

Jazz orchestras, evolution, and trillion dollar problems

David M. Rogers
University of South Florida
ACS FAME, 2018
COMP Session, Intro. Remarks



2013 Berklee Concert Jazz Orchestra, Greg Hopkins, Director



Theory

Experiment

Applied Research

Simulation

2013 Berklee Concert Jazz Orchestra, Greg Hopkins, Director





The Death of Socrates (1787), by Jacques-Louis David



WORLD'S BIGGEST MINECRAFT REDSTONE HOUSE!

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UnspeakableGaming
Published on Apr 4, 2016

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Minecraft: Biggest Redstone House w/ UnspeakableGaming. Today we take a look at a

Up next

AUTOPLAY



WORLD'S BIGGEST UNDERWATER

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WORLD'S BIGGEST UNDERWATER

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HILLSIDE MINECRAFT REDSTONE MANSION!

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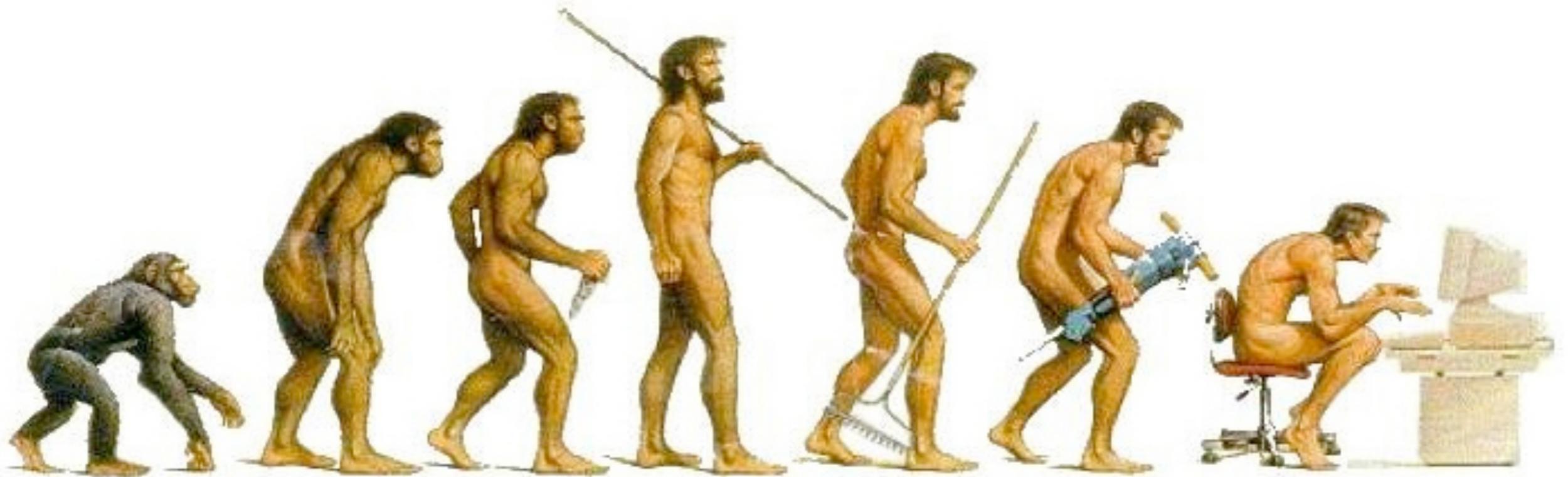
ULTIMATE MINECRAFT REDSTONE BUNKER!

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TOP 10 DEADLIEST TNT CANNONS!

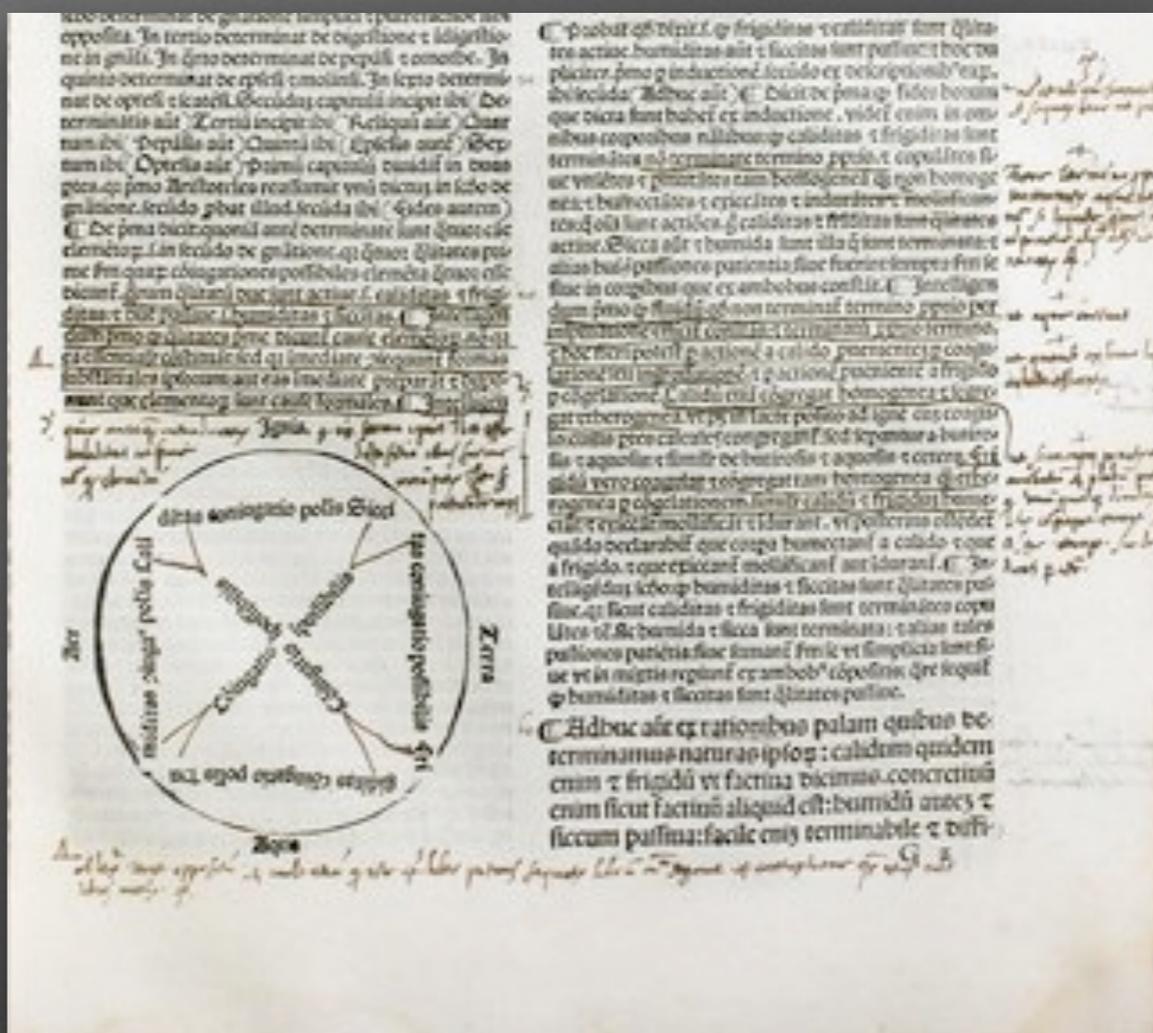
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Somewhere, something went terribly wrong

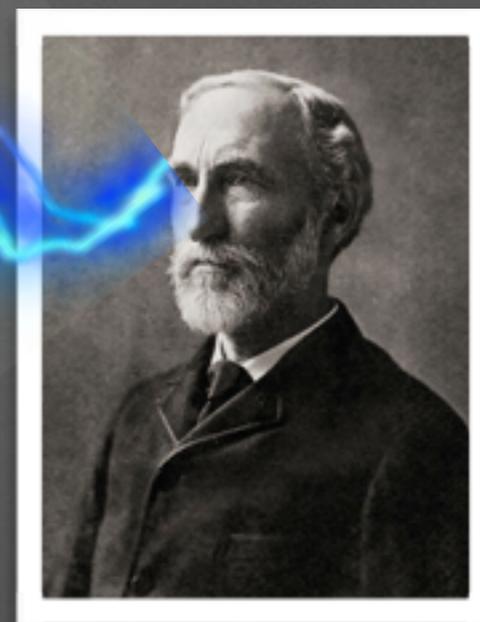
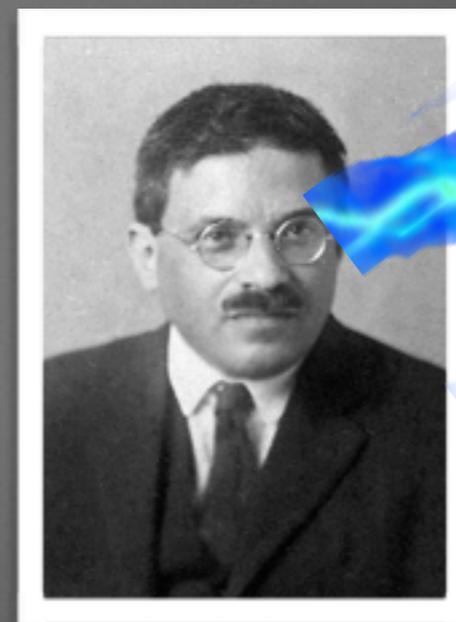


Democritus. Democritvs Abderita De arte magna, siue, De rebus naturalibus: nec non Synesii, & Pelagii, & Stephani Alexandrini, & Michaelis Pselli in eundem commentaria. Patavi: Apud Simon Galignanum, 1573.



Aristotle, Meteorology Course Notes by Kerry Magruder <http://kvmagruder.net/hsci/04-Pyth-Plato-Aristotle/aristotle/aristotle-earth.html>

A close look at this process of development shows that a systematic treatment, which W. Gibbs attempts to give in his *Elementary Principles in Statistical Mechanics*, covers only a small fraction of the ideas (and not even the most important ones) which have come into being through this process (cf. Sections 19–25).



The Conceptual Foundations of the Statistical Approach in Mechanics, P and T Ehrenfest, 1912

After Gibbs' work, however, the frequency view of probability took such absolute control over mens' minds that the ensemble became something physically real, to the extent that the following phraseology appears. Thermal equilibrium is defined as the situation where the system is "in a canonical distribution." Assignment of uniform prior probabilities was considered to be not a mere description of a state of knowledge, but a basic postulate of physical fact, justified by the agreement of our predictions with experiment.

Where do we stand on Maximum Entropy?, Jaynes, 1978

Circuit analysis by Laplace and Fourier Transforms

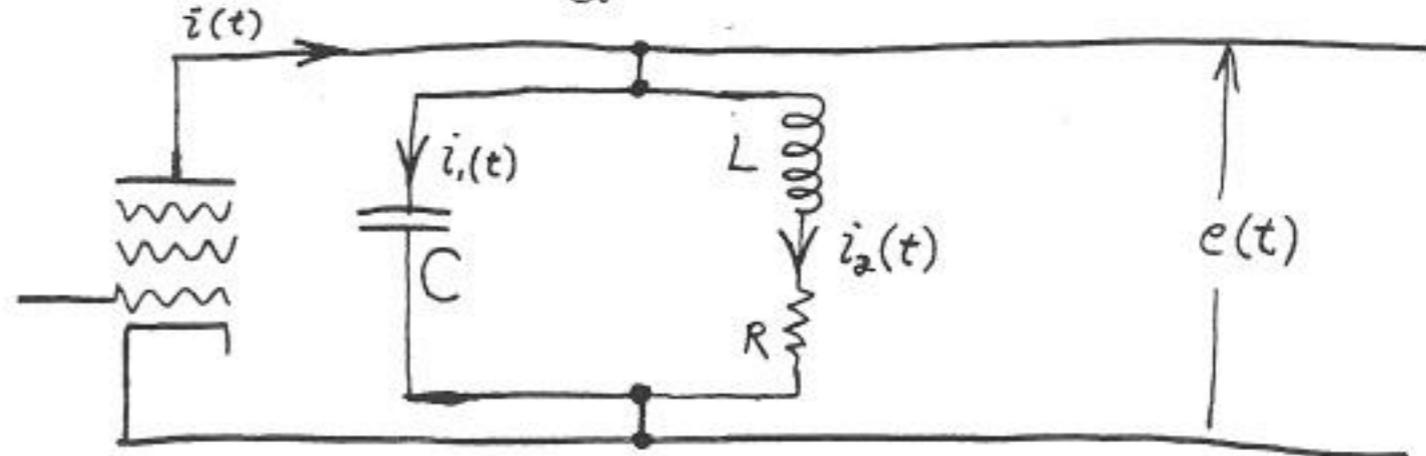
1945



$$i = 0, t < 0$$

$$i = i_0, t > 0$$

The circuit and terminology are as shown below:



The problem will be solved when we have found $e(t)$. The

Edwin T. Jaynes

Some Aspects of Maser Theory (ML 502)

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Count Basie

20s Basie Bio. by William Ruhlmann, allmusic.com

Vaudeville

performance music

30s Blue Devils / Page, Rushing

Moten

Barons of Rhythm

“Count” Basie

(+Green, Jones, Young)

(+/- many)

50s breakup to smaller
group (+Williams)

(-Williams,

+collaborations)

60s

Blues Inc. Jagger/Richards

70s Rolling Stones (+Jones)
(+Watts, Taylor) (-Jones)

(-Taylor) (+/- Wyman)

80s (+Cooder, -Richards)

(-Cooder)

90s

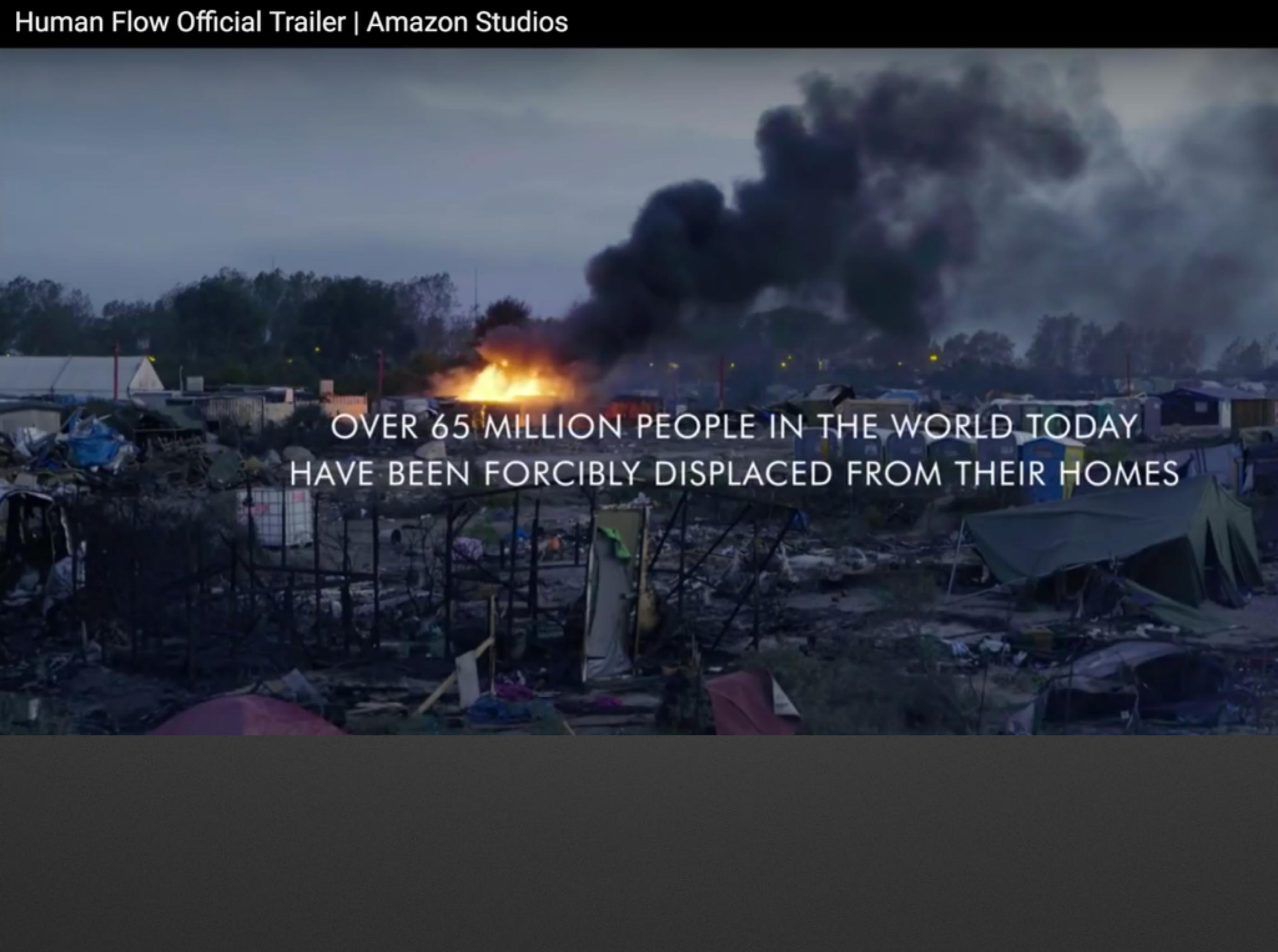
Solo (with guests)

y2k (+Richards)

10s

Super Heavy

/ Stewart, Stone, Marley

A night scene of a refugee camp. In the background, a large fire burns brightly, sending a thick plume of dark smoke into the dark, overcast sky. The camp itself is made of makeshift structures, including tents and shacks, some of which are illuminated by small lights. The overall atmosphere is somber and urgent.

OVER 65 MILLION PEOPLE IN THE WORLD TODAY
HAVE BEEN FORCIBLY DISPLACED FROM THEIR HOMES

Brandriet, Rupp, Lazenby and Becker, *Chem. Educ. Res. Pract.*, 2018, 19, 375

instead, to canvas the current state of introductory chemistry students' responses to a task that is frequently taught and tested in traditional courses. This analysis should provide insight to the effectiveness of current practices, and suggestions for supporting students' deeper engagement in the important practices of analyzing and interpreting data.

Editor's Page

January 31, 2005
Volume 83, Number 5
p. 3

Test Takers Or Scientists?

This guest editorial is by **Richard N. Zare**, Marguerite Blake Wilbur Professor in Natural Science at Stanford University's department of chemistry.

We all know that few americans are choosing careers in the sciences, yet we know how critical those careers are to economic growth. But why is that so and what can we do about it?

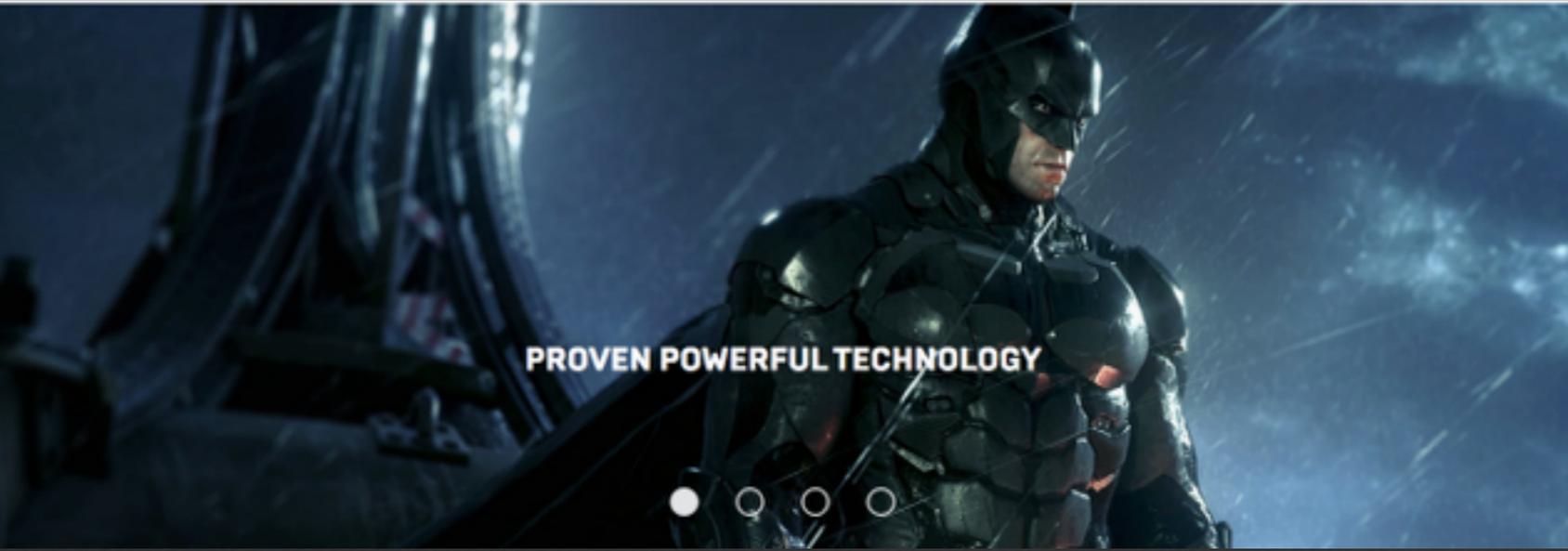


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SMM

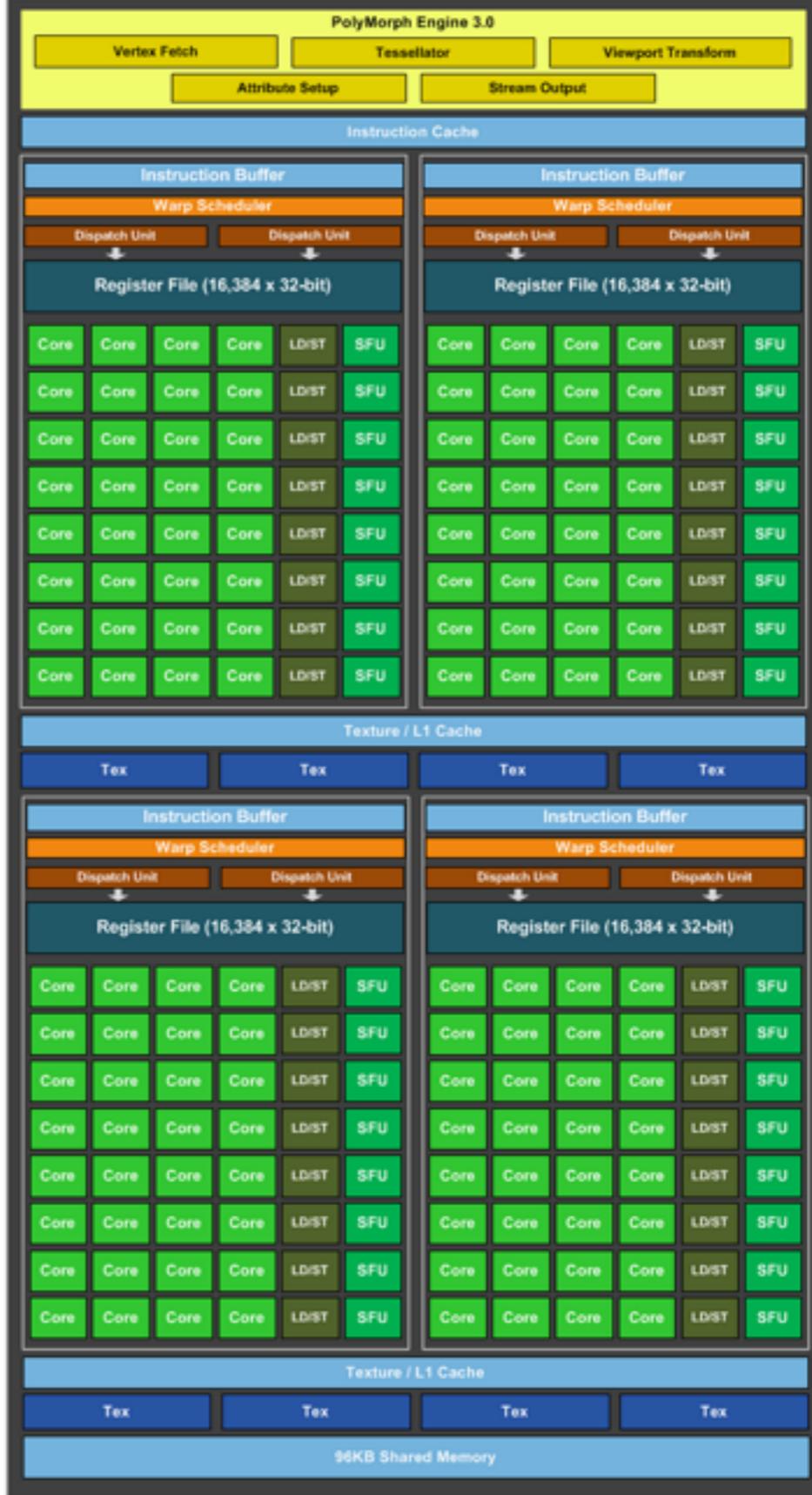


Figure 1: Maxwell's Multiprocessor, SMM
<https://devblogs.nvidia.com>

Computer "Experiments" on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules*

LOUP VERLET†

Belfer Graduate School of Science, Yeshiva University, New York, New York

(Received 30 January 1967)

The equation of motion of a system of 864 particles interacting through a Lennard-Jones potential has been integrated for various values of the temperature and density, relative, generally, to a fluid state. The equilibrium properties have been calculated and are shown to agree very well with the corresponding properties of argon. It is concluded that, to a good approximation, the equilibrium state of argon can be described through a two-body potential.

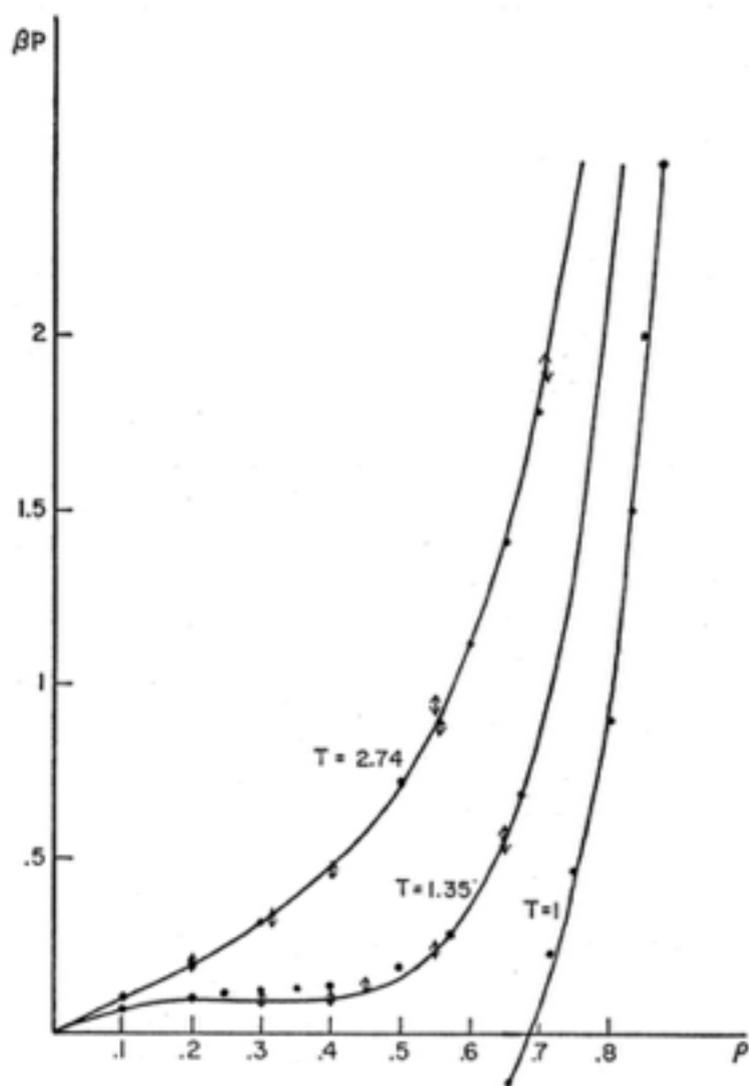


FIG. 2. For the isotherms $T=2.74$, $T=1.35$, and $T=1$, βP is represented as a function of ρ . The low-density parts of the curves were obtained with the help of the PY and PY II equations (Ref. 13). The arrows show the results of Monte Carlo calculations (Refs. 1, 13). The dots are the experimental results in argon (Refs. 10-12).

Molecular Dynamics Study of Liquid Water*

ANEESUR RAHMAN

Argonne National Laboratory, Argonne, Illinois 60439

AND

FRANK H. STILLINGER

Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey 07974

(Received 6 May 1971)

A sample of water, consisting of 216 rigid molecules at mass density 1 gm/cm^3 , has been simulated by computer using the molecular dynamics technique. The system evolves in time by the laws of classical dynamics, subject to an effective pair potential that incorporates the principal structural effects of many-body interactions in real water. Both static structural properties and the kinetic behavior have been examined in considerable detail for a dynamics "run" at nominal temperature 34.3°C . In those few cases where direct comparisons with experiment can be made, agreement is moderately good; a simple energy rescaling of the potential (using the factor 1.06) however improves the closeness of agreement considerably. A sequence of stereoscopic pictures of the system's intermediate configurations reinforces conclusions inferred from the various "run" averages: (a) The liquid structure consists of a highly strained random hydrogen-bond network which bears little structural resemblance to known aqueous crystals; (b) the diffusion process proceeds continuously by cooperative interaction of neighbors, rather than through a sequence of discrete hops between positions of temporary residence. A preliminary assessment of temperature variations confirms the ability of this dynamical model to represent liquid water realistically.

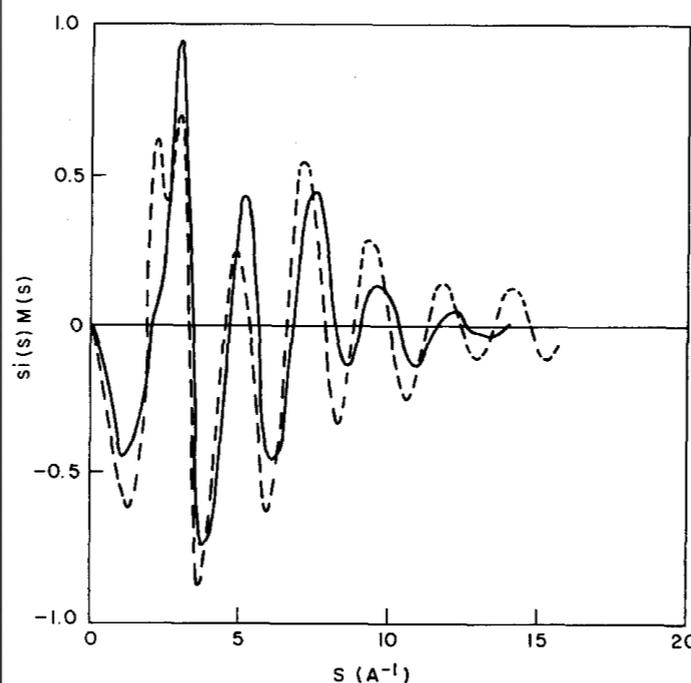


FIG. 7. Theoretical (solid line), and experimental (dotted line), x-ray scattering intensities for liquid water. The latter are taken from Narten, Ref. 29, and refer to 25°C .

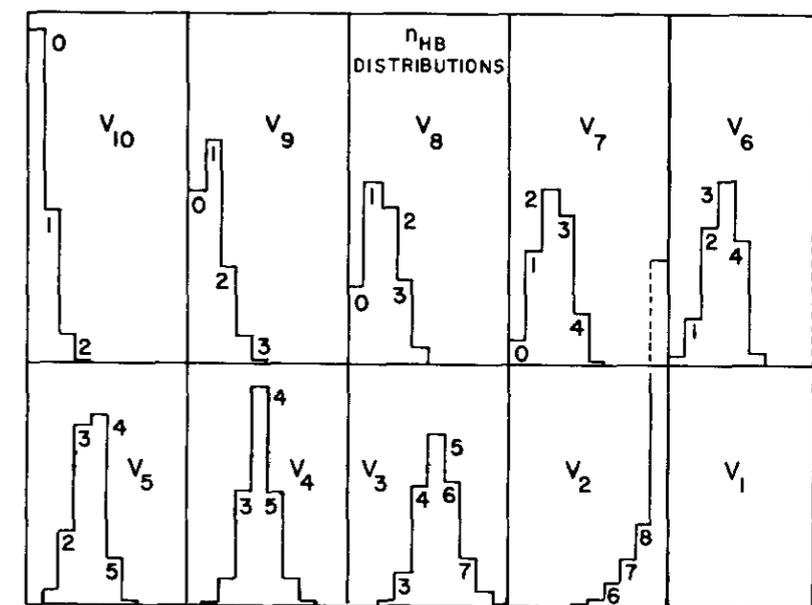


FIG. 19. Distribution of molecules according to the number of hydrogen bonds in which they engage. The set of cutoff energies V_{HB} used as alternative hydrogen-bond definitions is shown in Eq. (4.24).

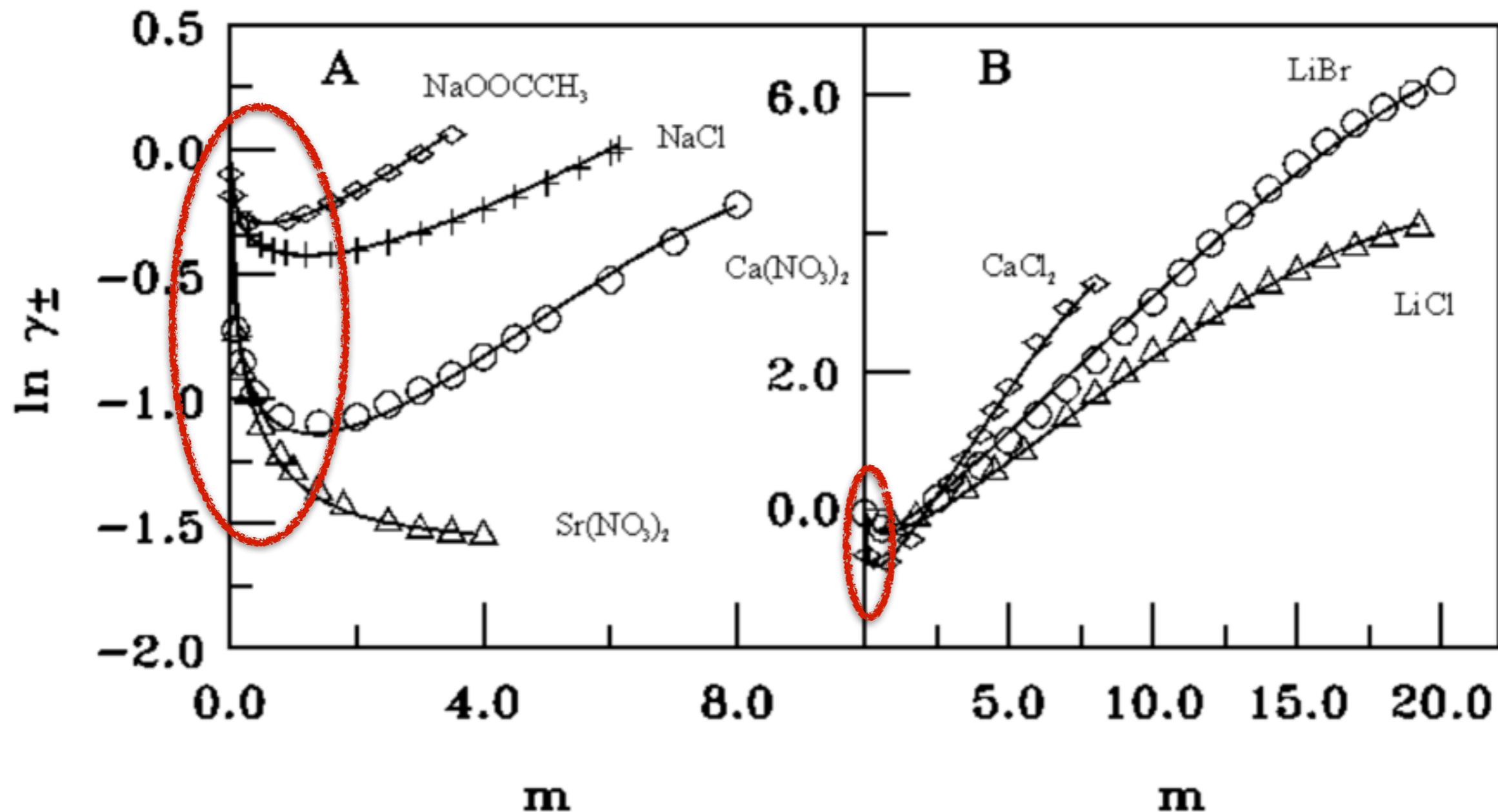
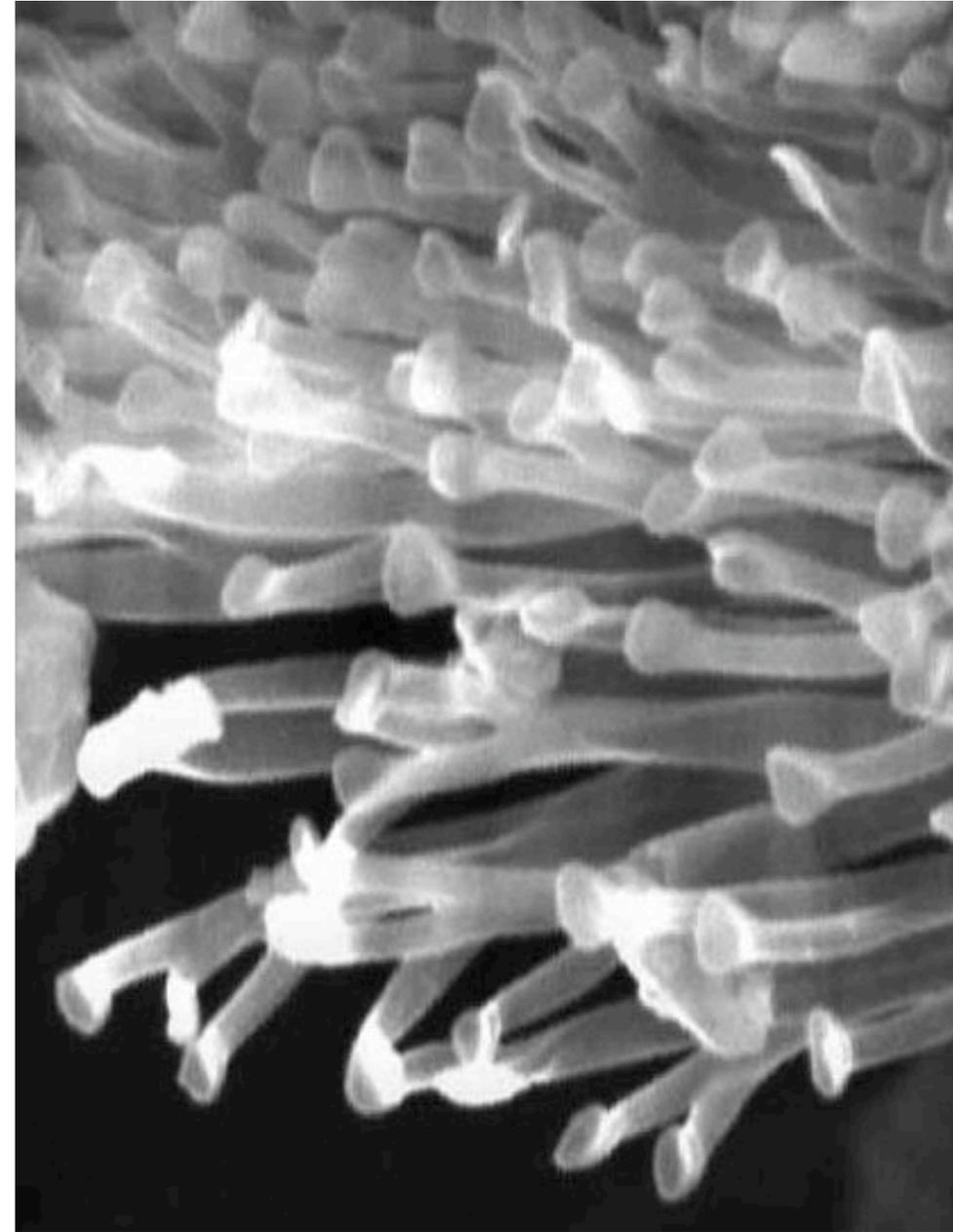


Fig. 4. Experimental and Predicted Mean Activity Coefficients for Aqueous Electrolyte Solutions at 25 °C. Salt molalities 0.0-20 mol \times kg⁻¹, $g \pm 0.2$ -500. ---, prediction (this work), (Δ , O , $+$) experimental values from (A) $\text{Na}(\text{OOCCH}_3)$ and NaCl , Hamer and Wu [57]; $\text{Ca}(\text{NO}_3)_2$ and $\text{Sr}(\text{NO}_3)_2$ Stokes [58]; (B) LiBr and LiCl , Hamer and Wu [57]; CaCl_2 , Stokes [58].

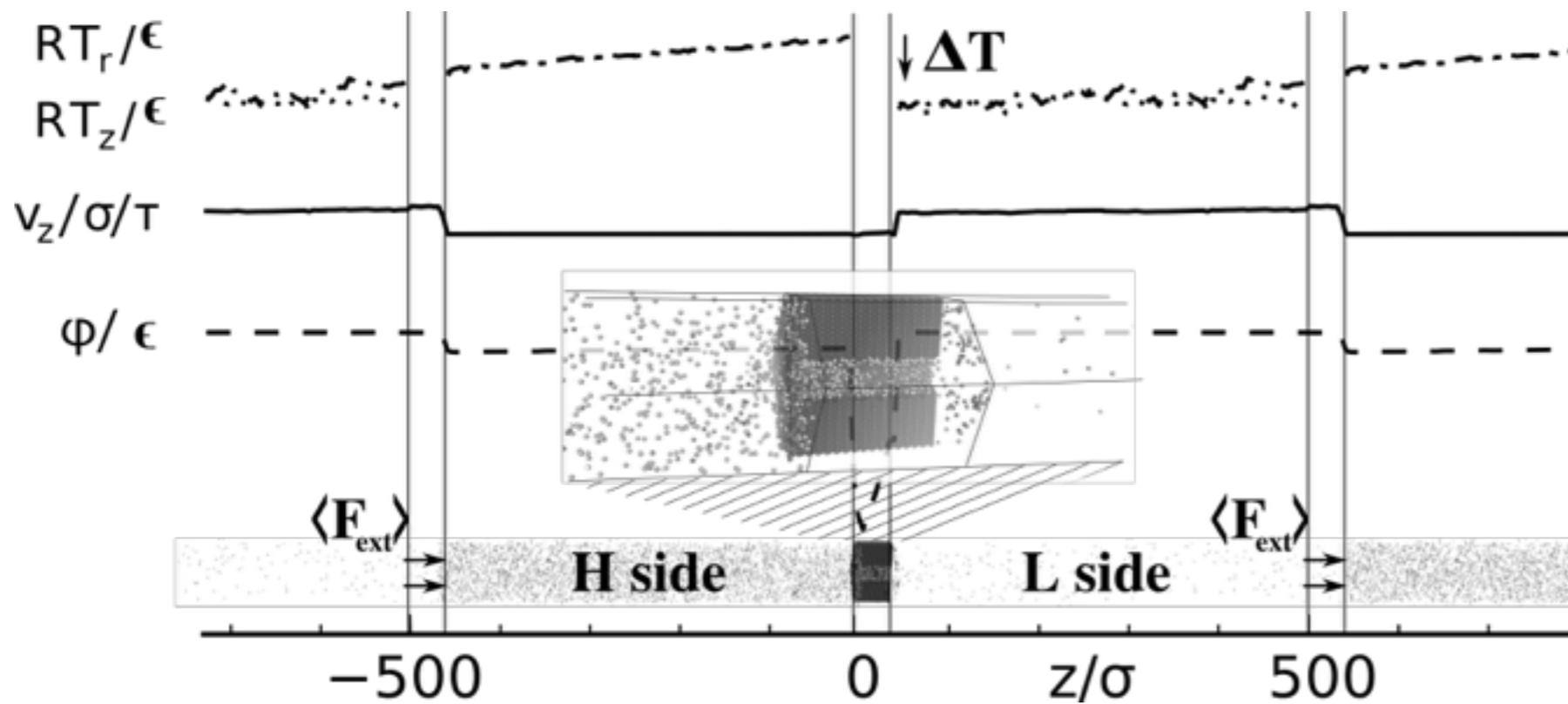
Gecko's grip grasped



K. Autumn, W.-P. Chang, R. Fearing, T. Hsieh, T. Kenny, L. Liang, W. Zesch, R.J. Full. Nature 2000.
Adhesive force of a single gecko foot-hair.

Lifted from a talk by A. Parsegian

<http://online.kitp.ucsb.edu/online/colloq/parsegian1/>



Dayhoff and Rogers, Mol. Sim. 43(5):467-477, 2017.

PHYSICAL REVIEW X 7, 011008 (2017)

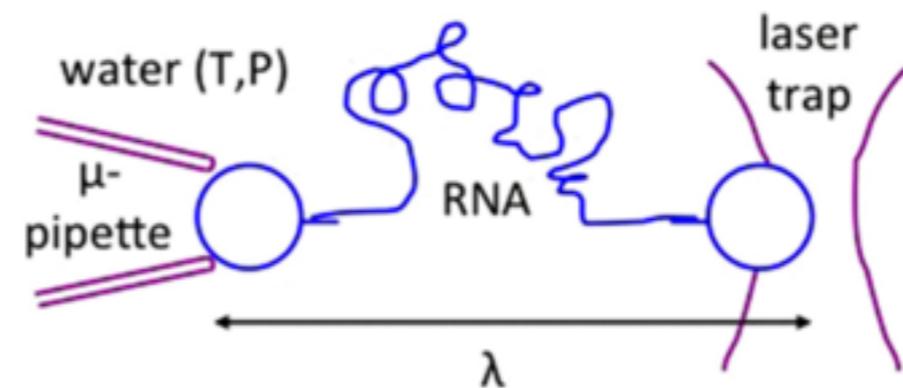
Stochastic and Macroscopic Thermodynamics of Strongly Coupled Systems

Christopher Jarzynski^{1,2,3}

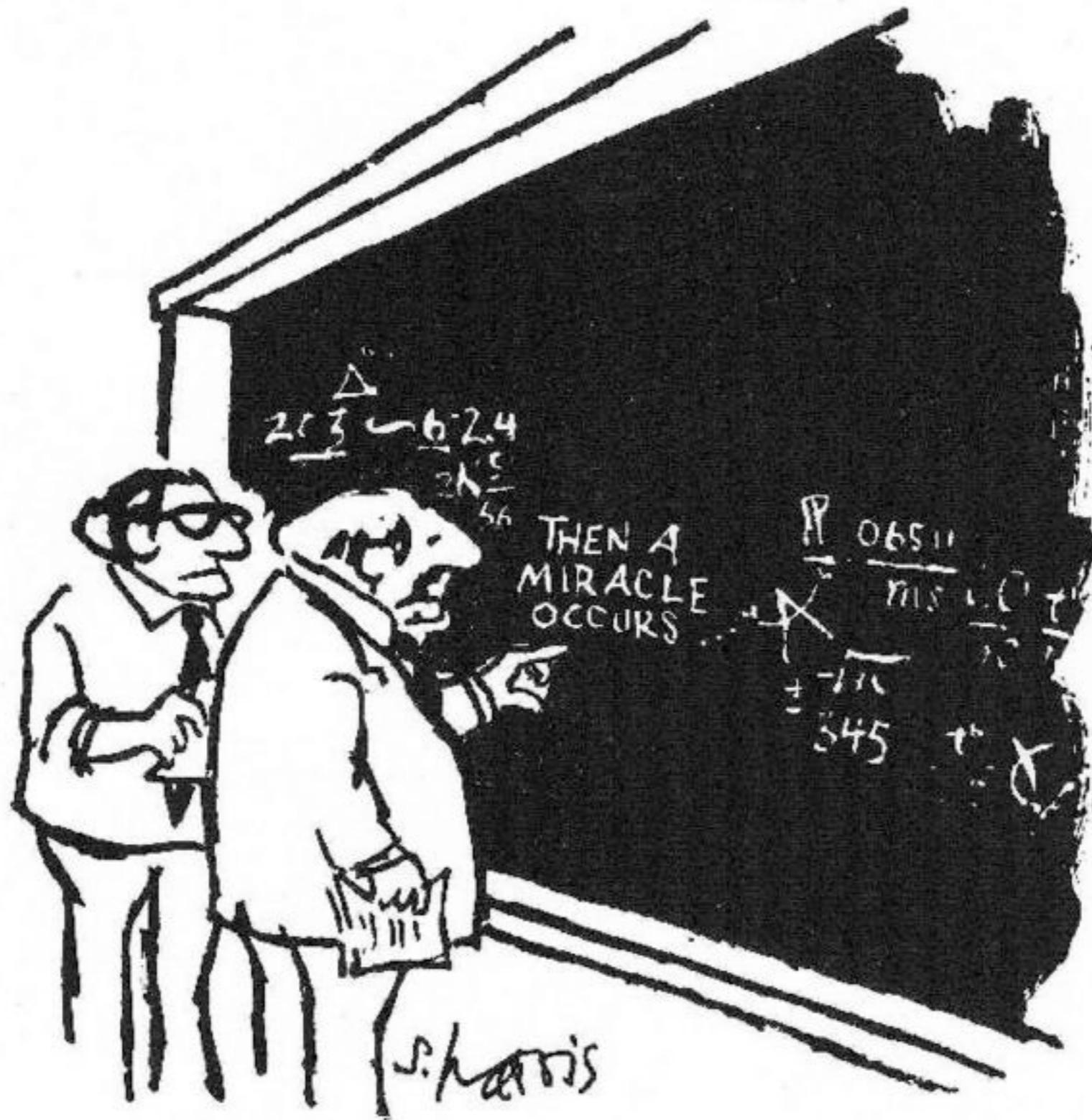
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²*Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland 20742, USA*

³*Department of Physics, University of Maryland, College Park, Maryland 20742, USA*
(Received 21 September 2016; published 24 January 2017)



We develop a thermodynamic framework that describes a classical system of interest \mathcal{S} that is strongly coupled to its thermal environment \mathcal{E} . Within this framework, seven key thermodynamic quantities—internal energy, entropy, volume, enthalpy, Gibbs free energy, heat, and work—are defined microscopically. These quantities obey thermodynamic relations including both the first and second law, and they



"I think you should be more explicit here in step two."

Sidney Harris, The New Yorker Magazine

<http://www.sciencecartoonsplus.com>

1,500 scientists lift the lid on reproducibility
Survey sheds light on the 'crisis' rocking research.
Monya Baker, *Nature* (News Feature), 25 May 2016.

IS THERE A REPRODUCIBILITY CRISIS?



SIL JOB QUE



David M.
Rogers

Projects:

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- [core.vector](#)
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False is unprovable

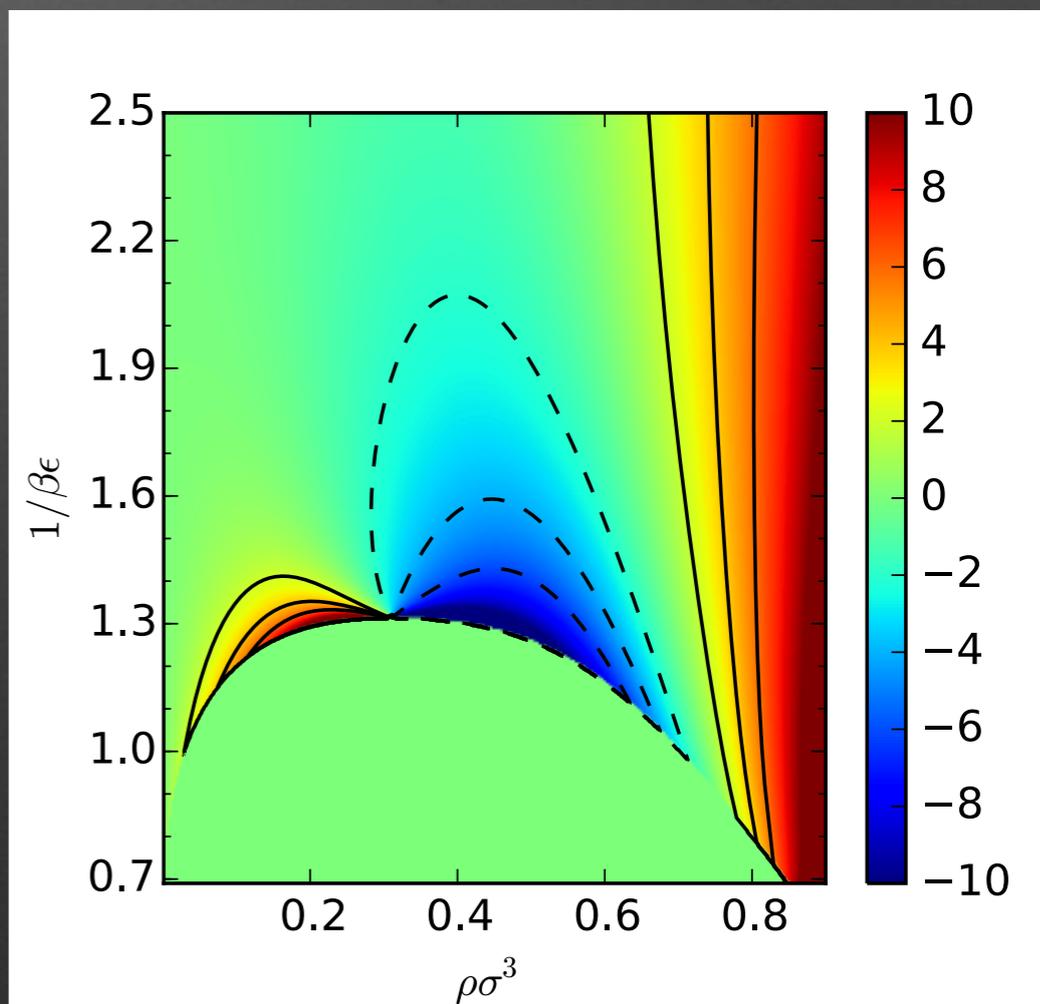
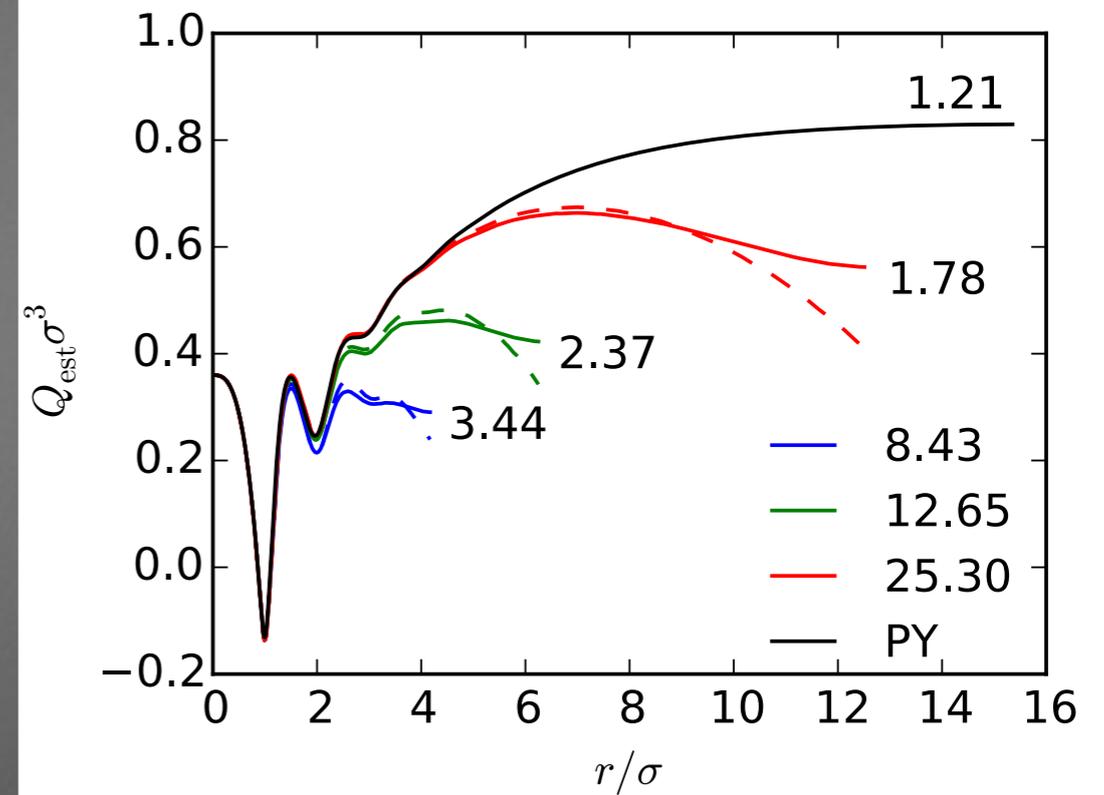
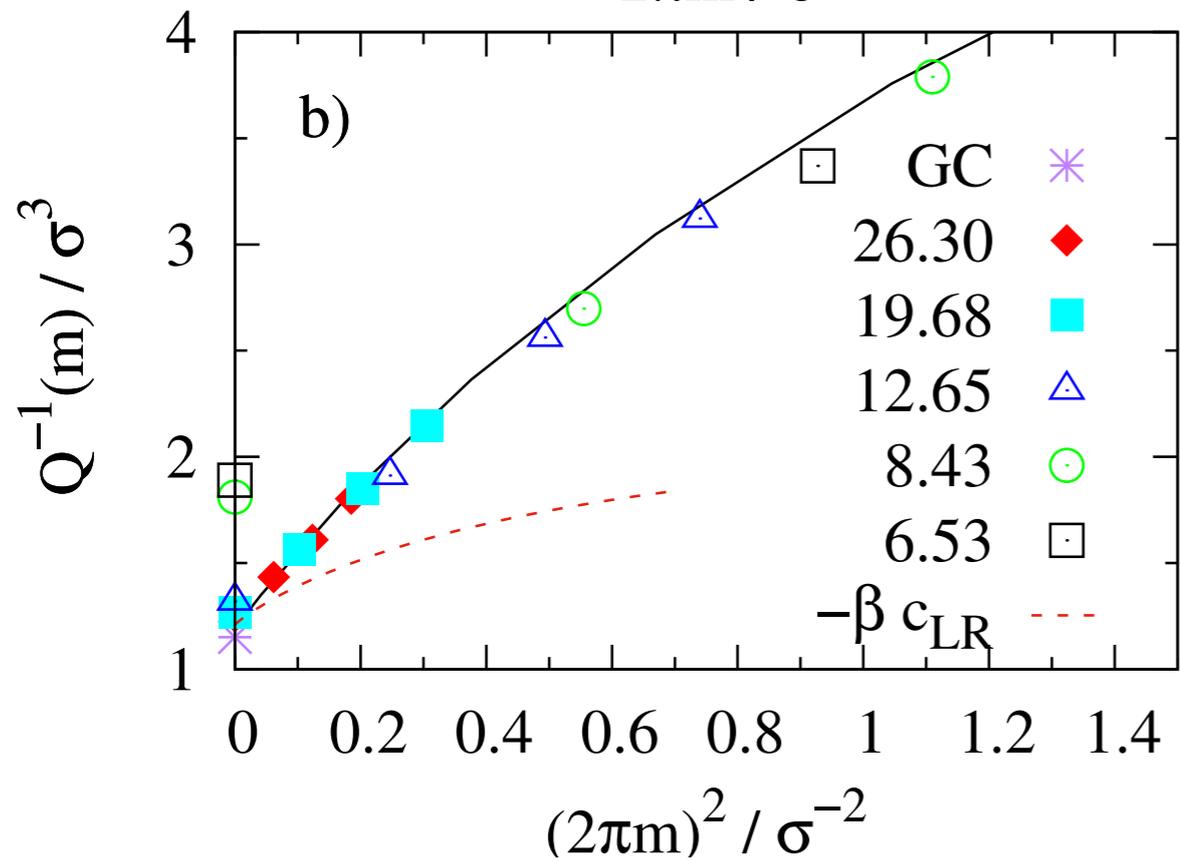
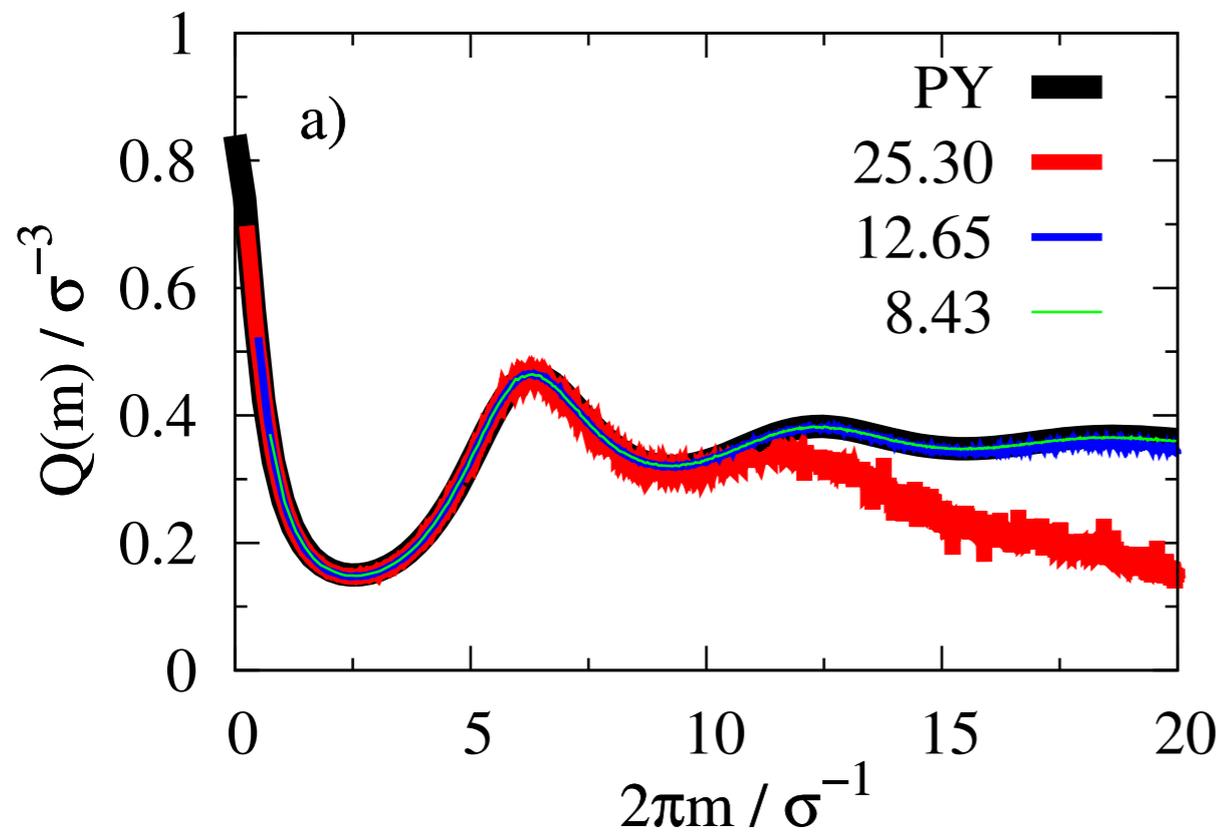
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Theorem False_cannot_be_proven : ~False.
Proof.
  unfold not.
  intros proof_of_False.
  exact proof_of_False.
Qed.
```

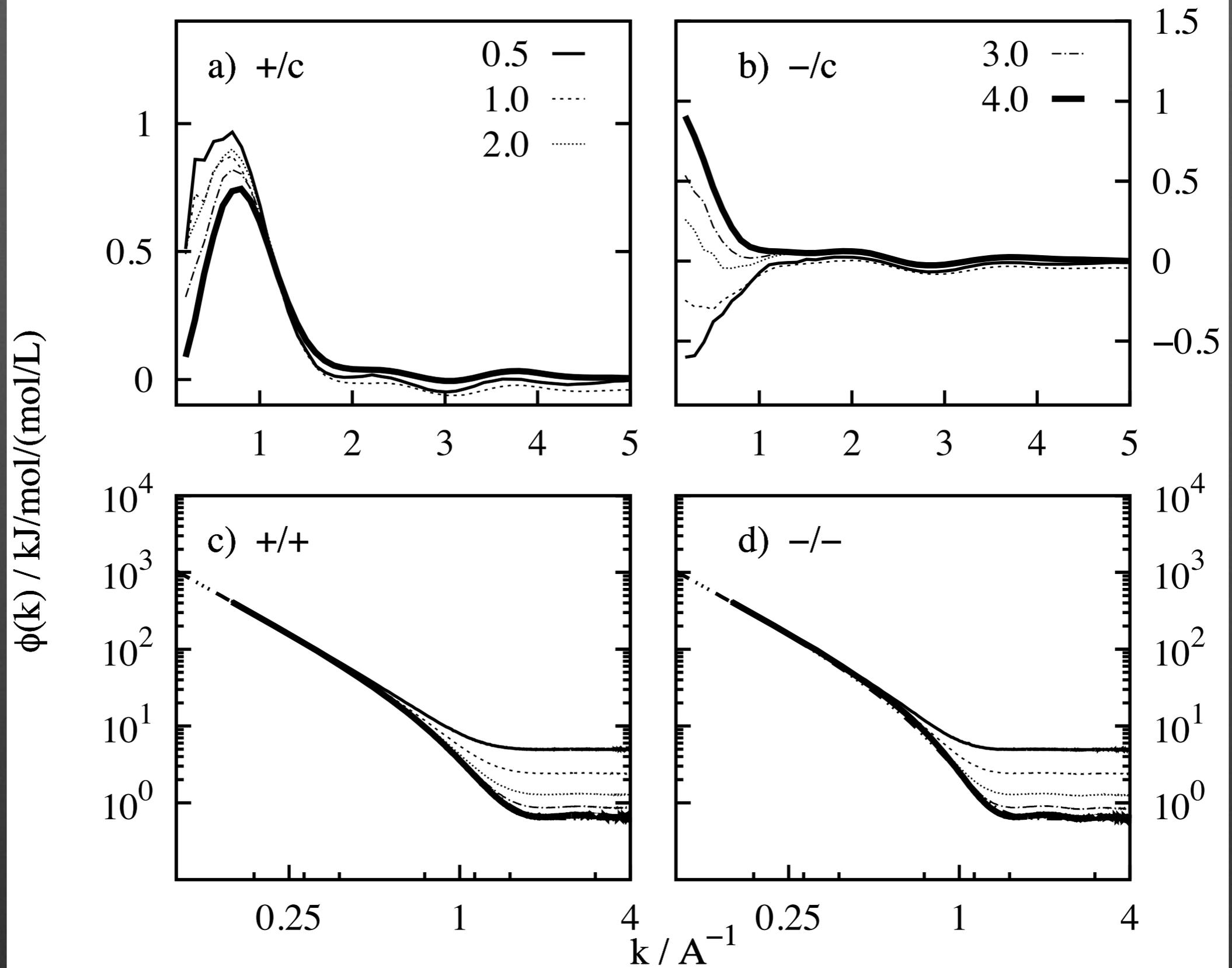
parallelsience.com

David Rogers

Coq proof assistant tutorial,
Mike Nahas

<https://coq.inria.fr/tutorial-nahas>





<http://moleculestothemax.com/>



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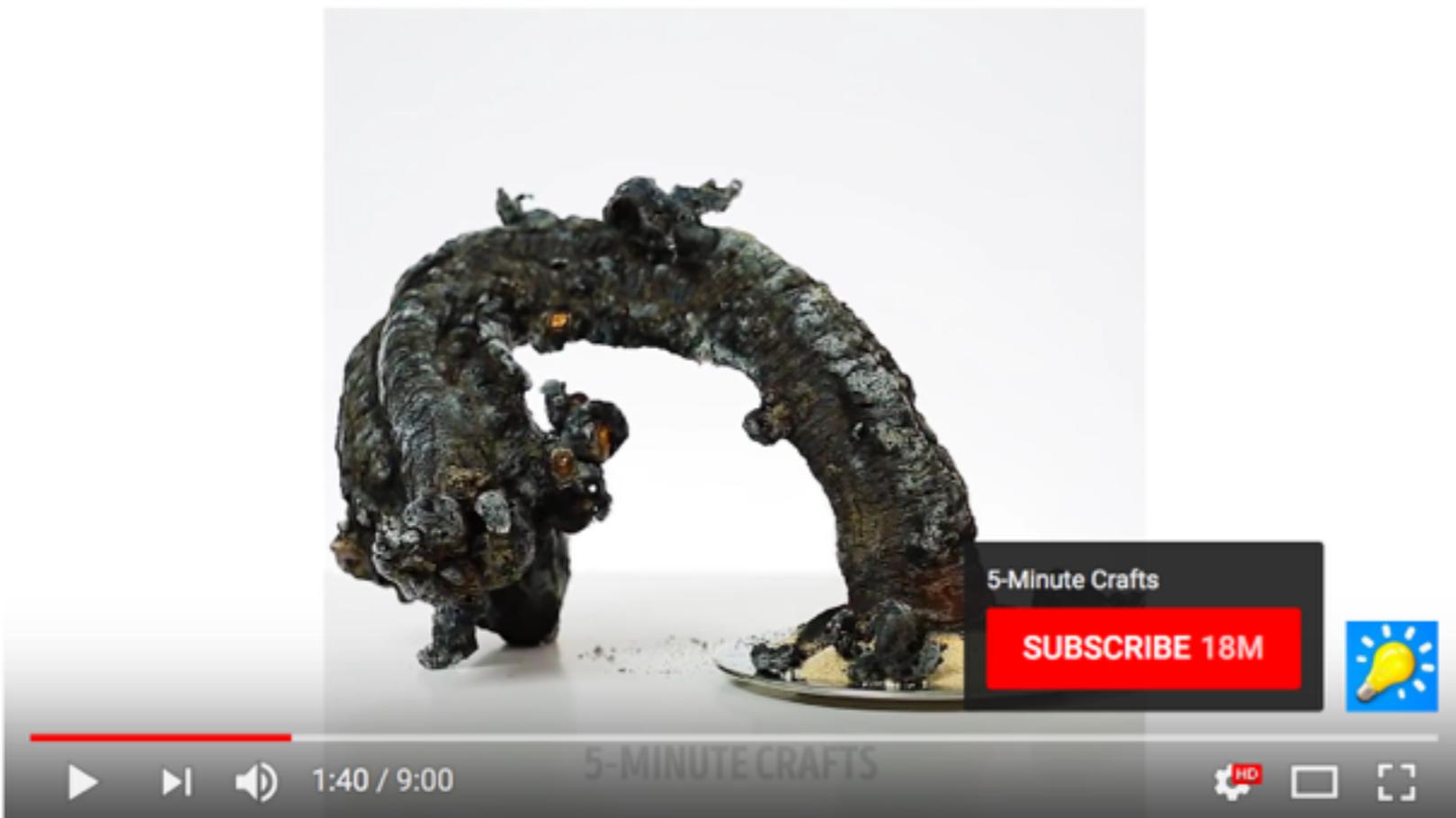
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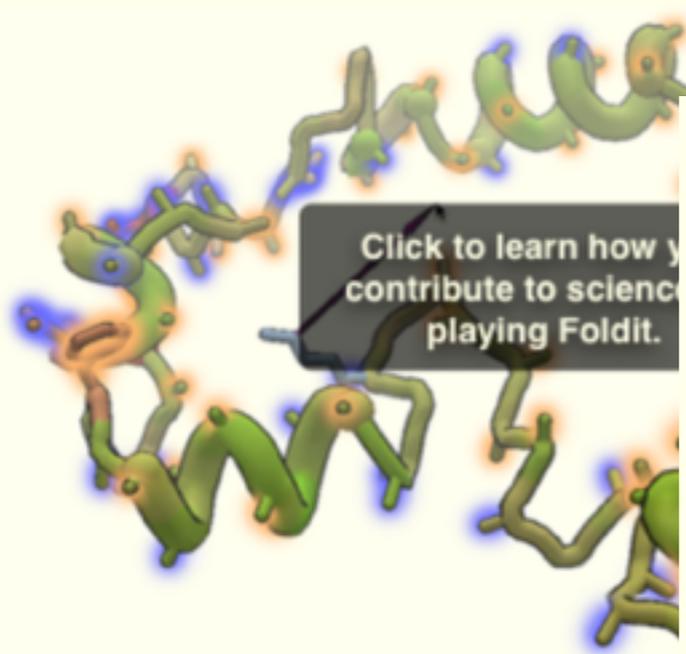
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TOP 10 INFORMATION - TTL ✓

19 Super Cool Science Experiments For Kids And Adults

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What's New

Electron Density for Foldit Player Design

We recently solved the crystal structure of a protein designed by **fiendish_ghoul** in Puzzle 1331! The crystal structure shows that the protein folds up exactly as **fiendish_ghoul** originally designed it, with a C α RMSD of 0.9 angstroms! Congratulations to **fiendish_ghoul**! We've uploaded the refined electron density map into **Puzzle 1516**, so players can try folding a model into the electron density. Check it out now!

Session Commences