Notes_Onsager Reciprocal Relation
Yining He

04/27/20
Paper 0) Dynamic density functional theory for microphase separation kinetics of block copolymer melts

1) Terminology
1.1 "Collective Diffusion"
(A) http://www.ifpan.edu.pl/ON-2/on26/on26sub/a2.html
"*Collective diffusion is a dynamic process that involves many particles and due to their cooperative movements leads to various interesting effects. Coefficient of the collective diffusion is a parameter that is a part of the equation describing local density diffusion process nearby the equilibrium state.*

*Diffusion coefficient as **a function** of a **particle density** and **other parameters of the system** describes dynamics of the diffusion processes in the system. Calculation of this parameter in the general case is not an easy task. Lately a new and very effective method has been worked out in our group. It is variational approach to the problem. According to this approach, calculation of the diffusion coefficient consists of the definition of the transition matrix in the given system, and definition of the proper variational eigenvector. Next, the parameters are found that minimalize the following formula that describes diffusion parameter.*

Finally, diffusion coefficient as a function of density, temperature and other physical condition is found. In this way we are able to describe various interesting and sometimes unexpected system behaviors. We show how the diffusion coefficient depends on the interaction strength between particles and on the interaction dependent barrier height. Interesting case of fractal like structure of the diffusion coefficient for a system with devil staircase phase diagram caused by long range interactions within medium. Diffusion on non-homogeneous potential has been calculated and 2-D systems are recently studied.

We show that an exponent of a power-like time domain growth is determined not only by the conservation or nonconservation of the order parameter, but also by the asymmetry of single particle jumps. Domains that have an anisotropic pattern, such as (2*1), have a tendency to grow faster in certain direction than they do in others. The rate of expansion in different directions depends on the barriers for single particle jumps. As a result, dynamical behavior of systems which start in the same configurations and eventually reach the same equilibrium states is completely different. We show how differences in microscopic dynamics in a 1-D Potts model lead to different rates of domain growth. We observe a similar effect for a two-dimensional (2*1) ordering by changing the way in which a barrier for a jump depends on the number of neighboring particles. We show examples of the domain power growth which are characterized by different exponents."

(B) "Molecular diffusion" https://en.wikipedia.org/wiki/Molecular_diffusion
(I) Intro
"Molecular diffusion, often simply called diffusion, is the thermal motion of all (liquid or gas) particles at temperatures above absolute zero. The rate of this movement is **a function of (i) temperature, (ii) viscosity of the fluid and (iii) the size (mass) of the particles**. Diffusion explains the net flux of molecules from a region of higher concentration to one of lower concentration. Once the concentrations are equal the molecules continue to move, but since there is no concentration gradient the process of molecular diffusion has ceased and is instead governed by the process of self-diffusion, originating from the random motion of the molecules. The result of diffusion is a gradual mixing of material such that the distribution of molecules is uniform. Since the molecules are still in motion, but an equilibrium has been established, the end result of molecular diffusion is called a "**dynamic equilibrium**". In a phase with uniform temperature, absent external net forces acting on the particles, the diffusion process will eventually result in complete mixing.

(II) Non-equilibrium system

Because chemical diffusion is a net transport process, the system in which it takes place is not an equilibrium system (i.e. it is not at rest yet). **Many results in classical thermodynamics are not easily applied to non-equilibrium systems.** However, there sometimes occur so-called quasi-steady states, where the diffusion process does not change in time, where classical results may locally apply. As the name suggests, this process is a not a true equilibrium since the system is still evolving.

Non-equilibrium fluid systems can be successfully modeled with Landau-Lifshitz fluctuating hydrodynamics. In this theoretical framework, diffusion is due to fluctuations whose dimensions range from the molecular scale to the macroscopic scale.

Chemical diffusion increases the entropy of a system, i.e. diffusion is a spontaneous and irreversible process. Particles can spread out by diffusion, but will not spontaneously re-order themselves (absent changes to the system, assuming no creation of new chemical bonds, and absent external forces acting on the particle).

(III) Concentration dependent "collective" diffusion
Collective diffusion is the diffusion of a large number of particles, most often within a solvent.

Contrary to brownian motion, which is the diffusion of a single particle, **interactions between particles may have to be considered**, unless the particles form an ideal mix with their solvent (ideal mix conditions correspond to the case where the interactions between the solvent and particles are identical to the interactions between particles and the interactions between solvent molecules; in this case, the particles do not interact when inside the solvent).

In case of an ideal mix, the particle diffusion equation holds true and the diffusion coefficient D, the speed of diffusion in the particle diffusion equation is independent of particle concentration. In other cases, resulting interactions between particles within the solvent will account for the following effects:

- The diffusion coefficient D in the particle diffusion equation becomes dependent of concentration. For an attractive interaction between particles, the diffusion coefficient tends to decrease as concentration increases. For a repulsive interaction between particles, the diffusion coefficient tends to increase as concentration increases.

- In the case of an attractive interaction between particles, particles exhibit a tendency to coalesce and form clusters if their concentration lies above a certain threshold. This is equivalent to a precipitation chemical reaction (and if the considered diffusing particles are chemical molecules in solution, then it is a precipitation).

1.2 Onsager Kinetic Coefficients
(A) Paper: Brownian motion and fluctuating hydrodynamics
(https://www.researchgate.net/publication/222595548_Brownian_motion_and_fluctuating_hydrodynamics)

Onsager and Machlup[2]) generalized the Langevin equation to serve as a basis for the discussion of linear fluctuation phenomena in nonequilibrium thermodynamics. This general theory was then applied to linear fluctuating hydrodynamics by Green and by Landau and Lifshitz[3]).

5. Discussion. In this paper we have applied a generalization of Faxén's theorem to derive from fluctuating hydrodynamics the Langevin equation for a spherical brownian particle. Faxén's theorem gives an explicit expression for the random force in terms of the fluctuating velocity field in the absence of the particle. The fluctuation-dissipation theorem then follows by straight forward evaluation of the random force-force correlation function. In section 4 we have also given an alter-

We conclude with the remark that it has thus been shown that fluctuating hydrodynamics, which is described by a gaussian and markovian stochastic process, leads for the velocity of brownian particle to a gaussian non-markovian process. Only when $m \gg \frac{4}{3}a^3\varrho$ this last process becomes approximately markovian again so that the classical Langevin equation holds. See also refs. 6 and 7 for a detailed discussion of this point.

(B) https://en.wikipedia.org/wiki/Onsager%E2%80%93Machlup_function
Onsager–Machlup function
"The Onsager–Machlup function is a function that summarizes the dynamics of a continuous stochastic process. It is used to define a probability density for a stochastic process, and it is similar to the Lagrangian of a dynamical system.

The dynamics of a continuous stochastic process X from time $t = 0$ to $t = T$ in one dimension, satisfying a stochastic differential equation

$$dX_t = b(X_t)\,dt + \sigma(X_t)\,dW_t$$

where W is a Wiener process, can in approximation be described by the probability density function of its value x_i at a finite number of points in time t_i:

$$p(x_1, \ldots, x_n) = \left(\prod_{i=1}^{n-1} \frac{1}{\sqrt{2\pi\sigma(x_i)^2 \Delta t_i}} \right) \exp\left(-\sum_{i=1}^{n-1} L\left(x_i, \frac{x_{i+1} - x_i}{\Delta t_i} \right) \Delta t_i \right)$$

where

$$L(x, v) = \frac{1}{2}\left(\frac{v - b(x)}{\sigma(x)} \right)^2$$

and $\Delta t_i = t_{i+1} - t_i > 0$, $t_1 = 0$ and $t_n = T$. A similar approximation is possible for processes in higher dimensions. The approximation is more accurate for smaller time step sizes Δt_i, but in the limit $\Delta t_i \to 0$ the probability density function becomes ill defined, one reason being that the product of terms

$$\frac{1}{\sqrt{2\pi\sigma(x_i)^2 \Delta t_i}}$$

diverges to infinity. In order to nevertheless define a density for the continuous stochastic process X, ratios of probabilities of X lying within a small distance ε from smooth curves φ_1 and φ_2 are considered:[2]

$$\frac{P\left(|X_t - \varphi_1(t)| \leq \varepsilon \text{ for every } t \in [0,T]\right)}{P\left(|X_t - \varphi_2(t)| \leq \varepsilon \text{ for every } t \in [0,T]\right)} \to \exp\left(-\int_0^T L\left(\varphi_1(t), \dot{\varphi}_1(t)\right)\, dt + \int_0^T L\left(\varphi_2(t), \dot{\varphi}_2(t)\right)\, dt\right)$$

as $\varepsilon \to 0$, where L is the **Onsager–Machlup function**.

Definition [edit]

Consider a d-dimensional Riemannian manifold M and a diffusion process $X = \{X_t : 0 \leq t \leq T\}$ on M with infinitesimal generator $\frac{1}{2}\Delta_M + b$, where Δ_M is the Laplace–Beltrami operator and b is a vector field. For any two smooth curves $\varphi_1, \varphi_2 : [0, T] \to M$,

$$\lim_{\varepsilon \downarrow 0} \frac{P\left(\rho(X_t, \varphi_1(t)) \leq \varepsilon \text{ for every } t \in [0,T]\right)}{P\left(\rho(X_t, \varphi_2(t)) \leq \varepsilon \text{ for every } t \in [0,T]\right)} = \exp\left(-\int_0^T L\left(\varphi_1(t), \dot{\varphi}_1(t)\right)\, dt + \int_0^T L\left(\varphi_2(t), \dot{\varphi}_2(t)\right)\, dt\right)$$

where ρ is the Riemannian distance, $\dot{\varphi}_1, \dot{\varphi}_2$ denote the first derivatives of φ_1, φ_2, and L is called the **Onsager–Machlup function**.

The Onsager–Machlup function is given by[3][4][5]

$$L(x, v) = \tfrac{1}{2}\|v - b(x)\|_x^2 + \tfrac{1}{2}\operatorname{div} b(x) - \tfrac{1}{12}R(x),$$

where $\|\cdot\|_x$ is the Riemannian norm in the tangent space $T_x(M)$ at x, $\operatorname{div} b(x)$ is the divergence of b at x, and $R(x)$ is the scalar curvature at x.

Examples [edit]

The following examples give explicit expressions for the Onsager–Machlup function of a continuous stochastic processes.

Wiener process on the real line [edit]

The Onsager–Machlup function of a Wiener process on the real line **R** is given by[6]

$$L(x, v) = \tfrac{1}{2}|v|^2.$$

Diffusion processes with constant diffusion coefficient on Euclidean space [edit]

The Onsager–Machlup function in the one-dimensional case with constant diffusion coefficient σ is given by[7]

$$L(x, v) = \frac{1}{2}\left|\frac{v - b(x)}{\sigma}\right|^2 + \frac{1}{2}\frac{db}{dx}(x).$$

In the d-dimensional case, with σ equal to the unit matrix, it is given by[8]

$$L(x, v) = \frac{1}{2}\|v - b(x)\|^2 + \frac{1}{2}(\operatorname{div} b)(x),$$

where $\|\cdot\|$ is the Euclidean norm and

$$(\operatorname{div} b)(x) = \sum_{i=1}^d \frac{\partial}{\partial x_i} b_i(x).$$

Generalizations [edit]

Generalizations have been obtained by weakening the differentiability condition on the curve φ.[9] Rather than taking the maximum distance between the stochastic process and the curve over a time interval, other conditions have been considered such as distances based on completely convex norms[10] and Hölder, Besov and Sobolev type norms.[11]

Applications

The Onsager–Machlup function can be used for purposes of reweighting and sampling trajectories, as well as for determining the most probable trajectory of a diffusion process.

(C) Onsager Reciprocal Relation
(i) https://www.sciencedirect.com/topics/chemistry/onsager-reciprocal-relation
"Onsager reciprocal relations are relationship between cross-effect coefficients of the linear phenomenological law in continuum mechanics, as Onsager said: "a reciprocal relation that is not necessary for fulfilling the requirements of thermodynamics", and completely out of thermodynamics."

(ii) https://en.wikipedia.org/wiki/Onsager_reciprocal_relations
"In thermodynamics, the Onsager reciprocal relations express the equality of certain ratios between flows and forces in thermodynamic systems out of equilibrium, but where a notion of local equilibrium exists.

"Reciprocal relations" occur between different pairs of forces and flows in a variety of physical systems. For example, consider fluid systems described in terms of temperature, matter density, and pressure. In this class of systems, it is known that temperature differences lead to heat flows from the warmer to the colder parts of the system; similarly, pressure differences will lead to matter flow from high-pressure to low-pressure regions. What is remarkable is the observation that, when both pressure and temperature vary, temperature differences at constant pressure can cause matter flow (as in convection) and pressure differences at constant temperature can cause heat flow. Perhaps surprisingly, the heat flow per unit of pressure difference and the density (matter) flow per unit of temperature difference are equal. This equality was shown to be necessary by Lars Onsager using statistical mechanics as a consequence of the time reversibility of microscopic dynamics (microscopic reversibility). The theory developed by Onsager is much more general than this example and capable of treating more than two thermodynamic forces at once, with the limitation that "the principle of dynamical reversibility does not apply when (external) magnetic fields or Coriolis forces are present", in which case "the reciprocal relations break down".

Though the fluid system is perhaps described most intuitively, the high precision of electrical measurements makes experimental realizations of Onsager's reciprocity easier in systems involving electrical phenomena. In fact, Onsager's 1931 paper refers to thermoelectricity and transport phenomena in electrolytes as well known from the 19th century, including "quasi-thermodynamic" theories by Thomson and Helmholtz respectively. Onsager's reciprocity in the thermoelectric effect manifests itself in the equality of the Peltier (heat flow caused by a voltage difference) and Seebeck (electrical current caused by a temperature difference) coefficients of a thermoelectric material. Similarly, the so-called "direct piezoelectric" (electrical current produced by mechanical stress) and "reverse piezoelectric" (deformation produced by a voltage difference) coefficients are equal. For many kinetic systems, like the Boltzmann equation or chemical kinetics, the Onsager relations are closely connected to the principle of detailed balance and follow from them in the linear approximation near equilibrium.

Experimental verifications of the Onsager reciprocal relations were collected and analyzed by D. G. Miller for many classes of irreversible processes, namely for thermoelectricity, electrokinetics, transference in electrolytic solutions, diffusion, conduction of heat and electricity in anisotropic solids, thermomagnetism and galvanomagnetism. In this classical review, chemical reactions are considered as "cases with meager"

(微不足道的情况) and inconclusive evidence. Further theoretical analysis and experiments support the reciprocal relations for chemical kinetics with transport.

For his discovery of these reciprocal relations, Lars Onsager was awarded the 1968 Nobel Prize in Chemistry. The presentation speech referred to the three laws of thermodynamics and then added "It can be said that Onsager's reciprocal relations represent a further law ==making a thermodynamic study of irreversible processes possible==." Some authors have even described Onsager's relations as the "Fourth law of thermodynamics".

Example: Fluid system [edit]

The fundamental equation [edit]

The basic thermodynamic potential is internal energy. In a simple fluid system, neglecting the effects of viscosity the fundamental thermodynamic equation is written:

$$dU = T\,dS - P\,dV + \mu\,dM$$

where U is the internal energy, T is temperature, S is entropy, P is the hydrostatic pressure, V is the volume, μ is the chemical potential, and M mass. In terms of the internal energy density, u, entropy density s, and mass density ρ, the fundamental equation at fixed volume is written:

$$du = T\,ds + \mu\,d\rho$$

For non-fluid or more complex systems there will be a different collection of variables describing the work term, but the principle is the same. The above equation may be solved for the entropy density:

$$ds = (1/T)\,du + (-\mu/T)\,d\rho$$

The above expression of the first law in terms of entropy change defines the entropic conjugate variables of u and ρ, which are $1/T$ and $-\mu/T$ and are intensive quantities analogous to potential energies; their gradients are called thermodynamic forces as they cause flows of the corresponding extensive variables as expressed in the following equations.

The continuity equations [edit]

The conservation of mass is expressed locally by the fact that the flow of mass density ρ satisfies the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J}_\rho = 0,$$

where $\mathbf{J}_\rho$ is the mass flux vector. The formulation of energy conservation is generally not in the form of a continuity equation because it includes contributions both from the macroscopic mechanical energy of the fluid flow and of the microscopic internal energy. However, if we assume that the macroscopic velocity of the fluid is negligible, we obtain energy conservation in the following form:

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{J}_u = 0,$$

where u is the internal energy density and $\mathbf{J}_u$ is the internal energy flux.

Since we are interested in a general imperfect fluid, entropy is locally not conserved and its local evolution can be given in the form of entropy density s as

$$\frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_s = \frac{\partial s_c}{\partial t}$$

where $\frac{\partial s_c}{\partial t}$ is the rate of increase in entropy density due to the irreversible processes of equilibration occurring in the fluid and $\mathbf{J}_s$ is the entropy flux.

The phenomenological equations [edit]

In the absence of matter flows, Fourier's law is usually written:

$$\mathbf{J}_u = -k\,\nabla T;$$

where k is the thermal conductivity. However, this law is just a linear approximation, and holds only for the case where $\nabla T \ll T$, with the thermal conductivity possibly being a function of the thermodynamic state variables, but not their gradients or time rate of change. Assuming that this is the case, Fourier's law may just as well be written:

$$\mathbf{J}_u = kT^2\,\nabla(1/T);$$

In the absence of heat flows, Fick's law of diffusion is usually written:

$$\mathbf{J}_\rho = -D\,\nabla\rho,$$

where D is the coefficient of diffusion. Since this is also a linear approximation and since the chemical potential is monotonically increasing with density at a fixed temperature, Fick's law may just as well be written:

$$\mathbf{J}_\rho = D'\,\nabla(-\mu/T)$$

where, again, D' is a function of thermodynamic state parameters, but not their gradients or time rate of change. For the general case in which there are both mass and energy fluxes, the phenomenological equations may be written as:

$$\mathbf{J}_u = L_{uu}\,\nabla(1/T) + L_{u\rho}\,\nabla(-\mu/T)$$
$$\mathbf{J}_\rho = L_{\rho u}\,\nabla(1/T) + L_{\rho\rho}\,\nabla(-\mu/T)$$

or, more concisely,

$$\mathbf{J}_\alpha = \sum_\beta L_{\alpha\beta}\,\nabla f_\beta$$

where the entropic "thermodynamic forces" conjugate to the "displacements" u and ρ are $f_u = (1/T)$ and $f_\rho = (-\mu/T)$ and $L_{\alpha\beta}$ is the Onsager matrix of transport coefficients.

The rate of entropy production [edit]

From the fundamental equation, it follows that:

$$\frac{\partial s}{\partial t} = (1/T)\frac{\partial u}{\partial t} + (-\mu/T)\frac{\partial \rho}{\partial t}$$

and

$$\mathbf{J}_s = (1/T)\mathbf{J}_u + (-\mu/T)\mathbf{J}_\rho = \sum_\alpha \mathbf{J}_\alpha f_\alpha$$

Using the continuity equations, the rate of entropy production may now be written:

$$\frac{\partial s_c}{\partial t} = \mathbf{J}_u \cdot \nabla(1/T) + \mathbf{J}_\rho \cdot \nabla(-\mu/T) = \sum_\alpha \mathbf{J}_\alpha \cdot \nabla f_\alpha$$

and, incorporating the phenomenological equations:

$$\frac{\partial s_c}{\partial t} = \sum_\alpha \sum_\beta L_{\alpha\beta}(\nabla f_\alpha) \cdot (\nabla f_\beta)$$

It can be seen that, since the entropy production must be greater than zero, the Onsager matrix of phenomenological coefficients $L_{\alpha\beta}$ is a positive semi-definite matrix.

The Onsager reciprocal relations [edit]

Onsager's contribution was to demonstrate that not only is $L_{\alpha\beta}$ positive semi-definite, it is also symmetric, except in cases where time-reversal symmetry is broken. In other words, the cross-coefficients $L_{u\rho}$ and $L_{\rho u}$ are equal. The fact that they are at least proportional follows from simple dimensional analysis (*i.e.*, both coefficients are measured in the same units of temperature times mass density).

The rate of entropy production for the above simple example uses only two entropic forces, and a 2x2 Onsager phenomenological matrix. The expression for the linear approximation to the fluxes and the rate of entropy production can very often be expressed in an analogous way for many more general and complicated systems.

Abstract formulation [edit]

Let $x_1, x_2, \ldots, x_n$ denote fluctuations from equilibrium values in several thermodynamic quantities, and let $S(x_1, x_2, \ldots, x_n)$ be the entropy. Then, Boltzmann's entropy formula gives for the probability distribution function $w = A \exp(S/k)$, A=const, since the probability of a given set of fluctuations $x_1, x_2, \ldots, x_n$ is proportional to the number of microstates with that fluctuation. Assuming the fluctuations are small, the probability distribution function can be expressed through the second differential of the entropy[6]

$$w = \tilde{A}e^{-\frac{1}{2}\beta_{ik}x_i x_k} ; \qquad \beta_{ik} = \beta_{ki} = -\frac{1}{k}\frac{\partial^2 S}{\partial x_i \partial x_k},$$

where we are using Einstein summation convention and β_{ik} is a positive definite symmetric matrix.

Using the quasi-stationary equilibrium approximation, that is, assuming that the system is only slightly non-equilibrium, we have[6] $\dot{x}_i = -\lambda_{ik}x_k$

Suppose we define *thermodynamic conjugate* quantities as $X_i = -\frac{1}{k}\frac{\partial S}{\partial x_i}$, which can also be expressed as linear functions (for small fluctuations): $X_i = \beta_{ik}x_k$

Thus, we can write $\dot{x}_i = -\gamma_{ik}X_k$ where $\gamma_{ik} = \lambda_{il}\beta_{lk}^{-1}$ are called *kinetic coefficients*

The *principle of symmetry of kinetic coefficients* or the *Onsager's principle* states that γ is a symmetric matrix, that is $\gamma_{ik} = \gamma_{ki}$[6]

1.3 "Landau-Lifshitz fluctuating hydrodynamics"
(Landau--Lifshitz equations for fluctuating linearized hydrodynamics)

(B) See Above

1.2 Onsager Kinetic Coefficients

(A) Paper: Brownian motion and fluctuating hydrodynamics
(https://www.researchgate.net/publication/222595548_Brownian_motion_and_fluctuating_hydrodynamics)

Onsager and Machlup[2]) generalized the Langevin equation to serve as a basis for the discussion of linear fluctuation phenomena in nonequilibrium thermo-dynamics. This general theory was then applied to linear fluctuating hydrodynamics by Green and by Landau and Lifshitz[3]).

Note: Constitutive equation (本构关系)
https://en.wikipedia.org/wiki/Constitutive_equation

In physics and engineering, a **constitutive equation** or **constitutive relation** is a relation between two physical quantities (especially kinetic quantities as related to kinematic quantities) that is specific to a material or substance, and approximates the response of that material to external stimuli, usually as applied fields or forces. They are combined with other equations governing physical laws to solve physical problems; for example in fluid mechanics the flow of a fluid in a pipe, in solid state physics the response of a crystal to an electric field, or in structural analysis, the connection between applied stresses or forces to strains or deformations.

04/30/20
Paper (0) Dynamic density functional theory for microphase separation kinetics of block copolymer melts
1) "Random Phase Approximation"
2) "Local Coupling Approximation"
3) "Cahn-Hilliard Analysis"

05/02/20
1) "Delta operator": https://en.wikipedia.org/wiki/Delta_operator

In mathematics, a **delta operator** is a shift-equivariant linear operator $Q\colon \mathbb{K}[x] \longrightarrow \mathbb{K}[x]$ on the vector space of polynomials in a variable x over a field $\mathbb{K}$ that reduces degrees by one.

To say that Q is **shift-equivariant** means that if $g(x) = f(x + a)$, then

$$(Qg)(x) = (Qf)(x + a).$$

In other words, if f is a "**shift**" of g, then Qf is also a shift of Qg, and has the same "**shifting vector**" a.

To say that *an operator reduces degree by one* means that if f is a polynomial of degree n, then Qf is either a polynomial of degree $n - 1$, or, in case $n = 0$, Qf is 0.

Examples:
- The forward difference operator
$$(\Delta f)(x) = f(x + 1) - f(x)$$
is a delta operator.

- Differentiation with respect to *x*, written as *D*, is also a delta operator.
- Any operator of the form

$$\sum_{k=1}^{\infty} c_k D^k$$

(where $D^n(f) = f^{(n)}$ is the nth derivative) with $c_1 \neq 0$ is a delta operator. It can be shown that all delta operators can be written in this form. For example, the difference operator given above can be expanded as

$$\Delta = e^D - 1 = \sum_{k=1}^{\infty} \frac{D^k}{k!}.$$

- The generalized derivative of time scale calculus which unifies the forward difference operator with the derivative of standard calculus is a delta operator.
- In computer science and cybernetics, the term "discrete-time delta operator" (δ) is generally taken to mean a difference operator

$$(\delta f)(x) = \frac{f(x + \Delta t) - f(x)}{\Delta t},$$

the Euler approximation of the usual derivative with a discrete sample time Δt. The delta-formulation obtains a significant number of numerical advantages compared to the shift-operator at fast sampling.