High Performance Computing for Accelerating Sustainable Transportation Innovations

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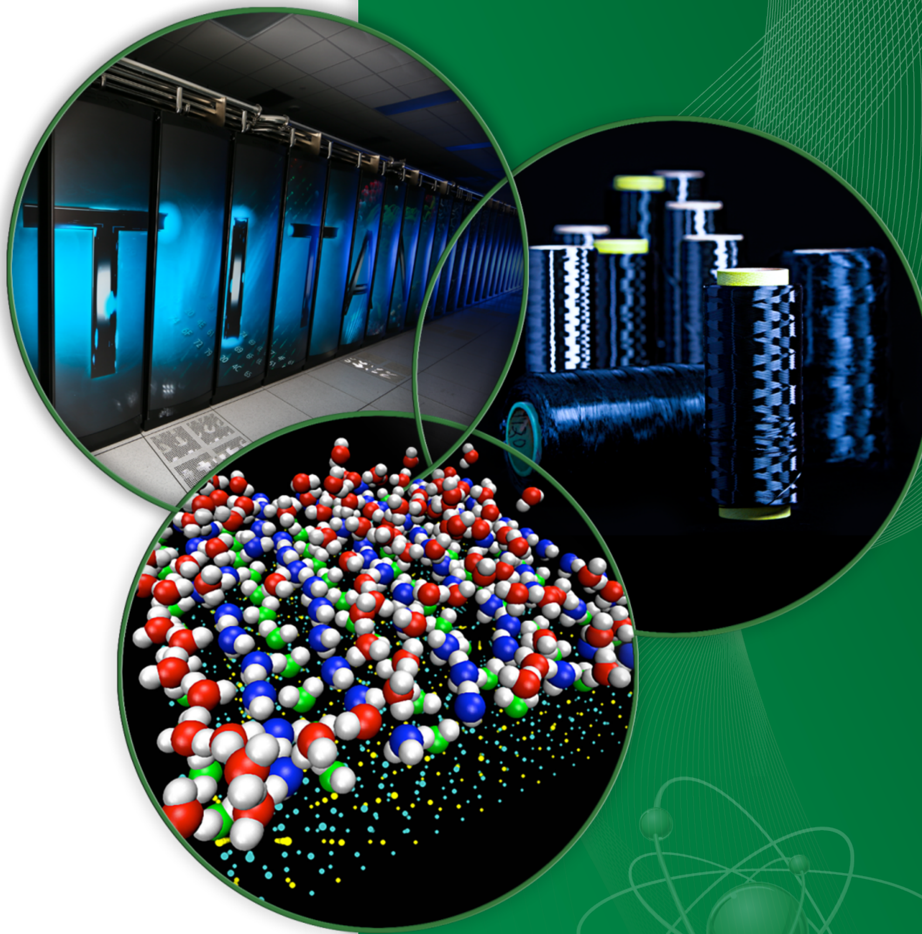

Sustainable Transportation Seminar

May 16, 2014

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE
National Laboratory

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And many others that make interdisciplinary research enjoyable at ORNL

Multiscale/Multiphysics Modeling for Clean Energy (M3E)
http://www.linkedin.com/groups?gid=1849998

M^3E ENERGY

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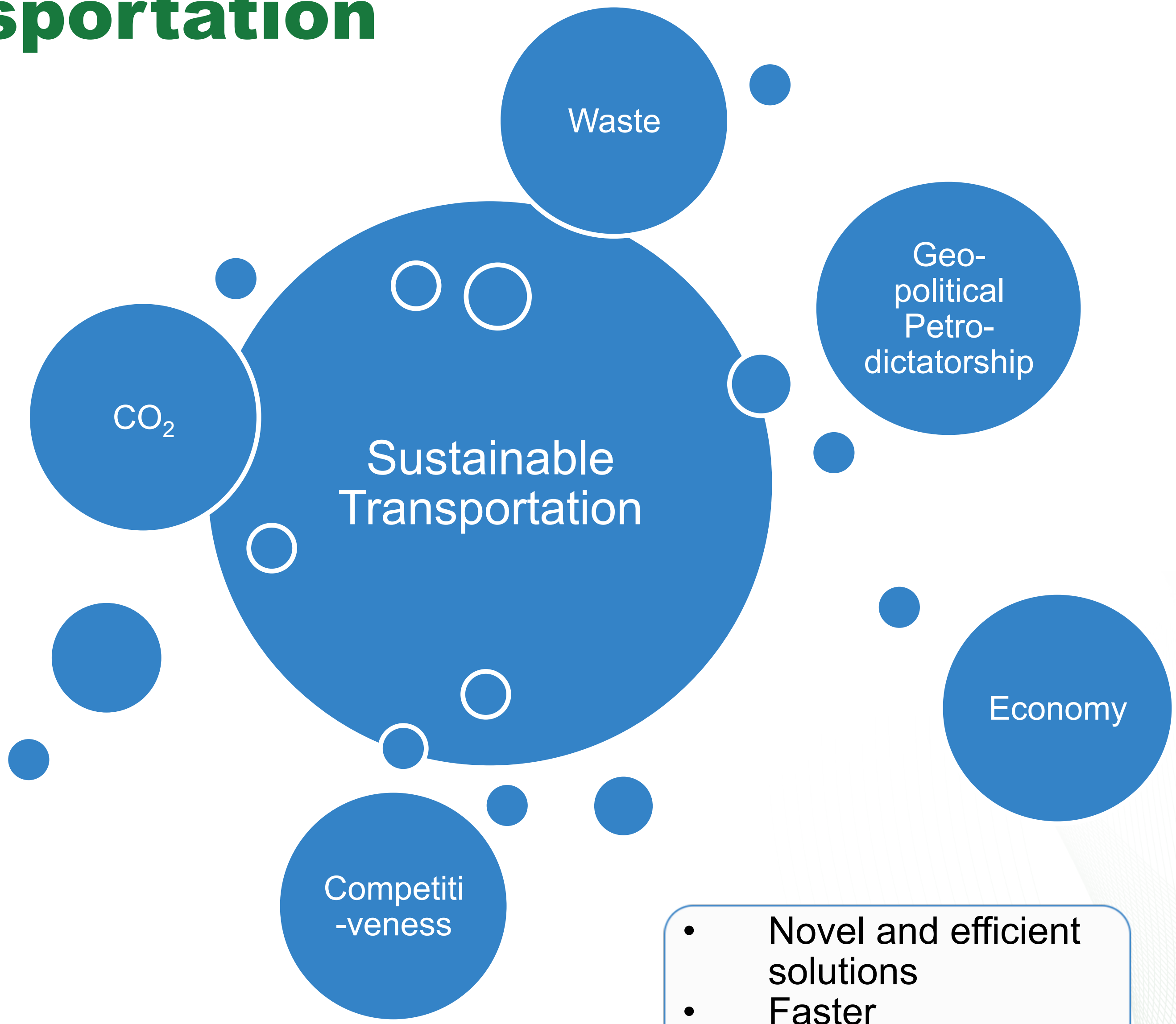
Outline

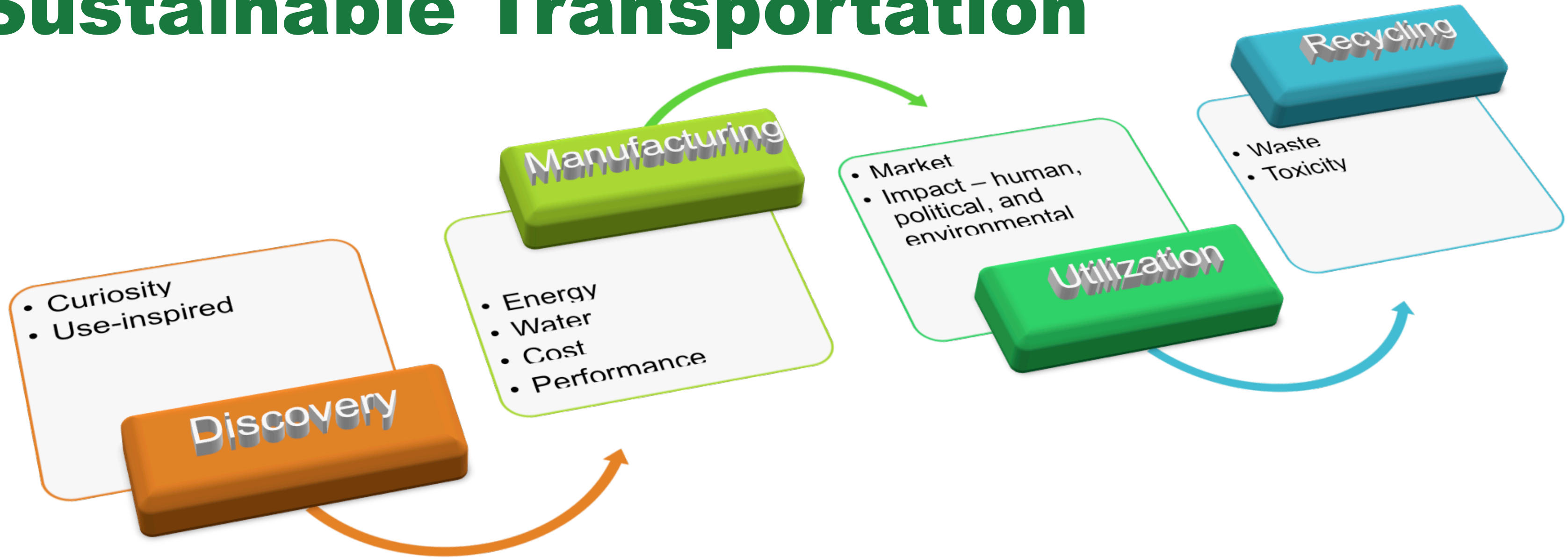
- Motivation
- Future of Innovation
  - Role of advanced computing
    - Sustainability by design
    - Connecting science to solutions
    - Essential ingredients
- Vision for Virtual Car/Vehicle
- Current/past efforts that we can build on
  - Batteries
  - Cycle-to-Cycle Variability (Ford, GE)
  - Injector optimization (GM)
  - Inverter cooling
  - Crashworthiness
  - Aerodynamics (SmartTruck and Ford projects at OLCF)
- Related activities
  - Computational Biomass Pyrolysis
- Opportunities/Challenges/Summary

Many Facets of Sustainable Transportation



- Novel and efficient solutions
- Faster
- Cheaper

Sustainable Transportation



- **We have to think about end-to-end solutions for materials/ chemicals/fuels**
  - **Can we turn the table upside down? – use-inspired**
- **It is very difficult to optimize – need for computational design**
  - **There are parts that can be cast *in silico***
  - **There are parts that will need human intervention in foreseeable future**
    - **Maybe with better understanding and concerted effort, some of these can also be posed as a computational problem**
- **Interdisciplinary**

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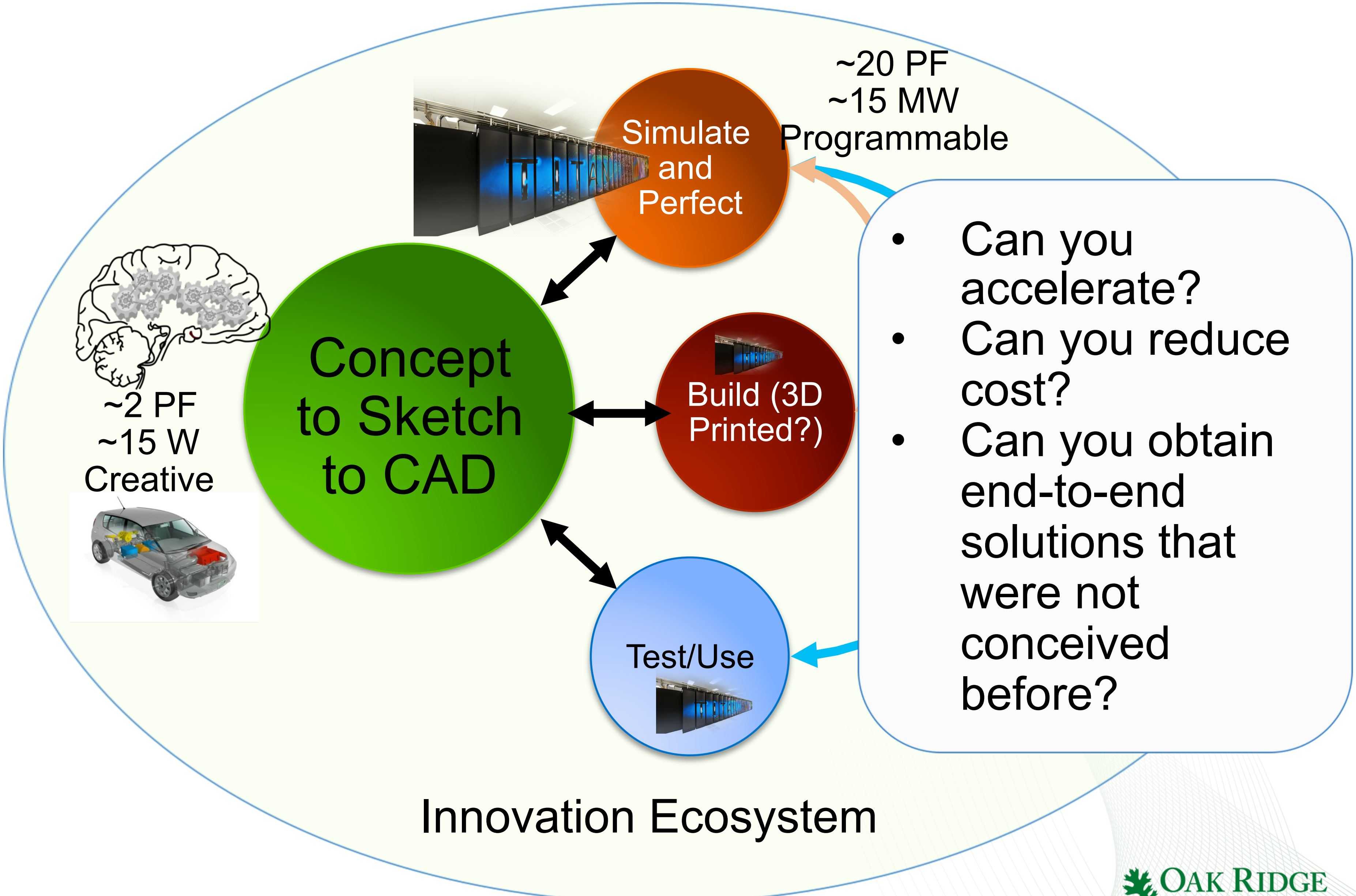
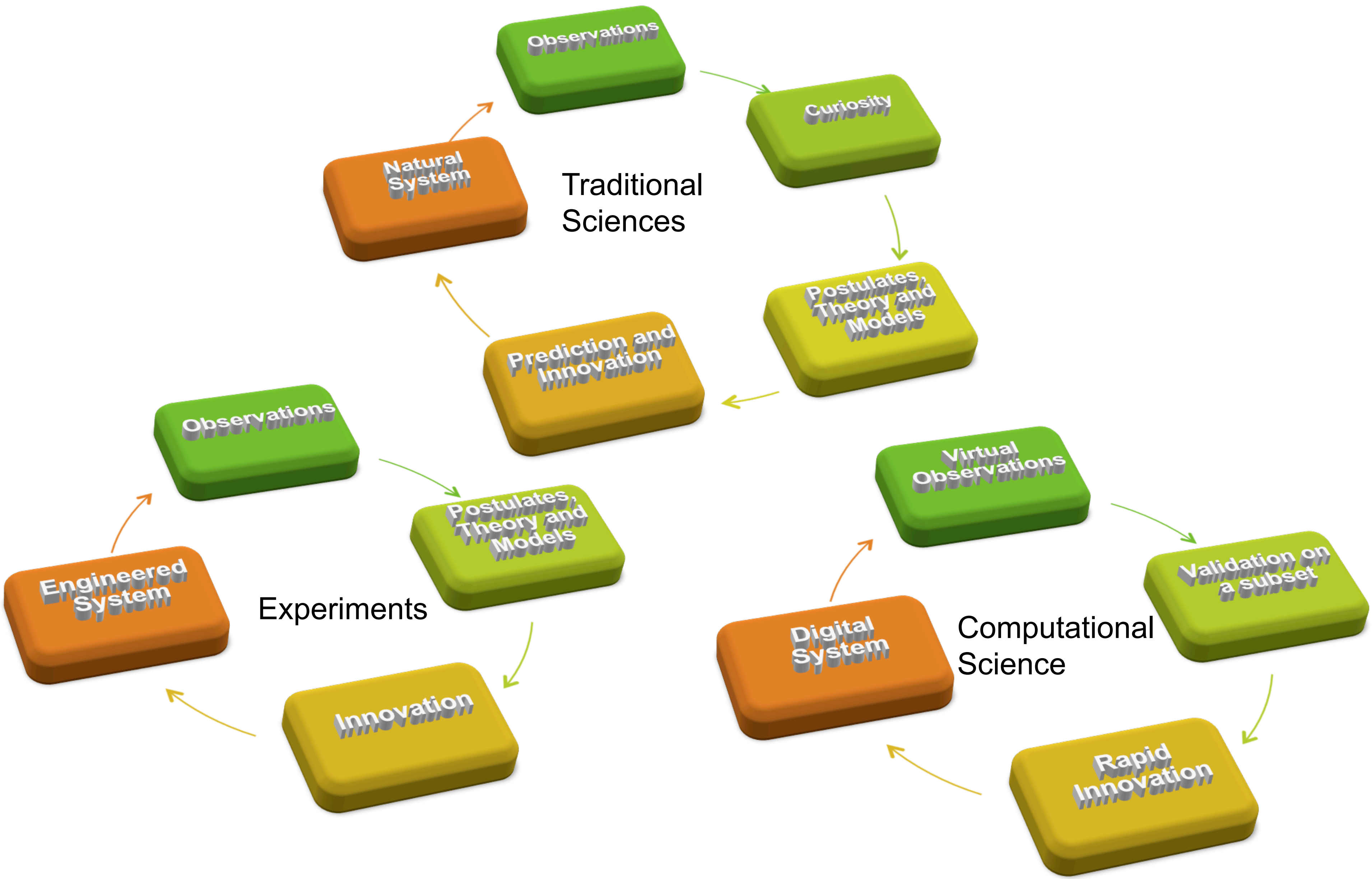
Future of Innovation



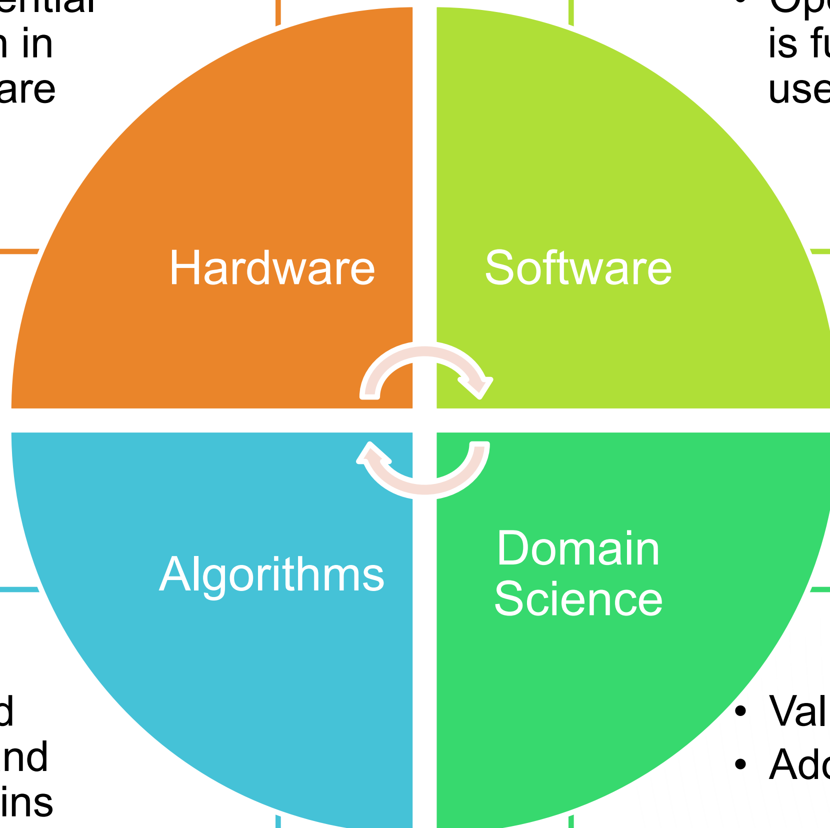
Bridging Science to Solutions



Essential Ingredients for advanced computing

- Exponential Growth in Hardware

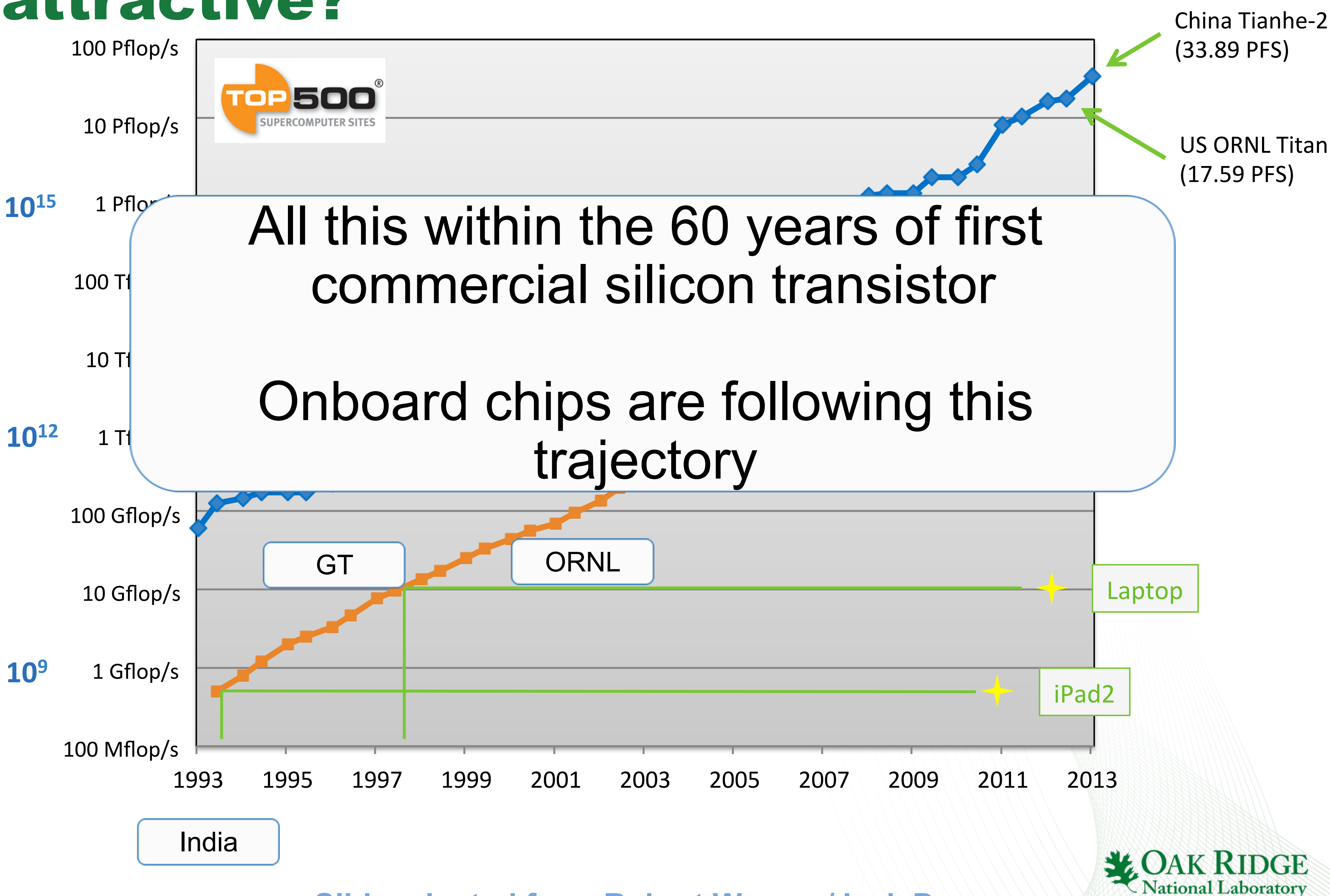
- Open source is fueling re-use



- Applied Math and CS Gains

- Validation
- Adoption

What makes advanced computing attractive?



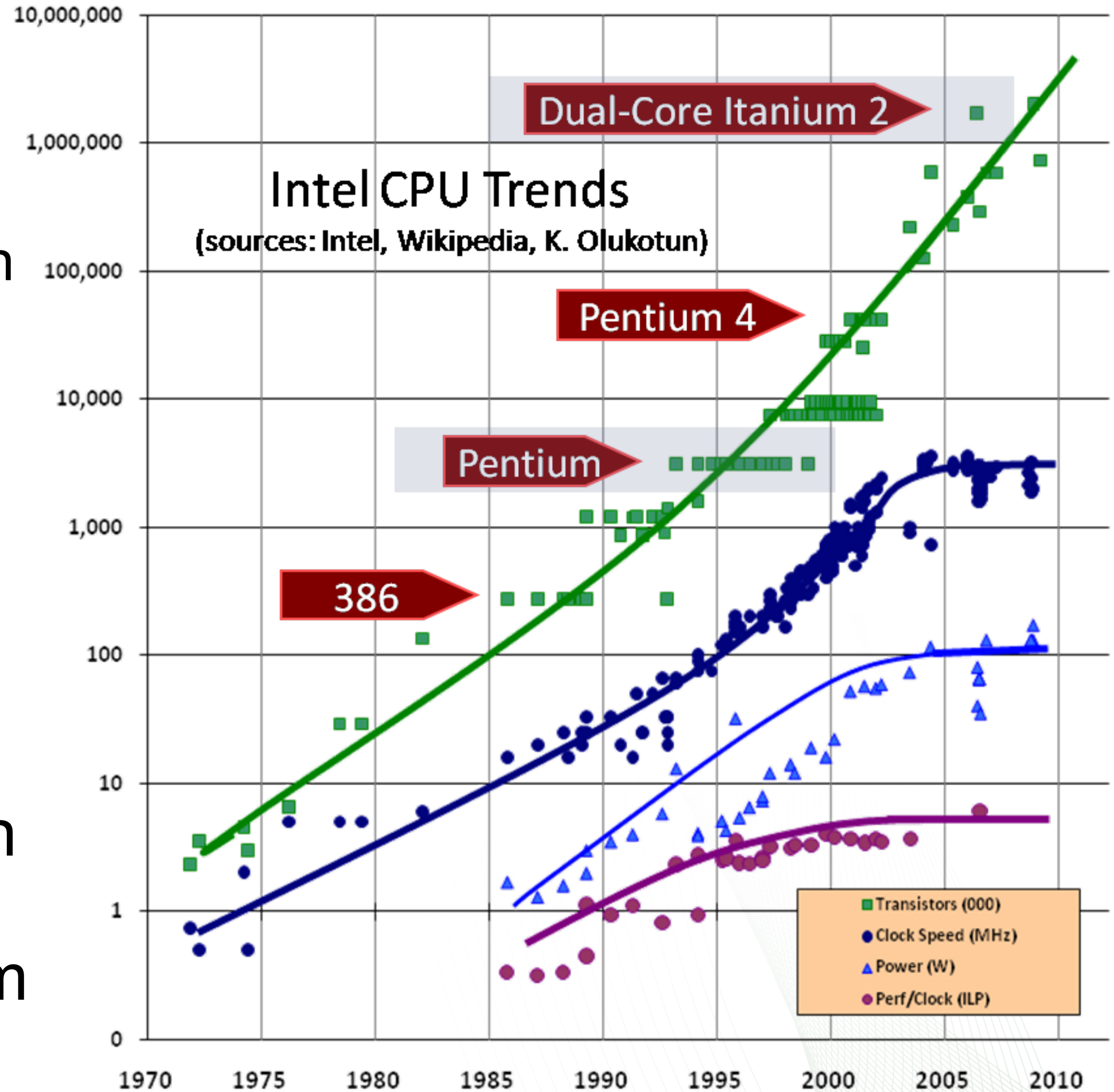
All this within the 60 years of first commercial silicon transistor

Onboard chips are following this trajectory

Slide adapted from Robert Wagner/Jack Dongarra

Architectural Trends – No more free lunch

- Moore's Law continues
  - CPU clock rates stopped increasing in 2003
  - power constraints
- Power is capped by heat dissipation and $$$
- Performance increases have been coming through increased parallelism



Herb Sutter: Dr. Dobb's Journal:
http://www.gotw.ca/publications/concurrency-ddj.htm

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Slide adapted from Jack Wells

Virtual Car/ Vehicle

Robert Wagner
Gil Weigand
Ron Graves
John Turner

Why do we have to do things differently?

Slow Development Cycle

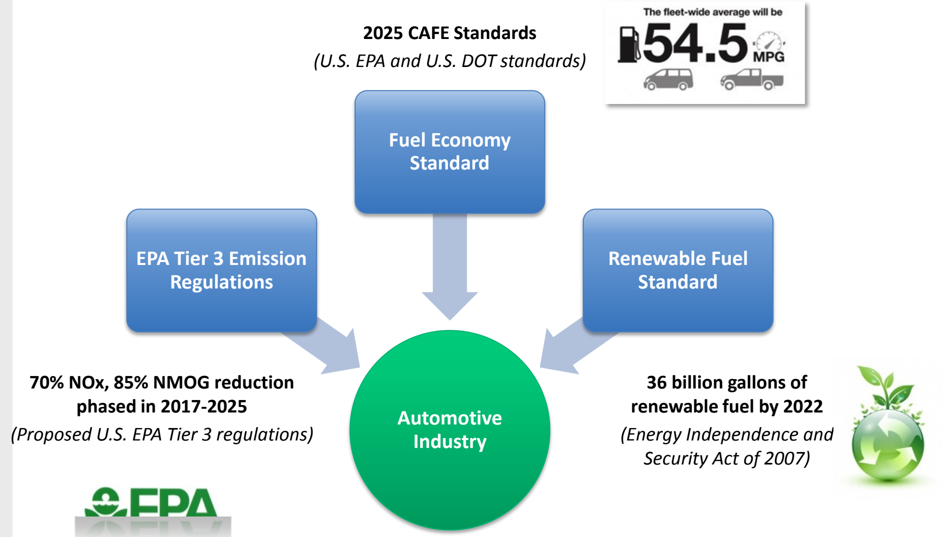
BMW 323i Model year 1983			BMW 325i Model year 2009
Fuel consumption[1]	10.3 l/100 km [~22 MPG]	- 31 %	7.1 l/100 km [~33 MPG]
Power output	102 kW	+ 57 %	160 kW
Torque	205 Nm	+ 32 %	270 Nm
Acceleration[2]	9.2 s	- 27 %	6.7 s
Emission quality	ECE R15-04	+ 95 %	EU 4
Weight	1080 kg	+ 39 %	1505 kg
Drag	$0.40 \times 1.85\ m^2$	- 21 %	$0.27 \times 2.17\ m^2$

Source: DEER 2009 presentation, BMW Group

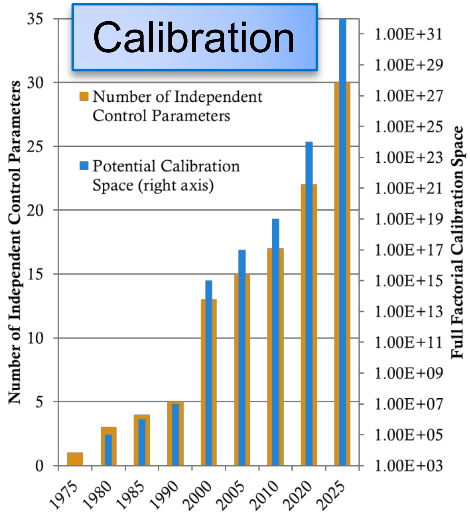
[1] EU fuel consumption MVEG

[2] 0 - 100 km/h

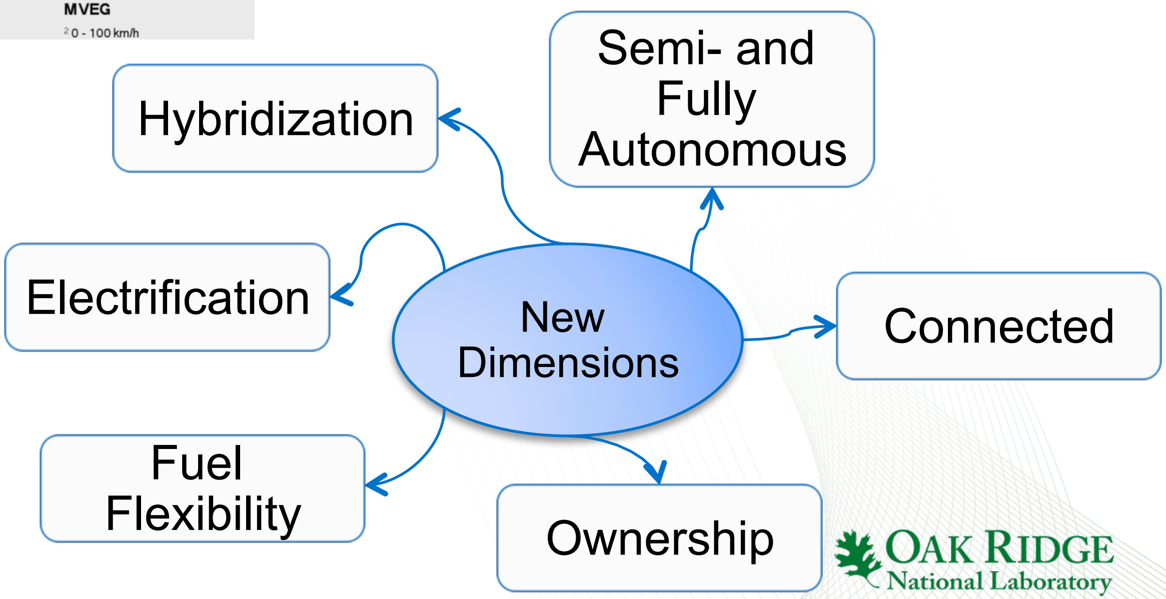
Regulations



Calibration



Source: Atkinson et al., 2013 SAE High Efficiency Engines Symposium



3D Virtual Vehicle Framework

Accelerating transportation efficiency

Today

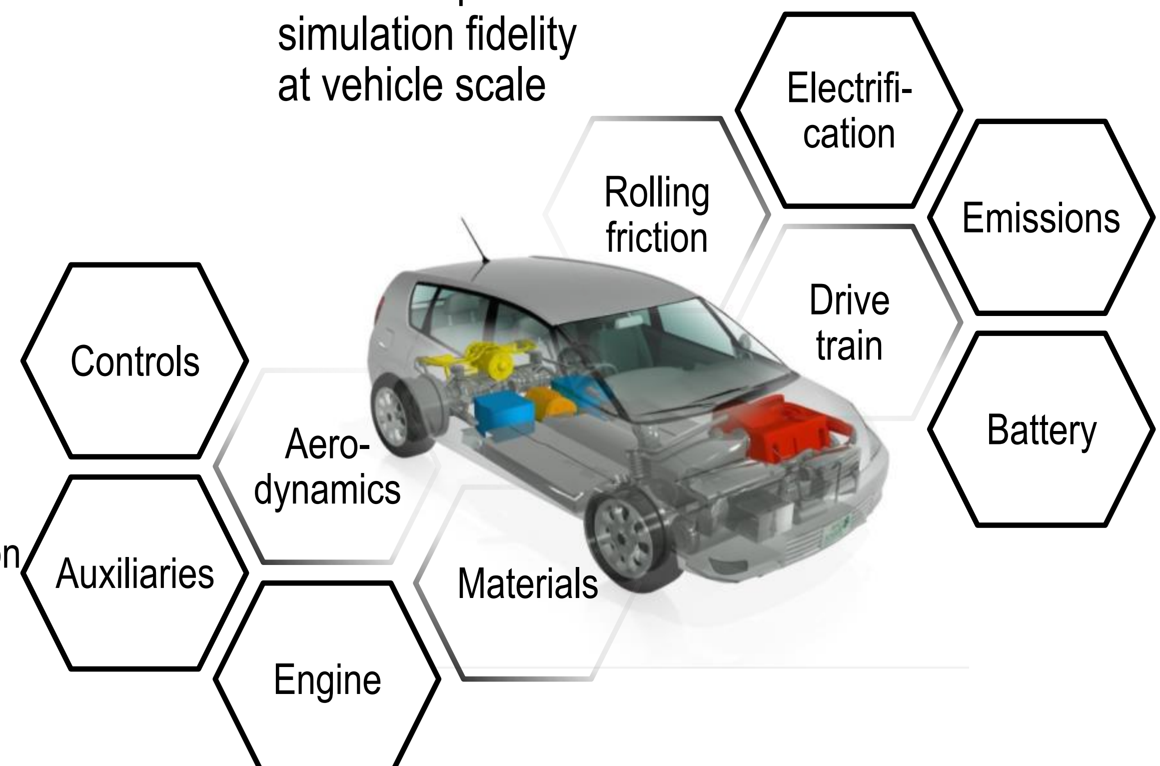
U.S. automotive industry is under unprecedented pressure

- New regulations, national agenda, and international competition drive demand for technology innovation
- Exponential increase in vehicle parameter and calibration space creates complexity
- Substantial HPC opportunities to meet industry needs can be realized only through:
  - Improved models for processes and systems
  - Integrated and scalable software (combustion, energy storage, aerodynamics, etc.)
- Virtualization made tremendous impact on subsystems in accelerating innovation
  - Crashworthiness
  - Optimizing aerodynamics

Big idea

Develop a **3D** Virtual Vehicle Framework to accelerate overall system optimization and innovation to enable efficient vehicles

- Span conventional, hybrid, and EV propulsion systems
- Deliver unprecedented simulation fidelity at vehicle scale



Opportunity

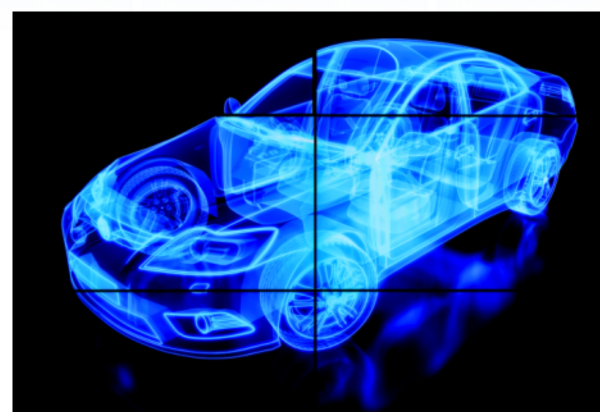
Integrate rapid advances in HPC with models and optimization methods to accelerate design of next-generation cars and trucks

RD&D targets

- Optimize propulsion systems to improve efficiency and reduce emissions
- Facilitate development, demonstration, and deployment of safe, lightweight materials
- Improve vehicle aerodynamics and reduce other frictional losses
- Provide adaptive controls customized to driver behavior to maximize efficiency
- Improve connectivity of vehicles with other vehicles and infrastructure
- Virtually evaluate social acceptability before manufacturing investment

Coordinated efforts across national labs, universities, and OEMs are key to expediting development of this framework and supporting component models

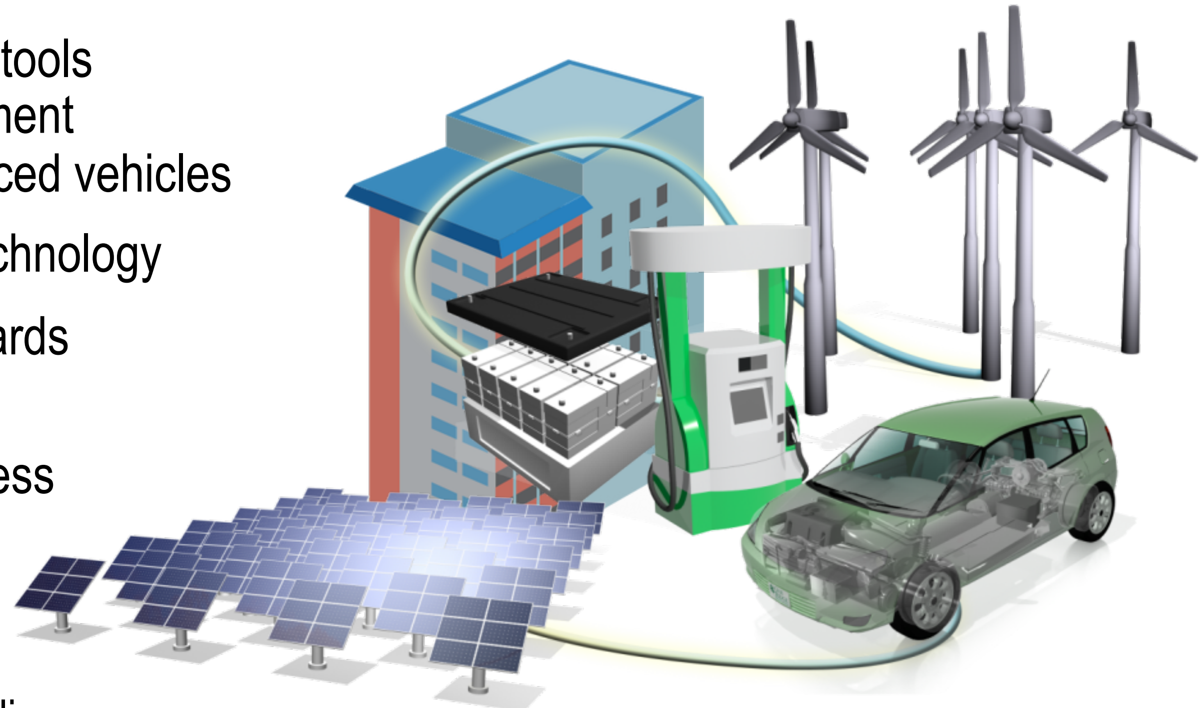
Argonne National Laboratory · NREL National Renewable Energy Laboratory · Oak Ridge National Laboratory · Sandia National Laboratories



Enduring benefits

Accelerated innovation to increase productivity and lower costs while meeting environmental goals

- World-leading computational tools that reduce time for development and final calibration of advanced vehicles
- Faster deployment of new technology
- Achievement of CAFE standards at lower cost
- Enhanced U.S. competitiveness
  - Adding flexibility to system integration
  - Providing new tools to small businesses and suppliers
  - Enabling more rapid identification and implementation of alternative technologies, power sources, integration with buildings, etc.

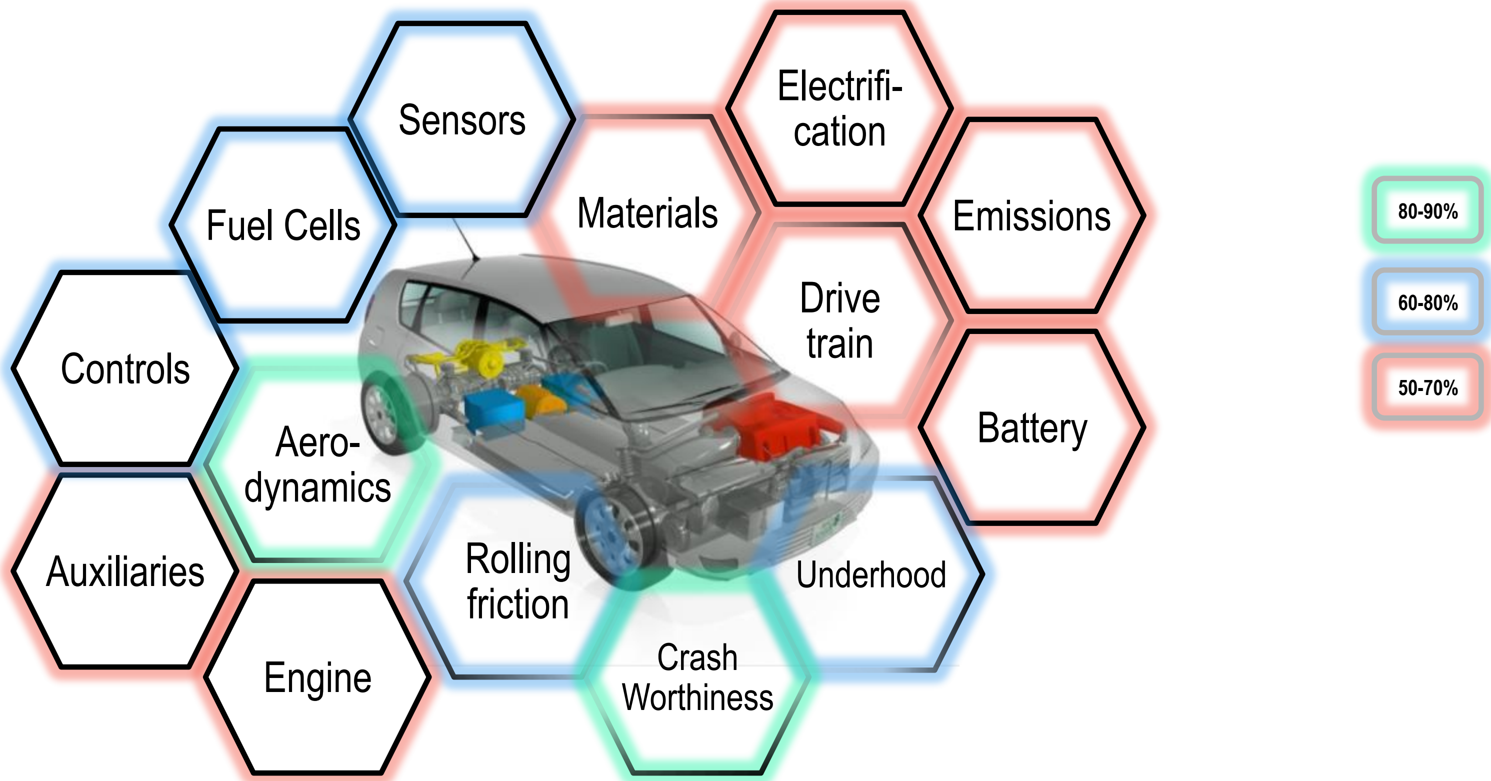


More effective integration of vehicle components, fuel/generation, storage, buildings, and connectivity to revolutionize sustainable transportation

What does it take?

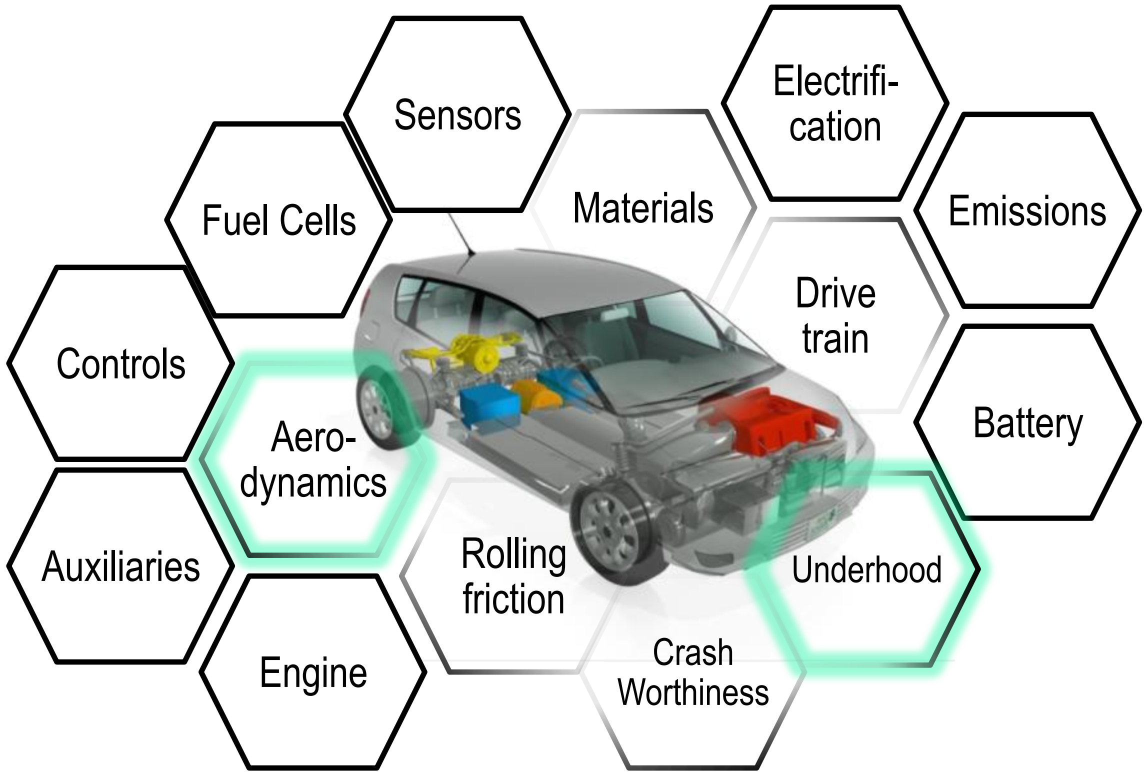
- Two Aspects
  - Maturity of the individual 3D computational tools
  - Maturity of the cross-component integration
- Strategy
  - Mature the components in view of the maximum impact on CAFE standards
  - Integrate all components as a single virtual-car design code
    - Utilize each component's current capability
    - Stage development and fidelity advancement of individual components based on industry needs/priority, e.g., shorter design cycle, reduce fleet CAFE
    - Deliver integrated code capability early, e.g., 2 years, then successively release versions with more capability for virtual car simulations
  - Mirrors the experience from the Nuclear Simulation Hub (CASL)

Current status of 3D computational tools



Colors to be updated with industry feedback!

Current status of integration of 3D computational tools



Need to be updated based on industry feedback

Electrochemical Energy Storage Modeling

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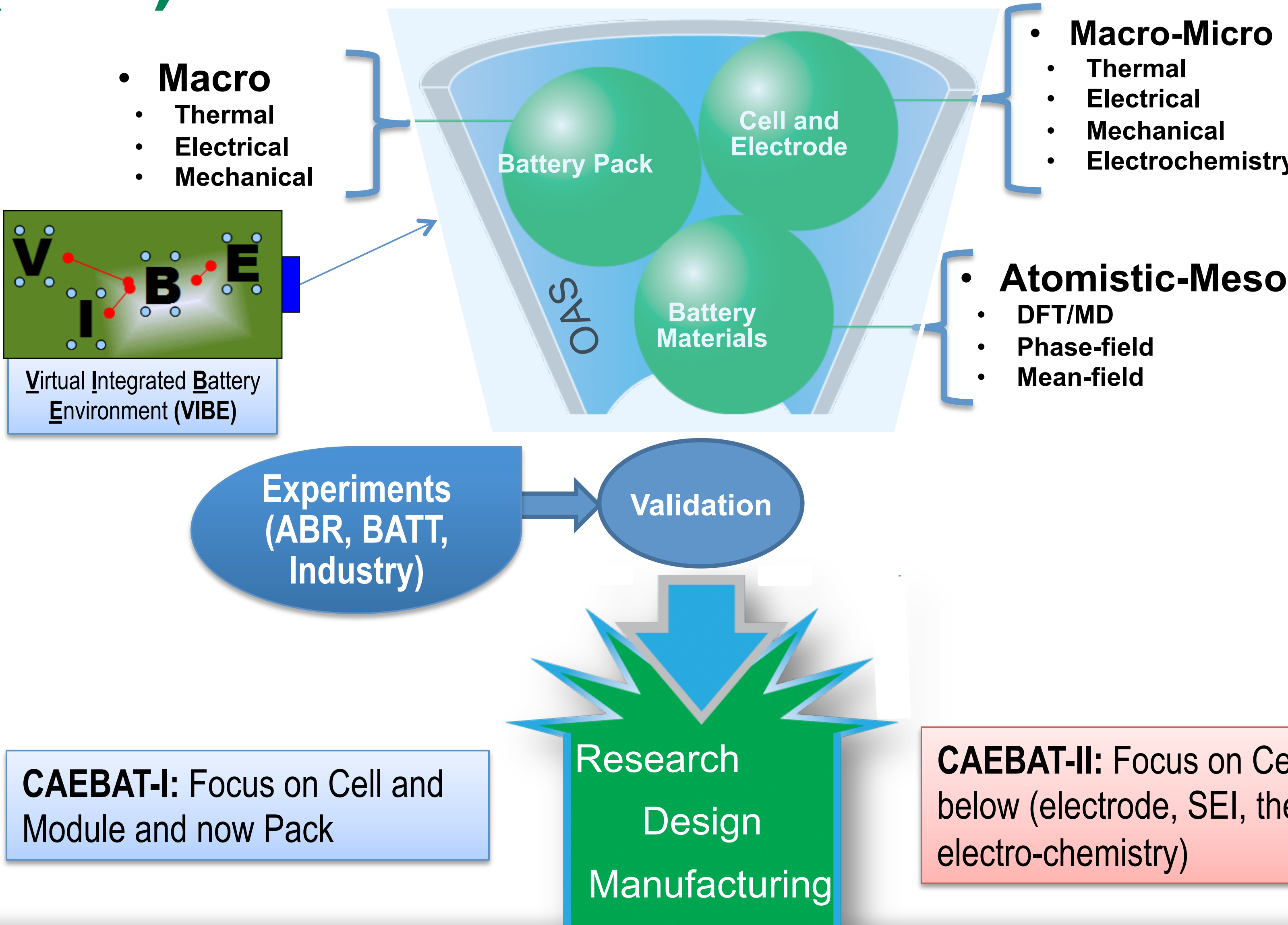
Jagjit Nanda
Hsin Wang
Andreas Malikopoulos
Damien Lebrun-Grandie

Farasis
ARPA-E
NHTSA
Oak Ridge National Laboratory
EERE
ANSYS
CD-adapco
NREL National Renewable Energy Laboratory
ASCR
EC-Power

Oak Ridge National Laboratory

CAEBAT Open Architecture Software (OAS) Vision – A Virtual Test Bed

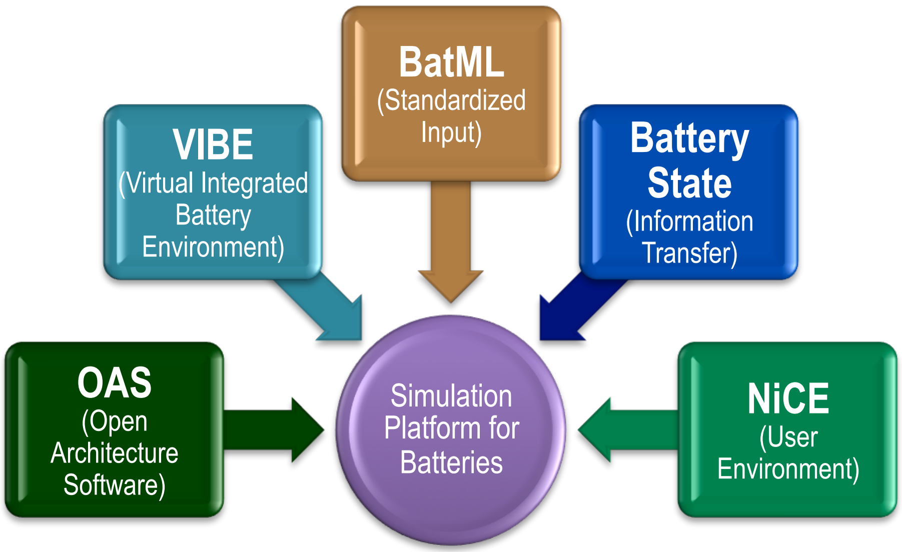


CAEBAT-I: Focus on Cell and Module and now Pack

CAEBAT-II: Focus on Cell and below (electrode, SEI, thermo-electro-chemistry)

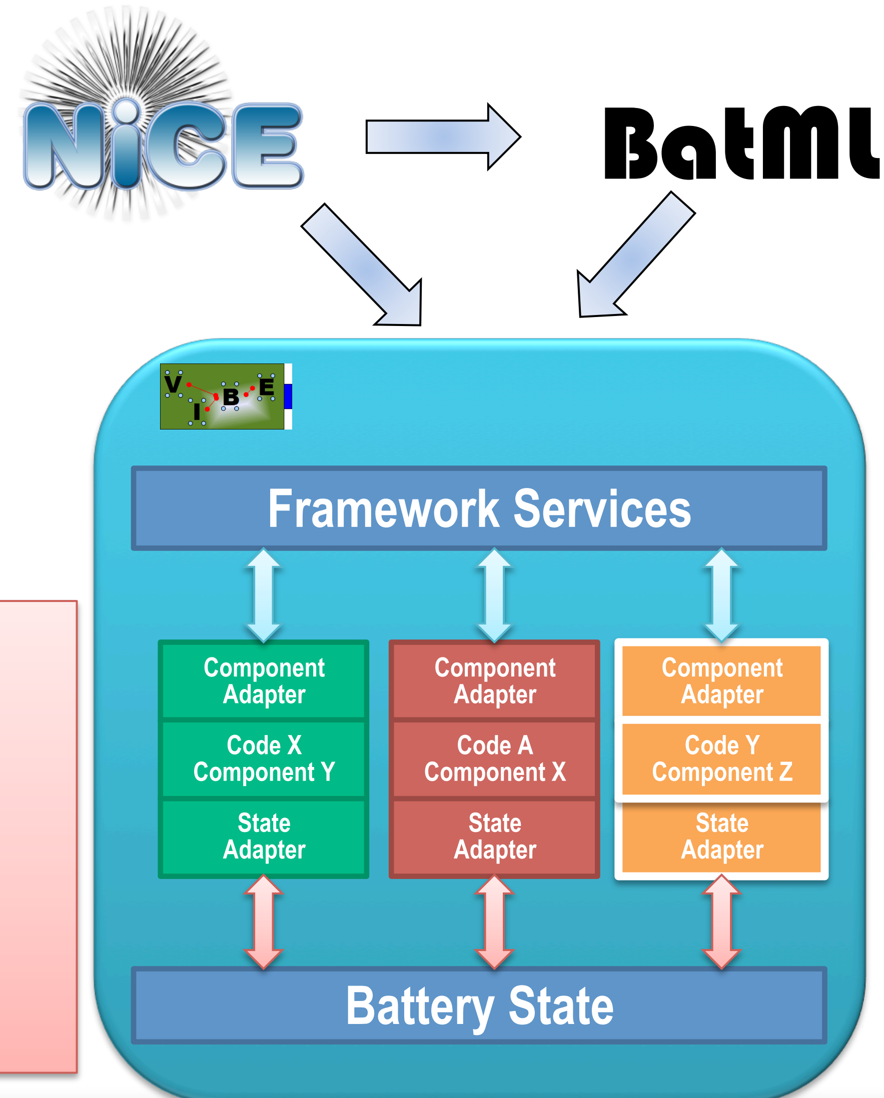
http://energy.ornl.gov/main.html

Components of fully integrated simulation platform for Batteries



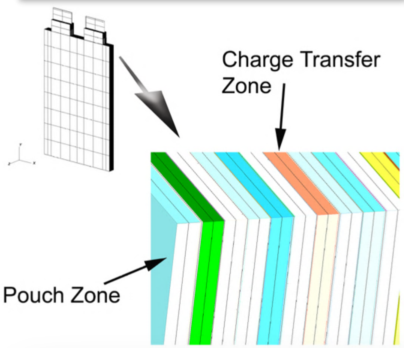
The CAEBAT simulation platform achieves multiple goals:

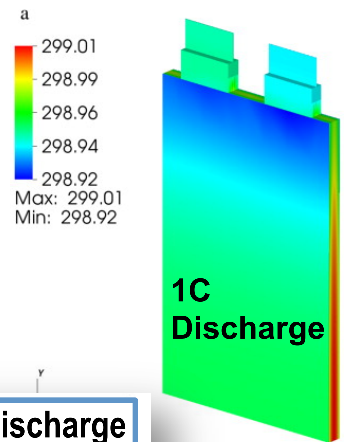
- Community software infrastructure
- Standardization to enhance leveraging
- Usability and re-use
- Scale bridging
- Scalability to many cores

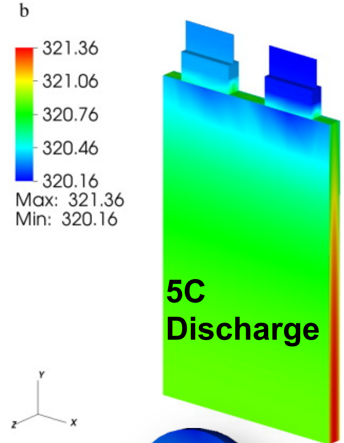


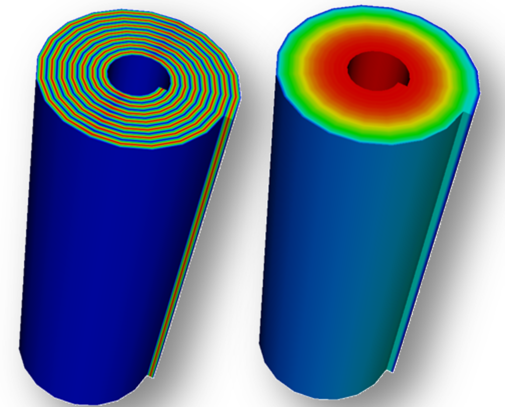
CAEBAT: Current status

Detailed 3D Modeling

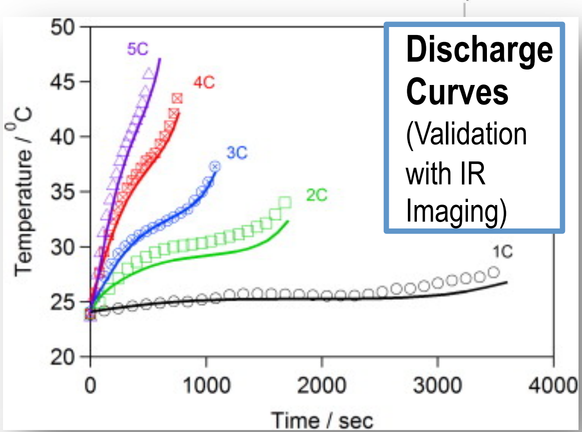




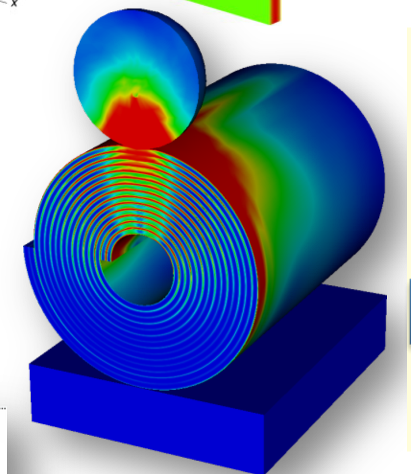




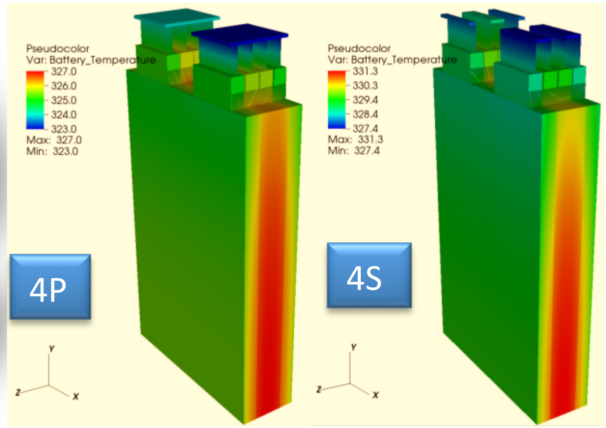
Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal - Electrical)



Discharge Curves (Validation with IR Imaging)



Mechanical Abuse of Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal – Electrical – Mechanical)



Temperature in 4P and 4S Module with Fully Coupled Electrochemical, Electrical and Thermal Simulations in CAEBAT OAS / VIBE

ELSEVIER

Journal of Power Sources

Available online 24 August 2013

In Press, Accepted Manuscript — Note to users

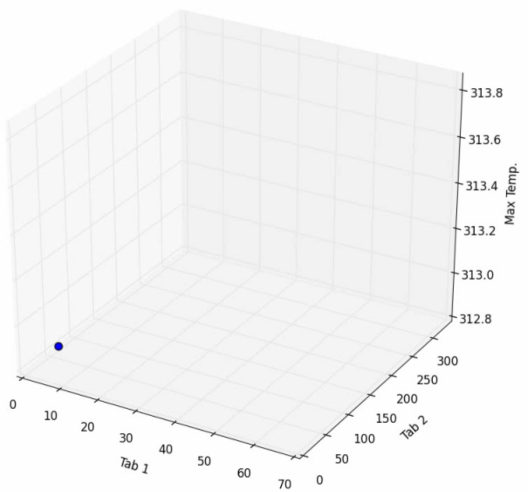
A new open computational framework for highly-resolved coupled 3D multiphysics simulations of Li-Ion Cells ☆

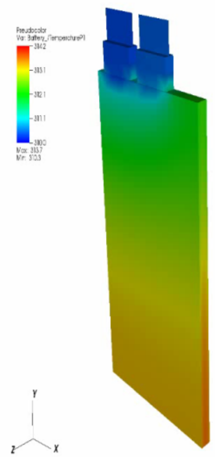
Srikanth Allu, Sergiy Kalnaus, Wael Elwasif, Srdjan Simunovic, John Turner, Sreekanth Pannala

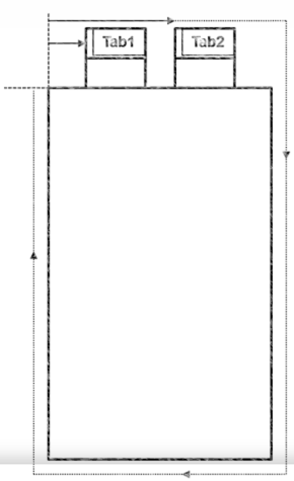
Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN-37831

Design Optimization

Optimal Placement of Tabs



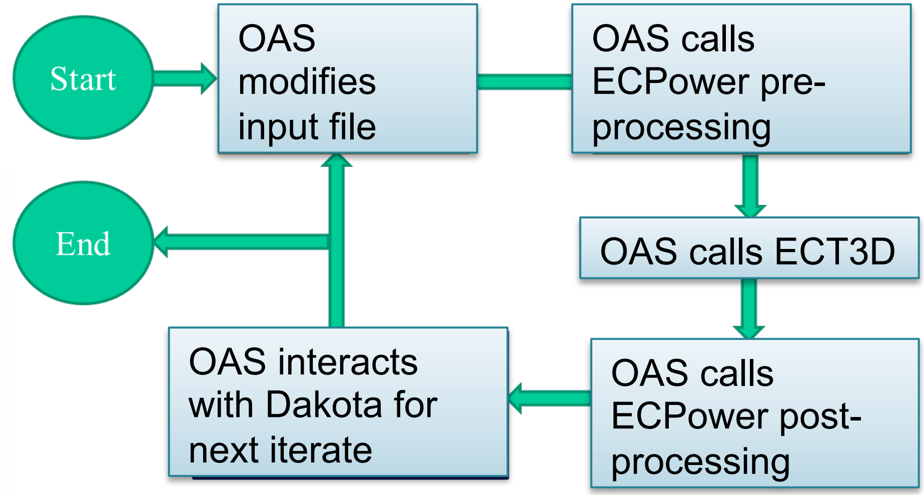


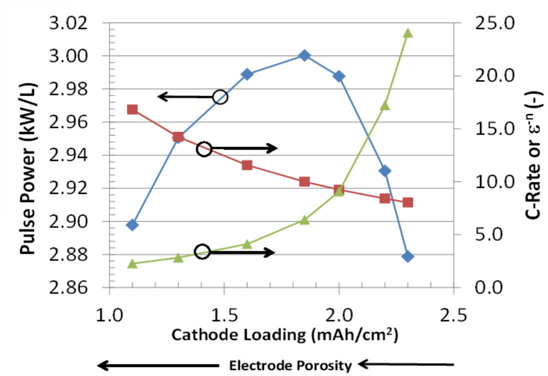


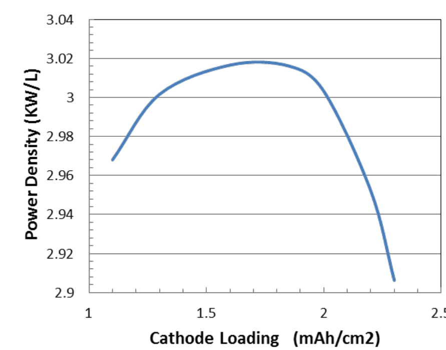
To reduce the peak cell temperature:

a) Increase the width of the tabs

b) Place them on opposite ends





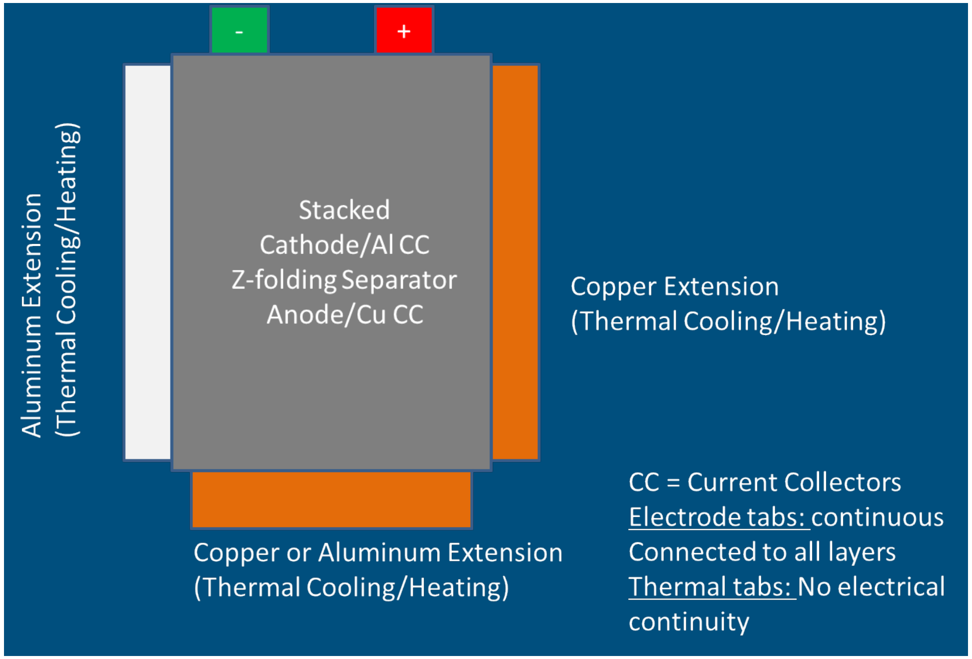


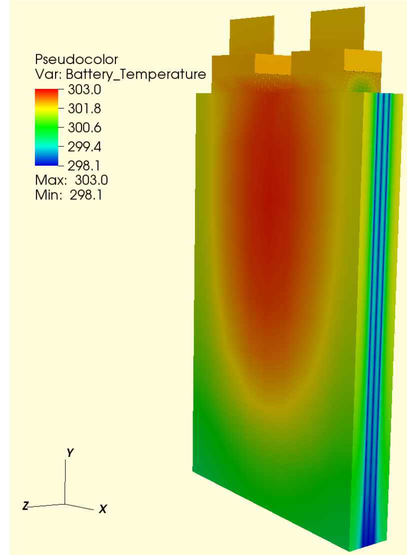
Previous 1D result (Blue curve)

OAS/ ECT3D result

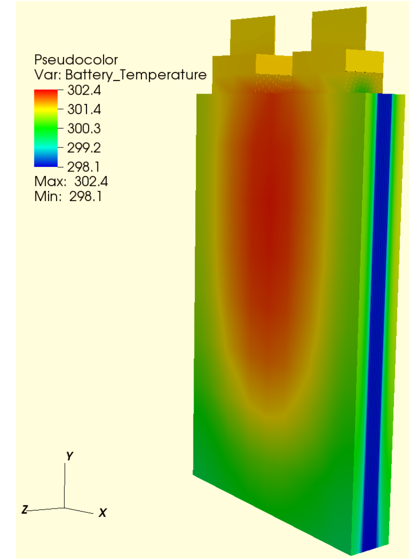
Optimizing the electrode properties

Novel Thermal Management (ARPA-E project)



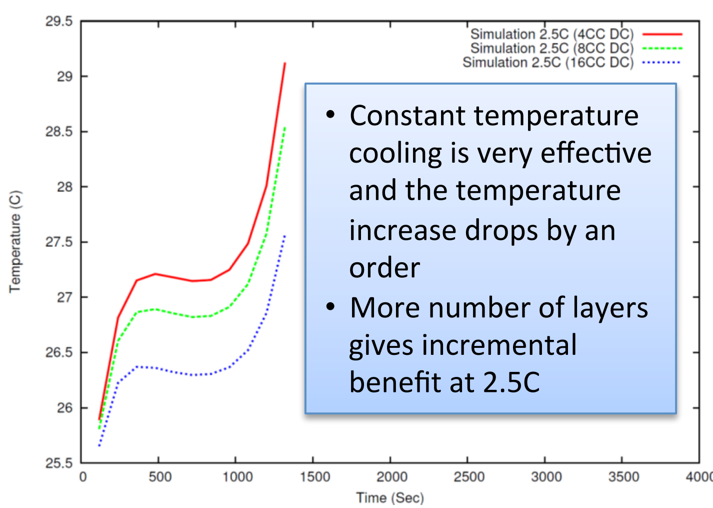


4 Anode CCs +
4 Cathode CCs



8 Anode CCs +
8 Cathode CCs

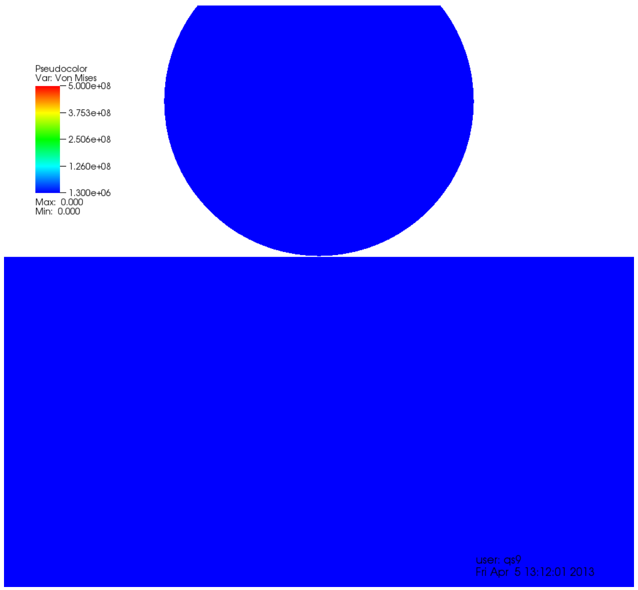
- Side cooling reduces the peak temperature dramatically
- The cooling is further improved for larger L/W formats



- Constant temperature cooling is very effective and the temperature increase drops by an order
- More number of layers gives incremental benefit at 2.5C

Modeling is used to evaluate different design scenarios so that only the most optimal configurations are built and tested – validation of the CAEBAT philosophy

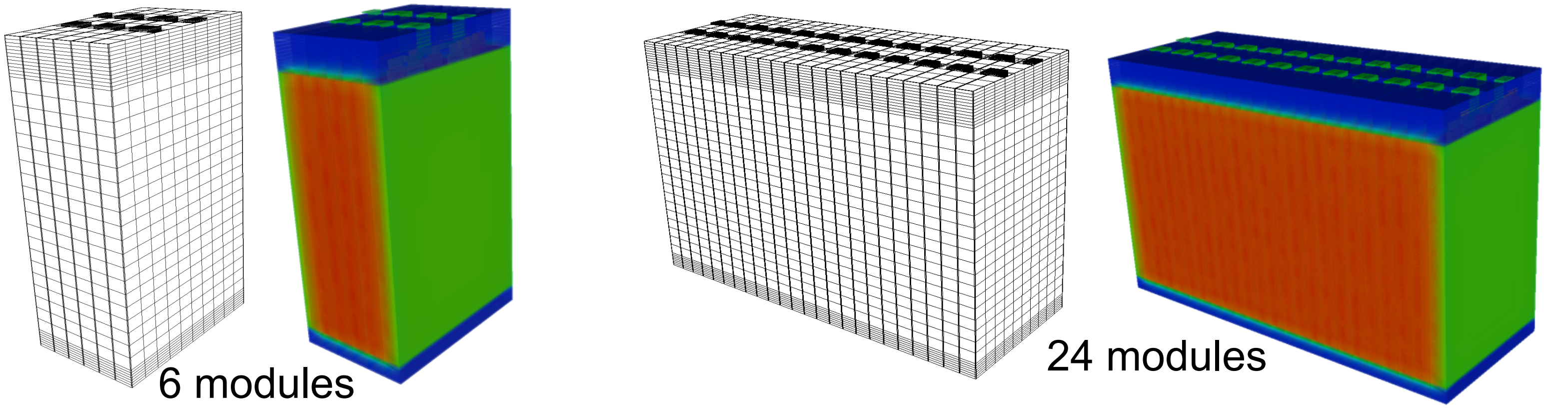
Mechanics of the cell



Dynamic Impact

Calendaring of Electrodes

VIBE – Facilitates Hierarchical Process to Construct Battery Packs

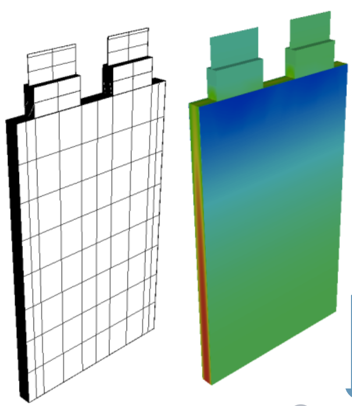


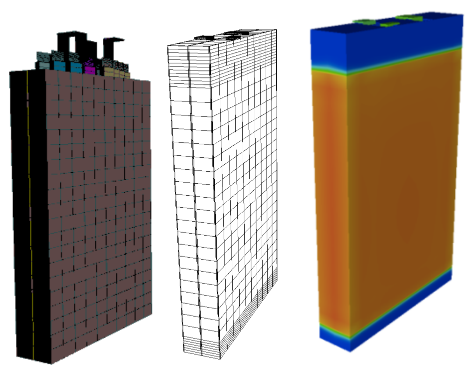
Pack

Module

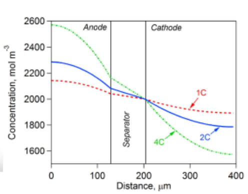
Cell

Cell Sandwich





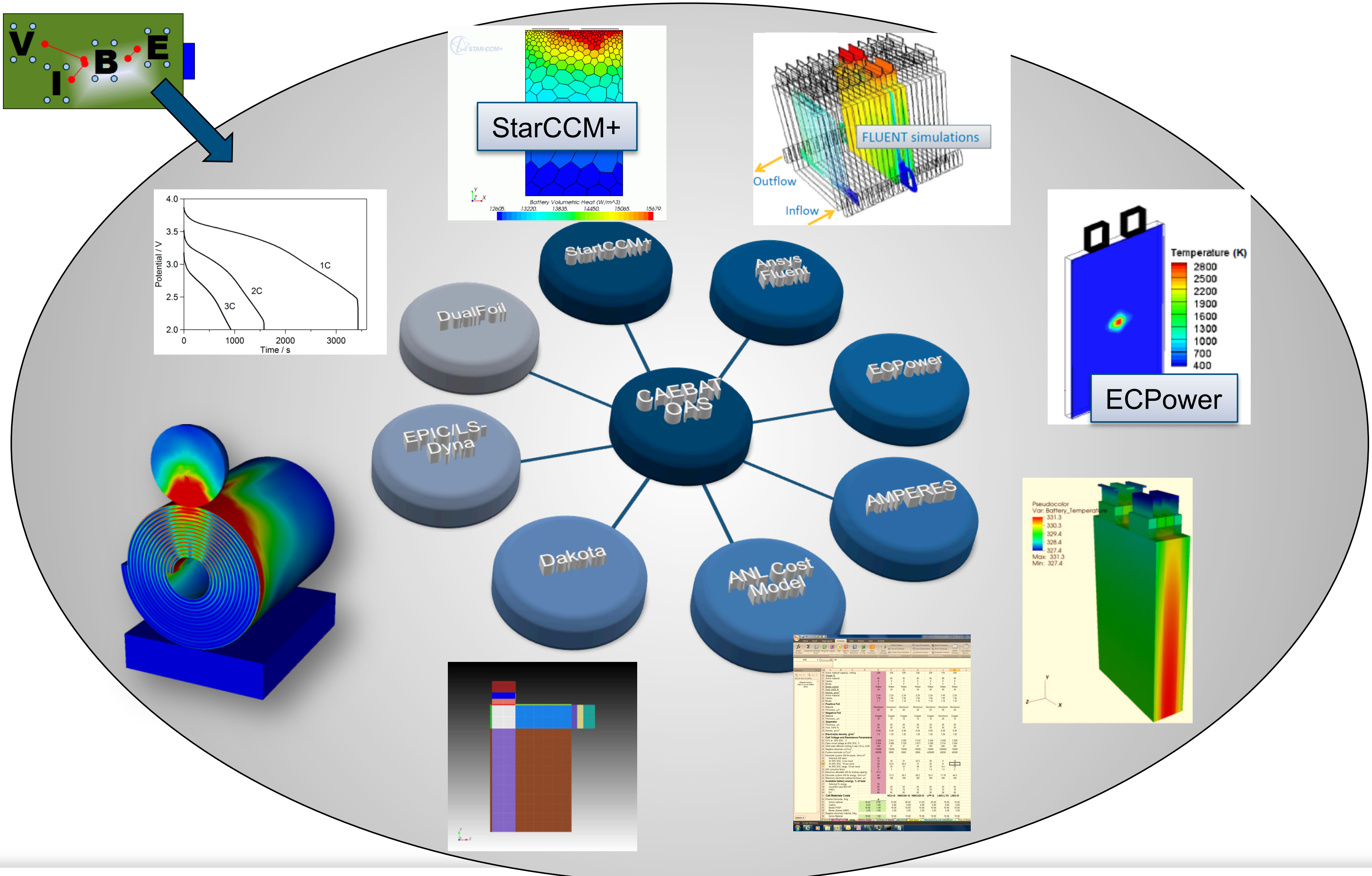
- Current module has 2 cells in series and 2 cells in parallel (similar to Nissan-Leaf)
- Each Cell has 17 cathode layers with 33 Ah capacity
- Dimensions ≈ 290mm × 210mm × 6mm
- Coarsest mesh for each module has ½ million degrees of freedom



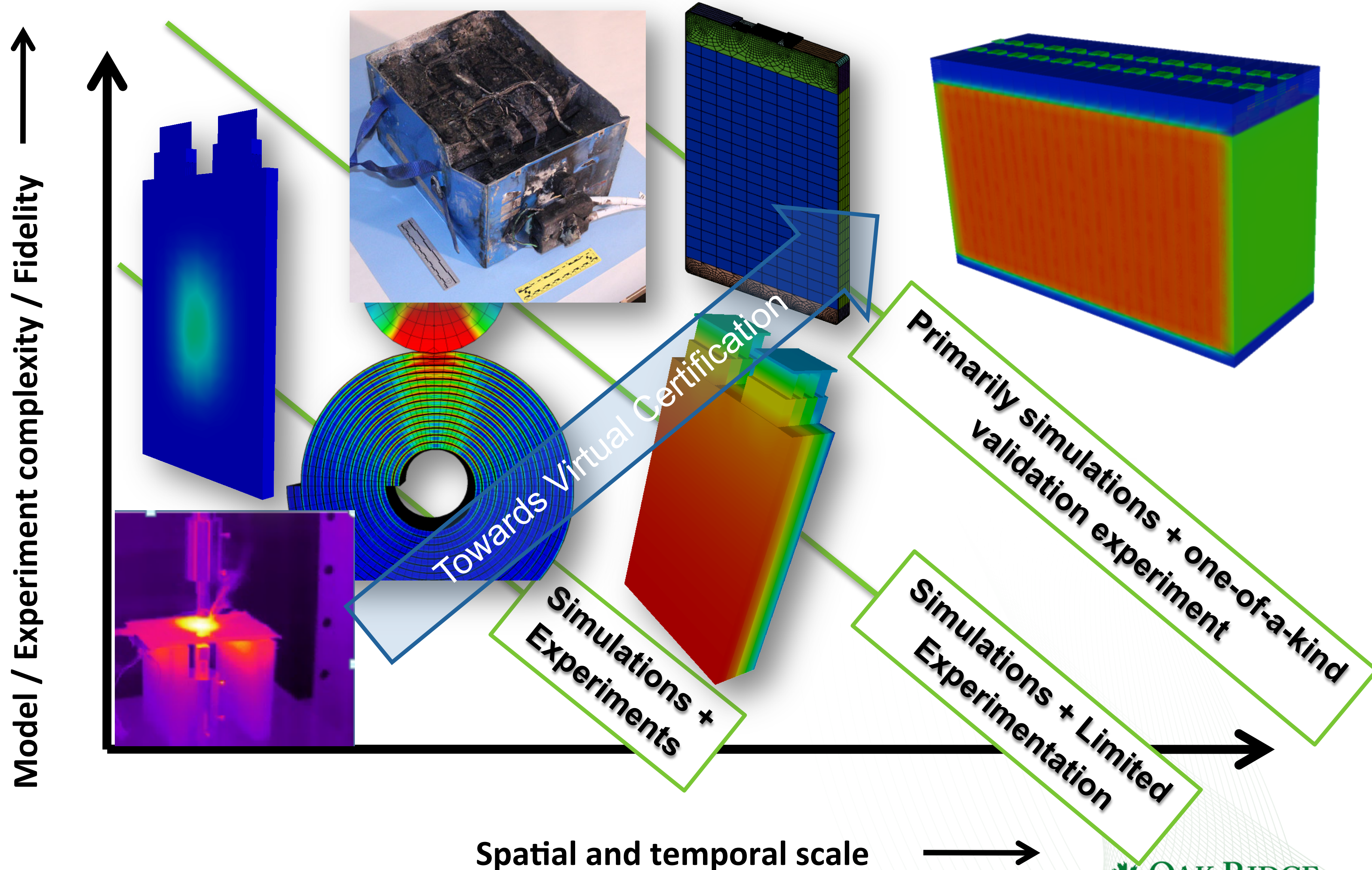
Advantages

- Test models sequentially
- Ability to stack cells and modules in series and parallel
- Both module and pack simulations can be performed
- Simulations can be distributed across multiple processors

VIBE Computational Ecosystem: Coupling open and proprietary components



Virtual Certification of Battery Packs
from cell to module to pack



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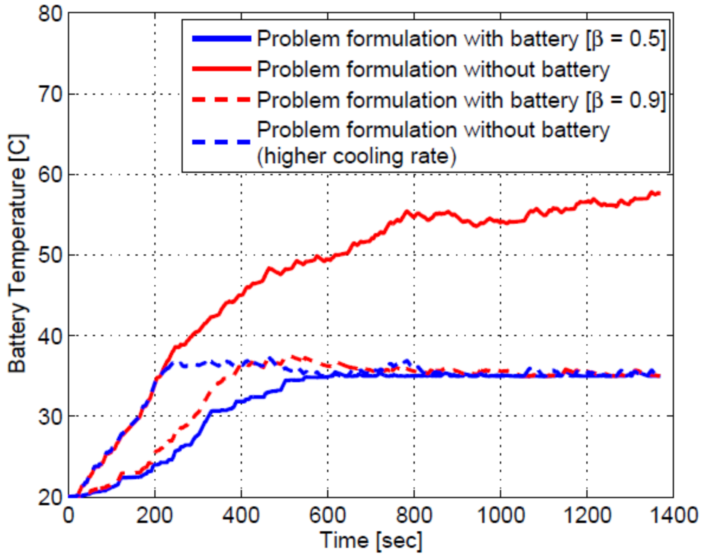
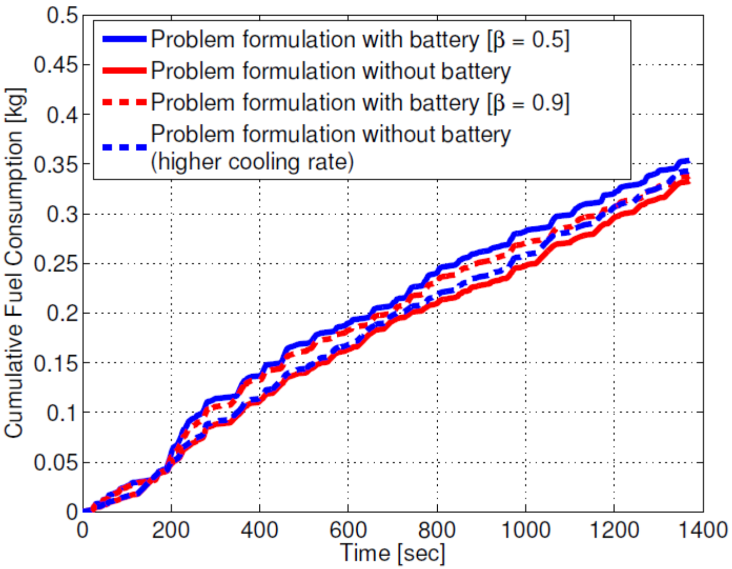
Controls and Optimization

- Battery temperature and life in the loop for (P)HEV optimization





Engine Modeling

Dean Edwards
Charles Finney
Robert Wagner
Stuart Daw
Johney Green
Miro Stoyanov
Wael Elwasif

Ongoing collaborative efforts

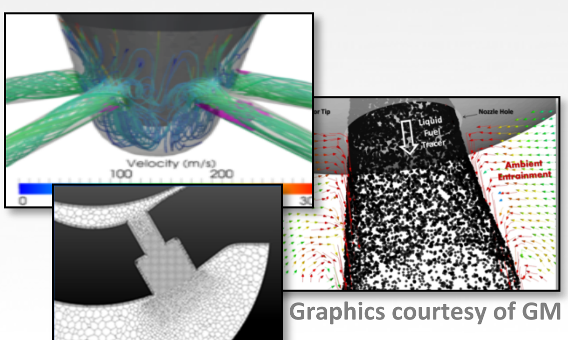
Gasoline DI fuel injector design optimization

Understand and optimize the design of GDI fuel injectors for improved efficiency and reduced emissions.

Computational framework to automate labor-intensive tasks through the iterative design process.

Coupling models of internal injector flow and cavitation with in-cylinder spray and combustion.

Enables massively parallel simulations for thorough and *rapid* investigation and optimization across *operational and geometric* design spaces.



Graphics courtesy of GM

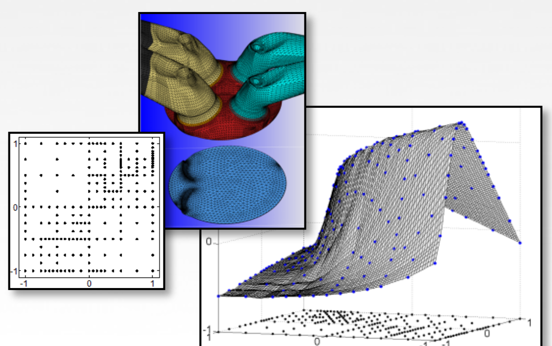
Cycle-to-cycle variation in highly dilute ICEs

Understand the stochastic and deterministic processes driving cyclic variability in highly dilute SI engines.

Novel approach to *parallel* simulation of a *serial* phenomena.

Detailed CONVERGE simulations at intelligently selected sample points in parameter space.

Enables creation of low-order metamodels that retain key dynamics of CFD model but greatly reduce computational time for thorough exploration of parameter space.



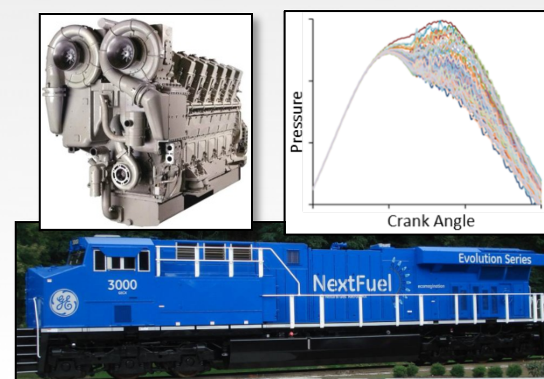
Cycle-to-cycle variation in dual-fuel locomotive engine

Investigate key factors promoting cyclic variability in a dual-fuel (NG/diesel) locomotive application.

Industry-driven with ORNL providing methodology, HPC resources, and limited support.

Similar approach to high-dilution effort with CONVERGE simulations feeding metamodel development.

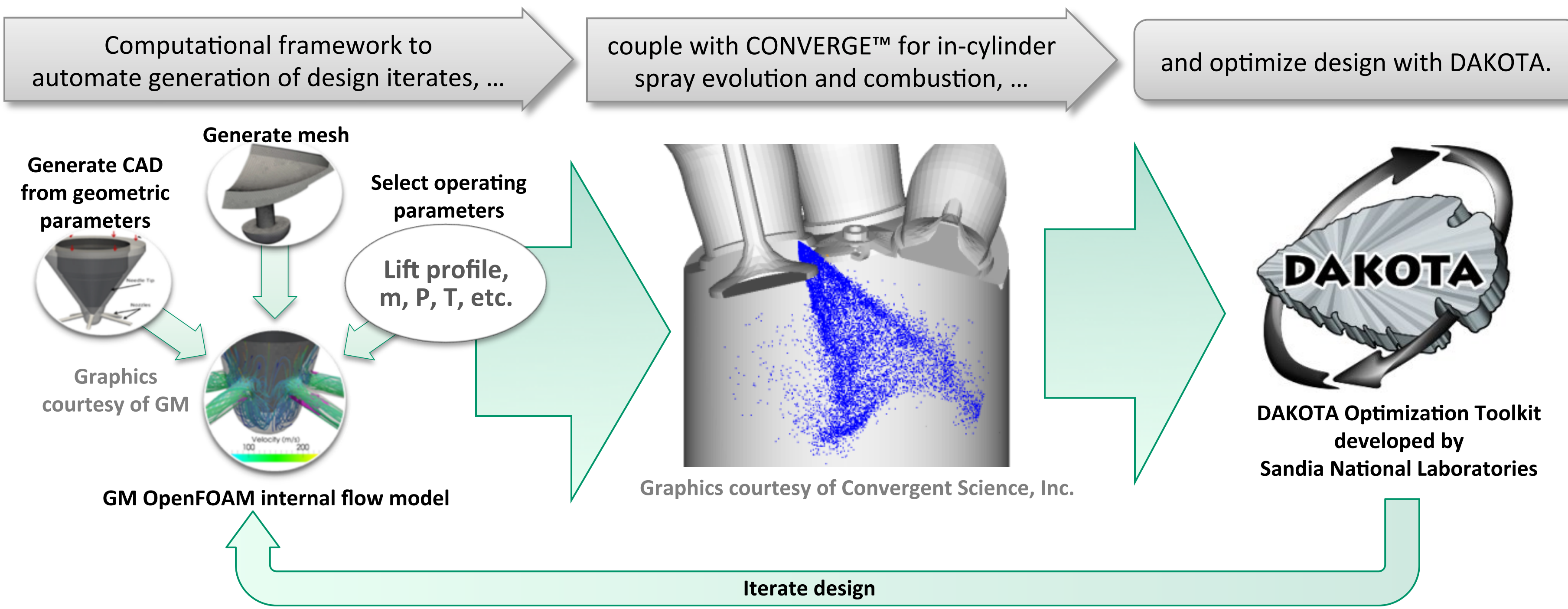
Stable dual-fuel operation will enable significant displacement of petroleum-based diesel fuel with NG.



Graphics courtesy of GE

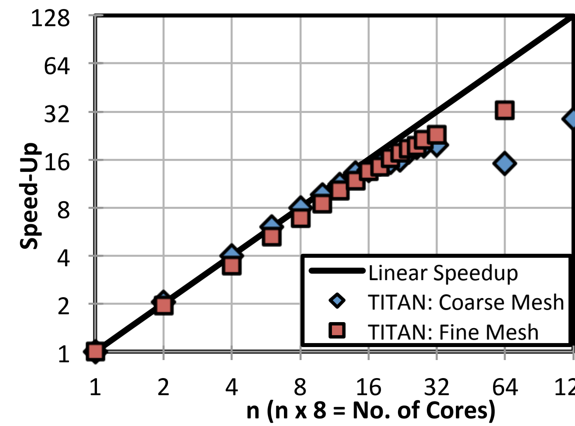
Injector design optimization – Relevance and Approach

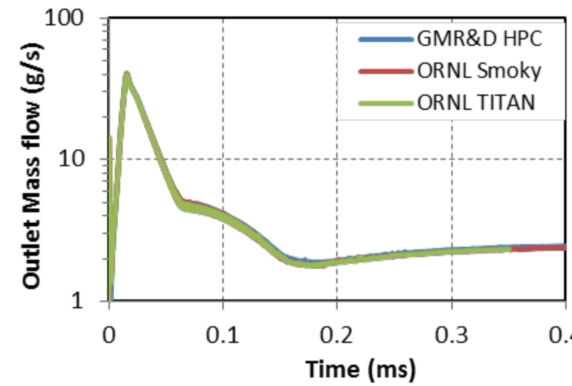
- **Collaborative effort with General Motors**
- **Injector design optimization is currently a lengthy, labor-intensive process**
  - Months of effort to minimally cover design space
- **HPC enables *thorough* & *rapid* investigation of *operational* & *geometric* design spaces**
  - From months to weeks *AND* more thorough coverage of design space
- **ORNL developing computational framework to automate model generation & design optimization**
  - Leveraging experience with CAEBAT for automotive batteries and IPS for fusion (ITER)

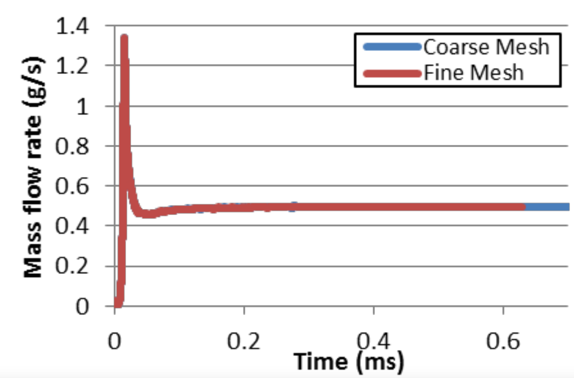


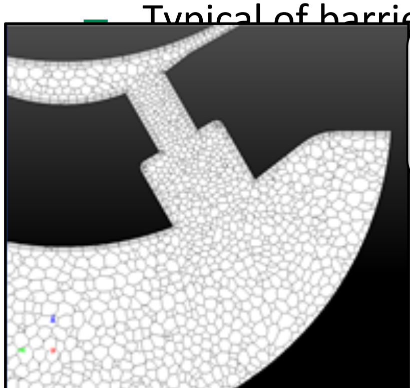
Model validation and grid optimization

- **Performed initial code validation and operating parameter sweeps**
  - 42 parallel cases using 5000+ cores on TITAN
  - Validated against GM simulations and *experimental data*
- **Repeated sweep with higher-resolution mesh in the nozzle area**
  - 256 cores/simulation => 10,000+ cores on TITAN
  - All cases showed good agreement with coarse grid results
  - Future runs will use the coarse grid
- **Initiated large-scale sweep of geometry and parameter space**
  - 7 nozzle designs at 42 reference operating points
  - 75,000 cores on TITAN
- **Identified file-write issues with OpenFOAM on HPC**
  - Each core writes an output directory, onerous for peta-scale HPC
    - 2.5M total files for our large-scale sweep
  - Typical of barriers encountered while adapting code for HPC



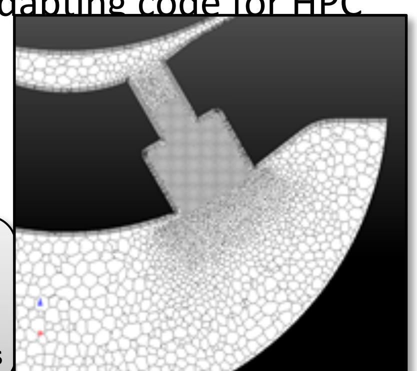






Coarse Grid
- 383k Total Cells
- Δx ≈ 30µm in counter bore
- 2 cells in 20µm prism layers

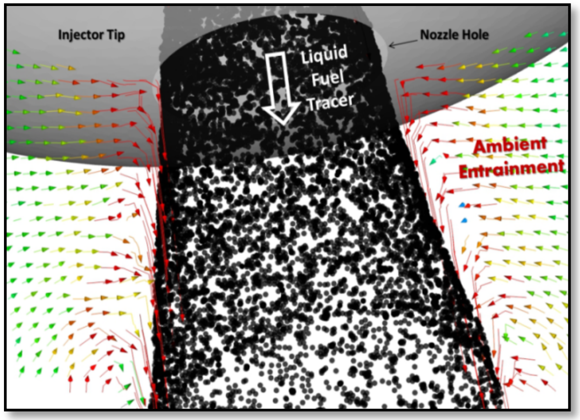
Fine Grid
- 688k Total Cells
- Δx ≈ 10µm in counter bore
- 4 cells in 20µm prism layers



Graphics provided by General Motors

Ongoing and future activities

- **<u>Remaining challenges and barriers:</u>**
  - Address file-write bottleneck with OpenFOAM
  - Couple internal flow model with in-cylinder spray evolution and combustion
  - Adapt codes for GPUs to take full advantage of TITAN's speed
- **Couple with CONVERGE™ for downstream spray evolution**
  - Validate with available experimental measurements
  - Fully coupled model for in-cylinder simulations with combustion
- **Improve scalability of OpenFOAM & CONVERGE™ models through use of GPUs**
  - Talking with NVIDIA, FluiDyna, Convergent Science
  - Possible collaboration with LLNL
- **Demonstrate automated optimization of injector geometry for…**
  - Improved fuel economy
  - Lower emissions
  - Lower shot-to-shot variability
- **Transfer of knowledge and methodology to GM for proprietary runs**

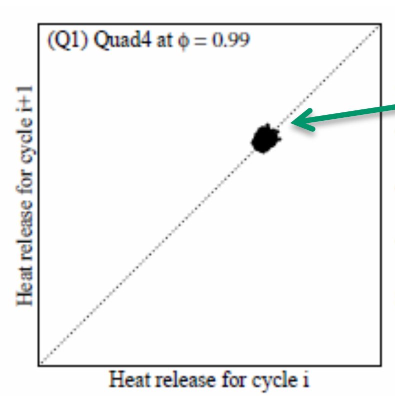


Graphics provided by General Motors

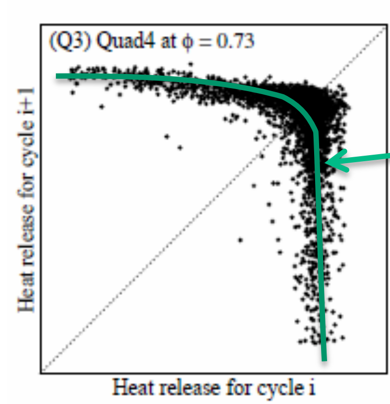
This project received 15M hours on Titan through an ALCC award

Highly dilute combustion stability – Relevance and Approach

- **Collaborative effort with Ford Motor Company and Convergent Science, Inc.**
- **Potential efficiency and emissions benefits of highly dilute (lean or high-EGR) operation are limited by combustion instability**
  - Instability driven by combined effects of stochastic and deterministic processes
  - Understanding the causes of instability enables potential for redesign and/or control
- **HPC and CFD models enable detailed study of key factors promoting instability**
  - Thousands of simulated cycles required to study problem with statistical accuracy
  - Previous analytical studies used low-order models to avoid excessive computation time
- **ORNL is using detailed HPC CFD simulations to feed development of low-order metamodels to improve understanding of stochastic and deterministic factors promoting combustion instability**



Low dilution
- Stochastic effects dominate
- Relatively low variability
- Minimize by design



High dilution
- Lean or high-EGR
- Deterministic effects dominate
- Stochastic effects produce additional "noise"
- High variability
- Minimize by active control

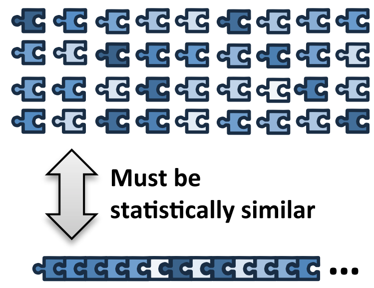
Approach

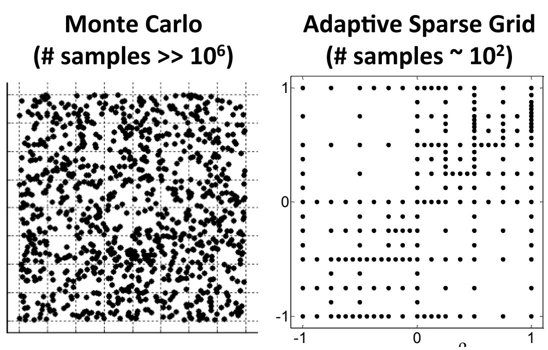
- **Parallel cycle simulations which cover the statistical behavior exhibited by serial combustion events**
  - Sampling of initial parameter space must match statistics of key feedback parameters to capture cycle-to-cycle interactions
- **Intelligent sampling of multi-dimensional parameter space**
  - Adaptive sparse grid sampling of multiple parameters
    - Iterative method concentrates samples in high-gradient regions
    - ~10^2 samples vs. >>10^6 samples for Monte Carlo
- **Detailed CFD combustion and kinetics simulations at sample points using CONVERGE™ on TITAN**
  - Must have control over all initial inputs (no randomness)
- **Create low-order metamodels of deterministic response**
  - Multi-dimensional mapping of CFD model's response at sample points
    - Continuous and differentiable set of basis functions
    - Uncertainty Quantification (UQ) and stochastic collocation using ORNL's TASMANIAN algorithm
  - Retains dominant features of detailed model's behavior
  - Allows rapid exploration of parameter space

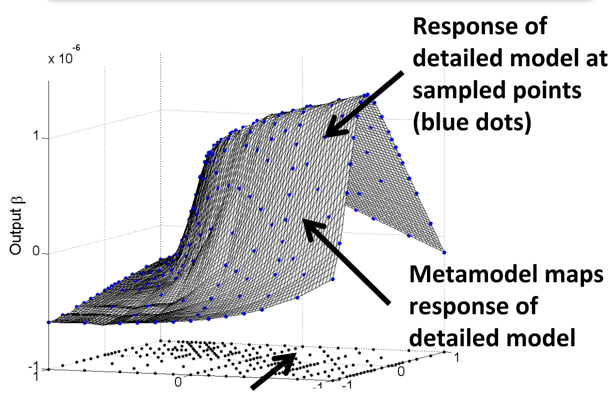
TASMANIAN

Toolkit for Adaptive Stochastic Modeling And Non-Intrusive ApproximatioN

Developed at ORNL with funding from the DOE Office of Science ASCR Program





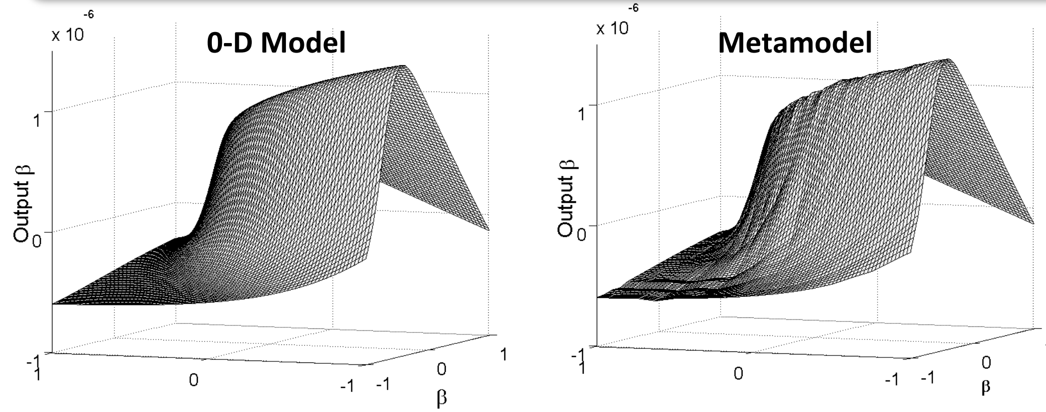


Detailed CFD simulations at sample points

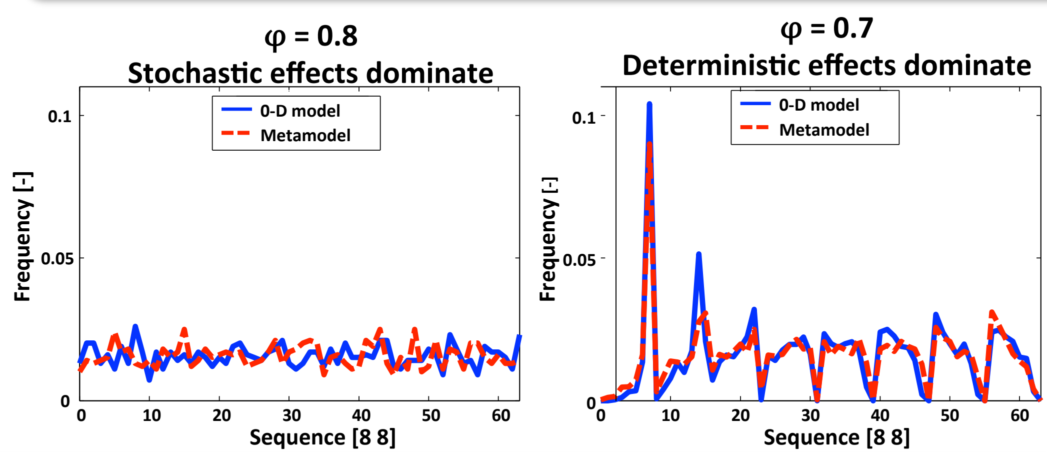
Proof of concept using simple, 0-D engine model

- **Successfully demonstrated our approach using simple SI model with cycle-to-cycle feedback**
  - 0-D, single-zone with prescribed (Wiebe) combustion
  - Combustion efficiency variation with dilution based on experimental observations and percolation theory
- **Metamodel created based on 8 sampled model parameters**
  - <u>No feedback</u>: SOC, φ, Wiebe exponent (m)
  - <u>With cycle feedback</u>: Fueling parameters (α and β), residual fraction and temperature, molar charge at IVC
- **Analysis shows metamodel retains key physics of original model**
  - Predicts transition from stochastic to deterministic behavior with φ

Metamodel captures steepness of response map with limited residual error (seen here as "wrinkles")

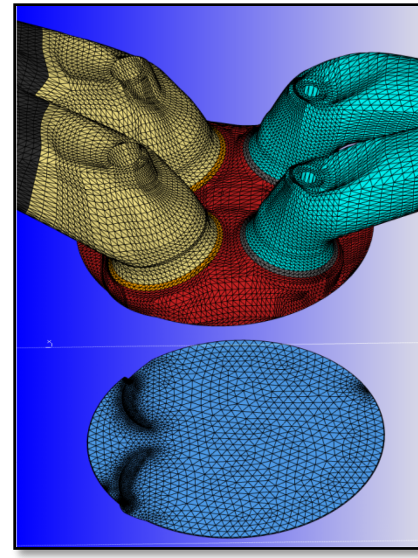


Symbol statistics show metamodel retains key physics of the original model. Residual fuel effects begin to dominate near the lean stability limit.



- **Finney, et al. 2012 International Conference on Theory and Applications of Nonlinear Dynamics (ICAND).**
- **Webster, et al. 2013 SIAM Computational Science and Engineering Conference.**

Transition to CFD simulations on TITAN



- **Ported CONVERGE™ to TITAN**
- **Non-proprietary geometry model provided by Ford**
- **Calibrated open model for high-EGR dilution**
  - Current open-source kinetic mechanisms appear to under-predict combustion performance at high dilution
- **Developed and validated supervisory framework for job management on TITAN**
  - Scripts to generate cases with parametric variations, monitor output quality, and manage restarts (~10-20+ restarts per simulation)
- **Completed initial sparse grid sampling on TITAN**
  - Nominal conditions: 1500 RPM, road load (~3.5-bar IMEP), 17% EGR
  - Sweep of 4 parameters:
    - Spray mass = 12.8-15.65 kg
    - Spark energy = 0.01-0.03 J
    - P in exhaust manifold = 85-110 kPa
    - T in exhaust m
  - 401 parallel simu
    cores and approx

CONVERGE™ simulation at lean conditions showing partial burn

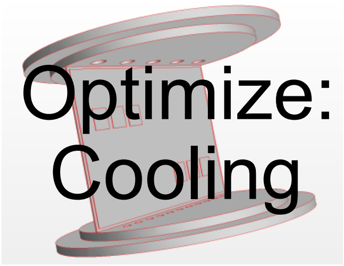
This project received 17.5M hours on Titan through an ALCC award

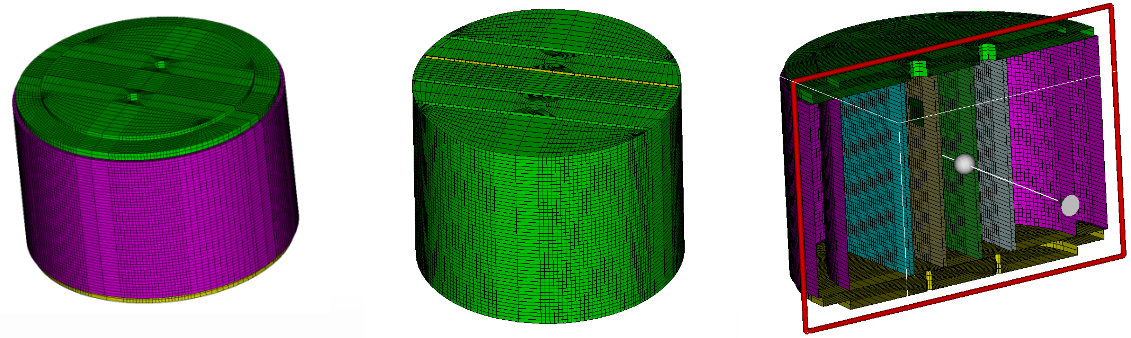
Inverter Thermal Management

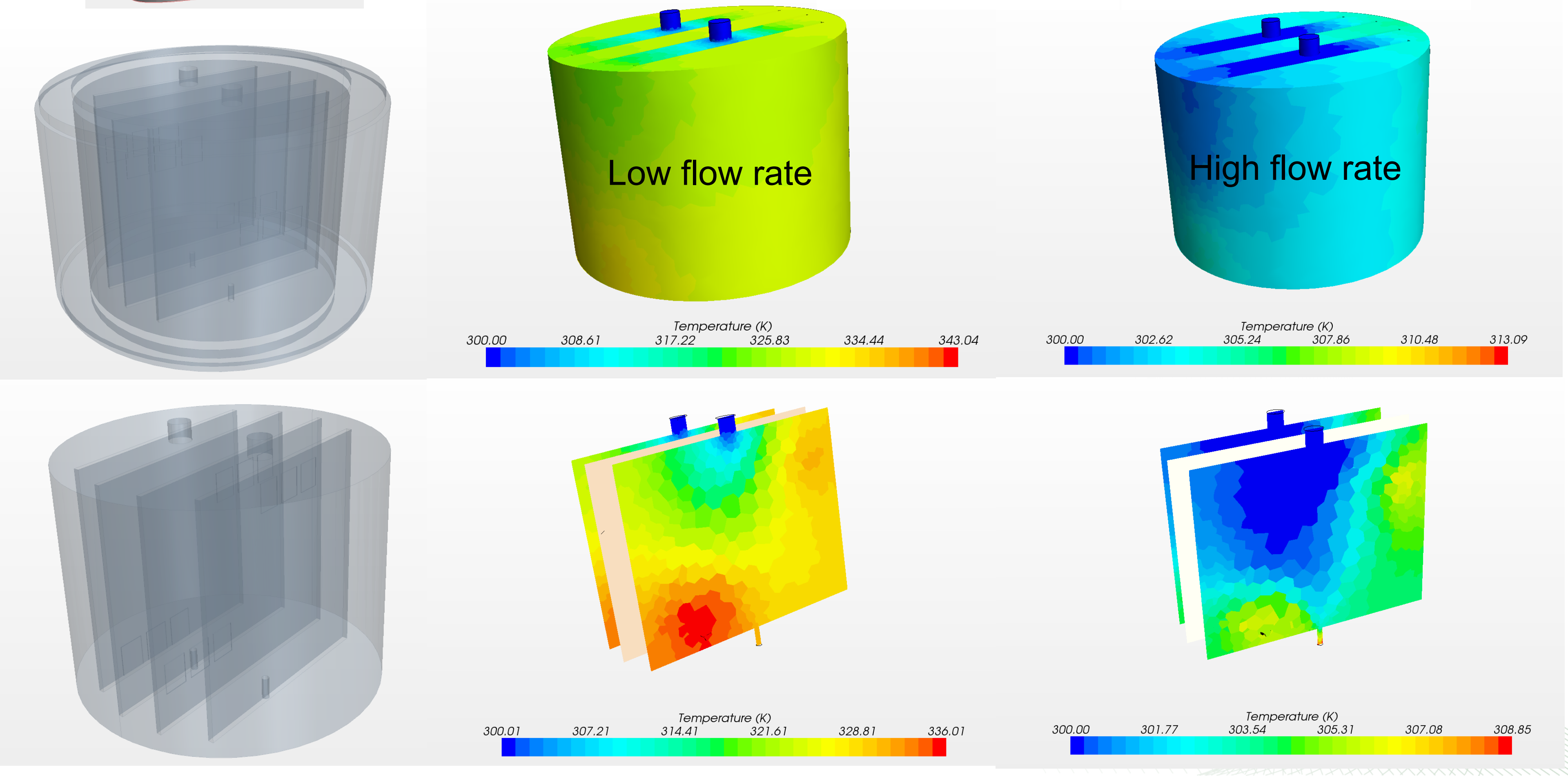
Srikanth Allu
Burak Ozpineci & Team

Oak Ridge National Laboratory

Thermal Management for Novel WBG Inverters





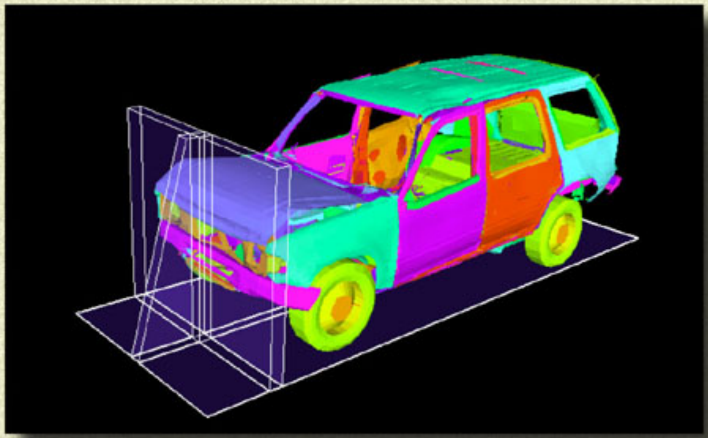


Crash Worthiness

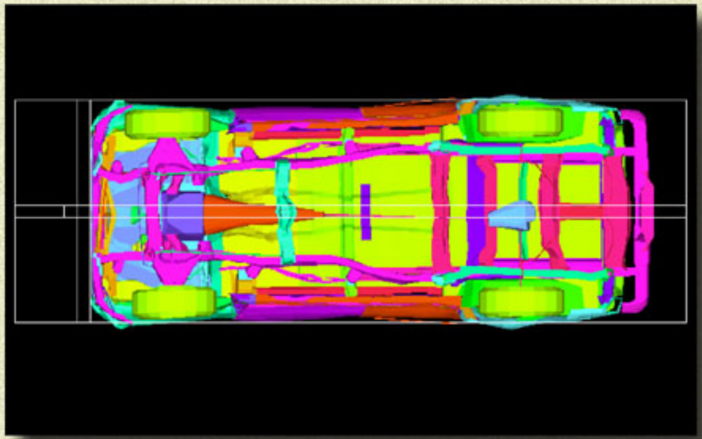
Srdjan Simunovic

Simulation Results

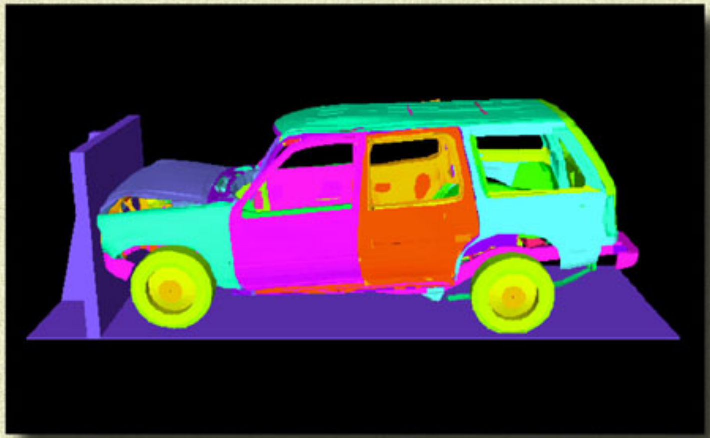
Full Frontal Impact with Rigid Barrier



Full Frontal Impact with Rigid Barrier
Bottom View



Full Frontal Impact with Rigid Barrier
Side View



Full Frontal Impact of an SUV
Cross Section through the Middle of the Vehicle

http://energy.ornl.gov/main.html

OLCF Projects (Aerodynamics)

SmartTruck
Ford

Computational Fluid Dynamics
"Smart Truck Optimization"

Science Objectives and Impact

- Apply advanced computational techniques from aerospace industry to improve fuel efficiency of Class 8 Long Haul Trucks
- New California Air Resources Board (CARB) requires 5% fuel efficiency increase on all Class 8 trucks; national drive to reduce emissions.
- Determine design of add-on parts to substantially reduce drag
- If all 1.3 million trucks operated with a passenger car's drag:
  - ✓ Save 1.5 billion gallons of diesel annually
  - ✓ Reduce 16.4 million tons CO_2 annually
  - ✓ Save $5 billion in fuel costs annually

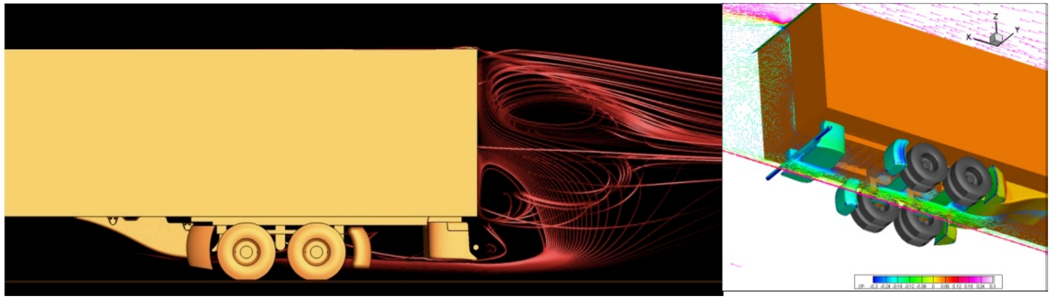
Science Results

Unprecedented detail and accuracy of a Class 8 Tractor-Trailer aerodynamic simulation.

UT-6 Trailer UnderTray System reduces Tractor/ Trailer drag by 12%.

- Minimizes drag associated with trailer underside components
- Compresses and accelerates incoming air flow and injecting high energy air into trailer wake
- Pulls high energy, attached air flow from the top of the trailer down into trailer wake

Application Performance



- CFD results using NASA's FUN3D within 1% of physical test results
- Access to Jaguar reduced single run times from 15 hours to less than 2 hours
- Stage set to do full Navier-Stokes-based optimization of large trucks

Competitiveness Impact

For BMI:

- Time from conception to manufacture reduced 50% (from 3 years to 1.5 years)
- Early-to- market advantage will result in earlier and greater revenue recognition

For BMI's customers

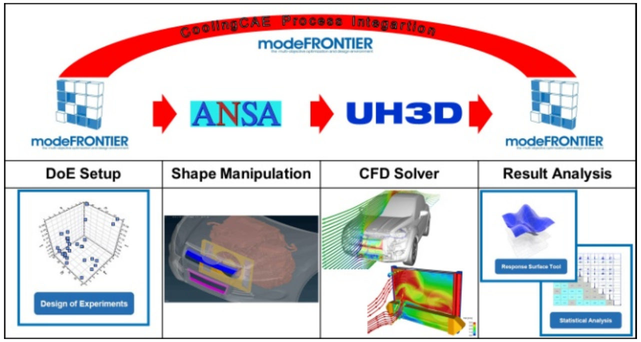
- Demonstrated fuel mileage improvements of 7% to 12% available 2011.
- Exceeds California CARB requirements.

Vehicle Engineering
Powertrain Cooling Optimization

Dr Burkhard Hupertz
Ford

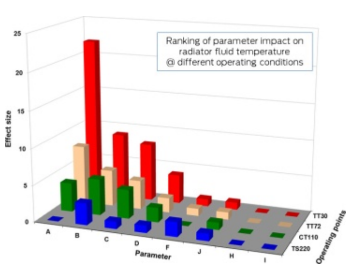
Science Objectives and Impact

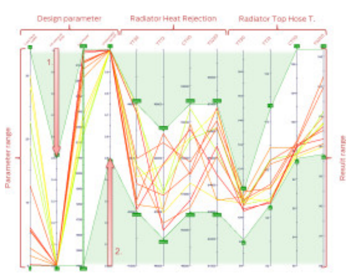
- Strategy: Develop a methodology to optimize the vehicle cooling package with respect to the cooling performance and the overall vehicle energy efficiency
- Driver: The continuous reduction of the fuel consumption of our vehicles is one of the key goals of the Ford product development team
- Objective: Develop an 3D CFD based optimization process which in an industrial environment enables the cooling package optimization while considering a large number of design parameters and several different vehicle operating conditions
- Impact: The new methodology will help to improve the energy efficiency and with that the fuel economy of our vehicles and in addition will enable a more cost and time efficient development process by reducing prototype testing

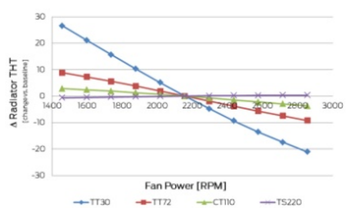


Process map of the analytical cooling package optimization process based on highly automated workflow management, sophisticated geometry morphing and full vehicle 3D CFD airflow analysis.

Application Performance







Statistical analysis of optimization results delivers an in depth understanding of the cooling system performance dependency on the design parameters and the parameter interactions.

Science Results

- Developed a new, efficient & automatic analytical cooling package optimization process running efficiently on large scale computer systems
- Running a cooling system optimization for the 1st time considering multiple objectives, a high number of design parameters and multiple vehicle operating conditions.
- Identify critical cooling system design parameters to deliver good cooling system performance and energy efficiency

Competitiveness Impact

- Deliver an industry leading analytical cooling system optimization process
- Enables development of more energy efficient cooling systems and with that helps to deliver even more fuel efficient vehicles to our customers
- New process will help to deliver more robust cooling pack concepts and with that enable further physical prototype and physical test reductions.

Computational Biomass Pyrolysis Consortium

Stuart Daw
Gavin Wiggins
Emilio Ramirez
Charles Finney

Argonne NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

OAK RIDGE National Laboratory

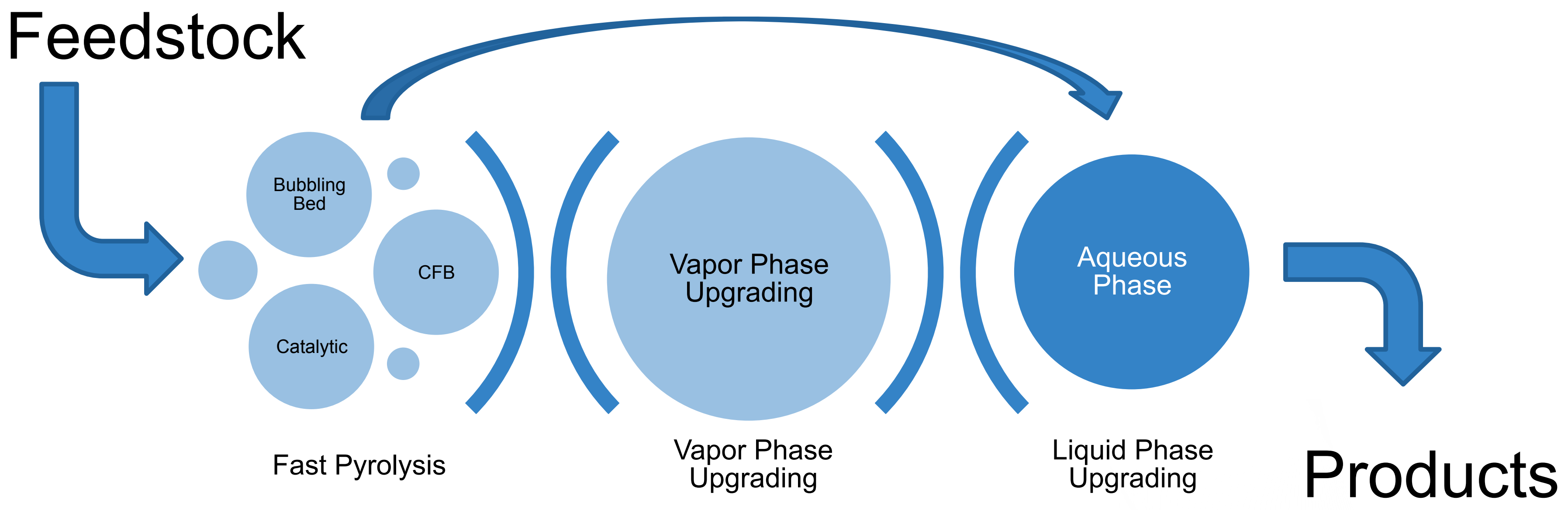
CPC

INL Idaho National Laboratory Operated by Battelle Energy Alliance

NREL NATIONAL RENEWABLE ENERGY LABORATORY

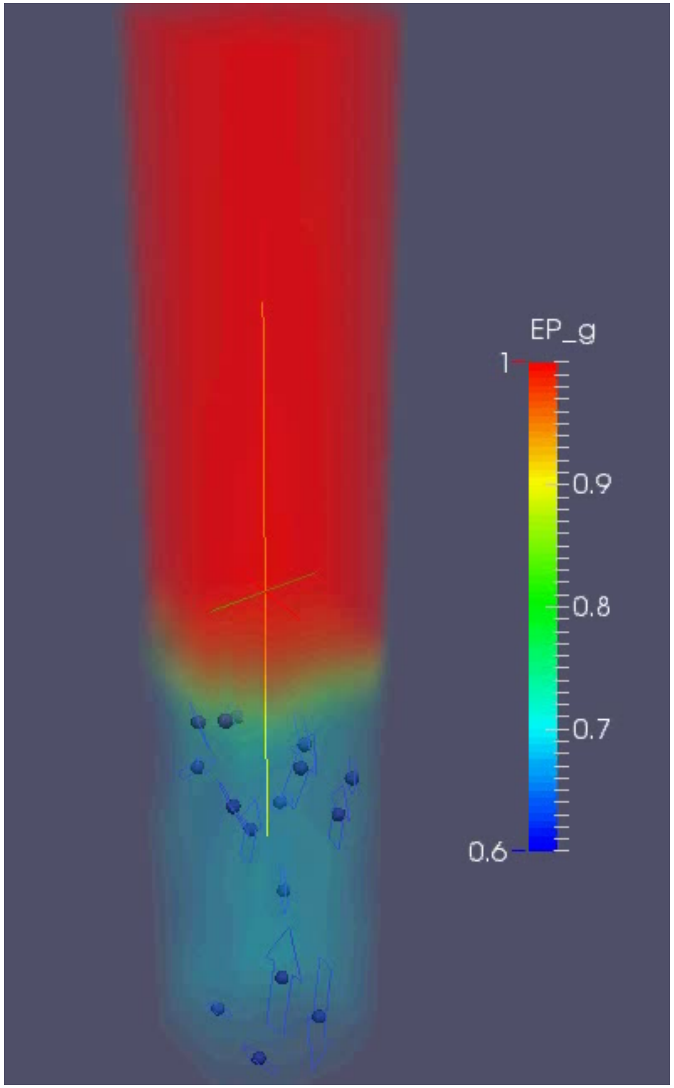
OAK RIDGE National Laboratory

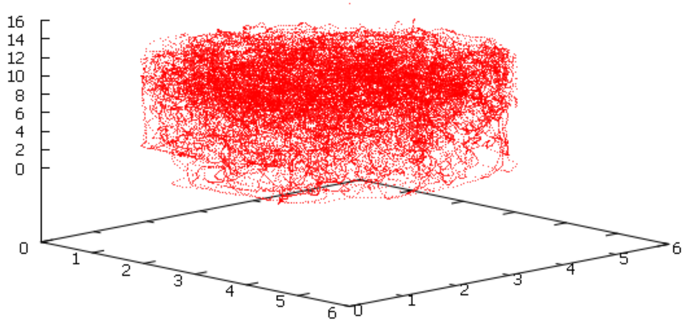
Process Diagram



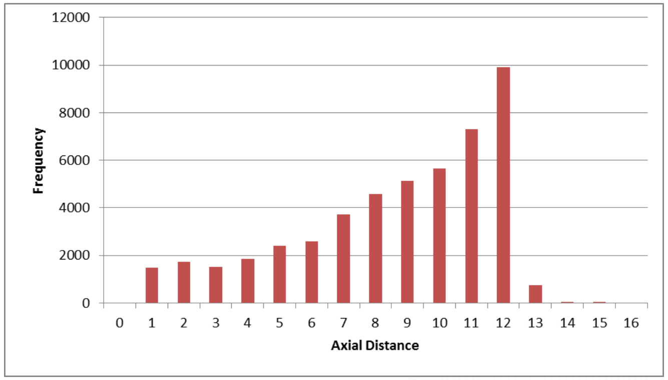
Objective: maximize (products); minimize (cost)

Biomass particles in a bubbling bed



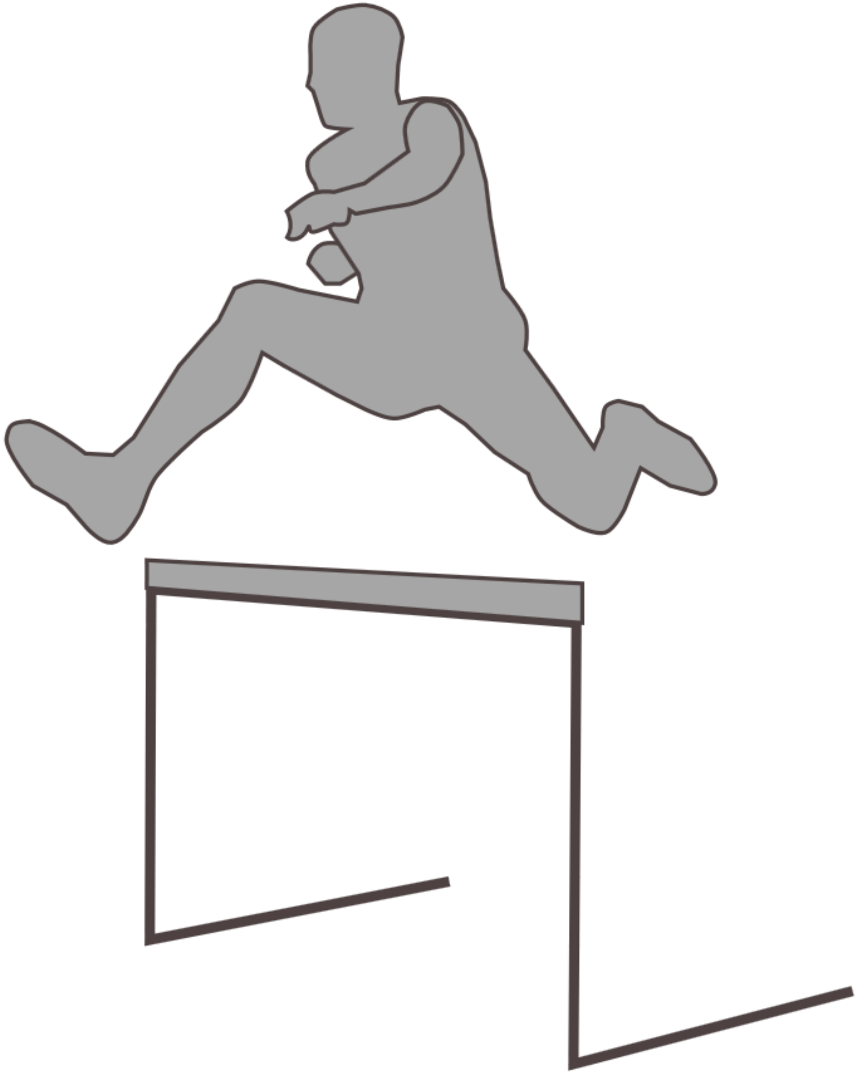


Spatial distribution of the biomass particle



Axial Frequency Distribution

Opportunities and Challenges



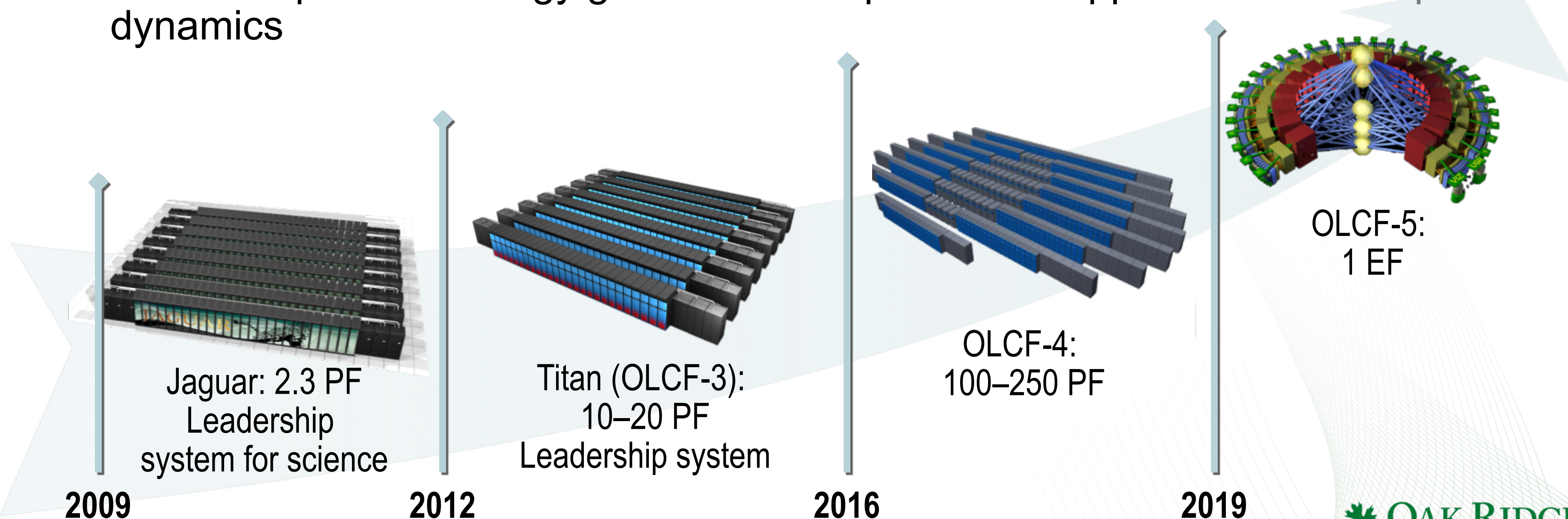
Exascale computational capability possible in this decade (ORNL Roadmap)

Mission: Deploy and operate the computational resources required to tackle global challenges

- Deliver transforming discoveries in climate, materials, biology, energy technologies, etc.
- Enabling investigation of otherwise inaccessible systems, from regional climate impacts to energy grid dynamics

Vision: Maximize scientific productivity and progress on largest scale computational problems

- World-class computational resources and specialized services for the most computationally intensive problems
- Stable hardware/software path of increasing scale to maximize productive applications development



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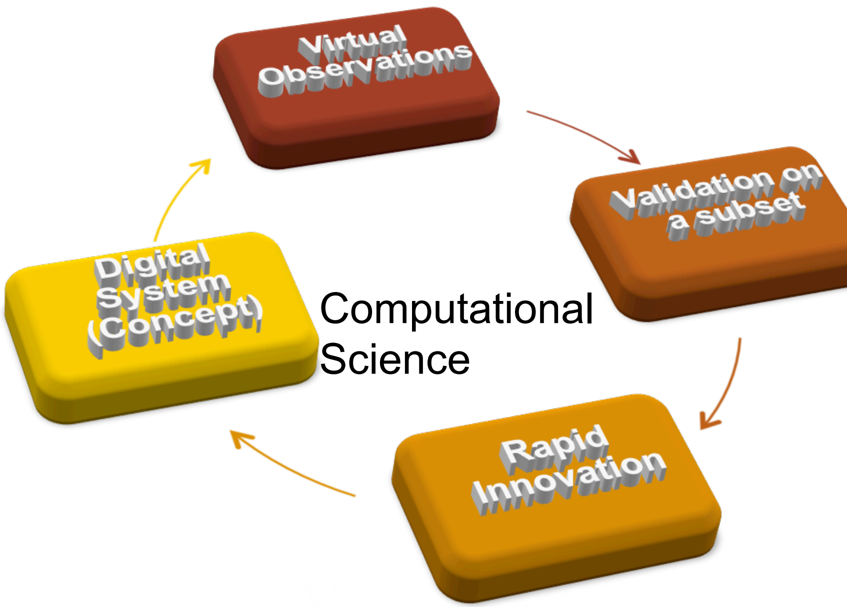
Slide adapted from Jack Wells

Opportunities

- Revolutionize the way simulation tools are used for sustainable transportation
- Develop new energy materials, devices, and vehicles through an integrated end-to-end solution
  - Most of the property-structure relationships are at the atomic and molecular scales
  - Most of the performance, safety, sustainability, and other considerations are at device and vehicle scales
  - Today the design process is totally decoupled – data is handed over from a group working at one scale to the other group at another scale in a sequential iterative process
- Develop feedback control systems to run devices in most optimal fashion

Computational Science Challenges

- Bringing a broad set of researchers working on materials and devices together to get their buy-in
  - Considerable investments are needed for software development and integration
- The future architectures are more conducive to locally coupled simulations
  - Many physical processes are globally coupled
  - Running multiple codes would need large and fast data movements across the processors/ cores
    - Need to have smart algorithms to overlap communications and computations
    - Minimize data movement
- Verification and Validation
  - Most validation is at steady state or subset of time-/space-trajectories
    - Very difficult to get all the data required to verify all the components of the simulations
    - Considerable investments need to be made in non-intrusive experimental techniques to obtain enough data
    - March towards the integration of "Theory, Experiment and Simulation" and Data?



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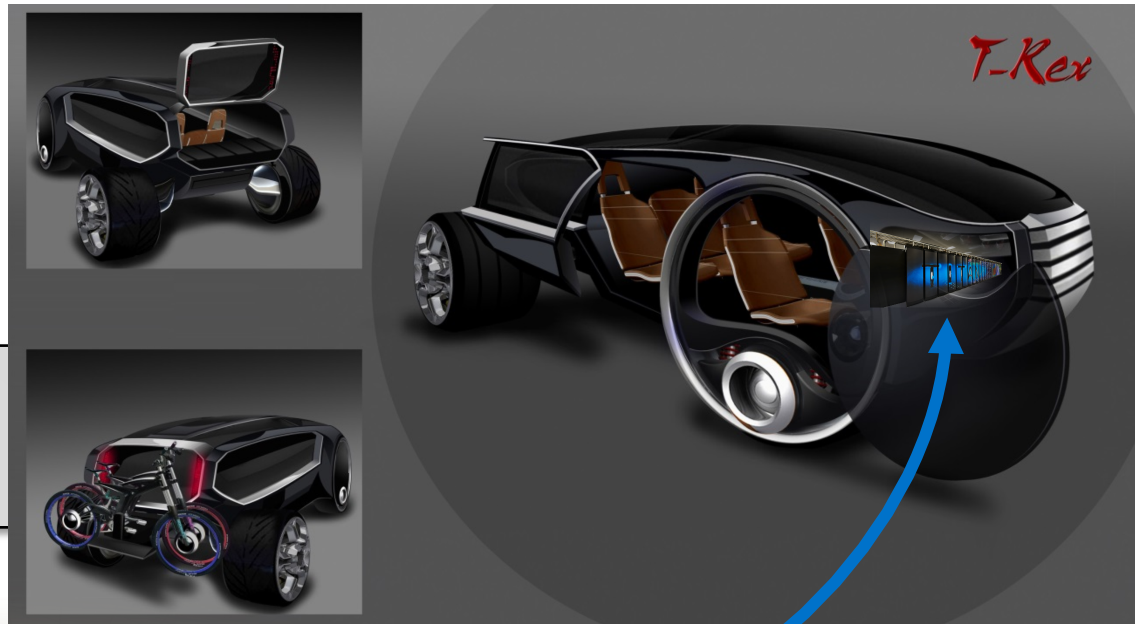
Summary

- Sustainable transportation is an urgent need in US and around the Globe!
- Integrated experiments and simulations at scale can revolutionize the design of transportation materials/fuels, devices, and vehicles
  - Cut down the current 4-10 year design cycle
  - Break cultural barriers
- Develop computations based feedback control systems to run devices in most optimal fashion
  - Adjust for fuels etc. online rather than offline adjustments with huge safety margins
  - Do not design the vehicles for the average person who does not exist in real-life
- Simulation science can and *has to* play a catalytic and important role in bringing innovation to sustainable transportation
  - Huge economic and societal impact

The end game is clean, efficient propulsion to move people and goods



Crowd-sourced?

3D-Printed?

HPC on the go! Autonomous, connected, comfortable, and efficient!

Picture from Local Motors

If you stretch your imagination?

Thank You!

OAK RIDGE National Laboratory