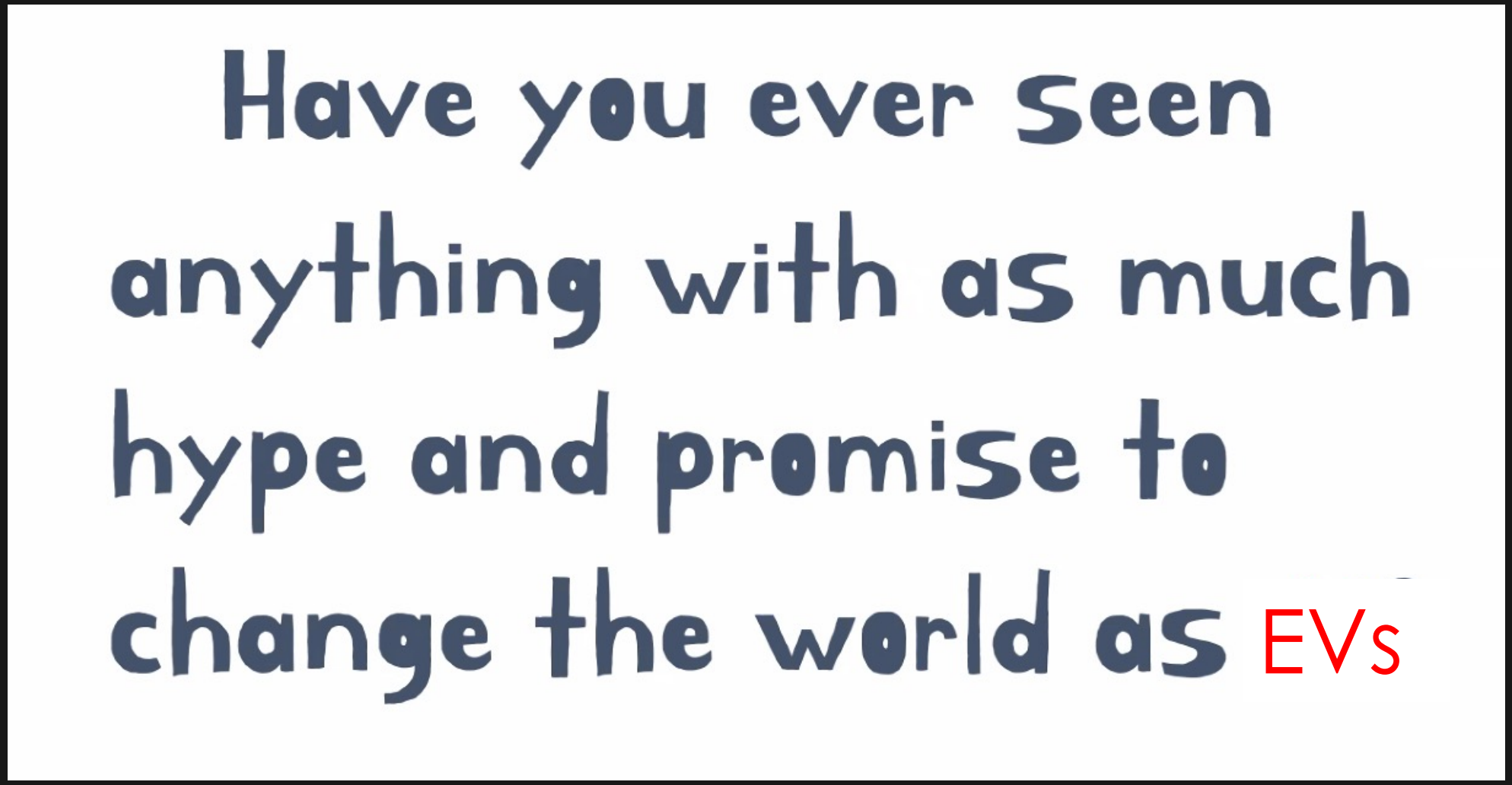
Driving Change Through High-Performance Computing

Kelly Senecal, Ph.D.

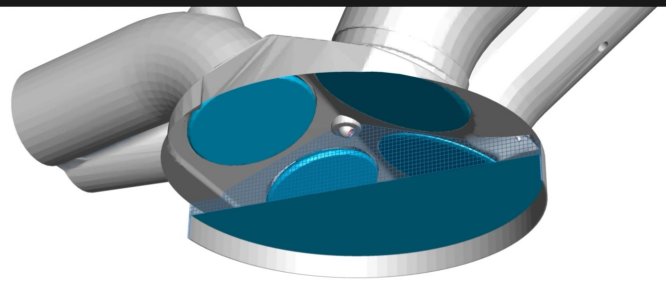
SHPCP Annual Meeting, Houston
April 25, 2024

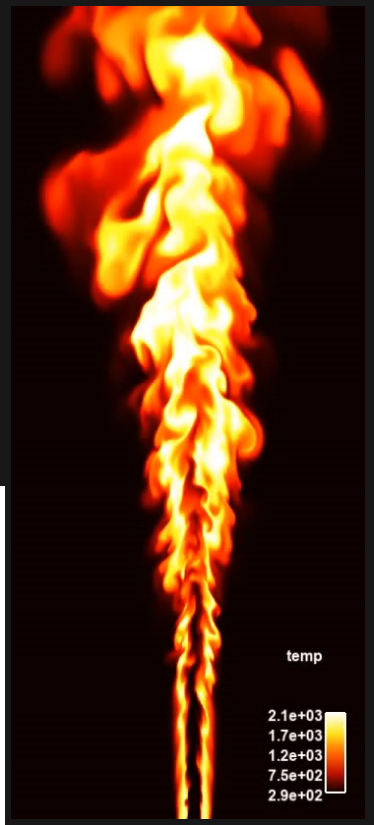
Question: What is the most climate friendly today, a car with an electric motor or a car with an IC engine?

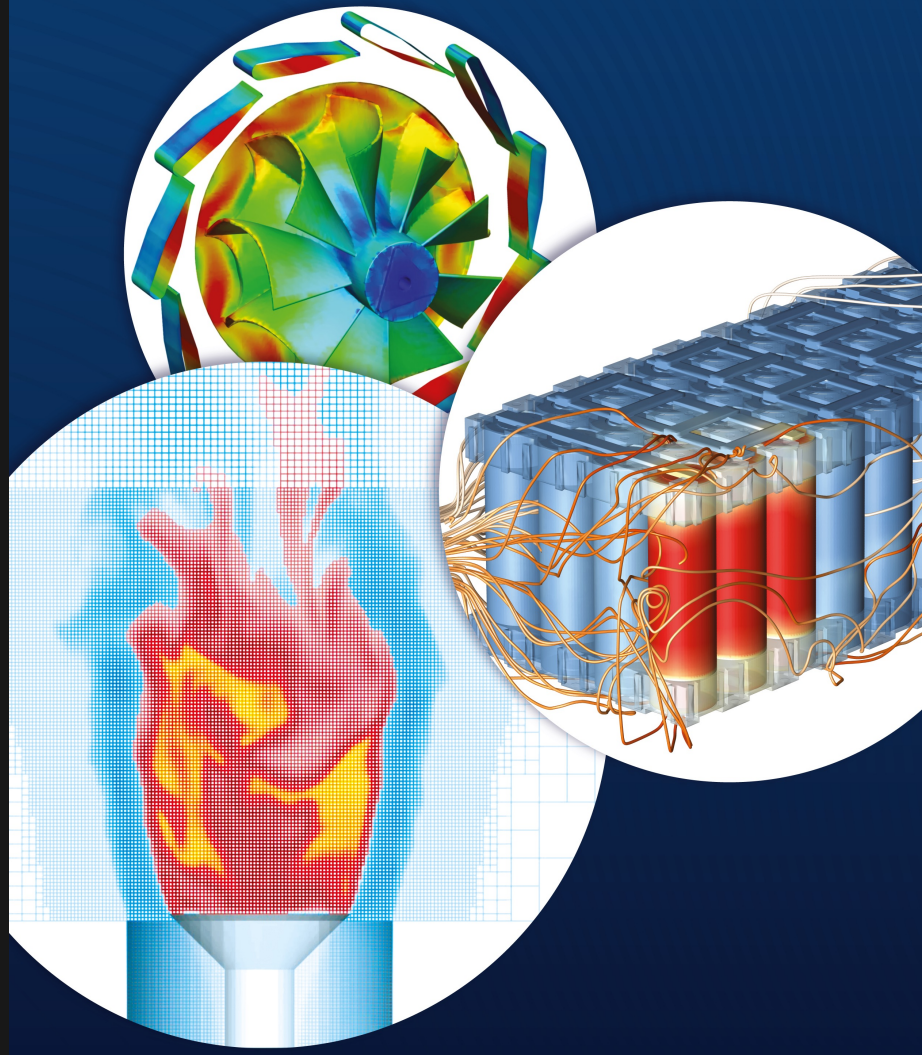


Original image courtesy of Addison Snell

My first passion is CFD





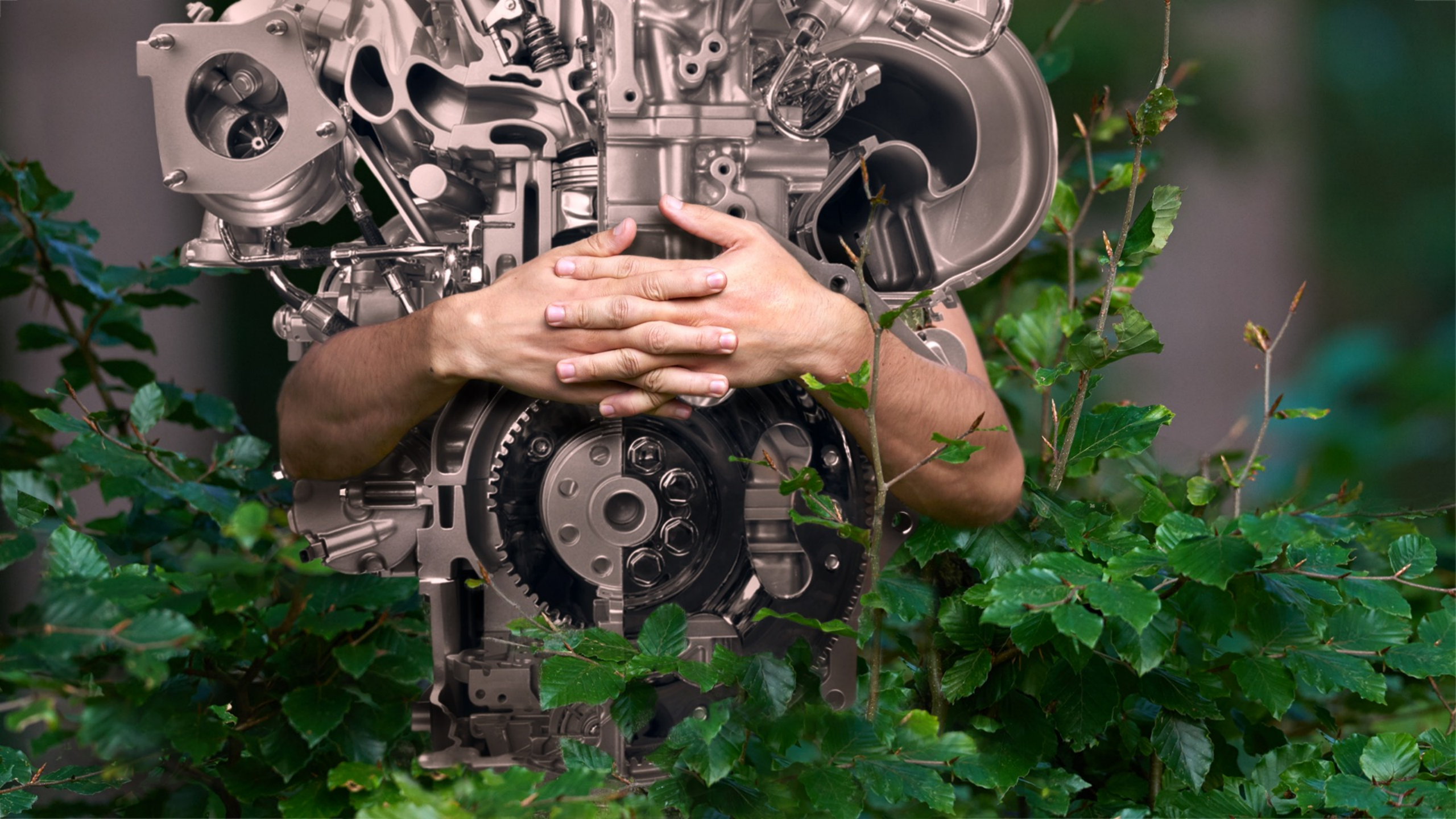


CONVERGE®
CFD SOFTWARE

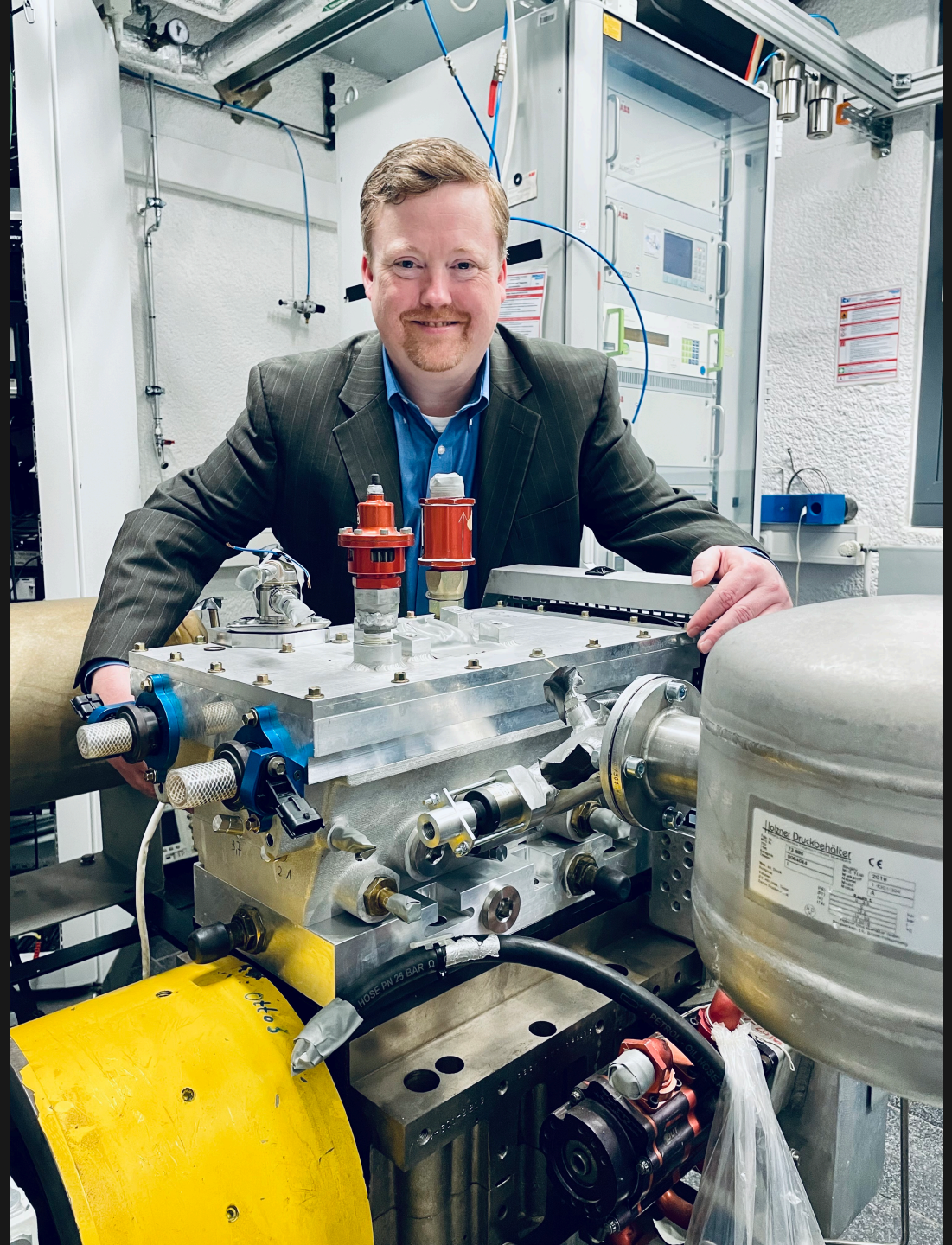
CONVERGECFD.COM

- My other passion is advocating for technology neutrality in transportation.
- Some (many?) of you may be surprised by my conclusions, which is OK!
- Let's have the debate. The jury is still out on the best approach for passenger cars.

I might be a little biased




Testarossa
Tipologia: 12 cilindri a V 180°
Cilindrata: 4943 cc (12 x 411,9 cc)
Potenza: 390 CV @ 6300 giri/min
F40
1984 | Testarossa
1985 | 3.2 Mondial Cabriolet
1987 | F40
1989 | 348 TB
FAMILY DAY


Holzner Druckbehälter
HOSE PN 25 BAR


Next-generation
electric motors,
powertrains,
and power electronics
for the industries
that move the w
ADVANCED
PHYSICAL
MODELS
CONVERGE
CFD SOFTWARE
enedym
Nithium HD e-Motorcycle
Magnet-Free SRM

Driving Change Through High-Performance Computing

What’s changing?

The landscape for transportation propulsion systems!

Engines, engines, and more engines!

Engines (with more and more alternative fuels), electric motors and batteries, and fuel cells.

So what's different now?

There is a major focus on decarbonization and sustainability

Sustainability consists of fulfilling the needs of current generations without compromising the needs of future generations, while ensuring a balance between economic growth, environmental care, and social well being.

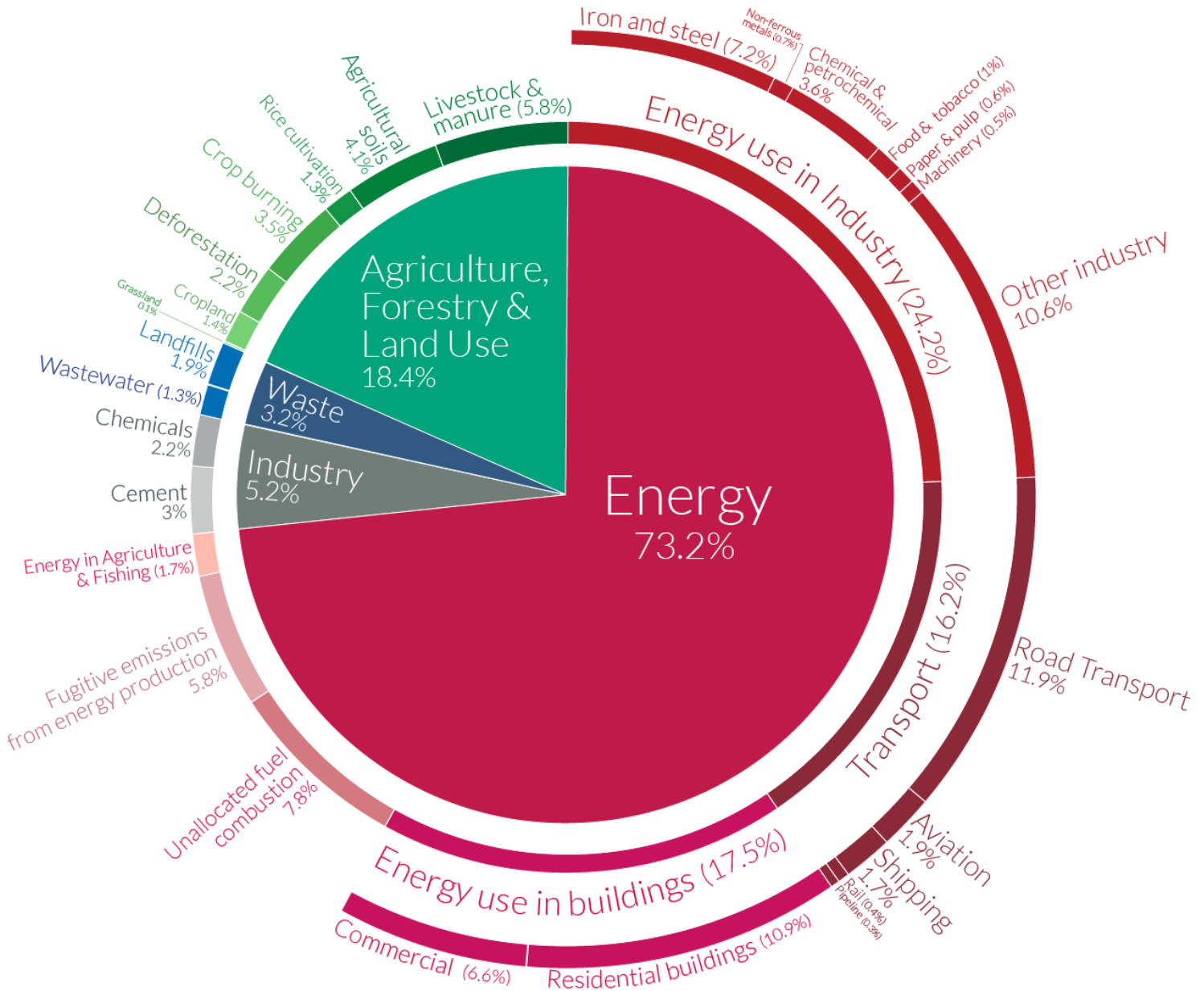
Sustainability consists of fulfilling the needs of current generations without compromising the needs of future generations, while ensuring a balance between economic growth, environmental care, and social well being.

Why is this important?

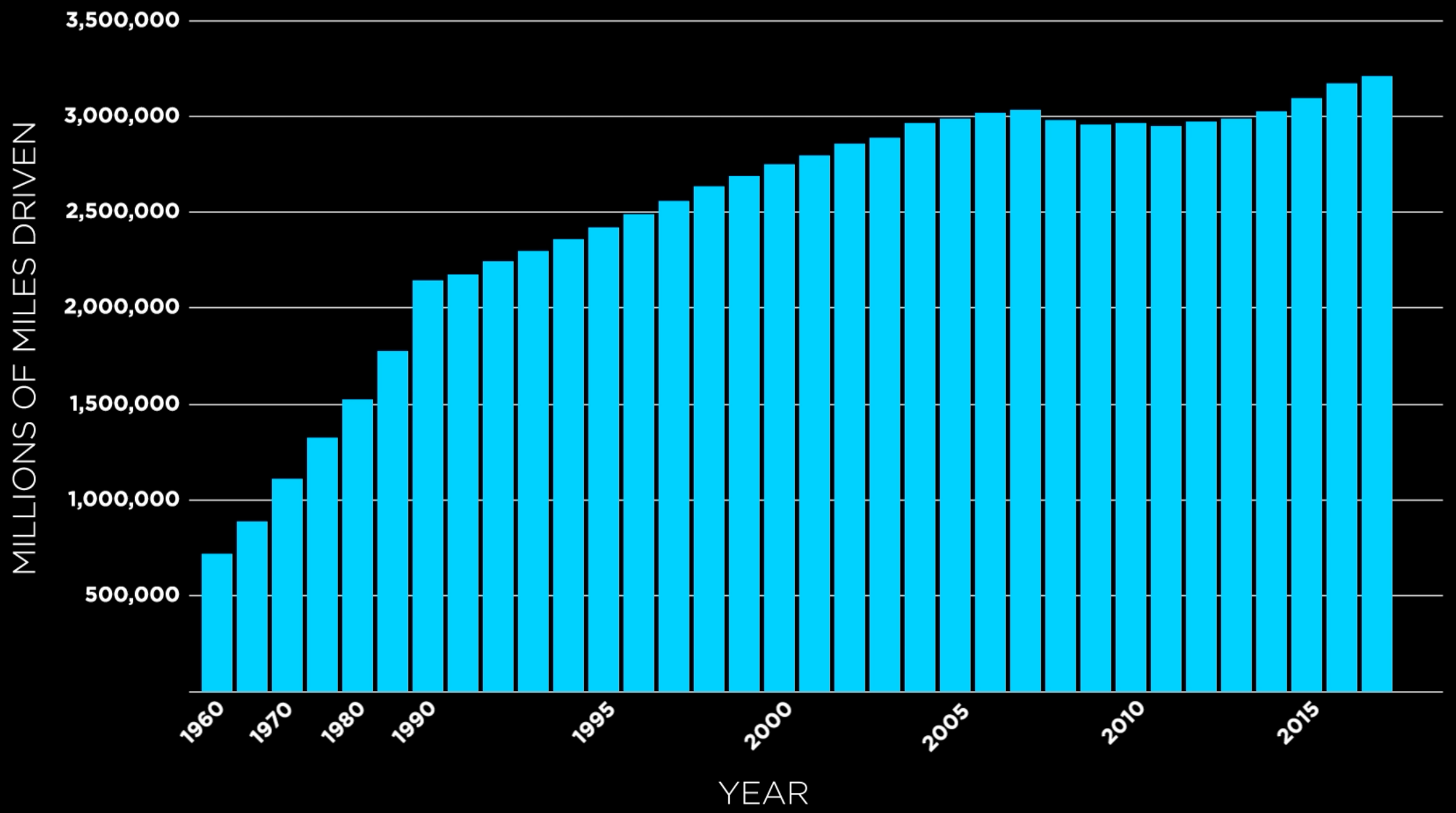
Global greenhouse gas emissions by sector

This is shown for the year 2016 – global greenhouse gas emissions were 49.4 billion tonnes CO_2eq.

Our World in Data



Source: Climate Watch, the World Resources Institute (2020).


3,500,000
3,000,000
2,500,000
2,000,000
1,500,000
1,000,000
500,000
MILLIONS OF MILES DRIVEN
1960
1970
1980
1990
1995
2000
2005
2010
2015
YEAR

The United States loves its cars

- Freedom
- Quality of life
- That's how the USA was designed!

Los Angeles Highway

What can we do?

What if there was a vehicle technology that offered:

- A substantial reduction of GHGs from driving over the lifetime of the vehicle, compared to conventional cars
- GHGs that scale with driving starting the day I drive off the lot (I drive less, I emit fewer GHGs, with a low upfront GHG penalty)
- Criteria pollutants well below the legal limits
- No change in consumer behavior
- No new infrastructure
- No significant price increase
- The need for only a small amount of battery resources
- The flexibility to use advanced sustainable fuels, with the potential to be net-zero GHGs

If this technology existed, wouldn’t it be clear that we should transition the fleet as soon as possible while we're working on more dramatic/disruptive technologies in parallel?

Meanwhile…

The Economist

AUGUST 12TH–18TH 2017

Fire and fury over North Korea

The Fed's runners and riders

Was Google right to sack him?

Competitive punning: game of groans

Roadkill

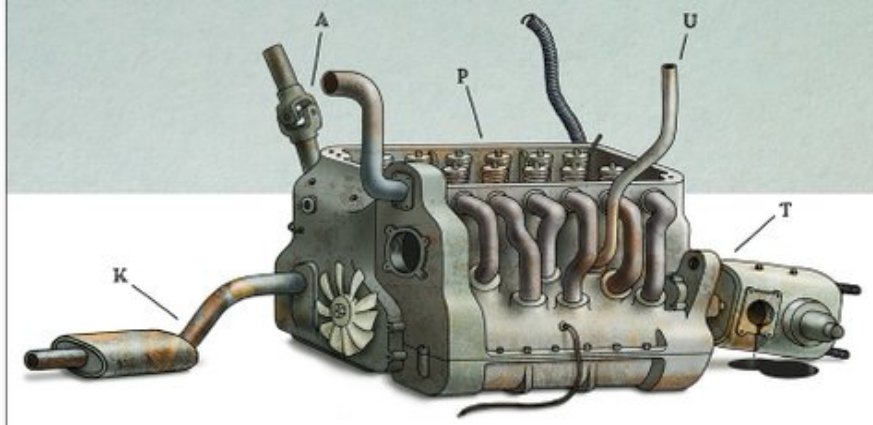
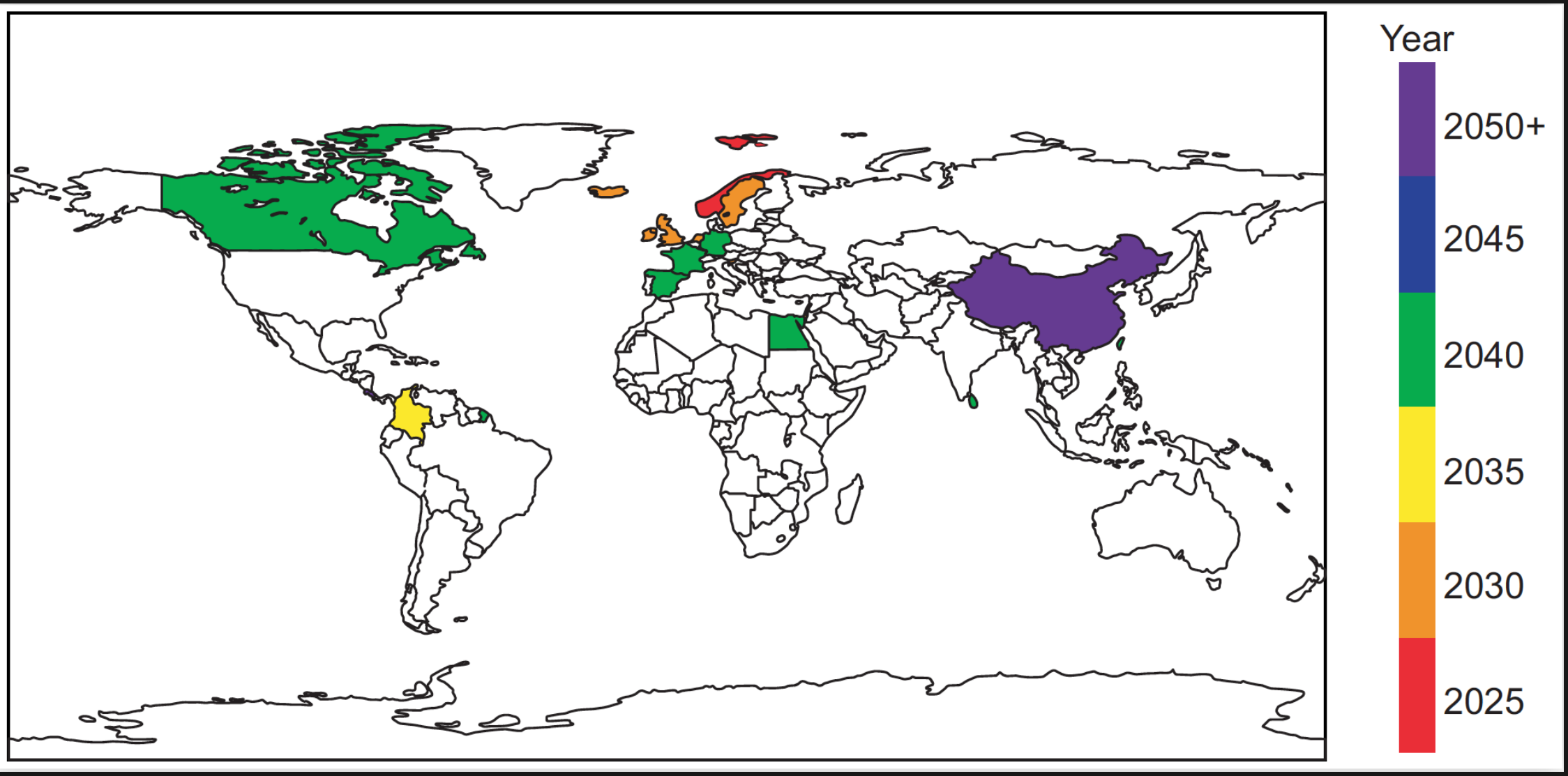


Fig.1 The Internal Combustion Engine


Year
2050+
2045
2040
2035
2030
2025

"… the President will sign an Executive Order that sets an ambitious new target to make half of all new vehicles sold in 2030 zero-emissions vehicles, including battery electric, plug-in hybrid electric, or fuel cell electric vehicles."

- Whitehouse.gov, August 5, 2021

EU Lawmakers Endorse Ban on Combustion-Engine Cars in 2035

European Union lawmakers have approved a proposed ban on cars with combustion engines in 2035 to step up the fight against global warming.

By Associated Press | June 8, 2022, at 1:25 p.m.

Save

Members of the parliament vote on plans to reduce carbon emissions, at the European Parliament, Wednesday, June 8, 2022 in Strasbourg, eastern France. The future of car transport in Europe may become clearer — and cleaner —on Wednesday when the European Parliament decides whether to ban vehicles with a combustion engine starting in the middle of the next decade. (AP Photo/Jean-Francois Badias) THE ASSOCIATED PRESS

GALLERIES

ELECTIONS
Political Cartoons on Joe Biden

PHOTOS
Photos You Should See - June 2022

If not combustion-engine cars, then what?

Regulations for Emissions from Vehicles and Engines Home

Onroad

Nonroad

Greenhouse Gas

Proposed Rule: Multi-Pollutant Emissions Standards for Model Years 2027 and Later Light-Duty and Medium-Duty Vehicles

On this page:

Rule Summary

On April 12, 2023, EPA announced new, more ambitious

Basic Information

Legal Authorities

- 42 U.S.C. §7401 - 7671q

Multi-Pollutant Emissions Standards for Model Years 2027 and Later Light-Duty and Medium-Duty Vehicles
AGENCY: Environmental Protection Agency (EPA).
ACTION: Proposed rule

Table 95. Comparison of proposed combined fleet targets to alternatives (CO_2 grams/mile)

Model Year	Proposed Stds	Alternative 1	Alternative 2	Alternative 3
2026 adjusted	186	186	186	186
2027	152	141	162	165
2028	131	121	141	148
2029	111	101	122	132
2030	102	92	112	115
2031	93	83	103	99
2032 and later	82	72	92	82

https://www.epa.gov/system/files/documents/2023-04/lmdv-multi-pollutant-emissions-my-2027-nprm-2023-04.pdf

Zero-emission vehicles

Multi-Pollutant Emissions Standards for Model Years 2027 and Later Light-Duty and Medium-Duty Vehicles
AGENCY: Environmental Protection Agency (EPA).
ACTION: Proposed rule

Table 99. Comparison of projected BEV penetrations for alternatives vs proposed standards (CO_2 grams/mile)

Model Year	Proposed Stds	Alternative 1	Alternative 2	Alternative 3
2027	36%	37%	33%	32%
2028	45%	46%	40%	39%
2029	55%	54%	52%	46%
2030	60%	63%	55%	54%
2031	63%	65%	59%	62%
2032	67%	69%	64%	68%

https://www.epa.gov/system/files/documents/2023-04/lmdv-multi-pollutant-emissions-my-2027-nprm-2023-04.pdf

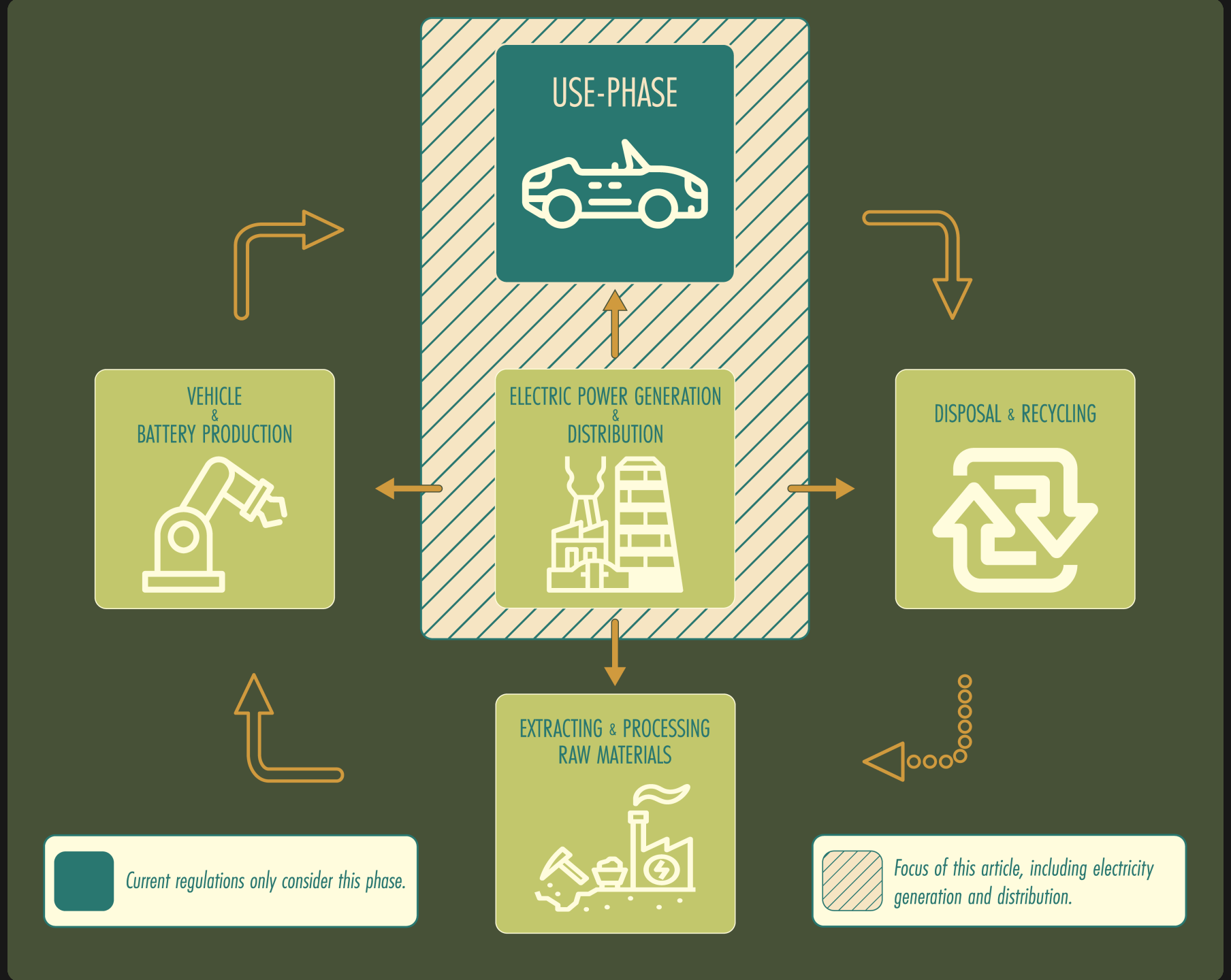
The problem with “zero-emission vehicles”

Clean Electric Car by Marian Kamensky, Austria

We have introduced new vehicle types (mainly BEVs) without proper methods to account for the environmental impact of driving them

- Regulations are based on tests measured at the tailpipe, but "zero-emissions vehicles" have no tailpipe
- Transportation thus makes the CO2 problem someone else's problem
- A "zero-emission vehicle" is counted as 0 CO2, and is sometimes even counted as more than one 0 CO2 vehicle
- Therefore, sales of "zero-emission vehicles" allow for more and more sales of large, low fuel economy vehicles – huh?

Life Cycle Analysis (LCA)


USE-PHASE
VEHICLE & BATTERY PRODUCTION
ELECTRIC POWER GENERATION & DISTRIBUTION
DISPOSAL & RECYCLING
EXTRACTING & PROCESSING RAW MATERIALS
Current regulations only consider this phase.
Focus of this article, including electricity generation and distribution.

ARTICLE INFO
Article ID: 14-12-01-0006

doi:10.4271/14-12-01-0006

A Data-Driven Greenhouse Gas Emission Rate Analysis for Vehicle Comparisons

Tristan Burton,[1] Scott Powers,[2] Cooper Burns,[1] Graham Conway,[3] Felix Leach,[4] and Kelly Senecal[1]

[1]Convergent Science, Inc, USA
[2]Los Angeles Dodgers, USA
[3]Southwest Research Institute, USA
[4]University of Oxford, UK

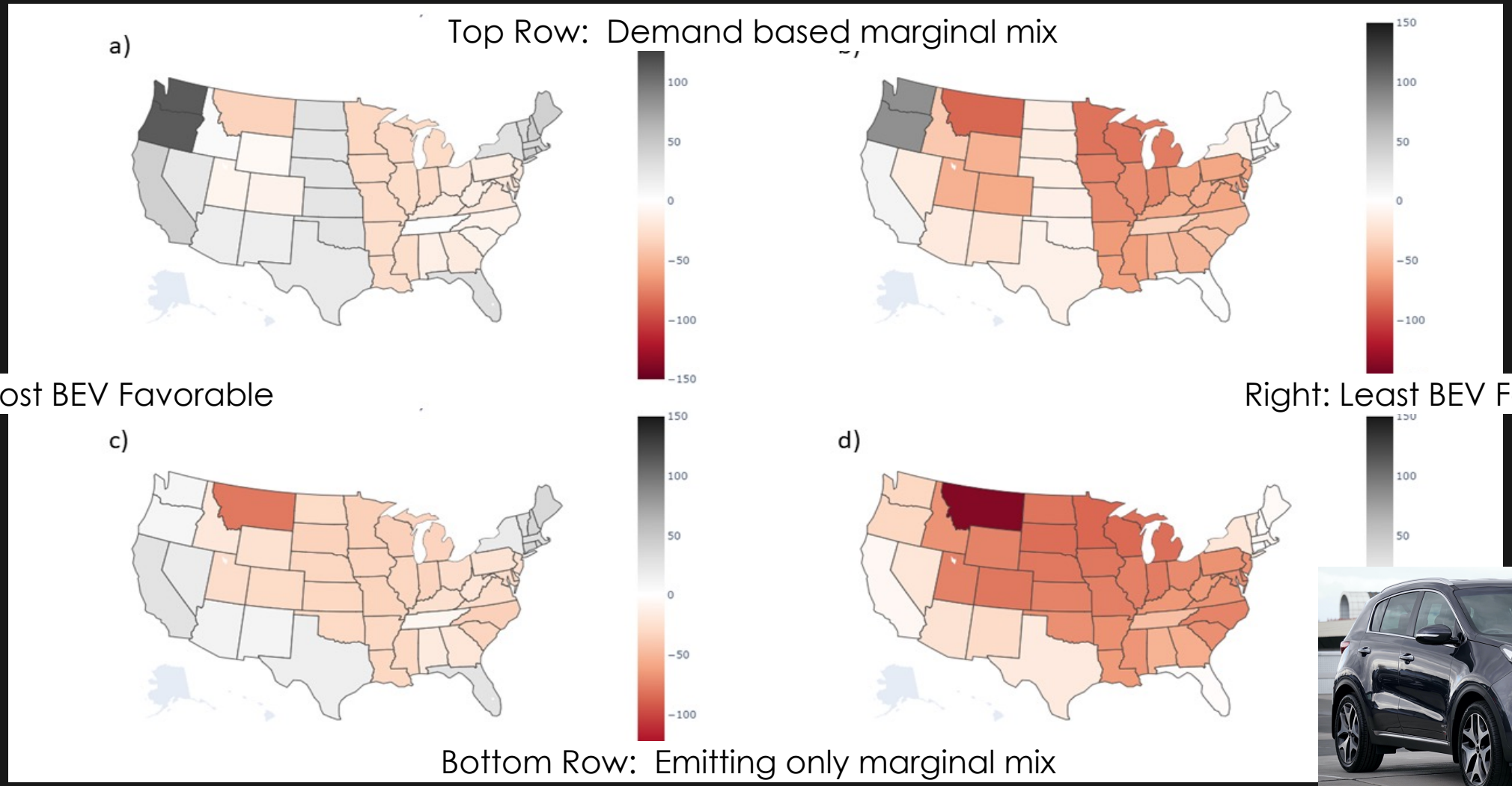
SAE International Journal of Electrified Vehicles

Example: BEV vs FHEV in the US

Burton et al., SAE JEV, 2023

Kia Niro (Small SUV)

$ER_{FHEV} - ER_{BEV}$ (gCO_2eq/km)



How can we use this methodology to inform policy?

An alternative blueprint for light-duty transportation decarbonization

Senecal, *SAE Update*, March 2023

An alternative blueprint for light-duty transportation decarbonization

What the U.S. got right — and wrong — with its joint strategy to transform transportation.

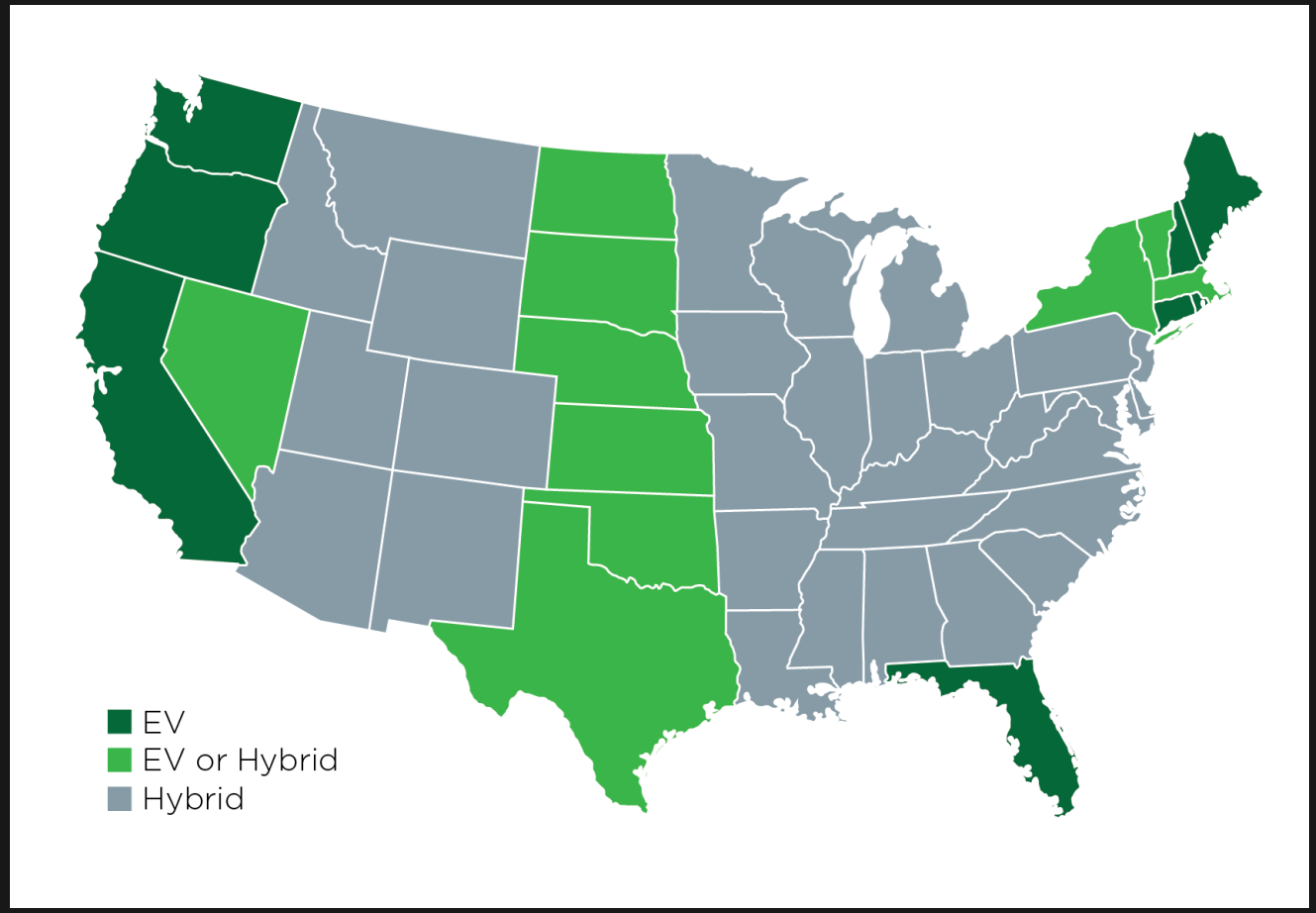
By KELLY SENECAL, PH.D., SAE Fellow and Visiting Professor, University of Oxford. Read more about Senecal at the end of this article.

Four U.S. federal agencies (DOE, DOT, EPA, and HUD) recently came together to publish "The U.S. National Blueprint for Transportation Decarbonization," a vision to build a clean transportation system to ensure a more sustainable future for generations to come. The document outlines the challenges we're facing, strategies to meet those challenges, and how the strategies should be applied to various modes of transportation, from passenger cars to long-haul trucks to aviation. The authors should be commended for taking on the enormous task of documenting an aspirational vision for a safe, affordable, equitable, and clean transportation system.

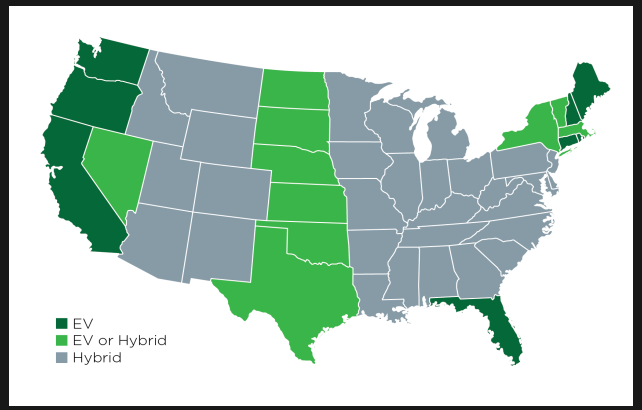
The document's executive summary nails

Alternative to what?

Step 1: Evaluate on a state-by-state basis which vehicle powertrain option has the lowest GHG impact, determined by an LCA analysis over a range of assumptions. An example for a Kia Niro small SUV/crossover vehicle is shown here.



Step 2: Roll out incentives in each state based on the vehicle powertrain type that produces the lowest GHGs. Also consider incentives by vehicle size (encouraging smaller vehicles when/where it makes sense). By promoting a combination of hybrids and EVs, we will use battery resources much more efficiently than if we convert the entire fleet to electric vehicles. This is especially important as resource bottlenecks have been identified throughout the supply chain.



Step 3: Ramp up charging infrastructure in the states where the study supports it.

Step 4: Reduce the fossil fuel content in liquid fuels through policy measures such as the Next Generation Fuels Act. The need for low-carbon/sustainable fuels is unassailable given the vast existing fleet.

It's not the engine, it's the fuel!

Step 5: Determine federal funding for batteries, engines, and fuels in proportion to our nation's projected needs for each technology.

Step 6: Revamp GHG regulations for cars and trucks based on LCA.

Step 7: Repeat steps 1–6 periodically (e.g., every five years).

Expected Outcomes

This plan will make substantial progress toward achieving net-zero emissions for light-duty transportation by 2050

It has the (huge) added benefit of minimizing GHG emissions as much as possible along the way

By investing in multiple technologies, these results will be achieved regardless of what happens with the US electrical grid in the future, safeguarding our decarbonization goals from unintended consequences and unforeseen events

As the grid becomes cleaner, the preferred technology choices in each state will be re-evaluated and updated

Technology diversity (with no bans!) is a deliberate part of this plan (we're not just getting diversity because it's taking EVs a long time to come up, we want it!)

Recommendations

Take a balanced approach to transportation, recognizing that there is no silver bullet solution. **We should have a well managed, diverse portfolio—we do this with our finances and we should be doing this with the fleet.**

Do not ban any particular technology. Set targets and let the best technology win, understanding that the best technology will likely vary depending on region.

Use LCA when comparing technologies. Including only the tailpipe emissions can significantly misrepresent a technology's environmental impact.

Continue to invest in ICE technology for three reasons:

- There is much untapped potential to still exploit
- ICEs are going to be present in electrified vehicles for years to come
- If we cease to invest in ICEs, there is danger that we will lose the opportunity to improve the technology, which would prove especially problematic if electric cars do not meet expectations.

Devote significant resources to investigating carbon-neutral fuels. Success in this area will not only allow us to make use of much of the current infrastructure, but will allow us to lower emissions in the current fleet.

Hybrids are the fastest way to reduce CO2 emissions from vehicles. They should be treated as such.

Engineering—not politics—should drive future transportation policy.

It’s starting to sink in

Home > News > News

February 14, 2023

EU Parliament Votes To Ban Sales Of New ICE-Powered Cars From 2035

The new law also includes intermediate emissions reduction targets for 2030: 55 percent for cars and 50 percent for vans.

https://insideevs.com/news/652486/eu-parliament-votes-ban-sales-ice-powered-cars-from-2035/

EU delays final vote on combustion engine ban, exposing growing dissent among member states

COMMENTS

By **Jorge Liboreiro** & **Vincenzo Genovese** • Updated: 03/03/2023

https://www.euronews.com/my-europe/2023/03/03/eu-delays-final-vote-on-combustion-engine-ban-exposing-growing-dissent-among-member-states

EU was set to ban internal combustion engine cars. Then Germany suddenly changed its mind

By Ivana Kottasová, CNN

Updated 2:06 PM EDT, Mon March 27, 2023

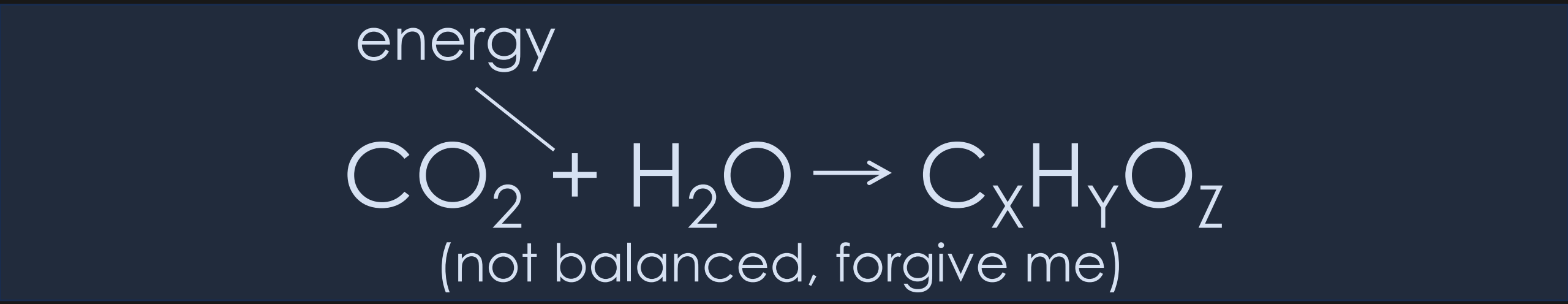
https://www.cnn.com/2023/03/24/cars/eu-combustion-engine-debate-climate-intl/index.html

What happened?

E-fuels

- E-fuels are made by converting electrical energy into chemical energy

- E-fuels are fuels made from CO_2, H_2O, and electricity



- If the electricity is renewable, e-fuels can be carbon-neutral

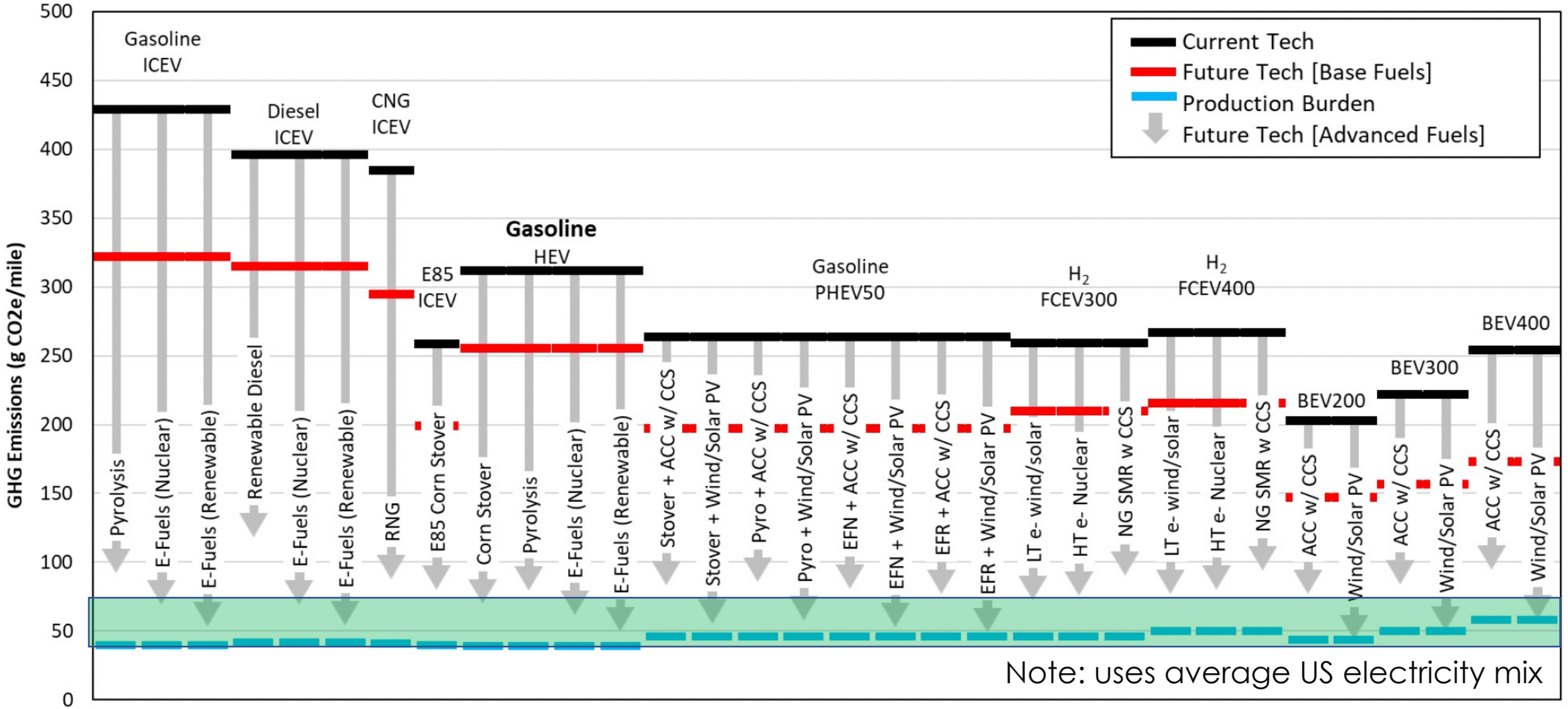
- The CO_2 can be sourced from a CO_2-rich exhaust (e.g., a power plant) or extracted from the atmosphere

RESULTS: GHG EMISSIONS

Slide courtesy of Jarod Kelly

Argonne NATIONAL LABORATORY

Finally, how can we decarbonize through different energy pathways?

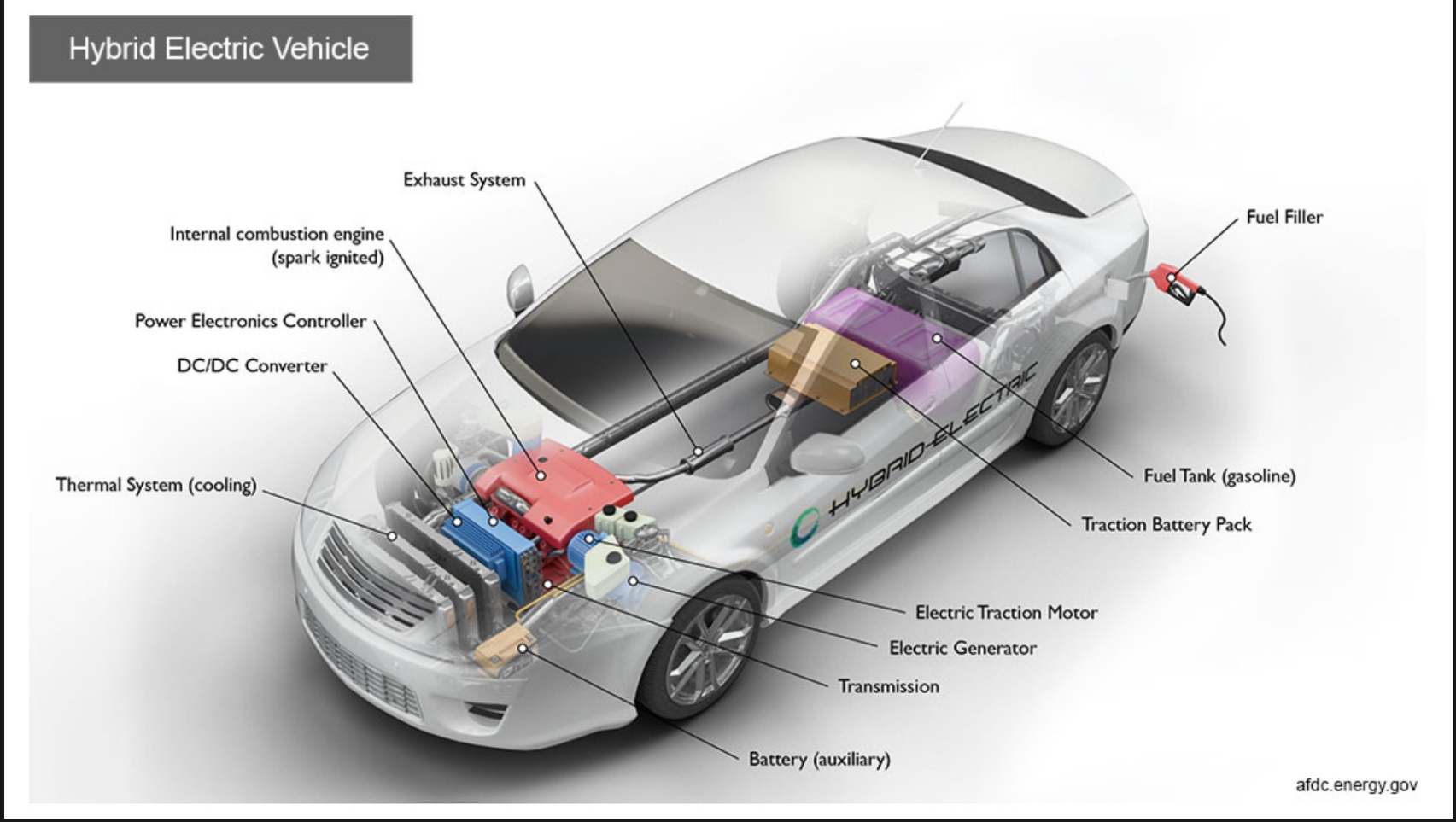


Note: uses average US electricity mix

What if there was a vehicle technology that offered:

- A substantial reduction of GHGs from driving over the lifetime of the vehicle, compared to conventional cars
- GHGs that scale with driving starting the day I drive the car off the lot (I drive less, I emit fewer GHGs, with a low upfront GHG penalty)
- Criteria pollutants well below the legal limits
- No change in consumer behavior
- No new infrastructure
- No significant price increase
- The need for only a small amount of battery resources
- The flexibility to use advanced sustainable fuels, with the potential to be net-zero GHGs

Full hybrid electric vehicle (FHEV or just “hybrid”)



Focus: Gas-electric hybrid vehicles get a boost in the US from Ford, others

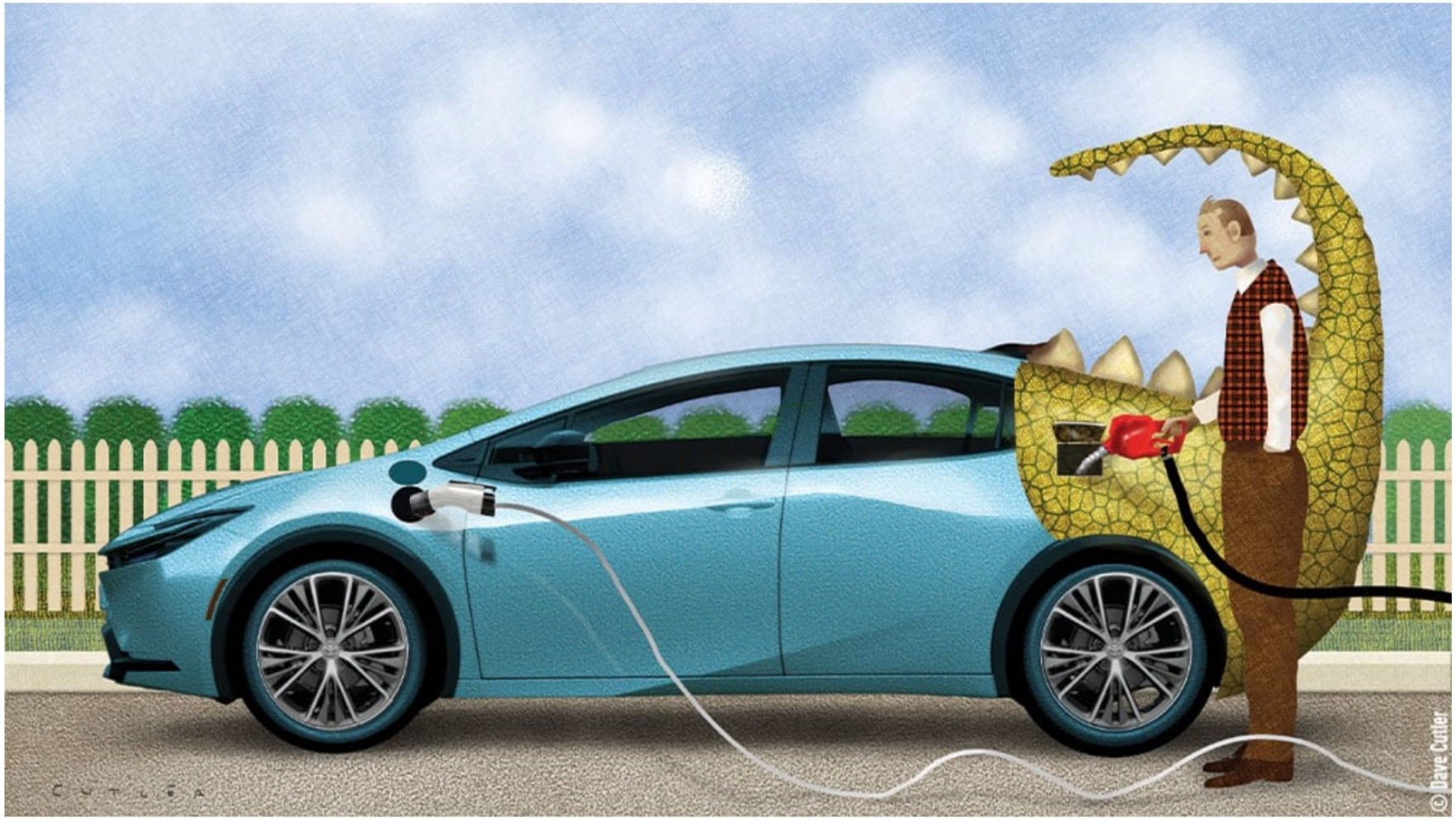
By **Paul Lienert** and **Ben Klayman**

August 23, 2023 1:08 PM CDT · Updated a day ago

[1/4] A view of the newly redesigned 2023 Prius unveiled by Japanese automaker Toyota prior to the start of the Los Angeles Auto Show in Los Angeles, California, U.S., November 16, 2022. REUTERS/Mike Blake/File Photo *Acquire Licensing Rights*

NEWS

Hybrid Cars Retake The Limelight As EV Sales Slow. What It Means For Ford, GM, Tesla.



Automakers are backtracking on massive EV commitments as consumers opt for the less stressful option of combined gas/electric hybrid cars. (© Dave Cutler)

How can HPC help?

Design cleaner engines using CFD

Mazda SKYACTIV-X Engine

- 20-30% efficiency improvement
- Extends range of HCCI using a spark
- SPCCI - Spark Plug Controlled Compression Ignition
- Combines benefits of both gasoline and diesel

Mazda SKYACTIV-X Engine

To find that perfect flame, we decided to expand our computing resources. Designing a new and complex method of combustion requires an accurate simulation of the combustion chamber. This was computer model-based development, where we determined the ideal combustion by calculation and then worked to achieve it in the real world. In the past our work was a time-consuming process that involved creating lots of prototype vehicles or engines and testing them repeatedly. But that approach would have gotten us nowhere when developing the present engine, since there were countless possible combinations. Computer model-based development increased our work efficiency dramatically.

We have also cooperated with academia and government to develop the fundamental technologies. As we increased the accuracy of our simulations, we found the right “flame” that would allow gasoline to combust vigorously. We used the simulation results to create something like a recipe that we then programmed into an engine control unit.

- Interview with Mazda lead engineer of SKYACTIV-X

https://www.mazda.com/en/csr/special/2017_01/

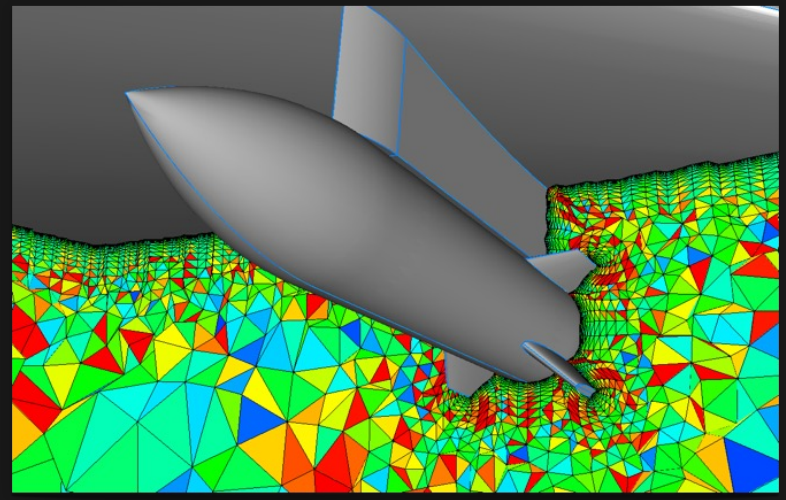
Since when is CFD this predictive?

- Autonomous meshing
- Grid convergence
- Scalability
- Accurate models

Autonomous Meshing

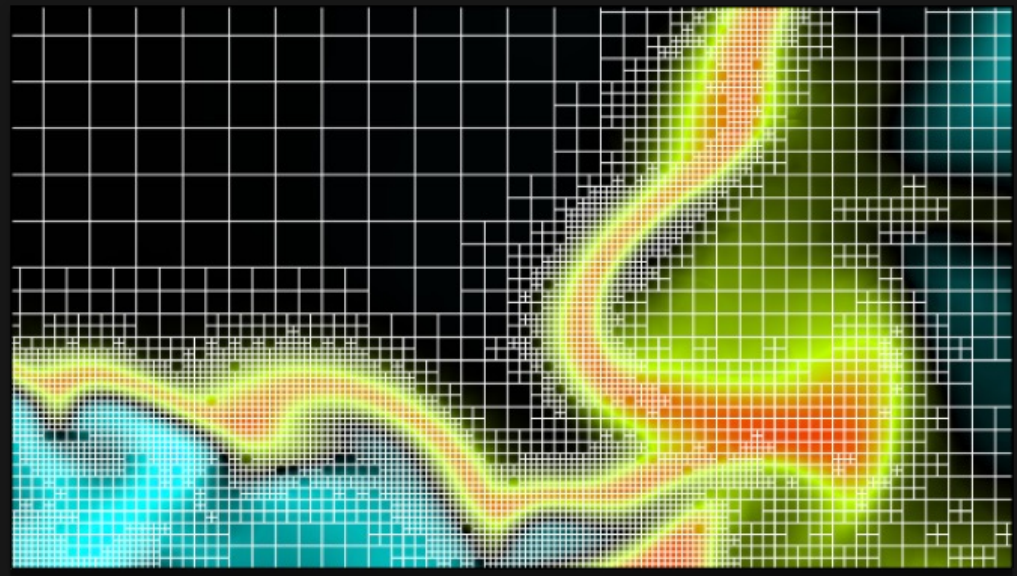
- Traditional Approach

  - Long meshing times
  - Meshing by guessing
  - Skewed cells
  - Grid convergence?

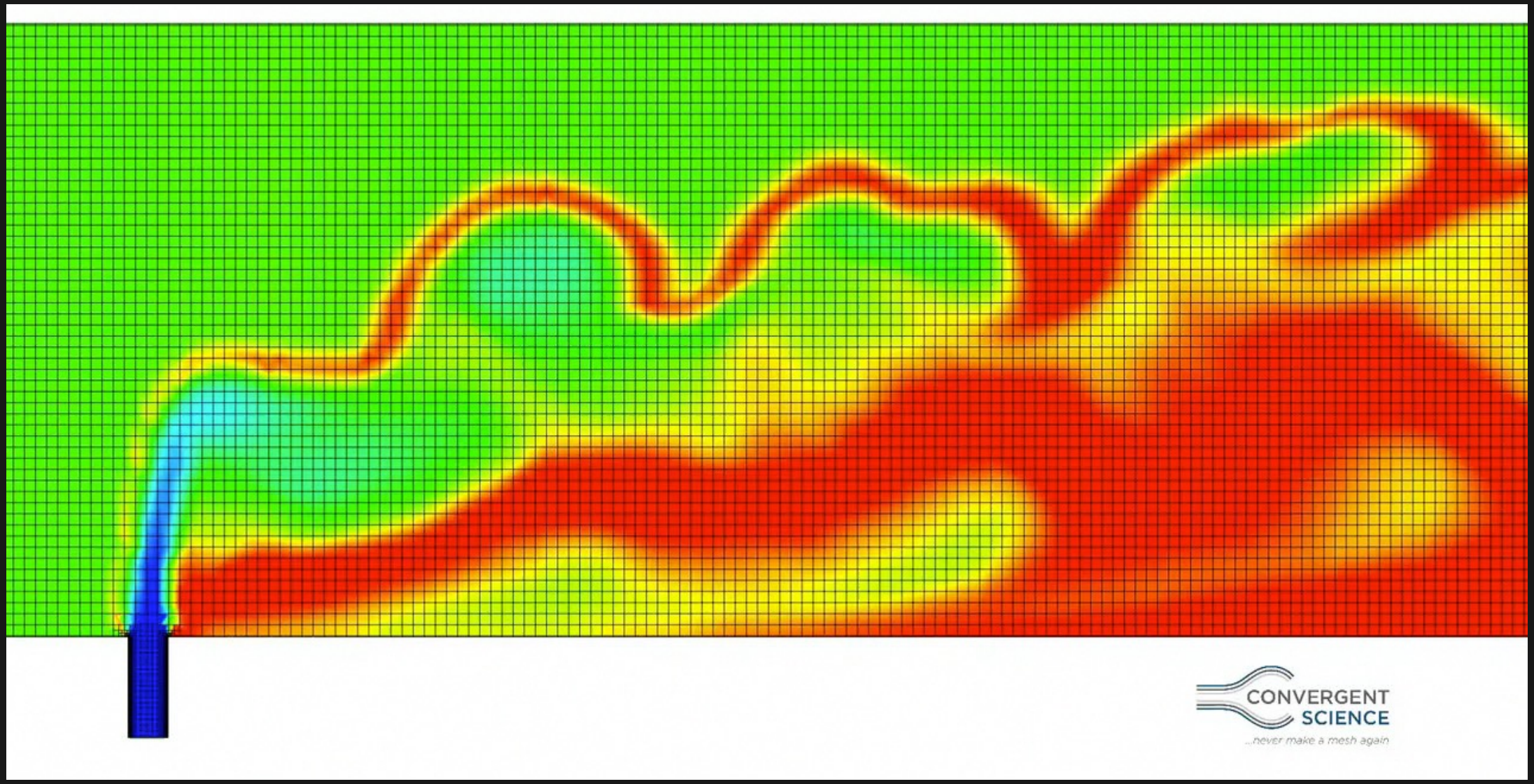


- Our Approach

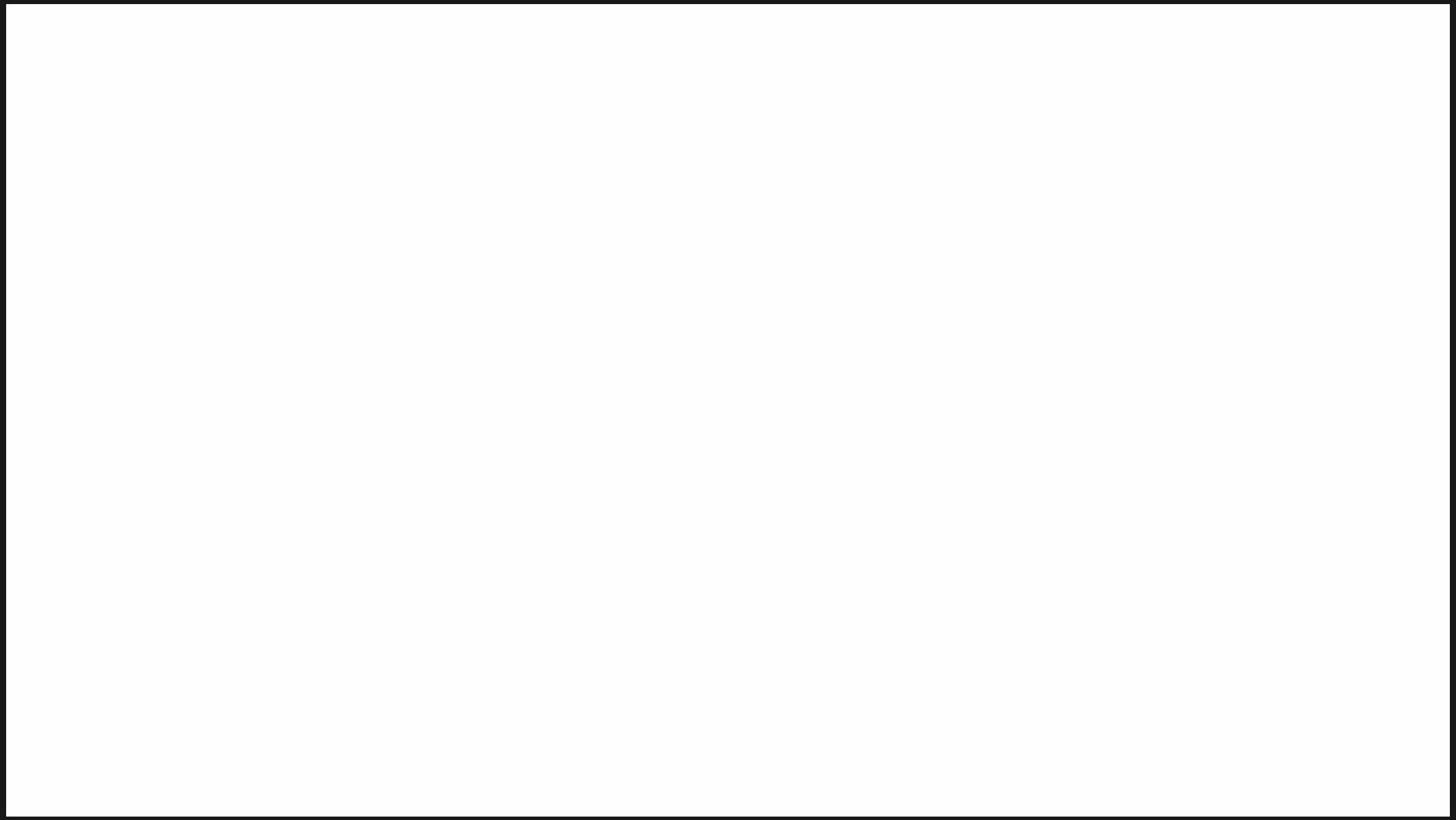
  - Automated meshing (no meshing time)
  - Adaptive Mesh Refinement (AMR) – no more guessing
  - Orthogonal cells
  - Easy to perform grid convergence studies



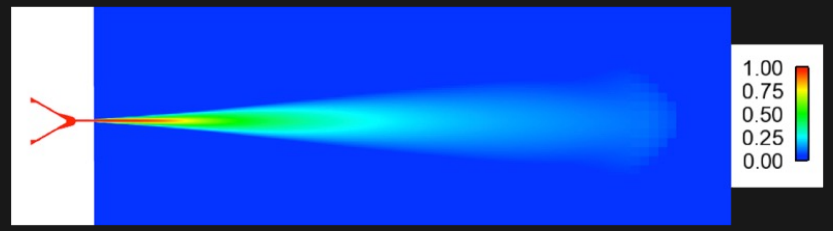
Autonomous Meshing



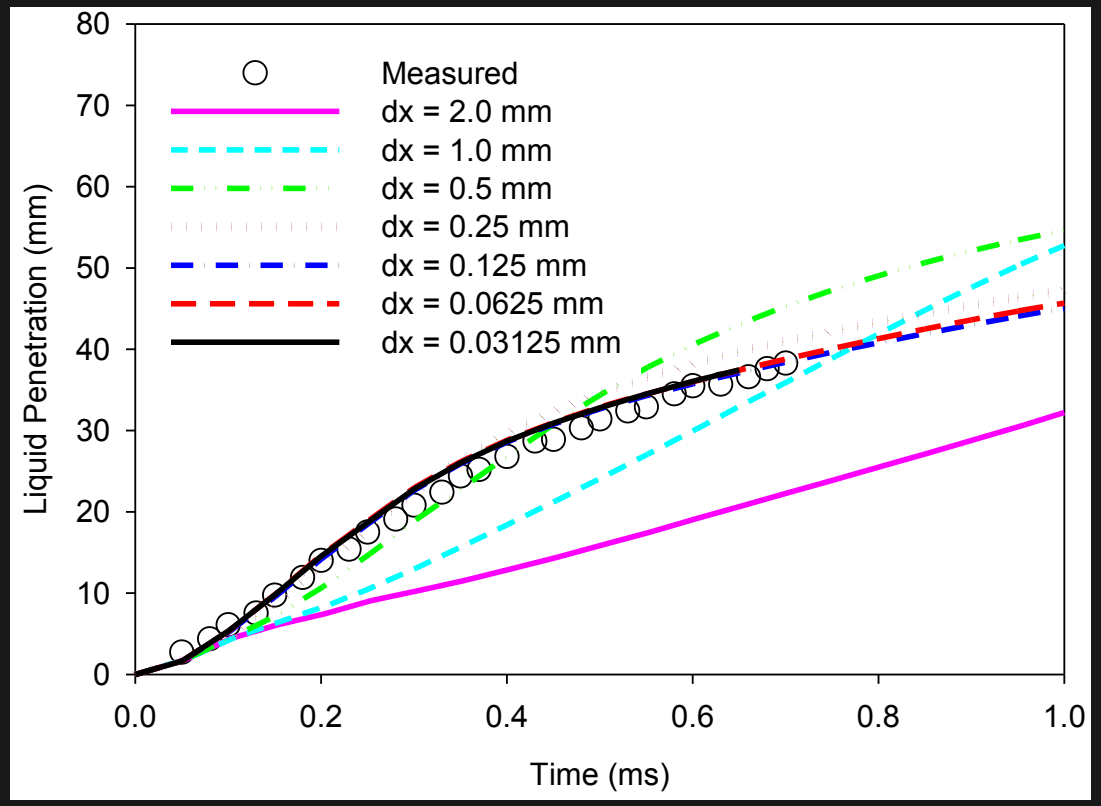
Autonomous Meshing

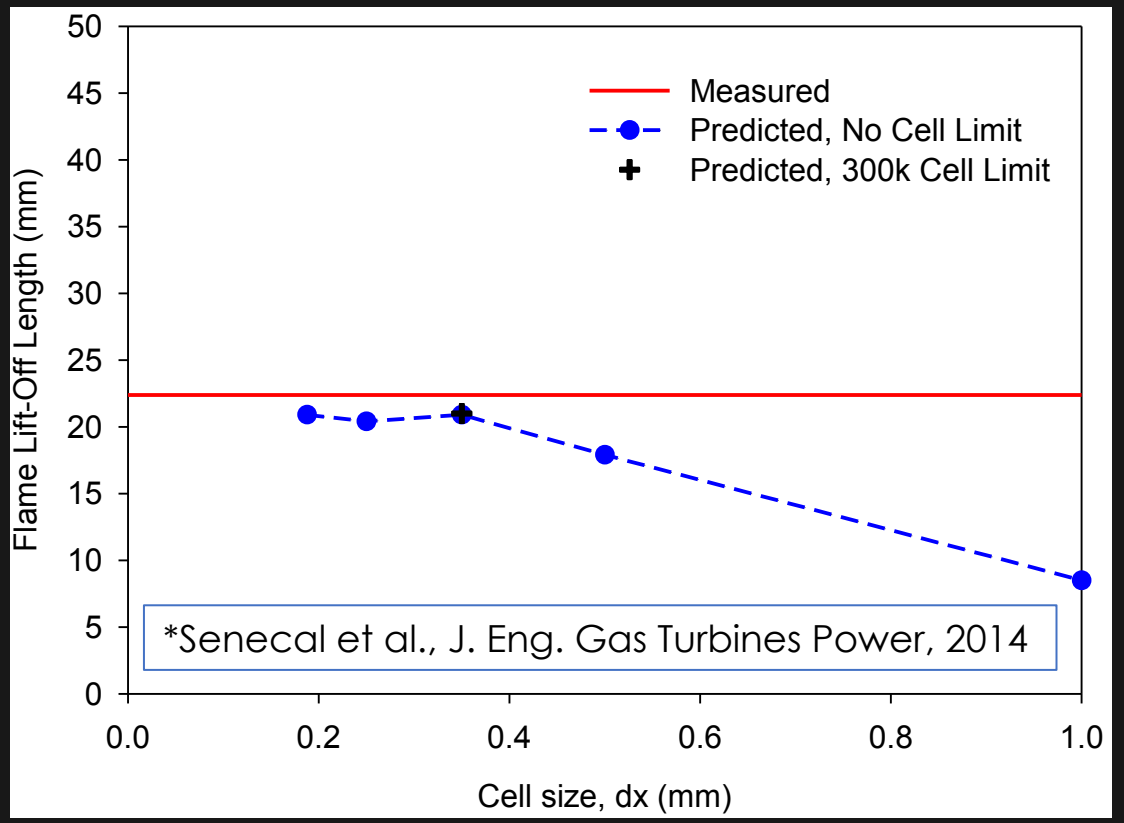


Grid Convergence



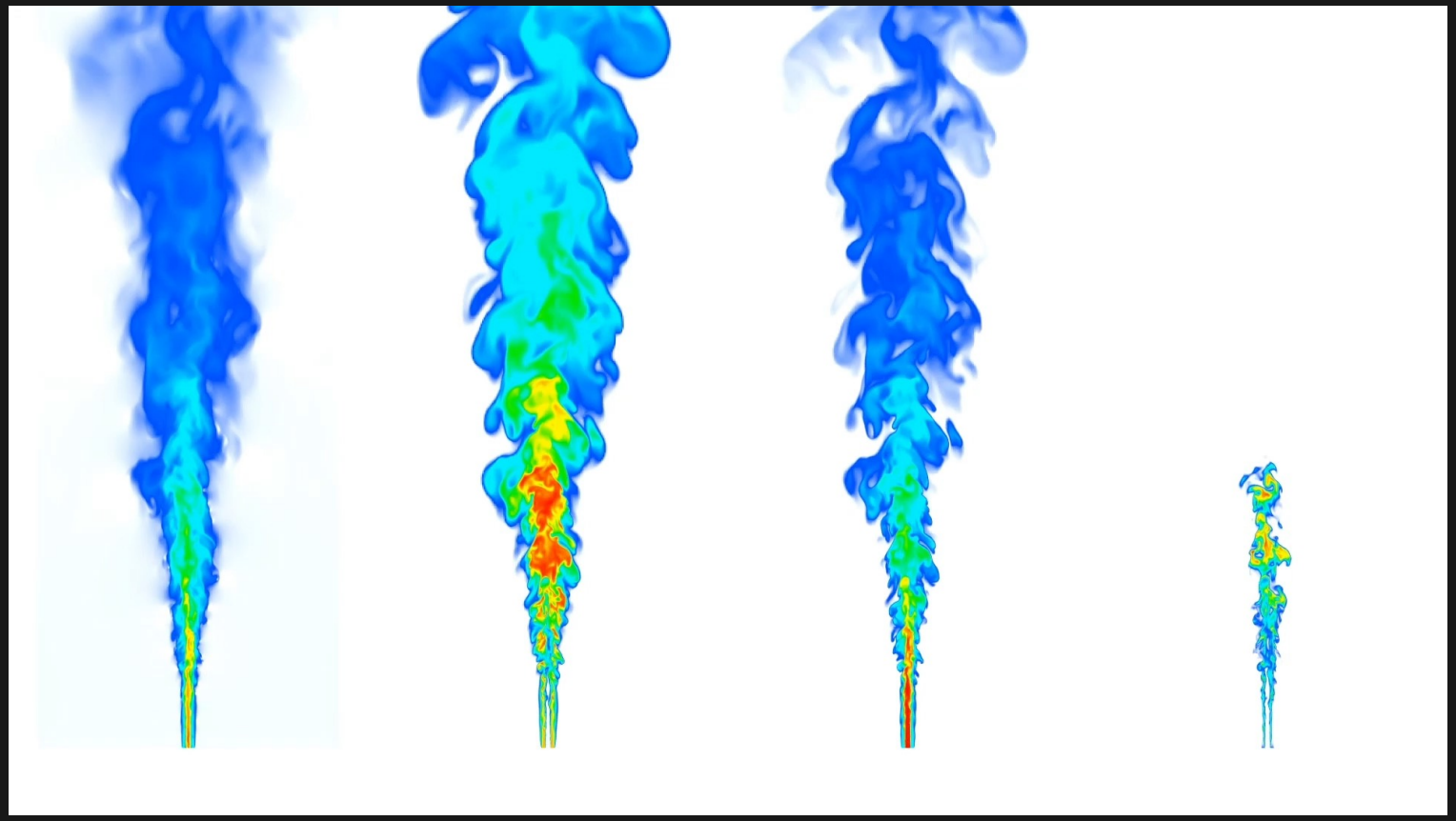
- If your answer is not grid converged, are errors due to the physical models or simply because you are under-resolved?



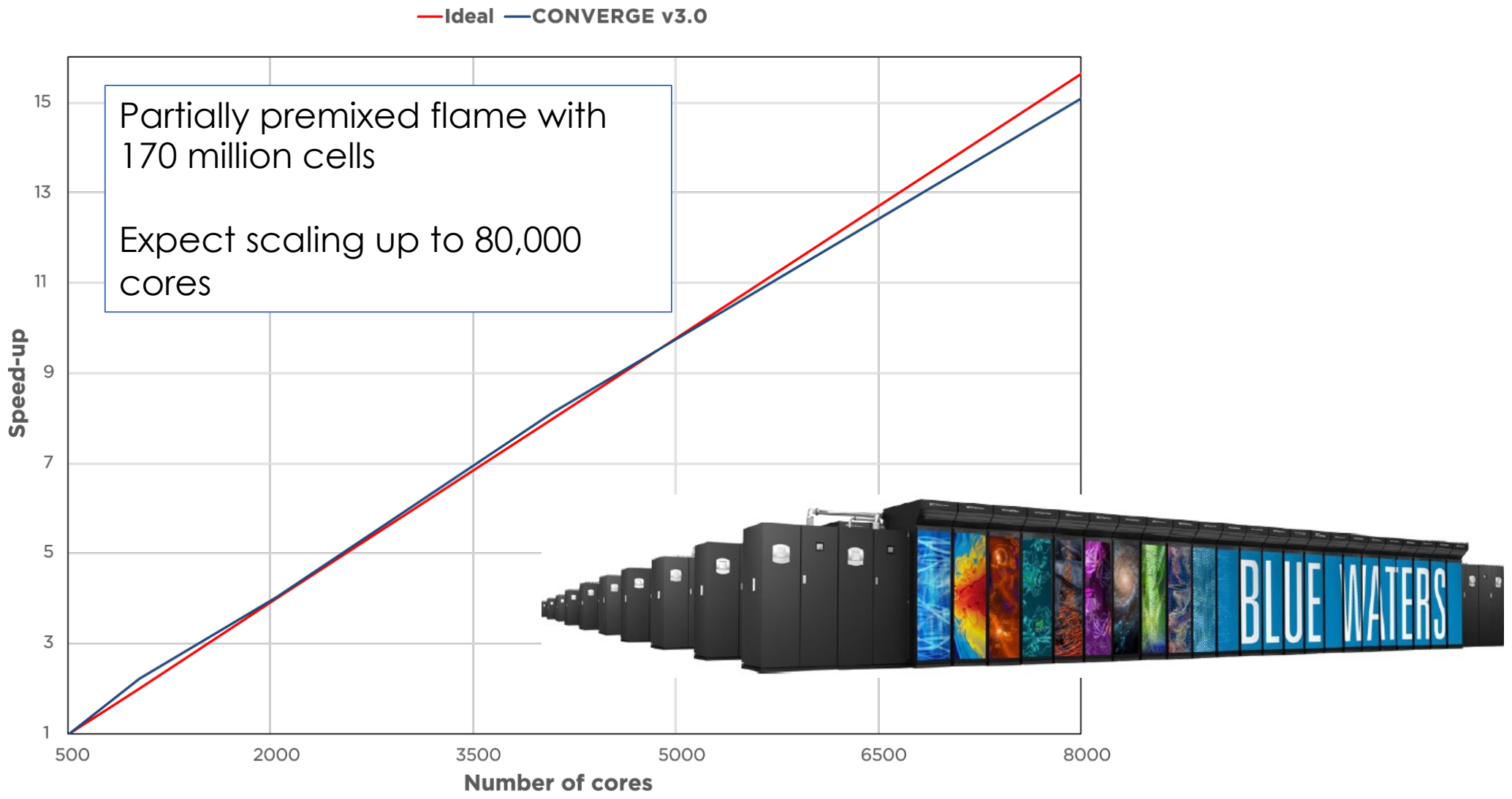


Scalability

- We need fine grids and fast turnaround for CFD to make a real impact on designing turbulent combustion devices

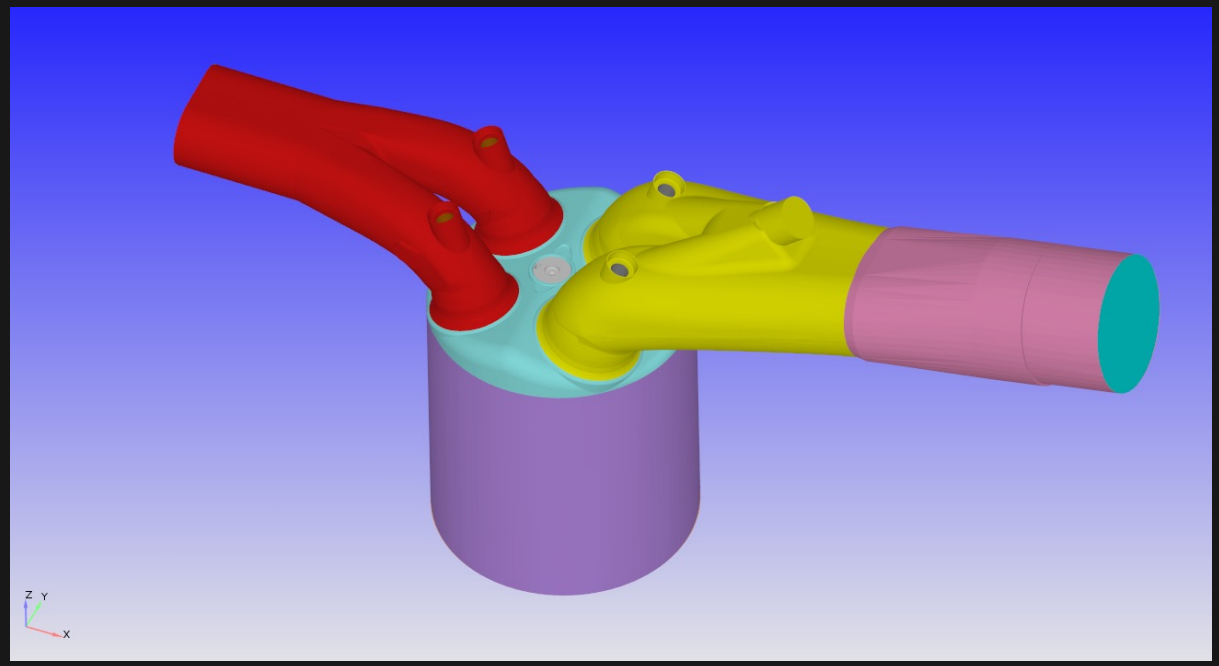


Scalability

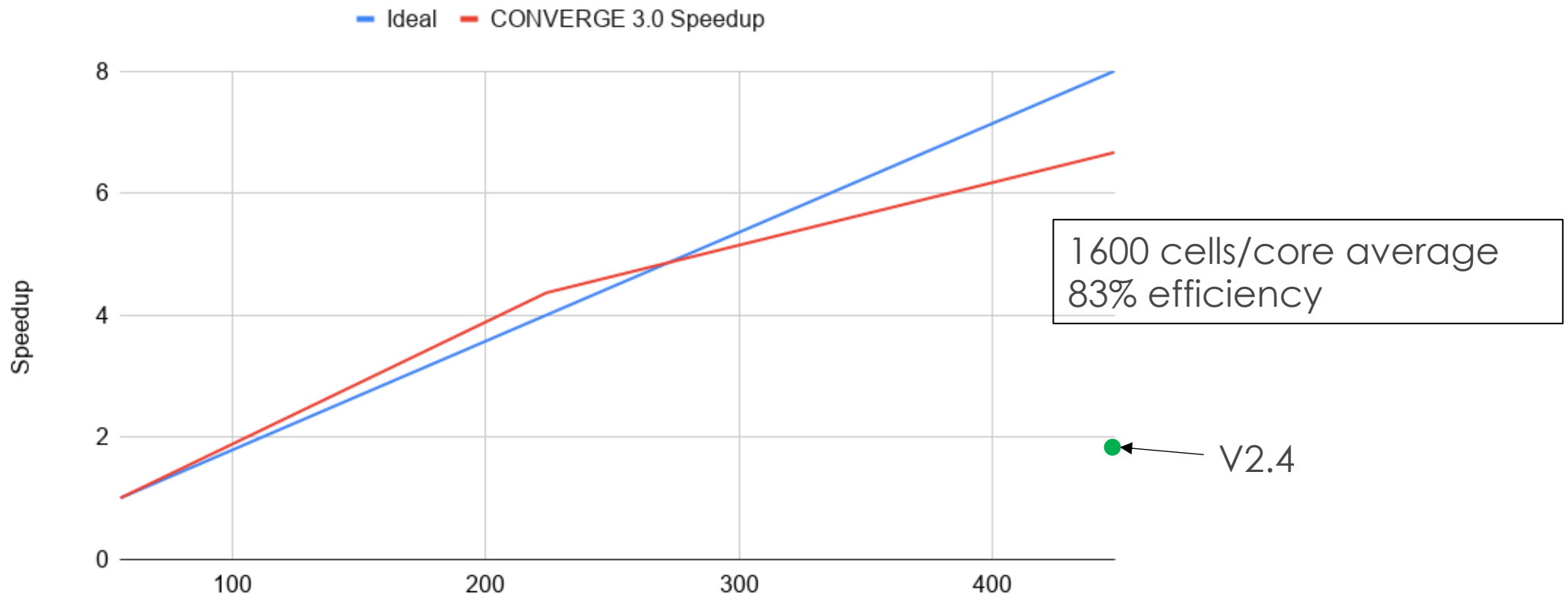


Scalability

- Standard gasoline engine case
  - spray, combustion, AMR, and moving geometry are all part of the simulation
  - restart files written every 5 CA
  - post files written as normal
  - max cell count is 1.3M, minimum is 230K
- Run on our internal cluster
  - 28 core 3.1 GHz Intel Skylake
  - single processor nodes
  - 100GB Infiniband interconnect
  - local attached SSD storage



Scalability

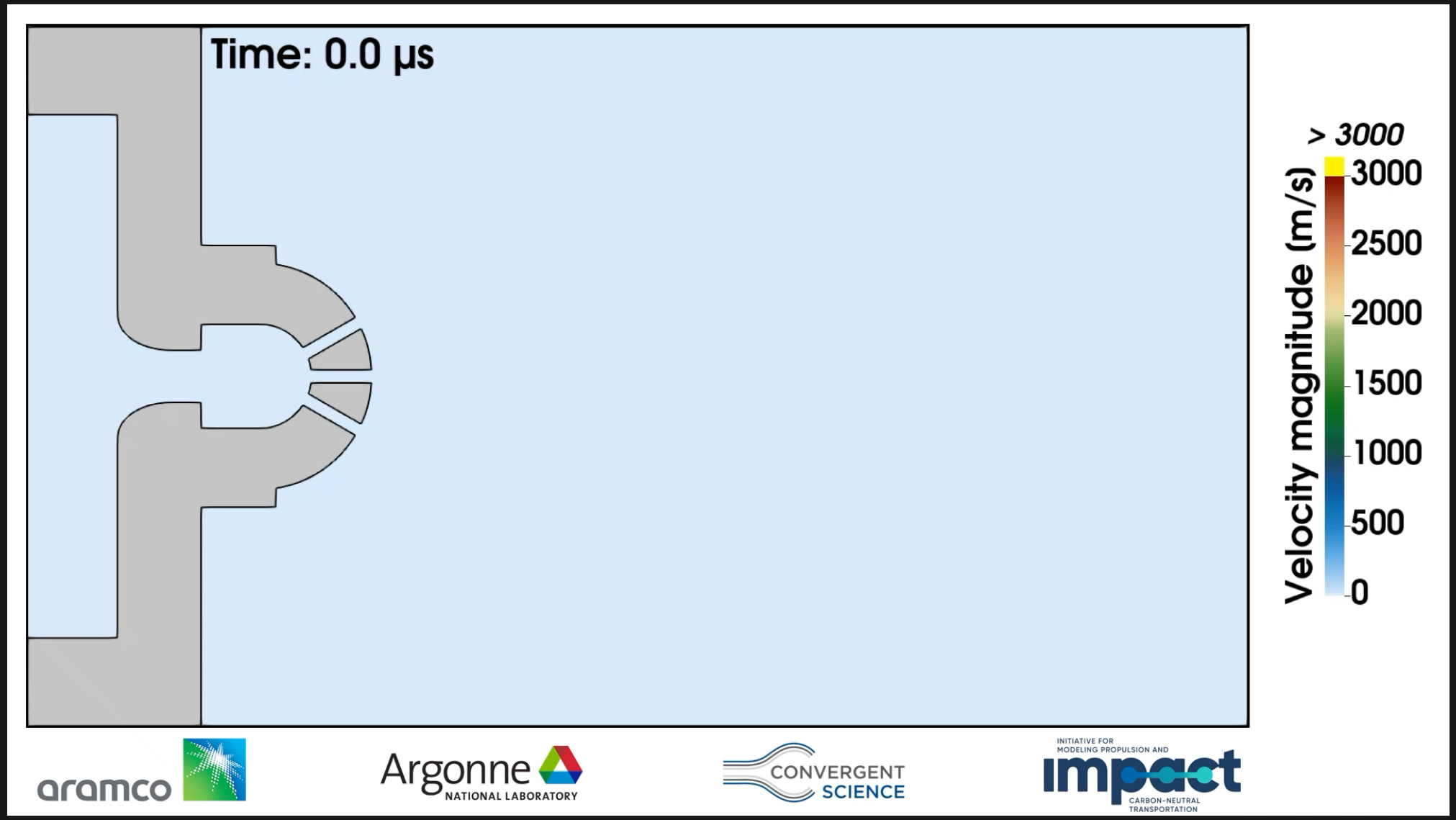


Cores	Time(h)	Speedup	Efficiency	Cells/core	Cycles/day
56	13.8	1	100%	12,500	1.7
224	3.16	4.37	109%	3,100	7.6
448	2.07	6.67	83%	1,600	11.6
896	1.62	8.51	53%	780	14.8

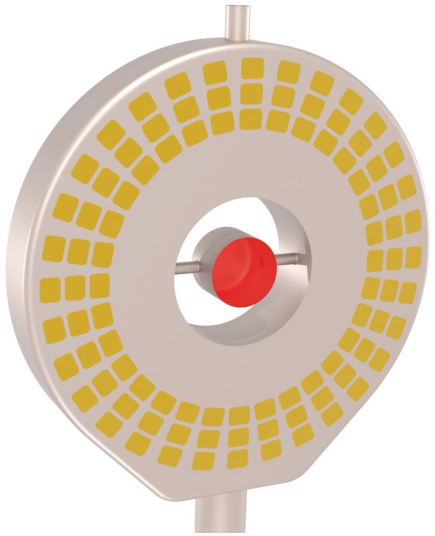
Accurate Models

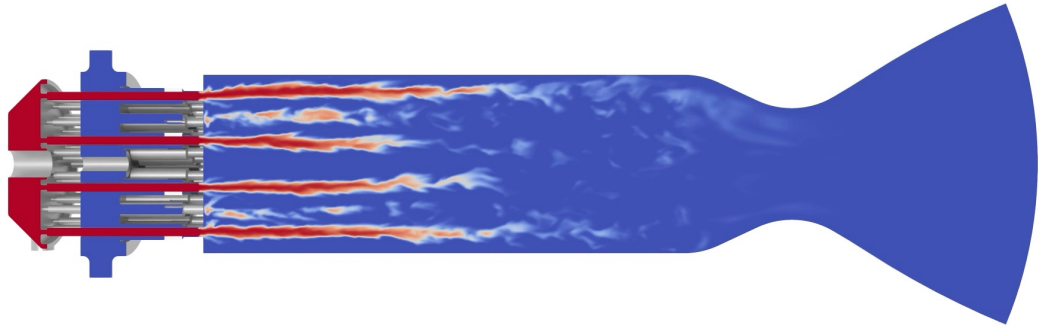
- Founded the Computational Chemistry Consortium (C3) to develop a single, consistent framework for simulating hydrocarbon chemistry including PAH and NOx with CFD
- High fidelity predictions of individual, surrogate, and dual fuels
- Version 3.3 of the master mechanism with around 4,000 species is available to the public

Accurate Models



Benefits to a wide range of applications





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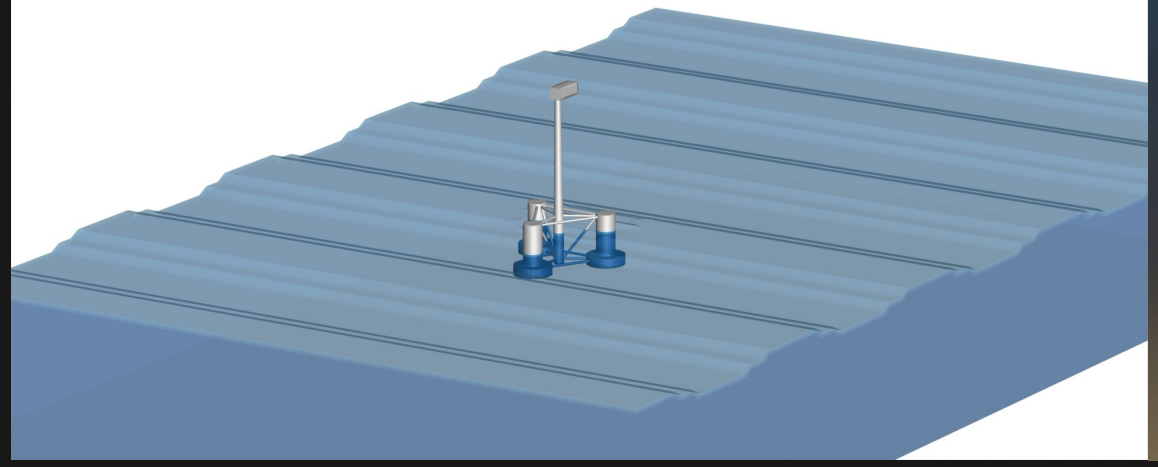
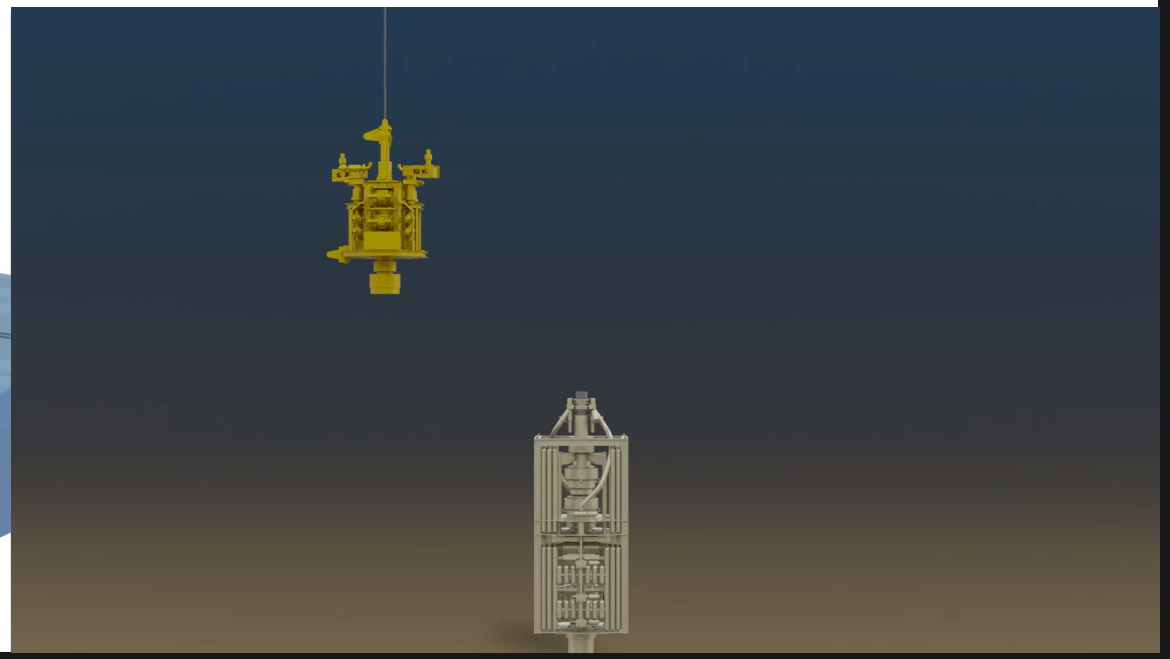
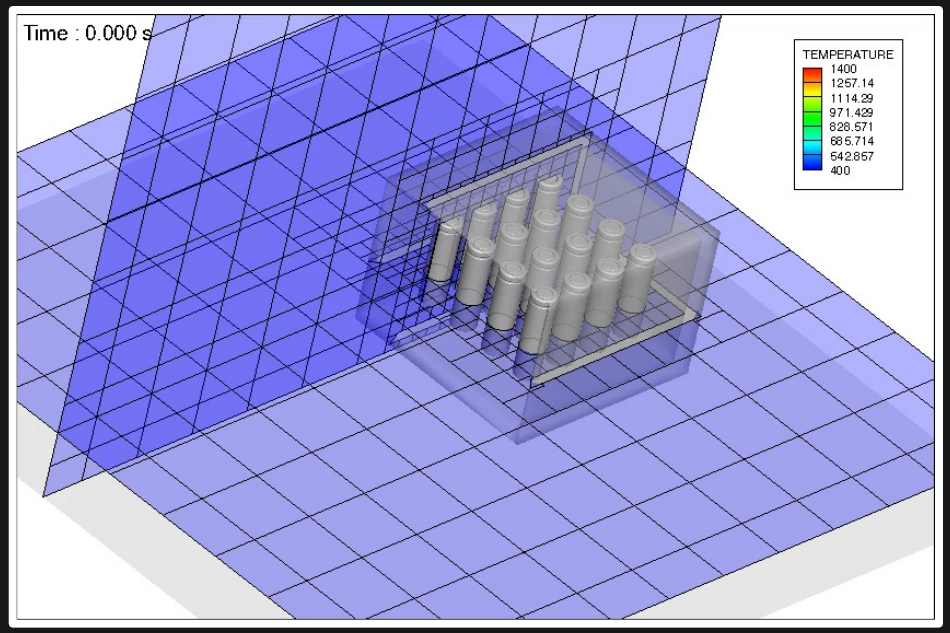
CFD SOFTWARE



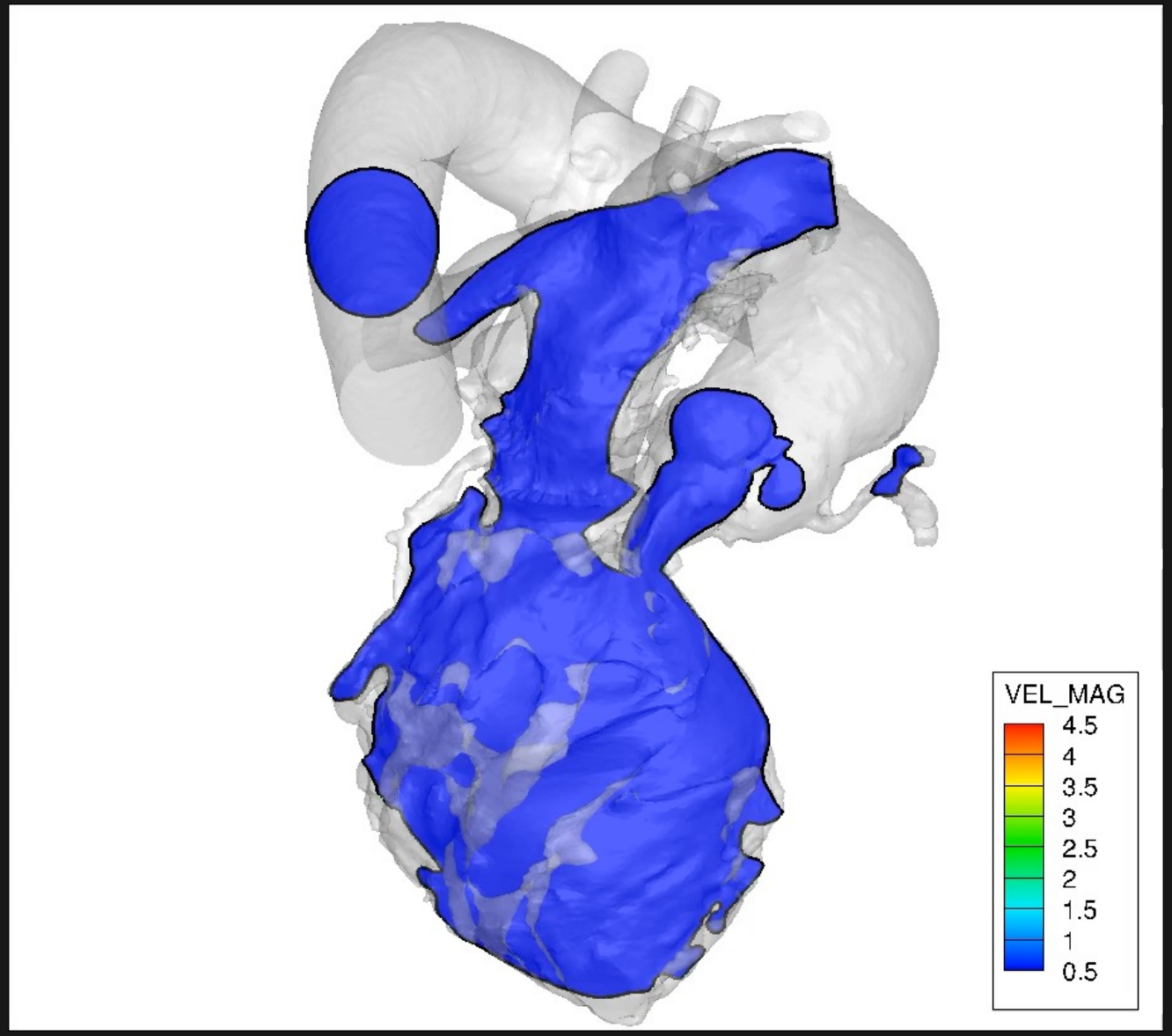


Benefits to a wide range of applications

University of Texas Fire Research Group
https://www.utfireresearch.com/battery-fires



Benefits to a wide range of applications



The future is ~~electric~~ eclectic

We are making a mistake in the transportation sector (including passenger cars) with this singular push toward battery electric vehicles (BEVs).

If our goal is to reduce transportation carbon emissions as fast as possible, hybrids and renewably fueled ICE (along with a growing number of electric vehicles) must make up a significant portion of the fleet for years to come.

Government and industry can educate, promote, and incentivize a diverse set of transportation technologies, not a "silver bullet". The best technology depends on location and application (and budget).

CFD and HPC can lead the way to more sustainable transportation technology.

Question: What is the most climate friendly today, a car with an electric motor or a car with an IC engine?

- Answer: It depends

Thank you

senecal@convergecfd.com

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