INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON

REPRODUCIBLE ENVIRONMENTAL HEAT TRANSFER

Christian Ghiaus

SCIENCE

Science: models of nature with testable explanations and reproducible predictions.

Causality: causal relations; the cause must precede the effect.

Relations = physical laws

Conservation (operation: addition $x_1 + x_2 = x_3$)

- Energy-mass ⇔ time symmetry (invariance)
- Linear momentum ⇔ translation symmetry (invariance)
- Angular momentum ⇔ rotation symmetry (invariance)
- …



Emmy Noether (1882-1935)

Universal laws (operation: multiplication $x = a\,y$)

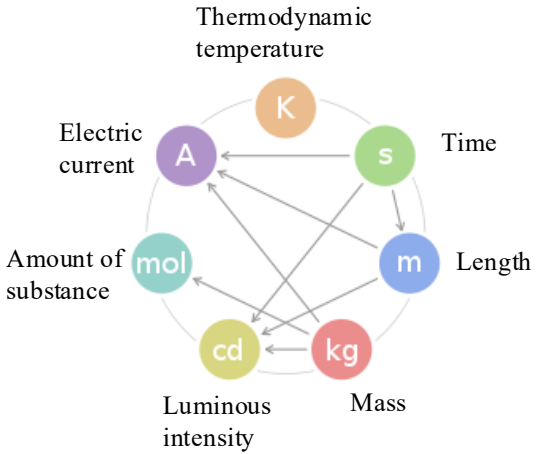
- Universal attraction (Newton) $F_1 = F_2 = G\frac{m_1 m_2}{d^2}$
- Plank-Einstein relation $E = h\,\nu$
- Thermal energy $E_{thermal} = k\,T$
- …

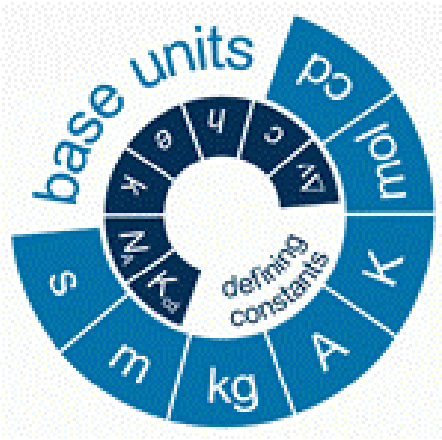
Phenomenological laws

- Ohm's law $u = R\,i$
- Hooke's law $F = k\,\Delta l$

2019 revision of the SI

NEW SI



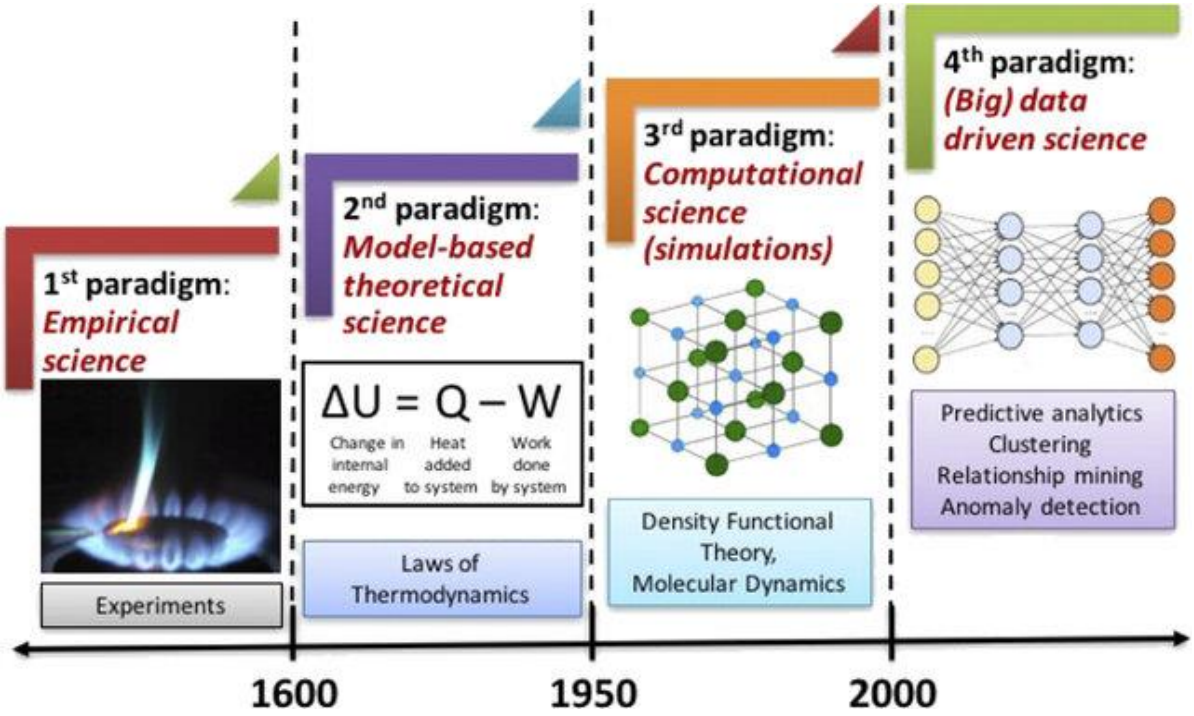


		Base Planck units
Name	**Dimension**	**Expression**
Planck length	Length (L)	$l_\mathrm{P} = \sqrt{\frac{\hbar G}{c^3}}$
Planck mass	Mass (M)	$m_\mathrm{P} = \sqrt{\frac{\hbar c}{G}}$
Planck time	Time (T)	$t_\mathrm{P} = \frac{l_\mathrm{P}}{c} = \frac{\hbar}{m_\mathrm{P} c^2} = \sqrt{\frac{\hbar G}{c^5}}$
Planck charge	Electric charge (Q)	$q_\mathrm{P} = \sqrt{4\pi\varepsilon_0 \hbar c}$
Planck temperature	Temperature (Θ)	$T_\mathrm{P} = \frac{m_\mathrm{P} c^2}{k_\mathrm{B}} = \sqrt{\frac{\hbar c^5}{G k_\mathrm{B}^2}}$

Table 1. The seven defining constants of the SI and the seven corresponding units they define

Defining constant	Symbol	Numerical value	Unit
hyperfine transition frequency of Cs	$\Delta\nu_{\mathrm{Cs}}$	9 192 631 770	Hz
speed of light in vacuum	c	299 792 458	m s^{-1}
Planck constant	h	$6.626\,070\,15 \times 10^{-34}$	J s
elementary charge	e	$1.602\,176\,634 \times 10^{-19}$	C
Boltzmann constant	k	$1.380\,649 \times 10^{-23}$	J K^{-1}
Avogadro constant	N_A	$6.022\,140\,76 \times 10^{23}$	mol^{-1}
luminous efficacy	K_{cd}	683	lm W^{-1}

4 SCIENTIFIC PARADIGMS



DOI: 10.1063/1.4946894

REPRODUCIBILITY CRISIS

Ioannidis, J. P. (2005). Why most published research findings are false. PLoS medicine, 2(8), e124.

- It can be proven that most claimed research findings are false.
- Most research findings are false for most research designs and for most fields.
- Claimed research findings may often be simply accurate measures of the prevailing bias.



Open access, freely available online

Essay

Why Most Published Research Findings Are False

John P. A. Ioannidis

Summary

There is increasing concern that most current published research findings are false. The probability that a research claim is true may depend on study power and bias, the number of other studies on the same question, and, importantly, the ratio of true to no relationships among the relationships probed in each scientific field. In this framework, a research finding is less likely to be true when the studies conducted in a field are smaller; when effect sizes are smaller; when there is a greater number and lesser preselection of tested relationships; where there is greater flexibility in designs, definitions, outcomes, and analytical modes; when there is greater financial and other interest and prejudice; and when more teams are involved in a scientific field in chase of statistical significance. Simulations show that for most study designs and settings, it is more likely for a research claim to be false than true.

factors that influence this problem and some corollaries thereof.

Modeling the Framework for False Positive Findings

Several methodologists have pointed out [9–11] that the high rate of nonreplication (lack of confirmation) of research discoveries is a consequence of the convenient, yet ill-founded strategy of claiming conclusive research findings solely on the basis of a single study assessed by formal statistical significance, typically for a *p*-value less than 0.05. Research is not most appropriately represented and summarized by *p*-values, but, unfortunately, there is a widespread notion that medical research articles

It can be proven that most claimed research findings are false.

is characteristic of the field and can vary a lot depending on whether the field targets highly likely relationships or searches for only one or a few true relationships among thousands and millions of hypotheses that may be postulated. Let us also consider, for computational simplicity, circumscribed fields where either there is only one true relationship (among many that can be hypothesized) or the power is similar to find any of the several existing true relationships. The pre-study probability of a relationship being true is $R/(R + 1)$. The probability of a study finding a true relationship reflects the power $1 - \beta$ (one minus the Type II error rate). The probability of claiming a relationship when none truly exists reflects the Type I error rate, α. Assuming that c relationships are being probed in the field, the expected values of the 2×2 table are given in Table 1. After a research finding has been claimed based on

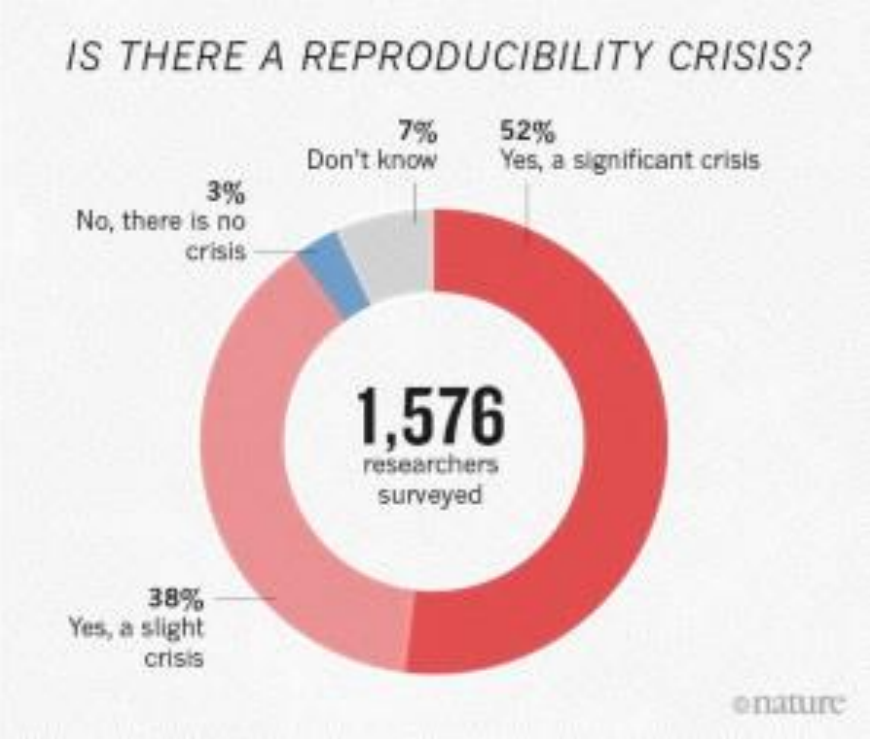
https://en.wikipedia.org/wiki/Why_Most_Published_Research_Findings_Are_False

Is Most Published Research Wrong? 6 M views, 2024

Is there a reproducibility crisis in science? 47 k views, 2017

The Replication Crisis: Crash Course Statistics #31, 107 k views, 2017

REPRODUCIBILITY CRISIS



The replication crisis

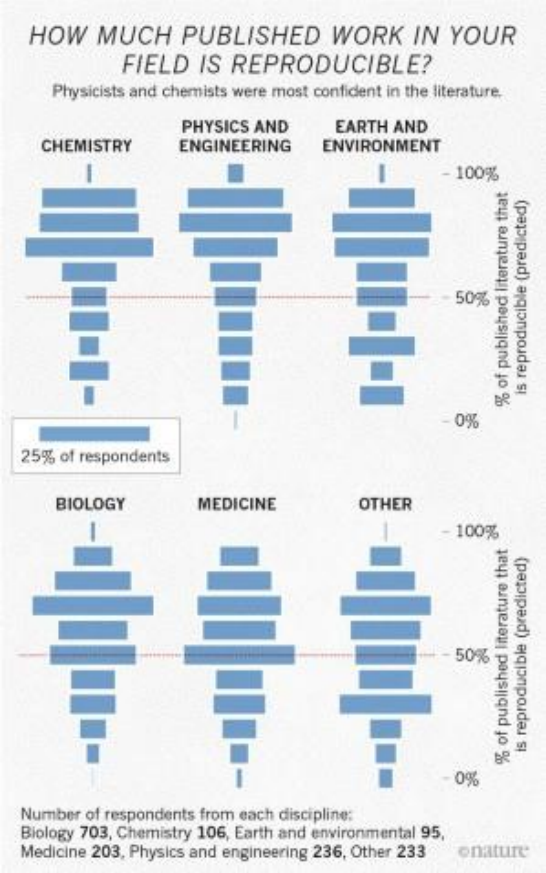
(also called the replicability crisis and the reproducibility crisis)

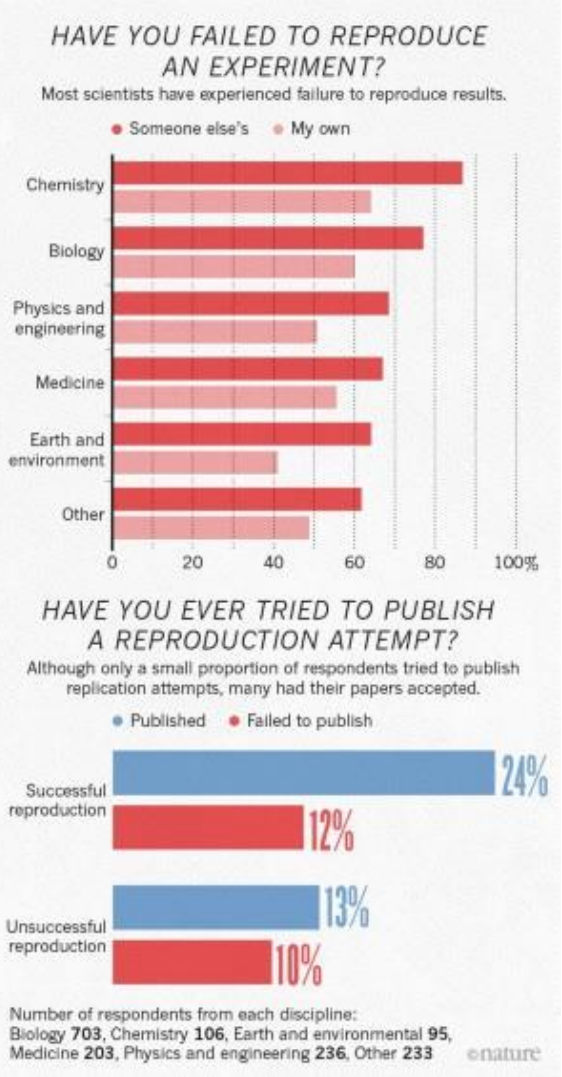
is an ongoing methodological crisis in which the results of many scientific studies are difficult or impossible to reproduce.

https://en.wikipedia.org/wiki/Replication_crisis

Baker, M. (2016). 1,500 scientists lift the lid on reproducibility. *Nature*, *533*(7604) link

REPRODUCIBILITY CRISIS





REPRODUCIBILITY CRISIS

Amgen (drug company) reproduced 6 out of 53 studies considered landmarks in basic science of cancer.
N.G. Beagley, L.M. Ellis (2012) Raise standards for preclinical cancer research, *Nature* 483, 531-533

Bayer HealthCare reproduced in house only ¼ of 67 seminal published studies.
F. Prinz et al. (2011) Believe it or not: how much can we rely on published data on potential drug targets? Nature Reviews Drug Discovery volume 10, page 712

F. Godlee, editor of *British Medical Journal:* paper with 8 important deliberate mistakes sent to 221 reviewers; not one spotted the 8 mistakes; on average, reported 2; 16%: none, 10%: 4 or more.
S. Schroter et al. (2008) What errors do peer reviewers detect, and does training improve their ability to detect them?, J R Soc Med. 2008 Oct 1; 101(10): 507–514

E. Wagner, T. Jeferson (2001) Shortcomings of peer review in biomedical journals, Learned Publishing, 14, 257-263

Pentaquark (human-made particle):
2002: a pentaquark discovered in Japan, confirmed by 10 labs but refuted by many.
2008: “a curious episode in the history of science” (*Review of Particle Physics*)
2012: another pentaquark confirmed by CERN
M. Chalmers (2015) Forsaken pentaquark particle spotted at CERN, Nature volume 523, pages 267–268 (2015)

SCIENTIFIC PUBLICATION BUSINESS

S. Buranyi (2017) Is the staggeringly profitable business of scientific publishing bad for science? The long read, *The Guardian*

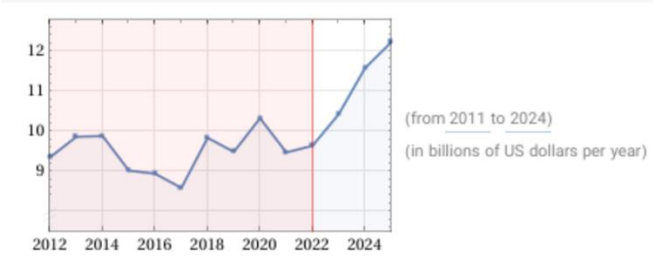
Elsevier

2010: revenue £2,000m, profit £724m, margin 36 %
margin higher than Google, Apple, Amazon
usual margin for journal: 12 – 15 %
2021: revenue £7,244m, profit £2,210m, margin 30 % (link)
2024: revenue £9,434m, profit £3,199m, margin 20.5 % (link)

Annual revenue 2022

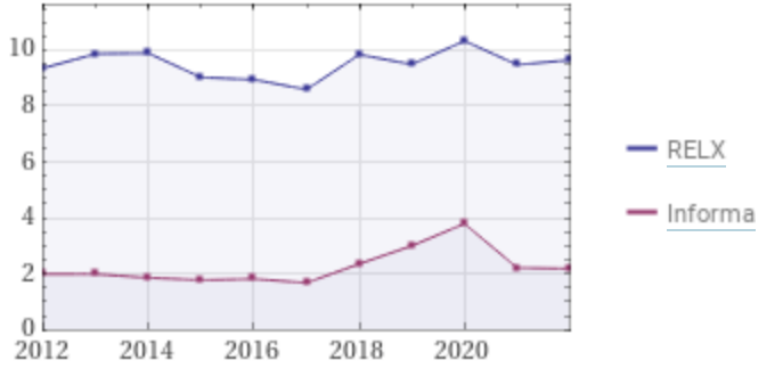
Siemens	€88.2 bn
Airbus	$70.4 bn
Renault	€20.6 bn
MGM	$9.8 bn
Elsevier (RELX)	$9.5 bn

Wolfram Alpha search: Reed Elsevier annual revenue 2000 to 2022 link.



Elsevier yearly revenue (link)

SCIENTIFIC PUBLICATION BUSINESS



(from 2011 to 2021) (in billions of US dollars per year)

Elsevier (RELX)

revenue	$9.835 billion per year
gross profit	$6.32 billion per year
net income	$1.972 billion per year
employees	33 500 people

Francis & Taylor (Informa)

revenue	$2.582 billion per year
gross profit	$1.224 billion per year
net income	$1.711 billion per year
employees	10 044 people

Wolfram Alpha search: reed elsevier vs informa plc annual revenue 2000 to 2022 link.

SCIENTIFIC PUBLICATION BUSINESS

S. Buranyi (2017) Is the staggeringly profitable business of scientific publishing bad for science? The long read, *The Guardian*

Business model:

Traditional publisher	Scientific publisher (e.g., Elsevier)
Pays writers for the articles	Scientists create work– funded largely by governments – and give it to publishers for free
Employs editors to commission, shape and check the articles	Peer review is done by working scientists on a volunteer basis
Pays to distribute the finished product to subscribers and retailers	Sells the product back to government-funded institutional and university libraries

Scientific publication is a “triple-pay” system, in which “the state funds most research, pays the salaries of most of those checking the quality of research, and then buys most of the published product”.

Deutsche Bank (2005)

SCIENTIFIC PUBLICATION BUSINESS

S. Buranyi (2017) Is the staggeringly profitable business of scientific publishing bad for science? The long read, *The Guardian*

Beginning of a success story



R. Maxwell

after 1945 – science financed by the Government
1951 – R. Maxwell buys Butterworth and Springer → Pergamon Press
convinces prominent academics: editor-in-chief of a new journal
1959: 40 journals;
1965: 150 journals;

Grand titles: *International Journal of* …
deals to publish for free
Russian Academy of Sciences' journals
Japanese scientific societies
"If a serious new journal appeared, scientists would simply request that their university library subscribe to that one as well."

"Oxford Polytechnic [now Oxford Brookes University] started a department of hospitality with a chef. We had to go find out who the head of the department was, make him start a journal. And boom – International Journal of Hospitality Management." Impact Factor: 10.427

SCIENTIFIC PUBLICATION BUSINESS

S. Buranyi (2017) Is the staggeringly profitable business of scientific publishing bad for science? The long read, *The Guardian*

Impact factor

before 1970: Scientists published to the journal best fitted for their research area.

1974 Cell: very high quality papers, rejected far more papers than it published
where you published became immensely important →
impact factor (E. Garfield, 1960, ISI Web of Science)

Science became a co-production between scientists and journal editors:
- avoid the prosaic work of confirming or disproving past studies
- favour of a middle ground: a topic popular with editors and likely to be published

PS. SCIENTIFIC PUBLICATION BUSINESS

Robert Maxwell

- 5 November 1991, Maxwell was found drowned off his yacht in the Canary Islands.

  fall, jumped, or pushed?
- had stolen more than £400m from the Mirror pension fund to service his debts

Ghislaine Maxwell

- 28/06/2022: 20 years in criminal prison (related to Jeffrey Epstein Wikipedia)
- 08/2022: former lawyer sued G Maxwell for failing to pay $878,000 in legal fees

REACTIONS

Profitability in Internet age

1998 “The Big Deal” of Elsevier: electronic access to all at a time (Cornell University paid £2m in 2009)

Share of journal: Elsevier 24% , Springer 12% Wiley 12%:
$20 - $30 consultation 1 article
Elsevier 1.5m articles per year, published 420k, of 800,000 scientists

Open access

since 2000
Alexandra Elbakyan, Kazhakstan:
Nature (2016) 10 people who most matter in science
Nature (2017) US court grants Elsevier [$15] millions in damages from Sci-Hub



PAPER PIRATE

The founder of an illegal hub for paywalled papers has attracted litigation and acclaim.

BY RICHARD VAN NOORDEN

It took Alexandra Elbakyan just a few years to go from information-technology student to famous fugitive.

In 2009, when she was a graduate student working on her final-year research project in Almaty, Kazakhstan, Elbakyan became frustrated at being unable to read many scholarly papers because she couldn't afford them. So she learnt how to circumvent publishers' paywalls.

Her skills were soon in demand. Elbakyan saw scientists on web forums asking for papers they couldn't access — and she was happy to oblige. "I got thanked many times for sending paywalled papers," she says. In 2011, she decided to automate the process and founded Sci-Hub, a pirate website that grabs copies of research papers from behind paywalls and serves them up to anyone who asks. This year, interest in Sci-Hub exploded as mainstream media cottoned on to it and usage soared. According to Elbakyan's figures, the site now hosts around 60 million papers and is likely to serve up more than 75 million downloads in 2016 — up from 42 million last year and, by one estimate, encompassing around 3% of all downloads from science publishers worldwide.

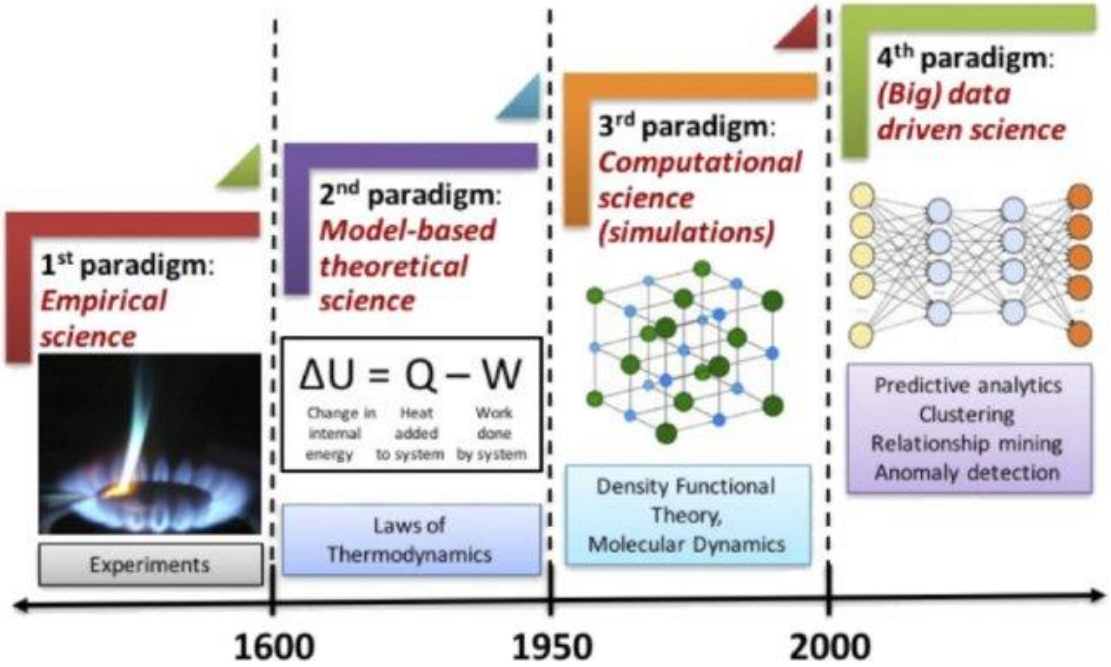
It is copyright-breaking on a grand scale — and has brought Elbakyan praise, criticism and a lawsuit. Few people support the fact that she acted illegally, but many see Sci-Hub as advancing the cause of the open-access movement, which holds that papers should be made (legally) free to read and reuse. "What she did is nothing short of awesome," says Michael Eisen,



Aaron Swartz, MIT
2010: download from JSTOR; settlement in 2011
2012: indictment 50 years imprisonment and $1m fines

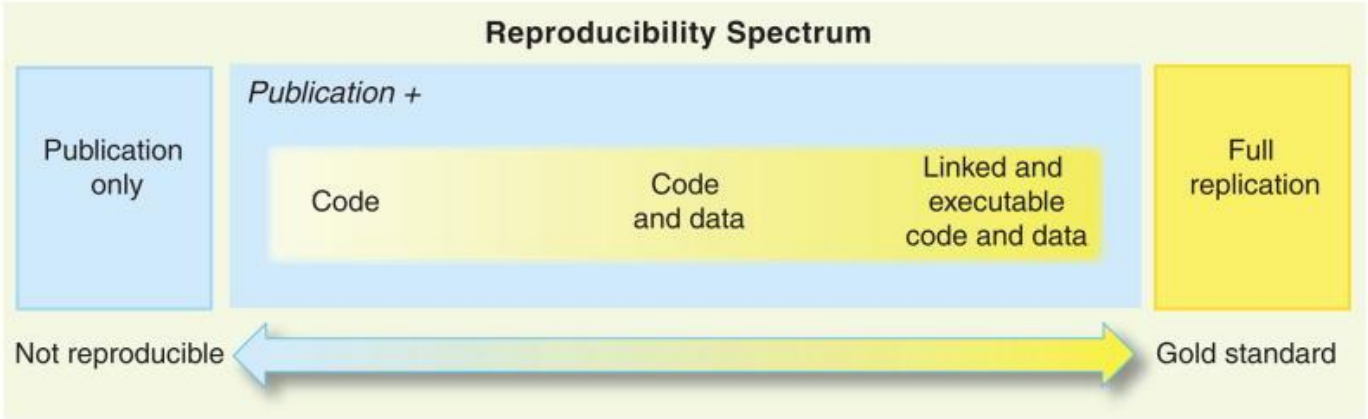
EC: Open Science Monitor: subcontractor Elsevier
Jon Tennant (2018) Elsevier are corrupting open science in Europe, The Guardian

FOUR PARADIGMS OF SCIENCE



Four paradigms of science:
empirical, theoretical, computational and data-driven (ref.)

REPRODUCTIBLE COMPUTATIONAL SCIENCE



Peng, R. D. (2011). Reproducible research in computational science. *Science*, *334*(6060), 1226-1227 link..

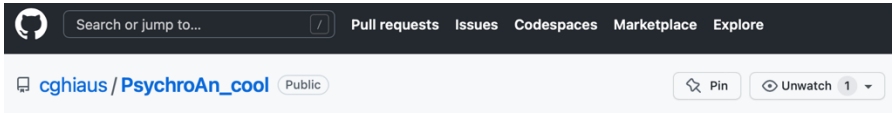
REPRODUCTIBLE SCIENCE ENVIRONMENT



Published paper



Open-access preprint



Open-access code & data

Python code and Jupyter notebooks accompanying the paper

> Christian Ghiaus (2022) Computational psychrometric analysis as a control problem: case of cooling and dehumidification systems, *International Journal of Building Performance Simulation*, 15(1), pp. 21-38, DOI: 10.1080/19401493.2021.1995498

dm4bem Dynamic Models for Building Energy Management



MOTIVATION

Dynamic thermal simulation software
(TRNSYS, EnergyPlus, IDA-ICE, Pleiades, etc.):

- widely used by professionals for building simulation

- limitations:
  - conventional models
  - use elements coupling
  - not adequate for control systems analysis and synthesis
  - reproducibility
    - graphical user interface
    - proprietary (not open source)

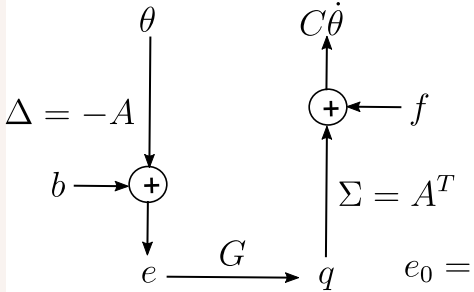
MOTIVATION

`dm4bem` (Dynamic Models for Building Energy Management):

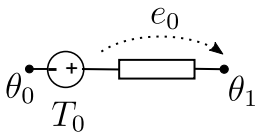
- Python module:
  - open source
  - reproducible computational science
  - computational eco-system
- uses model assembling
- extracts the state-space representation for the whole model: control systems analysis and synthesis



COMPUTATIONAL FRAMEWORK



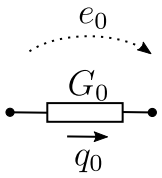
(a)



$$e_0 = (\theta_0 + T_0) - \theta_1 = (\theta_0 - \theta_1) + T_0$$

$$e = \Delta\theta + b = -A\theta + b$$

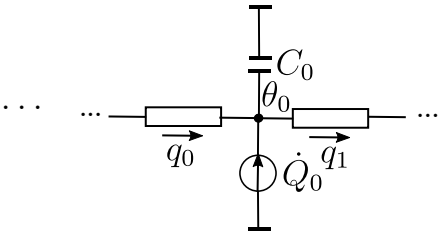
(b)



$$q_0 = G_0 e_0$$

$$q = Ge$$

(c)



$$C_0\dot{\theta}_0 = q_0 - q_1 + \dot{Q}_0$$

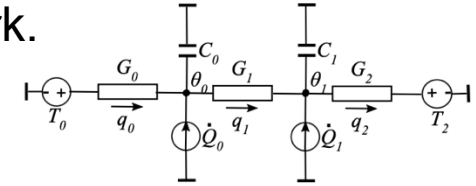
$$C\dot{\theta} = \Sigma q + f = A^T q + f$$

(d)

a) General framework.
b) Temperature differences (0 principle).
c) Flow rates by using constitutive laws (2nd principle).
d) Energy balance (1st principle).

MATRIX REPRESENTATION OF THERMAL CIRCUIT

a) Thermal network.



(a)

Legend

- conductances: G_0, G_1, G_2
- capacities: C_0, C_1
- temperature sources: T_0, T_2
- flow-rate source: $\dot{Q}_0, \dot{Q}_1$
- temperature reference
- temperature nodes: θ_0, θ_1
- flow-rate branches: q_0, q_1, q_2

b) Matrices and vectors.

$$A = \begin{array}{c} \\ q_0 \\ q_1 \\ q_2 \end{array} \begin{array}{c} \begin{array}{cc} \theta_0 & \theta_1 \end{array} \\ \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{bmatrix} \end{array} ; G = \begin{bmatrix} G_0 & 0 & 0 \\ 0 & G_1 & 0 \\ 0 & 0 & G_2 \end{bmatrix} ; b = \begin{bmatrix} T_0 \\ 0 \\ -T_2 \end{bmatrix}$$

$$C = \begin{bmatrix} C_0 & 0 \\ 0 & C_1 \end{bmatrix}$$

$$f = \begin{bmatrix} \dot{Q}_0 & \dot{Q}_1 \end{bmatrix}^T$$

$$y = \begin{bmatrix} 0 & 1 \end{bmatrix}^T$$

(b)

- A incidence matrix
- G conductance matrix
- C capacity matrix
- b temperature source vector
- f flow-rate source vector
- y output temperature vector

c) Differential-algebraic equations.

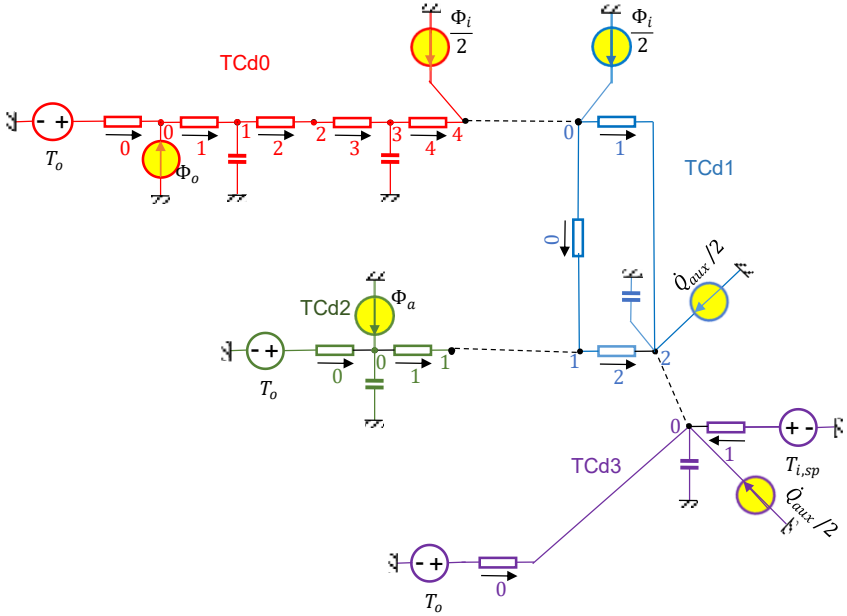
$$\begin{cases} C\dot{\theta} = -A^T G A\theta + A^T G b + f \\ q = G(-A\theta + b) \end{cases}$$

(c)

ASSEMBLING THERMAL CIRCUITS

Problem statement:

Given a number of thermal circuits, $TC_1, TC_2, \ldots, TC_n$ and knowing that some of their nodes are in common, find the assembled thermal circuit TC.



STATE SPACE REPRESENTATION

$$C\dot{\theta} = K\theta + K_b b + f \quad \Rightarrow \quad \begin{aligned} \dot{\theta}_C &= A_s\theta_C + B_s u \\ \theta_a &= C_s\theta_C + D_s u \end{aligned}$$

$$\begin{bmatrix} 0 & 0 \\ 0 & C_C \end{bmatrix} \begin{bmatrix} \dot{\theta}_0 \\ \dot{\theta}_C \end{bmatrix} = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_C \end{bmatrix} + \begin{bmatrix} K_{b1} \\ K_{b2} \end{bmatrix} b + \begin{bmatrix} I_{11} & 0 \\ 0 & I_{22} \end{bmatrix} \begin{bmatrix} f_0 \\ f_C \end{bmatrix}$$

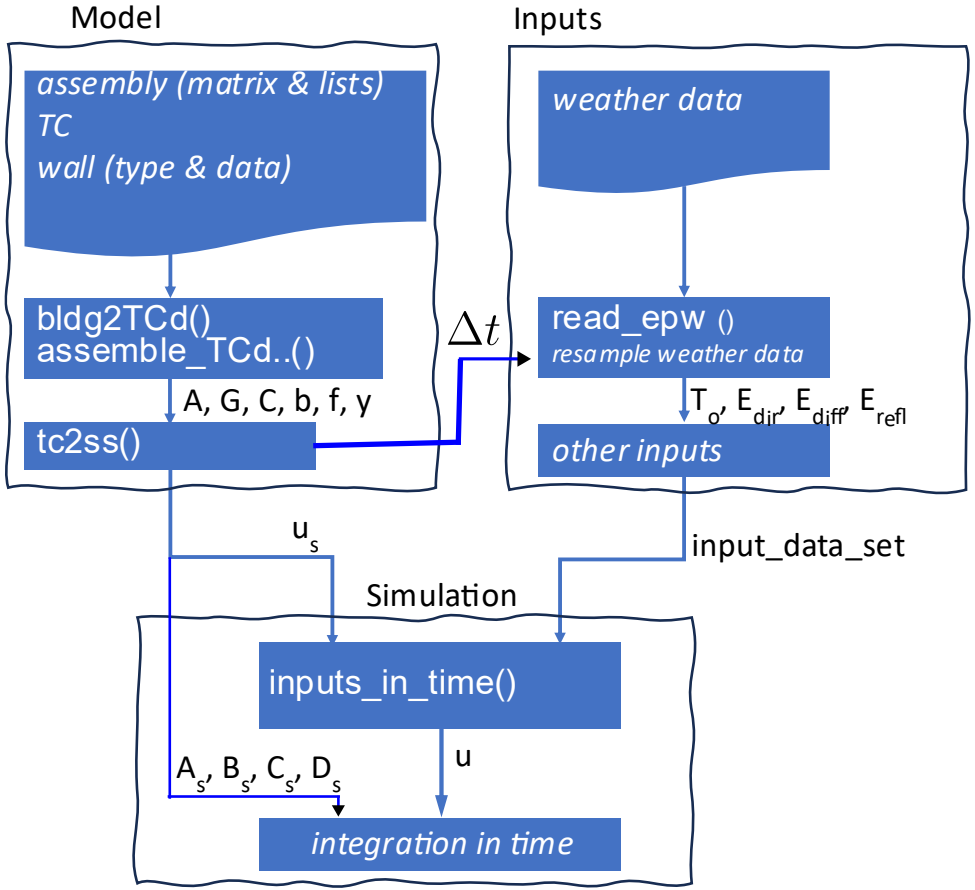
$$A_s = C_C^{-1}(-K_{21}K_{11}^{-1}K_{12} + K_{22})$$

$$B_s = C_C^{-1}\begin{bmatrix} -K_{21}K_{11}^{-1}K_{b1} + K_{b2} & -K_{21}K_{11}^{-1} & I_{22} \end{bmatrix}$$

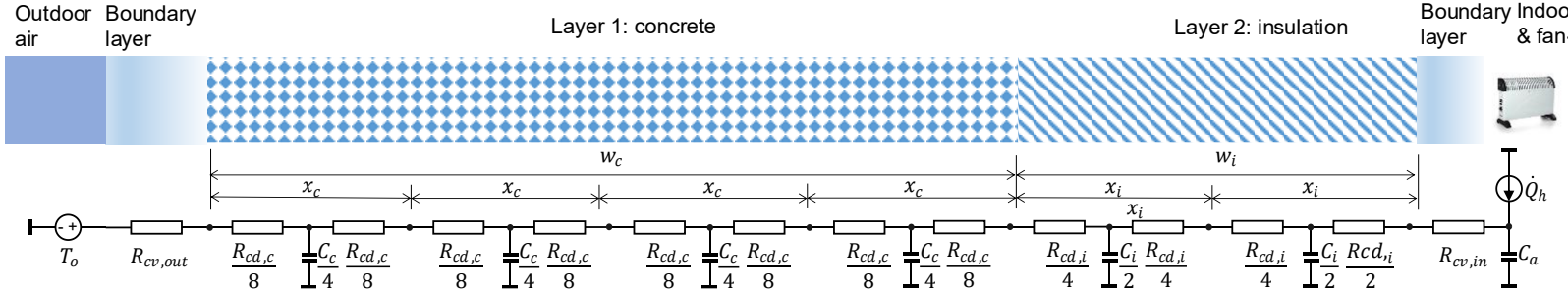
$$C_s = -K_{11}^{-1}K_{12}$$

$$D_s = -K_{11}^{-1}\begin{bmatrix} K_{b1} & I_{11} & 0 \end{bmatrix}$$

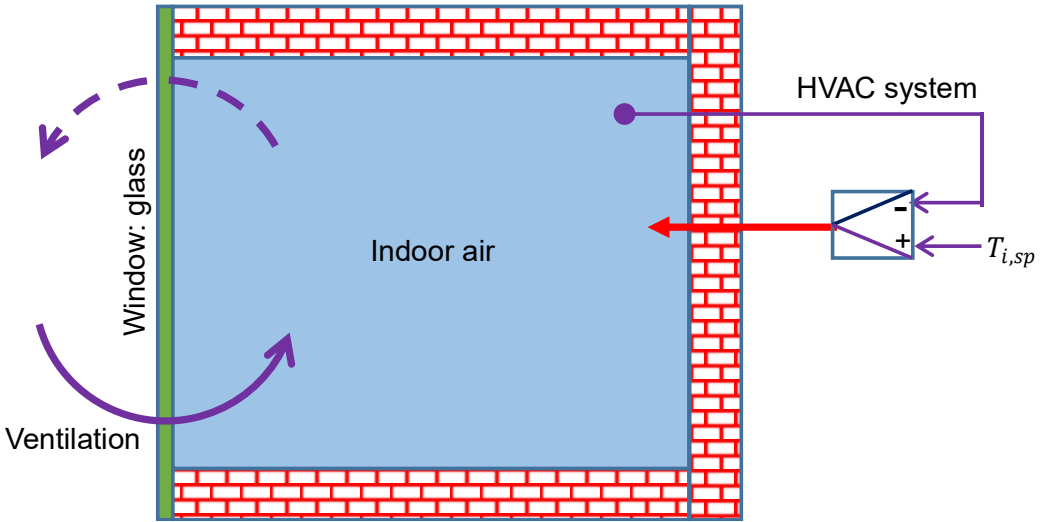
WORKFLOW


Model
Inputs
assembly (matrix & lists)
TC
wall (type & data)
weather data
bldg2TCd()
assemble_TCd..()
A, G, C, b, f, y
tc2ss()
Δt
read_epw ()
resample weather data
T_o, E_dir, E_diff, E_refl
other inputs
u_s
input_data_set
Simulation
inputs_in_time()
u
A_s, B_s, C_s, D_s
integration in time

EXAMPLES: SIMPLE WALL, TOY MODEL



Wall: concrete & insulation



INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON

THANK YOU FOR YOUR ATTENTION

Christian Ghiaus