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Sometimes Rigor is Overrated

Sometimes the Perfect is the Enemy of the Useful

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Outline

Physics view of rigorous analysis

Notion 1: Are We Ready for Rigor?

Notion 2: "First Principles" May Be Less Useful Than Expected

Notion 3: Commitment to Rigor May Make Us Timid

Notion 4: We Must Know When to Stop

Notion 5: Even Incomplete, Rigor May Have Value

Closing

Physics View of Rigorous Analysis

1. Begin with some very plausible and precise mathematical descriptions of nature (postulates & assumptions).
2. Accept a few principles – such as conservation laws
3. Employ mathematical rigor to deduce conclusions that must follow from general principles and those axioms.
4. From those mathematical conclusions, we obtain insight into the nature of nature.

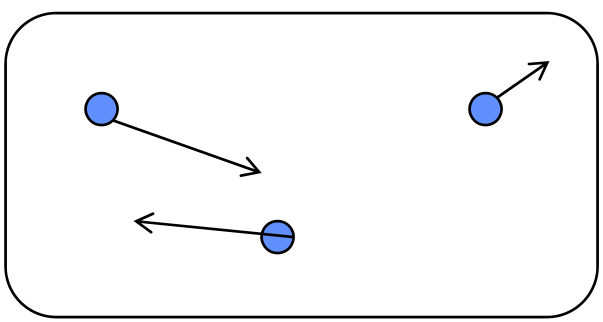
Notion 1: A Time for Everything

There is a time when deriving models in a rigorous manner makes sense.

Illustrated through a short review of the kinetic theory of gases.

Kinetic Theory of Gas – As We Like to See It

- **Begin with some reasonable assumptions**
  1. **A gas consists of a collection of small particles traveling in straight-line motion and obeying Newton's Laws.**
  2. **The molecules in a gas occupy no significant space**
  3. **Collisions between molecules are perfectly elastic**
  4. **There are no attractive or repulsive forces between the molecules.**



Kinetic Theory of Gas – As We Like to See It

- Perform cunning mathematical analysis
  - Calculate momentum transfer to container walls
  - Relate pressure to average kinetic energy of gas particles
  - ….
- Make keen insight into connection between statistical and continuum quantities
  - Deduce that absolute temperature can be defined in terms of average kinetic energy of gas particles.
  - ….

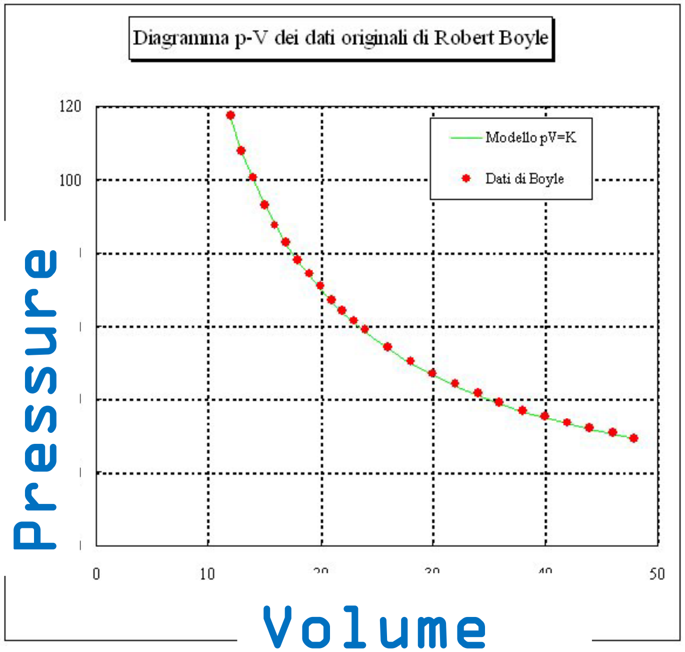
Some History on the Kinetic Theory of Gas[†]

[†] Largely taken from Stephen G. Brush, "History of the Kinetic Theory of Gases" *Storia della Scienza*

Experimental Precursor to the Kinetic Theory of Gas

- **Boyles's Law 1662: Rigorous experiments by Robert Boyle (and assistant Robert Hooke)**

For a fixed amount of an ideal gas‡ kept at a fixed temperature, P [pressure] and V [volume] are inversely proportional (while one increases, the other decreases).



PV=k

at constant temperature

‡ **Non-ideal gasses were unknown at the time**

Experimental Precursor to the Kinetic Theory of Gas

- **Charles's Law 1802: Rigorous experiments by Joseph Louis Gay-Lussac**

At constant pressure, the volume of a given mass of an ideal gas increases or decreases by the same factor as its temperature on the absolute temperature scale‡ (i.e. the gas expands as the temperature increases).

$$\frac{V_1}{V_2} = \frac{T_1}{T_2}$$ at constant pressure

‡ **The concept of absolute temperature derives from this law**

Experimental Precursor to the Kinetic Theory of Gas

- **Combine Boyle's Law and Charles' Law**

$$PV = K_N T$$

- **Consideration of several gasses yields**

$$PV = \frac{W}{V_0} T$$

Let's call $$M = \frac{W}{V_0}$$

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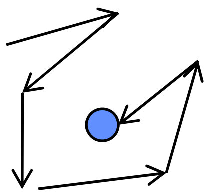
Experimental Precursor to the Kinetic Theory of Gas

- **Brownian Motion 1827: Robert Brown observed random motion of pollen and dye particles on water.**

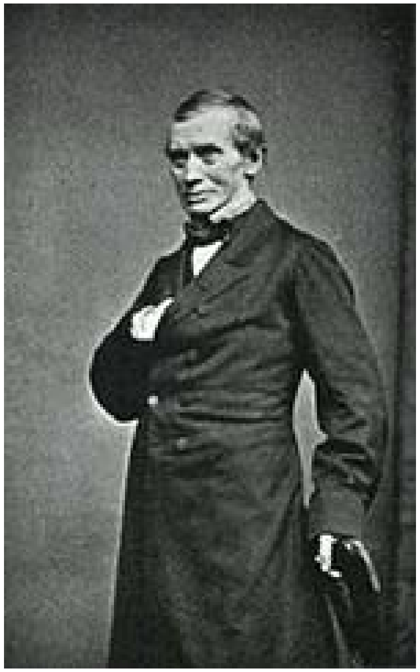


This seems relevant now, but it did not seem to imply anything about gasses at the time.

Experimental Precursor to the Kinetic Theory of Gas

- **Thomas Graham's Law of Effusion: 1831**

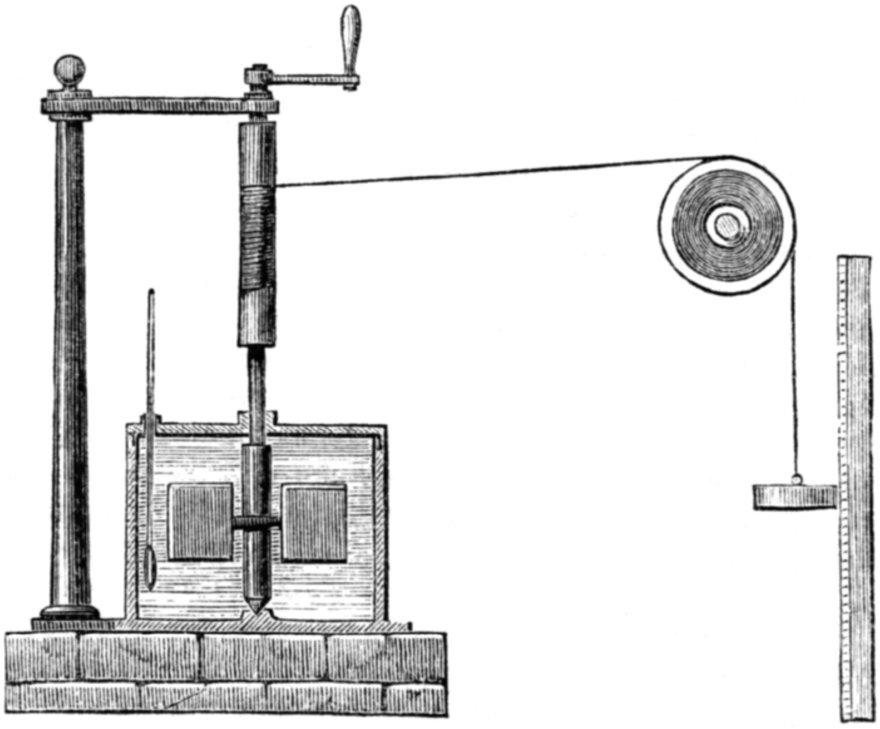
$$\frac{R_1}{R_2} = \frac{M_2}{M_1}$$



Connects a rate quantity to the density that shows up in the ideal gas law.

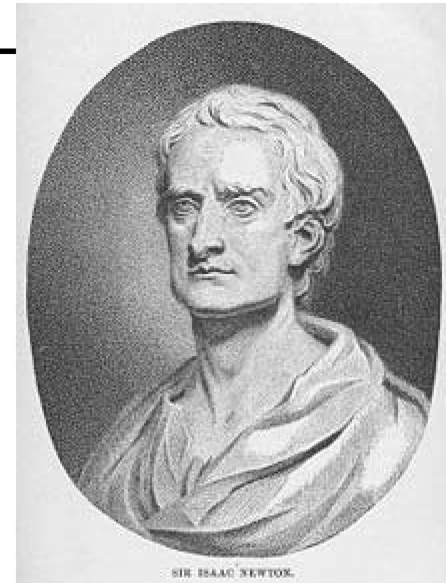
Experimental Precursor to the Kinetic Theory of Gas

- **James Prescott Joule, 1845, “The Mechanical Equivalent of Heat” brought an end to the caloric theory of heat.**



Early Speculation

- **Isaac Newton, 1687, Postulated a non-kinetic theory of gas:**
  - **Gas composed of particles**
  - **Particles repel each other with 1/r type forces**
  - **Static forces: impacts and velocities are not mentioned**



If a fluid be composed of particles fleeing from each other, and the density be as the compression, the centrifugal forces of the particles will be inversely proportional to the distances of their centres. And, conversely, particles fleeing from each other, with forces that are inversely proportional to the distances of their centres, compose an elastic fluid, whose density is as the compression.

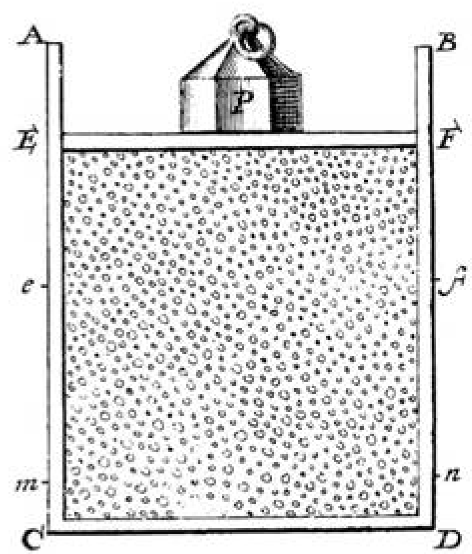
Later, widely integrated with the caloric theory of heat and transport/ether theory.

Yields Boyle's Law: PV=k

Early Speculation

- **Daniel Bernoulli, 1738, Postulated a kinetic theory of gas:**
  - **Gas composed of many particles**
  - **Pressure due to impacts on walls of container**
  - **Dynamic!**

"let the cavity contain very minute corpuscles, which are driven hither and thither with a very rapid motion; so that these corpuscles, when they strike against the piston and sustain it by their repeated impacts, form an elastic fluid which will expand of itself if the weight is removed or diminished…"



Yields Boyle's Law: PV=k

Early Speculation

- **Amadeo Avogadro 1811 postulated that equal volumes of different gases contain equal numbers of molecules.**

This was motivated from consideration of chemistry, rather than mechanics.

Did not seem to have much impact at the time on the theory of gases.

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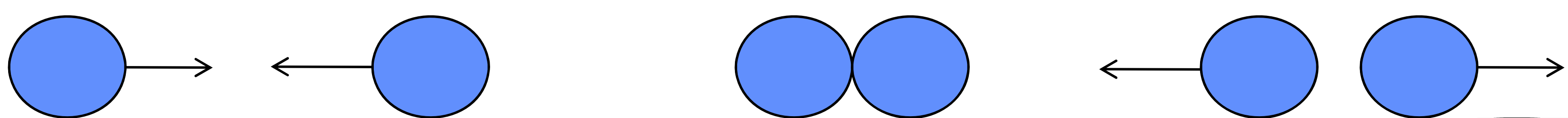
Early Speculation

- **John Herapath 1821, ignorant of Bernoulli's work, published derivation of kinetic theory (some errors). Largely ignored.**
- **Most serious criticisms:**
  - **Conflict with caloric theory - that it should not be possible to remove caloric from a body completely**
  - **Elasticity**
    - **What about drag against ether?**
    - **Proposed theory of atoms asserted that they were absolutely rigid. How is energy stored on impact?**



A **B** **C**

Early Speculation

- James Waterson, 1843, published a more complete kinetic theory of gasses
  - Derived Boyle's law and ideal gas equation.
  - Identified absolute temperature with mean square velocity
  - asserted the equipartition theorem.
- Largely ignored.
- Criticisms: same as those of the Herapath work

Picture Unavailable

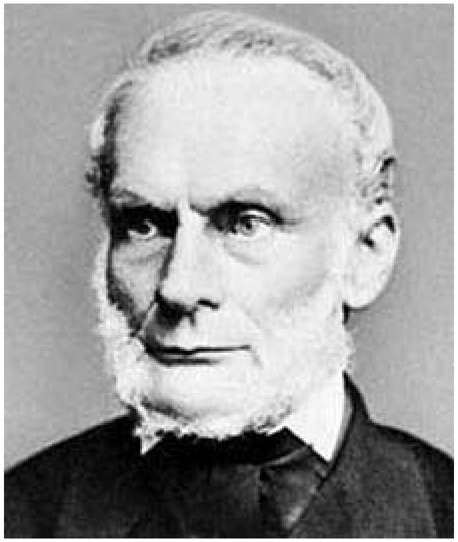
Honored Postumously

Timely Rigor

- August Carl Krönig, 1856, published a short article on the kinetic theory of gas
  - Largely reproducing the results of Waterson
  - Well received
  - Mild criticism by Clausius for not considering rotational and vibratory energy (remember equipartition)
  - Major criticism for prediction that diffusion occurred at the speed of sound

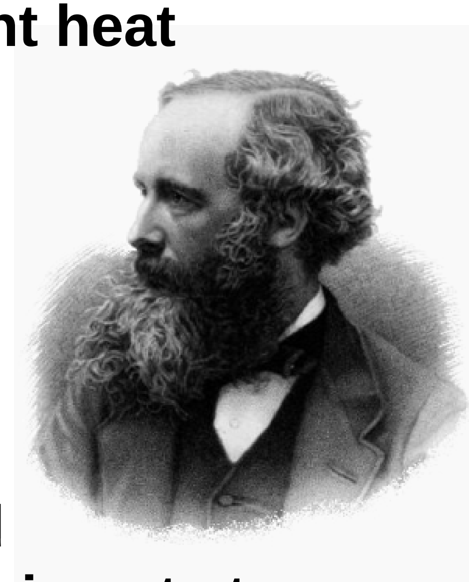
Timely Rigor

- **Julius Emanuel Clausius, 1857, extended kinetic theory**
  - **Accounting for rotational and vibratory energy**
  - **Explaining latent heat and changes of state**
  - **Incorporated Avagadro's hypothesis**
  - **Postulating a mean free path – resolving the diffusion problem**

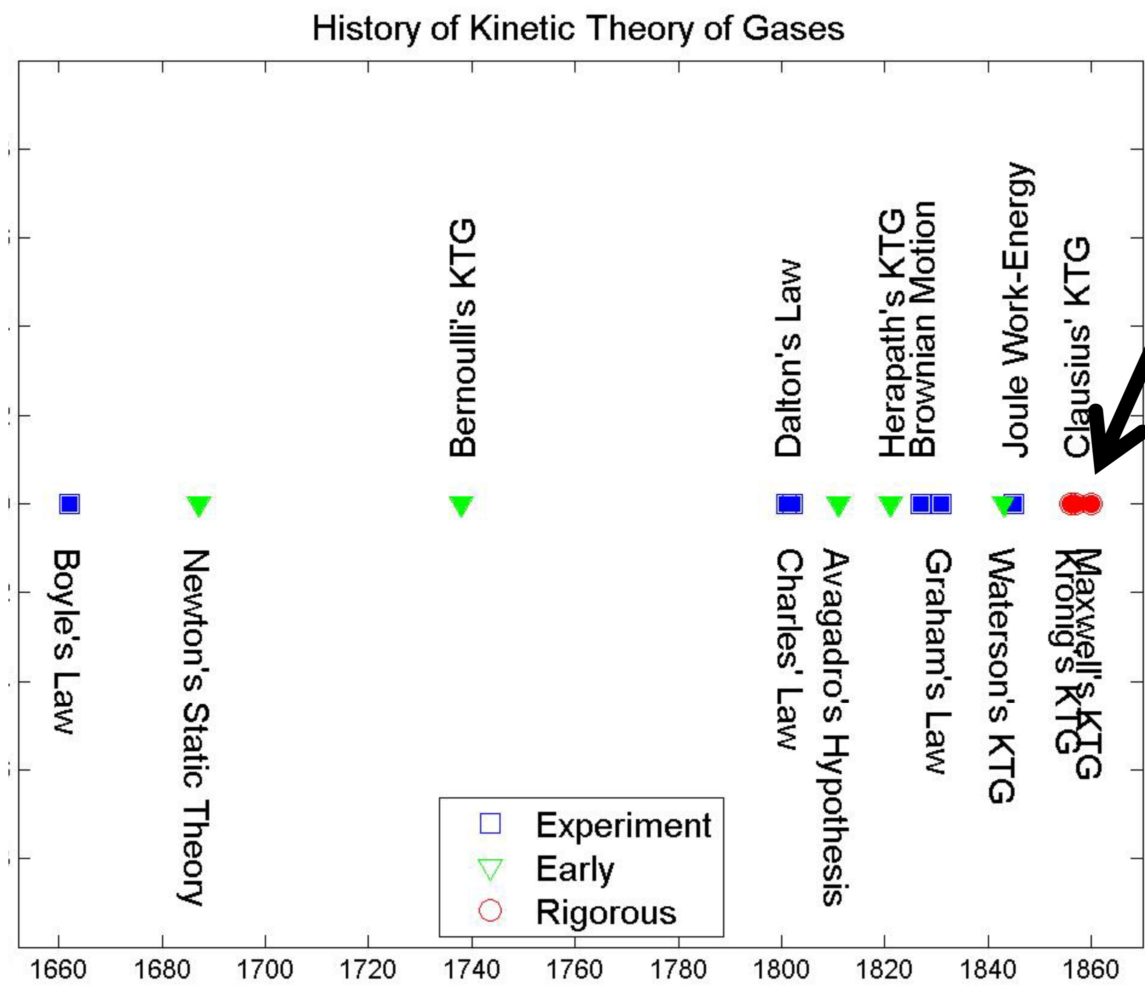


Timely Rigor

- James Clerk Maxwell, 1860, extended kinetic theory further
  - Derived expression for probability distribution of particle velocities using symmetry arguments
  - Made possible quantification of Clausius latent heat assertions
  - Related kinetic theory to transport properties
- A fairly complete, rigorously derived theory
  - Few basic postulates
  - Very few tunable parameters
  - Predicting most of what had been established experimentally and suggesting yet more experiments to test the theory

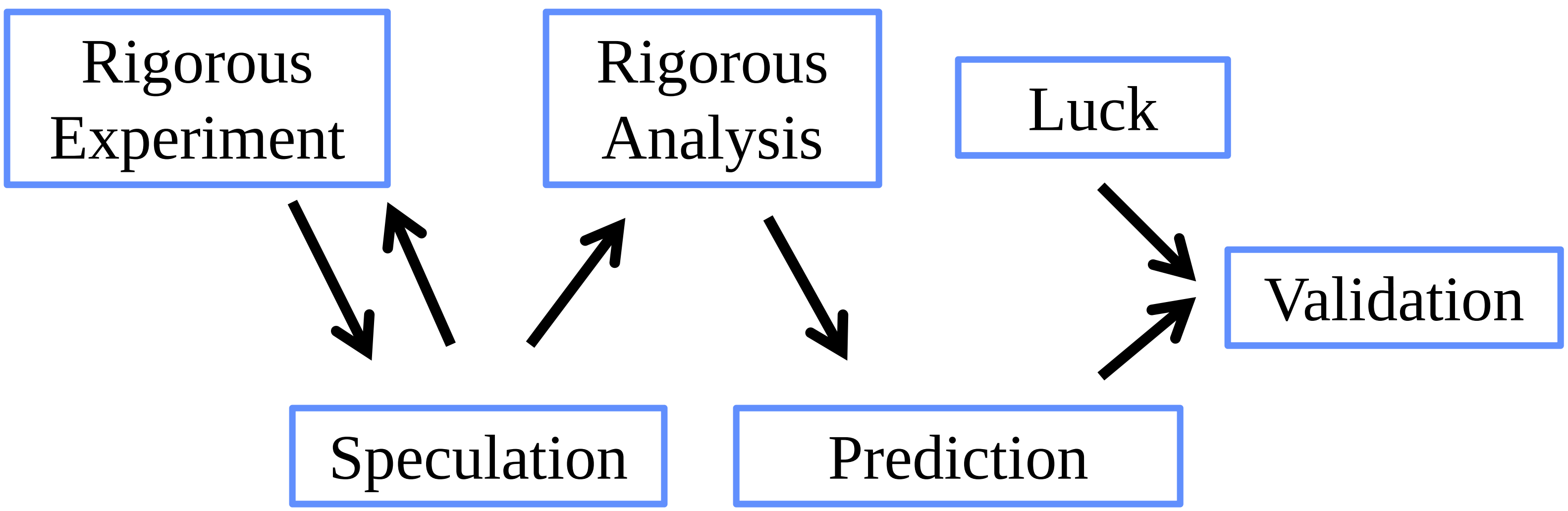


Put It All Together



What Happened?

How Things Seem to Work



Closure to Notion 1

There is an issue of timing. We may be ready for rigorous analysis:

- **Once there is enough empirical information to pose the questions that it might solve.**
- **Once there is enough empirical information to differentiate proposed models.**

Notion 2

- Rigor through “first principles” analysis can be less useful than it appears

What are First Principles (to mechanics folk)

- Conservation of Mass
- Conservation of Momentum
- Conservation of Energy
- Objectivity

And

Here comes a strong statement

- All the rest is empiricism or assumption

Example: Navier Stokes Equation

- **Conservation of Momentum**

$$\rho\left(\frac{\partial v}{\partial t} + v \bullet \nabla v\right) = \nabla \bullet T + f$$

- **Conservation of Mass**

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho v) = 0$$

- **Constitutive Equations – empirical:** $T = -pI + T_D$

where $\left(\frac{1}{\beta}\right)\dot{p} = \nabla \bullet v$ **and** $T_D = \frac{\mu}{2}\left(\nabla v + \nabla v^T\right)$

Notion 2

- First Principles analysis is no better than the empiricisms on which it is based.
- Rigor through “first principles” analysis can be less useful than it appears.

A Corollary from Notion 2

When Rigor and Reality Disagree

Choose Reality

Notion 3

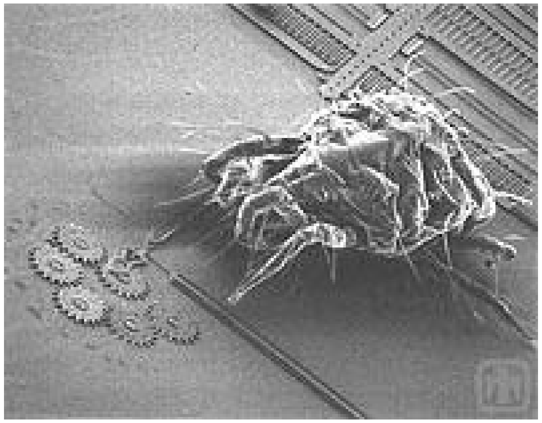
- **Sometimes our desire for rigorously derived models makes us timid about addressing messy problems.**
- **For instance, a large class of very messy problems**

  Consider almost any problem of chemical engineering:
  - **These usually include multiphysics processes, some components of which involve rigorous derivation and some of which are entirely empirical.**
  - **and they are combined in whatever ingenious manner yields a useful answer.**

Some Messy Problems

It is the transmission that makes things messy

Stress corrosion cracking



MEMS

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Notion 3: About Messy Problems

- Sometimes we shy away from these problems.
- Let's not be timid.

Closure to Notion 3

- Let's be sure that we are part of the team that investigates these problems
- Let's work to make each component model as rigorous a possible.
- With an eye continuously on the data, let's attempt to develop model elements that bring sense to the problem

Notion 4

- **Sometimes rigorous models yield different but similar results.**
- **We need to know when to stop.**

Range of predictions of various models

Range of values found experimentally

Thanks to Tom Hahn of composites fame for making this point.

Notion 5: In the Right Cases, Even Incomplete but Rigorous Models Have Value

- Rigorously derived models – even entailing oversimplifications – can have value:
  - Simplicity
  - Diagnostics
  - Understanding
  - Direction

Consider A Typical Large Multi-Physics Computer Model

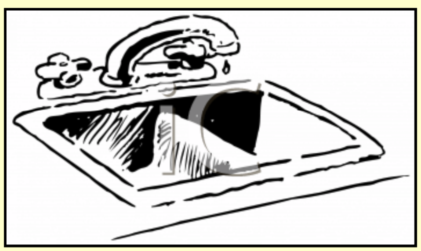
Multi-Scale Models

Monte Carlo Quantum Atomistics

Postulated Statistical Distributions

Operator Splitting

Mean-Quadrature Elements



Stability-Enhancing, Non-Physical Algorithms

Such Models Have Value and Limitations

- **Who really understands these?**
- **How does one use sparse experimental data to refine these models?**
- **How does one use sparse experimental data to identify wrong components?**

On the Other Hand

- **Small, rigorously-derived models whose assumptions and simplifications capture 80% of the physics**
  - **Have design utility**
  - **Facilitate understanding**
  - **Can suggest new areas for exploration**
- **Even wrong models can be useful**

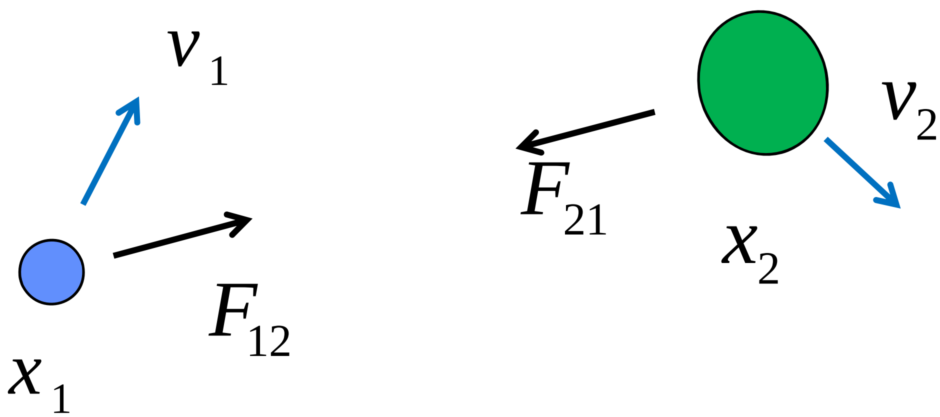
Consider Calculation of Orbits of the Planets

- **Very complicated N-Body problem**
  - **planets,**
  - **dwarf planets,**
  - **asteroids,**
  - **…**

$$\ddot{x}_k = \sum_{n=0, n \neq k} F_{kn} = \sum_{n=0, n \neq k} \frac{x_n - x_k}{\left| x_n - x_k \right|^3} g m_k m_n$$

- **Simplifications derive from the mass of the sun**
  - **The motion of each planet can be approximated as that of a single planet rotating around the sun.**

Consider Calculation of Orbits of the Planets



$$\ddot{x}_1 = F_{12} = \frac{x_2 - x_1}{|x_2 - x_1|^3} g m_1 m_2 \qquad \ddot{x}_2 = F_{21} = -\frac{x_2 - x_1}{|x_2 - x_1|^3} G m_2 m_1$$

$$R = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \qquad r = x_2 - x_1$$

$$\ddot{R} = 0 \qquad \ddot{r} = 2F_{21} = -\frac{x_2 - x_1}{|x_2 - x_1|^3} 2 G m_2 m_1$$

Closed-Form Solutions

$$u_{12}(\theta) = 1/r_{12}(\theta) = \frac{G(m_1 + m_2)}{h_{12}^2}\left(1 + e_{12}\cos(\theta - \theta_{12}^0)\right)$$

$$|r|^2 \dot{\theta} = C$$

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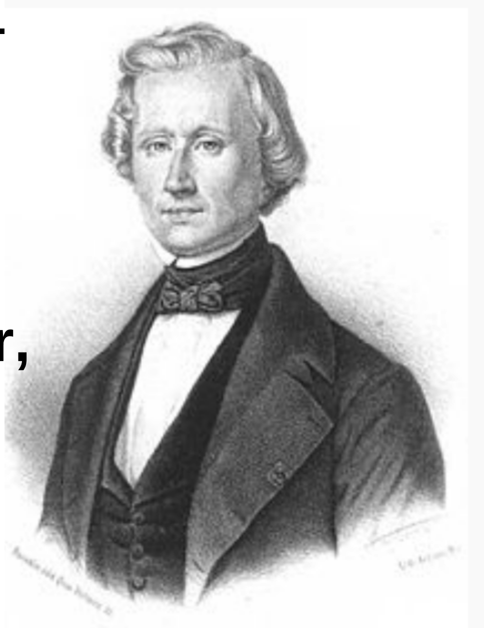
Yields

- The well known results for the 2-body problem: Kepler's Laws of planetary motion
- First term in perturbation solution for N-body problem – we can explore the interaction of orbits of all planets.
- A simple tool to understand a preponderance of the problem of planetary motion.

Yields (continued)



- **A tool to look for anomalies:**
  - **Urbain Le Verrier (1845) noted that irregularities in orbit of Uranus could be explained by the existence of another larger, more remote planet. He predicted location and mass of Neptune.**
  - **Le Verrier also computed that anomalous precession of the perihelion of Mercury could not be explained entirely by precession of the equinoxes, the pull of other planets, and the oblateness of the Sun.**

  This was resolved ultimately by general relativity.

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Closure to Notion 5

Rigorously derived models are most valuable where they lead to understanding.

Closing

- Rigorously performed experiments are almost always a prerequisite to rigorously derived models.
- It is futile to try to develop rigorous theory until there is enough experimental data to distinguish one theory from another.
- For the constituent postulates of a theory to be accepted, there must be some background of experimental evidence to make them plausible.

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Closing

- Even when problems are not ready for our kind or rigorous analysis, lets get on board anyway.
- A good, rigorously derived model provides both understanding and predictive value.
- Thank you for this honor.

Backup

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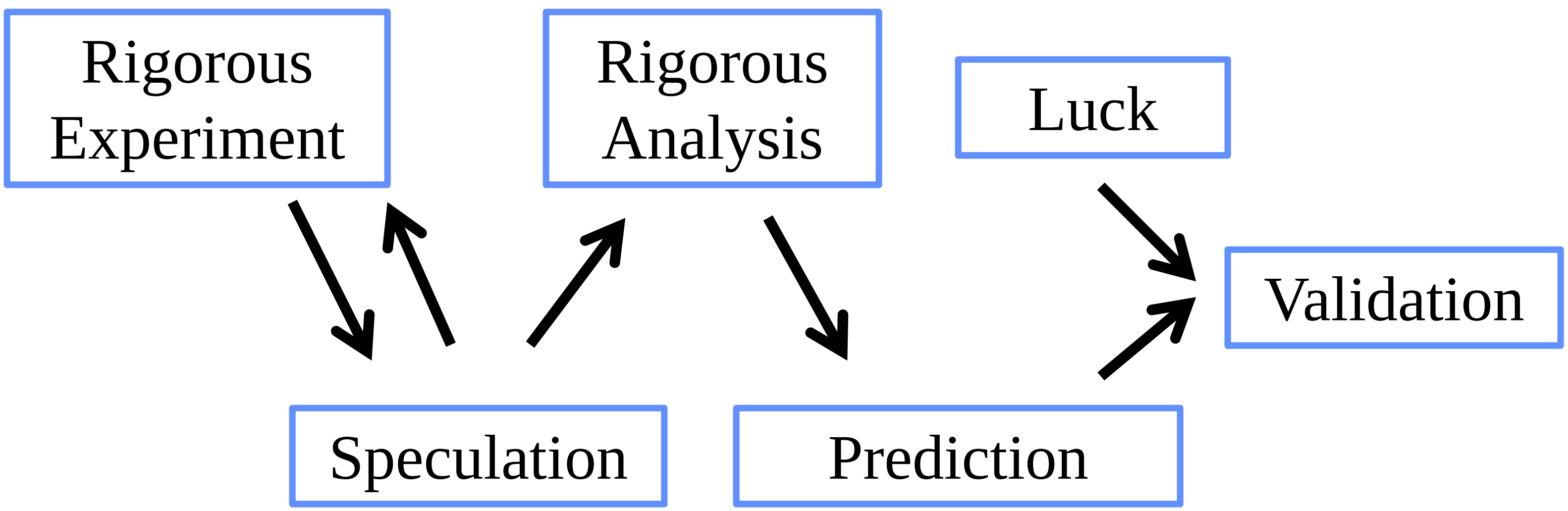
Rigorous Experiment
Rigorous Analysis
Luck
Validation
Speculation
Prediction

Conclusions from Experience with KTG

- It is futile to try to develop rigorous theory until there is enough experimental data to distinguish one theory from another.
- For Rigorous Analysis to have value, it must answer questions.
- For the constituent postulates of a theory to be accepted, there must be some background of experimental evidence to make them plausible.

Conclusions from Experience with KTG

- It is only once a version of the theory is taken seriously that the community will work to make it rigorous:
  - Fully self consistent
  - Consistent with preponderance of experimental data
  - That there are more predictions than parameters.

It is easier to write simulation code than it is to use it intelligently

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