Notes About Phase Space

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1.9 “Coarse-grained modeling”: Wiki (https://en.wikipedia.org/wiki/Coarse-grained_modeling)

Coarse-grained modeling

From Wikipedia, the free encyclopedia

Coarse-grained modeling, **coarse-grained models**, aim at simulating the behaviour of complex systems using their coarse-grained (simplified) representation. Coarse-grained models are widely used for molecular modeling of biomolecules[1][2] at various granularity levels. A wide range of coarse-grained models have been proposed. They are usually dedicated to computational modeling of specific molecules: proteins,[1][2] nucleic acids,[3][4] lipid membranes,[2][5] carbohydrates[6] or water.[7] In these models, molecules are represented not by individual atoms, but by "pseudo-atoms" approximating groups of atoms, such as whole amino acid residue. By decreasing the degrees of freedom much longer simulation times can be studied at the expense of molecular detail. Coarse-grained models have found practical applications in molecular dynamics simulations.[1]

The coarse-grained modeling originates from work by Michael Levitt and Ariel Warshel in 1970s.[8][9][10] Coarse-grained models are presently often used as components of multiscale modeling protocols in combination with reconstruction tools[11] (from coarse-grained to atomistic representation) and atomistic resolution models.[1] Atomistic resolution models alone are presently not efficient enough to handle large system sizes and simulation timescales.[1][2]

Software packages [edit]

- Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
- Extensible Simulation Package for Research on Soft Matter ESPReSo (external link)

1.10 “Configuration space (physics)”: Wiki (https://en.wikipedia.org/wiki/Configuration_space_(physics))

In classical mechanics, the parameters that define the configuration of a system are called *generalized coordinates*, and the vector space defined by these coordinates is called the **configuration space** of the physical system. It is often the case that these parameters satisfy mathematical constraints, such that the set of actual configurations of the system is a manifold in the space of generalized coordinates. This manifold is called the **configuration manifold** of the system.

Example: a particle in 3D space [edit]

The position of a single particle moving in ordinary Euclidean 3-space is defined by the vector $q = (x, y, z)$, and therefore its *configuration space* is $Q = \mathbb{R}^3$. It is conventional to use the symbol q for a point in configuration space; this is the convention in both the Hamiltonian formulation of classical mechanics, and in Lagrangian mechanics. The symbol p is used to denote momenta; the symbol $\dot{q} = dq/dt$ refers to velocities.

A particle might be constrained to move on a specific manifold. For example, if the particle is attached to a rigid linkage, free to swing about the origin, it is effectively constrained to lie on a sphere. Its configuration space is the subset of coordinates in $\mathbb{R}^3$ that define points on the sphere S^2. In this case, one says that the manifold Q is the sphere, *i.e.* $Q = S^2$.

For *n* disconnected, non-interacting point particles, the configuration space is $\mathbb{R}^{3n}$. In general, however, one is interested in the case where the particles interact: for example, they are specific locations in some assembly of gears, pulleys, rolling balls, *etc.* often constrained to move without slipping. In this case, the configuration space is not all of $\mathbb{R}^{3n}$, but the subspace (submanifold) of allowable positions that the points can take.

Formal definition [edit]

In classical mechanics, the configuration of a system consists of the positions had by all components subject to kinematical constraints.[2]

Phase space [edit]

The configuration space is insufficient to completely describe a mechanical system: it fails to take into account velocities. The set of velocities available to a system defines a plane tangent to the configuration manifold of the system. At a point $q \in Q$, that tangent plane is denoted by $T_q Q$. Momentum vectors are linear functionals of the tangent plane, known as cotangent vectors; for a point $q \in Q$, that cotangent plane is denoted by $T_q^* Q$. The set of positions and momenta of a mechanical system forms the cotangent bundle $T^* Q$ of the configuration manifold Q. This larger manifold is called the phase space of the system.

State space [edit]

In quantum mechanics, the analogous concept is called the state space. A rather different set of formalisms and notation are used in this case. The analog of a "point particle" becomes a single point in $\mathbb{CP}^1$, the complex projective line, also known as the Bloch sphere. It is complex, because a quantum-mechanical wave function has a complex phase; it is projective because the wave-function is normalized to unit probability. That is, given a wave-function ψ one is free to normalize it by the total probability $\int \psi^* \psi$, thus making it projective.

位形空间 [编辑]

维基百科，自由的百科全书

经典力学中，**位形空间**（或译**组态空间**）是一个物理系统可能处于的所有可能状态的空间，可以有外部约束。一个典型系统的位形空间具有流形的结构；因此，它也称为**位形流形**。

例如，运动在普通欧几里得空间中的单个粒子的位形空间就是$\mathbf{R}^3$。对于N个粒子的系统，组态空间就是$\mathbf{R}^{3N}$，或者说它的没有两个位置重叠的子空间。更一般地，可以将在一个流形M中运动的N个粒子的系统的位形空间看作函数空间 M^N。

要同时考虑位置和动量，就必须转到位形空间的余切丛中。这个更大的空间称为系统的相空间。简单说来，一个位形空间通常是一个相空间（参看拉格朗日分布）从函数空间构造的“一半”。

在量子力学中，路径积分表述强调了位形的历史。

位形空间也和辨理论相关，因为一条弦不穿过本身的条件可以表述为将函数空间的对角线切除。

1.11 “Phase space”: Wiki (https://en.wikipedia.org/wiki/Phase_space)

“*In dynamical system theory, a phase space is a space in which all possible states of a system are represented, with each possible state corresponding to one unique point in the phase space. For mechanical systems, the phase space usually consists of all possible values of **position** and **momentum** variables.*”

Thermodynamics and statistical mechanics [edit]

In thermodynamics and statistical mechanics contexts, the term phase space has two meanings: for one, it is used in the same sense as in classical mechanics. If a thermodynamic system consists of N particles, then a point in the $6N$-dimensional phase space describes the dynamic state of every particle in that system, as each particle is associated with three-position variables and three momentum variables. In this sense, as long as the particles are distinguishable, a point in phase space is said to be a microstate of the system. (For indistinguishable particles a microstate will consist of a set of $N!$ points, corresponding to all possible exchanges of the N particles.) N is typically on the order of Avogadro's number, thus describing the system at a microscopic level is often impractical. This leads to the use of phase space in a different sense.

The phase space can also refer to the space that is parameterized by the *macroscopic* states of the system, such as pressure, temperature, etc. For instance, one may view the pressure-volume diagram or entropy-temperature diagrams as describing part of this phase space. A point in this phase space is correspondingly called a macrostate. There may easily be more than one microstate with the same macrostate. For example, for a fixed temperature, the system could have many dynamic configurations at the microscopic level. When used in this sense, a phase is a region of phase space where the system in question is in, for example, the liquid phase, or solid phase, etc.

Since there are many more microstates than macrostates, the phase space in the first sense is usually a manifold of much larger dimensions than in the second sense. Clearly, many more parameters are required to register every detail of the system down to the molecular or atomic scale than to simply specify, say, the temperature or the pressure of the system.

Phase integral [edit]

In classical statistical mechanics (continuous energies) the concept of phase space provides a classical analog to the partition function (sum over states) known as the phase integral.[4] Instead of summing the Boltzmann factor over discretely spaced energy states (defined by appropriate integer quantum numbers for each degree of freedom) one may integrate over continuous phase space. Such integration essentially consists of two parts: integration of the momentum component of all degrees of freedom (momentum space) and integration of the position component of all degrees of freedom (configuration space). Once the phase integral is known, it may be related to the classical partition function by multiplication of a normalization constant representing the number of quantum energy states per unit phase space. This normalization constant is simply the inverse of Planck's constant raised to a power equal to the number of degrees of freedom for the system.[5]