Large Deviations and Statistical Inference in Phased Materials

Dalton A R Sakthivadivel

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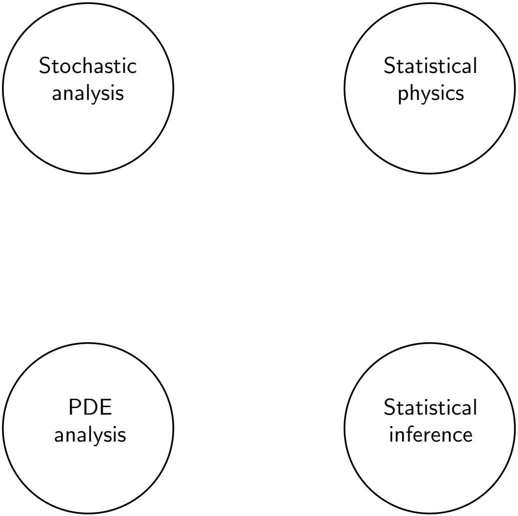
Stony Brook University

A diagram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Statistical physics
PDE analysis
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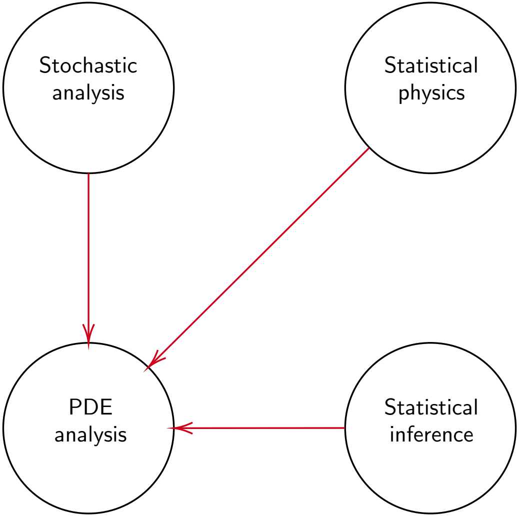
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Phases (sketch)

In physics, a *phase* is a region of state space with distinct qualitative behaviour

Usually determined via symmetry: the *disordered phase* has a global symmetry under a representation of some Lie group (transformations are 'idempotent' in the face of disorder), whilst the *ordered phase* breaks this symmetry (transformations destroy order)

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Phases (motivation: Ising model)

Consider a family of random variables $\{X_i\}_{i\in[1:N^2]}$ valued in $\{-1,1\}$, and a joint random variable $X = |X_1X_2X_3\dots X_{N^2}\rangle$

Suppose X satisfies a stochastic differential equation with a parameter T

Moreover, suppose T controls the variance of the joint probability measure. In particular, for $0 \leq T < 1$, $P(x)$ concentrates around the *ground state* $|(-1)(-1)(-1)\dots(-1)\rangle$

In physics this is called an *Ising model*. Here X_i is a *spin state*, X is a *field configuration*, and T is *temperature*

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Arrange X on a two-dimensional lattice with N vertices in each direction

The probability measure for X is given by

$$P(X = x) \propto e^{-\frac{1}{T}E(x)}$$

where $E(x) = -\sum_{ij} x_i x_j$

Notice that the quantity $E(x)$ is invariant under a $\mathbb{Z}_2$ action

However, the state x itself is not. Example:
$|(-1)(-1)(-1)\ldots(-1)\rangle \mapsto |111\ldots1\rangle$ (ground state degeneracy)

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Under a global rotation of the ground state, m goes from -1 to 1

So the physics changes, even though the energy level doesn't

Ground state degeneracy = 'spontaneously broken symmetry'

There exists an ordered phase ($m = -1$ or $m = 1$) and a disordered phase ($m \in (-1, 1)$)

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Generalised phases

Not all systems have macroscopic properties based on SSB or order-disorder transitions

Examples: set-points in control systems, turbulence in fluid flows, patterns in reaction-diffusion systems, hurricane formation in the atmosphere... and so forth

However, these are still systems with distinct behaviours dependent on some parameter

How can we generalise the idea of a phase to cover the physics of control and pattern formation?

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Generalised phases

Notice that

(i) the low-T regime of the Ising model is a point attractor

(ii) when T is large, the probability of the system being in the ground state is low

$\therefore$ The quantity T controls the behaviour of the system near an attractor

This suggests the Ising model is well-approximated by fluctuations in a lower dimensional, parametric system

Generalised phases

How do we carve up the state space into distinct regions whose *occupation probability* depends on some parameter? Under what conditions do those regions correspond to *patterns*?

We want the following:

(i) When $0 \leq T < 1$, $m = -1$ or $m = 1$, satisfying $\arg\min E(x)$

(ii) When $T > 1$, m fluctuates with probability $P(m)$, where $P(m = -1)$ is small

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SPDEs

Ansatz: X can be described by the SPDE

$$\partial_T x(T) = -\partial_x E(x) + \sqrt{T}\xi$$

Fix a ground state. Taking fluctuations $\sqrt{T}\xi$ as $(x - m)$, we have

(i) a system which fluctuates away from an attractor with magnitude proportional to T

(ii) a stochastic Allen-Cahn equation (a 'model A system')

(iii) Glauber-like dynamics for the Ising model (Hohenberg and Halperin 1977, Rev Mod Phys)

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Main results

Our main result is that dynamics near a *normally hyperbolic slow manifold* lie in the model A universality class, describing phased materials with well-defined effective descriptions

In this way it is possible to define a notion of a phase that has nothing to do with a system's symmetries

This canonical form is a simple stochastic (partial) differential equation derived partially from a large deviations principle for fluctuations near a slow manifold

Why is this interesting? Extends the theory of 'patterns' to very general dynamics (~~conjecture~~ total speculation to follow)

Main results

Suppose a slow manifold $(x, h(x))$ exists, such that $\partial_t u = f(x, h(x))$ for small u.

Let $f(x, h(x))$ satisfy the Euler-Lagrange equation for some quantity F

Suppose also that fluctuations in u are fast (*i.e.*, $u - (x, h)$ has timescale $\varepsilon^{-1} t$)

Incorporate a correction term to $\partial_t u$ which keeps track of fluctuations off of $(x, h(x))$

Main results

The following expansion of the flow near the slow manifold holds for arbitrary large u and $\nu > 0$:

$$\partial_t u = f(x, h(x)) + (u - (x, h(x))))$$

Adiabatic theorem $\implies$ fast variables behave like noise

We obtain $\partial_t u(t) = f(x(t), h(x(t)) + \nu\xi$

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Main results

Let c_ν be a divergent ν-dependent constant (*i.e.*, for which $c_\nu \to \infty$ when $\nu \to 0$)

The flow obeys a large deviations principle with rate function F where $f = \delta F / \delta u$

Instanton solution is slow manifold

In L^2, stationary measure (if it exists) is

$$p(u) \propto \exp\{-c_\nu F(u)\}.$$

Example:

$$p(u) \propto \exp\left\{-\frac{1}{T} E(u)\right\}$$

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Since $h(x)$ minimises F, a more general expression is obtainable:

$$\begin{aligned}\partial_t u(t) &= c_\nu \nabla F(u(t)) + \nu\xi \\ &= -\nabla \log p(u(t)) + \nu\xi\end{aligned}$$

$\Longrightarrow$ if we don't know F, we can just infer $p(u(t))$

Total speculation

Patterns in fluid flow are sometimes described using space-dependent attractor-repellor configurations called Lagrangian coherent structures (see *e.g.* Lekien, Shadden, Marsden, 2007, J Math Phys; Haller 2015, Ann Rev Fluid Mech)

Is there a straightforward generalisation of this result that provides a description of dynamics with low-dimensional space-dependent patterns?

Total speculation

Suppose we have an A-model for $h(x)$ coupled to the fluctuations near a disjoint slow manifold $k(x)$

This describes an LCS where the flow off of one slow manifold enters the neighbourhood of another

This introduces interaction terms, which are usually challenging

For simple equations, one may be more optimistic... however, in the general case, not much hope *a priori* of doing this rigorously

Dimension reduction; Bayesian inference of order parameters

Because slow manifolds are difficult to describe analytically, a question naturally arises: is there an alternative road to producing slow manifolds?

We are now asking about the inference of low-dimensional descriptions of a system (*i.e.*, of an order parameter)

So is there an algorithm that carves a dynamical system into slow and fast subsystems?

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Dimension reduction; Bayesian inference of order parameters

One approach to this lies in the study of structure vs function in neural networks

Dynamic causal modelling infers the coupling constants between different subsystems of a random dynamical system for purposes of causal inference (Friston, Li, Daunizeau, Stephan, 2011, NeuroImage)

Weak or sparse coupling approximation leads to the spontaneous identification of order parameters in a network of oscillators

DCM / LCS

Known to carve up signals from networks of neural cells into slow dynamics and fluctuations / stable and unstable phases. Example: epilepsy (Jafarian et al, 2021, NeuroImage)

Likely a useful tool in understanding systems like LCSs numerically

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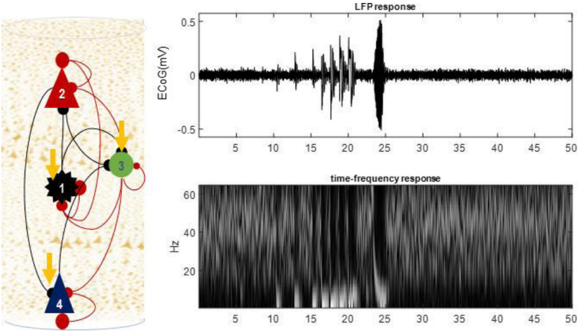

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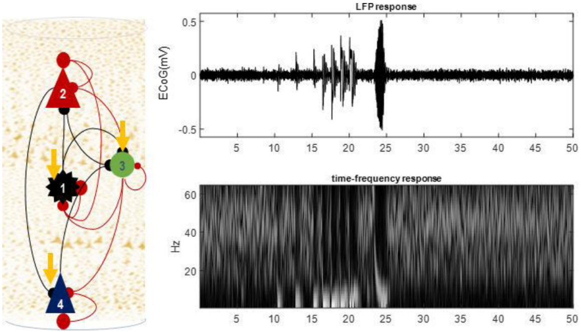

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Concluding remarks

- We can understand phases as low-dimensional descriptions of a system (patterns) in distinct areas of phase space
- We can understand a system spreading out in its state space (instability) as a disordered, high-noise phase
- Generalisations to more complex systems may exist
- Tools already designed for problems in this universality class exist, and will likely be useful in numerical analysis of such systems