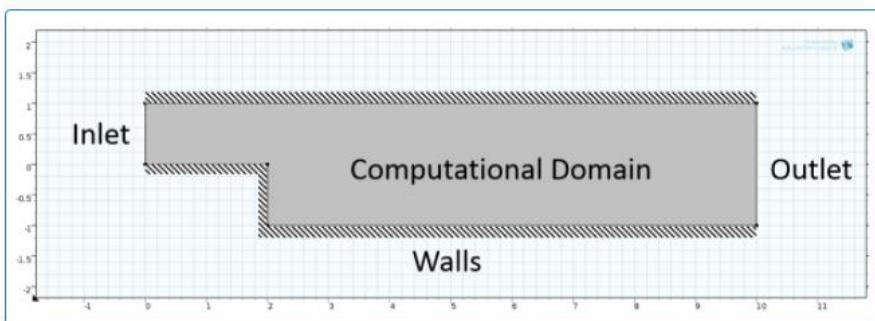
纳维-斯托克斯方程表示动量守恒，而连续性方程则表示质量守恒。

纳维-斯托克斯方程在建模仿真中的应用

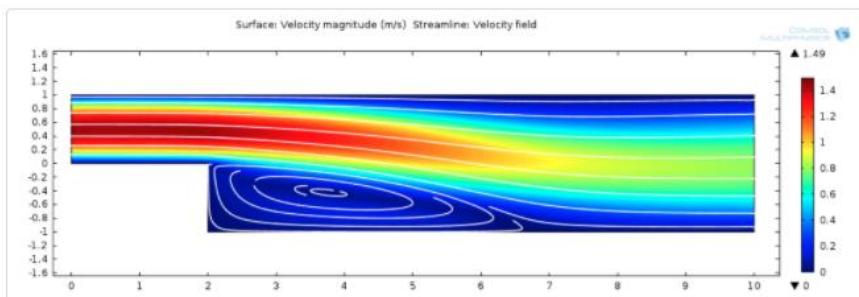
纳维-斯托克斯方程是流体流动建模的核心。在特定的边界条件（如入口、出口和壁）下求解这些方程，可以预测给定几何体中的流体速度和压力。由于这些方程本身的复杂性，我们只能得到非常有限的解析解。例如，对于两个平行板之间的流动或圆管内的流动，方程的求解会相对容易一些；但对于更为复杂的几何结构，求解方程会非常困难。

示例：流经后台阶的层流

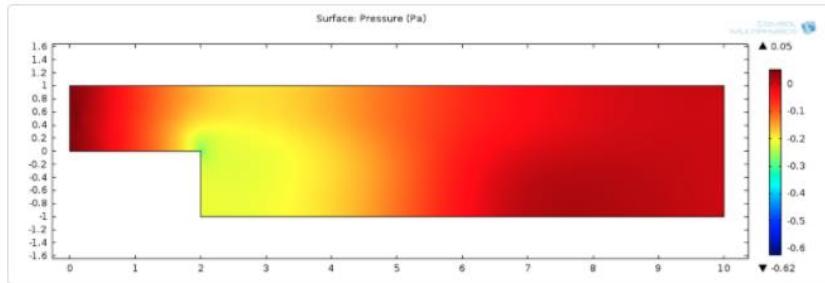
在下面的例子中，我们对一个计算域中的纳维-斯托克斯方程（以下简称“NS 方程”）和质量守恒方程进行数值求解，为此需要一组边界条件：



模型中，在入口指定了流体速度，在出口指定了压力，并指定了无滑移壁面边界条件（即，速度为零）。在层流流态和恒定边界条件下，稳态 NS（(1) 中的时间相关导数设为零）和连续性方程的数值解如下：



速度大小分布和流线图。



压力场。

纳维-斯托克斯方程的各种形式

根据研究的流态，我们通常可以将这些方程进行简化。在某些情况下，可能还需要附加方程。在流体动力学领域，人们常使用无因次数（例如雷诺数和马赫数）对不同的流态进行分类。

关于雷诺数和马赫数

雷诺数 $Re = \rho UL/\mu$ 是惯性力（1）与黏性力（3）的比值，用于测量流体的湍流程度。低雷诺数的流动是层流，高雷诺数的流动为湍流。

马赫数 $M = U/c$ 是流体速度 U 与该流体中声速 c 的比值，用于测量流体的压缩性。

在后台阶流动示例中， $Re = 100$ 且 $M = 0.001$ ，表明这是一个层流，并且几乎不可压缩。对于不可压缩流，由连续性方程可得：

$$\nabla \cdot \mathbf{u} = 0$$

对于不可压缩流的情况，由于速度散度等于零，我们可以将

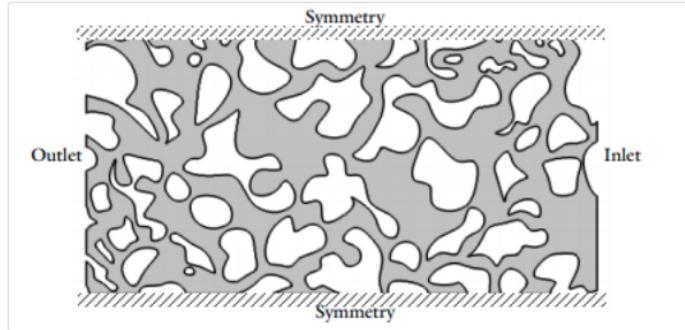
$$-\frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$$

这一项从 NS 方程的黏性力项中去除。

在下一节，我们将研究一些特殊的流态。

低雷诺数/蠕动流

当雷诺数非常小 ($Re \ll 1$) 时, 与黏性力 (3) 相比, 惯性力 (1) 会很小, 在求解 NS 方程时可以将这些力忽略。为了对这一流态进行说明, 我们来看一看美国加州大学圣塔芭芭拉分校的 Arturo Keller、Maria Auset 和 Sanya Sirivithayapakorn 进行的孔隙尺度流动实验。



图形显示孔隙尺度的流动实验中的边界条件。

关于该实验

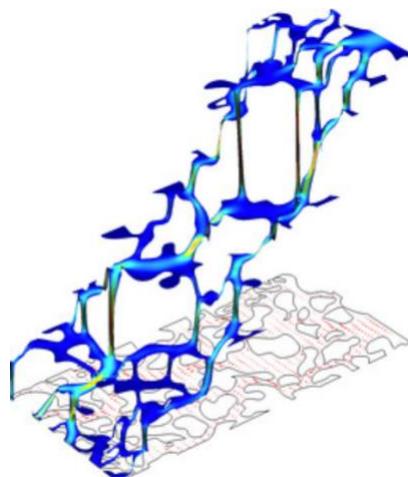
实验研究的区域大小为 $640 \mu\text{m} \times 320 \mu\text{m}$ 。水从右向左流动, 穿过整个几何体。孔隙中的水流不会渗透固体部分 (上图中的灰色区域)。入口和出口的流体压力为已知条件。由于通道的最大宽度为 0.1 毫米, 并且最大速度小于 10^4 m/s , 因此最大雷诺数小于 0.01。因为没有外力作用 (重力忽略不计), 所以力项 (4) 也等于零。

由此可以将 NS 方程简化为:

$$0 = \underbrace{-\nabla p}_{2} + \underbrace{\nabla \cdot (\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))}_{3}$$

实验建模

下图显示仿真得到的等流速线和压力场 (高度)。



由于入口的压力比出口高，这就产生了压力驱动的流体流动。这些结果表明，NS 方程中的压力（2）和黏性力（3）之间存在平衡。在沿较小通道的位置，其黏性扩散的影响更加明显，从而导致压降也更大。

高雷诺数/湍流

在雷诺数非常高的工程应用中，惯性力（1）远大于黏性力（3）。这种湍流问题在本质上是瞬态的；需要使用足够精细的网格，才能求解最小涡流的大小。

使用 NS 方程计算此类问题，往往会超出当今大多数计算机和超级计算机的计算能力。因此，我们可以改用纳维-斯托克斯方程的雷诺平均纳维-斯托克斯（RANS）公式，对速度和压力场取时间平均值。

如此一来，我们便能够基于相对粗糙的网格以静态方式计算这些时均方程，从而大大降低此类仿真对计算能力的要求，并显著缩短计算时间（通常，二维流动需要几分钟，三维流动则需要几分钟到几天不等）。

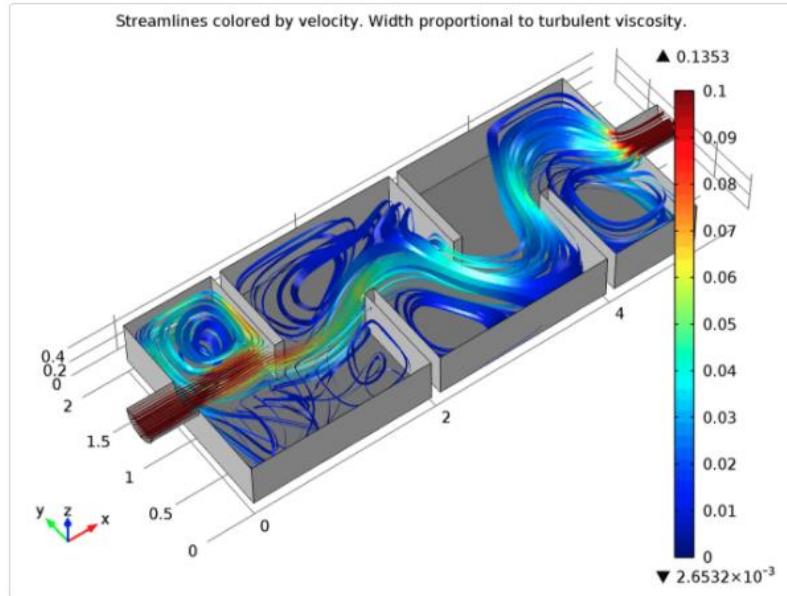
雷诺平均纳维-斯托克斯（RANS）公式如下：

$$\underbrace{\rho(\mathbf{U} \cdot \nabla \mathbf{U}) + \nabla \cdot (\mu_T(\nabla \mathbf{U} + (\nabla \mathbf{U})^T) - \frac{2}{3}\mu_T(\nabla \cdot \mathbf{U})\mathbf{I})}_{1} = \underbrace{-\nabla P + \nabla \cdot (\mu(\nabla \mathbf{U} + (\nabla \mathbf{U})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{U})\mathbf{I})}_{2} + \underbrace{\mathbf{F}}_{4}$$

其中， \mathbf{U} 和 P 分别是时均速度和压力。 μ_T 项表示湍流黏度，即小尺度的瞬态速度波动的影响，RANS 方程不会求解这种波动。

湍流黏度 μ_T 通过湍流模型进行计算，最常用的是 k- ϵ 湍流模型（众多 RANS 湍流模型之一）。由于这个模型不仅具有较好的稳定性，还能有效节省计算资源，因此常被用于工业应用领域。该模型还求解两个附加方程：湍流动能 k 的传递和湍流耗散 ϵ 。

为了进一步说明这一流态，我们来看看在一个比孔隙尺度流动大得多的几何体中的流动情况：一个典型的臭氧净化反应器。这个反应器长约 40 米，看起来像一个迷宫，其中使用部分墙壁或挡板将空间分成房间大小的多个隔间。根据入口速度和直径（本例中分别为 0.1 m/s 和 0.4 m），相应的雷诺数为 400,000。通过该模型可以求解时均速度 \mathbf{U} 、压力 P 、湍流动能 k 以及湍流耗散 ϵ ：



仿真结果显示了流型、流速和湍流黏度 μ_T 。

流体压缩性

流体压缩性可以通过马赫数进行测量。前面的所有例子都是弱可压缩流体，也就是说马赫数小于 0.3。

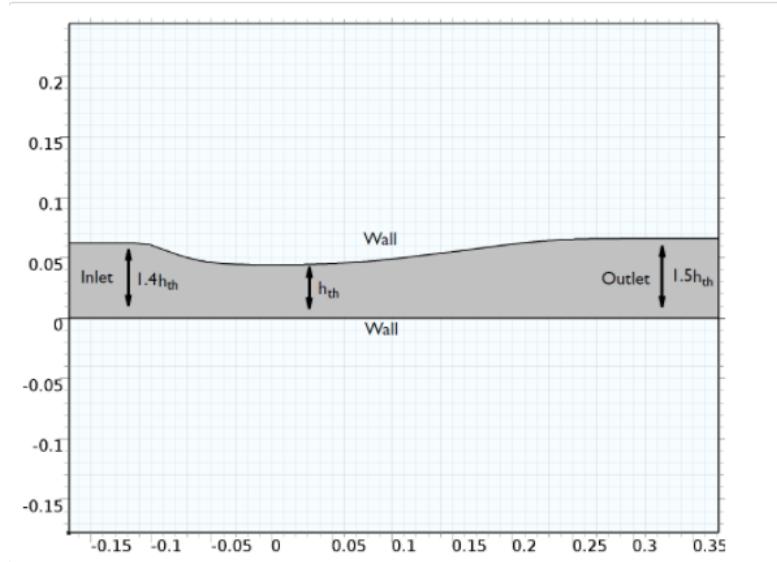
不可压缩流

当马赫数很低时，我们可以假设流体是不可压缩的。对于压缩性比气体小得多的液体来说，这通常是一个良好的近似。在这种情况下，假设密度恒定，连续性方程可以简化为 $\nabla \cdot \mathbf{u} = 0$ 。在蠕动流例子中，水以低速流经多孔介质，这就是一个很好的不可压缩流示例。

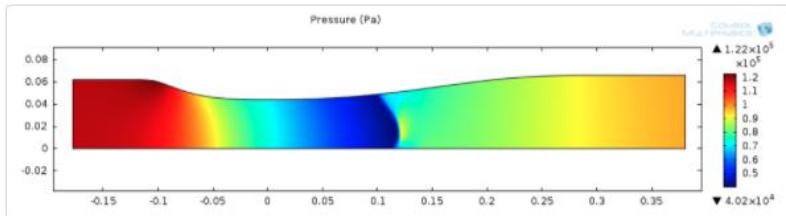
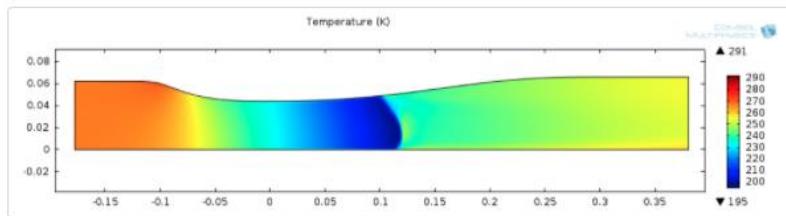
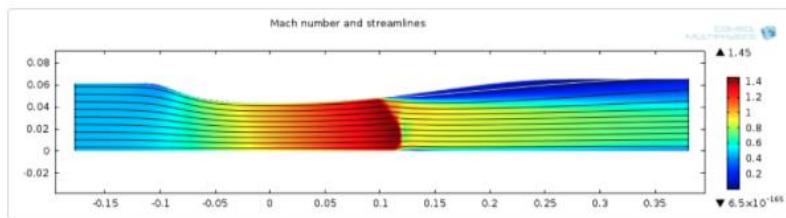
可压缩流

在某些情况下，流速非常大，并引起流体的密度和温度发生显著变化。当 $M < 0.3$ 时，这些变化可以忽略不计。然而，当 $M > 0.3$ 时，速度、压力和温度场之间的耦合会变得非常强，此时需要同时求解纳维-斯托克斯方程、连续性方程以及能量方程（流体传热方程）。通过能量方程，我们可以预测流体中的温度，这是计算温度相关的材料属性所需的参数。

可压缩流既可以是层流，也可以是湍流。在下一个示例中，我们来看看扩散器（一个收缩和扩散的喷嘴）中的高速湍流气流。



扩散器是一个跨音速流动环境，从这个意义上来说，尽管入口的气体是亚音速流动，但由于收缩和较低的出口压力，流动会加速并在喷嘴喉部变为音速流动 ($M = 1$)。



以上三个绘图的结果表现出很强的相似性，证实了速度、压力和温度场之间的强耦合关系。在一小段区域的超音速流动 ($M > 1$) 之后，气流通过正激波，流速再次变回亚音速。M. Sajben 及其同事已通过大量的实验和数值仿真对这一体系进行了研究 [1-6]。

纳维-斯托克斯方程无法求解的流态



仅当系统的特征物理长度尺度远大于流体分子的平均自由程时，纳维-斯托克斯方程才成立。这种情况下流体称为连续介质。平均自由程 λ 与特征长度尺度 L 的比值称为克努森数 $Kn = \lambda/L$ 。

当 $Kn < 0.01$ 时，NS 方程成立。当 $0.01 < Kn < 0.1$ 时，这些方程仍然适用，但需要施加特殊的边界条件。当 $Kn > 0.1$ 时，方程不成立。例如，在环境压力为 1 atm 的情况下，空气分子的平均自由程是 68 纳米。因此，模型的特征长度应大于 6.8 μm ，NS 方程才能成立。

6) <https://www.zhihu.com/question/27405114>

如何形象地理解纳维斯-托克斯方程？

作者：毛博 链接：<https://www.zhihu.com/question/27405114/answer/36629624>



毛博

业余PhD

991 人赞同了该回答

谢邀。

其实本来看了其他的答案，我是打算点个赞了事的，因为就是 $F=ma$ 嘛。不过后来看了问题描述，发现题主的疑惑不源自这个，加上题主要求形象的来解释，那么我就尝试着形象地来分析一下 NS 方程。

一步一步来。

1. 欧氏描述 v.s 拉氏描述。

作为学习传统流体力学的人，有一个必需知道的常识，那就是当描述流体流动时，我们采用的是欧拉描述。与其对应的是在固体力学中使用的拉格朗日描述。通俗的说，拉氏描述关注对象是物体，比如高中物理中的的神物——斜坡上的小木块。而欧氏描述的对象是场，是空间位置。这个就比较抽象了，形象地说就是你研究一根水柱，你看到的其实是一个水柱形状的空间。当水流时，这根水柱里的水（一群连续的质点）每时每刻都是不同的，但是空间是固定的（水柱状）。这里要提醒题主，传统牛顿三定律都是拉氏描述，而且拉氏描述下的牛顿定律在低速条件下是普适的。为什么会出现这两种不同的描述呢？传统固体力学的对象是固体，方法是线性的。线性固体力学的对象是一群位置相对不变的连续质点，外部力向内部传递的方式是相对固定的（这是线性固体力学的小形变假设，没有这个假设，非线性固体力学和流体力学本质上是一样的），所以受力分析相对简单。也就是说，整个计算过程，我们关注的是某一个或者某一群质点，从头到尾

我们都是在分析这群质点的受力。而流体力学无法这样分析，因为流体的形变是很大的，当你对一坨流体做受力分析，实在太复杂。而且当你对不同形状的流体做受力分析，外部力向内部的传递方式是不一样的。因此，欧拉描述就有了大作用：与其关注一群质点，我关心的是一个固定的空间（控制体） 不同的质点可以进出这个控制体 但是质量守恒与动量、能量平衡在控制体内必须得到满足：流经这个控制体的流体，在期间收到多少力，动量就改变多少；收到多少功、热量，能量就改变多少；而流进流出的流体质量必须守恒。换言之，我不关心某一个特定的质点了，我关心的是在某个时间点，位于某个目标位置的质点。质点 A 这一刻在我的目标位置，我研究它，下一刻它流到了一个我不关心的位置，而质点 B 流了进来，那我就研究质点 B。受力分析无法运作了，因为你研究的质点时刻在变。在这里，回答题主的第一个疑惑：为什么流体力学中没有 Freebody Diagram（受力分析）这种东西？对于质点的受力分析是拉氏描述特有的，欧氏描述不具备这样的特征。因为拉氏描述关注的是物体（质点），欧氏描述关注的是空间（控制体）。你的目标质点时刻在变，而你对空间本身做受力分析是木有意义的。

-----更新前说一点-----

评论里有同学在纠结流体里拉氏和欧氏的应用面。我统一回复：根据我的理解，从连续体力学和张量分析的角度，这两者是互通的。根据研究对象要求随时变换使用。我在上面的回答也说到了，小形变或者无形变时，比如静止液体、等液面分析，拉氏描述是更占优的，因为它避开了 NS 方程中随流项带来的非线性从而使问题线性化（后面会介绍），解决了解的存在性和唯一性问题。但是，对于我这种做航空发动机进气道内流的人，几百米每秒的速度流动，用拉氏描述分析问题，臣妾做不到啊。所以，具体问题具体分析，两者一样好，都是棒棒哒！另外，高校流体力学的教材中，对欧氏描述介绍比较多，因为拉氏描述大家从高中就知道。着重介绍，仅仅因此而已。

-----继续拖更新-----

2. 雷诺输运定理。

提到欧氏与拉氏描述，就必须讲雷诺输运定理。简单地说，雷诺输运定理是连接拉氏描述与欧氏描述的桥梁。直接摆公式：

$$\frac{d}{dt} \int_{\Omega} m dV = \int_{\Omega} \frac{\partial}{\partial t} m dV + \oint_{\partial\Omega} m \bar{v} \cdot d\bar{A}$$

等号左边是物质导数，拉氏描述。而等号右边，就是典型的控制体分析。用通俗的语言来说，就是：

物理量 m 的变化量=控制体内物理量 m 的当地变化量 + 物理量 m 流入/流出控制体的量。

很多人不理解为什么左边的 d/dt 项要在积分外而等号右边的 d/dt （偏微分）项要在等号内。这其实也是拉氏与欧氏描述的差异与精髓所在。搞清这点，才算真正的对两种描述有了一定的认识。正如之前所说，拉氏描述关注质点，那么等号左边的时间导数是针对某些特定的质点而言的，那么当时间变化，这些质点移动后，他们所在的位置是改变的，换言之，由这些质点组成的空间也是随时间改变的。所以，将时间导数放在积分号外，是因为拉氏描述下，对象空间也是随时间改变的，时间导数需要将空间的变化也考虑进去。而等号右边的时间导数，因为是欧氏描述，目标空间（控制体）固定，所以空间不是时间的函数，于是时间导数符号就放在了积分号的里面。雷诺输运定理的重要性体现在其桥梁作用以及在欧氏描述下的普适性。传统流体力学的 NS 方程就是由雷诺输运定理结合牛顿三定律与质能守恒律推导出来的。

3. NS 方程。

鉴于篇幅，只推导动量方程了，质量与能量方程请大家自己看教科书。**在之前说过，欧氏描述下的控制体分析，精髓在于流量守恒。**对于一个固定的控制体，以质量为例，在没有源的前提下，流进和流出控制体的质量，必须是相等的。类似的还有动量与能量的平衡。但是，数学描述是怎样的呢？我在开头介绍欧氏与拉氏描述时，提到过一点，牛顿三定律是拉氏描述，而且牛顿定律是低速下普适的。任何其他动量方程必须以满足牛顿三定律为前提。所以，以动量方程为例，推导就应该从牛顿定律开始，也就是：

$$\frac{dm\bar{v}}{dt} = \bar{F}.$$

考虑到流体不是一个质点，而是一个连续体，所以：

$$\frac{d}{dt} \int_{\Omega} \rho \bar{v} dV = \int_{\Omega} \bar{f} dV.$$

其实 \bar{f} 表示单位体积的力。到这里，我没有使用任何欧氏描述，一切都是拉氏描述，没有任何变换。接下来，就要引入欧氏描述了。等号的左边是不是特别眼熟？雷诺输运定理：

$$\frac{d}{dt} \int_{\Omega} \rho \bar{v} dV = \int_{\Omega} \frac{\vartheta}{\vartheta t} \rho \bar{v} dV + \oint_{\partial\Omega} \rho \bar{v} (\bar{v} \cdot d\bar{A}) = \int_{\Omega} \bar{f} dV.$$

利用高数里的高斯散度定理，上述方程的第三项流量项可替换为散度的体积积分，于是：

$$\int_{\Omega} \frac{\vartheta}{\vartheta t} \rho \bar{v} dV + \oint_{\partial\Omega} \text{Div} \cdot (\rho \bar{v} : \bar{v}) dV = \int_{\Omega} \bar{f} dV.$$

第二项内的两点表示张量积。这不是重点，重点在于，整个方程变成了一个关于 \bar{v} 的积分方程。因为控制体的选择是任意的，所以上述等式满足的必要条件是：

$$\frac{\vartheta}{\vartheta t} \rho \bar{v} + \text{Div} \cdot (\rho \bar{v} : \bar{v}) = \bar{f}.$$

等号左边的项，是一个三维矢量，其 x 方向的投影就是题主在问题描述中的 x 方向动量方程的等号左边部分。

我已经提到过，NS 方程本身就是一个针对牛顿流体的模型。原因在于，牛顿流体的应力是与其应变率成正比的：
★

$$[\sigma] = [C][\tau] + [\delta_{ij}]p.$$

其中 $[\tau]$ 就是应变率矩阵，其元素定义如下：

$$\tau_{ij} = \frac{\vartheta u_i}{\vartheta x_j}.$$

而 $[C]$ 是一个 $3 \times 3 \times 3 \times 3$ 的张量，但是因为我们的理论学习多假设各项同性和泊松效应，所以就简化成一个 3×3 的矩阵了，其性质类似弹簧的刚度系数或者材料力学力的材料的剪切系数、泊松比之类的，总而言之，就是一系列与流体本身性质相关的常数。再根据：

$$\bar{f} = \operatorname{Div} \cdot ([\sigma]).$$

另外，如果在考虑重力，结合上述，一项一项代入，你看到的就是完整的NS方程组。具体细节我就懒得写了。

4、关于 NS 方程组形象的物理意义。

上面的推导，基本上把 NS 方程基本的物理意义介绍了一遍。而题主要形象地介绍 NS 方程，那我就从以下几个点再补充一些：

(a) 随流项。

NS 方程组的至今无解的原因，是因为方程本身是非线性的。而非线性的源头就是等号左边的第二项，即：

$$\operatorname{Div} \cdot (\rho \bar{v} : \bar{v}).$$

众所周知，对于非线性偏微分方程，除了少数极简单的方程外，普遍意义上来说还没找到有效的普遍的求解析解的方式。而且 NS 方程组的本身还是二阶非线性的，而且还是方程组，这就更无法解了。虽然无解，但是随流项的物理意义却非常重要：它表征了流体中物理量在空间中的信息传递。首先，随流项是在拉氏描述向欧氏描述转换时产生的，这说明随流项是欧氏特有的。拉氏没有这样的非线性项。那么回到欧氏描述。欧氏描述的特征是目标空间。在欧拉描述下，研究对象时正好位于目标空间的物质。举个不恰当的例子，一帮运动员绕着田径场跑长跑。而我研究他们的速度，我盯着的是 200 米处这个位置，任何经过这个位置的人，我都记下他/她的速度。这是欧氏的描述方式。那么随流项在欧氏描述下起到的作用是什么呢？正如我之前所说，信息传递。还是这群长跑的运动员，我想知道其中某个运动员在 300 米处时的速度，我知道运动员的速度随着距离的增加而减小的规律，同时知道他们在 200 米处的速度，那么 300 米处的速度怎么求？不就是 200 米处的速度 + 300 米处到 200 米处的速度变化吗？写成数学公式：

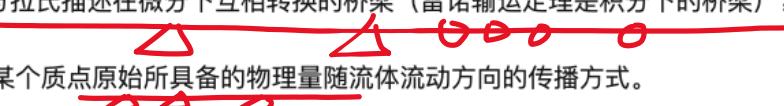
$$v_{300} = v_{200} + \Delta v$$

如果每个运动员经过 200 米处的速度随时间变化：

$$\frac{d}{dt} v_{300} = \frac{\vartheta}{\vartheta t} v_{200} + \frac{\Delta v}{\Delta t} = \frac{\vartheta}{\vartheta t} v_{200} + \frac{\Delta v}{(\Delta s/v)} = \frac{\vartheta}{\vartheta t} v_{200} + v \frac{\vartheta v}{\vartheta s}$$

是不是就是随流项？  

通俗地说：

- i) 随流项是欧氏与拉氏描述在微分下互相转换的桥梁（雷诺输运定理是积分下的桥梁）；

- ii) 随流项描述了某个质点原始所具备的物理量随流体流动方向的传播方式。

- iii) 流体中任意一个质点的物理量，不仅与它当前的状态有关，也与它之前的状态相关，两者之间的连系方式就是随流项。

(b) \bar{f} 的应用范围。

一句话：

\bar{f} 本身是没有限制的，如果你研究的流体有自己的特性，那么等号右边的 \bar{f} 项会有不同的表达方式，但是大体的推导过程和上面没啥差别。

05/16/20

任务(I) Dissipative Particle Dynamics (DPD)

1) 看 Notability 上的 Notes

2) Wikipedia 中文

耗散粒子动力学 (Dissipative particle dynamics, DPD) 是一种粗粒化的分子模拟算法，用于模拟复杂流体的行为。DPD 方法首先由 Hoogerbrugge 和 Koelman 于 1992 年提出，用于解决格状自动机方法与实际的差异和分子动力学 (MD) 所无法解决的介观的时间与空间尺度上的流体问题。之后被 Espanol 改写，使其符合热平衡状态的条件。此后，一些列扩展的和经过优化的的 DPD 算法被提出。DPD 是一种非格子模型的方法，模拟粒子在连续的空间和间断的时间中运动。**DPD 方法中单个粒子代表整个分子或包含多个分子，或高分子的一个片段的流体区域，而不是单个原子，并且不考虑原子的行为细节，认为其与过程无关**。粒子自身的自由度被整合，粒子间的受力由一对保守力、耗散力与随机力表示，并以此保证动量守恒与正确的流体动力学行为。这些近似的结果使得 DPD 方法能模拟更大空间和时间尺度的系统。与全原子模拟相比，**DPD 方法虽然不能提供原子尺度的描述，但其因为把数个溶剂分子“捆绑”成一个 DPD 粒子的处理，使得粒子间有有效的摩擦相互作用和涨落，反而能得到较为准确的流体动力学性质**。DPD 方法与传统的 MD 模拟方法相比，主要优势在于可实现更大时间与空间尺度的模拟计算。100 nm 尺寸的聚合物流体在几十微秒时间尺度的模拟现已普遍使用。

方程：

DPD将两个不成键粒子*i*与*j*之间的作用力分为三种，分别是保守力(F_{ij}^C)，耗散力(F_{ij}^D)和随机力(F_{ij}^R): [5]

$$f_i = \sum_{j \neq i} (F_{ij}^C + F_{ij}^D + F_{ij}^R)$$

为了减少计算时间，设有截断半径 r_c ，仅当两粒子间距离小于截断半径时才计算两者间的作用力。

保守力代表粒子的化学性质，不同种类粒子保守力的作用参数不同，以此区分不同粒子之间的亲疏性。保守力是软排斥作用：

$$F_{ij}^C = a_{ij} \left(1 - \frac{r_{ij}}{r_c}\right) \hat{r}_{ij}$$

其中 a_{ij} 是两种粒子间的相互作用参数，与Flory-Huggins作用参数有关。

耗散力与随机力的值通过涨落-耗散定理相关联，并使其统计值符合系统温度：

$$F_{ij}^D = -\gamma \omega_D^2 (\hat{r}_{ij} \cdot \vec{v}_{ij}) \hat{r}_{ij}$$

$$F_{ij}^R = \sigma \omega_R \theta_{ij} \hat{r}_{ij}$$

其中 γ 是控制耗散力的摩擦系数， σ 是控制随机力的噪声振幅，两者间满足 $\sigma^2 = 2\gamma k_B T$ 。 θ_{ij} 是随机波动变化因子，是与积分时间元有关的正态分布函数，期望值为0。 ω 是依赖于距离的权重函数，耗散力和随机力的权重因子选取是任意的，但两者间应当满足 $\omega_D = \omega_R^2$ 以符合玻尔兹曼统计。最基本的DPD方法中通常选取：

$$\omega_R = \begin{cases} 1 - \frac{r_{ij}}{r_c} & (r_{ij} < r_c) \\ 0 & (r_{ij} \geq r_c) \end{cases}$$

此外，根据实际模型中粒子间的成键，还加入以弹簧振子为模型的键张力，和用于维持一定键角的角张力等。

3) Wikipedia English https://en.wikipedia.org/wiki/Dissipative_particle_dynamics

Dissipative particle dynamics (DPD) is a stochastic simulation technique for simulating the dynamic and rheological properties of simple and complex fluids. It was initially devised by Hoogerbrugge and Koelman to avoid the lattice artifacts of the so-called lattice gas automata and to tackle hydrodynamic time and space scales beyond those available with molecular dynamics (MD). It was subsequently reformulated and slightly modified by P. Español[3] to ensure the proper thermal equilibrium state. A series of new DPD algorithms with reduced computational complexity and better control of transport properties are presented. The algorithms presented in this article choose randomly a pair particle for applying DPD thermostating thus reducing the computational complexity.

DPD is an off-lattice mesoscopic simulation technique which involves a set of particles moving in continuous space and discrete time. Particles represent whole molecules or fluid regions, rather than single atoms, and atomistic details are not considered relevant to the processes addressed. The particles' internal degrees of freedom are integrated out and replaced by simplified pairwise dissipative and random forces, so as to conserve momentum locally and ensure correct hydrodynamic behaviour. The main advantage of this method is that it gives access to longer time and length scales than are possible using conventional MD simulations. Simulations of polymeric fluids in volumes up to 100 nm in linear dimension for tens of microseconds are now common.

(1) Equations

The total non-bonded force acting on a DPD particle i is given by a sum over all particles j that lie within a fixed cut-off distance, of three pairwise-additive forces:

$$f_i = \sum_{j \neq i} (F_{ij}^C + F_{ij}^D + F_{ij}^R)$$

where the first term in the above equation is a conservative force, the second a dissipative force and the third a random force. The conservative force acts to give beads a chemical identity, while the dissipative and random forces together form a thermostat that keeps the mean temperature of the system constant. A key property of all of the non-bonded forces is that they conserve momentum locally, so that hydrodynamic modes of the fluid emerge even for small particle numbers. Local momentum conservation requires that the random force between two interacting beads be antisymmetric (反对称, unaltered in magnitude but changed in sign by exchange of two variables or by a particular symmetry operation). Each pair of interacting particles therefore requires only a single random force calculation. This distinguishes DPD from Brownian dynamics in which each particle experiences a random force independently of all other particles. Beads can be connected into ‘molecules’ by tying them together with soft (often Hookean) springs. The most common applications of DPD keep the particle number, volume and temperature constant, and so take place in the NVT ensemble. Alternatively, the pressure instead of the volume is held constant, so that the simulation is in the NPT ensemble.

(2) Parallelization

In principle, simulations of very large systems, approaching a cubic micron for milliseconds, are possible using a parallel implementation of DPD running on multiple processors in a Beowulf-style cluster. Because the non-bonded forces are short-ranged in DPD, it is possible to parallelize a DPD code very efficiently using a spatial domain decomposition technique. In this scheme, the total simulation space is divided into a number of cuboidal regions each of which is assigned to a distinct processor in the cluster. Each processor is responsible for integrating the equations of motion of all beads whose centres of mass lie within its region of space. Only beads lying near the boundaries of each processor's space require communication between processors. In order to ensure that the simulation is efficient, the crucial requirement is that the number of particle-particle interactions that require inter-processor communication be much smaller than the number of particle-particle interactions within the bulk of each processor's region of space. Roughly speaking, this means that the volume of space assigned to each processor should be sufficiently large that its surface area (multiplied by a distance comparable to the force cut-off distance) is much less than its volume.

(3) Applications

A wide variety of complex hydrodynamic phenomena have been simulated using DPD, the list here is necessarily incomplete. The goal of these simulations often is to relate the macroscopic non-Newtonian flow properties of the fluid to its microscopic structure. Such DPD applications range from modeling the rheological properties of concrete to simulating liposome (脂质体) formation in biophysics to other recent three-phase phenomena such as dynamic wetting. The DPD method has also found popularity in modeling heterogeneous multi-phase flows containing deformable objects such as blood cells and polymer micelles (胶束).

(4) Further reading

The full trace of the developments of various important aspects of the DPD methodology since it was first proposed in the early 1990s can be found in "Dissipative Particle Dynamics: Introduction, Methodology and Complex Fluid Applications – A Review".

The state-of-the-art in DPD was captured in a CECAM workshop in 2008. Innovations to the technique presented there include DPD with energy conservation; non-central frictional forces that allow the fluid

viscosity to be tuned; an algorithm for preventing bond crossing between polymers; and the automated calibration of DPD interaction parameters from atomistic molecular dynamics. Recently, examples of automated calibration and parameterization have been shown against experimental observables. Additionally, datasets for the purpose of interaction potential calibration and parameterisation have been explored. Swope et al, have provided a detailed analysis of literature data and an experimental dataset based on Critical micelle concentration (CMC) and micellar mean aggregation number (Nagg). Examples of micellar simulations using DPD have been well documented previously.

Note: 先了解到这里，如有需要进一步了解就看下面的两个资料：

(i) Review Paper

Moeendarbary; et al. (2009). "Dissipative Particle Dynamics: Introduction, Methodology and Complex Fluid Applications - A Review". International Journal of Applied Mechanics. 1 (4): 737–763. Bibcode:2009IJAM....1..737M. doi:10.1142/S1758825109000381.

Link:

<https://www.semanticscholar.org/paper/DISSIPATIVE-PARTICLE-DYNAMICS%3A-INTRODUCTION%2C-AND-%E2%80%94-Moeendarbary-Ng/3565ba6ec0f15871b56ccbe2d7341996036e307a>

(ii) Workshop Article

Dissipative Particle Dynamics: Addressing deficiencies and establishing new frontiers Archived 2010-07-15 at the Wayback Machine, CECAM workshop, July 16–18, 2008, Lausanne, Switzerland.

link: <https://web.archive.org/web/20100715071125/http://www.cecams.org/workshop-0-188.html>

任务(II) Lattice Gas Automaton (LGA)

1) “**Lattice gas automaton**” (LGA)

(i) 中文

格子气自动机 [编辑]

维基百科，自由的百科全书

格子气自动机或格子气细胞自动机是一种用来模拟液体流动的**细胞自动机**。他们是Lattice Boltzmann方法的前身。通过格子气自动机，我们可能得出宏观的纳维－斯托克斯方程^[1] 对于格子气自动机方法的兴趣在20世纪90年代早期趋于稳定，Lattice Boltzmann方法开始流行。^[2]

(ii) English

https://en.wikipedia.org/wiki/Lattice_gas_automaton

Lattice gas automata (LGA), or lattice gas cellular automata, are a type of cellular automaton used to simulate fluid flows. They were the precursor to the **lattice Boltzmann methods**. From lattice gas automata, it is possible to derive the macroscopic Navier-Stokes equations. Interest in lattice gas automaton methods levelled off in the early 1990s, as the interest in the lattice Boltzmann started to rise.

(1) Basic principles

As a cellular automaton, these models comprise a lattice, where the sites on the lattice can take a certain number of different states. In lattice gas, the various states are particles with certain velocities. Evolution of the simulation is done in discrete time steps. After each time step, the state at a given site can be determined by the state of the site itself and neighboring sites, before the time step. **The state at each site is purely boolean. At a given site, there either is or is not a particle moving in each direction. At each**

time step, two processes are carried out, propagation and collision. In the propagation step, each particle will move to a neighboring site determined by the velocity that particle had. Barring (禁止, 阻拦) any collisions, a particle with an upwards velocity will after the time step maintain that velocity, but be moved to the neighboring site above the original site. The so-called exclusion principle prevents two or more particles from travelling on the same link in the same direction. **In the collision step, collision rules are used to determine what happens if multiple particles reach the same site.** These collision rules are required to maintain mass conservation, and conserve the total momentum; the block cellular automaton model can be used to achieve these conservation laws. Note that the exclusion principle does not prevent two particles from travelling on the same link in opposite directions, when this happens, the two particles pass each other without colliding.

(2) Early attempts with a square lattice

In papers published in 1973 and 1976, Hardy, Pomeau and de Pazzis introduced the first Lattice Boltzmann model, which is called the HPP model after the authors. HPP model is a two-dimensional model of fluid particle interactions. In this model, the lattice is square, and the particles travel independently at a unit speed to the discrete time. The particles can move to any of the four sites whose cells share a common edge. Particles cannot move diagonally. If two particles collide head-on, for example a particle moving to the left meets a particle moving to the right, the outcome will be two particles leaving the site at right angles to the direction they came in.[5] The HPP model lacked rotational invariance, which made the model highly anisotropic. This means for example, that the vortices (旋涡) produced by the HPP model are square-shaped.

(3) Hexagonal grids

The hexagonal grid model was first introduced in 1986, in a paper by Uriel Frisch, Brosl Hasslacher and Yves Pomeau, and this has become known as the FHP model after its inventors. The model has six or seven velocities, depending on which variation is used. In any case, **six of the velocities represent movement to each of the neighboring sites.** In some models (called FHP-II and FHP-III), a seventh velocity representing particles "at rest" is introduced. The "at rest" particles do not propagate to neighboring sites, but they are capable of colliding with other particles. The FHP-III model allows all possible collisions that conserve density and momentum. Increasing the number of collisions raises the Reynolds number, so the FHP-II and FHP-III models can simulate less viscous flows than the six-speed FHP-I model. The simple update rule of FHP model proceeds in two stages, chosen to conserve particle number and momentum. The first is collision handling. The collision rules in the FHP model are not deterministic, some input situations produce two possible outcomes, and when this happens, one of them is picked at random. Since random number generation is not possible through completely computational means, a pseudorandom process is usually chosen. After the collision step a particle on a link is taken to be leaving the site. If a site has two particles approaching head-on, they scatter. A random choice is made between the two possible outgoing directions that conserve momentum. The hexagonal grid does not suffer as large anisotropy troubles as those that plague the HPP square grid model, a fortunate fact that is not entirely obvious, and that prompted Frisch to remark that "the symmetry gods are benevolent".

(4) Obtaining macroscopic quantities

The density at a site can be found by counting the number of particles at each site. If the particles are multiplied with the unit velocity before being summed, one can obtain the momentum at the site. However, calculating density, momentum, and velocity for individual sites is subject to a large amount of noise, and in practice, one would average over a larger region to obtain more reasonable results. Ensemble averaging is often used to reduce the statistical noise further.

(5) Advantages and disadvantages

The main assets held by the lattice gas model are that the boolean states mean there will be exact computing without any round-off error due to floating-point precision, and that the cellular automata system makes it possible to run lattice gas automaton simulations with parallel computing.

Disadvantages of the lattice gas method include the lack of Galilean invariance, and statistical noise. Another problem is the difficulty in expanding the model to handle three dimensional problems, requiring the use of more dimensions to maintain a sufficiently symmetric grid to tackle such issues.

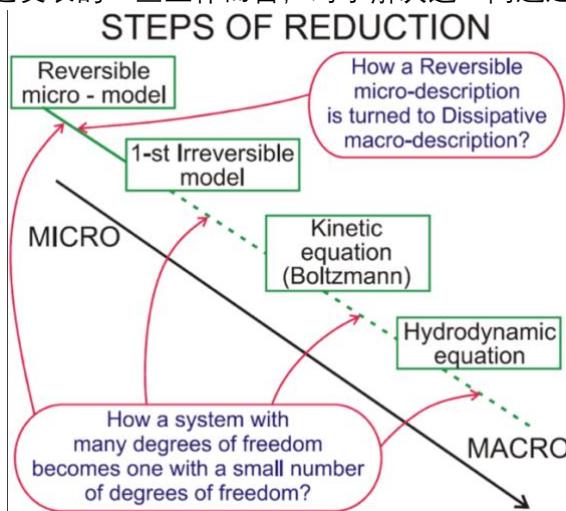
任务(III) Lattice Boltzmann

任务 III.1 --- Boltzmann Equation.

1) 看 Notability App 上的 Notes.

2) Wikipedia 中文 --- 玻尔兹曼方程

玻尔兹曼方程或玻尔兹曼输运方程 (Boltzmann transport equation, BTE) 是由玻尔兹曼于 1872 年提出的一个方程，用于描述非平衡状态热力学系统的统计行为。具有温度梯度的流体即为这类系统的一个经典的例子：构成流体的微粒在系统中通过随机而具有偏向性的运动让热量从较热的区域流向较冷的区域 而这一过程可用玻尔兹曼方程来描述。在现今的论文中，“玻尔兹曼方程”这个术语常被用于更一般的意义上，它可以是任何涉及描述热力学系统中宏观量（如能量、电荷或粒子数）的变化的动力学方程。玻尔兹曼方程并不去确定流体中每个粒子的位置和动量，而是求出具有特定位置和动量的粒子的概率分布。具体而言，考虑某一瞬间，以位置矢量 \vec{r} 末端为中心的无穷小区域内，动量无限接近动量矢量 \vec{p} (即这些粒子在动量空间中也处于无穷小区域 $d^3\vec{p}$ 内) 的粒子的概率分布。玻尔兹曼方程可用于确定物理量是如何变化的，例如流体在输运过程中的热能和动量；还可由此推导出其他的流体特征性质，例如黏度、热导率，以及电阻率（将材料中的载流子视为气体），详见对流扩散方程。玻尔兹曼方程是一个非线性的积微分方程。方程中的未知函数是一个包含了粒子空间位置和动量的六维概率密度函数。方程解的存在性和唯一性问题仍然没有完全解决，但就最近发表的一些工作而言，对于解决这一问题还是有一定希望的。



玻尔兹曼动力学方程在众多近似模型（从微观动力学到宏观连续介质动力学）中所处的位置 (The place of the Boltzmann kinetic equation on the stairs of model reduction from microscopic dynamics to macroscopic continuum dynamics (illustration to the content of the book))

(1) 概述

(i) 相空间与密度函数

系统中所有可能的位置 \mathbf{r} 和动量 \mathbf{p} 组成的集合被称作此系统的相空间，其中位置坐标记为 x, y, z ，动量坐标记为 p_x, p_y, p_z 。整个空间是六维的：空间中某一点的坐标可表示为 $(\mathbf{r}, \mathbf{p}) = (x, y, z, p_x, p_y, p_z)$ ，每个坐标均通过时间 t 参数化。微元（或微分体积元）可写作：

$$d^3 \mathbf{r} d^3 \mathbf{p} = dx dy dz dp_x dp_y dp_z$$

波尔兹曼方程的核心是“ f ”函数，它表示的是在一段极短的时间内，每一相空间单位体积中的 N 个分子在微元 $d^3 \mathbf{r} d^3 \mathbf{p}$ 中，位置都为 \mathbf{r} 且动量都为 \mathbf{p} 的概率。通过定义，我们可使概率密度函数 $f(\mathbf{r}, \mathbf{p}, t)$ 满足以下条件：

$$dN = f(\mathbf{r}, \mathbf{p}, t) d^3 \mathbf{r} d^3 \mathbf{p}$$

dN 被定义为在时间 t ，位于 (\mathbf{r}, \mathbf{p}) 的空间元 $d^3 \mathbf{r} d^3 \mathbf{p}$ 中的粒子总数^{[5]:61-62}。对坐标空间与动量空间的一个区域积分即可得该区域内所有具有对应位置和动量的粒子的总数：

$$N = \int_{\text{positions}} d^3 \mathbf{r} \int_{\text{momenta}} d^3 \mathbf{p} f(\mathbf{r}, \mathbf{p}, t) = \iiint_{\text{positions}} \iiint_{\text{momenta}} f(x, y, z, p_x, p_y, p_z, t) dx dy dz dp_x dp_y dp_z$$

虽然 f 是和一群粒子相关的，但此相空间是对于单一粒子的（而不是像多体系统中考虑全部粒子）。这里不使用 $\mathbf{r}_1, \mathbf{p}_1$ 表示粒子1， $\mathbf{r}_2, \mathbf{p}_2$ 表示粒子2，……， $\mathbf{r}_N, \mathbf{p}_N$ 表示粒子N。

系统中的粒子被假定是相同的（因此他们均有相同的质量 m ）。对于具有超过一种化学组分的混合物，每一种成分都需要有一个分布函数，见下文。

(ii) 一般形式

方程的一般形式可以写作：^[6]

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t} \right)_{\text{force}} + \left(\frac{\partial f}{\partial t} \right)_{\text{diff}} + \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

这里“force”一词指的是外部对粒子施加的力（而不是粒子间的作用），“diff”表示粒子的扩散，“coll”表示粒子的碰撞，指的是碰撞中粒子间相互的作用力。上述三项的具体形式将会在下文给出。^[6]

注意，一些作者会使用粒子的速度 \mathbf{v} ，来代替上文的 \mathbf{p} ；这两个物理量可以通过定义 $\mathbf{p} = m\mathbf{v}$ 来联系。

(2) “force”项和“diff”项

考虑一群以 f 分布的粒子。每个粒子均受到外力 \mathbf{F} 的作用（不包括粒子间作用力。粒子间的作用见后面对“coll”项的处理）。

假设在时间 t ，一定数量的粒子都有位置 \mathbf{r} （于微元 $d^3 \mathbf{r}$ 内），和动量 \mathbf{p} （于微元 $d^3 \mathbf{p}$ 内）。如果此时有一个力 \mathbf{F} 在这一瞬间作用在每个颗粒上，那么在时间 $t + \Delta t$ ，它们的位置将会是 $\mathbf{r} + \Delta \mathbf{r} = \mathbf{r} + \mathbf{p}\Delta t/m$ ，动量将变成 $\mathbf{p} + \Delta \mathbf{p} = \mathbf{p} + \mathbf{F}\Delta t$ 。在没有碰撞的情况下， f 必须满足

$$f \left(\mathbf{r} + \frac{\mathbf{p}}{m} \Delta t, \mathbf{p} + \mathbf{F} \Delta t, t + \Delta t \right) d^3 \mathbf{r} d^3 \mathbf{p} = f(\mathbf{r}, \mathbf{p}, t) d^3 \mathbf{r} d^3 \mathbf{p}$$

这里，注意到相空间元 $d^3 \mathbf{r} d^3 \mathbf{p}$ 是恒定的这个事实可以从哈密顿方程（见刘维尔定理）得知。然而，由于存在碰撞，相空间元 $d^3 \mathbf{r} d^3 \mathbf{p}$ 中的粒子密度是可变的，所以

$$\begin{aligned} dN_{\text{coll}} &= \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \Delta t d^3 \mathbf{r} d^3 \mathbf{p} \\ &= f \left(\mathbf{r} + \frac{\mathbf{p}}{m} \Delta t, \mathbf{p} + \mathbf{F} \Delta t, t + \Delta t \right) d^3 \mathbf{r} d^3 \mathbf{p} - f(\mathbf{r}, \mathbf{p}, t) d^3 \mathbf{r} d^3 \mathbf{p} \\ &= \Delta f d^3 \mathbf{r} d^3 \mathbf{p} \end{aligned} \quad (1)$$

其中 Δf 指的是 f 的总变化量。(1) 式除以 $d^3 \mathbf{r} d^3 \mathbf{p} \Delta t$ 并取极限 $\Delta t \rightarrow 0$ 和 $\Delta f \rightarrow 0$ 可得

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \quad (2)$$

f 的全微分：

$$\begin{aligned} df &= \frac{\partial f}{\partial t} dt + \left(\frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz \right) + \left(\frac{\partial f}{\partial p_x} dp_x + \frac{\partial f}{\partial p_y} dp_y + \frac{\partial f}{\partial p_z} dp_z \right) \\ &= \frac{\partial f}{\partial t} dt + \nabla f \cdot d\mathbf{r} + \frac{\partial f}{\partial \mathbf{p}} \cdot d\mathbf{p} \\ &= \frac{\partial f}{\partial t} dt + \nabla f \cdot \frac{\mathbf{p} dt}{m} + \frac{\partial f}{\partial \mathbf{p}} \cdot \mathbf{F} dt \end{aligned} \quad (3)$$

其中 ∇ 为梯度算符， \cdot 为点积，

$$\frac{\partial f}{\partial \mathbf{p}} = \hat{\mathbf{e}}_x \frac{\partial f}{\partial p_x} + \hat{\mathbf{e}}_y \frac{\partial f}{\partial p_y} + \hat{\mathbf{e}}_z \frac{\partial f}{\partial p_z} = \nabla_{\mathbf{p}} f$$

是 ∇ 的动量类比的一个简写， $\hat{\mathbf{e}}_x, \hat{\mathbf{e}}_y, \hat{\mathbf{e}}_z$ 为笛卡尔坐标系下的单位矢量。

最终形式：

对 (3) 两边同除以 dt 并代入 (2) 可得：

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

这里， $F(\mathbf{r}, t)$ 为流体中作用在粒子上的力场， m 为粒子质量。右边的一项用于描述粒子间相互碰撞产生的影响；如果此项为零，则说明粒子之间没有碰撞。无碰撞情况下的玻尔兹曼方程常被称为弗拉索夫方程。

这个方程比上一节“主要论述”中的一般形式更加有用。然而这个方程依旧是不完整的：除非已知 f 中的碰撞项，否则 f 是解不出来的。这一项并不像其他项一样可以简单地或一般地得到——这一项是表示粒子的碰撞的统计项，需要知道粒子遵守怎样的统计规律，例如麦克斯韦-玻尔兹曼分布，费米-狄拉克分布或玻色-爱因斯坦分布。

(3) 碰撞项 (Stosszahlansatz) 和分子混浊

玻尔兹曼的一个关键见解就是对碰撞项的确定。他假设的碰撞项完全是由假定在碰撞前不相关的两个粒子的相互碰撞得到的。这个假设被波尔兹曼称为“Stosszahlansatz”，也叫做“分子混沌假设”。根据这一假设，碰撞项可以被写作单粒子分布函数的乘积在动量空间上的积分：[2]

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \iint g I(g, \Omega) [f(\mathbf{p}'_A, t) f(\mathbf{p}'_B, t) - f(\mathbf{p}_A, t) f(\mathbf{p}_B, t)] d\Omega d^3 \mathbf{p}_A d^3 \mathbf{p}_B.$$

其中 \mathbf{p}_A 和 \mathbf{p}_B 表示碰撞前任意两个粒子的动量（为了方便而标记为 A 和 B ）， \mathbf{p}'_A 和 \mathbf{p}'_B 表示碰撞后的动量

$$g = |\mathbf{p}_B - \mathbf{p}_A| = |\mathbf{p}'_B - \mathbf{p}'_A|$$

指对应动量的大小（此概念参考相对速度）， $I(g, \Omega)$ 是碰撞的微分散射截面。

(4) 对碰撞项的简化

求解波尔兹曼方程时，许多挑战都来自于其复杂的碰撞项；因此我们会做一些对碰撞项“建模”和简化的尝试。现知最好的模型是由Bhatnagar, Gross和Krook作出的（BGK近似）[7]。BGK近似中假设分子的碰撞会迫使一个物理空间中的某一点的非平衡分布函数回到麦克斯韦平衡分布函数，且其发生率正比于分子碰撞频率。于是，波尔兹曼方程可被写作以下的BGK形式：（也叫做“驰豫时间近似”，relaxation time approximation[8]）

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \nu(f_0 - f)$$

其中 ν 是分子碰撞频率，和驰豫时间 τ 具有倒数关系： $\nu = 1/\tau$ 。 f_0 是此处局域的麦克斯韦分布函数，由空间中这一点的气体温度给定。

(5) 普适方程（对于混合物）

对于具有多种化学组分的混合物，我们以 $i = 1, 2, 3, \dots, n$ 标记各种成分。则对于组分 i 的方程是：[2]

$$\frac{\partial f_i}{\partial t} + \frac{\mathbf{p}_i}{m_i} \cdot \nabla f_i + \mathbf{F} \cdot \frac{\partial f_i}{\partial \mathbf{p}_i} = \left(\frac{\partial f_i}{\partial t} \right)_{\text{coll}}$$

其中 $f_i = f_i(\mathbf{r}, \mathbf{p}_i, t)$ 。碰撞项为

$$\left(\frac{\partial f_i}{\partial t} \right)_{\text{coll}} = \sum_{j=1}^n \iint g_{ij} I_{ij}(g_{ij}, \Omega) [f'_i f'_j - f_i f_j] d\Omega d^3 \mathbf{p}'.$$

其中 $f' = f'(\mathbf{p}'_i, t)$ ，相对动量的大小是

$$g_{ij} = |\mathbf{p}_i - \mathbf{p}_j| = |\mathbf{p}'_i - \mathbf{p}'_j|$$

I_{ij} 是粒子 i 和粒子 j 之间的微分散射截面。此积分的和描述的是某一相空间元中，组分 i 粒子的进出。

(6) 应用和推广

(i) 守恒方程

玻尔兹曼方程可用于推导流体动力学中的质量守恒，电量守恒，动量守恒，以及能量守恒定律^{[9]:p 163}。对于只含有一种粒子的流体，粒子数密度 n 为：

$$n = \int f d^3 p$$

算符 A 的期望值由下式给出：

$$\langle A \rangle = \frac{1}{n} \int A f d^3 p$$

由于守恒方程中包含张量，以下使用爱因斯坦求和约定简化标记，即 $\mathbf{x} \rightarrow x_i$ 且 $\mathbf{p} \rightarrow p_i = m w_i$ ，其中 w_i 为粒子速度矢量。定义某函数 $g(p_i)$ ，使得其唯一的自变量为动量 p_i （碰撞中动量守恒）。假设力 F_i 为位置的函数，且对于 $p_i \rightarrow \pm\infty$ ， f 为0。对玻尔兹曼方程两边同乘 g ，并对动量积分可得如下四项：

$$\begin{aligned} \int g \frac{\partial f}{\partial t} d^3 p &= \frac{\partial}{\partial t} (n \langle g \rangle) \\ \int \frac{p_j g}{m} \frac{\partial f}{\partial x_j} d^3 p &= \frac{1}{m} \frac{\partial}{\partial x_j} (n \langle g p_j \rangle) \\ \int g F_j \frac{\partial f}{\partial p_j} d^3 p &= -n F_j \left\langle \frac{\partial g}{\partial p_j} \right\rangle \\ \int g \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} d^3 p &= 0 \end{aligned}$$

因为 g 在碰撞中守恒，所以最后一项为零。

令 $g = m$ ，即粒子质量，积分后的玻尔兹曼方程化为质量守恒方程^{[9]:pp 12,168}：

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_j} (\rho V_j) = 0$$

$\rho = mn$ 为质量密度， $V_i = \langle w_i \rangle$ 为平均流体速度。

令 $g = mw_i$ ，即粒子动量，积分后的玻尔兹曼方程化为动量守恒方程^{[9]:pp 15,169}：

$$\frac{\partial}{\partial t} (\rho V_i) + \frac{\partial}{\partial x_j} (\rho V_i V_j + P_{ij}) - n F_i = 0$$

$P_{ij} = \rho \langle (w_i - V_i)(w_j - V_j) \rangle$ 为压强张量（粘性应力张量加上流体静力学压强）。

令 $g = \frac{1}{2}mw_i w_i$ ，即粒子动能，积分后的玻尔兹曼方程化为能量守恒方程^{[9]:pp 19,169}：

$$\frac{\partial}{\partial t} (u + \frac{1}{2} \rho V_i V_i) + \frac{\partial}{\partial x_j} (u V_j + \frac{1}{2} \rho V_i V_i V_j + J_{qj} + P_{ij} V_i) - n F_i V_i = 0$$

$u = \frac{1}{2} \rho \langle (w_i - V_i)(w_i - V_i) \rangle$ 为动力热能密度（kinetic thermal energy density），

$J_{qi} = \frac{1}{2} \rho \langle (w_i - V_i)(w_k - V_k)(w_k - V_k) \rangle$ 热通量矢量。

(ii) 哈密顿力学

在哈密顿力学中, 波尔兹曼方程通常写作

$$\hat{\mathbf{L}}[f] = \mathbf{C}[f],$$

其中 \mathbf{L} 是刘维尔算子(这里定义的刘维尔算子和链接文章中的定义不一致), 它描述了相空间体积的演化; \mathbf{C} 是碰撞算子。

非相对论下的 \mathbf{L} 写作

$$\hat{\mathbf{L}}_{\text{NR}} = \frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{p}}.$$

(7) 波尔兹曼方程的解

直到2010年, 波尔兹曼方程的准确解才在数学上被证明是良好 (well-behaved) 的。这意味着, 如果对服从波尔兹曼方程的系统施加一个微扰, 此系统最终将回到平衡状态, 而不是发散到无穷, 或表现出其他的行为^{[10][11]}。然而, 这种存在性证明是无助于我们在现实问题中求解该等式的。事实上, 这个结论只告诉我们某种特定条件下的解是否存在, 而不是如何找到他们。在实践中, 数值计算方法被用于寻找各种形式的波尔兹曼方程的近似解, 应用范围从稀薄气流中的高超音速空气动力学^[12], 到等离子体的流动^[13]中都可以见到。

3) Boltzmann equation --- Wikipedia (English https://en.wikipedia.org/wiki/Boltzmann_equation)
(跟中文基本对照一致, 所以仅摘录一开始的介绍部分)

The Boltzmann equation or Boltzmann transport equation (BTE) describes the statistical behavior of a thermodynamic system not in a state of equilibrium. The classic example of such a system is a fluid with temperature gradients in space causing heat to flow from hotter regions to colder ones, by the random but biased transport of the particles making up that fluid. In the modern literature the term Boltzmann equation is often used in a more general sense, referring to any kinetic equation that describes the change of a macroscopic quantity in a thermodynamic system, such as energy, charge or particle number.

The equation arises not by analyzing the individual positions and momenta of each particle in the fluid but rather by considering a probability distribution for the position and momentum of a typical particle—that is, the probability that the particle occupies a given very small region of space (mathematically the volume element $d^3\vec{r}$) centered at the position \vec{r} , and has momentum nearly equal to a given momentum vector \vec{p} (thus occupying a very small region of momentum space $d^3\vec{p}$), at an instant of time. The Boltzmann equation can be used to determine how physical quantities change, such as heat energy and momentum, when a fluid is in transport. One may also derive other properties characteristic to fluids such as viscosity, thermal conductivity, and electrical conductivity (by treating the charge carriers in a material as a gas). See also convection–diffusion equation. The equation is a nonlinear integro-differential equation, and the unknown function in the equation is a probability density function in six-dimensional space of a particle position and momentum. The problem of existence and uniqueness of solutions is still not fully resolved, but some recent results are quite promising.

任务 III.2 --- Lattice Boltzmann Method.

1) 看 Notability App 上的 Notes

2) Wikipedia https://en.wikipedia.org/wiki/Lattice_Boltzmann_methods

Lattice Boltzmann methods (LBM), originated from the lattice gas automata (LGA) method (Hardy-Pomeau-Pazzis and Frisch-Hasslacher-Pomeau models), is a class of computational fluid dynamics (CFD) methods for fluid simulation. Instead of solving the Navier-Stokes equations directly, a fluid density on a lattice is simulated with streaming and collision (relaxation) processes. The method is versatile as the model fluid can straightforwardly be made to mimic common fluid behavior like vapor/liquid coexistence, and so fluid systems such as liquid droplets can be simulated. Also, fluids in complex environments such as porous media can be straightforwardly simulated, whereas with complex boundaries other CFD methods can be hard to work with.

Qadyan method is a new lattice Boltzmann method using combination of semi-discrete schemes to create a system of ordinary differential equation and differential quadrature method (微分求积法).

(1) Algorithm

LBM is a relatively new simulation technique for complex fluid systems and has attracted interest from researchers in computational physics. Unlike the traditional CFD methods, which solve the conservation equations of macroscopic properties (i.e., mass, momentum, and energy) numerically, LBM models the fluid consisting of fictive (虚构的) particles, and such particles perform consecutive propagation and collision processes over a discrete lattice mesh. Due to its particulate nature and local dynamics, LBM has several advantages over other conventional CFD methods, especially in dealing with complex boundaries, incorporating microscopic interactions, and parallelization of the algorithm. A different interpretation of the lattice Boltzmann equation is that of a discrete-velocity Boltzmann equation. The numerical methods of solution of the system of partial differential equations then give rise to a discrete map, which can be interpreted as the propagation and collision of fictitious particles.

In an algorithm, there are collision and streaming steps. These evolve the density of the fluid $\rho(\vec{x}, t)$, for \vec{x} the position and t the time. As the fluid is on a lattice the density has a number of components $f_i, i = 0, \dots, a$ equal to the number of lattice vectors connected to each lattice point. As an example, the lattice vectors for a simple lattice used in simulations in two dimensions is shown here. This lattice is usually denoted D2Q9, for two dimensions and nine vectors: four vectors along north, east, south and west, plus four vectors to the corners of a unit square, plus a vector with both components zero. Then, for example vector $\vec{e}_4 = (0, -1)$, i.e., it points due south and so has no x component but a y component of -1 . So one of the nine components of the total density at the central lattice point, $f_4(\vec{x}, t)$, is that part of the fluid at point \vec{x} moving due south, at a speed in lattice units of one.

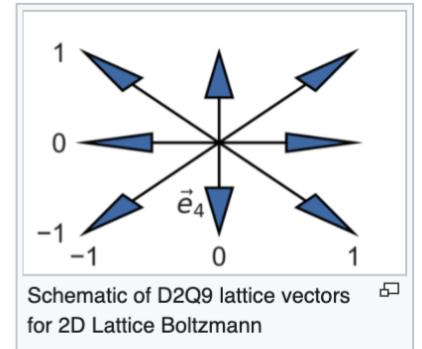
Then the steps that evolve the fluid in time are^[1]:

$$\text{Collision step: } f_i(\vec{x}, t + \delta_t) = f_i(\vec{x}, t) + \frac{f_i^{eq}(\vec{x}, t) - f_i(\vec{x}, t)}{\tau_f}$$

which is the Bhatnagar Gross and Krook (BGK)^[2] model for relaxation to equilibrium via collisions between the molecules of a fluid. $f_i^{eq}(\vec{x}, t)$ is the equilibrium density along direction i at the current density there. The model assumes that the fluid locally relaxes to equilibrium over a characteristic timescale τ_f . This timescale determines the kinematic viscosity, the larger it is, the larger is the kinematic viscosity.

$$\text{Streaming step: } f_i(\vec{x} + \vec{e}_i, t + 1) = f_i(\vec{x}, t)$$

As $f_i(\vec{x}, t)$ is, by definition, the fluid density at point \vec{x} at time t , that is moving at a velocity of \vec{e}_i per time step, then at the next time step $t + 1$ it will have flowed to point $\vec{x} + \vec{e}_i$.



(2) Advantages

- The LBM was designed from scratch to run efficiently on massively parallel architectures, ranging from inexpensive embedded **FPGAs** and **DSPs** up to **GPUs** and heterogeneous clusters and supercomputers (even with a slow interconnection network). It enables complex physics and sophisticated algorithms. Efficiency leads to a qualitatively new level of understanding since it allows solving problems that previously could not be approached (or only with insufficient accuracy).
- The method originates from a molecular description of a fluid and can directly incorporate physical terms stemming from a knowledge of the interaction between molecules. Hence it is an indispensable instrument in fundamental research, as it keeps the cycle between the elaboration of a theory and the formulation of a corresponding numerical model short.
- Automated data pre-processing and mesh generation in a time that accounts for a small fraction of the total simulation.
- Parallel data analysis, post-processing and evaluation.
- Fully resolved multi-phase flow with small droplets and bubbles.
- Fully resolved flow through complex geometries and porous media.
- Complex, coupled flow with heat transfer and chemical reactions.

(3) Limitations

Despite the increasing popularity of LBM in simulating complex fluid systems, this novel approach has some limitations. At present, high-Mach number flows in aerodynamics are still difficult for LBM, and a consistent thermo-hydrodynamic scheme is absent. However, as with Navier–Stokes based CFD, LBM methods have been successfully coupled with thermal-specific solutions to enable heat transfer (solids-based conduction, convection and radiation) simulation capability. For multiphase/multicomponent models, the interface thickness is usually large and the density ratio across the interface is small when compared with real fluids. Recently this problem has been resolved by Yuan and Schaefer who improved on models by Shan and Chen, Swift, and He, Chen, and Zhang. They were able to reach density ratios of 1000:1 by simply changing the equation of state. It has been proposed to apply Galilean Transformation to overcome the limitation of modelling high-speed fluid flows. Nevertheless, the wide applications and fast advancements of this method during the past twenty years have proven its potential in computational physics, including microfluidics. LBM demonstrates promising results in the area of high Knudsen number flows.

(4) Development from the LGA method

LBM originated from the lattice gas automata (LGA) method, which can be considered as a simplified fictitious molecular dynamics model in which space, time, and particle velocities are all discrete. For example, in the 2-dimensional FHP Model each lattice node is connected to its neighbors by 6 lattice velocities on a triangular lattice; there can be either 0 or 1 particles at a lattice node moving with a given lattice velocity. After a time interval, each particle will move to the neighboring node in its direction; this process is called the propagation or streaming step. When more than one particle arrives at the same node from different directions, they collide and change their velocities according to a set of collision rules. Streaming steps and collision steps alternate. Suitable collision rules should conserve the particle number (mass), momentum, and energy before and after the collision. LGA suffer from several innate (先天的) defects for use in hydrodynamic simulations: lack of **Galilean invariance** for fast flows, statistical noise

and poor Reynolds number scaling with lattice size. LGA are, however, well suited to simplify and extend the reach of reaction diffusion and molecular dynamics models.

The main motivation for the transition from LGA to LBM was the desire to **remove the statistical noise by replacing the Boolean particle number in a lattice direction with its ensemble average, the so-called density distribution function**. Accompanying this replacement, **the discrete collision rule is also replaced by a continuous function known as the collision operator**. In the LBM development, **an important simplification is to approximate the collision operator with the Bhatnagar-Gross-Krook (BGK) relaxation term**. This lattice BGK (LBGK) model makes simulations more efficient and allows flexibility of the transport coefficients. On the other hand, it has been shown that the LBM scheme can also be considered as a special discretized form of the continuous Boltzmann equation. From Chapman-Enskog theory, one can recover the governing continuity and Navier-Stokes equations from the LBM algorithm. In addition, as also directly available from the density distributions and hence there is no extra Poisson equation to be solved as in traditional CFD methods.

(5) Lattices and the DnQm classification

Lattice Boltzmann models can be operated on a number of different lattices, both cubic and triangular, and with or without rest particles in the discrete distribution function. A popular way of classifying the different methods by lattice is the DnQm scheme. Here "Dn" stands for "n dimensions", while "Qm" stands for "m speeds". For example, D3Q15 is a 3-dimensional lattice Boltzmann model on a cubic grid, with rest particles present. Each node has a crystal shape and can deliver particles to 15 nodes: each of the 6 neighboring nodes that share a surface, the 8 neighboring nodes sharing a corner, and itself. (The D3Q15 model does not contain particles moving to the 12 neighboring nodes that share an edge; adding those would create a "D3Q27" model.) **Real quantities such as space and time need to be converted to lattice units prior to simulation. Nondimensional quantities, like the Reynolds number, remain the same.**

(6) Lattice units conversion

In most Lattice Boltzmann simulations δ_x is the basic unit for lattice spacing, so if the domain of length L has N lattice units along its entire length, the space unit is simply defined as $\delta_x = L/N$. Speeds in lattice Boltzmann simulations are typically given in terms of the speed of sound. The discrete time unit can therefore be given as $\delta_t = \frac{\delta_x}{C_s}$, where the denominator C_s is the physical speed of sound.^[5]

For small-scale flows (such as those seen in porous media mechanics), operating with the true speed of sound can lead to unacceptably short time steps. It is therefore common to raise the lattice Mach number to something much larger than the real Mach number, and compensating for this by raising the viscosity as well in order to preserve the Reynolds number.

(7) Simulation of mixtures

Simulating multiphase/multicomponent flows has always been a challenge to conventional CFD because of the moving and deformable interfaces. More fundamentally, the interfaces between different phases (liquid and vapor) or components (e.g., oil and water) originate from the specific interactions among fluid molecules. Therefore, it is difficult to implement such microscopic interactions into the macroscopic Navier-Stokes equation. However, in LBM, the particulate kinetics provides a relatively easy and consistent way to incorporate the underlying microscopic interactions by modifying the collision operator. Several LBM multiphase/multicomponent models have been developed. Here phase separations are generated automatically from the particle dynamics and no special treatment is needed to manipulate the interfaces as in traditional CFD methods. Successful applications of multiphase/multicomponent LBM models can be found in various complex fluid systems, including interface instability, bubble/droplet dynamics, wetting on solid surfaces, interfacial slip, and droplet electrohydrodynamic deformations.

A lattice Boltzmann model for simulation of gas mixture combustion capable of accommodating significant density variations at low-Mach number regime has been recently proposed. To this respect, it is worth to notice that, since LBM deals with a larger set of fields (as compared to conventional CFD), the simulation of reactive gas mixtures presents some additional challenges in terms of memory demand as far as large detailed combustion mechanisms are concerned. Those issues may be addressed, though, by resorting to (诉诸) systematic model reduction techniques.

(8) Thermal lattice-Boltzmann method

Currently (2009), a thermal lattice-Boltzmann method (TLBM) falls into one of three categories: the multi-speed approach, the passive scalar approach, and the thermal energy distribution.

(9) Derivation of Navier-Stokes equation from discrete LBE

Starting with the discrete lattice Boltzmann equation (also referred to as LBGK equation due to the collision operator used). We first do a 2nd-order Taylor series expansion about the left side of the LBE. This is chosen over a simpler 1st-order Taylor expansion as the discrete LBE cannot be recovered. When doing the 2nd-order Taylor series expansion, the zero derivative term and the first term on the right will cancel, leaving only the first and second derivative terms of the Taylor expansion and the collision operator:

$$f_i(\vec{x} + \vec{e}_i \delta_t, t + \delta_t) = f_i(\vec{x}, t) + \frac{\delta_t}{\tau_f} (f_i^{eq} - f_i).$$

For simplicity, write $f_i(\vec{x}, t)$ as f_i . The slightly simplified Taylor series expansion is then as follows, where ":" is the colon product between dyads:

$$\frac{\partial f_i}{\partial t} + \vec{e}_i \cdot \nabla f_i + \left(\frac{1}{2} \vec{e}_i \vec{e}_i : \nabla \nabla f_i + \vec{e}_i \cdot \nabla \frac{\partial f_i}{\partial t} + \frac{1}{2} \frac{\partial^2 f_i}{\partial t^2} \right) = \frac{1}{\tau} (f_i^{eq} - f_i).$$

By expanding the particle distribution function into equilibrium and non-equilibrium components and using the Chapman-Enskog expansion, where K is the Knudsen number, the Taylor-expanded LBE can be decomposed into different magnitudes of order for the Knudsen number in order to obtain the proper continuum equations:

$$\begin{aligned} f_i &= f_i^{eq} + K f_i^{neq}, \\ f_i^{neq} &= f_i^{(1)} + K f_i^{(2)} + O(K^2). \end{aligned}$$

The equilibrium and non-equilibrium distributions satisfy the following relations to their macroscopic variables (these will be used later, once the particle distributions are in the "correct form" in order to scale from the particle to macroscopic level):

$$\begin{aligned} \rho &= \sum_i f_i^{eq}, \\ \rho \vec{u} &= \sum_i f_i^{eq} \vec{e}_i, \\ 0 &= \sum_i f_i^{(k)} \quad \text{for } k = 1, 2, \\ 0 &= \sum_i f_i^{(k)} \vec{e}_i. \end{aligned}$$

The Chapman-Enskog expansion is then:

$$\begin{aligned}\frac{\partial}{\partial t} &= K \frac{\partial}{\partial t_1} + K^2 \frac{\partial}{\partial t_2} \quad \text{for } t_2 \text{ (diffusive time-scale)} \ll t_1 \text{ (convective time-scale)}, \\ \frac{\partial}{\partial x} &= K \frac{\partial}{\partial x_1}.\end{aligned}$$

By substituting the expanded equilibrium and non-equilibrium into the Taylor expansion and separating into different orders of K , the continuum equations are nearly derived.

For order K^0 :

$$\frac{\partial f_i^{\text{eq}}}{\partial t_1} + \vec{e}_i \nabla_1 f_i^{\text{eq}} = -\frac{f_i^{(1)}}{\tau}.$$

For order K^1 :

$$\frac{\partial f_i^{(1)}}{\partial t_1} + \frac{\partial f_i^{\text{eq}}}{\partial t_2} + \vec{e}_i \nabla f_i^{(1)} + \frac{1}{2} \vec{e}_i \vec{e}_i : \nabla \nabla f_i^{\text{eq}} + \vec{e}_i \cdot \nabla \frac{\partial f_i^{\text{eq}}}{\partial t_1} + \frac{1}{2} \frac{\partial^2 f_i^{\text{eq}}}{\partial t_1^2} = -\frac{f_i^{(2)}}{\tau}.$$

Then, the second equation can be simplified with some algebra and the first equation into the following:

$$\frac{\partial f_i^{\text{eq}}}{\partial t_2} + \left(1 - \frac{1}{2\tau}\right) \left[\frac{\partial f_i^{(1)}}{\partial t_1} + \vec{e}_i \nabla_1 f_i^{(1)} \right] = -\frac{f_i^{(2)}}{\tau}.$$

Applying the relations between the particle distribution functions and the macroscopic properties from above, the mass and momentum equations are achieved:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} &= 0, \\ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \Pi &= 0.\end{aligned}$$

The momentum flux tensor Π has the following form then:

$$\Pi_{xy} = \sum_i \vec{e}_{ix} \vec{e}_{iy} \left[f_i^{\text{eq}} + \left(1 - \frac{1}{2\tau}\right) f_i^{(1)} \right],$$

where $\vec{e}_{ix}\vec{e}_{iy}$ is shorthand for the square of the sum of all the components of \vec{e}_i (i. e. $(\sum_x \vec{e}_{ix})^2 = \sum_x \sum_y \vec{e}_{ix}\vec{e}_{iy}$), and the equilibrium particle distribution with second order to be comparable to the Navier–Stokes equation is:

$$f_i^{\text{eq}} = \omega_i \rho \left(1 + \frac{\vec{e}_i \vec{u}}{c_s^2} + \frac{(\vec{e}_i \vec{u})^2}{2c_s^4} - \frac{\vec{u}^2}{2c_s^2} \right).$$

The equilibrium distribution is only valid for small velocities or small [Mach numbers](#). Inserting the equilibrium distribution back into the flux tensor leads to:

$$\begin{aligned} \Pi_{xy}^{(0)} &= \sum_i \vec{e}_{ix}\vec{e}_{iy} f_i^{\text{eq}} = p\delta_{xy} + \rho u_x u_y, \\ \Pi_{xy}^{(1)} &= \left(1 - \frac{1}{2\tau} \right) \sum_i \vec{e}_{ix}\vec{e}_{iy} f_i^{(1)} = \nu (\nabla_x (\rho \vec{u}_y) + \nabla_y (\rho \vec{u}_x)). \end{aligned}$$

Finally, the Navier–Stokes equation is recovered under the assumption that density variation is small:

$$\rho \left(\frac{\partial \vec{u}_x}{\partial t} + \nabla_y \cdot \vec{u}_x \vec{u}_y \right) = -\nabla_x p + \nu \nabla_y \cdot (\nabla_x (\rho \vec{u}_y) + \nabla_y (\rho \vec{u}_x)).$$

This derivation follows the work of Chen and Doolen.^[14]

[14]: Chen, S., and Doolen, G. D., "Lattice Boltzmann Method for Fluid Flows", *Annual Review of Fluid Mechanics*, vol. 30, p. 329–364, 1998.

(10) Mathematical equations for simulations

The continuous Boltzmann equation is an evolution equation for a single particle probability distribution function $f(\vec{x}, \vec{e}_i, t)$ and the internal energy density distribution function $g(\vec{x}, \vec{e}_i, t)$ (He et al.) are each respectively:

$$\begin{aligned} \partial_t f + (\vec{e} \cdot \nabla) f + F \partial_v f &= \Omega(f), \\ \partial_t g + (\vec{e} \cdot \nabla) g + G \partial_v f &= \Omega(g), \end{aligned}$$

where $g(\vec{x}, \vec{e}_i, t)$ is related to $f(\vec{x}, \vec{e}_i, t)$ by

$$g(\vec{x}, \vec{e}_i, t) = \frac{(\vec{e} - \vec{u})^2}{2} f(\vec{x}, \vec{e}_i, t),$$

F is an external force, Ω is a collision integral, and \vec{e} (also labeled by $\vec{\xi}$ in literature) is the microscopic velocity.

The external force F is related to temperature external force G by the relation below. A typical test for one's model is the [Rayleigh–Bénard convection](#) for G .

$$\begin{aligned} F &= \frac{\vec{G} \cdot (\vec{e} - \vec{u})}{RT} f^{\text{eq}}, \\ \vec{G} &= \beta g_0 (T - T_{\text{avg}}) \vec{k}. \end{aligned}$$

Macroscopic variables such as density ρ , velocity \vec{u} , and temperature T can be calculated as the moments of the density distribution function:

$$\begin{aligned}\rho &= \int f d\vec{e}, \\ \rho\vec{u} &= \int \vec{e} f d\vec{e}, \\ \frac{\rho DRT}{2} &= \rho\epsilon = \int g d\vec{e}.\end{aligned}$$

* The lattice Boltzmann method discretizes this equation by limiting space to a lattice and the velocity space to a discrete set of microscopic velocities (i. e. $\vec{e}_i = (\vec{e}_{ix}, \vec{e}_{iy})$). The microscopic velocities in D2Q9, D3Q15, and D3Q19 for example are given as:

$$\begin{aligned}\vec{e}_i &= c \times \begin{cases} (0, 0) & i = 0 \\ (1, 0), (0, 1), (-1, 0), (0, -1) & i = 1, 2, 3, 4 \\ (1, 1), (-1, 1), (-1, -1), (1, -1) & i = 5, 6, 7, 8 \end{cases} \\ \vec{e}_i &= c \times \begin{cases} (0, 0, 0) & i = 0 \\ (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1) & i = 1, 2, \dots, 5, 6 \\ (\pm 1, \pm 1, \pm 1) & i = 7, 8, \dots, 13, 14 \end{cases} \\ \vec{e}_i &= c \times \begin{cases} (0, 0, 0) & i = 0 \\ (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1) & i = 1, 2, \dots, 5, 6 \\ (\pm 1, \pm 1, 0), (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1) & i = 7, 8, \dots, 17, 18 \end{cases}\end{aligned}$$

The single-phase discretized Boltzmann equation for mass density and internal energy density are:

$$\begin{aligned}f_i(\vec{x} + \vec{e}_i \delta_t, t + \delta_t) - f_i(\vec{x}, t) + F_i &= \Omega(f), \\ g_i(\vec{x} + \vec{e}_i \delta_t, t + \delta_t) - g_i(\vec{x}, t) + G_i &= \Omega(g).\end{aligned}$$

The collision operator is often approximated by a BGK collision operator under the condition it also satisfies the conservation laws:

$$\begin{aligned}\Omega(f) &= \frac{1}{\tau_f} (f_i^{\text{eq}} - f_i), \\ \Omega(g) &= \frac{1}{\tau_g} (g_i^{\text{eq}} - g_i).\end{aligned}$$

In the collision operator f_i^{eq} is the discrete, equilibrium particle probability distribution function [clarify]. In D2Q9 and D3Q19, it is shown below for an incompressible flow in continuous and discrete form where D , R , and T are the dimension, universal gas constant, and absolute temperature respectively. The partial derivation for the continuous to discrete form is provided through a simple derivation to second order accuracy.

$$\begin{aligned} f^{\text{eq}} &= \frac{\rho}{(2\pi RT)^{D/2}} e^{-\frac{(\vec{e}-\vec{u})^2}{2RT}} \\ &= \frac{\rho}{(2\pi RT)^{D/2}} e^{-\frac{(\vec{e})^2}{2RT}} e^{\frac{\vec{e}\vec{u}}{RT} - \frac{\vec{u}^2}{2RT}} \\ &= \frac{\rho}{(2\pi RT)^{D/2}} e^{-\frac{(\vec{e})^2}{2RT}} \left(1 + \frac{\vec{e}\vec{u}}{RT} + \frac{(\vec{e}\vec{u})^2}{2(RT)^2} - \frac{\vec{u}^2}{2RT} + \dots \right) \end{aligned}$$

Letting $c = \sqrt{3RT}$ yields the final result:

$$f_i^{\text{eq}} = \omega_i \rho \left(1 + \frac{3\vec{e}_i \vec{u}}{c^2} + \frac{9(\vec{e}_i \vec{u})^2}{2c^4} - \frac{3(\vec{u})^2}{2c^2} \right)$$

$$g^{\text{eq}} = \frac{\rho(\vec{e} - \vec{u})^2}{2(2\pi RT)^{D/2}} e^{-\frac{(\vec{e}-\vec{u})^2}{2RT}}$$

$$\omega_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1, 2, 3, 4 \\ 1/36 & i = 5, 6, 7, 8 \end{cases}$$

$$\omega_i = \begin{cases} 1/3 & i = 0 \\ 1/18 & i = 1, 2, \dots, 5, 6 \\ 1/36 & i = 7, 8, \dots, 17, 18 \end{cases}$$

As much work has already been done on a single-component flow, the following TLBM will be discussed. The multicomponent/multiphase TLBM is also more intriguing and useful than simply one component. To be in line with current research, define the set of all components of the system (i. e. walls of porous media, multiple fluids/gases, etc.) Ψ with elements σ_j .

$$f_i^\sigma(\vec{x} + \vec{e}_i \delta_t, t + \delta_t) - f_i^\sigma(\vec{x}, t) + F_i = \frac{1}{\tau_f^\sigma} (f_i^{\sigma, \text{eq}}(\rho^\sigma, v^\sigma) - f_i^\sigma)$$

The relaxation parameter, $\tau_f^{\sigma_j}$, is related to the kinematic viscosity, $\nu_f^{\sigma_j}$, by the following relationship:

$$\nu_f^{\sigma_j} = (\tau_f^{\sigma_j} - 0.5)c_s^2 \delta_t.$$

The [moments](#) of the f_i give the local conserved quantities. The density is given by

$$\rho = \sum_{\sigma} \sum_i f_i$$

$$\rho\epsilon = \sum_i g_i$$

$$\rho^{\sigma} = \sum_i f_i^{\sigma}$$

and the weighted average velocity, \vec{u}' , and the local momentum are given by

$$\vec{u}' = \left(\sum_{\sigma} \frac{\rho^{\sigma} \vec{u}^{\sigma}}{\tau_f^{\sigma}} \right) / \left(\sum_{\sigma} \frac{\rho^{\sigma}}{\tau_f^{\sigma}} \right)$$

$$\rho^{\sigma} \vec{u}^{\sigma} = \sum_i f_i^{\sigma} \vec{e}_i.$$

$$v^{\sigma} = \vec{u}' + \frac{\tau_f^{\sigma}}{\rho^{\sigma}} \vec{F}^{\sigma}$$

In the above equation for the equilibrium velocity v^{σ} , the \vec{F}^{σ} term is the interaction force between a component and the other components. It is still the subject of much discussion as it is typically a tuning parameter that determines how fluid-fluid, fluid-gas, etc. interact. Frank et al. list current models for this force term. The commonly used derivations are Gunstensen chromodynamic model, Swift's free energy-based approach for both liquid/vapor systems and binary fluids, He's intermolecular interaction-based model, the Inamuro approach, and the Lee and Lin approach.[\[15\]](#)

The following is the general description for \vec{F}^{σ} as given by several authors.[\[16\]\[17\]](#)

$$\vec{F}^{\sigma} = -\psi^{\sigma}(\vec{x}) \sum_{\sigma_j} H^{\sigma\sigma_j}(\vec{x}, \vec{x}') \sum_i \psi^{\sigma_j}(\vec{x} + \vec{e}_i) \vec{e}_i$$

$\psi(\vec{x})$ is the effective mass and $H(\vec{x}, \vec{x}')$ is Green's function representing the interparticle interaction with \vec{x}' as the neighboring site. Satisfying $H(\vec{x}, \vec{x}') = H(\vec{x}', \vec{x})$ and where $H(\vec{x}, \vec{x}') > 0$ represents repulsive forces. For D2Q9 and D3Q19, this leads to

$$H^{\sigma\sigma_j}(\vec{x}, \vec{x}') = \begin{cases} h^{\sigma\sigma_j} & |\vec{x} - \vec{x}'| \leq c \\ 0 & |\vec{x} - \vec{x}'| > c \end{cases}$$

$$H^{\sigma\sigma_j}(\vec{x}, \vec{x}') = \begin{cases} h^{\sigma\sigma_j} & |\vec{x} - \vec{x}'| = c \\ h^{\sigma\sigma_j}/2 & |\vec{x} - \vec{x}'| = \sqrt{2c} \\ 0 & \text{otherwise} \end{cases}$$

The effective mass as proposed by Shan and Chen uses the following effective mass for a *single-component, multiphase system*. The [equation of state](#) is also given under the condition of a single component and multiphase.

$$\psi(\vec{x}) = \psi(\rho^\sigma) = \rho_0^\sigma \left[1 - e^{(-\rho^\sigma / \rho_0^\sigma)} \right]$$

$$p = c_s^2 \rho + c_0 h[\psi(\vec{x})]^2$$

So far, it appears that ρ_0^σ and $h^{\sigma\sigma_j}$ are free constants to tune but once plugged into the system's [equation of state](#)(EOS), they must satisfy the thermodynamic relationships at the critical point such that $(\partial P / \partial \rho)_T = (\partial^2 P / \partial \rho^2)_T = 0$ and $p = p_c$. For the EOS, c_0 is 3.0 for D2Q9 and D3Q19 while it equals 10.0 for D3Q15.[\[18\]](#)

It was later shown by Yuan and Schaefer[\[19\]](#) that the effective mass density needs to be changed to simulate multiphase flow more accurately. They compared the Shan and Chen (SC), Carnahan-Starling (C–S), van der Waals (vdW), Redlich–Kwong (R–K), Redlich–Kwong Soave (RKS), and Peng–Robinson (P–R) EOS. Their results revealed that the SC EOS was insufficient and that C–S, P–R, R–K, and RKS EOS are all more accurate in modeling multiphase flow of a single component.

For the popular isothermal Lattice Boltzmann methods these are the only conserved quantities. Thermal models also conserve energy and therefore have an additional conserved quantity:

$$\rho\theta + \rho uu = \sum_i f_i \vec{e}_i \vec{e}_i.$$

(11) Applications

During the last years, the LBM has proven to be a powerful tool for solving problems at different length and time scales. The behavior of fluid flow through porous media can be analyzed using the lattice Boltzmann method. Moreover, its easy handling of complex geometries has made it an excellent tool to study biofluid dynamics in complex anatomical geometries. Recent literature has also applied LBM based DNS for the study of transitional and turbulent flows in simple and complex geometries. In summary some of the applications of LBM include:

- Earth sciences (Soil filtration).
- Energy Sciences (Fuel Cells[\[20\]](#)).
- Biofluid Dynamics [\[21\]](#)
- Transitional and Turbulent Flows [\[22\]](#)

(3) “Lattice Boltzmann Method” http://www.scholarpedia.org/article/Lattice_Boltzmann_Method

[Contents \[hide\]](#)

- 1 Fluids, atoms and kinetic theory
- 2 The Lattice Boltzmann equation: history
- 3 The Lattice Boltzmann equation: mathematical formulation
 - 3.1 Hydrodynamics from LBE
- 4 Boundary conditions
- 5 Post-classical LBE's
 - 5.1 Restoring the second principle: Entropic Models
 - 5.2 Lattice Boltzmann from Boltzmann: the Hermite-Gauss connection
 - 5.3 Multi-time relaxation LBE
- 6 Idiosyncrasies, lucky strikes and some misbeliefs
 - 6.1 Weak compressibility and pressure drops
 - 6.2 The mirage of zero viscosity
 - 6.3 LB is -not- a dilute-gas approximation
- 7 LBE for non-ideal fluids
- 8 LB beyond Navier-Stokes: meso and nano-hydrodynamics
- 9 Whither LB?
- 10 References
- 11 Further reading and www links

具体的看 Notability APP 上的 Notes

05/25/20

(I) Cahn-Hilliard-Cook (CHC) nonlinear diffusion equation

(II) Cell-Dynamic Method (CDM)

(III) Dynamic DFT

05/31/20

1) Paper (01) Multiscale modeling and simulation of polymer nanocomposites

(1) Notes: <https://www.tandfonline.com/doi/abs/10.1080/AMP-200068646?journalCode=lmmp20>

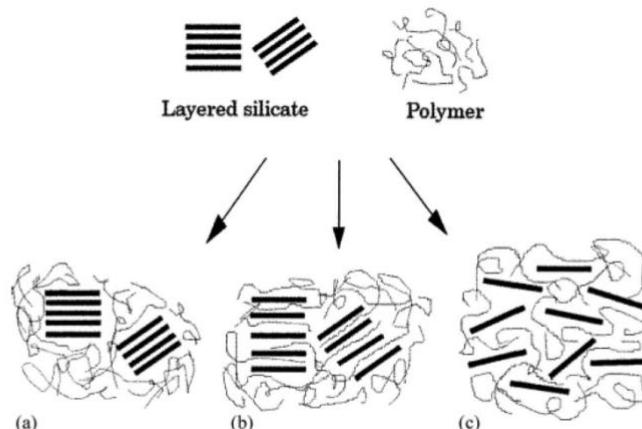


FIGURE 2.—Schematic of three main types of polymer/layer structure composite morphologies: (a) microcomposites, (b) intercalated nanocomposites, and (c) exfoliated nanocomposites (reproduced with permission from [25]).

06/06/20

任务 I) Stress relaxation time difference (between nanoparticles and polymers)

(1) https://en.wikipedia.org/wiki/Stress_relaxation

(2)

<https://www.google.com/search?q=stress+relaxation+time&oq=stress+relaxation+time&aqs=chrome..69i57j0l7.4807j0j7&sourceid=chrome&ie=UTF-8>

(3) <https://www.whoi.edu/fileserver.do?id=28331&pt=10&p=17274>

06/11/20

1) Percolation threshold

https://en.wikipedia.org/wiki/Percolation_threshold

The percolation threshold is a mathematical concept in percolation theory that describes the formation of long-range connectivity in random systems. Below the threshold a giant connected component does not exist; while above it, there exists a giant component of the order of system size. In engineering and coffee making, percolation represents the flow of fluids through porous media, but in the mathematics and physics worlds it generally refers to simplified lattice models of random systems or networks (graphs), and the nature of the connectivity in them. The **percolation threshold** is the critical value of the occupation probability p , or more generally a critical surface for a group of parameters p_1, p_2, \dots , such that infinite connectivity (percolation) first occurs.

(i) Percolation models

The most common percolation model is to take a regular lattice, like a square lattice, and make it into a random network by randomly "occupying" sites (vertices) or bonds (edges) with a statistically independent probability p . At a critical threshold p_c , large clusters and long-range connectivity first appears, and this is called the **percolation threshold**. Depending on the method for obtaining the random network, one distinguishes between the **site percolation threshold** and the **bond percolation threshold**. More general systems have several probabilities p_1, p_2, \dots , and the transition is characterized by a critical surface or manifold. One can also consider continuum systems, such as overlapping disks and spheres placed randomly, or the negative space (Swiss-cheese models).

In the systems described so far, it has been assumed that the occupation of a site or bond is completely random—this is the so-called Bernoulli percolation. For a continuum system, random occupancy corresponds to the points being placed by a Poisson process. Further variations involve correlated percolation, such as percolation clusters related to Ising and Potts models of ferromagnets, in which the bonds are put down by the Fortuin-Kasteleyn method.[1] In bootstrap or k-sat percolation, sites and/or bonds are first occupied and then successively culled (扑灭) from a system if a site does not have at least k neighbors. Another important model of percolation, in a different universality class altogether, is directed percolation, where connectivity along a bond depends upon the direction of the flow.

Over the last several decades, a tremendous amount of work has gone into finding exact and approximate values of the percolation thresholds for a variety of these systems. Exact thresholds are only known for certain two-dimensional lattices that can be broken up into a self-dual array, such that under a triangle-triangle transformation, the system remains the same. Studies using numerical methods have led to numerous improvements in algorithms and several theoretical discoveries.

Simply duality in two dimensions implies that all fully triangulated lattices (e.g., the triangular, union jack, cross dual, martini dual and asanoha or 3-12 dual, and the Delaunay triangulation) all have site thresholds of 1/2, and self-dual lattices (square, martini-B) have bond thresholds of 1/2.

The notation such as (4,8₂) comes from Grünbaum and Shephard,[2] and indicates that around a given vertex, going in the clockwise direction, one encounters first a square and then two octagons (八边形). Besides the eleven Archimedean lattices composed of regular polygons with every site equivalent, many other more complicated lattices with sites of different classes have been studied.

Error bars in the last digit or digits are shown by numbers in parentheses. Thus, 0.729724(3) signifies 0.729724 ± 0.000003 , and 0.74042195(80) signifies $0.74042195 \pm 0.00000080$. The error bars variously represent one or two standard deviations in net error (including statistical and expected systematic error), or an empirical confidence interval.

06/16/20

1) “Polydispersity” and “Dispersity Index”

Wikipedia: “Dispersity”: <https://en.wikipedia.org/wiki/Dispersity>

In chemistry, the dispersity is a measure of the heterogeneity of sizes of molecules or particles in a mixture. A collection of objects is called uniform if the objects have the same size, shape, or mass --- monodisperse. A sample of objects that have an inconsistent size, shape and mass distribution is called non-uniform. The objects can be in any form of chemical dispersion, such as particles in a colloid, droplets in a cloud, crystals in a rock, or polymer macromolecules in a solution or a solid polymer mass. Polymers can be described by molecular mass distribution; a population of particles can be described by size, surface area, and/or mass distribution; and thin films can be described by film thickness distribution.

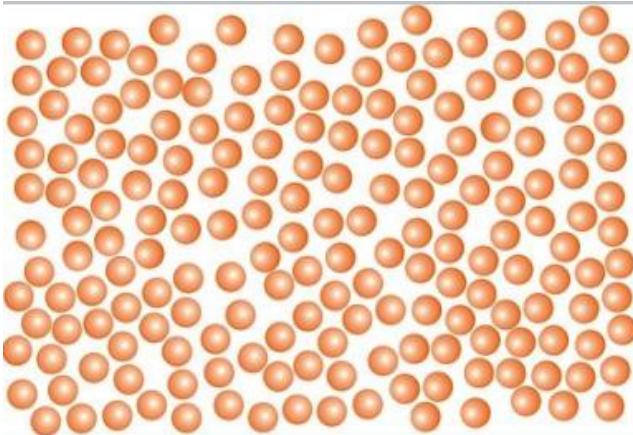
IUPAC has deprecated the use of the term **polydispersity index**, having replaced it with the term **dispersity**, represented by the symbol D (pronounced D-stroke^[4]) which can refer to either molecular mass or degree of polymerization. It can be calculated using the equation $D_M = M_w/M_n$, where M_w is the weight-average molar mass and M_n is the number-average molar mass. It can also be calculated according to degree of polymerization, where $D_X = X_w/X_n$, where X_w is the weight-average degree of polymerization and X_n is the number-average degree of polymerization. In certain limiting cases where $D_M = D_X$, it is simply referred to as D . IUPAC has also deprecated the terms **monodisperse**, which is considered to be self-contradictory, and **polydisperse**, which is considered redundant, preferring the terms **uniform** and **non-uniform** instead.

IUPAC definition

$$D_M = M_w/M_n$$

where M_w is the mass-average molar mass (or molecular weight) and M_n is the number-average molar mass (or molecular weight).

Pure Appl. Chem., 2009, 81(2), 351-353 ↗



A uniform (monodisperse) collection



A non-uniform (polydisperse) collection

2) “Polymer storage modulus”

<https://www.google.com/search?q=polymer+storage+modulus&oq=polymer+storage&aqs=chrome.4.0j69i57j0l6.7834j1j7&sourceid=chrome&ie=UTF-8>

a) <https://www.eag.com/wp-content/uploads/2017/09/M-022717-Characterization-of-Polymers-using-Dynamic-Mechanical-Analysis.pdf>

Storage modulus corresponds to the mechanical energy **stored** by the material during a loading cycle. Consequently, the **storage modulus** is related to the stiffness and shape recovery of the **polymer** during loading.

www.eag.com › wp-content › uploads › 2017/09 › M-02... [PDF](#)

Characterization of Polymers using Dynamic Mechanical ...

b) https://en.wikipedia.org/wiki/Dynamic_mechanical_analysis

The **storage modulus** measures the stored energy, representing the elastic portion, and the loss modulus measures the energy dissipated as heat, representing the viscous portion.^[4] The tensile storage and loss moduli are defined as follows:

- **Storage modulus:** $E' = \frac{\sigma_0}{\varepsilon_0} \cos \delta$

任务: “Polymer Relaxation” ---> Mechanical Properties

ccc