Lecture Notes on Hydrometeorology
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Simple physical principles for complex systems

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Common misconceptions about physics—and their remedies

- Misconceptions:
  - Laws of complex physical systems can be inferred by synthesizing detailed representations of their elements (the reductionism approach).
  - Physical laws are mathematically expressed only by equations.
  - Physical laws are deterministic and mechanistic.
- Remedies:
  - The principle of parsimony.
  - Variational principles and the extremization approach.
  - Recognition of the fundamental character of uncertainty and use of stochastic approaches.

What is the principle of parsimony?

- A principle that advises us to prefer the simplest theory among those that fit the data equally well.
- Alternative names: **principle of parsimony**, **principle of simplicity**, **principle of economy**, **Ockham's razor**.
- Example of a parsimonious natural law:
  - Dogs bark.
- Examples of non-parsimonious laws:
  - Black, white and spotted dogs bark.
  - Dogs bark on Mondays, Wednesdays and Fridays.
- Intuitively, the above law does not exclude that a particular dog is mute.
  - We should not understand it as "there is no dog that does not bark".
- In other words, laws of complex systems (e.g. the biological system "dog") are necessarily probabilistic in nature:
  - "Dogs bark" means "any dog is very likely to bark".

Failure to recognize the probabilistic character of parsimony in complex systems may create confusion (see e.g. Courtney and Courtney, 2008, and the "all crows are black" example).

Parsimony: historical reference

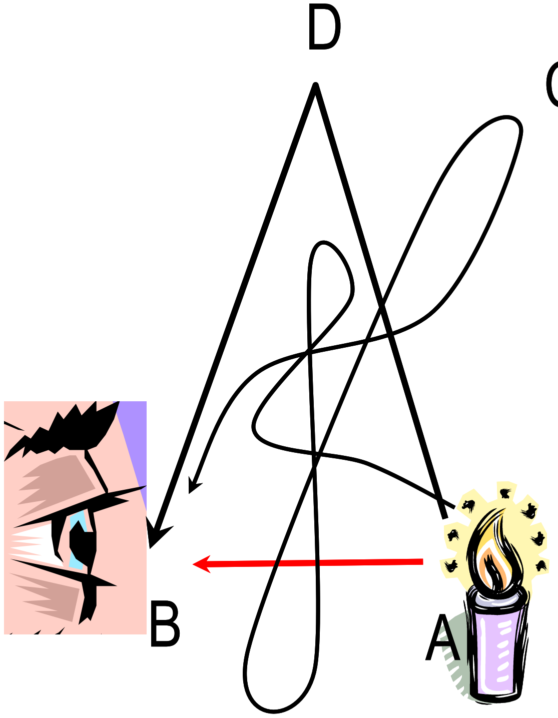
- Aristotle (384–322 BC):
  - [Αναλυτικά Ύστερα, I, 25] “*Ἔστω γὰρ αὕτη ἡ ἀπόδειξις βελτίων τῶν ἄλλων τῶν αὐτῶν ὑπαρχόντων, ἡ ἐξ ἐλαττόνων αἰτημάτων ἢ υποθέσεων ἢ προτάσεων.*”
  - [Posterior Analytics, I, 25] “*We may assume the superiority, other things being equal, of the demonstration which derives from fewer postulates or hypotheses or propositions.*”

    [Περί Ουρανού, III, 4] “*Φανερὸν ὅτι μακρῷ βέλτιον πεπερασμένας ποιεῖν τὰς ἀρχὰς, καὶ ταύτας ὡς ἐλαχίστας πάντων γε τῶν αὐτῶν μελλόντων δείκνυσθαι, καθάπερ ἀξιοῦσι καὶ οἱ ἐν τοῖς μαθήμασιν.*”
  - [On the Heavens, III, 4] “*Obviously, it is much better to assume a finite number of principles, as few as possible yet sufficient to prove what has to be proved, like in what mathematicians demand.*”
- Medieval philosophers: Robert Grosseteste (c. 1168-1253), Thomas Aquinas (c. 1225-1274), William of Ockham (c. 1285-1347; “*Plurality is not to be posited without necessity*”).
- Nicolaus Copernicus (1473-1543), Galileo Galilei (1564-1642), Isaac Newton (1642-1727)—all used parsimony in developing their theories.
- Albert Einstein’s formulation of parsimony: “*Everything should be made as simple as possible, but not simpler*”.

For more information on history and philosophy of parsimony and the scientific method, see Gauch (2003).

Is the principle of parsimony epistemological or ontological?

- Ockham put parsimony as an epistemological principle for choosing the best theory.
- However, earlier philosophers, from Aristotle to Grosseteste had interpreted parsimony also as an ontological principle, thus expecting Nature to be simple.
- A simple example can help us to see the ontological basis of the principle: Light follows the simplest path from A to B (the red line) and not other more complex ones (e.g. the black lines ACB, ADB)?
- But what does "**simplest**" mean?



Were Nature not parsimonious (e.g. were paths ACB, ADB materialized) it would be difficult to understand her and life would be hard.

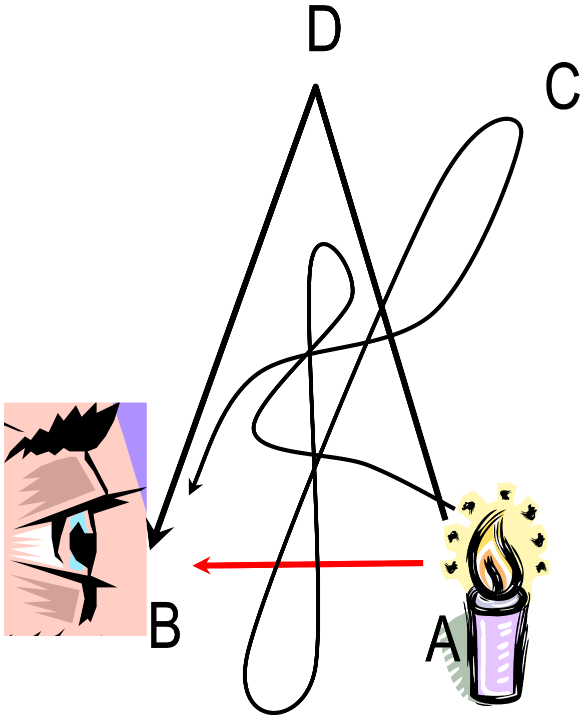
Quantification of simplicity

- The traditional approach to physics is based on writing equations, which express conservation laws; these govern the following quantities only:
  - Mass (scalar equation);
  - Linear momentum (vector equation);
  - Angular momentum (vector equation);
  - Energy (scalar equation);
  - Electric charge (scalar equation).
- However, to find states or paths which are "**as simple as possible**", it seems more natural to formulate the problem in terms of optimization rather that using equations.
- Mathematically, extremizing is much more powerful than equating:
  - A system of equations "$\boldsymbol{g}(\boldsymbol{s}) = \mathbf{0}$" can work if the number of equations equals the number of unknowns.
  - A single extremizing expression like "maximize $f(\boldsymbol{s})$" can work irrespective of the number of unknowns (it is equivalent to as many equations as needed).

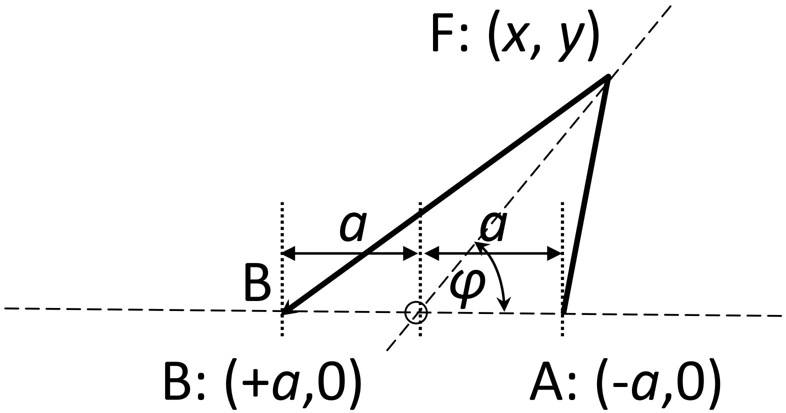
Nature is an **extremizer**—not an **equalizer.**

The simplicity of light trajectory: Attempt 1

- Light follows the shortest possible path from A to B.
  - A parsimonious law for a parsimonious natural behaviour.
  - Further investigation will show that it is not correct (formulation simpler than “as simple as possible”).



The light trajectory: Quantification for attempt 1

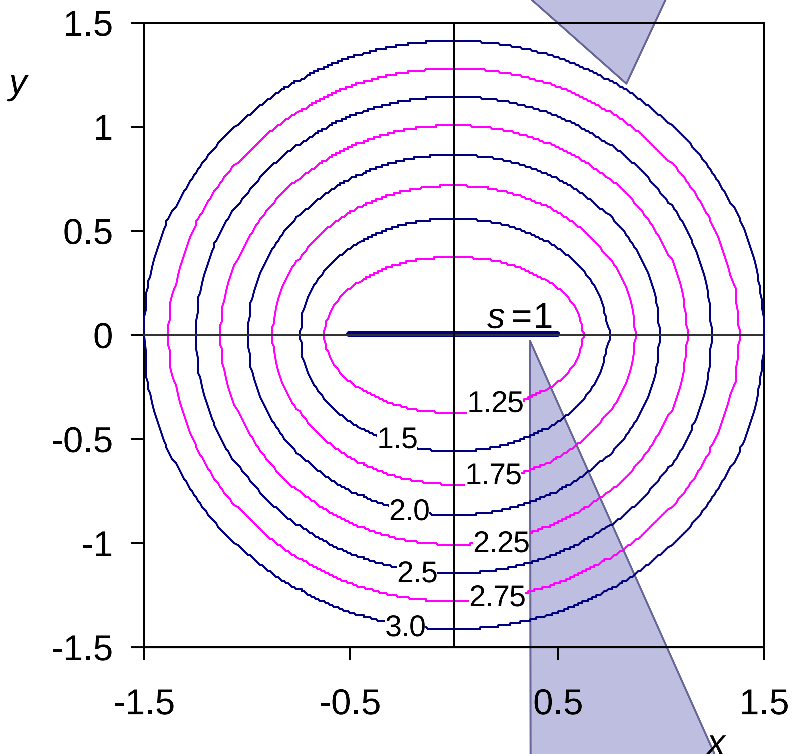


- Assume that light can travel from A to B along a broken line with a break point F with coordinates (x, y).
  This is not restrictive: we can add a second, third, … break point (homework).
- The travel distance is $s(x, y)$ = AF + FB, where:

$$\mathrm{AF} = \sqrt{(x-a)^2 + y^2}$$

$$\mathrm{FB} = \sqrt{(x+a)^2 + y^2}$$

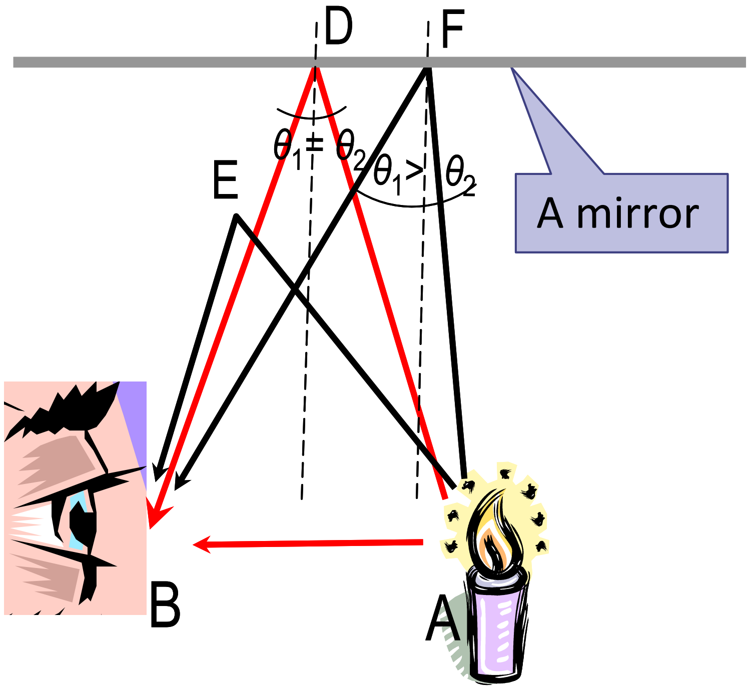
Contours of the distance $s(x, y)$ assuming $a = 0.5$



Line of minimum distance $s(x, y) = 1$
Infinite points F essentially describing the same path

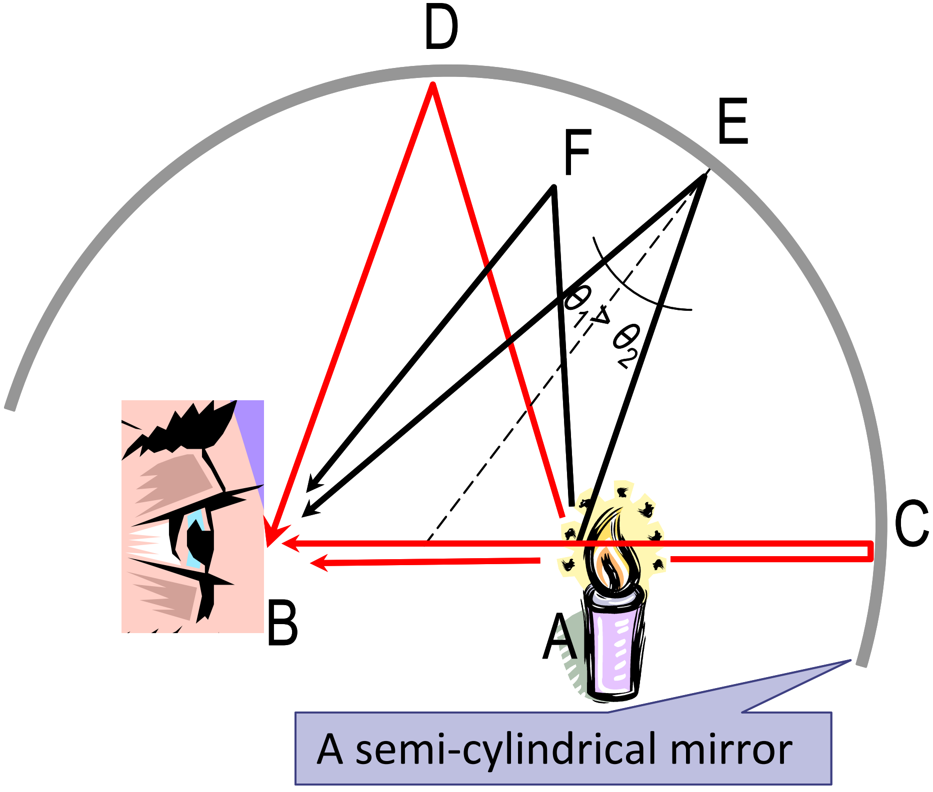
The simplicity of light trajectory: Attempt 2

- In the presence of a mirror, light follows both red paths from A to B (AB, ADB)—but not other (the black) ones (e.g. AEB, AFB).
- The previous formulation of the law is not valid.
- Replacement: Light follows the shortest path, but when there is a mirror, it also follows a second path with a reflection by the mirror such that the angle of incidence equals the angle of reflection.
  - A wordy law, not parsimonious ("equalizer" thinking…).
- We observe that the mirror has imposed an inequality constraint to possible paths (by disallowing light to go through it) and thus generated a second minimum in the 'shortest path' problem.
- **The paths followed by light have minimum length** (either global or local minimum).
- Parsimonious law—Principle of Hero of Alexandria (~1st cent. BC)—but not perfect.



The simplicity in light trajectory: Attempt 3

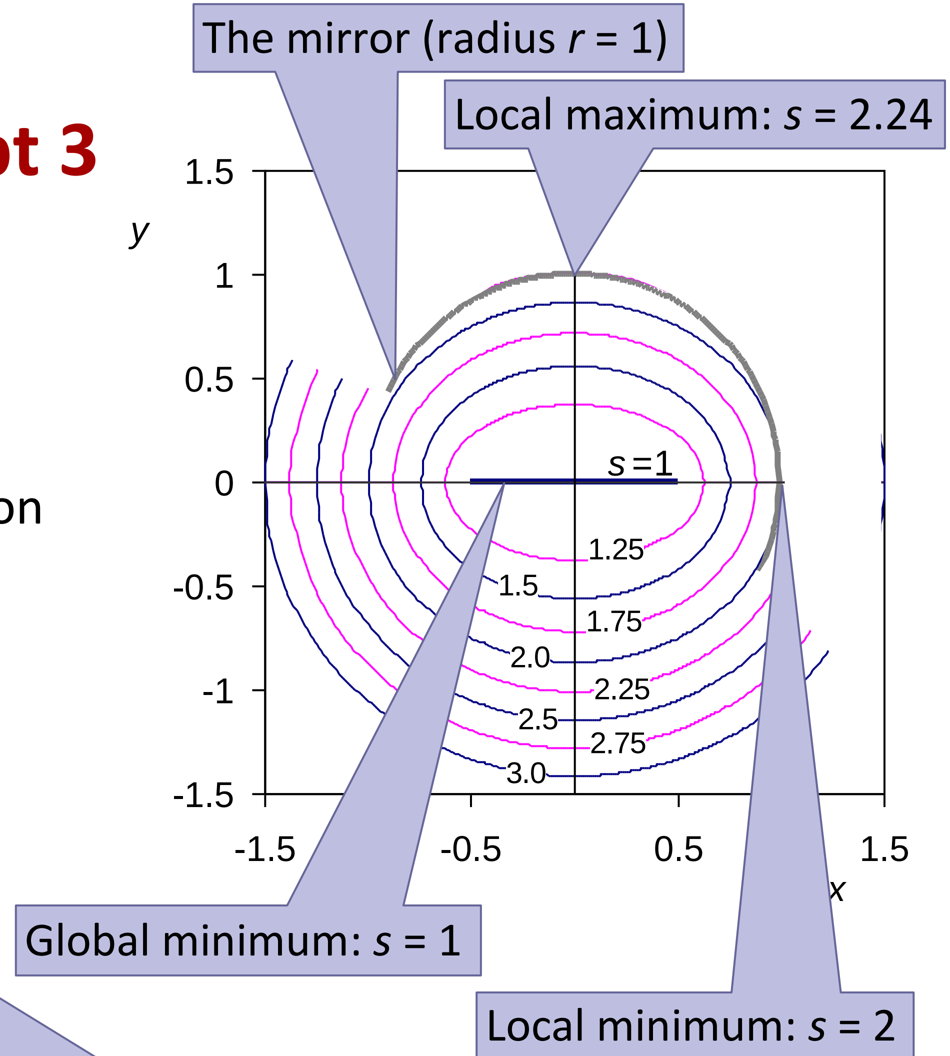
- If we replace the flat mirror with a cylindrical mirror, the light follows several paths from A to B, including the red lines AB, ACB, ADB—but not the black ones, e.g. AEB, AFB.
- Of these, AB is the global minimum, ACB is a local minimum and ADB is a local maximum.
- **The paths followed by light have extremal length** (either global or local minimum or maximum)—still not a perfect law.

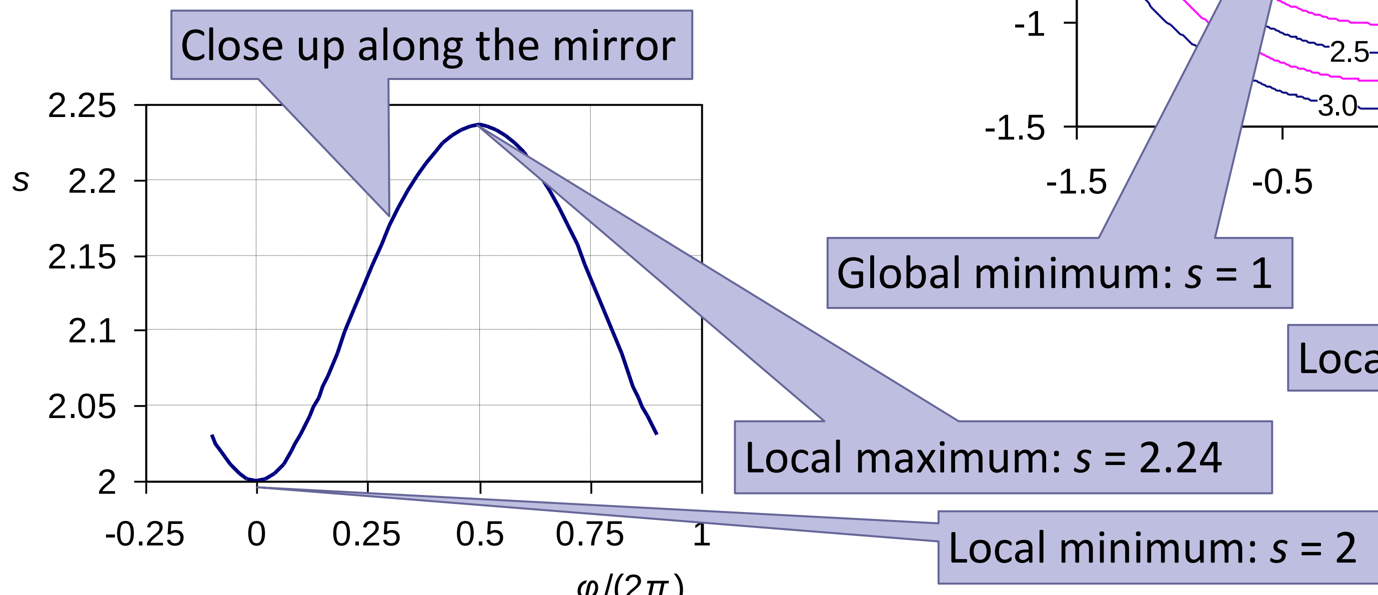


Nature is a skilful extremizer, as she finds all local minima and maxima (put many mirrors to see lots of paths materializing). Failure to observe this makes things difficult to explain, as indicated for instance in the debate by Gaertner (2003) and Schoemaker (2003).

The light trajectory: Quantification for attempt 3

- The mirror introduces an inequality constraint in the optimization: the point F should not be behind the mirror.
- Two points of local optima emerge on the mirror surface (the curve where the constraint is binding).





The simplicity of light trajectory: Attempt 4

- Refraction makes clear that light does not always follow the shortest (straight line) path.
- This is related to the fact that the light speed in liquids is smaller than in air.
- The broken line ACB, rather than the straight line AB, has the least travel time. The point C is determined so as to minimize the total travel time. Assuming an *x* axis at the level of the liquid (so that $x_C = 0$) and denoting the light speed c_A and c_B in the liquid and air, respectively, the travel time is:

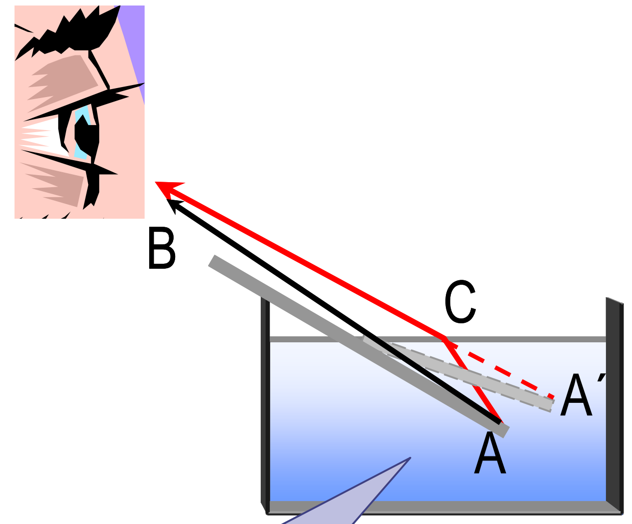
$$t_{ACB} = \frac{\sqrt{(x_A - x_c)^2 + y_A{}^2}}{c_A} + \frac{\sqrt{(x_c - x_b)^2 + y_B{}^2}}{c_B}$$

- Extremization of t_{ACB} yields:

$$\frac{1}{c_A}\frac{x_A - x_c}{\sqrt{(x_A - x_c)^2 + y_A{}^2}} = \frac{1}{c_B}\frac{x_C - x_B}{\sqrt{(x_C - x_B)^2 + y_B{}^2}}$$

(notice, the rightmost fractions of the two sides are the sinuses of the angles of incidence and refraction).

- Final law (Fermat’s principle, corrected for extremal—instead of minimal):
Light follows paths that have extremal travel time.

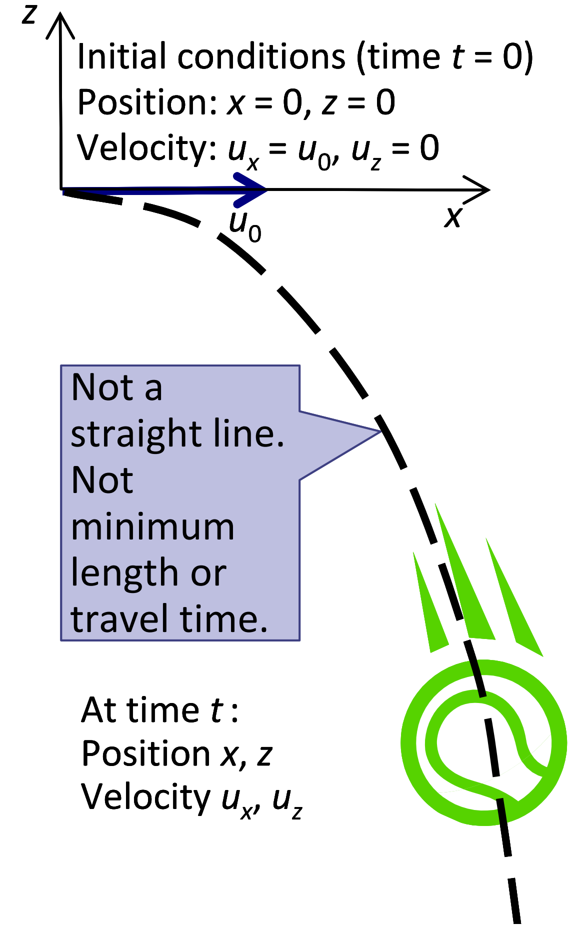


Refraction by water

Nature is indeed parsimonious (ontological parsimony).
The law is parsimonious (epistemological parsimony), reflecting the parsimony of Nature.

Generalization to the trajectory of a weight
The principle of extremal (stationary) action

- Quantities involved:
  - Potential energy: $V = m\,g\,z$;
  - Kinetic energy: $T = (1/2)m\,u^2 = (1/2)m\,(u_x^2 + u_z^2)$;
  - Lagrangian: $L = T - V = (1/2)m\,(u_x^2 + u_z^2) - m\,g\,z$;
  - Action: $S = \int_\Pi L\,\mathrm{d}t$ along the path Π.
- **Principle of extremal action** (Hamilton; applicable both in classical and in quantum physics):
  - **From all possible motions between two points, the true motion has extremal (stationary) action.**
  - Credit for the principle is given to Pierre-Louis Moreau de Maupertuis, who wrote about it in 1744; Leonhard Euler discussed it in 1744, whereas Gottfried Leibniz preceded both by 39 years.
- Solution
  - Extremization of action results in the Euler-Lagrange equation: $\frac{d}{dt}\left(\frac{\partial L}{\partial u_x}\right) - \frac{\partial L}{\partial x} = 0, \quad \frac{d}{dt}\left(\frac{\partial L}{\partial u_z}\right) - \frac{\partial L}{\partial z} = 0$



The trajectory of a weight
Application of the principle of extremal action

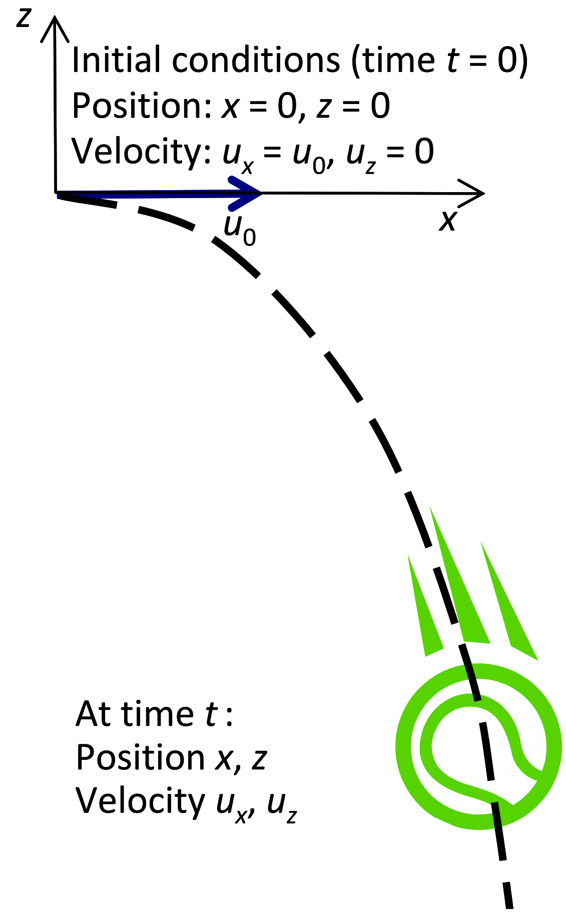
- The Euler-Lagrange equation results in a single (global) minimum (**least action**):

  $u_x = u_0$ (= constant), $u_z = -g\,t$

  from which we obtain:

  $x = u_0\,t$, $z = -g\,t^2/2$ or $z = -(g\,/\,2u_0^{\,2})\,x^2$

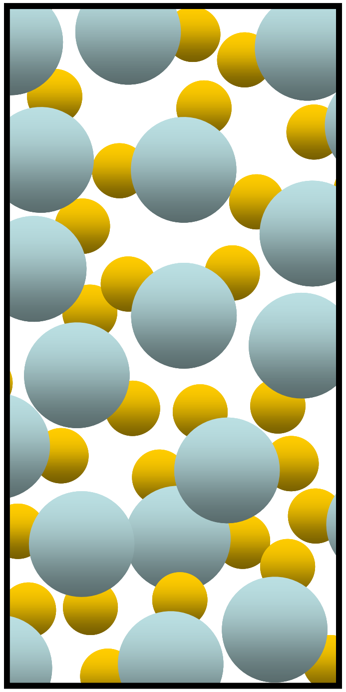
  (parabola; going down).
- In the above formulation, we have not used Newton's laws, not even the conservation of energy.
  - Rather, the conservation of total energy $E = T + V$ results from the least action solution.
- The solution gives not only the geometry (parabola) and direction (down) of the trajectory but the full description of the movement of the weight.



A single principle (Hamilton's with Fermat's as a special case) describes diverse phenomena in optics and classical mechanics—but works well only in simple systems.

From simple to complex systems

- When we investigate a system of many “bodies” e.g. particles (such the molecules of water in solid, liquid or gaseous phase; see figure), we are not interested on the properties (position, momentum) of each particular particle.
- Even if we were interested, it would be difficult (and extremely non-parsimonious) to know them; e.g. 1 m^3 of a gas at room conditions contains 2.7×10^{25} molecules.
- Only macroscopic/statistical (or thermodynamic) properties of the system are of interest.
- Macroscopic properties are state variables such as pressure, internal energy, entropy, temperature, and characteristic constants such as specific heat and latent heat.
- Inevitably—albeit often not stated explicitly—macroscopic descriptions rely on probability and involve uncertainty.
- However, when the system components are very many and identical, due to the applicability of the laws of large numbers, uncertainty becomes near certainty.



When we move from single to complex systems, parsimony demands replacement of microscopic with macroscopic properties and of deterministic with probabilistic descriptions.

What does Nature extremize in complex systems?

- The quantity that gets extremized is the *entropy*[*] (or the *entropy production* when time is involved; Koutsoyiannis, 2011).
- The scientific term[†] is due to Clausius (1850-1865) and the concept was fundamental to formulate the Second Law of thermodynamics.
- Boltzmann (1866) showed that the entropy of a macroscopic stationary state is proportional to the logarithm of the number *W* of possible microscopic states that correspond to this macroscopic state.
- Gibbs (1902) studied the concept further in a statistical mechanical context.
- Shannon (1948) generalized the mathematical form of entropy and explored it further.
- Kolmogorov (1956, 1958) founded the concept on the basis of the measure theory and introduced entropy to the theory of dynamical systems.
- Jaynes (1957) introduced the principle of maximum entropy as a tool for logical inference (to infer unknown *probabilities* from known *information*).
- In modern terms, entropy is a probabilistic concept and is a measure of uncertainty.

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* The word is ancient Greek: ἐντροπία (a feminine noun; also ἐντροπή) meaning a turning towards, twist—also a trick, dodge; it springs from the preposition verb ἐν (in) and the verb τρέπειν (to turn or direct towards a thing, to turn round or about, to alter, to change, to overturn); related ancient Greek words: ἐντροπαλισμός (turning round); ἐντροπαλίζεσθαι (to turn round often).

† As in composition the preposition ἐν- often expresses the possession of a quality, the scientific meaning of the term ἐντροπία is the possession of the potential for change.

What is the mathematical tool to reconcile the complexity of natural systems with parsimony?

- A consistent theory for complex systems should necessarily be based on probability—but in an enhanced setting.
- The tool is **Stochastics = Probability theory + Statistics + Stochastic processes**.
- Probability theory provides the theoretical basis for:
  - moving from a microscopic to a macroscopic view of phenomena by mapping sets of diverse elements and events of complex systems to single numbers (a probability or an expected value);
  - making induction.
- Statistics provides the empirical basis for:
  - summarizing data;
  - making inference from data;
  - supporting decision making.
- Stochastic processes and Monte Carlo simulations provide the means for:
  - probabilistic predictions;
  - uncertainty estimation;
  - design and management of complex systems.

A note on the “enhanced setting” of stochastics

- Classical statistics is based on the prototype of independence and repeatability (the “coin-tossing” prototype).
- This prototype works well for systems with many *identical* particles for which *independence* can be assumed (this is the case e.g. for ideal gases).
- However, more complex natural (real-world) systems evolving in time may behave differently from the classical prototype (e.g. turbulent flows, hydrometeorological and climatic processes).
- In such cases, stochastic models admitting dependence in time/space are necessary.
- Typical stochastic models (particularly the multivariate ones) are often not parsimonious themselves.
- A more advanced stochastic approach is necessary to make models more consistent with:
    - observed natural behaviours, and
    - the principle of parsimony.

Conclusions

- Nature seems to be naturally parsimonious.
- It is then natural to try to build parsimonious models for natural processes.
- Simple systems can be parsimoniously modelled by deterministic approaches.
- In complex systems parsimony should necessarily be combined with stochastic approaches.
- Recently mainstream research invested hopes in detailed approaches by building complicated models.
- However, comparisons of complicated models with parsimonious ones indicate that the latter:
  - can facilitate insight and comprehension;
  - improve accuracy, efficiency and predictive capacity;
  - require fewer data to achieve the same accuracy with the former.
- Parsimonious formulations and solutions of problems are more reasonable and rational, and easier to apply and monitor in practice.

References

- Boltzmann, L., *Über die Mechanische Bedeutung des Zweiten Hauptsatzes der Wärmetheorie*, Wiener Berichte, 53, 195–220, 1866.
- Clausius, R., *Mechanical Theory of Heat – with its Applications to the Steam Engine and to Physical Properties of Bodies*, London: John van Voorst, 1850-1865.
- Courtney, A., and M. Courtney, Comments Regarding “On the Nature of Science”, *Physics in Canada*, 64(3), 7-8, 2008.
- Gaertner, H.-M., Huygens’ Principle: A case against optimality, *Behavioral and Brain Sciences*, 26, 779–781, 2003.
- Gauch, H. G., Jr., *Scientific Method in Practice*, Cambridge University Press, Cambridge, 2003.
- Gibbs, J. W., *Elementary Principles in Statistical Mechanics*, Yale University Press, New Haven, Connecticut, 1902.
- Jaynes, E. T., Information theory and statistical mechanics, *Phys. Rev.*, 106(4), 620–630, 1957.
- Kolmogorov, A. N., The theory of transmission of information, Session of the USSR Academy of Sciences on Scientific Problems of Automating Production, Plenary Meetings 66-99, *Izd. Akad. Nauk SSSR*, Moscow (In Russian), 1956.
- Kolmogorov, A. N., A new metric invariant of transitive dynamical systems and automorphisms of Lebesgue spaces, *Dokl. Akad. Nauk SSSR*, 119, 861-864 (in Russian), 1958.
- Koutsoyiannis, D., Hurst-Kolmogorov dynamics as a result of extremal entropy production, *Physica A: Statistical Mechanics and its Applications*, 390 (8), 1424–1432, 2011.
- Schoemaker, P. J. H., Huygens versus Fermat: No clear winner, *Behavioral and Brain Sciences*, 26, 781–783, 2003.
- Shannon, C. E., A mathematical theory of communication, *Bell Systems Tech. J.*, 27(379), 623-656, 1948.