Introduction to Fractional Calculus and its Applications
Summer 2013

Instructor: Gary Bohannan
WSB 313

Schedule

- BH 212 is reserved for tutorial time 10 am -12 pm Monday, Wednesday, and Friday. We'll use the days we need.
  - Topics will vary
    - Fractional dynamics modeling
    - Control Theory
    - Impedance Spectroscopy
    - Statistics
  - I will attempt to announce topics in advance
  - The intent is to introduce the math in varying contexts
- BH 320 is reserved on 1 pm – 3 pm on Mondays for work on numerical methods.
  - Modeling and data analysis

An admittedly biased point of view

- Laser applications and other ultra-fast systems are quite the rage.
  - Fun and exciting.
- But the real problem we face now is not understanding the slow stuff.
- In particular, energy storage – e.g. batteries.
  - The entire Boeing Dreamliner fleet was grounded recently due to failure of their batteries.
  - Lead acid batteries are still the most economical.(?)
- So, I'm going to focus some of the discussion on electrochemistry and impedance spectroscopy.
- This will not restrict your freedom to explore ideas of interest.

A very nontraditional approach

- We’ll meet for tutorial sessions in BH 212.
- We’ll use BH 320 for introduction to “M-word” programs.
- We’ll break up fairly quickly into areas of interest.
  - The subject is as broad as mathematics in general, so you aren’t going to “get it” all at once. (Actually, no author seems to fully “get it”.)
  - You may work in groups or individually, or both if you have more than one area of interest.
  - Areas of interest will necessarily overlap.
- Yes, there are lots of tough questions and problems to be tackled, but that’s what makes it fun.
- Grading is based on level of interest and effort and how much progress you’ve made over the summer.

General Session Format

- Session I will be focused on introducing the basic ideas.
  - Definitions of fractional order operators
  - Setting up differential equations
  - Analyzing data and making fractional dynamics models

- Session II will focus on some particular application(s) of interest.
  - Making fractors
  - Critiquing some topic in the literature
  - Designing experiments and/or building test apparatus
  - Measuring and modeling, e.g. viscoelastic deformation
  - Coding numerical simulations
  - …

- Session timing is flexible.
  - (We just have to act like we are following the rules.)

Why fractional calculus?

- A good question: Is there anything pushing math in this particular direction?
- The answer comes from both Physics and Statistics.
- All macroscopic responses in materials are the result of gazillions of contributions from constituent particles.
  - Such as electrons or ions contributing to electric current
  - Or photons coming from a light bulb
- The resulting response is then the sum of all the contributions.
- It is very unlikely that all the constituent particles behave in identical ways. Thus, we have a distribution of contributions.

The sum distribution

- Statistically, we refer to the macroscopic response as having a “sum distribution”.
- The most famous of these is the Gaussian.
  - If you have a sum of “nearly independent” contributions and the second moment of the distributions exists, then the law of large numbers says the sum will have a Gaussian, or Normal distribution.
- The assumptions going in are rarely tested.
  - What if the particles aren’t all that independent of one another?
  - What if the second moment of the data doesn’t converge?
    - The standard deviation tends toward infinity.
- We don’t need to give up. There is a much stronger Generalized Law of Large Numbers.

Generalized law of large numbers

- If you have a sum distribution with the individual contributors having distributions bounded by a power law, then the sum distribution will be α-stable.
- This is good news for us.
- Example, if the waiting time distribution for recombination-regeneration and trapping of charge carriers in a dielectric material is just bounded by power-law, then the dielectric will exhibit a power-law impedance spectrum.
- One rather big extra problem: there are typically more than one trapping and other processes going simultaneously.
- We may be able to isolate these processes. This is where the research into the fractor is headed.

More generally

- The theorem from the Generalized Law of Large Numbers gives us confidence that power-law is the law.
- So, we want a branch of mathematics that accounts for the power-law tails.
  - But it must also converge to our simpler integer order views.
- Enter the **Calculus of Arbitrary Order**, better known as the **Fractional Calculus**.
  - Generally accounts for power-law interactions while converging to the traditional integer order.
  - Handles both space and time dimensions.

But with a big challenge

- It’s one thing to go from a general set of relations, say Maxwell’s equations, and work out the specifics.
- It’s quite another to start from specifics and try to deduce the more general relations.
- So it is with the Fractional Calculus.
  - There are several competing definitions.
- The difficult comes from the non-local implications.
  - If all past time is included, can you define an initial condition?
  - How do you handle boundary conditions?
- This is where physics comes back into the game.
  - What does nature do?

A common thread?

- The limiting behavior of stress-strain response is power-law, not exponential.
- The general limiting sum distribution is power-law, not exponential.
- The description of electrical (or mechanical) response in matter is primarily statistical.
  - We are looking at the bulk or summed response.
- Nanoparticle response can be much different from bulk due to the differences in interactions among particles.

Also

- In many systems, responses aren't proportional to generalized "velocity," but to a non-integer power of "velocity."
- We would write the differential equation with a derivative of non-integer order.

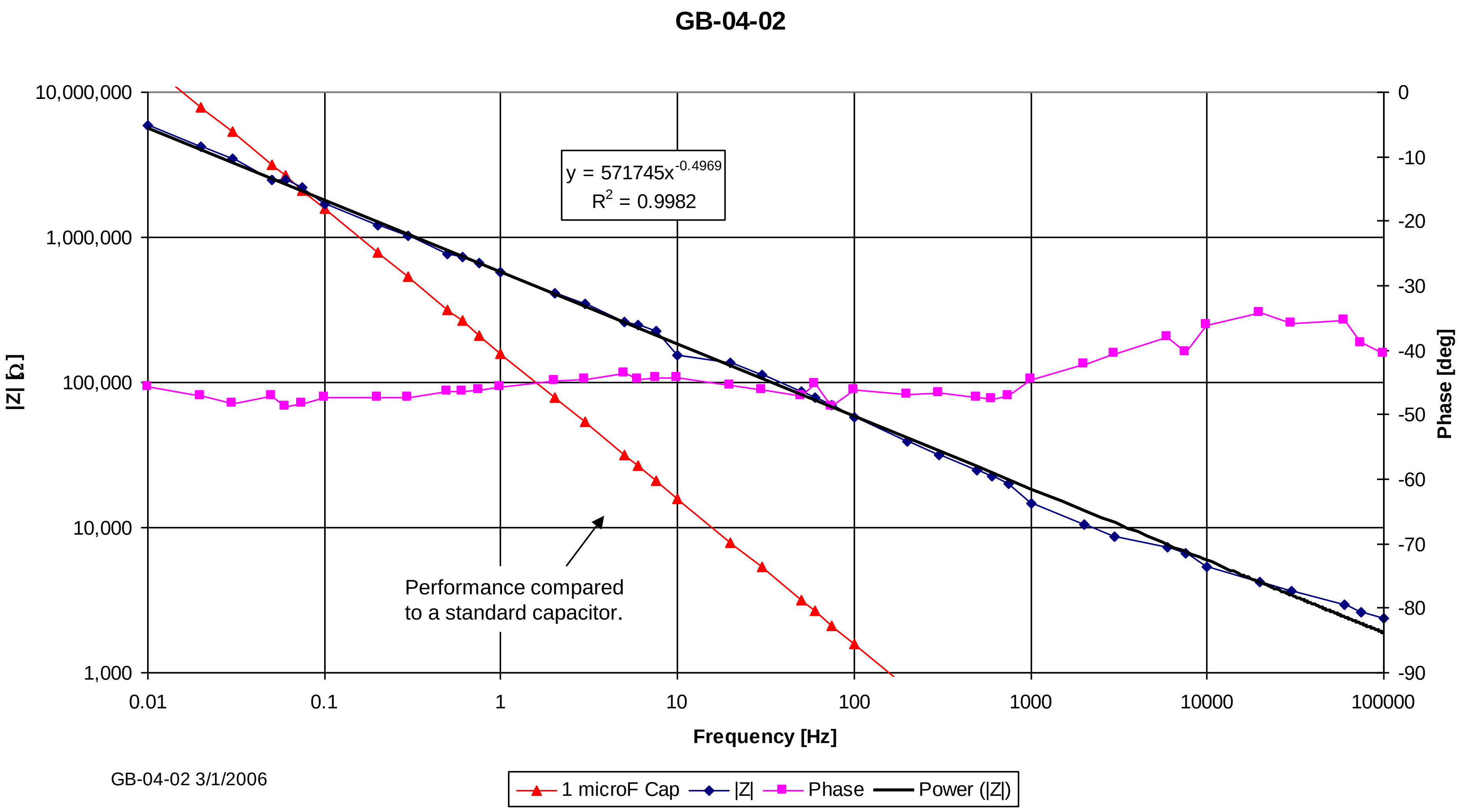
$$\text{e.g.} \Rightarrow \tau^{\alpha} \frac{d^{\alpha}}{dt^{\alpha}} f(t) + f(t) = g(t)$$

With α = 0.932 or 1.26 or …

What about fractional units?

- The simple, but correct, answer: You never actually have to deal with fractional units.
- There will always be some scaling effect that takes care of the units.
- Unfortunately, many (most?) authors insist on using fractional order units, but this has had several nasty results.
  - Few people want to deal with silly fractional units.
  - You have a very hard time measuring and designing to fractional units.
- What we are actually dealing with is magnitude scaling and phase shifts.
- Let’s look at a real example.

Example impedance spectrum



Impedance Description

$$Z(s) \cong \frac{K}{(s\tau)^{\alpha}} \quad or \quad Z(\omega) \cong \frac{K}{\left(i\dfrac{\omega}{\omega_C}\right)^{\alpha}}$$

Where $\boldsymbol{K}$ is the impedance magnitude at calibration frequency $\boldsymbol{\omega_c} = 1/\boldsymbol{\tau}$ and $\boldsymbol{\alpha}$ is a real number $0 < \boldsymbol{\alpha} < 1$. The phase is $\phi = -90^\circ \times \boldsymbol{\alpha}$.
This describes "fractance". It is in units of Ohms.

Resistance is the limiting case $\boldsymbol{\alpha} \rightarrow 0$,
Capacitance is the limiting case $\boldsymbol{\alpha} \rightarrow 1$.

Fractional order integral

The inverse Laplace transform of that impedance leads to the fractional order integral:

$$v(t) = \left(\frac{K}{\tau^{\alpha}}\right)\ {}_{a}I_{t}^{\alpha} i(t) \equiv \left(\frac{K}{\tau^{\alpha}}\right) \int_{a}^{t} \underbrace{\left(\frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)}\right)}_{\text{memory kernel}} i(\tau)\, d\tau$$

The Grünwald-Letnikov Definition

- The Grünwald-Letnikov definition of the fractional derivative:

$$ {}_aD_t^q f(t) = \lim_{N\to\infty} \left\{ \frac{[dt]^{-q}}{\Gamma(-q)} \left[\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(t - j[dt]) \right] \right\} $$

where $dt = {(t-a)}/{N}$

Notes:

1. The order q can be positive, negative, or even complex.
2. Even derivatives are computed over a finite interval.

The Grünwald-Letnikov Definition

- Applying the idea of a fractional integral, that is, a negative order.

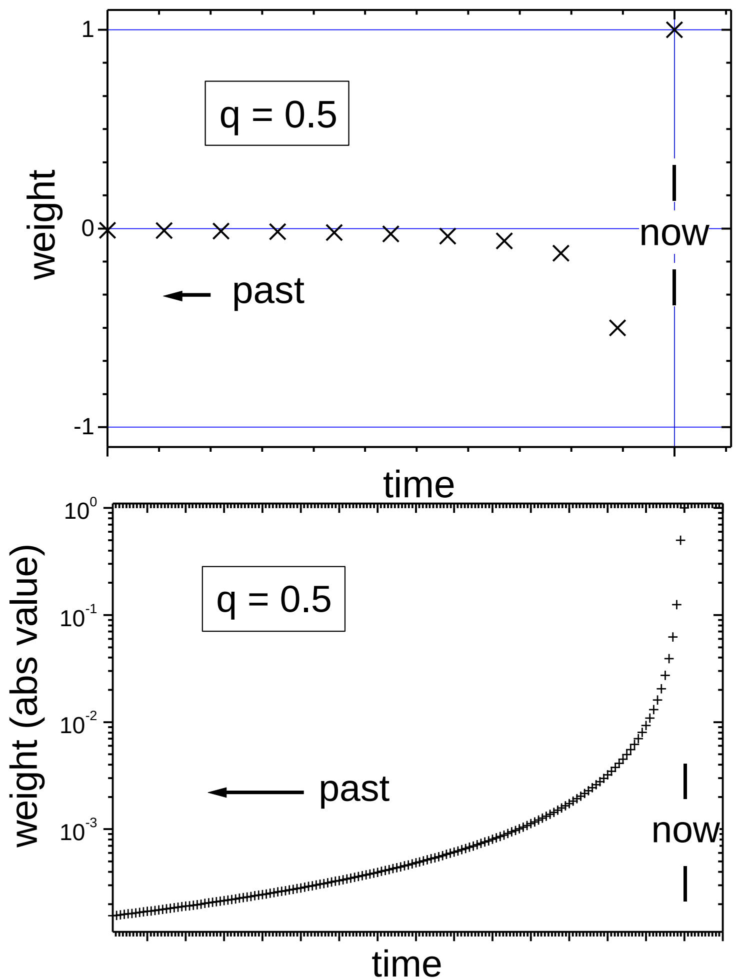
$$v(t) = \left(\frac{K}{\tau^q}\right) {}_aD_t^{-q} i(t) = K \lim_{N\to\infty} \left\{ \left(\frac{dt}{\tau}\right)^q \sum_{j=0}^{N-1} W_j i(t - j\,dt) \right\}$$

where $dt = [t-a]/N$,

and $W_j = \Gamma(j+q)/\big(\Gamma(q)\Gamma(j+1)\big)$

- Major point: The scaling is absorbed in the differential.
- Additional point: You can use the factorial properties of the Gamma function to calculate all the weights without actually computing a Gamma function value.

Weighted History



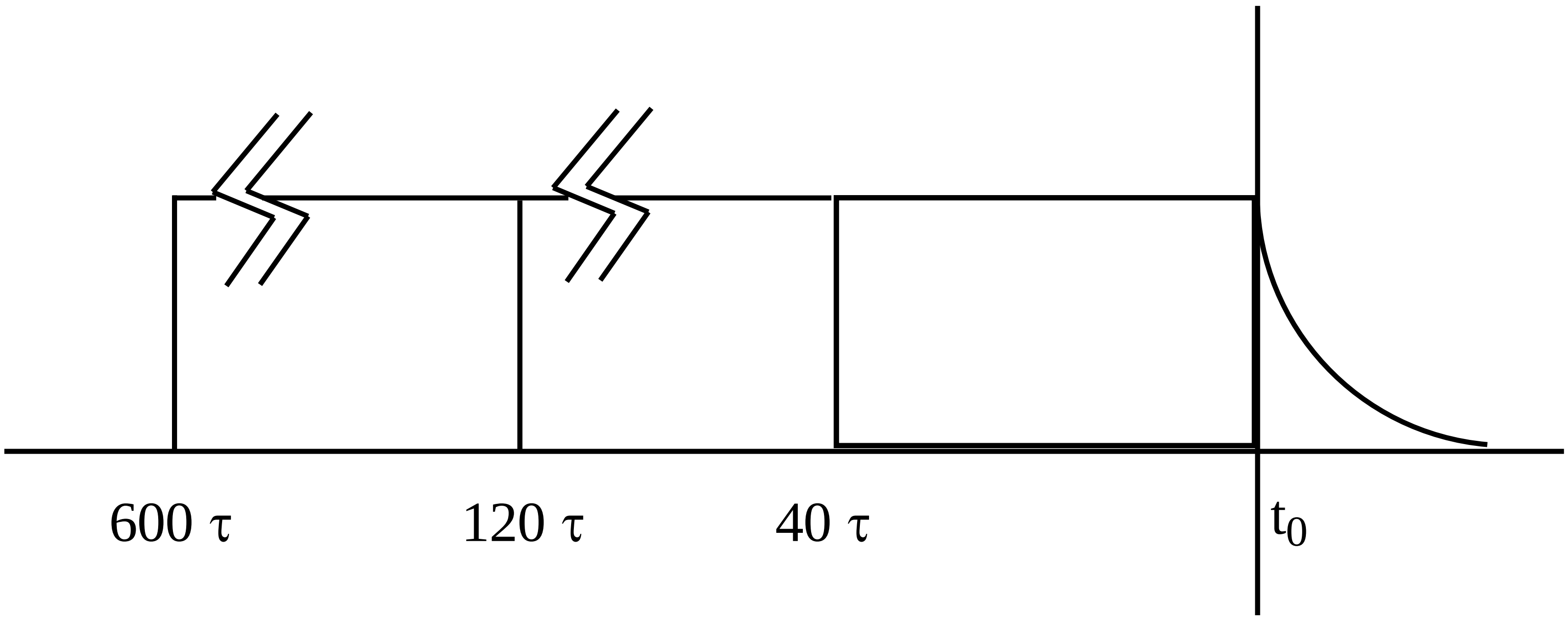
The fractional derivative, or integral, includes past history weighted by a term which becomes power-law at long times.

The example weights shown here are for the half-order derivative.

Experimental challenge

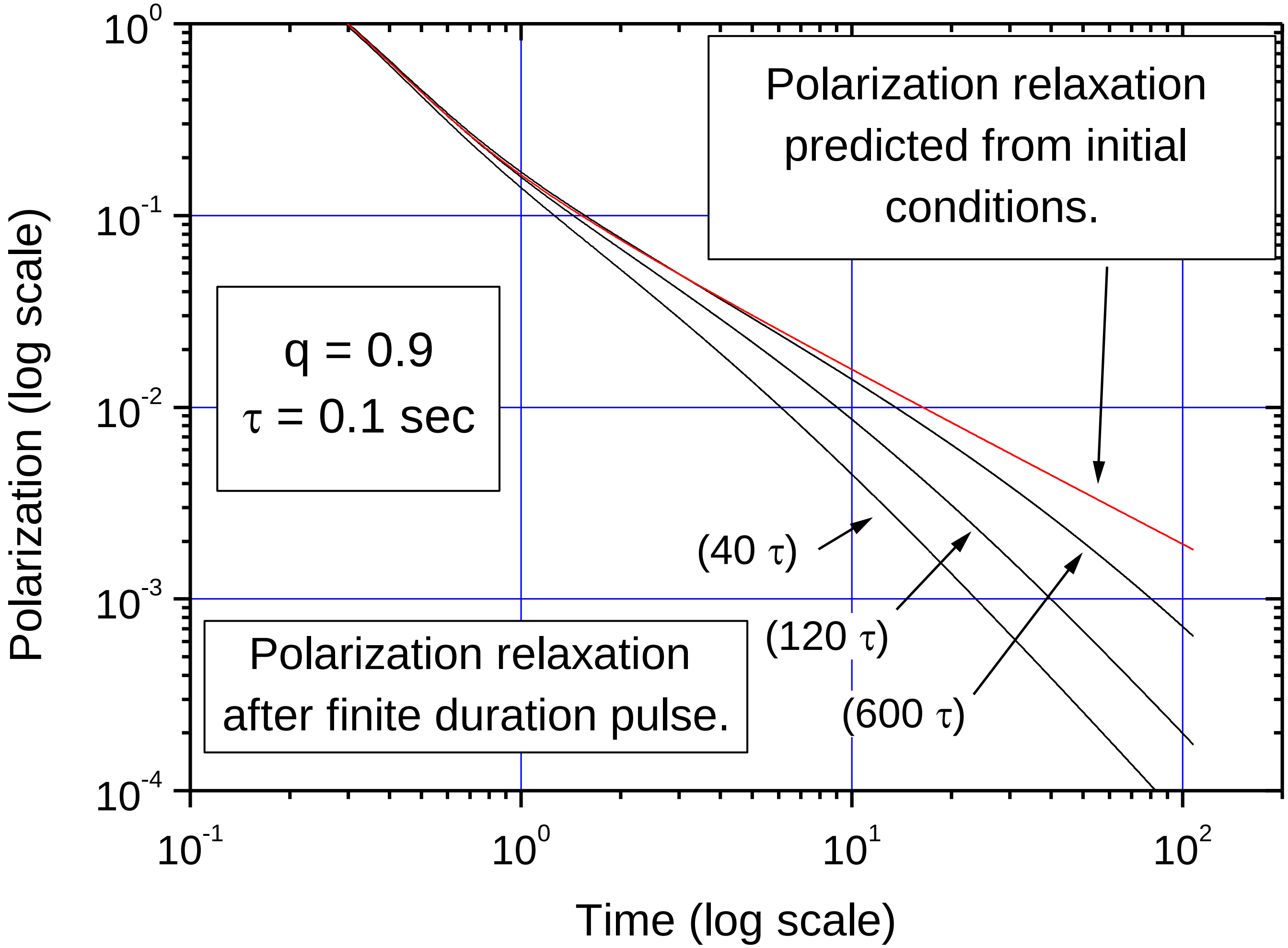
- We need to determine the state of any system before we start an experiment.
- How much affect will we see from past history?
- How could it contaminate our data and interpretation?
- Using dielectric materials as an example:
  - Does response to a an applied voltage produce the same response as the relaxation after the voltage is removed?
  - Integer order models say you get the same exponential shape to the response curves.
- As always in physics, we’re looking for the math that best fits the actual measured results.
  - We just have to make sure we know what we measured.

Pulse History



- Three pulses, duration 600, 120, and 40 units.
- Plus the "initial condition" loading at t_0.

History Dependent Relaxation



Some functions we'll use

- The Gamma function Γ(z):

$$\Gamma(n+1) = n!$$

$$\Gamma(x+1) = x\Gamma(x)$$

$$\Gamma(z) = \int_0^\infty t^{z-1}\, e^{-t} dt$$

- Related functions:

The incomplete upper gamma function

$$\Gamma(s,x) = \int_x^\infty t^{s-1} e^{-t} dt$$

The incomplete lower gamma function

$$\gamma(s,x) = \int_0^x t^{s-1}\, e^{-t} dt$$

The limiting function

$$\gamma^*(s,z) = \gamma(s,z)/z^s\, \Gamma(s)$$

Some functions we'll use

- Mittag-Leffler E-Function:

$$E(a,b,z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(ak+b)}$$

- Special cases:

$$E(2,1,-z^2) = \cos(z)$$

$$E(1,1,z) = e^z$$

$$E(1,2,z) = \frac{e^z - 1}{z}$$

$$E(2,2,z^2) = \frac{\sinh(z)}{z}$$

Some functions we'll use

- Error function

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$$

- Complimentary error function

$$\mathrm{erfc}(z) = 1 - \mathrm{erf}(z)$$

Notation

- Oldham and Spanier (1975) used

$$\frac{d^q}{d[t-a]^q} f(t)$$

to indicate that the process included the interval a to t.

- More modern notation is

$${}_aD_t^q f(t) = {}_aI_t^{-q} f(t)$$

- However, you will still see

$$\frac{d^q}{dt^q} f(t)$$

which leaves the interval ambiguous.

Basics

- We'll start with some basic assumptions about how the "differ-integral" should work.

- These are based on the idea that the results should be continuous in order and converge to the integer order case.

- The exponential

$$_{-\infty}D_t^q e^{kt} = k^q e^{kt}$$

  - Note that we have to take all of past history into account to get this neat result. Starting from $t = 0$ gives a different result, as we'll see.

- Powers of t, starting at $t = 0$ in this case

$$_0D_t^q t^k = \frac{\Gamma(1+k)}{\Gamma(1+k-q)} t^{k-q}$$

An apparent contradiction

- But can’t you write an exponential as a power series?

$$\exp(t) = 1 + t + \frac{t^2}{2} + \cdots + \frac{t^n}{n!} + \cdots$$

- Why the difference?

- Power series with only non-zero positive exponents all evaluate to zero at $t = 0$. This means we can assume that the input function was zero for all time prior to $t = 0$. (Valid?)

- This is not true for the exponential. It has a value of one at $t = 0$ and has had a very long non-zero history up this point. The trouble comes with that constant 1 at the start of the power series expansion.

The derivative of a “constant”

- This issue gets at the very heart of the interpretation of fractional calculus operators.
- If we take a constant to mean t^0, then we can apply the rule for differentiating a power

$$ {}_0D_t^q t^0 = \frac{\Gamma(1+0)}{\Gamma(1+0-q)} t^{0-q} = \frac{1}{\Gamma(1-q)} t^{-q} $$

- That the derivative of a constant might not evaluate to zero has raised much discussion, but actually has a simple explanation.
- By starting the process at $t\ = 0$, we are implicitly assuming that the “function” was zero prior to that moment. Meaning there was a jump from zero to 1 at $t = 0$.
- The derivative of a jump is a singularity that decays over time.

The Caputo definition

- Caputo seems to have missed this simple idea and simply demanded that the derivative of a constant is zero, no matter.

- As a result, his formula doesn't give the derivative of the exponential as an exponential. Instead

$$ {}_{0}^{C}D_t^q e^t = t^{1-q} E(1,2-q,t) $$

  – A generalized Mittag-Leffler function that asymptotically approaches the exponential for large t.

- We'll investigate this a bit further when we power up the computers.

Comparing the Liouville and Caputo definitions

- The Liouville fractional derivative

$$
{}_{-\infty}^{\ L}D_t^q f(t) = \frac{d}{dt}\, {}_{-\infty}^{\ L}I_t^{1-q} f(t)
$$

$$
= \frac{d}{dt}\frac{1}{\Gamma(1-q)}\int_{-\infty}^{t}(t-\tau)^{-q} f(\tau)\, d\tau
$$

- The Caputo fractional derivative

$$
{}_0^C D_t^q f(t) = {}_0^R I_t^{1-q} \frac{d}{dt} f(t)
$$

$$
= \frac{1}{\Gamma(1-q)}\int_{0}^{t}(t-\tau)^{-q} \frac{df(\tau)}{d\tau}\, d\tau
$$

$$
= \frac{1}{\Gamma(1-q)}\int_{0}^{t}(t-\tau)^{-q} f'(\tau)\, d\tau
$$

Comparing the definitions

- And there are mixtures of definitions
  - Riemann-Liouville
  - Liouville-Caputo
- But, in the end, we'll be forced to use the definition that produces a match with actual measurements.
- So far, that seems to be the Liouville form, starting at $t = -\infty$ to take in all prior history.
- That implies that we don't really have "initial conditions".
- It also says that a perfect calculation is impossible since we can't know all of the prior history.
- What to do?

An what about the spatial forms?

- In the time domain, we have to be causal. We don't think that memory of future events plays a role in what happens now.
- In space, same definitions apply (plus some), but we can now use "centered" differentials and not worry about causality.
- Conversion of these definitions to spherical coordinates has not yet been accomplished.
  - What does a Jacobian look like in fractional form?
  - Fractional order tensors?
- Now we have another problem with non-locality.
  - What happens when we really do have a spatial boundary condition such as an insulating wall?

The grand challenge

- Assuming we do find which definition to use under given conditions, what happens when the order changes?
  - Does a system have memory of its memory function?
  - What changes the order of the operator?
- We do know that the order does change with environmental conditions. How and why is uncertain.
- Will we be able to write anything like the Riemann, Liouville, Caputo, etc. formula? What would it look like?

$$v(t) = \frac{K}{\tau_o^{q(?)}} \int_{-\infty}^{t} \frac{(t-\tau)^{q(?)-1}}{\Gamma(q(?))} i(\tau) d\tau$$

Session II ideas

- We’ll discuss some of the ideas for the Grand Challenge in Session I.
  - How we might set up experiments
  - How to take and analyze data
  - This will undoubtedly take quite a bit of teamwork

- That may open up Session II (and beyond?) activity to start attacking the questions.

- For now, we’ll back up and take some elementary steps to see what the math says and maybe how to interpret the results.

Start with a different way of thinking

- I'll violate my own rules here and drop the units. We'll just focus on how the math can help us think about physics in different ways. You'll put the units in as part of HW#1.

- Examples:

- Harmonic oscillator

$$\frac{d^2}{dt^2}x(t) + x(t) = f(t)$$

- First order relaxation

$$\frac{d}{dt}x(t) + x(t) = f(t)$$

We’ll write these in new format

- We’ll let $x^{(\alpha)} \equiv {}_0D_t^{\alpha} x(t)$, where we have set the beginning of the interval of interest to be $t = 0$. Initial condition of $x(t) = 0$ for $t \leq 0$.
- The function $f(t)$ will be a unit step turned on at $t = 0$.
- Harmonic oscillator

$$\frac{d^2}{dt^2} x(t) + x(t) = f(t)$$

$$x^{(2)} + x = f(t)$$

- First order relaxation

$$\frac{d}{dt} x(t) + x(t) = f(t)$$

$$x^{(1)} + x = f(t)$$

The model

- $x(t)$ is some kind of generalized "displacement".
- In the model we have a "restoring force", such as a spring in Hook's law, proportional to the displacement.
- $f(t)$ is some kind of externally applied force, maybe gravity or an electric field.
- $x^{(\alpha)}$ represents a change in the displacement in time.
  - With $\alpha = 1$ representing first derivative, e.g. modeling capacitor discharge through a resistor. Pure dissipation of energy.
  - And $\alpha = 2$ representing second derivative, e.g. modeling harmonic oscillation. Pure energy conservation.

A note from Newton

- The two differential equation forms just presented are typical of conventional integer order thinking.
- If you stick to integer order, they give approximately accurate predictions.
- Their form is generally wrong in a very fundamental way.

$$F = ma = m\ddot{x}$$

- Read this as a “force causes a mass to accelerate”.
- This is not a correct mathematical statement.
  - Forces are **not** accelerations and ma is **not** a force.
- So the two sides are not truly equal in the mathematical sense.
- Look back at the equations and see that we’ve mixed cause and effect.

Not just a pedantic issue

- In order to determine how something changes, we need to put together all the causes for the change.
  - Simple Newtonian thinking that we ignore at our own risk.
- The idea now being accepted, but not yet universally applied, is that you need to put the highest order derivative on the left and everything else on the right.
- Harmonic oscillator

$$x^{(2)} = f(t) - x$$

- First order relaxation

$$x^{(1)} = f(t) - x$$

Then integrate

- Then carry out formal integration to accumulate all of the changes to the system.

- Harmonic oscillator

$$x(t) = \int \int \{f(t') - x(t')\}\, dt'dt''$$

- First order relaxation

$$x(t) = \int \{f(t') - x(t')\} dt'$$

- As mentioned, this is pedantic for integer order operations.

Critical for fractional order processes

- In fractional order, we are taking history into account.
  - History of what?
  - How is that history accumulated?
  - How does the memory decay?

- In arbitrary order

$$x(t) = {}_aI_t^{\alpha}\{f(t') - x(t')\}$$

where ${}_aI_t^{\alpha}\{\,\}$ is the anti-derivative ${}_aD_t^{-\alpha}\{\,\}$.