Maxwell's Core Equations

Exact, Universal, and Scary

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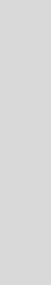
COMPUTATIONAL AND APPLIED MATH SEMINAR

Presented March 29, 2021

Thanks to

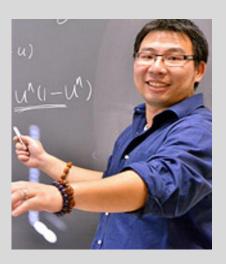
Arkadz Kirshtein, James Alder and Xiaozhe Hu for the invitation and interest

Tufts Math Department









Abstract

DOI: 10.13140/RG.2.2.24122.31687

When the Maxwell equations are written without a dielectric constant, they are universal and exact, for biological and technological applications, from inside atoms to between stars. Dielectric and polarization phenomena need then to be described by stress strain relations for charge, that show how charge redistributes when the electric field is changed, in each system of interest.

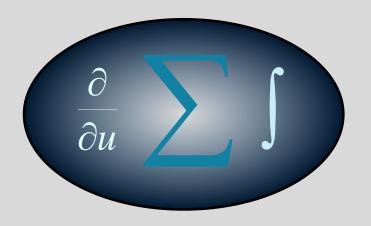
Conservation of total current (including the ethereal displacement current $\varepsilon_0 \partial E/\partial t$) is then as exact as the Maxwell equations themselves and independent of any property of matter. It is a consequence of the Lorentz invariance of the elementary charge, a property of all locally inertial systems, described by the theory of relativity.

Exact Conservation of Total Current allows a redefinition of Kirchhoff's current law that is itself exact. In unbranched systems like circuit components or ion channels, conservation of total current becomes equality. Spatial dependence of total current disappears in that case. Hopping phenomena disappear. Spatial Brownian motion disappears. The infinite variation of a Brownian model of thermal noise becomes the zero spatial variation of total current.

Maxwell's Core Equations become a perfect (spatial) low pass filter.

An Exact and Universal theory of Electrodynamics is a scary challenge to scientists like me, trained to be skeptical of all sweeping claims to perfection.

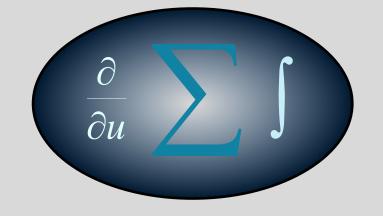
April 11, 2021 3



Mathematics describes only a tiny part of life,







Mathematics* Creates
our
Standard of Living

Electronics, Electricity, Computers, Mobile Phones, TV, Games

and Fluid Dynamics, Optics, Structural Mechanics,

Essence of Electrodynamics is Maxwell's Core Equations

Flows and Forces of Charge and Current in matter and space

Nearly Exact and Universal from Stars to inside atoms

Eisenberg, Oriols, and Ferry (2017) Dynamics of Current, Charge, and Mass.

Molecular Based Mathematical Biology 5:78-115 and arXiv preprint https://arxiv.org/abs/1708.07400.

Maxwell's Core Equations

Describe Electricity with errors <10-6

in biological and technological applications

$$\operatorname{div} \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

$$div B = 0$$

$$\mathbf{curl}\,\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\mathbf{curl} \; \mathbf{B} = \mu_0 \left(\mathbf{J} + \, \varepsilon_0 \, \frac{\partial \mathbf{E}}{\partial t} \right)$$

E is electric field, B is magnetic field

J is the current of all mass, including brief dielectric transients of the **P** and **D** fields

 ρ is charge density (of all types, including dielectric charge of the **P** and **D** fields)

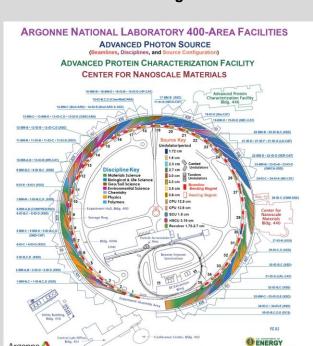
 ε_0 is the permittivity of a vacuum

 μ_0 is the permeability of a vacuum

$$(\mu_0 \varepsilon_0)^{-0.5}$$
 = velocity of light (!)



Advanced Photon Source Argonne National Laboratory



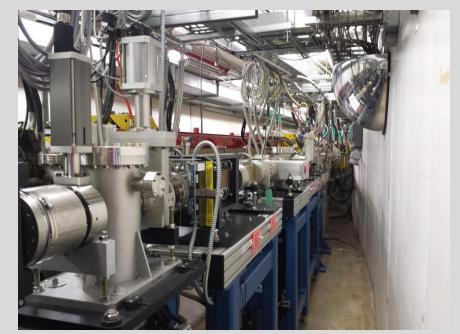
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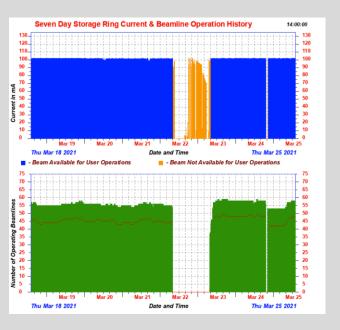
Argonne 📤

$\begin{array}{c} \text{Error in Theory} \\ < 10^{-10} \end{array}$

Beam $\sim 10^{10}$ eV Beam length 10^3 m Tolerance $< 10^{-7}$ m Beam Current 100 mA Beam Power 10^9 watts







Source Internet

8

Richard Feynman

"Whenever you see a **sweeping statement** that a tremendous amount can come from a very small number of assumptions, **You always find that it is False**

There are usually a large number of **Implied Assumptions**that are far from obvious if you think about them sufficiently carefully."

Section 26-1.

The Feynman Lectures on Physics, Mainly Electromagnetism and Matter 1963 also at http://www.feynmanlectures.caltech.edu/II_toc.html

CHALLENGE TO THE AUDIENCE

Find and Discuss the Implied Assumptions in this Talk

Contact me at Bob.Eisenberg@gmail.com

April 11, 2021 9

Maxwell's Core Equations are Universal and Exact

But they are Complicated Differential Equations

need very complicated mathematics to describe universal physics

Electro 'statics'

$$abla \cdot \mathbf{E} = \frac{oldsymbol{
ho}}{oldsymbol{arepsilon}_0}$$

Electrodynamics

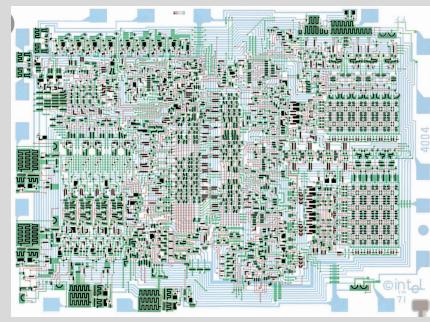
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

Magneto 'statics'

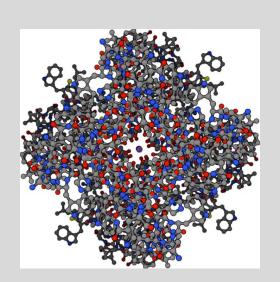
$$\nabla \cdot \mathbf{B} = 0$$

Magnetodynamics

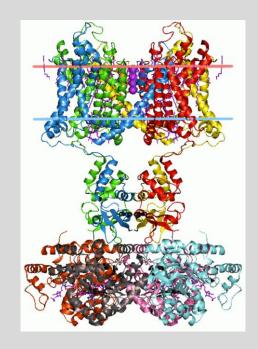
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$$



Integrated Circuit



Potassium Ion Channel $K_{V_{1,2}}$ PDB: 1BL8



or

Don't Recognize these Maxwell Equations?

" ... if we exhibit in every case all the charges, whatever their origin, the equations are always correct ...

The fundamental equations for *E* ... represent our deepest and most complete understanding of electrostatics."

Section 10-4 Feynman, Leighton, and Sands (1963) *The Feynman: Lectures on Physics, Vol. 2 Mainly Electromagnetism and Matter*.

http://www.feynmanlectures.caltech.edu/II_toc.html

$$div E = \frac{\rho}{\varepsilon_0}$$

$$div B = 0$$

Relativistic
Property of
Space
NOT matter

$$\mathbf{curl} \; \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\mathbf{curl} \; \mathbf{B} = \mu_0 \left(\mathbf{J} + \; \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$$

E is electric field, B is magnetic field

J is the current of all mass, including brief dielectric transients of the **P** and **D** fields ρ is charge density (of all types)

Where is the dielectric constant ε_r ? more later

Corollaries of Maxwell's Core Equations

Derivation of the **Continuity Equation** Linking Flux and Content

curl
$$\mathbf{B} = \mu_0 \underbrace{\int \mathbf{J}(x,t) + \varepsilon_0 \, \partial \mathbf{E}/\partial t}$$

div curl $\mathbf{B} = 0 = \mu_0 \, \mathbf{div}(\mathbf{J}(x,t) + \varepsilon_0 \, \partial \mathbf{E}/\partial t)$
div $\mathbf{J}(x,t) = -\varepsilon_0 \, \mathbf{div} \, (\partial \mathbf{E}/\partial t) = -\varepsilon_0 \, \partial (\mathbf{div} \, \mathbf{E})/\partial t$
But $\mathbf{div} \, \mathbf{E} = \rho/\varepsilon_0$

$$\mathbf{div} \, \mathbf{J} = -\partial \rho/\partial t$$

Corollaries of Maxwell's Core Equations

Continuity Equation

Linking Flux and Content

$$\mathbf{div}\,\mathbf{J} = -\frac{\partial \rho}{\partial t}$$

Question for Students
This is not a useful equation on atomic scale
Why?

Continuity Equation

Linking Flux and Content

Feynman's Hidden Implications



$$\mathbf{div}\,\mathbf{J} = -\frac{\partial \rho(x,y,z|t)}{\partial t}$$

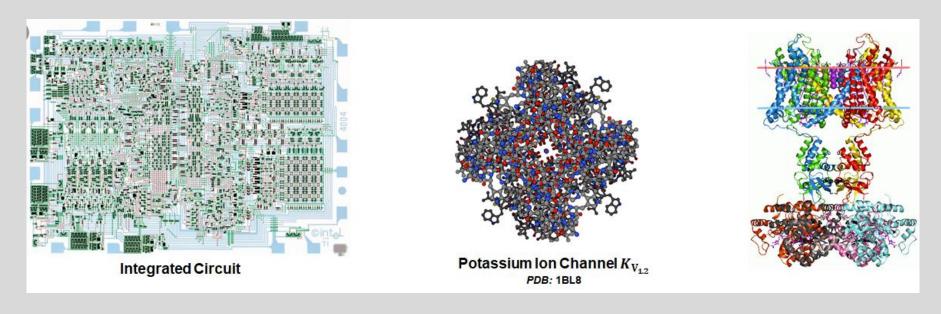
Must know all charges $\rho(x, y, z|t)$

at all times

Continuity Equation Feynman's Hidden Implications

Must know all charges and how they move

$$\mathbf{div}\,\mathbf{J} = -\frac{\partial \mathring{\rho}(x,y,z|t)}{\partial t}$$



15

Hopeless, if one must

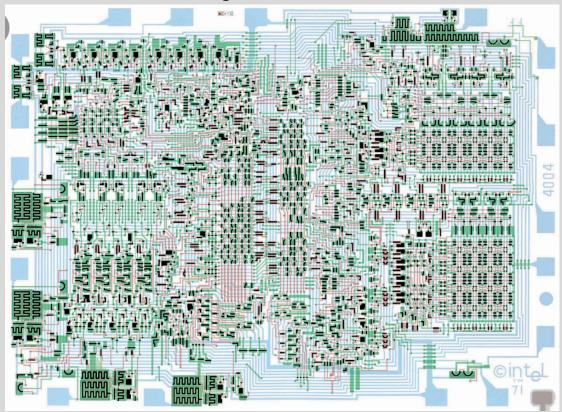
"... exhibit in every case all the charges, whatever their origin" at all times

Section 10-4 of Feynman, Leighton, and Sands (1963) vol. 2 *Electromagnetism and Matter*

Without Conservation of Current Need to Know ALL charges at all times!!

Hopeless in large systems where all ions interact with each other!

integrated circuit



Source: textbooks and internet

Seems Hopeless

Fortunately, it is not hopeless

Stay Tuned

Kirchhoff's Current Law Brings hope

It is NOT necessary in computers to know all the charges!

Kirchhoff's Current law is (almost) enough

April 11, 2021 19

Corollaries of Maxwell Equations

Conservation of Current

Linking Current and Electric Field

curl
$$\mathbf{B} = \mu_0 (\mathbf{J} + \varepsilon_0 \partial \mathbf{E} / \partial t)$$

div curl
$$\mathbf{B} = \mathbf{0} = \mu_0 \mathbf{div} (\mathbf{J} + \varepsilon_0 \partial \mathbf{E} / \partial t)$$

Total Current = J_{total}

$$div J_{total} = 0$$

J = Flux of All Charges with mass, however small or transient

Corollaries of Maxwell Equations Conservation of Total Current

$$div J_{total} = 0$$

Notice: there are ZERO adjustable or vaguely defined parameters J, E, J_{total} are routinely measured in laboratories

Scary



Scientists are Taught to be Skeptical

Particularly of Universal Exact Theories as they should be!





Richard Feynman

"Whenever you see a **sweeping statement** that a tremendous amount can come from a very **small number of assumptions**, **You always find that it is False.**

There are usually a large number of **Implied Assumptions**

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The Feynman Lectures on Physics Vol 2 (1963) also at http://www.feynmanlectures.caltech.edu/II_toc.html





Challenge to Audience What are implied assumptions? in Conservation of Total Current and Core Maxwell Equations

Contact Bob. Eisenberg @gmail.com



Challenge to Audience

What are implied assumptions?

Hint:

Look at usual formulation of Maxwell Equations

Textbook formulation of Maxwell Equations Depends on Dielectric Properties

$$\operatorname{div} \mathbf{D} = \operatorname{div} \boldsymbol{\varepsilon_r} \varepsilon_0 \mathbf{E} = \rho_f$$

$$\frac{1}{\mu_0} \operatorname{curl} \mathbf{B} = \tilde{\mathbf{J}} + \boldsymbol{\varepsilon_r} \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$
Relativistic Property of Space NOT matter

Bold red means dangerously oversimplified: \mathbf{D} , $\tilde{\mathbf{J}}$, $\boldsymbol{\varepsilon_{\mathbf{r}}}$, ρ_f

What is a Dielectric? What is Polarization?

Mechanical Systems need model of how force changes mass distribution

Stress Strain Relation is needed in mechanics

Hooke's law or its time dependent and nonlinear generalizations

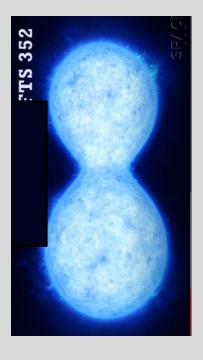
Electrical Systems need model of how electrical force changes charge distribution

Polarization is Stress Strain of Charge

Model of dielectric and its time dependent and nonlinear generalizations

Mechanical Systems need Model of how Force changes Mass distribution

STRESS STAIN RELATION is needed in models of mechanics

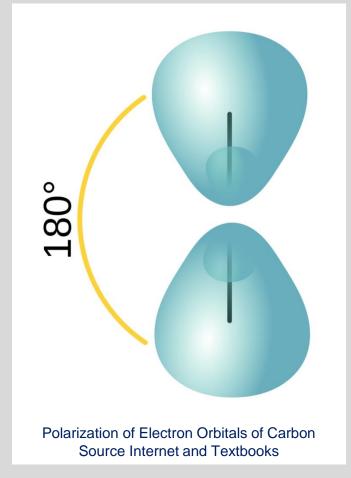


Gravitational Field Distorts Shape of Stars

Double Star VFTS 352

Source Internet

Electric Force Moves Charge so Electric Force Changes ρ Polarization is Stress Strain of Charge



Polarization is almost never ideal It always depends strongly on time It often depends on the electric field

Source Internet

Polarization

is the Electrical Analog of the STRESS STRAIN relationship of Mechanics

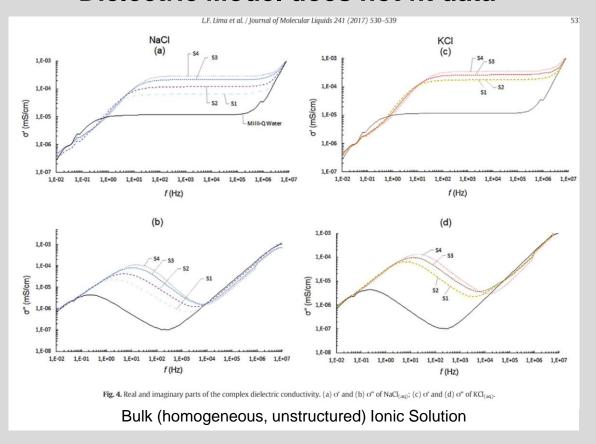
Polarization is the change in Charge Distribution when Electric Force changes

Polarization depends on time

because charge takes time to move

Polarization cannot be described by a dielectric constant independent of time

Dielectric Model does not fit data



Electrical Systems need Models of how electrical force changes charge distribution

Electrical Systems need Model of How Electrical Force changes Charge Distribution

Dielectric Model does <u>not</u> fit data from Proteins

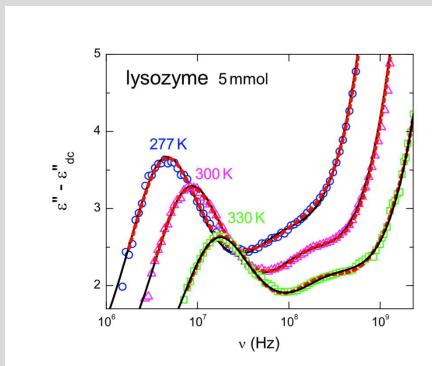
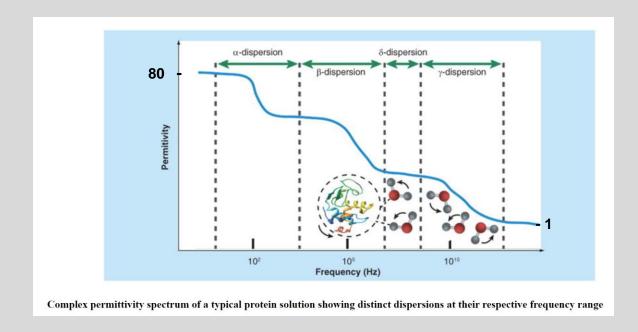


Fig. 3. Dielectric-loss spectra of a 5 mmol lysozyme solution in the region of the β - and δ -relaxations at different temperatures. The solid lines are fits using the sum of a Debye function for the β -relaxation and two Cole–Cole functions for the δ - and γ -relaxations. Dashed lines represent fits with four Debye functions according to Ref. [4].

Wolf, Gulich, Lunkenheimer & Loidl. 2012. Biochimica et Biophysica Acta (BBA) – Proteins and Proteomics 1824:723-730.



Move the physics of dielectrics into J and ρ to make Maxwell's Core Equations

$$\operatorname{div} \mathbf{E} = \frac{\rho}{\varepsilon_0} \qquad \operatorname{div} \mathbf{D} = \operatorname{div} \underbrace{\varepsilon_r \varepsilon_0 \mathbf{E}} = \rho_f$$

$$\frac{1}{\mu_0} \mathbf{curl} \, \mathbf{B} = \mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \qquad \frac{1}{\mu_0} \mathbf{curl} \, \mathbf{B} = \mathbf{J} + \boldsymbol{\varepsilon_r} \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

Polarization is part of J and ρ

When nothing is known about polarization, it is customary and appropriate to include the dielectric constant ε_r as a single real positive constant $\varepsilon_r \ge 1$

Maxwell's Core Equations

Describe Electricity with no errors, <10-6

in any technological situation

$$\operatorname{div} \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

$$\mathbf{curl} \, \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$div B = 0$$

$$\mathbf{curl} \; \mathbf{B} = \mu_0 \left(\mathbf{J} + \, \varepsilon_0 \, \frac{\partial \mathbf{E}}{\partial t} \right)$$

Implicit Assumptions are ONLY in ho

Relativistic Property of Space NOT matter

NO Implicit Assumptions in Conservation of Total Current

$$\mathbf{div} \, \mathbf{J_{total}} = 0$$

 $\operatorname{div}\left(\mathbf{J}+\,\varepsilon_0\,\partial\mathbf{E}/\partial t\right)=0$

Flux of all charge with mass

ρ does not appear No adjustable parameters

J and E and J_{total} are routinely measured in laboratories!!!

Relativistic Property of Space NOT matter

Conservation of Total Current

 $div J_{total} = 0$

ρ does not appear No adjustable parameters

J and E and J_{total} are routinely measured in laboratories!!!

Scary: nothing to Adjust

No implicit parameters or assumptions are visible Audience:

Can you find any? Contact Bob. Eisenberg @gmail.com



Scientists are Taught to be Skeptical

Particularly of Universal Exact Theories as they should be

but

Conservation of Total Current appears to be Universal and Exact

Independent of all properties of matter and charge

Conservation of Total Current is NOT a theory of everything

Conservation only describes **Total Current** J_{total}

When flux J of charge is important, conservation of current is not enough

$$\operatorname{div}\left(\underbrace{\frac{\partial \mathbf{E}}{\mathbf{J} + \varepsilon_0} \frac{\partial \mathbf{E}}{\partial t}}_{\mathbf{J}_{total}}\right) = 0$$

$$\implies$$
 div J \neq 0

Conservation only describes **Total Current** J_{total}

When flux J of charge or charge movement is important, conservation of current is not enough

$$\operatorname{div}\left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right) = 0 \quad \Longrightarrow \quad \operatorname{div} \mathbf{J} \neq \mathbf{0}$$

$$\operatorname{div} \mathbf{J} = -\operatorname{div}\left(\varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right) \neq \mathbf{0}$$

Flux J of charged matter is NOT NOT NOT conserved

$$\operatorname{div}\left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right) = 0 \quad \Longrightarrow \quad \operatorname{div} \mathbf{J} \neq \mathbf{0}$$

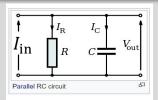
Maxwell core Equations imply that

Charge and Matter accumulate because $\varepsilon_0 \frac{\partial E}{\partial t} \neq 0$

$$\operatorname{div} \mathbf{J} = -\varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \neq 0$$

In physical language of electronics,

Some charge accumulates in the 'stray capacitance'
of space
independent of matter

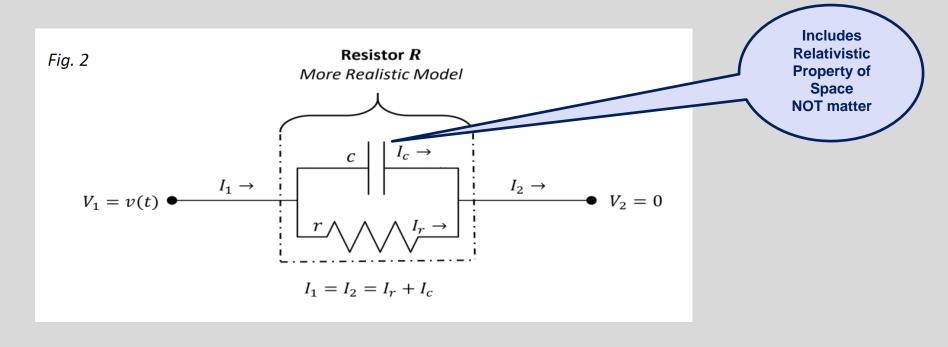


$$V_{out} = I_{in}(1 - e^{-t/RC})$$

Relativistic Property of Space NOT matter

In language of electronics Flux of electrons into a Resistor does NOT equal Flux of electrons out of Resistor

Total Current I_1 into a Resistor DOES EQUAL the **Total** Current I_2 out of a Resistor

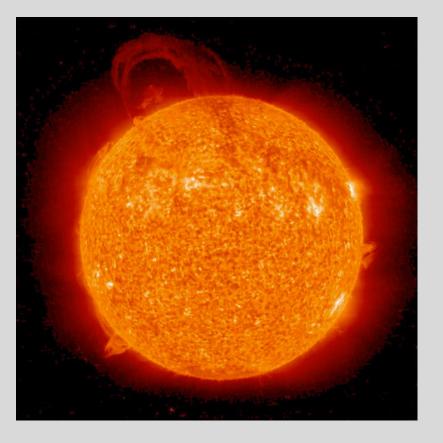


Eisenberg, B., N. Gold, Z. Song, and H. Huang. 2018. What Current Flows Through a Resistor? arXiv preprint arXiv:1805.04814. Eisenberg, R. S. 2019. Kirchhoff's Law can be Exact. arXiv preprint available at https://arxiv.org/abs/1905.13574.

Electromagnetic Field Exists in Vacuum

where $\rho = 0$ and J = 0 and c = 0 velocity of light because of the relativistic properties space

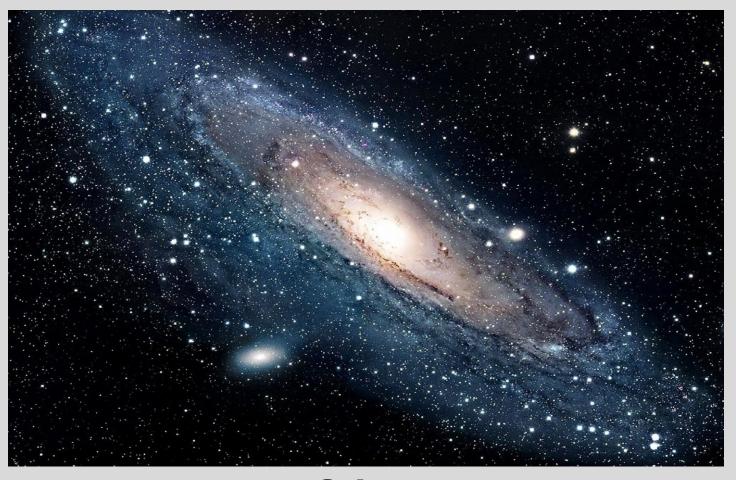
$$\begin{array}{ll} \operatorname{\mathbf{div}} \mathbf{E} = \mathbf{0} & \operatorname{\mathbf{div}} \mathbf{B} = \mathbf{0} \\ \\ \operatorname{\mathbf{curl}} \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} & \operatorname{\mathbf{curl}} \mathbf{B} = \underbrace{\mu_0 \varepsilon_0}_{\text{Ethereal Current}} \underbrace{\partial \mathbf{E}/\partial t}_{\text{Ethereal Current}} = c^{-2} \underbrace{\partial \mathbf{E}/\partial t}_{\text{Space NOT matter}} \\ \\ \operatorname{\mathbf{Derivation}} \text{ of Wave Equation is in every textbook, starting with curl curl E} \end{array}$$



The Sun with Prominence

Source Internet

Light travels through the Vacuum of Space



Conservation of Total Current J_{total}

S

Universal and Exact because

It is a Property of Space

 $\partial E/\partial t$ in a perfect vacuum produces B field

Not a property of matter It arises from the Principle of Relativity

every textbook and Dunstan, D. (2008) Phil Trans Roy Soc A: 366 1861

Charge does not vary when velocity → speed of light Length, time, and (relativistic) Mass, do vary

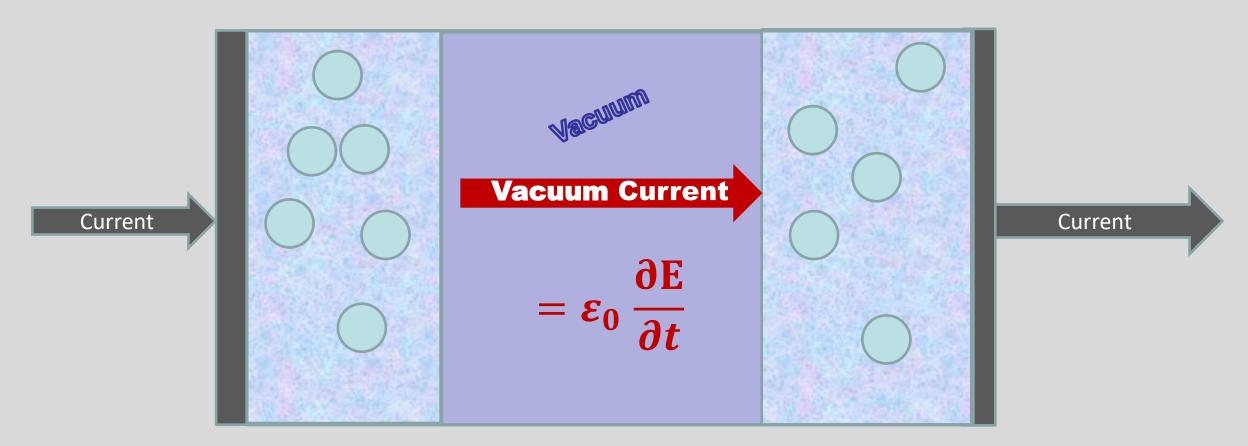
Conservation of Total Current J_{total}

An example of Feynman's Hidden Factor Property of Space not matter

That is why it is Universal and Exact

Well known Example

Taught,
or should be taught,
In First Year of Physics



Vacuum current = Ethereal current = Displacement Current All are names for the same thing $\varepsilon_0 \partial E/\partial t$

Conservation of Current is Exact and Universal **So what?**

Total Current J_{total} must always be described by Continuum Equations

Particle motion J itself does NOT define Current J_{total}

Contradicts Intuition

Current $J_{total} \neq Flux$ of charge JFlux J is defined by only particle motion Total Current J_{total} is not defined by particle motion alone Not Widely Known
Not Widely Known

Contradicts Intuition

Small Systems REQUIRE

Continuum Description

of

Electric Current

Total Current J_{total} does NOT flow by hopping

Current is independent of location in series systems

Particle Motion can be hopping, not current

Well known in Electronics

"Hopping Models Ignore Capacitive Currents"

Paraphrase from Landauer (1992)
Conductance from transmission: common sense points.
Physica Scripta 1992 p.110



Eisenberg, B., N. Gold, Z. Song, and H. Huang. 2018. What Current Flows Through a Resistor? arXiv preprint arXiv:1805.04814.
Eisenberg, R. S. 2019. Kirchhoff's Law can be Exact. arXiv preprint available at https://arxiv.org/abs/1905.13574.

Contradicts Intuition

Small Systems REQUIRE

Continuum Description

Total Current J_{total} does NOT flow by hopping

Current J_{total} is independent of location in series systems

Particle Motion J can be hopping, not total current J_{total}

Well known in Electronics

"Hopping Models Ignore Capacitive Currents"

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Conservation of Total Current J_{total} is EQUALITY of Total Current in a Channel or Series System

Well known in Electronics

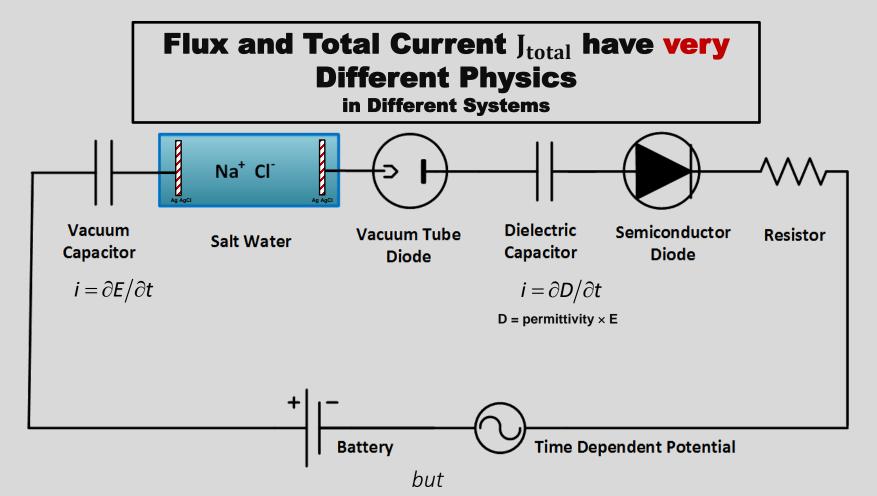
"It is, after all, the **sum** of electron current and **displacement** current which has **no divergence**.

One of those two components can take over from the other."

Landauer (1992) Physica Scripta T42 p 110.

"Electrodynamic fields are endowed by unique features, including an exquisite spatial nonlocality"

Slight paraphrase of Lundeberg *et a*l (2017) Tuning quantum nonlocal effects plasmonics Science 357:187-191



Continuity of Total Current J_{total} is Exact

 $J_{\text{total in Device 1}} = J_{\text{total in Device 2}} = J_{\text{total in Device 3}} \dots$

no matter what carries the current J at all times and all locations!

Eisenberg (2016) Mass Action and Conservation of Current.

Hungarian Journal of Industry and Chemistry Posted on arXiv.org with paper ID arXiv:1502.07251 44:1-28.

Conservation of Total Current J_{total} is Exact

even though
Physics of Charge Flow
Varies Profoundly

How can that possibly be?

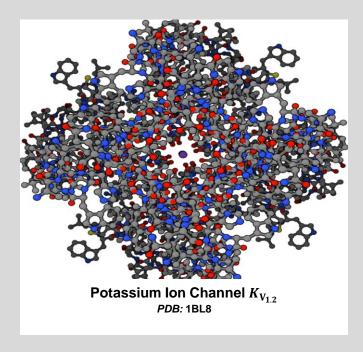
Electrodynamic Fields E, B take on the Values that Conserves total Current J_{total} This is NOT mysterious E is the force field that moves atoms

so total current $J(x,t) + \varepsilon_0 \partial E/\partial t$ is always conserved

Details and PROOF
including quantum mechanics at
Eisenberg, Oriols, and Ferry. 2017. Dynamics of Current, Charge, and Mass.
Molecular Based Mathematical Biology 5:78-115
and arXiv https://arxiv.org/abs/1708.07400

E is a force field that moves atoms

because atoms have charge



so total current $J_{total} = J(x,t) + \varepsilon_0 \partial E/\partial t$ is always conserved

Details and PROOF

including quantum mechanics at

Eisenberg, Oriols, and Ferry. 2017. Dynamics of Current, Charge, and Mass.

Molecular Based Mathematical Biology 5:78-115

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EQUALITY of Total Current J_{total} is an Enormous Simplification

Eisenberg, B., N. Gold, Z. Song, and H. Huang. 2018. What Current Flows Through a Resistor? arXiv preprint https://arxiv.org/abs/1805.04814.

Eisenberg, R. S. 2019. Kirchhoff's Law can be Exact. arXiv preprint available at https://arxiv.org/abs/1905.13574.

Current flow is very smooth in spatial coordinate

Differential equation in x is not needed for J_{total}

 $J_{total} = J + \varepsilon_0 \, \partial E / \partial t$

What does this mean for theory and simulations?

Opportunity to Simplify Algorithms and Codes perhaps dramatically

Spatial Dependence is Already Known
Only have to average the time dependence
Ma, Li and Liu (2016). arXiv:1605.04886; Ma, Li and Liu (2016). arXiv:1606.03625.

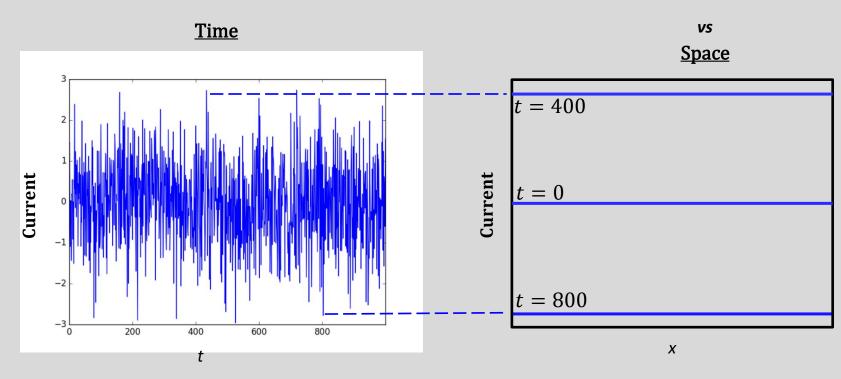
Current flow is very smooth in spatial coordinate Differential equation in x is not needed for $J_{total} = J + \epsilon_0 \partial E / \partial t$

What does this mean for theory and simulations? Opportunity to Simplify Algorithms and Codes

perhaps dramatically

Spatial Dependence is Already Known
Only have to average the time dependence
Ma, Li and Liu (2016). arXiv:1605.04886; Ma, Li and Liu (2016). arXiv:1606.03625.

Current Noise J_{total} is Zero in Space



One Dimensional Systems like Channels or Circuit Components

Current Noise

HUGE in time

Jtotal

EQUALITY of Total Current J_{total} is an Enormous Simplification

It can create a **Perfect Low Pass Filter**It can **Convert Chaos** of Brownian Motion into a **Constant**

What does this mean for Mathematical Models?

The image of total current flow J_{total} is very different VERY SMOOTH in space

Total Current J_{total} does not vary in space so Spatial Derivatives are not needed to describe total current

But they are needed to describe everything else.

Revolution in Biophysics

Total Current flow J_{total} is equal everywhere in a one dimensional channel

Thermal Motion in Space does <u>not</u> appear in equations for flow of total current J_{total} in a one dimensional channel

Thermal motion appears ONLY in time

Eisenberg (2020)
Electrodynamics Correlates Knock-on and Knock-off: Current is Spatially Uniform in Ion Channels.

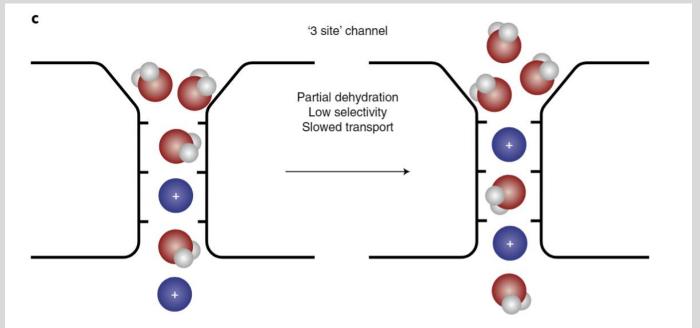
Preprint on arXiv at https://arxiv.org/abs/2002.09012.

What does this mean for Ion Channels?

Knock On and Knock Off of Ions is

IRRELEVANT for the Total Current J_{total} Through the Channel

Paradigm Change



Corry (2018) The naked truth about K⁺ selectivity. Nature Chemistry 10:799-800.

Eisenberg (2020)
Electrodynamics Correlates Knock-on and Knock-off: Current is Spatially Uniform in Ion Channels.

Preprint on arXiv at

https://arxiv.org/abs/2002.09012.

View of Channels has been focused on movements of individual ions in channels,

But

Total Current J_{total} is equal everywhere in a one dimensional channel



Position does <u>not</u> appear in equations for total current J_{total} in a one dimensional channel

References and Proofs in

Eisenberg (2019) Kirchhoff's Law can be Exact. arXiv: 1905.13574

Eisenberg, Gold, Song, and Huang (2018) What Current Flows Through a Resistor? arXiv:1805.04814

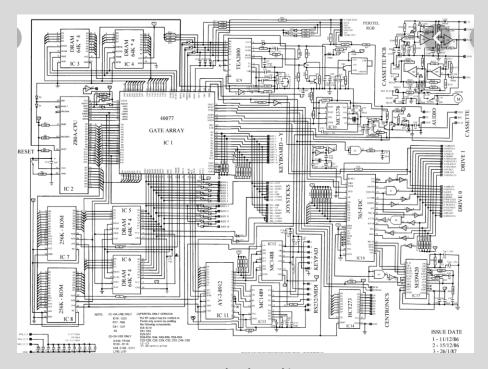
Turn from Biophysics to Electricity and Electronics And then Back to Biology

Kirchhoff's Current Law Should be for TOTAL CURRENT

References and Proofs in

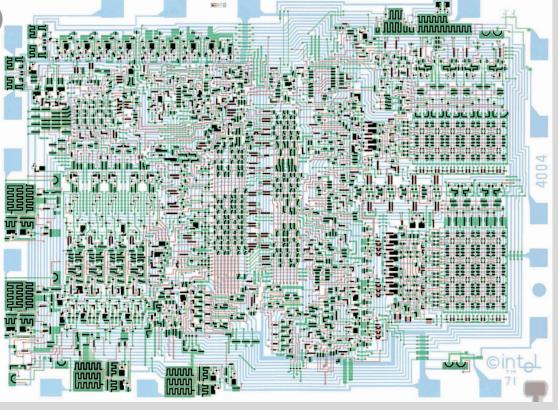
Eisenberg (2019) Kirchhoff's Law can be Exact. arXiv: 1905.13574

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What Current Flows Through a Resistor?
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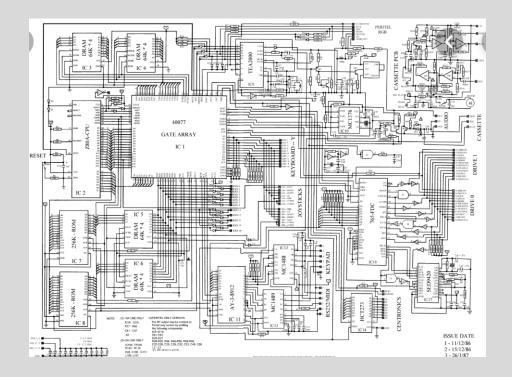


Source: textbooks and internet

It is NOT necessary in our computers to know all the charges! Kirchhoff's law is (almost) enough



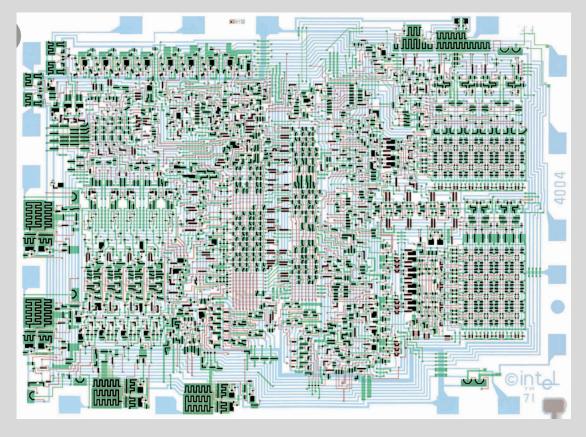
Source: textbooks and internet





Integrated Circuits are Designed with Kirchhoff's Current Law and little else!!!

Hard as that is to believe



How can that possibly be?

Usual Derivation of Kirchhoff's law is on Long Time Scale $\gg 10^{-6} sec$

NOT AT ALL at 10^{-10} sec

How can that possibly be?

Usual Derivation of Kirchhoff's law is about fluxes

BUT

FLUXES ARE NOT CONSERVED

according to experiment or Maxwell equations NOT AT ALL at $10^{-10}\,\text{sec}$

How can that be?

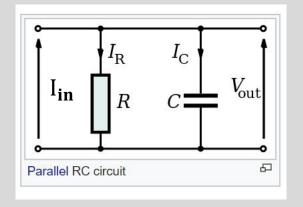
 $\begin{aligned} & \text{Maxwell div } J_{total} = 0 \\ & \text{and} \\ & \text{Kirchhoff div } J \neq 0 \end{aligned}$



DISAGREE

in usual derivation of Kirchhoff using flux J of charges

How can that possibly be?



$$V_{out} = I_{in}(1 - e^{-t/RC})$$

RC = charging time = 10^{-12} farads \times 10^{3} ohm = 10^{-9} sec FLUXES J ARE NOT CONSERVED

Kirchhoff's Laws Describe TOTAL CURRENT J_{total} Not flux JValid whenever branched network is valid And Maxwell's Core Equations are Valid

References and Proofs in

Eisenberg (2019) Kirchhoff's Law can be Exact. arXiv: 1905.13574

Eisenberg, Gold, Song, and Huang (2018)
What Current Flows Through a Resistor?
arXiv:1805.04814

Deriving Kirchhoff's Laws from Maxwell Equations

and conservation of current

is

Trivial if you use Total Current J_{total}

References and Proofs in

Eisenberg (2019) **Kirchhoff's Law can be Exact**.

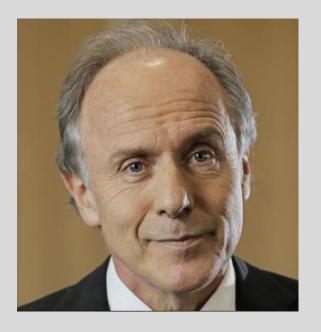
arXiv: 1905.13574

Eisenberg, Gold, Song, and Huang (2018)

What Current Flows Through a Resistor?

arXiv:1805.04814

All is obvious to a fine practicing engineer and old friend



Alan Finkel
Co-designer* of AxoPatch
Amplifier
Founder Axon Instruments,
Recently
Chief Scientist
Australian Government

"Bob, why do you need all that math?

Everyone knows how to use Kirchhoff.

Everyone knows you have to include the displacement current.

No one would try to keep track of all the charges"

Paraphrase of email exchange, with permission

Conservation of Total Current

is important in

Biology

Conservation of Current

is

Practically Important

in

Understanding

Transporters

Oxidative

Phosphorylation

Photosynthesis

main processes in life

Applying Maxwell to Transporters

Sum of Currents in a Transporter = zero in 'small cell', mitochondrion, HHK, etc.

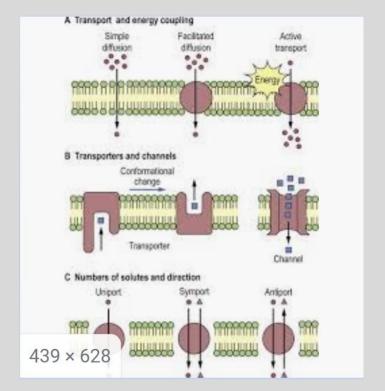
SO

Currents are Coupled in a Transporter in a 'small cell'

Currents are NOT coupled by Conservation of Current in standard bilayer setup

Liu, Hsieh, and Eisen

Source internet



Conservation of Total Current

$$\operatorname{div}\left(\operatorname{J}(x,t) + \varepsilon_0 \frac{\partial \operatorname{E}(x,t)}{\partial t}\right) = \mathbf{0}$$

Liu, Hsieh, and Eisenberg (2016)
J Phys Chem B 120:2658-2669

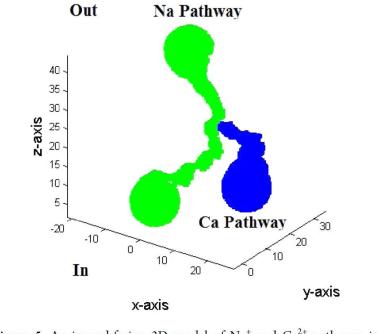
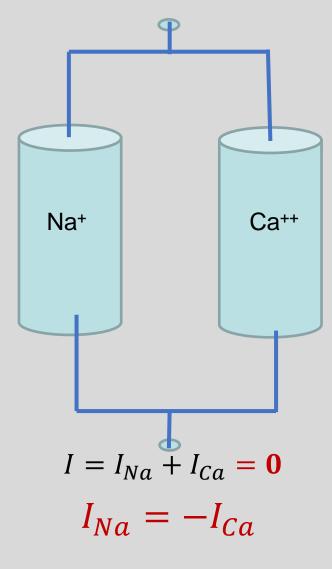


Figure 5. An inward-facing 3D model of Na⁺ and Ca²⁺ pathways in NCX.

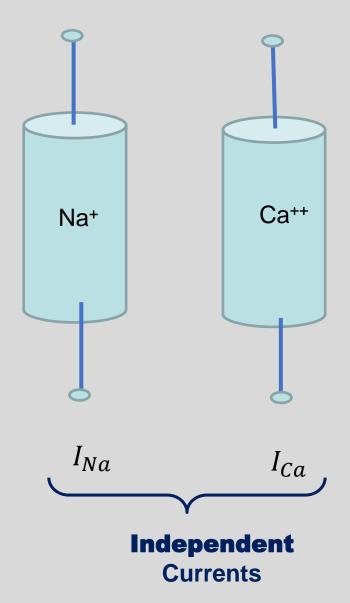
Natural Setup: small cell, etc.

Homogeneous Neumann Boundary Condition for total current Fig. 10 of Hodgkin Huxley Katz 1952



Bilayer Setup 'voltage clamp'

Inhomogeneous Dirichlet Condition for <u>Classic Voltage Clamp</u> Hodgkin Huxley 1952



Biophysical Prediction

Coupling of Transporters Depends on Setup

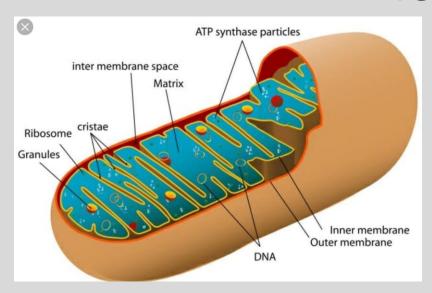
not just the transporter itself

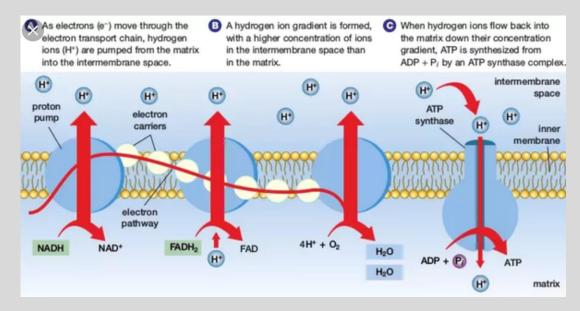
Ratio of Fluxes J_{Ca}/J_{Na} is Different in Vesicle (e.g., mitochondrion) and Bilayer

Eisenberg (2020)
Electrodynamics Correlates Knock-on and Knock-off: Current is Spatially Uniform in Ion Channels.

Preprint on arXiv at https://arxiv.org/abs/2002.09012.

Applying Maxwell To Mitochondrion





Source Internet

Depends on Conservation of Current



Without Conservation of Current Need to Know ALL charges at all times!!

Hopeless in large systems where all ions interact with each other!

NOTE

Chemical Kinetics does not conserve current, in its usual form

Does Molecular Dynamics conserve current?

With Conservation of Current no more difficult than large circuit problems

Any Questions?

April 11, 2021

Extra Slides

What are the problems with textbook Maxwell Equations?

$$\varepsilon_r \varepsilon_0$$
 is a hybrid

Polarization of Matter
$$(\epsilon_r - 1)\epsilon_0$$

 $arepsilon_r$ involves all movements of matter that do not translate mass, roughly speaking

$$(\varepsilon_r-1)\varepsilon_0$$
 is as complex as the motion of matter itself.

Seems hopeless to make a general theory

$\partial E/\partial t$ creating B field in a vacuum

is Mysterious

Electric & Magnetic Fields takes on the Value that Conserves Current

Specifically,

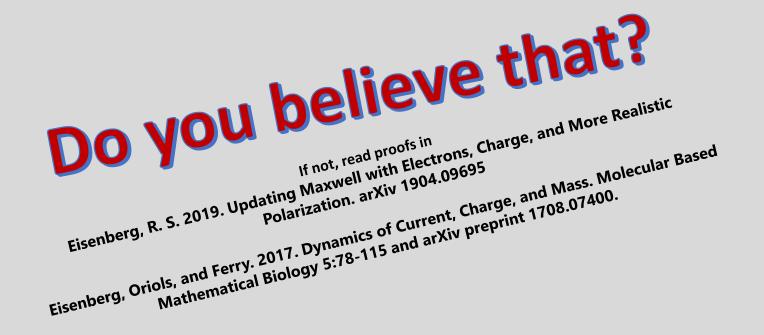
E & B moves atoms

Creates the 'ethereal' current $\varepsilon_0 \partial E/\partial t$ So total current $J + \varepsilon_0 \partial E/\partial t$ is always conserved

Details and PROOF including quantum mechanics at https://arxiv.org/abs/1609.09175

Profound Implications of One Dimensional Systems for atomic view of ion channels

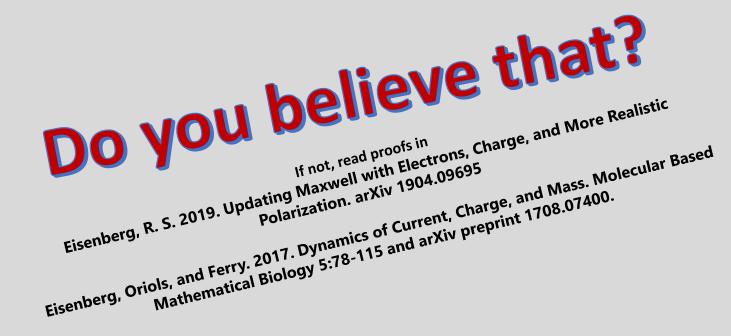
Spatial Variable does NOT appear in description of current in a one dimensional channel



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Hopping Model is COMPLETELY INAPPROPRIATE

for current that is uniform in x



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Spatial Variable <u>does</u> appear in description of ion movement in a one dimensional channel

How take advantage of this enormous simplication?

April 11, 2021

How take advantage of this enormous simplication?

We need a Molecular Dynamics that

- 1) conserves current
- 2) has one dielectric constant
- 3) extends to biological time scales

How take advantage of this enormous simplication?

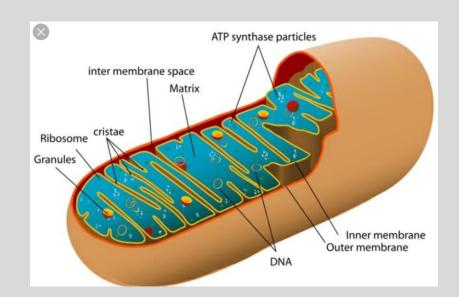
Quasi-particle for current CONDUCTON

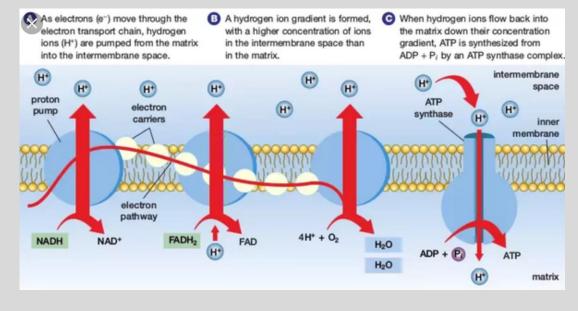
left over is DIFFUSON + POLARON. $\Sigma = PERMION^*$

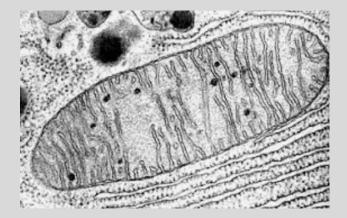
*Elber, Chen, Rojewska, and Eisenberg. 1995. Sodium in gramicidin: An example of a permion. Biophys. J. 68:906-924.

With Conservation of Current mitochondria are no more difficult than large circuit problems

Applying Maxwell to Mitochondria





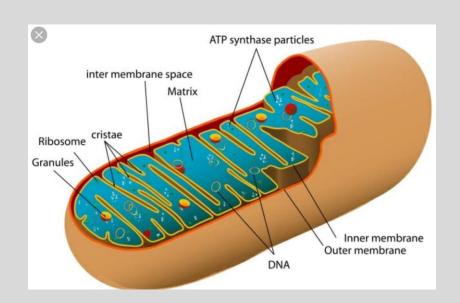


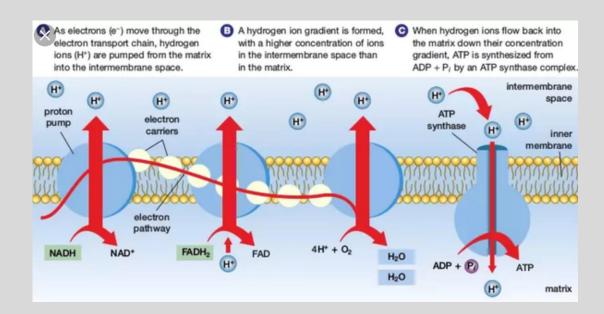
Seems Hopeless

But Stay Tuned for Future Work

Source: textbooks and internet

Applying Maxwell To Mitochondrion





Depends on Conservation of Current

and depends on collaboration of Oscar Juarez, Chun Liu, and Bob Eisenberg

With Conservation of Current no more difficult than large circuit problems

How take advantage of this enormous simplication?

Another way is to include <u>equality of current</u> as a constraint in time averaging schemes

e.g., of Ma and Liu
Ma, Li, and Liu. 2016.. arXiv:1605.04886.
Ma, Li, and Liu. 2016. arXiv:1606.03625.

Derivation of Kirchhoff's Law is at DC Derivation of Kirchhoff's law is about fluxes

How can that work in a computer at 10^{-10} sec?

References and Proofs in

Eisenberg (2019) Kirchhoff's Law can be Exact. arXiv: 1905.13574

Eisenberg, Gold, Song, and Huang (2018) What Current Flows Through a Resistor?

arXiv:1805.04814

Traditional Form of Maxwell Equations Cannot be Used

Maxwell's equations do not deal with Diffusion Convection Complex materials Complicated dielectric properties

Eisenberg, 2019. **Dielectric Dilemma**. arXxiv: 1901.10805.

It is necessary to update Maxwell's Equations to see how

Kirchhoff's law & Conservation of Current

apply to

Complex Liquids

and

Complex Biological Systems

Eisenberg, R. S. 2019. Updating Maxwell with Electrons, Charge, and More Realistic Polarization. arXiv 1904.09695

Eisenberg, Oriols, and Ferry. 2017. Dynamics of Current, Charge, and Mass. Molecular Based Mathematical Biology 5:78-115 and arXiv preprint 1708.07400.

It is necessary to update Maxwell's Equations

https://arxiv.org/abs/1904.09695

Not just my opinion

This is the opinion* of Nobel Prize winners in Physics,

Richard Feynman

(quantum electrodynamics) and

Edward Purcell

(nuclear magnetic resonance)

*p. 10-7 of Feynman, Leighton, and Sands. 1963. *Mainly Electromagnetism and Matter*

*p. 506 of Purcell and Morin. 2013. *Electricity and Magnetism*

What are the PHYSICAL problems with traditional Maxwell Equations?

Maxwell's equations do not deal with

Diffusion

Convection

Complex materials

Complicated dielectric properties

Indeed, Maxwell's original equations do not include ions or electrons or their movement! Textbook treatments do not deal with other forces like diffusion or convection at all.

Eisenberg, 2019. **Dielectric Dilemma**. arXxiv: 1901.10805.

NOT hopeless, **Maxwell Predicts Important Biophysics** Independent of details of the Mitochondrion if a branched **One-dimensional Formulation** is appropriate

Inside Channels PROFOUND SIMIPLIFICATION

If we can figure out how to exploit it

Profound Implications of One Dimensional Systems for atomic view of ion channels

Current is equal everywhere in a channel At all times and under all conditions that the Maxwell Equations Apply

Paradigm Change

What are the problems with textbook Maxwell Equations?

$$\varepsilon_r \varepsilon_0$$
 is a hybrid

Polarization of Matter
$$(\epsilon_r - 1)\epsilon_0$$

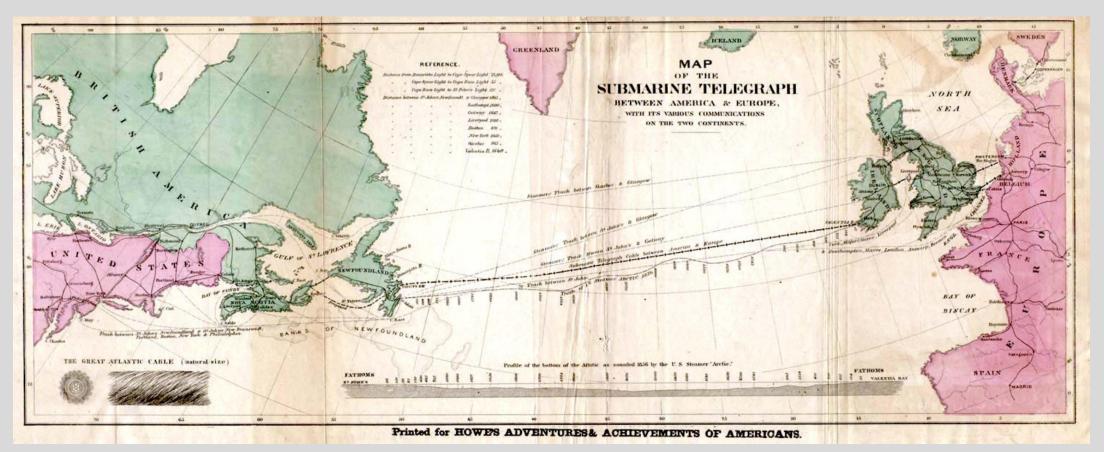
 $arepsilon_r$ involves all movements of matter that do not translate mass, roughly speaking

$$(arepsilon_r-1)arepsilon_0$$
 is as complex as the motion of matter itself.

Seems hopeless to make a general theory

Continuity of Current is Exact in Kelvin's Submarine Telegraph

 $i_{Newfoundland} = i_{Ireland}$



How can that possibly be true?

It is NOT necessary to know the charges to understand one crucial property of current.

Total Current is conserved independent of any property of charge or matter

Conservation of Current

$$\mathbf{div}\,\mathbf{J}_{total}\,=0$$

Applying Maxwell to Transporters

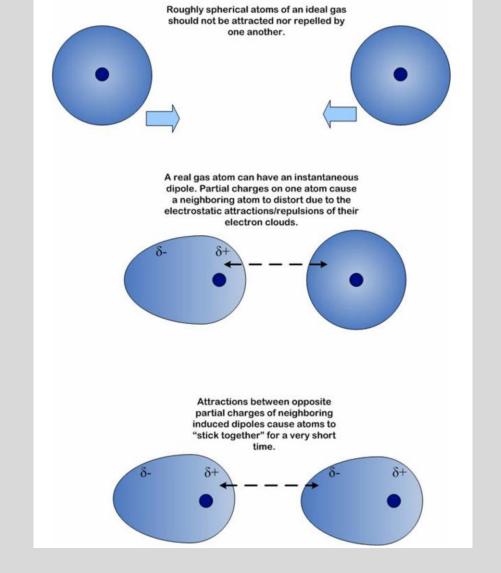
Natural Setting

- 1) Sum of Currents in a Transporter is zero in 'small cell', mitochondrion, etc.
- 2) Currents are Coupled in a Transporter in a natural setting by Maxwell

Experimental Setting

- 3) Bilayer set up does NOT require currents to sum to zero.

 Bilayer setup sets voltage across transporter, currents are not controlled.
- 4) So transporter currents are NOT coupled by Conservation of Current in standard bilayer setup



Source Internet

Polarization of Electron Orbitals