LaVA MEETING @ECT*

23/02/2023

Algorithms (2)

presented by

Francesco Di Renzo (University of Parma & INFN)

DISCLAIMER this will not look like a (piece of) syllabus, nor I will present a talk (lecture)

I will be alluding to both…

This is intended to provide material for a couple (maybe more) of videos within the structure sketched by Mike. There are quite a number of ties to other sections (not a problem).

Algorithms, Physics and Computational Strategies

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Having discussed autocorrelation and integrated autocorrelation time, a natural question arises: are there cases in which

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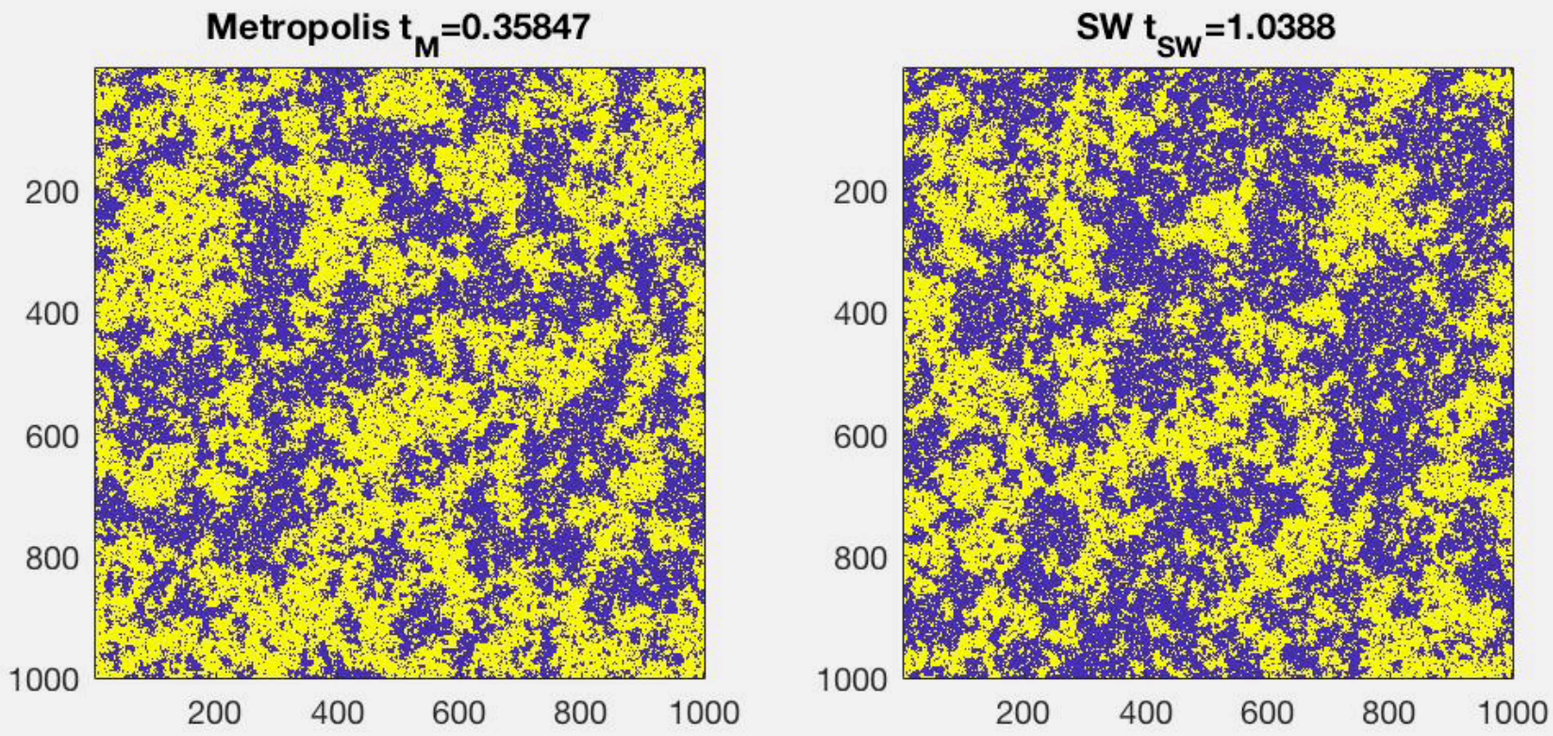
$$\tau_{int} \to \infty \quad ?$$

Ising 2d (h=0)

YES! … and for very good reasons!



II order phase transitions ... relevant picture is correlation over all length scales ... local VS global algorithms ...

This is an example of a VIRTUOUS LOOP gluing everything together

SIGN PROBLEMS: the tough problem par excellence

$$Z(\beta,\mu) = \int [D\phi]\, \mathrm{e}^{-\beta\, S[\phi] + i\mu\, Q[\phi]}$$

… i.e. living without a probability distribution …

… and we know that $\quad \left\langle \mathrm{e}^{i\mu\, Q} \right\rangle = \dfrac{Z(\beta,\mu)}{Z(\beta,0)} = \mathrm{e}^{-V\, \Delta F}$

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Any possible VIRTUOUS LOOP like before?

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Meron-Cluster Solution of Fermion Sign Problems

Shailesh Chandrasekharan[†] and Uwe-Jens Wiese[‡]
[†] *Department of Physics, Box 90305, Duke University, Durham, NC 27708, U.S.A.*
[‡] *Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.*
(February 10, 1999)

We present a general strategy to solve the notorious fermion sign problem using cluster algorithms. The method applies to various systems in the Hubbard model family as well as to relativistic fermions. Here it is illustrated for non-relativistic lattice fermions. A configuration of fermion world-lines is decomposed into clusters that contribute independently to the fermion permutation sign. A cluster whose flip changes the sign is referred to as a meron. Configurations containing meron-clusters contribute 0 to the path integral, while all other configurations contribute 1. The cluster representation describes the partition function as a gas of clusters in the zero-meron sector.

The QCD phase diagram according to the center group

Ydalia Delgado Mercado[a], Hans Gerd Evertz[b], Christof Gattringer[a]
[a] *Institut für Physik, Karl-Franzens Universität, Graz, Austria*
[b] *Institute for Theoretical and Computational Physics, Technische Universität Graz, Austria*

We study an effective theory for QCD at finite temperature and density which contains the leading center symmetric and center symmetry breaking terms. The effective theory is studied in a flux representation where the complex phase problem is absent and the model becomes accessible to Monte Carlo techniques also at finite chemical potential. We simulate the system using a generalized Prokof'ev-Svistunov worm algorithm and compare the results to a low temperature expansion. The phase diagram is determined as a function of temperature, chemical potential and quark mass. Shape and quark mass dependence of the phase boundaries are as expected for QCD. The transition into the deconfined phase is smooth throughout, without any discontinuities or critical points.

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Still, you will see quite a number approaches to taming/evading/mitigating the SIGN PROBLEM and they can (to a certain extent) enable (finite density QCD) computations!

- Density of states
- Lefschetz Thimbles / holomorphic flow / sign-optimised manifolds
- complex Langevin
- tensor networks

- Imaginary chemical potential simulations
- Taylor expansions at zero chemical potential

… with (analytic) continuation, (various) summation schemes needed (with Padè coming back to popularity…)

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What's going on with thimbles …

Suppose you want to compute the *functional integral* $\frac{1}{Z}\int_{-\infty}^{\infty} \mathrm{d}x\, O(x)\, e^{-S(x)}$

with the *action* $S(x) = \mu\, x^2 + \lambda\, x^4 \qquad \mu, \lambda \in \mathbb{C} \qquad S = S_R + S_I$

On the real axis the action is in general COMPLEX. Try to change the integration domain, going to the COMPLEX PLANE

$$x \quad \rightarrow \quad z = x + iy$$

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along which (because of Cauchy Riemann) $\begin{cases} \dot{S}_I = 0 \\ \dot{S}_R \geq 0 \end{cases}$ … PERFECT!

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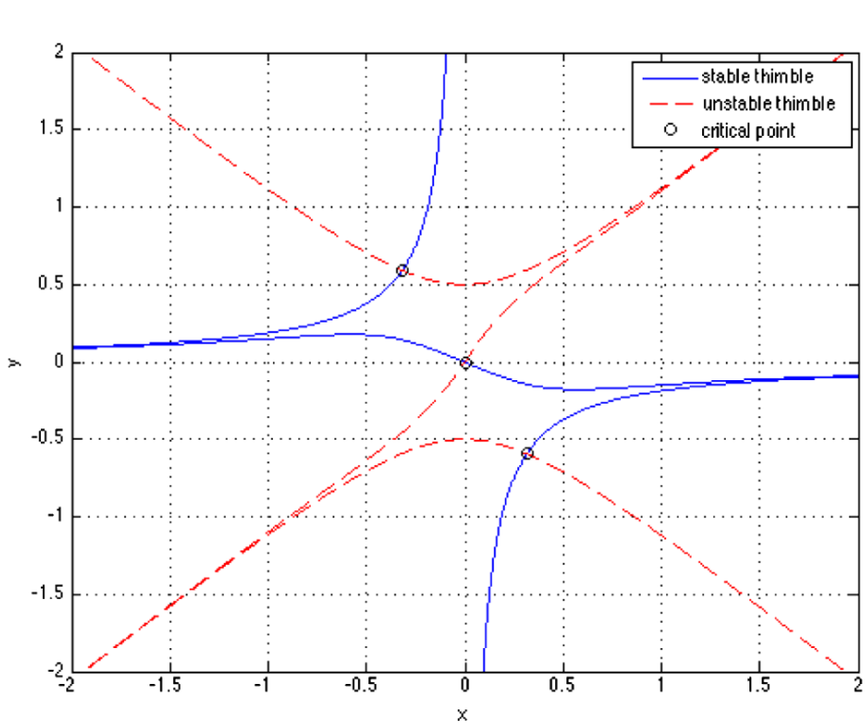
In particular, let's take the ones which (at infinite time!) go through critical points

$$\partial_x S_R|_{z_c} = \partial_y S_R|_{z_c} = 0$$

For a given choice of parameter …



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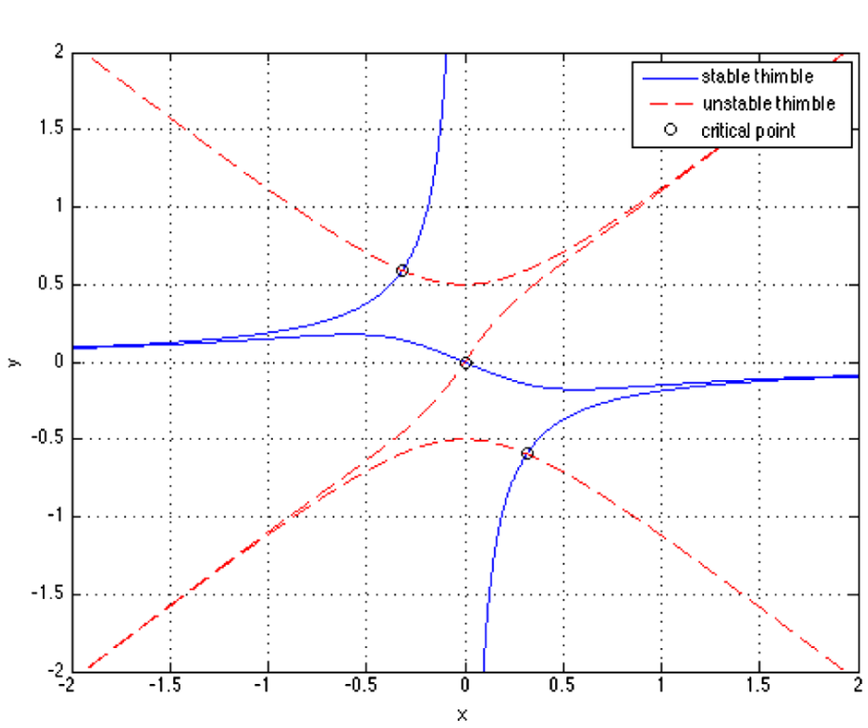

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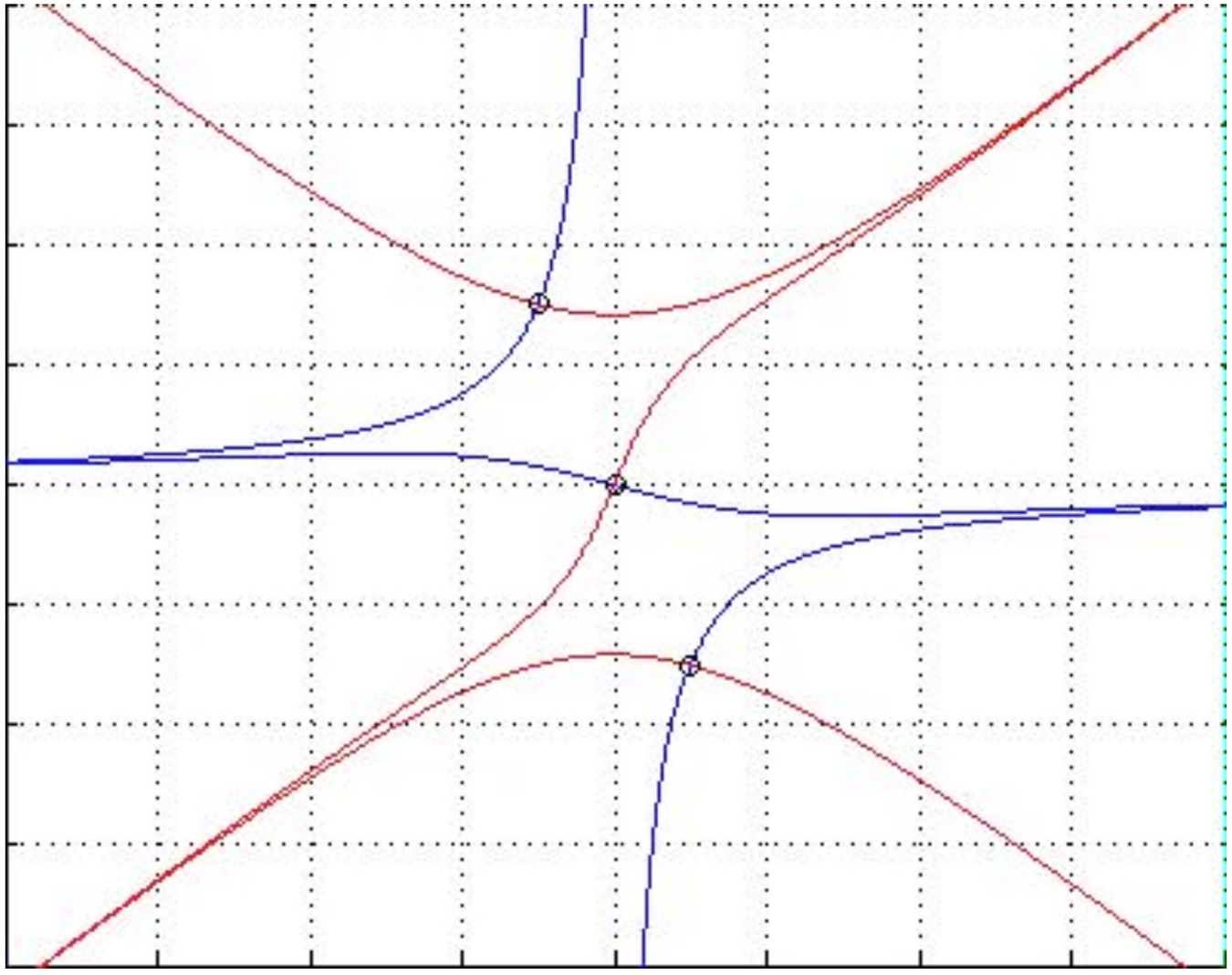
Perfect …There is a very good reason: thimbles always provide a BASIS to decompose any contour!

The SIGN PROBLEM is always nasty…

There are different decompositions as you move in parameter space!



Yust to mention one tricky point…

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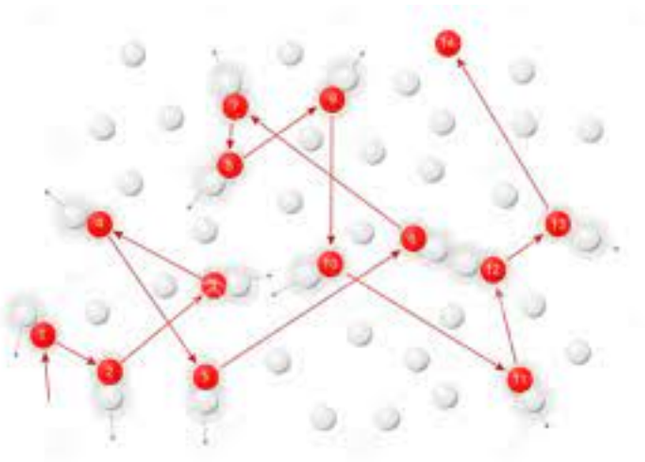

Brownian motion (BM)

$$m\frac{d}{dt}\vec{v}(t) = -\alpha\,\vec{v}(t) + \vec{\eta}(t) \qquad \langle \eta_i(t) \rangle = 0$$

$$\langle \eta_i(t)\,\eta_k(t') \rangle = 2\,\lambda\,\delta_{ik}\,\delta(t-t')$$

$$\langle\, f(v(t))\,\rangle = \int dv\, f(v)\, P(v,t)$$ with (… solution of Fokker Planck eqn …) $$P^{eq} \sim \mathrm{e}^{-\frac{m\alpha v^2}{2\lambda}}$$

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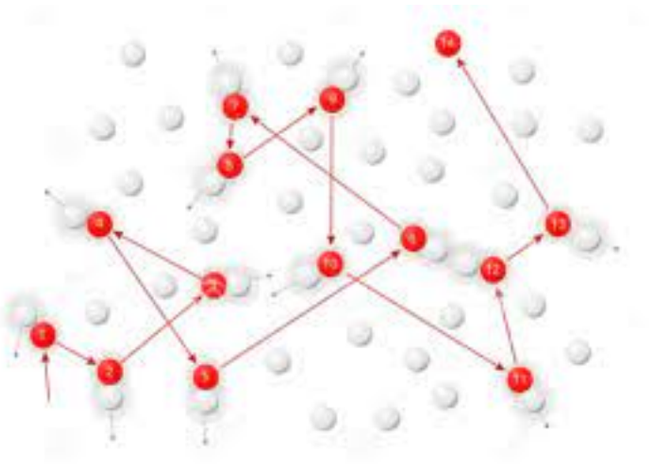

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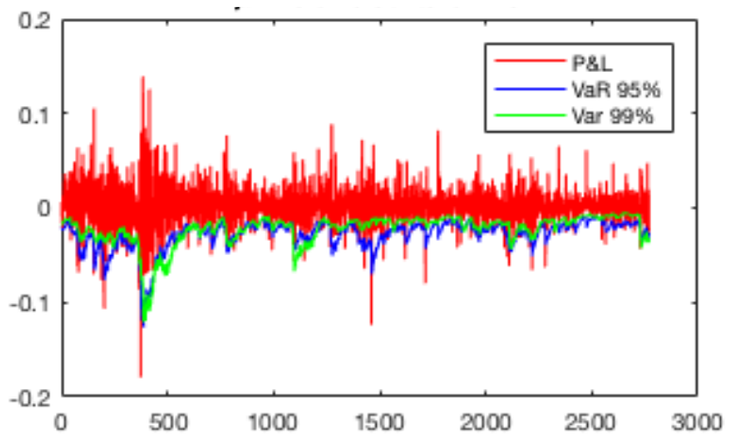
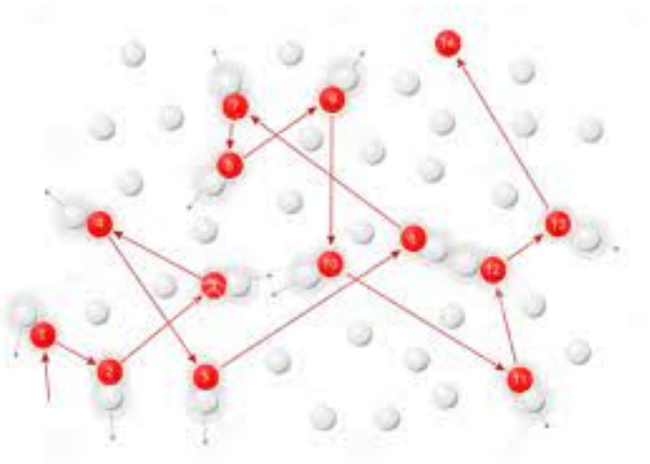
Quite interestingly … (FINANCE) returns (log price change of a security) undergo BM…



The main goal is to reliably estimate the Value at Risk (VaR)

Langevin algorithms, in a sense Simon's simulations/computations issue



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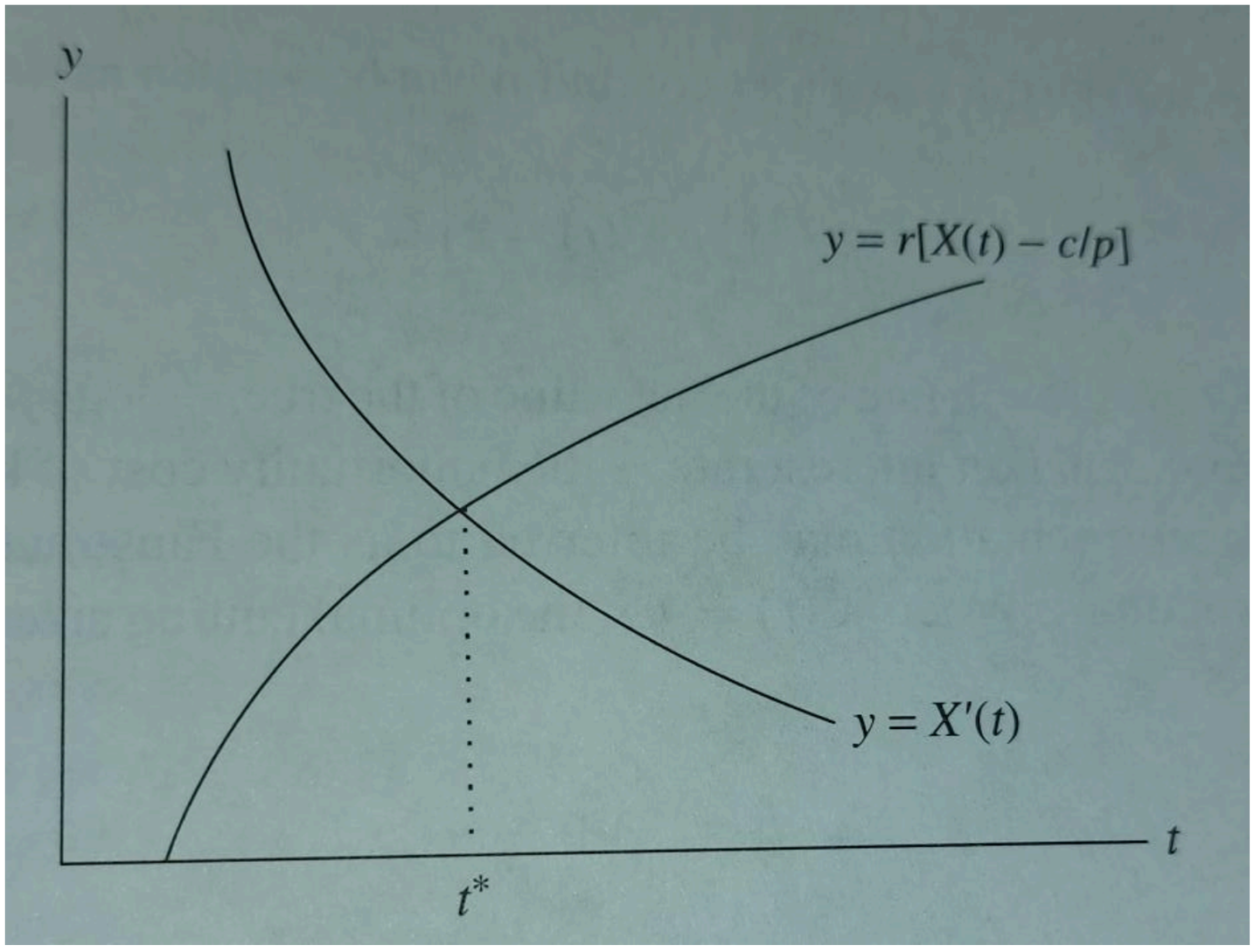
Perhaps less known, but maybe more interestingly, another example of "non-Physics Langevin" is the TREE CUTTING PROBLEM

i.e. When is the best time to cut a tree so that its net present value is maximised?

$$\max_t \left[\, \mathrm{e}^{-rt}\,[\,p\,X(t) - c\,]\right]$$

X(T) the *size* of your tree
p the *price* at which you sell it - *c* the *cost* of cutting
r>0 the rate of *interest* the bank pays to you

$$\max_t \left[\mathrm{e}^{-rt} \left[p\,X(t) - c \right] \right]$$ with first order condition $$X'(t) = r\left[X(t) - c/p \right]$$



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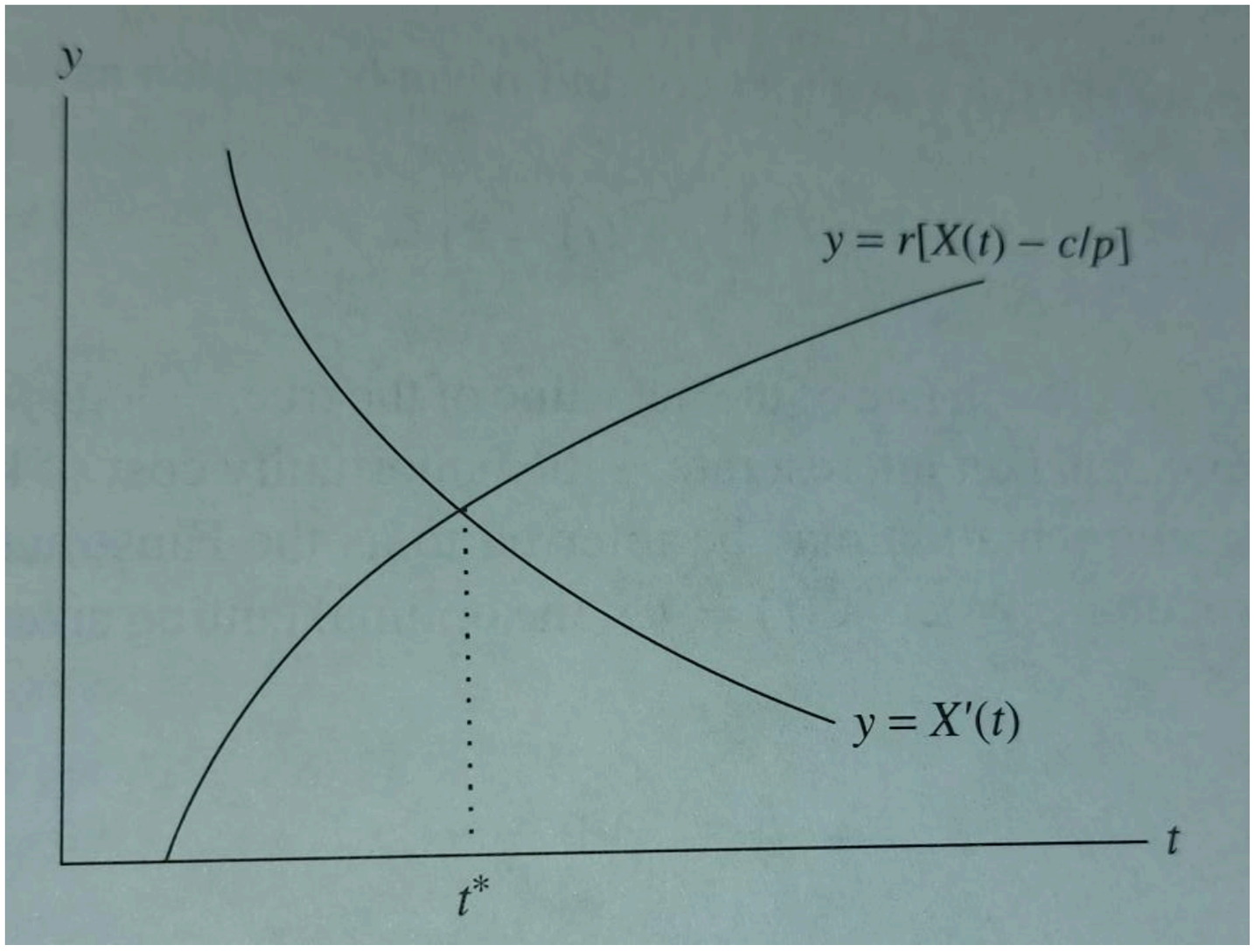

but growth is subject to "noise" … so … $$dX(t) = f(t)\,dt + \sigma dz$$

Langevin and Stochastic Quantisation

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$$\langle O[\phi]\rangle = \frac{\int D\phi\ O[\phi]\ e^{-S[\phi]}}{\int D\phi\ e^{-S[\phi]}} \qquad \phi(x) \mapsto \phi_\eta(x;t)$$

You have a field theory and you add a degree of freedom

This is a fictitious time in which Langevin evolution takes place

$$\frac{d\phi_\eta(x;t)}{dt} = -\frac{\partial S[\phi]}{\partial \phi_\eta(x;t)} + \eta(x;t)$$

Natural expectation values are now wrt the random (gaussian) noise

$$\langle \eta(x,t)\ \eta(x',t')\rangle_\eta = 2\,\delta(x-x')\,\delta(t-t') \qquad \langle \dots \rangle_\eta = \frac{\int D\eta(z,\tau)\ \dots\ e^{-\frac{1}{4}\int dzd\tau\eta^2(z,\tau)}}{\int D\eta(z,\tau)\, e^{-\frac{1}{4}\int dzd\tau\eta^2(z,\tau)}}$$

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Main assertion is

$$\langle O[\phi_\eta(x_1;t)\dots\phi_\eta(x_n;t)]\rangle_\eta \to_{t\to\infty} \langle O[\phi(x_1)\dots\phi(x_n)]\rangle$$

A proof can go through the definition of a time-dependent probability distribution of the fields

$$\langle O[\phi_\eta(t)]\rangle_\eta = \frac{\int D\eta\, O[\phi_\eta(t)]\, e^{-\frac{1}{4}\int dzd\tau\eta^2(z,\tau)}}{\int D\eta\, e^{-\frac{1}{4}\int dzd\tau\eta^2(z,\tau)}} = \int D\phi\ O[\phi]\, P[\phi,t]$$

for which we can derive

$$\dot{P}[\phi,t] = \int dx\ \frac{\delta}{\delta\phi(x)}\left(\frac{\delta S[\phi]}{\delta\phi(x)} + \frac{\delta}{\delta\phi(x)}\right) P[\phi,t]$$

the Fokker Planck equation

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$$\lim_{t\to\infty} P[\phi,t] \equiv P^{eq}[\phi] = \frac{e^{-S}}{\int D\phi \exp -S}$$

A first interesting feature: you can go for complex actions!

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When the action is complex, Langevin equations amounts to complexifying the degrees of freedom

$$\partial_\tau x = -\mathrm{Re}\left.\frac{\partial S(z)}{\partial z}\right|_{z=x+iy} + \eta_\tau,$$

$$\partial_\tau y = -\mathrm{Im}\left.\frac{\partial S(z)}{\partial z}\right|_{z=x+iy}$$

This amounts to averaging on a manifold which is different from the original one, but does not mean we are doubling the number of degrees of freedom

A first interesting feature: you can go for complex actions!

When the action is complex, Langevin equations amounts to complexifying the degrees of freedom

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The probability distribution of the fields in time now reads $\langle O\rangle_{P(t)} = \int dxdyP(x,y,t)O(x+iy)$

What we are mostly interested in reads

$$\langle O\rangle_\rho = \int dxO(x)\rho(x) = \lim_{t\to\infty}\langle O\rangle_{\rho(t)} = \lim_{t\to\infty}\int dxO(x)\rho(x,t)$$

The strategy of the proof is formally the same, i.e. going through Fokker Planck. In exponential notation this reads $\rho(x,t) = \exp(L_c^T)\rho_0(x)$

A formal argument for correctness is still there, even if care is needed because we can not rule out convergence to a wrong result, but there are progress (at least) in the direction of spotting an incorrect convergence.

A second interesting feature: prototype of Numerical Stochastic Perturbation Theory

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Since we now formally have a continuous stochastic process, we can think the Langevin equation solution as a function of the coupling constant of the theory and write a formal expansion

$$\phi_\eta(x,t) = \phi_\eta^{(0)}(x,t) + \sum_{n>0} g^n \phi_\eta^{(n)}(x,t)$$

which we now have to plug into our Langevin equation

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The result is a hierarchy of equations of increasing order, which we can exactly truncate at any given one

Perturbative orders for a given observable come almost from free: take the appropriate order when averaging over the evolution of the resulting process

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Langevin was the prototype, but one can also play the same game with other stochastic processes, i.e.

- Hybrid Molecular Dynamics
- Kramer equation

The main advantage is that you can reach much higher orders than you could afford in a standard, diagrammatic computation. (Remember: the computer is integrating the system for you)