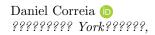
# Maxwell's Silver Hammer: On the application of pulsed microwave acoustic resonant viral inactivation \*

Based primarily on exceptional work by

May 2020



#### Abstract

We extend this landmark work rather trivially by:

Aims: this is primarily bookkeeping.

- Establishing the time dependence of inactivation
- Demonstrating a modulation scheme that decreases the inactivation threshold to below current safety levels in surrogate bacteriophage
- Demonstrating a prototype emitter in an "electromagnetic mask" form-factor, costing about \$5 in prototype quantities, which can reasonably be produced in 10 million-of quantities
- Testing power thresholds in various conditions; biological fluids of various conductivities and pHs
- Using a coarse-grained molecular-dynamics simulation to optimize the impulse
- Using a virus-in-the-loop optimization with a centrifugal microfluidic system
- Discussing the biological basis for the safety of the device
- Showing that the deviation from the expected the shold could be explained by variance in the Perhaps notable that a completely free and open-source tool chain was used for the entire project, including FDTD microwave antenna optimization. This work can be replicated with \$500 in equipment.

<sup>\*</sup>I would be delighted to include any criticisms or comments anyone may have, both on substance and comprehensibility; preferably leave them on the GitHub issues page, or email therobotist@gmail.com, @0xDBFB7 on Twitter, or irc.0xDBFB7.com:6667 #covid.

#### autem

This work was prepared by an undergraduate and has not been peer-reviewed. Additionally, the author has no prior experience with either biology or microwave design.

While our study is very simple, biological research is of such complexity that a tremendous amount of care must be taken before any conclusion can be drawn at all. It is not likely that we have taken sufficient care.

This is especially true with RF biophysics. The literature is littered with otherwise impeccably perormed research which is both difficult to find fault in, and faulty.

This paper does not contribute to the state of the art at all, except perhaps in the obvious avenue of time-domain modulation; [Hung 2014] have already demonstrated a reflectarray, and the rest of our discussion is anything but novel.

Though the original research used Inf. A, our testing was only performed with a surrogate bacteriophage. All experiments must be repeated with SARS-NCoV-2.

Additionally, other sterilization techniques may produce superior results with less faffing about and should be evaluated in the same context. For instance, data on far UV [Buonanno 2017] indicates safety.

Accurate microwave measurements are rife with parasitics and sensitivities. It has occurred before that otherwise striking resonances were detected, and further replication found them to be artifacts of the measurement equipment. [Foster 1987] even offers this disclaimer:

"To detect the DNA resonances with the probe technique requires correction for system errors that are potentially much larger than the effect to be studied and lead to resonance-like artifacts. This is true even with the more precise instrumentation used in this study. Such data are easily misinterpreted".

The direct inactivation plaque and PCR data in the referenced papers are somewhat convincing corroboration that this effect is not an artifact; but hundreds of convincing and wrong papers exist in the literature.

Our data is crude and imprecise, our equipment hastily constructed, and should not be considered validation of this effect even existing.

Even if this effect exists and is as effective as it appears, it could still be impractical to apply for any number of reasons.

Please consider all claims with appropriate skepticism.

**To-do list** We see the following steps that must be undertaken before production can be started:

- $\bullet\,$  Re-run the experiment with
- Verify
- Failure-tree to ensure that power levels can never go above specified values.
- Obtain special permission from the FCC?

We've got a thing that's called Radar Love We've got a wave in the air

The phased-array techdemo.

## the gist

The chain of literature [Fröhlich 1968]  $\rightarrow$  [Fröhlich 1980]  $\rightarrow$  [Liu 2009]  $\rightarrow$  ([Hung 2014] || [Yang 2015] || [Sun 2017])<sup>1</sup> apparently culminates in the flagship work we focus on in this paper,

Efficient Structure Resonance Energy Transfer from Microwaves to Confined Acoustic Vibrations in Viruses [Yang 2015].

estabilishes that - unique to certain viruses, and apparently unlike human cellular structures, as we shall see - coincidentally have just the right size, shape, stiffness, and net charge distribution to form a weak (Q=2) spherical dipole resonance mode which couples well to the microwave spectrum at approximately 8 GHz.

More critically, [Yang 2015] (and, in parallel, [Hung 2014]) theoretically model and then experimentally validate in various strains of Influenza A that - due to this acoustic-resonance effect - the power density levels required to crack the lipid envelope are near the safety limits for continuous exposure to humans.<sup>2</sup>

They demonstrate this with both a plaque and PCR assay, finding good agreement with the theoretical model.<sup>3</sup>

Like pumping a swing, this effect allows an otherwise inconsequential field magnitude to store energy over a small number of cycles until the virus is destroyed.

If this mechanism exists, it would seem to provide significant advantages over existing UV or cold-plasma sterilization.

If the extensions made in our paper are valid, this is a non-ionizing, non-thermal  $^4$ , non-chemical technique, harmless for continuous exposure to tissue, which can sterilize air and surfaces alike, including skin, eyes, and within hair; it evolves no ozone, can readily be generated with \$1 USD - scale devices, acts instantaneously, and perhaps most critically - could be made to act within infected tissues.

The X-band is also minimally absorbed by air, allowing action in the far-field and scaling to square-kilometer areas with single installations.

autem

The previous paragraph may cut an impressive figure; but it hinges on all the rest of this paper being correct.

It cannot be overstated how unexpected and positively dubious this finding appears to be -at least, based on our limited research and experience to date.

For even the RF power limits set by standards organizations appear to be based on the observation that few significant resonance modes exist in biological tissues, and (as we shall see), this is grounded in solid *in vitro* (albeit more limited *in vivo*) evidence.

This may account for why this paper has been ignored.

The precise structure and charge of the virion appears to be a singular anomaly in this otherwise catagorical non-existence.

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#### Ramifications

<sup>&</sup>lt;sup>1</sup>We have not conducted a thorough review; many more papers are probably involved.

<sup>&</sup>lt;sup>2</sup>Sort of. See below and supplemental.

<sup>&</sup>lt;sup>3</sup>As we will discuss, there are a few issues with the experimental technique.; sham, blinding, and dosimetry demanded by [Vjl.] are not mentioned

<sup>&</sup>lt;sup>4</sup>It may be useful to define 'non-thermal'; it caused us some confusion. Certainly the proteins of the virion locally absorb energy and increase in temperature. The key is that, when excited in this manner, the energies in the envelope are poorly modelled by a Maxwell-Boltzmann distribution; they are not given sufficient time to 'thermalize'. In contrast, with typical 2.4 GHz microwave exposure, sterilization can only occur by aggregate heating of the fluid and tissue.

<sup>&</sup>lt;sup>5</sup>It should be noted that this *confined* acoustic resonance is subtly distinct from common-and-garden pipe-organ acoustic resonance; this is apparently not a strictly classical phenomenon. Besides standard Coulomb-like and Lennard-Jones-like interactions between constituent particles, if Fröhlich is to be believed at these nanoscopic scales there are also wave-function interactions among the particles of the virus which can shift storage to modes not otherwise expected.

We confess to not yet understanding this phenomenon; fortunately, while helpful, the details of how this mode appears are not critical to implementing this technique.

<sup>&</sup>lt;sup>6</sup> "[B]elow about 6 GHz, where EMFs penetrate deep into tissue (and thus require depth to be considered), it is useful to describe this in terms of specific energy absorption rate (SAR), which is the power absorbed per unit mass (W/kg). Conversely, above 6 GHz, where EMFs are absorbed more superficially (making depth less relevant), it is useful to describe exposure in terms of the density of absorbed power over area  $W/m^2$ , which we refer to as absorbed power density" [ICNIRP 2020  $\square$ ]

<sup>&</sup>lt;sup>7</sup>All values have been converted to  $W/m^2$  to avoid confusion. 100  $W/m^2 = 10 \text{ mW/cm}^2 = 10 \text{ dBm/cm}^2$ .

A poignant summary of the consensus is found in [IEEE C95.1-2005], Annex B, "Identification of levels of RF exposure responsible for adverse effects: summary of the literature".

Further examination of the RF literature reveals no reproducible low level (non-thermal) effect that would occur even under extreme environmental exposures. The scientific consensus is that there are no accepted theoretical mechanisms that would suggest the existence of such effects. This consensus further supports the analysis presented in this section, i.e., that harmful effects are and will be due to excessive absorption of energy, resulting in heating that can result in a detrimentally elevated temperature. The accepted mechanism is RF energy absorbed by the biological system through interaction with polar molecules (dielectric relaxation) or interactions with ions (ohmic loss) is rapidly dispersed to all modes of the system leading to an average energy rise or temperature elevation. Since publication of ANSI C95.1-1982 [B6], significant advances have been made in our knowledge of the biological effects of exposure to RF energy. This increased knowledge strengthens the basis for and confidence in the statement that the MPEs and BRs in this standard are protective against established adverse health effects with a large margin of safety.

Unfortunately, the power levels required by

However, there is an obvious avenue of optimization. If the virus is destroyed in a few dozen nanoseconds via an electric field amplitude incidentally caused by an instantaneous power P, but tissue damage requires a temperature rise due to an energy deposition P dt, then we should minimize dt.

We thus turn the CW microwave signal into a series of effectively instantaneous pulses.

The human body contains proteins with all sorts of net charges.

All known non-thermal physiological effects, including changes in the permeability of membranes, direct nerve stimulation are accounted for in the time-domain equation and the 6-minute averaging period.

To drive home this point, apparently the best-quality evidence available fulfills sham requirements [Vijayalaxmi 2006] provide in-vitro. They expose blood lymphocytes to pulse power in precisely the regime required in this work; 8.2 GHz, 8 ns duration and 50 khz repetition rate, pulse power densities of  $250,000 \text{ W/m}^{28}$ , average power  $100 \text{ W/m}^2$  9, for 2 hours, finding no change in any of the measured quantities. [Chemeris 2004] use 8.8 GHz, 180 ns pulse width, peak power 65,000 W, repetition rate 50 Hz, exposure duration 40 min, on frog etheyrocytes, and find genotoxicity only from the temperature rise.

So it appears that this is not merely rules-lawyering to exploit a loophole in the regulations; it is a physically-informed effect.

These papers (the best quality we are aware of) were extensively cherry-picked from the literature based on the results of a meta-analysis [Vj. 2019], listing the requirements for reliable in-vitro RF experiments.

How sensitive this research is, [Chemeris 2004] mention:

The increase in DNA damage after exposure of cells to HPPP EMF shown in Table 2 was due to the temperature rise in the cell suspension by  $3.5\pm0.1^{\circ}$ C. This was confirmed in sham-exposure experiments and experiments with incubation of cells for 40 min under the corresponding temperature conditions."

There are a substantial number of papers in the literature which show positive effect sizes; these are listed in the bibliography.

The literature reviews conducted by standards organizations.

We are not aware of any past uses of these microwave en-masse. We do not have the

[?]

#### References

<sup>&</sup>lt;sup>8</sup>computed from average power / duty cycle

<sup>&</sup>lt;sup>9</sup>the safety limit

#### Talkin' 'bout the Variation

To re-cap, [Yang 2015] theoretically model the virus to determine the minimum electric field required to destroy it.

They assume that the virus is a simple damped harmonic oscillator, where the 'core' and 'shell' oscillate in opposition.

They determine the net charge experimentally from microwave absorption measurements.

Since [Yang] try to compute the *threshold*, they use a value of 400 pN for the breaking strength of the envelope, obtained from [Li 2011]. However,

<sup>"95</sup>

| Col1 | Col2 | Col2  | Col3 |
|------|------|-------|------|
| 1    | 6    | 87837 | 787  |
| 2    | 7    | 78    | 5415 |
| 3    | 545  | 778   | 7507 |
| 4    | 545  | 18744 | 7560 |
| 5    | 88   | 788   | 6344 |
|      |      |       |      |

Of course, this application is hardly much better than an N95 mask, except that it is non-disposable and provides protection for eyes and skin.

#### Vomit

[Vj] mention the importance of precise dosimetry. Even simple structures can produce hot-spots Yang et al use both a plastic cuvette, and a single drop of solution on a glass slide; in either case, a sharp change dielectric constant is present.

To the extreme, some papers have used

#### Time dependence

The fact that the viral inactivation is non-thermal

Both [Yang 2015] and [Hung 2014] use an apparently arbitrary 15-minute exposure in their tests - a very reasonable decision, given the focus of their paper.

The effectiveness against airborne particles, and to minimize the power required in a dwelling phased-array beam, we must establish the required duration of exposure.

#### speculative hypothesizing {

In contrast to chemical inactivation, where the time dependence appears to be dominated by viscous fluid dynamic effects [Hirose 2017], or UV inactivation, where a certain quantized dose of photons must be absorbed, we expected RF to act instantaneously.

As a damped, driven oscillator, the ring-up time of the virus depends on the Q factor. Yang et al. state the Q of Inf. A as between 2 and 10, so at 8 GHz the steady-state amplitude should be reached in well under 100 nanoseconds.?????????FIXME

[] found a significant mechanical fatigue effect in phage capsids, where a small strain applied repetitively eventually causes a fracture. Such a mechanism could perhaps extend the exposure required to break the capsid or membrane. Other mechanisms could include some sort of lipid denaturation, requiring an absolute amount of energy absorption to break or twist bonds and modify the properties before the envelope fractures.

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## Safety

Because this is an ostensibly novel and niche mechanism, it may behoove us to breifly review the biological basis for the safety limits set by standards organizations. <sup>10</sup> a loophole in the guidelines

WHEN YOU SEE A CLAIM THAT A COMMON DRUG OR VITAMIN "KILLS CANCER CELLS IN A PETRI DISH,"



SO DOES A HANDGUN.

There are also things.

For instance, it is reasonable to wonder why we might not see such resonances in bodily tissues. Approximately similar nanoscopic structures exist in humans, such as nuclear pores (120 nm) and the famous microtubules (10x50 nm).

While from which epidemiological data could be derived.  $^{11}$ 

What we find is a messy affair. Biology is hard.

There are some 20,000 papers on the topic of RF safety, with solid in vitro, in vivo and epidemiological evidence of safety in the 2.4 GHz and 5.8 GHz bands.

However, "There are limited experimental human data upon which to set limits on exposures above 6 GHz" [Chan 2019]. Only 2% of the above papers are on frequencies > 6 GHz [Vijayalaxmi 2018].

In addition, what data remains in this category is of varying quality.

As has been starkly demonstrated in the recent hydroxychloroquine contradictions [Gautret 2020] [Geleris 2020], biological research must be essentially perfect to have any meaning at all.

The IEEE standard which the flagship paper [Yang 2015] references [IEEE C95.1-2005] was recently overhauled [IEEE C95.1-2019] with new metrics.

[Vijayalaxmi 2018] is a remarkable meta-analysis of in vitro data. They synthesize a quality score, rating bindedness, sham controls, dosimetry, and sample size. Qual-

ity was inversely, monotonically related to the effect size. An example of the subtle effects that can call into question superfically reasonable results are [

They additionally find a publication bias of incredible magnitude in the positive (harm) direction in this field, further degrading the usefulness of statistical analyeses.

An example of a relevant study that they grade as "quality 1" [Karaca 2011]. This study's conclusion is that However, in figure 5, one can see that only 1 out of 11 genes tested had a statistically significant difference in expression. Given the N=6 cultures,

[Adair 2002] demonstrate theoretically that acoustic resonances are, in general, highly unlikely in biological solvents, primarily focusing on DNA. All resonance modes are strongly overdamped by the surrounding solvent, and no amplitude amplification can take place.

This analysis would seem to disagree with the viral resonance apparently conclusively demonstrated by [Yang 2015] - the PCR result seems especially inarguable. This could be explained by the large charge on the virus compared to the molecules analyzed in Adair. [Yang 2015] find a charge of order  $10^7 e$ , whereas Adair analyzes a very different regime, "assume coupling to the field through single charges q = e at each end".

[Liu 2009] cite [Edwards, Swicord 1984], saying: "It was proposed that a hydration layer surrounding DNA molecules could lower the viscoelastic transition frequency, raise the quality factor of confined acoustic vibrations, and result in a microwave resonant absorption".

But [Adair 2002]'s [Foster 1987] seem to quite conclusively put the kibosh on that idea, demonstrating no resonances in DNA with 20x higher precision than previous work, showing previous results to be an artifact of the measurement equipment.

The supplemental material to [Vijayalaxmi 2018] has a table of studies on this topic. High-quality research invitro concurs with.

#### [Manikowska 1979]

9.4 GHz pulsed / in vivo, mouse,  $0.1 - 10 \text{mW/m}^2$  over the whole body for 2 weeks. N=16.

This is a particularly concerning result, especially given their p < 0.001. [Servantie 1989] discusses the (admittedly circuituious) route by which birth defects could occur.

<sup>&</sup>lt;sup>10</sup>The idea of biological microwave resonances appears to have originated in [Frohlich 1968, 1980].

<sup>&</sup>lt;sup>11</sup>The cloud service [scite.ai] was irreplaceable during this. It's like a mirror to an alternate universe where literature made sense.

Work by [Manikowska 1985] in the 2.4 GHz range has been contradicted [Beechey 1986], but the 9 GHz range does not appear to have been repeated.

More modern research [Juutilainen 2011], [Chemeris], [Vijayalaxmi 2006], does not tend to agree with these concerns. As cited by [ICNIRP 2020]'s excellent literature review, expose lymphocyte blood cells to 8 ns pulsed 8.2 GHz radiation for 2 hours at an average power of  $10 \text{mW/cm}^2$ . They find no change in any of the parameters measured, including various chromosomal parameters. They further discuss previous results.

In the frequency range of interest, there seems to be good-quality in-vitro evidence using lymphocytes of lack of harm. We are not aware of any high-quality in vivo or epidemeological data from which useful conclusions can be drawn.

We must defer to health experts for interpretation of these data.

Please contact the author if you are aware of other salient research, or have a different interpretation.

## The Experiment

#### Centrifugal microfluidics

The field of centrifugal microfluidics is accelerating.

Many CD microfluidics systems use standard CD molding techniques for the channels and machining techniques, using either acrylic or silicone. The turbidity sensor is most sensitive if the plastic is clear. Sterilization does not seem to be discussed.

Polypropylene is the ideal material, being almost indefinitely autoclavable. It is quite difficult to machine.

## Modes of application

Personal 'electromagnetic mask'

Even with judicious use of phased-arrays, spatial power-combining, etc, each transistor can only reasonably maintain sterility in approx.  $0.1~\mathrm{m}^3$ .

We therefore demonstrate this form factor because, superficially, there are fewer people than there are places.

On the other hand, a personal device may present issues with participation and production volume.

#### Direct treatments at the fundamental

Via [Hand 1982], the  $E_{mag} = 1/e$  penetration depth<sup>12</sup> is approximately 40 mm for 'dry' tissues and 5 mm for 'wet'.

SARS is found widely distributed throughout many of the most favoured organs [Ding 2004], shielded by an average of 4 cm of chest wall [Schroeder 2013]; so safe external treatment of the body is unlikely.

However, destruction of lung tissue appears to be significant in the lethality of SARS [Nicholls 2006].

A bronchoscopic technique may therefore be effective, very similarly to that demonstrated by [Yuan 2019]: in adults, the bronchi are less than 2 mm thick [Theriault 2018] and the lungs themselves are only on the order of 7 mm thick [Chekan 2016].

The main bronchus is about 8 mm in diameter, which is smaller than the patch antenna used here; a monopole (or multiple, phased monopoles) like is probably more suitable.

#### **Subharmonics**

The 8 GHz wave need not be the fundamental. A modulated carrier wave with a more deeply penetrating wavelength which then locally interferes to produce the 8 GHz tone within the tissue could be useful.

The penetration depth shortens as frequency increases, until the so-called 'optical windows' in the absorp-

tion spectra of tissues, particularly in the near-IR range.

#### More fanciful concepts

Many systems operate in these X-band frequency ranges; and precision

It is easy to produce megawatts of power at these frequency ranges using Klystrons. Assuming an appropriate antenna, a single 50MW SLAC XL-class klystron with a PRF of 180 Hz could sanitize almost a square kilometer every second.  $^{13}$ 

On the other hand, if this is conducted in outdoor free-space, sunlight

Existing marine, weather, and aviation radar systems often use the X-band; depending on the focusing power

**Sensing** Surprisingly, there is little discussion on microwave virus detection, with the notable exception of [Mehrotra 2019]. Such scholarly silence is usually an indicator that a technique is impossible for reasons so obvious they scarcely bear repeating.

However, [Oberoi 2012] find that - in controlled conditions - they can detect a single E. Coli bacterium in 50 uL of broth via a microwave cavity.

Of course, discriminating miniscule returns in free-space is not easy; but with precise knowledge of this resonance mode, it may become somewhat easier. Frequency-domain measurements can be made with incredible precision; and there are many parameters by which virions could be discriminated; ring-up time of the resonance, excitation non-linearity, etc.

It has been shown that virions can effect large-scale changes in the electric charges of their [].

Use of this technique will provide a selection bias towards immunity to electromagnetic fields, which could perhaps be effected by preferring extreme-sized mutants (shifting the resonance away from the applied field).

We do not have the biological knowledge to know if this is plausible; it simply seemed worth mentioning.

<sup>12&</sup>quot;skin skin depth?"

<sup>&</sup>lt;sup>13</sup>Giving 'asceptic field' new meaning.

## Microwave Musings

#### Toolchain:

- Failed oscillator feedback-loop optimization toolchain: QUCS 0.0.20 + python-qucs + scipy's 'basinhopper'
- Successful A slightly modified ngspice + ngspyce + pyEVTK
- gprMax for FDTD EM simulation
- KiCAD, wcalc, scikit-rf, ngspice

Microwave design has a reputation for being the purview of wizards. Modern RF software packages like HFSS, Microwave Office, Agilent's ADS, and Mathworks' RF toolbox, for which; component models

Luckily, this project falls perfectly within the subset of

microwave technologies that do not require a goatee. The vast majority of the behavior of most circuits can be accurately modelled with the very same SPICE tools as one would use at low frequencies. With judicious application of reference designs, it seems to be possible to design

Before about 2005, however, it seems to have been somewhat the norm to write a simple numerical code to solve the problem at hand based on underlying principles.

We are also aided by the fact that what took a \$150,000 computing cluster a single decade ago can now be done in a few minutes by a single budget GPU.

#### Interference

## Mass production

Almost all components on the device can be replicated with fully vertically-integrated first-principles. Capacitors can be

If this 'electromagnetic mask' form is the ideal (not nearly),

The largest RFID plants can produce

a minimum of 5 GaAs or SiGe:C transistors will be required. Without SOI or, it does not appear that

As a lower bound, there are 1 million hospital beds in the U.S. [AHA 2018]; and as an upper bound obtaining global herd immunity would take 1.75 billion units.

It is difficult to determine the supply capacity for these semiconductor processes; information is not forthcoming from the manufacturers. Fermi estimates  $^{14}$ 

It is possible to use common Si-based devices at these frequencies, especially with second-harmonic techniques [Winch 1982]. However, obtaining the required gain and output power is not a trivial matter.

The techniques and equipment required to produce these devices are extremely complex; load-lock UHV,

Figures are not forthcoming,

Given the supply difficulties of comparatively simple materials such as Tyvek at pandemic scales, it is difficult to imagine that RF semiconductor production can be immediately re-tasked and scaled to this degree.

#### Vacuum RF triode

Especially combined with an integrated titanium sorption pump,

One concern is the large filament heater power, which prevents the use of low-cost button cells for power. Use of cold-cathode field-emitter arrays would alleviate this issue, but at the cost of complexity.

Small tungsten incandescent lights are available down to 0.05 watts. With a suitable high-efficiency cathode coating, a pulsed heater power of less than 0.02

 $<sup>^{14}\</sup>mathrm{GaAs}$  MMIC market of \$2.2 Bn USD / random sample of MMIC prices = about 2 Bil devices / yr, 3e9 wifi connected devices produced each year,

#### Acknowledgements

This paper is not novel enough to deserve this chapter, but those to be acknowledged are.

The authors of the original papers deserve the credit for this entire work; it is rare that such a monumental finding is served on a silver platter.

Professor Shahramian's excellent video blog *The Signal Path* inspired this work.

Dr. Dainis' videos on microbiological technique were also useful.

Thanks to the professors at York and beyond for returning my emails.

Thanks to L.H. for wisdom regarding this project.

Thanks to P.B and H.P. for tolerating ramblings and M. for the hug.

Special thanks to all the people - most equally capable of writing this paper if provided the opportunity - who work menial shifts at the component suppliers that remained open that were so critical. Hopfstader be damned; despite the name below the abstract, this paper is of course entirely the result of circumstance and luck.

Chiefly among the enablers are of course my parents, Doris and Brian, without whom this work would have been done by someone else, and who also supported this work financially.

The authors acknowledge the Computational Electromagnetics Group at The University of Texas at Austin for developing and making the AustinMan and AustinWoman human body models available at https://sites.utexas.edu/austinmanaustinwa

One Very Important Thought

i3

## Captain's Log, Supplemental

#### Molecular dynamics simulation

It was originally expected that a large part of this work would be done in-silico, as we did not anticipate having access to suitable RF test equipment.

Some time was spent attempting to set up a molecular dynamics toolchain capable of simulating an entire virus.

Having an approximate simulation of the this technique would be useful for a number of reasons:

We would have a better idea of the transferability to SARS, without wasting the time of experts with BSL-3/4 labs.

The impulse could be subjected to the same optimization as the RF feedback loop. A number of parameters (such as phase, polarization)

Coarse-graining also greatly increases the allowable timestep.

We also did not understand the \*confined\* part in the \*confined\* acoustic resonance.

Simulating the aggregate bose condensate wavefunction is well beyond us.

## optical\_centrifuge

June 28, 2020

Optical centrifuges rotate the polarization axis of an electromagnetic field, spinning up polarized molecules until centrifugal forces rip them apart. This has been demonstrated with simple molecules [Villeneuve 2000], [Karczmarek 1999].

The oscillating electric field in our technique induces a slight dipole polarization on the virus, giving us a foothold through which a torque could be applied.

Modulating the polarization axis of microwave transmitters is an established technique, and can be accomplished in a number of ways:

- Switching the antenna feedport location using PiN diodes [Medina-Sanchez], [Silveira 2018] (limiting the switching frequency to a few KHz)
- Modulating the phase shift between feed-ports so as to produce circular polarization
- Mechanically rotating the antenna
- Using four or more standard linearly-polarized antennas at various angles, modulating the power to buffer amplifiers.

There is also the concern that biological tissues could exhibit the same effect.

This sounds plausible, but then most wrong ideas do.

A first-order Fermi estimate:

We will need the dipole moment, and for this we need the charge separation.

Here we make our first assumption; that the charge separation is the same as the mechanical displacement. This is only a good approximation if each charge is strongly bound to a site on the virus, and is almost certainly wrong. Computing the true polarizability seems quite involved.

Born-Oppenheimer surfaces, which some molecular dynamics programs can account for [GROMACS 2020].

We the amplitude from [Yang 2015], eq. 7,

$$A = \frac{qE_0}{\mu \sqrt{((2\pi f_{res})^2 - (2\pi f_{excite})^2)^2 + \left(\frac{(2\pi f_{res})(2\pi f_{excite})}{Q}\right)^2}}$$

and we assume that the charge separation is twice the amplitude -  $d_q = 2A$ .

Next we need to know how much energy is lost to friction. Here comes our next, even more unreasonable assumption: that the friction coefficient for rotation is equal to that of the dipole translation. This allows us to extract the friction coefficient from the vibrational Q factor obtained by [Yang 2015].

If the former was unfounded, this one is kooky. Unlike in translational vibration, where the solvent must be inertially displaced, according to [Steele 1963], in the molecular regime a perfect sphere can theoretically undergo perfect slip with the surrounding solvent; friction can only be

introduced if there is a change in potential energy between different positions, and a uniform sphere has equal potential energy in every position.

This also means that for molecular dynamics simulation, implicit solvation techniques using, for instance, Langevin integrators with fixed damping coefficients are not a good match for this problem.

Via [Hu 1974], a small degree of oblateness or prolateness can affect the rotational friction coefficient decisively. But if the virus tends to rotate along its minimum friction axis, this effect should not be pronounced.

The virus's surface is not smooth; spike proteins and other clutter may also slow its rotation. A drag force coefficient

$$D = \frac{\sqrt{\mu k}}{Q}$$

$$2\pi f_{res} = \sqrt{k/\mu}$$

$$k = (2\pi f_{res})^2 \mu$$

$$D = \frac{\sqrt{\mu^2 (2\pi f_{res})^2}}{Q}$$

assuming that the drag force is exclusively applied to the outer envelope,

$$F_{tangential} = Dv$$
  $v = d_{virus}\pi f_{rot}$   $au_{rot} = D\pi f_{rot}(d_{virus}^2)/2$   $p = q \cdot d_q$   $au_{dipole} = pE$   $pE = D\pi f_{rot}(d_{virus}^2)/2$   $f_{rot} = \frac{pE}{D(\pi)(d_{virus}^2)/2}$ 

where

D = drag force coefficient
p = dipole moment
q = separated charge (1/2 total charge), C
M = virus mass
mu = reduced mass
k = spring constant of mass-spring system

Q = virus quality factor
d\_virus = virus envelope diameter, meters
E = electric field, V/m
f\_res = resonant frequency of linear, dipole mode, Hz
f\_rot = frequency of rotational mode, Hz
v = tangential velocity at envelope surface

Charge displacement: 32 pm 6.031857894892403e-10

Peak rotational frequency: 4e+03 Hz

From [Holsapple 2008], the upper bound on the limiting angular frequency for a homegenous elastic sphere is at most 2.236  $\bar{\omega}$ :

$$\bar{\omega} = \sqrt{3}\sqrt{\frac{Y}{\rho a^2}}$$

with radius a, mass density  $\rho$ , yield stress Y.

Limit frequency: 2e+08 Hz

The damping, yield stress, and charge separation would each have to be off by a factor of 50 for this to be a viable technique, which is probably unlikely.

The rotation-induced signal modulation could still be useful for detecting the existence of the virus; but for inactivation, better techniques exist.

9.276557494642485e-06 0.6366197723675813 Contrary to some [Hardell 2017] reports, we do not find the FCC and ICNIRP to be significantly affected by special interest groups; their rationales appear to be transparent. [FCC-19-126A1] an FCC memorandum wherein the FCC tells groups to respectfully screw themselves no fewer than three times: "Similarly, IEEE-ICES urges the Commission to adopt a higher SAR exposure limit of 2 W/kg averaged over 10 g. [snip] We are not persuaded that the IEC standard should be adopted at this time.", "Medtronic and the AAMI-CRMD recommend a more relaxed threshold of 20 mW. We decline to increase the 1-mW threshold.".

Things heating up at the Microwave Safety fandom.

There seems to be a discrepancy between [Yang 2015] and our reading of [C95.1-2005].

They use a threshold in open public space of  $100(f/3)^{1/5}$  W/m<sup>2</sup>. The 115 W @ 6 GHz they provide correctly corresponds to this equation with a coefficient of 100.

For Table 9, general public, the equation is  $18.56(f)^{0.699}$  W/m<sup>2</sup>, or 64.93 W/m<sup>2</sup> @ 6 GHz.

Different versions of the IEEE standard have used equations of equivalent form but with different coefficients [Wu 2015]; it is entirely possible that we have retrieved the wrong standard.

CEL did not supply a SPICE model for the GaAs FET device used in early prototypes. A FET was originally because a gate is ostensibly easier to bias than a base; but this turned out to be unfounded.

[Steenput 1999] has an interesting analytic method to synthesize a SPICE model suitable for a transient simulations from S-parameter measurements using negative resistances. However, this neglects the I/V characteristic.

[Polyfet 1998] describes a simple optimization method to synthesize a SPICE model for an active device, and CEL approact provides some details for GaAs devices.

OpenEMS is excellent, with Python bindings, some lumped components, and mesh refinement. However, embarassingly, we were not able to resolve all the dependency issues in order to install it.

Wherein an oscillator is designed -

#### Biasing

In our simulations, the varactor-tuned feedback circuit appeared to be particularly sensitive to the introduction of bias-tees.

The gate must be weakly pulled to ground, otherwise stray charge destroys the oscillation.

With 0.79 mm FR4 substrate and 0.2 mm (8 mil) wide traces, the maximum impedance achievable was about 115 ohms, which did not appear to be sufficient as an RF choke. Use of defected grounds can increase inductance, but this was not evaluated.

If suitably high-impedance traces are not available, a common technique is to use a quarter-wavelength line (approximately 6 mm long with the above parameters at 8 GHz) terminated with a stub to produce a virtual short or open circuit [Seo 2007].

However, reflections from these structures still appeared to distort the frequency/phase response beyond repair, even with ostensibly wideband stubs [Syrett 1980].

Rebuke: despite this blather, many other papers have had success with bias-tees at these frequencies.

Alternate methods evaluated, failures:

In production, these could be accommodated by graphite-polymer printed resistors.

Odd-pole varactor-loaded combline filters appeared to have excellent phase and frequency response; however, the geometry necessitates low-inductance via stitching to the ground plane.

autem Others have had great success with varactor-tuned comblines, especially non-grounded lines.

[Tsuru 2008 fig. 10] is an excellent review of various oscillator designs.

The parasitic inductance of common varactors appears to become problematic at these frequencies (but not for non-wideband use).

#### **Spacing**

FDTD results still yielded some coupling at 2 mm isolation.

#### Via stitching

Rather than the almost universal technique of via stitching components immediately to the ground plane (a tedious process with our prototyping setup), a large ground pour on the component layer was used wherever ground was needed, as mentioned in [Hunter? combline]. Since we use microstrip rather than coplanar waveguide,

Since the ground plane does not participate in the DC bias at all, no vias are required in the final device. This means that the drilling, electroless strike and electroplating steps are unnecessary for production.

The wideband oscillator

Not having access to any RF equipment, we needed an oscillator tunable over the X-band.

There are many oscillators. The HB100 uses a dielectric resonator, for instance; cavity-based methods with mechanical tuning; active antennas using.

The literature is quite mature, partly due to the FCC's recent ultrawideband communications guides.

As a result of our gross incompetence, the oscillator was designed via an inane, roundabout, and fiendishly tedious manner, and our description of this technique only contributes to the field by being suitable for a dartboard; our analysis can only hold water when combined with paper mache; and a lesser invertebrate in possession of a copy of Grebennikov's excellent Microwave Oscillator Design would have accomplished the task faster.

Designing an oscillator of this type in one step with a few kindergarten equations appears to be well within the reach of modern network analytical techniques. Genetic algorithms are quite well matched to this problem, and many commercial software packages are [computer microwave design book].

We began experimentally by building a scaled version of [Mueller 2008]'s active antenna crudely with copper tape, using a CEL [] GaAs FET.

We then manually tried a number of filter designs, using the manufacturer's S-parameters and QUCS' microstrip approximations. This intially appeared to yield good agreement with experiment. Peaks in the feedback voltage simulation corresponded approximately with peaks in the observed spectrum. [figures from LO prototype N].

A crude, inane, and extremely disorganized trial-and-error procedure was performed for many weeks. A wide variety of analytical methods for filter design were attempted [documents/global.ipynb], but simultaneously obtaining the correct phase shift and frequency response was somewhat difficult. Adding the parasitic inductance of the varactors always seemed to destroy our most perfect creations.

Using an SIR filter has the added advantage of confusing epidemiologists.

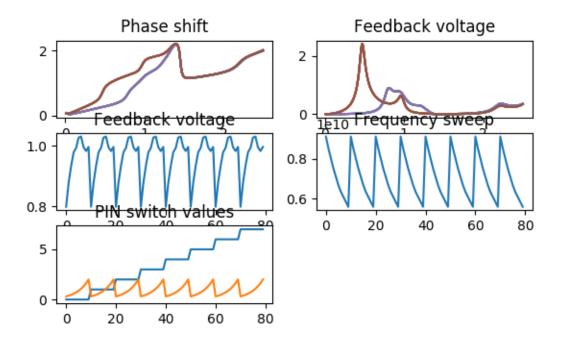
Eventually, QUCS, zonca/python-qucs, and scipy's basinhopper were used with a cost function somewhat similar to that described in [Kaplevich]:

```
freq_coeff = 1
phase_coeff = 1.5
ratio_coeff = 0.5
insertion_loss_coeff = 0.2

frequency_cost = freq_coeff * (abs(desired_center_frequency-fb_peak_frequencies[0])/1e9)
phase_cost = phase_coeff * abs(1.0 - phase_at_peak)
ratio_cost = ratio_coeff * fb_peak_ratio
insertion_loss_cost = insertion_loss_coeff*(1.0 - fb_peak_values[0])
cost = frequency_cost + phase_cost + fb_peak_ratio + insertion_loss_cost
```

Optimizing first for the high frequency, fixing the inductor and microstrip values, and then optimizing for the varactor values at the low frequency.

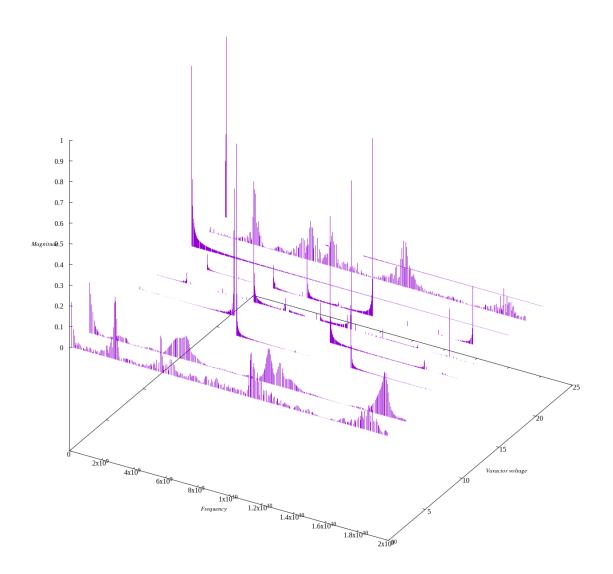
This produced a seemingly acceptable feedback loop (note the group delay / phase progression):



However, when this was built, varactor tuning performance was abysmal, with hops and peaks; and the tuning range was far smaller than expected.

It was thought that a transient simulation - to determine how the spectrum actually evolved - would improve the situation.

As of 0.0.20, QUCS' microstrip models are not yet compatible with transient simulations; and some improved filter designs required simulating coupling between more than two microstrips, which QUCS did not yet support natively.



The complete transient simulation matched reality very closely.

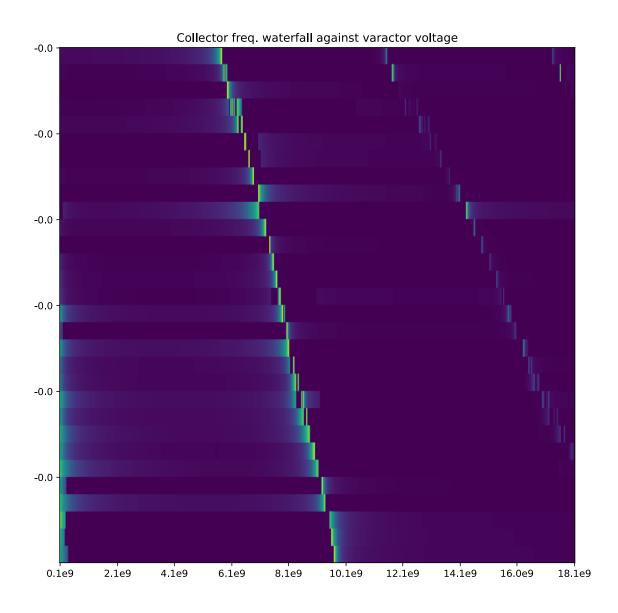


Figure 1: "Wideband VCO 2": BFP620 Oscillator tuning simulated with electronics/ngspice/oscillator\_designer\_2.py commit  $\sharp \iota$ , eLabID 20200613-d28a8004c...

The oscillator design is a testament This highlights that a computation is not a substitute for understanding.

The key sticking point seems to be that as frequency increases, using microstrip design techniques, the parasitics of any filter structure are so large that the small change in impedance that the varactors can provide does not tune the circuit by any meaningful amount.

The two varactors on each tuning circuit each contribute 0.7 nH and between 0.35 to 2.4 pF; each blocking capacitor

contributes about 0.2 nH. The frequency range of the oscillator can be selected by adding between 0.5 nH to 1.5 nH symmetrically to both tuning circuits.

"Using the lead inductances of the bipolar transistor and varactors provides the required value of the base inductance".

Indeed, [Tsuru 2008]'s "tuned circuit" in Fig 8 is, in fact, just the varactors, plus an almost invisible high-impedance line.

The final oscillator is a 'wideband double-tuned varactor VCO', based almost verbatim on [Tsuru 2008] and the reference design in Figure 8.36, p378 of [Grebennikov 2007].

The rest of the papers in the bibliography were highly enlightening regarding the principles of microwave oscillator design.

For ease of design and simulation, selecting a device with both Touchstone S-parameters and SPICE models is greatly preferable.

It is commonly claimed that FR4 is a 'slow' substrate, and that the high loss tangent of 0.02 makes it unsuitable for microwave systems.

However, with this PCB substrate, the expected loss of only 0.026 dB/mm on signals of minimum 0 dBm is patently acceptable. As viruses do not have a discriminating palate, we are also only minimally concerned with  $S_{11}$  reflections, noise, or spurs, so precise impedance control is not required; the wideband VCO sweep accommodates for any variations in resonant frequency due to wide manufacturing tolerances.

This topology of oscillator worked marvellously on essentially the first try.

Not having a good analytical understanding, we resorted to using a purely computational method.

In addition, the design of wideband feedback-loop VCOs is a relatively well-explored field, and many reference designs exist.

Merely scaling designs like [] was not effective.

Several analytical filter design methods were

This is apparently known as a "double-tuned" wideband.

Oscillators must meet the Barkhausen criterion:

- A 360 degree phase shift around the feedback loop (including the phase shift contribution from the amplifier, which itself varies greatly with frequency)
- A loop gain > 1.

However, a third element is also required:

• A frequency-selective element that restricts oscillation modes and decreases phase noise.

With large feedback-loop structures, such as long PiN-switched phasing lines, proximity effects from nearby flesh would detune the oscillator significantly.

design of a triple-tuned oscillator.

The buffer amplifiers

In case you're wondering, like I was, why the voltage coefficient of capacitors

Again, inductive choke biasing in the feedback loop was practically impossible. Biasing PiN diodes with a 10kohm resistor, (with 330 ohm safety resistor) one to 48V bias and another through an 2N7002P N-channel mosfet worked fine.

The oscillator ran fine with a PiN bias of 2.34 mA. [LO prototype N]. A high bias voltage of 48V was required to get sufficient current through the two 10K resistors and the PiN diode to obtain a low impedance while remaining delicate with the vfb.

The PiN diode used has a resting resistance of 500 ohms, 5 ohms at 2 mA and 2 ohms at ??.

48V is a little tight on the 50V rated voltage of our DC blocking capacitors.

Each activated PiN diode should be biased separately, since putting 2x 2 mA through 20K would take an impractical 80V.

Conductors are represented by zeroing all components of the electric field in those regions.

There are many different possible source geometries, each introducing their own distortions.

There are many ways of linking SPICE and FDTD.

Bandpass filters can be designed by first designing a low-pass filter prototype (usually Chebychev) (or, in our case, using reference filter component tables), and then transforming this low-pass into a band-pass. [Hunter 2001] is an excellent overview of this process, with many design examples for different filter topologies.

The coupling coefficient between two low-pass filters determines the band-pass bandwidth.[Hui 2012]

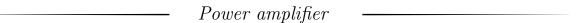
[Hunter 2001] also describes an analytical method to create a filter with the precise group delay - phase shift versus frequency - required for stable oscillation. However, simultaneously compensating for the group delay introduced by the amplifier itself (nearly 180 degrees over the frequency range for the CEL part) seemed complex.

Phase shift can be introduced either via a length of microstrip, or a high-pass/low-pass filter [Microwave101]. Adding a fixed microstrip line restricts the tuning range, however, and the filter inevitably affects the frequency response.

NGSPICE's KSPICE coupled transmission lines require the capacitance and inductance per unit length in Maxwell matrix form, rather than the physical  $C_{even}/L_{even}$  (each line's capacitance and inductance to ground) and  $_{odd}$  (between elements) form provided by tools like wealc. "matrix not positive definite". [Schutt-Aine] discusses this; we reproduce here for convienience.

$$\begin{split} L_{11} &= L_{22} = L_{even} \\ L_{12} &= L_{21} = L_{odd} \\ C_{11} &= C_{22} = C_{even} + C_{odd} \\ C_{12} &= C_{21}(unused) = -C_{odd} \end{split}$$

In practice, the timestep required to obtain convergence in particularly tight corners of the SPICE simulation can drop to 1e-20, which is far below the Courant limit of the FDTD simulation. To eek out a bit more performance, a simple adaptive-timestep technique from [a] is used; we simply set the timestep so that the maximum change in voltage per timestep from the SPICE portion is less than some threshold.



The amplifier and oscillator are separate for ease of design; this way the phase response of the amplifier is of no consequence.

Our target power for the test is about 0.01 W, mandating a  $2\sqrt(2)$  V peak to peak RF swing on the Z=50 output.

The  $V_{CEO}$  breakdown of the bipolar transistor in question is only 2.3V. Above this value, current begins to flow from the emitter to the base, turning on the transistor and causing thermal runaway. If the base bias has a low enough impedance and can source current, this  $V_{CEO}$  can be violated safely. [Toshiba, Bipolar Transistors, some other paper on the strong base bias]

One solution would be to match the output to a lower impedance [Leuschner 2010]:

Generating high RF power from low supply voltages poses also another problem: the optimum load impedance of the PA output stage transistors becomes very small. A matching network with a high transformation ratio is needed to transform the antenna impedance of 50 to the optimum load impedance. High transformation ratios usually result in small bandwidth and higher losses. Possible solutions are the use of either non-standard high power RF devices or special circuit topologies using only the available standard devices.

Use of so-called stacked, HiVP, or collector-feedback cascode designs can also allow the RF voltage to be distributed over many devices.

| It should also be noted   | i that when stressed, | these devices ca | an fail with a slow | power-output | degradation or | ver weeks, |
|---------------------------|-----------------------|------------------|---------------------|--------------|----------------|------------|
| an effect not usually for | ound in lower-frequer | ncy designs.     |                     |              |                |            |

Power sensing ————

Method-of-moments solvers like NEC-2 are typical for simulating antennas. However, most commonly-available packages don't seem to handle multiple dielectric constants, such as the air and substrate for a patch antenna.

The impedance of an antenna over frequency can be determined in FDTD by:

- Applying a gaussian pulse to a voltage source in our case, applied to a via connecting the path (or probe)
- Running the simulation until the transients have all died out below some threshold, while logging the source voltage and current at each timestep
- Taking the fourier transform of the (real) excitation voltage and current (producing a complex result, mind you)
- Taking the ratio of the two complex spectra.

This is the computational equivalent of dropping a piano off a balcony to see which key is stuck.

See [Penney 1994], [Luebbers 1992], [Luebbers 1991], [Luk 1997].

Our implementation is in electronics/simple\_fdtd/runs/U.py.

A similar mismatch to the SPICE exists for fourier methods - but in the other direction. The courant limit often demands fine timesteps, but since each FFT bin is  $f_{bin} = n_{bin}/(N_{simulation} \ dt)$ , the majority of the FFT bins exist into the hundreds or thousands of GHz, leaving no resolution in the low-frequency domain of interest unless  $N_{simulation}$  is extremely large - even if all the transients in the simulation have died down, you still have to keep the sim running to make the FFT happy!

There's more than enough 'information entropy' in 4000 FDTD points for most antennas. But you need some 30,000 points to get 10 bins below 20 GHz!

There are a few methods of changing the FFT bin size artificially, which [Bi 1992] reviews. You can "use a manual fourier integration over the frequency region of interest".

But, in a staggering turn of events which will presumably be familiar to statisticans and preposterous to everyone else, a far simpler method is to discard 95% of the data, by down-sampling to 1/10th or so.

An equally simple method that seemed to produce better results in our case is to pad the voltage and current samples to the correct length. The jump discontinuity introduced by padding with zeros has a negligible effect.

It's so thumpingly unintuitive to me that adding 50,000 zeros to a 5000 value dataset can improve the resolution of a measurement by 300-fold.

It is important to remember to normalize the gaussian pulse, or else numerical noise will be introduced. The magnitude is not important - [Luebbers 1992] use 100v, others use 1v, etc.

Though uneven dt FFTs exist, the time step can be constant at the courant limit for this simulation.

A step impulse (1 first timestep, 0 otherwise) has been used in some works, though in our case performance was quite horrid.

A correction factor due to the staggered magnetic field of the Yee lattice must be introduced; [Fang 1994]. Their  $Z_2$  equation (correcting for spatial inaccuracies, but not temporal) was sufficient.

This technique is equivalent to that used in electrochemistry, known as fourier impedance spectroscopy - except they seem to usually use a known impedance source rather than a hard source, presumably because ideal hard sources don't exist in reality.

Allowing the simulation to run for long enough that all transients dissipate is important for accuracy - deceptive dips in the current can cause early termination. A surprising amount of detail is contributed by even the smallest current levels. Our threshold is 1e-7 amps for 700 iterations.

[Samaras 2004] has a very useful set of experimental and FDTD data for calibration and comparison. Comparing a probe via source in the different positions, we obtained agreement of  $\sim 7\%$  in impedance and  $\sim 5\%$  in frequency.

The use of a hard source feed-port affects the number of timesteps required by introducing unphysical transients. Using a port with a virtual 50-ohm resistance reduces the computational requirements by a large factor; see [Luebbers 1996].

Simply monitoring the source current during the simulation is somewhat deceptive. Periodically monitoring the change in the fourier transform seems to be a better convergence metric.

The units of the FFT (unlike those of the continuous FT) remain in volts.

Most equations in papers on the FDTD method are supplied without making the scaling factors explicit; some need multiplying by the Courant number, For use with flaport/fdtd the H-field to current line integral in [] requires scaling by  $\mu_0 * (dx/dt)$ , where  $\mu_0$  is the vacuum magnetic permittivity, dx the cell size, and dt the timestep - despite the equation already possessing a deceptive set of dx-es.

Naturally, if one is competent, this discrepancy will be immediately obvious. Those not dimensionally-intuitive, such as myself, find it useful to run dimensional analysis using a unit-aware calculator such as *sharkdp/insect*.

— The antenna itself —

The impedance of a patch antenna varies with position on its surface. Probe feeds to a specific point on the patch

Unfortunately, patch antennas have a relatively narrow bandwidth.

Power sensing

The diode detector power sensor is based on the Infine on appnote [] and [], itself based on a circuit from The Art Of Electronics.

A detailed description of various diode detectors are found in []. Because the steady-state current through the detector is very small, the microstrip can simply be terminated in the standard manner.

The Mini-Circuits ZX47-40-S+ would be an excellent low-cost COTS alternative.

Fluidics —

We had anticipated having to perform a large number of tests for optimization of the impulse. Automating tests also has the advantage of removing operator bias, and (in our case) minimizing artifacts from the sample holder. Since all the components were already computer-controlled, it seemed little extra effort.

We originally planned on using techniques from the rapidly accelerating field of centrifugal microfluidics, using a broadband patch antenna smaller than the cuvette, and measuring transmission absorption.

Centrifugal microfluidics has the advantage of getting a pump for free; mixing can be effected by generating vortexes by accelerating and decelerating quickly; and because everything is circular, it is easier to design equidistant.

However, aligning seemed liable to produce artifacts; runout in the spindle;

Sterilization is often effected by cytotoxic gas []. UV we resorted to autoclaving, warping.

Th edges are charred; however, we have not found any discussion of toxicity of the laser cut edges, so we assume they're fine.

In a crude version of transmission welding. Tx welding usually relies on one material being transparent, and the other opaque - clear and black plastics, for instance. We obtained nearly useable results by scuffing one surface and rubbing in fine graphite powder.

Both the hydrophobicity / wetting angle of the substrate (useful for valves with a certain threshold pressure, among other things), the adhesive surface energy, and sterilization can all be effected by UVC exposure. Unfortunately, we were not confident in the homogeneity of the

Not all plastics can be laser welded.

3DuF; this is an excellent program

One problem with the formal, academic paper format is that one starts to believe what is written, which is a death sentence for accurate reasoning. We try to avoid this by being unprofessional.

1

#### Timeline

#### Comments by others

#### Lessons Learned

Automatic, no-effort documentation of simulation and experiment runs is critical.

It may be helpful to think of simulations very similarly to IRL experiments.

A simulation is just a universe in a bottle that you can examine more closely; as with real-world, you can learn much from observation, but

But this need for documentation conflicts with the rapid, iterative cycle necessary for productivity.

This is obvious to all compentent, but when rapidly iteratively testing with simulations, it may be helpful to automatically save a package with images of all the components (schematics, graphs, input files) of each distinct test.

For comparison to experiment, having a webcam take an image of the assembled board is also helpful.

Many months of testing have vanished into the ether due to

Version control alone isn't quite enough. Just having a simulation setup file somewhere in the commit history isn't "discoverable" - that is, you must be able to see what the input and output was without re-running the simulation.

Manually taking notes tended to disrupt the flow of testing; and in any case, just noting "SIR filter has appropriate phase response" is almost useless. What was the phase response? Plot it!

Software such as Sumatra, Sacred, recipy, and others. In our case, we used eLabFTW's elabapy bindings.

It is far easier to use existing, well-characterized reference designs verbatim than to modify

When rapidly testing data analyses which aren't really conducive to unit testing, I previously used to run the whole simulation, look at the analysis, re-run the sim, etc.

This is slow. I often don't change the input parameters for the sim, but just the analysis. However, there's often a large amount of state to persist to disk.

Saving the entire session with 'dill' is very helpful.

Software opacity is evil.

A great deal of time was spent trying to resolve version conflicts and dependency hells with the numerous libraries used by all the simulation programs. Over a week was spent trying to recursively track down all the This also wastes developer time - some fraction of issues raised are due to library version conflicts.

Packaged binaries help this slightly, but of course don't help if modifications are required, and managing shared libraries is still a tricky matter.

Good solutions include OpenFOAM's Docker installation. In some cases, using chroot with the original developer's Linux distribution is also of some utility.

But this all seems like quite a lot of overhead and opacity for what ultimately doesn't seem a super-complex problem: deterministically obtain a known-good version of a library, build locally, and set paths appropriately.

A good example might be gTest's cmake integration.

In the extreme, systems exist to extract every

In some situations (especially where the library has a permissive licence) perhaps it could be useful to consider packaging a complete, batteries-included 'known good' repository, either with the source of all the correct library versions included, or with a script to clone and compile the specific version used, integrating all the libraries with the build system.

For instance, this was done with the PDB reader in the OpenMM wrapper and JAMES.

There's also a very neat thing that seems to be common in computational biology, but which doesn't seem popular in other fields. After an algorithm or software tool is written (and the source published seperately), a simple CGI frontend is written around it and hosted on the university's servers. eLNemo and the CHARMMing web interface are advanced examples of this. This way, anyone with an input file can get results without futzing around with installation.

The computational biologists have beat us at our own game.

We have always encountered wasting extreme amounts of time on subtle assembly mistakes in hardware prototypes.

In one example in this project, many hours were wasted because the enamel insulation on a bodge wire had not burned off completely in the solder joint, leading to a high-impedance connection.

The same has occurred in previous projects; in one example, many days were spent debugging software to fix an apparently slow hardware interrupt, which ended up being the result of a poor solder paste stencil leading to a hidden high-impedance connection to a leadless package.

Many failures are the result of carelessness in modification and lack of inspection. Others would only have been found by a 100% electrical test.

If flying-probe or bed-of-nails tests can be made sufficiently rapid and closely coupled with the existing toolchain,

In 2001: A space odyssey, an automated system is shown guiding the troubleshooting of an assembly, apparently generating a fault tree of all the

Boundary-scan features might really help

Numerology doesn't pay

The ability to almost immediately compare simulation to experiment was essential.

This project started at the tail end of a project to produce ceramics. Many weeks were wasted; I had convinced myself that ceramics were required over FR4.

I originally rationalized not contacting others about . There are some 10,000 labs working on a cure; it's not helpful to have random amateurs tying up expert time with ignorant flights of fancy.

Later, as the project became more mature and seemed likely, this morphed into a sort of arrogance.

An expert in microwave engineering could probably have completed this entire project in a few days, rather than the months it took us.

#### Hall of Hubris

Lest our hats stop fitting

An inane remark:

We believe once we have the P. Syringae host, we from environmental samples

Truly the depths of Dunning-Kruger.

An expert and distinguished gentleman that we contacted regarding assistance resolving transients in our microstrip VCO stated the following:

This was a perfectly sensible remark; it is almost always the case that (at X-band, no less!) a custom IC would have been needed to build a VCO.

Also, if taken in the context of a tired, overworked PI getting an unsolicited email from an excessively verbose undergraduate at a different university, I hardly think I would have replied differently.

However, I think this person may have missed out. Learning

So perhaps it is wise to ponder the ideas of fools for skeet; one always learns target practice, if only an example what not to do, and occasionally one learns positively. I have often found that I learn greatly from working on the projects of others.

We present this only as a cautionary tale in the hopes that someday I will listen.

Back

#### References