Future Development of CONVERGE: A Roadmap to Increasing the Predictive Capability of Engine Simulations

Daniel Lee, Ph.D.

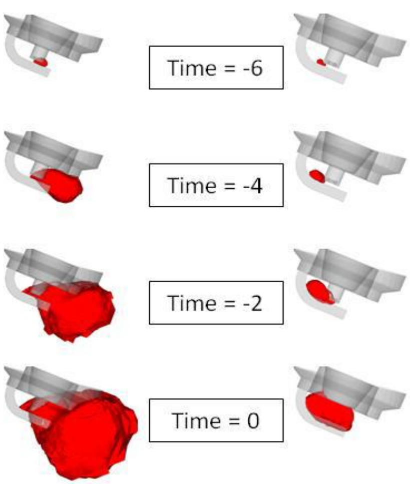
Convergent Science, Inc.

IDAJ CAE Solution Conference 2013

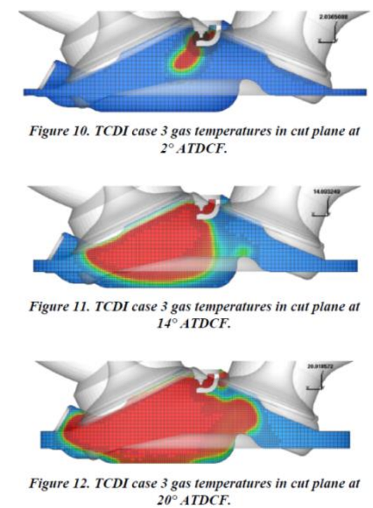
CONVERGE Conference Day

November 7th, 2013

Yokohama, Japan



Comparison of initial flame development from two different spark location
Courtesy Prometheus Applied Technology



Gasoline Combustion Modeling of Direct and Port-Fuel Injected Engines using a Reduced Chemical Mechanism

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...never make a mesh again

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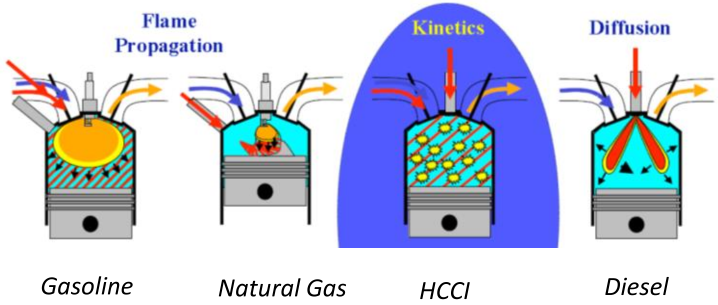
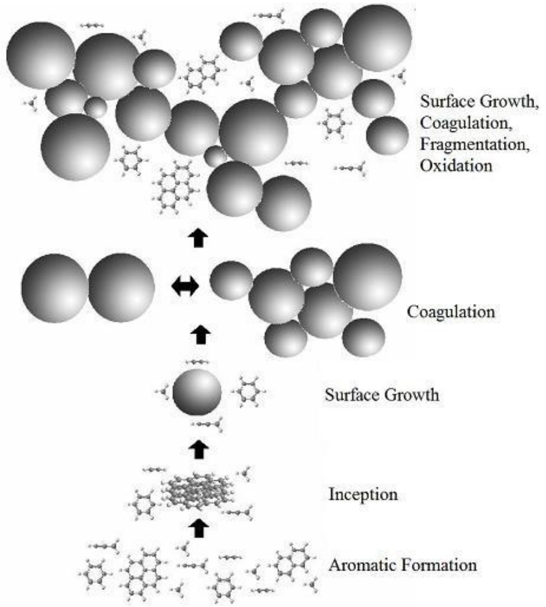
Overview of Presentation

- Company Overview
- Technology Overview
- Combustion Modeling
- Spray/nozzle modeling
- Emissions modeling
- Conjugate heat transfer





Convergent Science Inc. (CSI): Summary

- Founded in 1997, headquartered in suburbs of Madison, Wisconsin
- Experts in CFD flow, spray, combustion
- Developed CONVERGE CFD which is widely used in the automotive industry
- Rapidly growing and stable organization with many satisfied customers
- CSI currently has 40 employees and maintains distributors throughout the world
- Recently purchased a ~40,000 square foot office and will be relocating in early 2014
- Maintains a strong academic program with an installed base of over 50 universities
- Maintain strategic partnerships with thought leaders for technology improvement.
  - Lawrence Livermore, Argonne, Sandia, Oak Ridge, Sandia etc

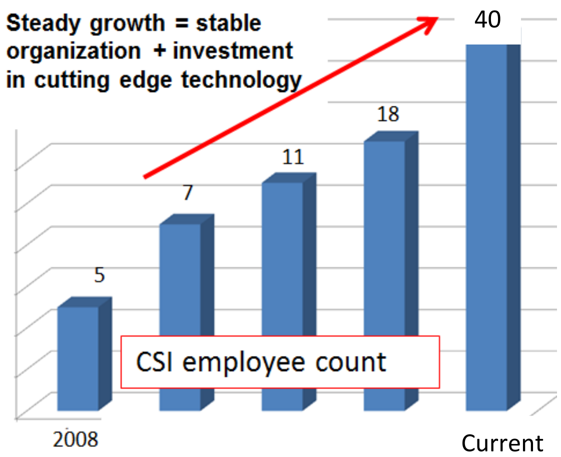
Lawrence Livermore National Laboratory

Argonne NATIONAL LABORATORY Transportation Technology R&D Center

OAK RIDGE National Laboratory

Current Convergent Science Inc. headquarters in Wisconsin USA

Future Convergent Science Inc. headquarters in Wisconsin USA



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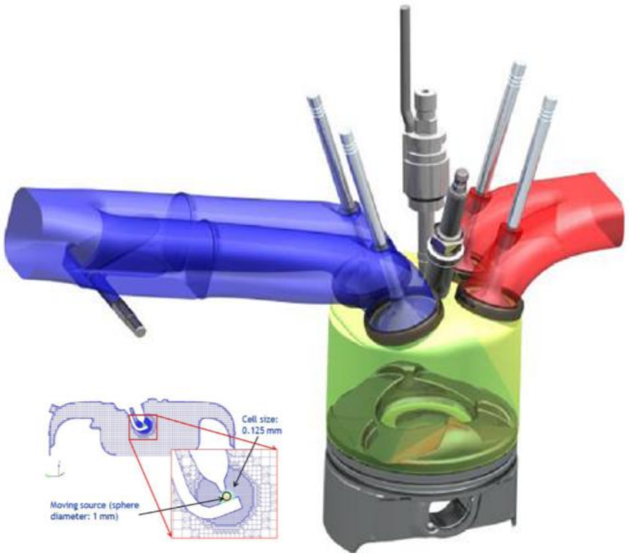
CONVERGE CFD Software

- CONVERGE CFD software was developed with the goal of increasing both productivity and accuracy for modeling flow, spray and combustion:
    - Generates a high quality mesh automatically at runtime thus eliminating all user meshing
    - Adds mesh refinement based upon gradients using adaptive mesh refinement (AMR)
    - Extensive parallel processing technologies for high performance computing
    - Rich suite of physical models for spray, combustion and turbulence
        - Lagrangian models include spray breakup, collision, coalescence and wall film
        - SAGE detailed chemistry solver
        - Extensive suite of RANS and LES models
        - State of the art suite of emissions models
- CONGO genetic algorithm included which automatically spawns CONVERGE simulations for optimization



Ignition and Combustion Simulations of Spray-Guided SIDI Engine using Arrhenius Combustion with Spark-Energy Deposition Model

SAE technical paper 2012-01-0147
Couresy General Motors

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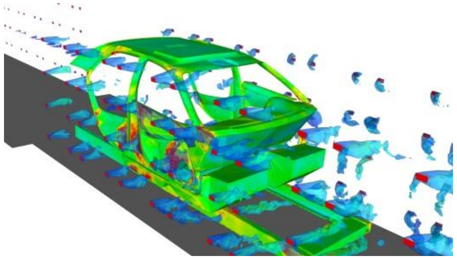
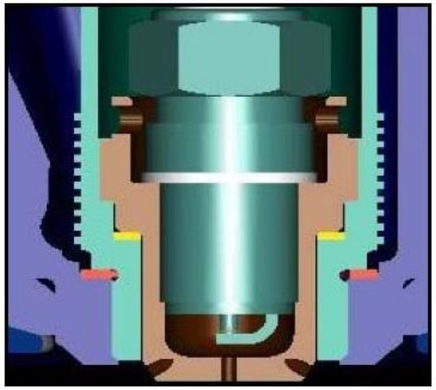
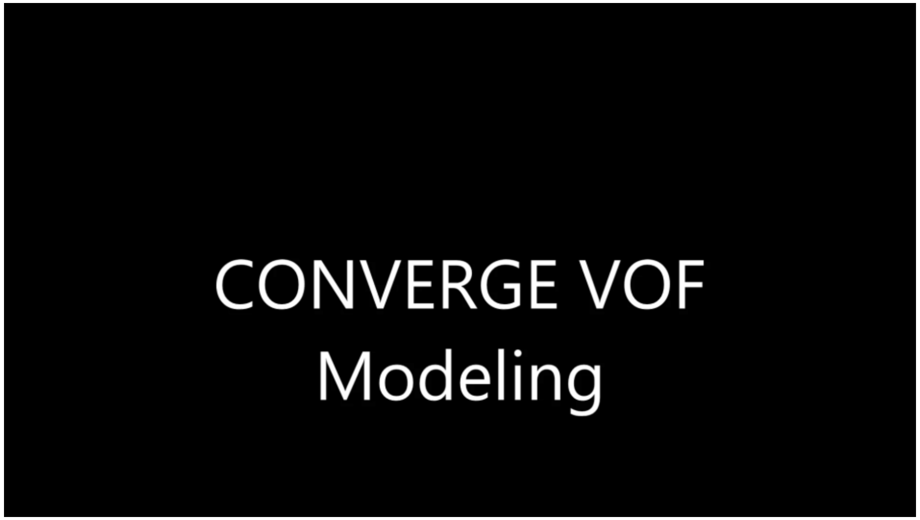
Spray combustor simulated with LES and detailed chemistry. All meshing 100% automated

CONVERGE Philosophy

- 100% eliminate all user meshing time
- Add more mesh resolution in key areas (Adaptive mesh refinement & embedding)
- Detailed chemistry with large mechanisms
- State of the art spray models
- State of the art turbulence models (LES)
- High performance computing
- Optimization (let the computer do the work whenever possible)
- Run more cycles and more cylinders whenever possible







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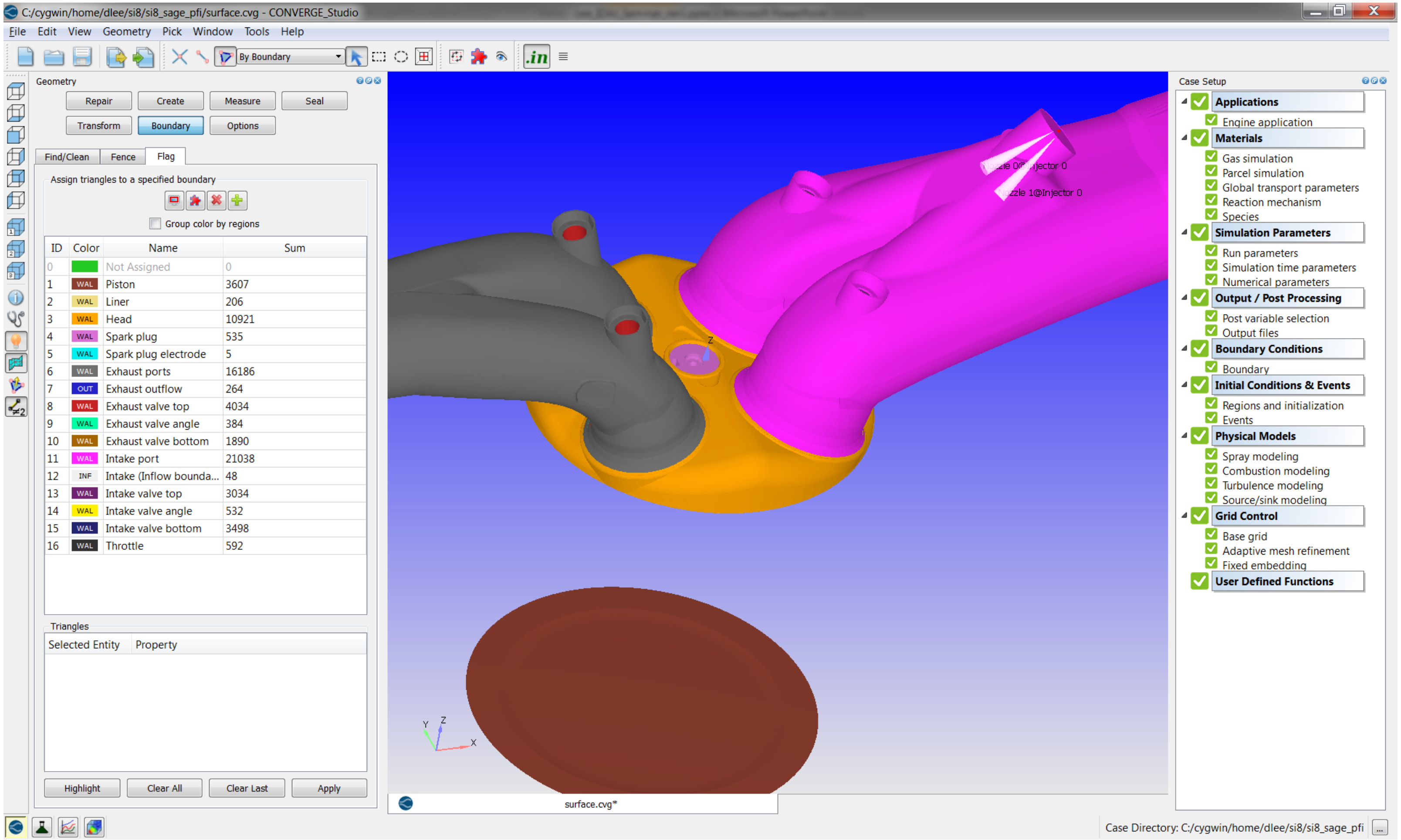
VOF modeling test case with moving components

CONVERGE Studio



- Full case setup (mesh, spray, combustion etc) with error checking
- Plotting utility
- Chemistry reduction environment
- Designed for quick and easy case setup

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Ensight Desktop for CONVERGE

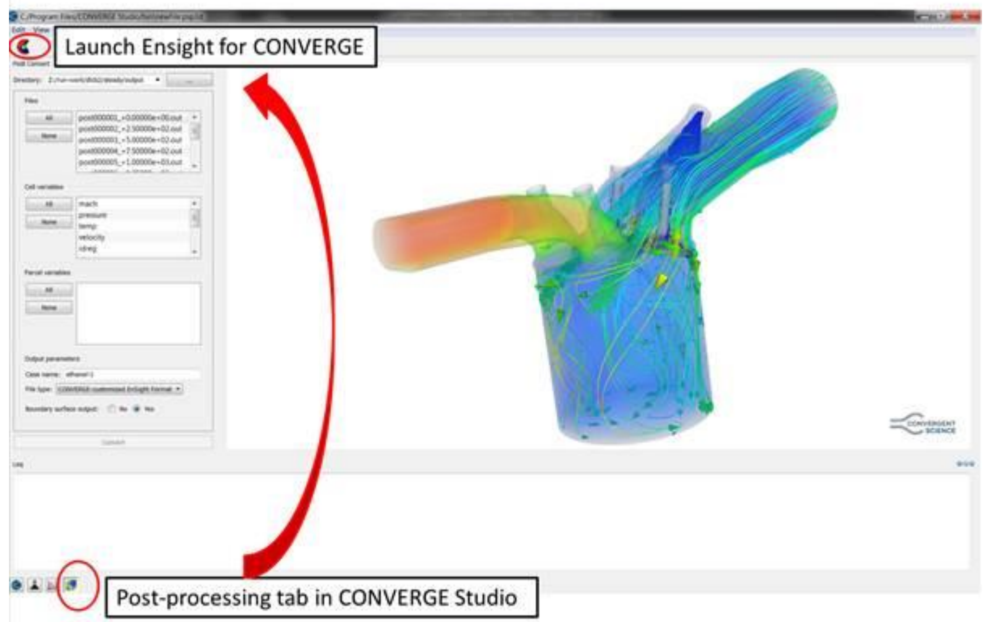
Convergent Science and Computational Engineering International (CEI) announce partnership to offer an integrated CFD visualization solution

July 15, 2013 – Convergent Science Inc. has announced that they have partnered with Computational Engineering International, Inc. to offer CEI's flagship product EnSight-Desktop fully integrated into CONVERGE™ Studio. CONVERGE™ Studio is the graphical user interface for the innovative CFD solver CONVERGE™.

Rob Kaczmarek, Director of Sales and Marketing at Convergent Science stated "*We are very pleased to partner with CEI to bundle EnSight-Desktop with CONVERGE™ Studio. Having CEI's post-processor integrated with CONVERGE™ Studio will offer our CFD users an industry leading option for visualizing their CONVERGE™ results.*"

Darin McKinnis, VP of Sales & Marketing at CEI Software commented "*EnSight has been used to post-process and visualize CONVERGE™ results for several years, but the past two years as our companies have worked more closely together we've made greater strides than ever in better serving CONVERGE™ users. We expect that progress to accelerate due to this partnership.*"

CONVERGE™ Studio allows users to cleanup geometries, setup cases, prepare chemical mechanism reduction, create plots, and post process all in one easy to use environment. With CONVERGE™ Studio getting from CAD to CFD just got even faster.



Ensight Desktop for CONVERGE now comes bundled as a standard feature of CONVERGE.

If the user prefers, other postprocessors can definitely be used as well.

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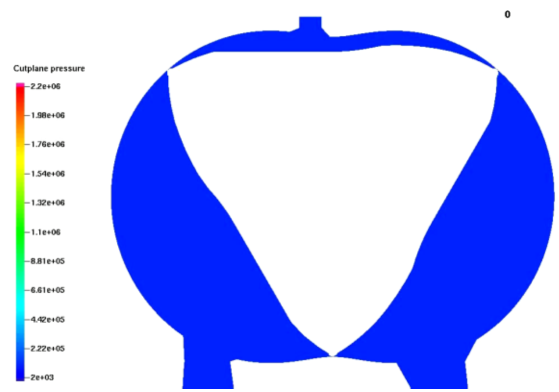
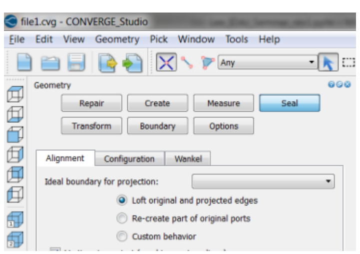
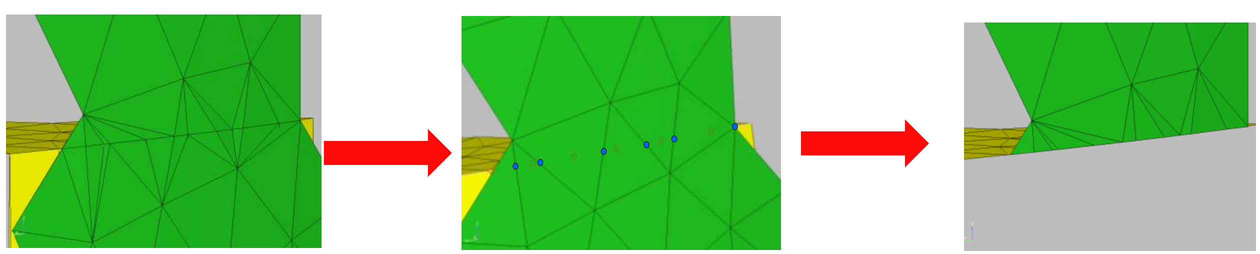
Sealing Feature

- In older versions of CONVERGE, moving components couldn't touch
- In v2.1, a sealing feature was introduced which eliminates this restriction
- The sealing feature automatically re-triangulates the surface during the simulation allowing surfaces to come into contact (i.e., "sealing")
- This feature is very useful for two stroke engine transfer ports as well as rotary engines
- Sealing capability can be set up in CONVERGE-Studio "sealing" tab



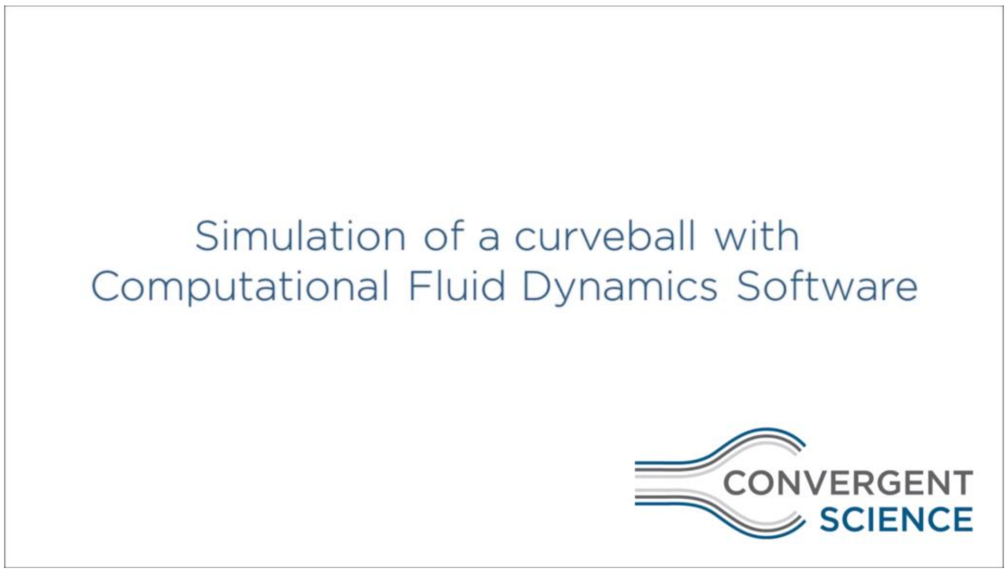
Two stroke (above) and rotary engine (left) simulations utilizing sealing feature



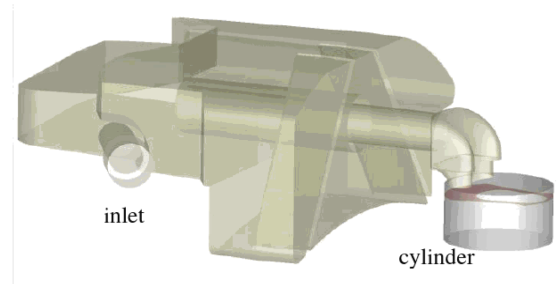


Fluid Structure Interaction

- With CONVERGE, moving body problems are easy to set up
  - Moving boundaries aren't a problem as new mesh is automatically generated every timestep so
- The motion of moving bodies is often specified (valves and pistons)
- A six degree of freedom (6-DOF) solver has been implemented for fluid structure interaction
  - The pressure and viscous forces are integrated to used to determine the motion of moving components
- The 6-DOF solver has many applications including valves and compressors



Fluid structure interaction in CONVERGE



(a)

Representative compressor geometry from "A Simplified Computational Fluid Dynamics Model for the Suction Process of Reciprocating Compressors"

$$I_1\dot{\omega}_1 + (I_3 - I_2)\omega_2\omega_3 = M_1$$
$$I_2\dot{\omega}_2 + (I_1 - I_3)\omega_3\omega_1 = M_2$$
$$I_3\dot{\omega}_3 + (I_2 - I_1)\omega_1\omega_2 = M_3$$

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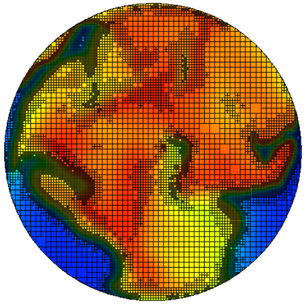
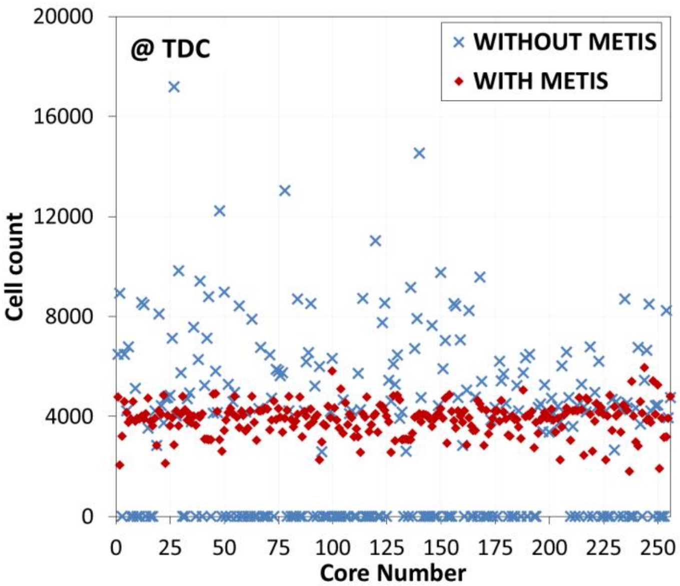
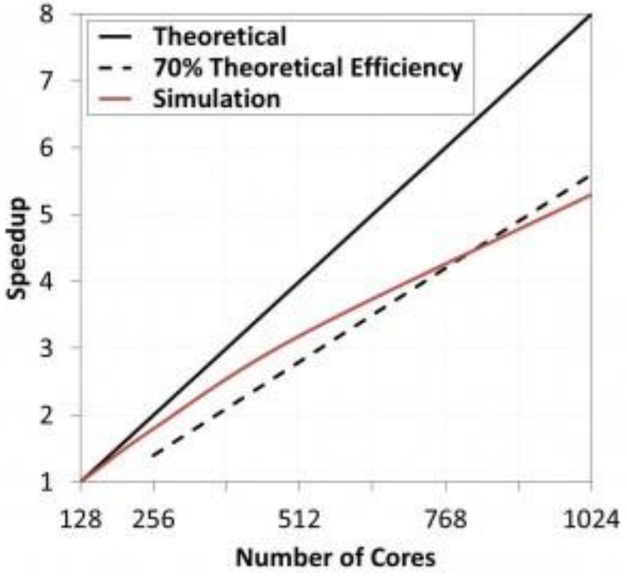
High Performance Computing

- CONVERGE is widely used in HPC
- SAGE parallelizes independently from the flow
- Dynamic load balancing is available
- METIS is now available which improves load balancing
- Load balancing improves with more cells and more chemistry





Significant improvement in load-balancing using METIS



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Collaboration with Caterpillar Inc. and Argonne National Laboratory

*Som et al. SAE 2013

Convergent Science in the News

The Science of Combustion

Achates Power uses CFD simulation and optimization to find the best opposed-piston engine design.

BY KENNETH WONG

Fabien Redon, VP of technology development at Achates Power (pronounced A-*kay*-tees), is currently prevented from revealing the recognizable commercial vehicle makers working with his company by confidentiality agreements. But if I want to get a sense of the energy and efficiency of his company's flagship products, opposed-piston engines (OPE), Redeon suggests that all I have to do is observe the stream of delivery trucks pulling in and out of large grocery chains.

Dubbed "An Engine That Uses One-Third Less Fuel" in *MIT Technology Review* (Jan. 14, 2013, TechnologyReview.com), Achates' engine bypasses the need for cylinder heads, "which are a major contributor to heat losses in conventional engines," according to the company. The OPE contains two pistons per cylinder, working in opposite reciprocating action. In a paper authored by Achates' staff, the company states that its opposed-piston, two-stroke diesel engine design "provides a step-function improvement in brake thermal efficiency compared to conventional engines while meeting the most stringent, mandated emissions requirements."

That significant advantage is one the reasons the trucking industry has been quick to adopt it. Other sectors deploying the same technology include military (for tanks), aerospace and marine ("Eight Companies Determined to Change Diesel Engines Forever," March 2012, *Diesel Power*, DieselPowerMag.com). Whereas Achates' clients rely on the company's OPE technology, Achates relies on CONVERGE Computational Fluid Dynamics (CFD), computer-aid flow simulation software, to study and perfect its engine design.

The Chemistry of Combustion

In the software the company was previously using, and in many other commercial codes available, using a combustion model including detailed chemical kinetic mechanisms wasn't an option, noted Rishikesh Venugopal, Achates' senior staff engineer. "CONVERGE is one of the earliest adopters of detailed chemistry," he adds. "It took too much time to simulate with detailed chemistry [in other software]. CONVERGE uses an automatic adaptive meshing technique, which lets us use not only detailed chemistry, but also reduces computing time."

Observing detailed chemical reactions in engine operations is important for Achates because the company is "not only trying to optimize engine performance but also emissions," says Venugopal. "Studying detailed chemistry reactions lets us understand, for instance, the oxidation of fuel through several reaction steps. If the chemistry is not detailed, then we can't capture the sensitivity of the emissions, such as nitrogen oxides and soot, when the engine's operating conditions change."

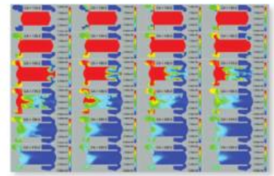
Adaptive Meshing

The simulation usually begins with a Pro/ENGINEER CAD model, converted into .STL format. Other than fixing a few triangulation problems that occur during the conversion process, Achates engineers seldom do any other additional work on the .STL model.

"We refined the process of developing the Pro/E model to make the .STL implementation into CONVERGE software easy," explains Redon. "It has taken us some time to refine that process to understand the characteristics of the Pro/E model we can readily use when converting to .STL."

"With CONVERGE, we don't need to clean up the .STL model as much as in other software," adds Rodrigo Zermeño, Achates' development engineer. "The automatic mesher takes care of the small features [details such as rounded corners, small holes and fasteners not needed for simulation]."

The adaptive mesher also makes the job easier by automatically using an appropriate degree of details for each region of the



To study the best possible configuration of its engine, Achates uses CONVERGE CFD software.

model. The software doesn't blindly apply fine meshes on the entire model, explains Venugopal. This method keeps the number of elements as low as possible, thus reducing computing time during simulation.

Known and Unknown

From experience and years of R&D, Achates has developed fairly accurate engine combustion data, such as the inside temperature of the engine walls — critical for calculating heat transfer in digital simulation. For the rest of the data needed for simulation, engineering judgment has to be used, Venugopal says

"Take, for instance, the spray characteristics," Venugopal continues. "It requires very detailed breakup time-scale and droplet-dynamics related constants, which cannot easily be measured." For those, Achates relies on real-world tests conducted with fuel injectors in its state-of-the-art fuel lab to obtain the right approximations. "Physical lab tests guiding simulation" is the only way to remove uncertainties, Venugopal says.

Finding the Best Way to Combust

The purpose of simulating the engine is to "optimize combustion," Redon says. "We have so many combinations we can lay out our engine. So it's critical to use simulation tools to study the options we have."

During simulation of the engine scavenging process, Achates encountered a scenario the software couldn't faithfully replicate. The OPE has two sets of ports: one set for exhaust, another set for the intake.

"In an opposed-piston two-stroke diesel engine, the areas of the ports change as the pistons move past them, and this is a geometric feature that CONVERGE initially couldn't capture," explains Redon.

As robust as the software is, "when you have very thin regions with high-pressure flows, it's difficult to simulate the event in a mathematically stable manner," Venugopal says. So, in collaboration with CONVERGE, Achates engineers came up with a workaround. They shrank the pistons' diameter by 0.1% and added a thin layer of cells — called liner gaps — between the ports and the pistons. This allowed the fluid motion to occur.

"Using the disconnect triangle feature [in the software] and the liner gaps, we were able to simulate where the flow was occurring and where it was blocked when the ports were uncovered by the pistons," says Venugopal. "That was significant because we were able to observe the gas exchange happening in the open-cycle scavenging."

The workaround didn't compromise the fidelity of the simulation, but it did require diligent monitoring of the process, notes Venugopal. "We had to use two sets of geometry — with liner gaps, and without. So we couldn't run the entire scavenging cycle as one cycle. We split it into two simulations," he said. "We had to use good bookkeeping to make sure we were using the right geometry for the right phase."

This workaround is no longer needed because CONVERGE CFD now has a sealing feature that resolves the issue, according to Rob Kaczmarek, director of sales and marketing, CONVERGE.

Injection Innovation

The use of optimization driven by CONVERGE software's genetic algorithm (GA) has allowed Achates to find the best configuration of injectors, among others.

"Even though the solution was what we anticipated and it made sense, we also saw how far we could push it," Venugopal reflects. "It also showed that, even as we were pushing the design's limits, the engine was still giving good performance."

In keeping with its biological metaphor, the GA optimization begins with a set number of design options, and then spawn a greater number by varying different parameters.

"In one such GA run, I believe we ran about 200 to 300 designs before arriving at the desired solution," Venugopal recalls. "But the software wasn't running all [parameter] combinations at all times; it was only running those that were favorable, so it didn't waste time."

Achates uses a Linux cluster and Windows cluster to run the software. For optimization jobs, Achates relies on the Linux cluster because, Venugopal explained, the code is deeply rooted in the Linux environment, as it's often the case with combustion CFD codes. At Achates, a typical combustion simulation involves 100,000 to 200,000 elements, running on eight to 16 CPU cores. In larger jobs, it could involve a few million cells, running on 32 cores. The jobs can take anywhere from eight hours to five days.

"CONVERGE possesses extensive technologies to minimize the runtimes on high-performance computing platforms," says Kaczmarek. The company is also working with Lawrence Livermore National Laboratory, Cummins Inc., Indiana University and NVIDIA, and will be releasing CONVERGE with GPU

The design of Achates' opposed-piston engine in a rendered 3D model.

support later this year, he adds.

"Keep in mind that, after a certain number of cores, the performance benefits are no longer proportional to the number of cores you add because there'll be increased chatter," notes Venugopal, referring to communication between cores. "So it's really about balancing the number of licenses you have, the cores, and the job. We tried to take into account all these factors."

CONVERGE CFD's licensing policy is multicore-friendly, he says.

Reality and Simulation

"Our engine technology is much more complicated than conventional engines, so some of our strategies cannot be applied blindly," says Achates' Redon. "It's very important to anchor simulation in physical tests."

CONVERGE's Kaczmarek agrees: "While it's our goal to provide our customers with the most advanced CFD tools on the market, it's important to remember that simulation and validation must always coexist."

As the use of simulation gains popularity, there's a risk that designers might place unwarranted trust in simulation results. Achates' philosophy — always make sure simulation stays close to the physical response of the engine — serves as a good reminder not to lose touch with reality. DE

Kenneth Wong *is Desktop Engineering's resident blogger and senior editor. Email him at kennethwong@deskeng.com or share your thoughts on this article at deskeng.com/facebook.*

INFO → Achates Power: AchatesPower.com

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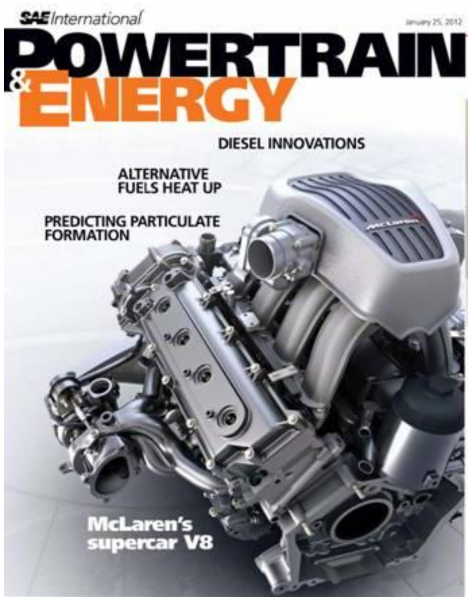
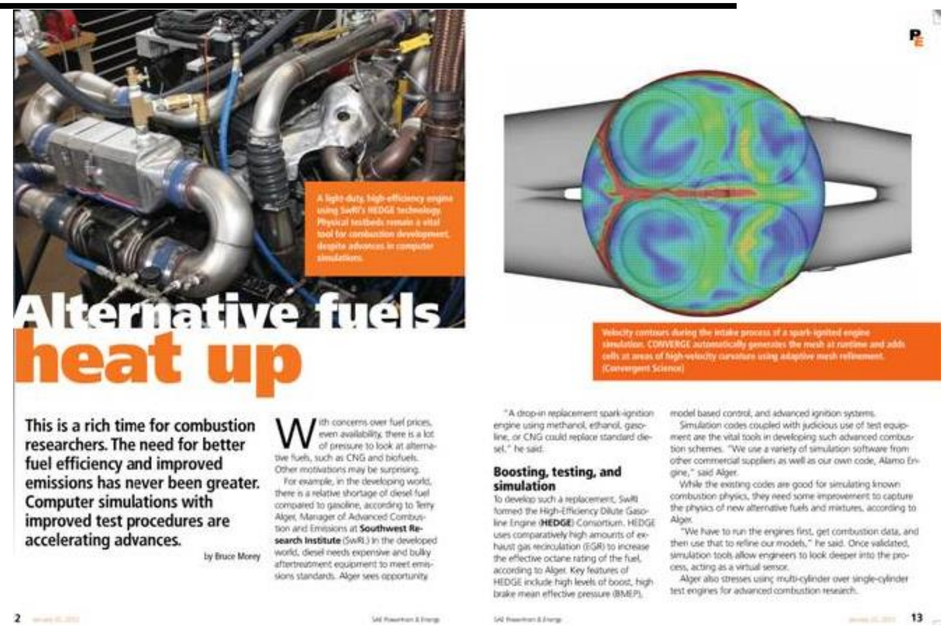
CONVERGENT SCIENCE

CONVERGE and CONGO used by Achates Power to design a two stroke opposed piston Diesel engine

Convergent Science in the News

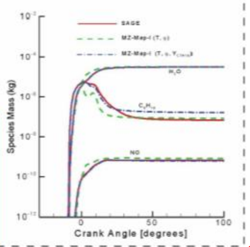




CONVERGE used for alternative fuel research

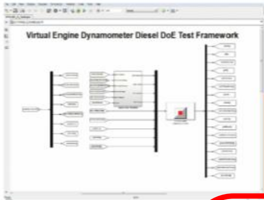
CONVERGENT SCIENCE

Convergent Science in the News



Comparisons of traditional and fast approximations that reduce computational load show close agreement. Such methods are reducing the trade-off between speed and accuracy in emissions predictions. (Convergent Science)

describes V-SIM as a parametric model constructed in MATLAB/Simulink or EASY5. Some see a trend in this. "Until recently, engineers tended to optimize individual components, integrate them, and then expect them to work," explained Wensi Jin to *SOHE*. He is the Automotive Industry Manager for **MathWorks**, the company that supplies MATLAB/Simulink products used in many simulations such as V-SIM. "Now, engineers are working more toward optimizing the system as a whole, using system models with 'reduced level of detail' but more completeness to understand system trade-offs," he said. While hybridization is forcing this in the light-duty sector, he believes the new emissions standards are driving system optimization in the off-highway industry. "Software is driving practically every component now. Not only do you have an engine control but a fuel system control, a DPF control, and an SCR control. So, these individual controls have to be brought together in order to have a system-level design that is truly optimal," said Jin.



A diesel engine virtual dynamometer test framework for Design of Experiments illustrates how system calibration work is migrating to simulation. (MathWorks)

CAE is helping in other ways. Jin is observing a tendency toward doing powertrain system calibration much earlier in the development, even to the point of getting a first pass calibration using CAE-modeled data rather than experimental data. "There are still questions about tools, accuracy, and computational power, but in a number of areas we have seen 'no touch' calibration. That is, using CAE to generate calibration values that eventually went into production without any physical calibration," he stated, noting these were in component parts of powertrains, such as an air intake system.

Back to fundamentals—controlling engine-out emissions

Simulating the combustion process inside a cylinder means creating a complex model of combined CFD and reacting kinematic chemistry. Improving simulations at this stage will provide more insight and, possibly, reduce development cost. "Everything with CFD is a balance between accuracy and practical limits on runtime," explained Dr. Daniel Lee, Director of Business Development of **Convergent Sciences**.

CAE providers such as Lee's company are tackling these practical limits, reducing runtimes and improving accuracy by

eliminating sources of error. One well-known source is poor computational meshes. His company's software, CONVERGE, reduces mesh-induced error through orthogonal and stationary cells, which he claims as being optimal. The software also automatically refines the mesh in key areas using adaptive mesh refinement. They also use improved meshing methods that produce stable answers while the grid is refining, something he calls "grid convergence."

Beyond the mesh, of course, is getting the physics right "with as little empirical input as possible," explained Lee. This means modeling the charge preparation correctly, the CFD modeling of the spray, and a good combustion model. Since actual fuels are composed of many thousands of species, calculating the reactions within each computational cell is

Digital engineering for Tier 4

by Bruce Morey

While engines such as this EcoMaxT4 Tier 4 will meet the rigorous emissions standards, the next round of development will focus on balancing attributes with an eye toward future regulations. (Ricardo)

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October 11, 2012

CONVERGE used for emissions modeling

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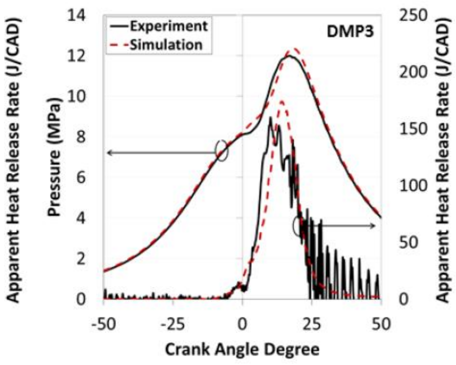
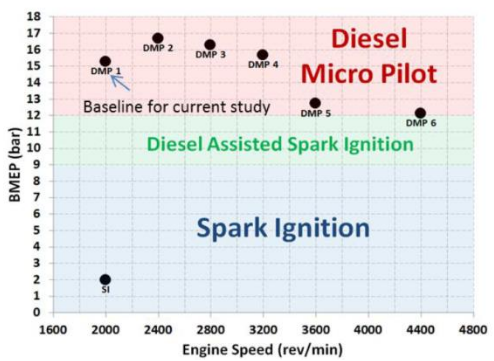
ASME Fall Technical Conference

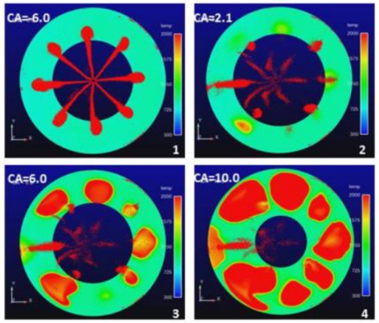
• At the ASME 2013 IC Engine Conference (October 2013), there were 13 technical papers presented which utilized CONVERGE CFD Software

• Authors include: Cameron Compression Systems, Argonne National Lab, Caterpillar, Sandia National Lab, Chrysler Group LLC, General Motors, University of Perugia Italy, Mississippi State University, Carnegie Melon University, Cummins

• Topics covered a wide range including: Large bore natural gas combustion modeling, nozzle flow and cavitation, bio-diesel chemical kinetics, Diesel combustion, Diesel micro Pilot ignited DI Gasoline Engine modeling, spark ignited thermal load prediction, RANS vs LES modeling for IC engine flows, LES spray modeling, HCCI combustion







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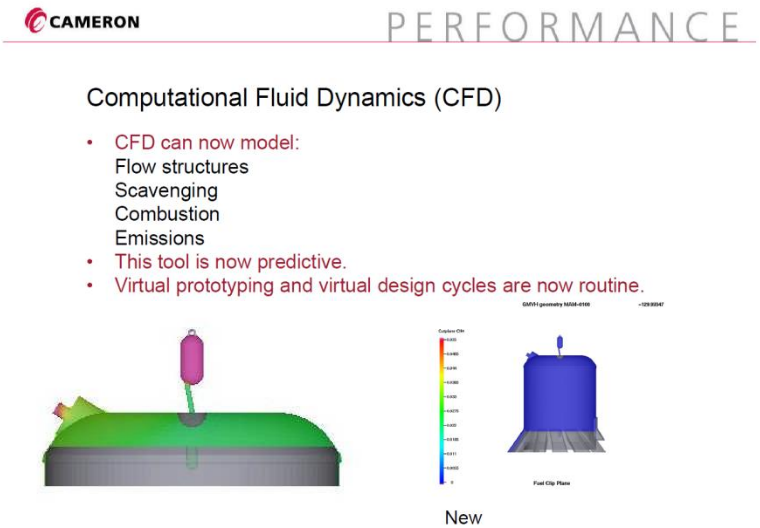
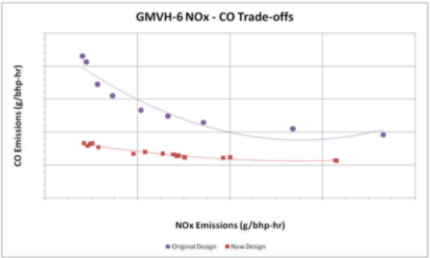
http://asmeconferences.org/ICEF2013

Natural Gas Engine Simulations

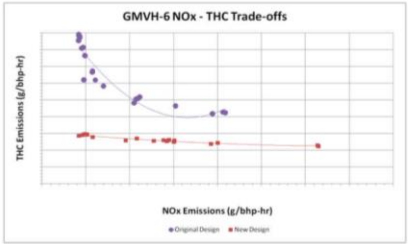


http://www.gaselectricpartnership.com/HCAMERON021213.pdf

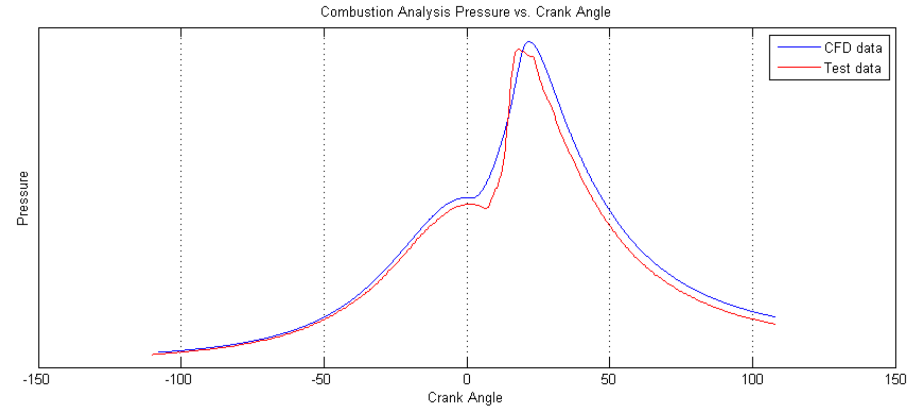
NO$_x$ and CO Emissions

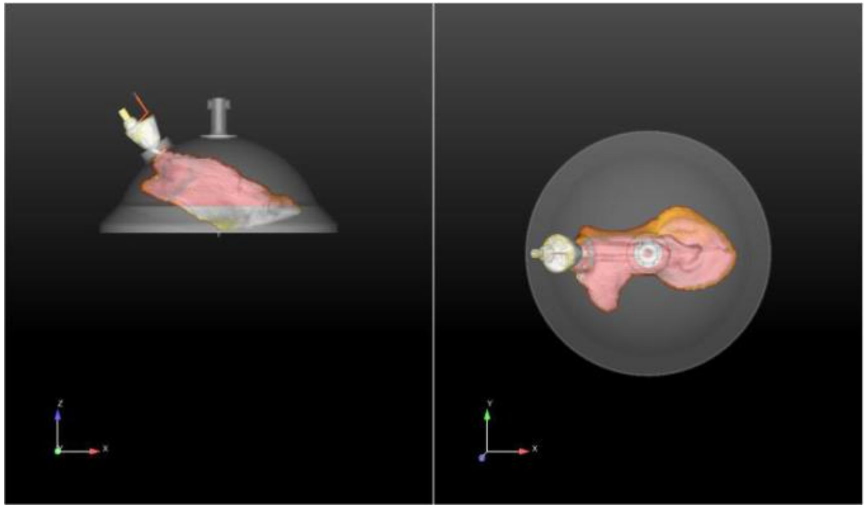


Unburned Hydrocarbon Emissions



CONVERGE is used for modeling natural gas engines

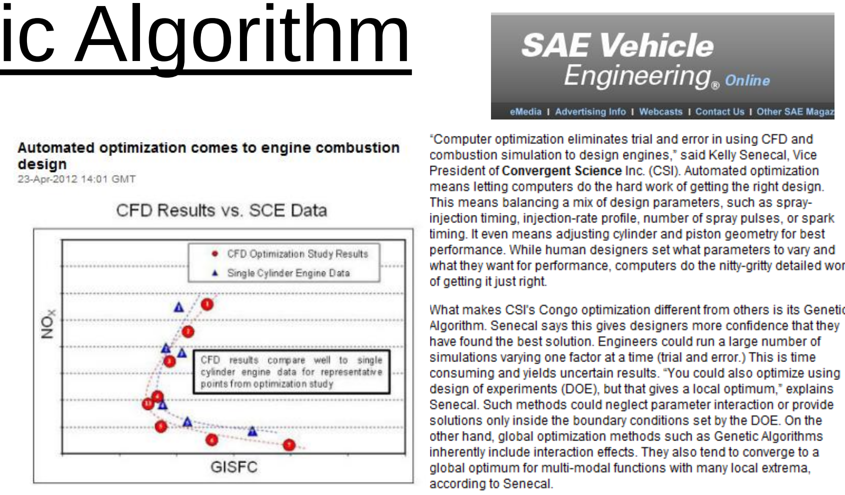




Pressure trace (top) and flame location for large bore natural gas engine
VIRTUAL DESIGN OF AN INDUSTRIAL, LARGE-BORE, SPARK-IGNITED, NATURAL GAS, INTERNAL COMBUSTION ENGINE FOR REDUCTION OF REGULATED POLLUTANT EMISSIONS ICEF2013-19138

CONVERGENT SCIENCE

CONGO Genetic Algorithm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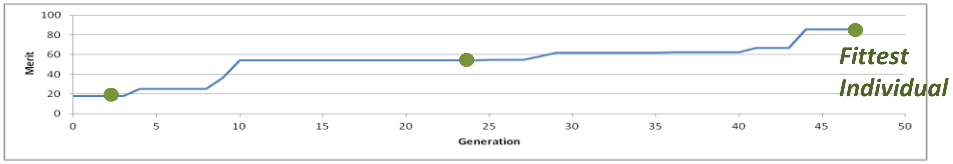
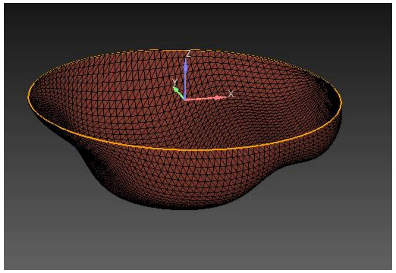
Automated optimization comes to engine combustion design
23-Apr-2012 14:01 GMT

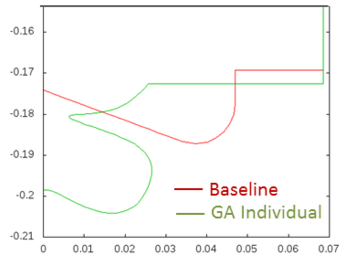
"Computer optimization eliminates trial and error in using CFD and combustion simulation to design engines," said Kelly Senecal, Vice President of **Convergent Science** Inc. (CSI). Automated optimization means letting computers do the hard work of getting the right design. This means balancing a mix of design parameters, such as spray-injection timing, injection-rate profile, number of spray pulses, or spark timing. It even means adjusting cylinder and piston geometry for best performance. While human designers set what parameters to vary and what they want for performance, computers do the nitty-gritty detailed work of getting it just right.

What makes CSI's Congo optimization different from others is its Genetic Algorithm. Senecal says this gives designers more confidence that they have found the best solution. Engineers could run a large number of simulations varying one factor at a time (trial and error.) This is time consuming and yields uncertain results. "You could also optimize using design of experiments (DOE), but that gives a local optimum," explains Senecal. Such methods could neglect parameter interaction or provide solutions only inside the boundary conditions set by the DOE. On the other hand, global optimization methods such as Genetic Algorithms inherently include interaction effects. They also tend to converge to a global optimum for multi-modal functions with many local extrema, according to Senecal.

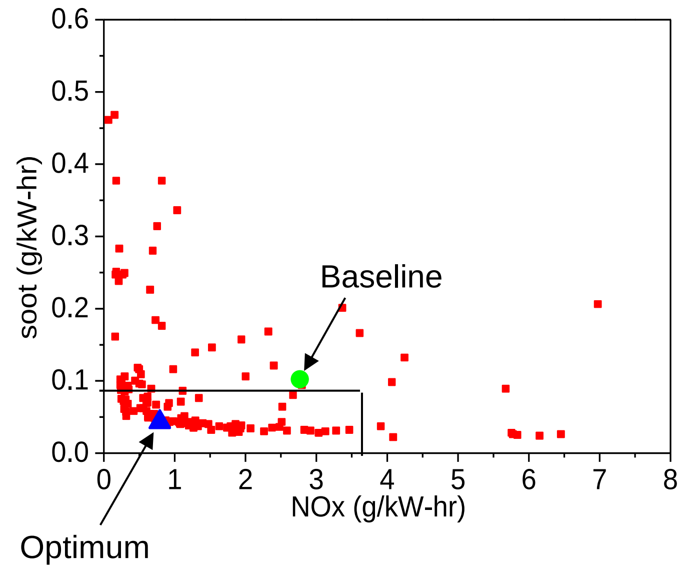
- CONVERGE has an on-board genetic algorithm called CONGO which takes a "survival of the fittest" approach to optimize a design
- A merit function (e.g., a combination of NOx, soot and fuel consumption) is defined to rate the fitness of each design – this is what CONGO will optimize
- The variables CONGO can vary is specified by the user.
- Number of processors and the total search time are specified
- CONGO initiates a population of designs automatically searching for the one which optimizes the merit function
- Optimization of input parameters and geometry is possible







Piston optimization study



Example GA Results

CONVERGENT SCIENCE

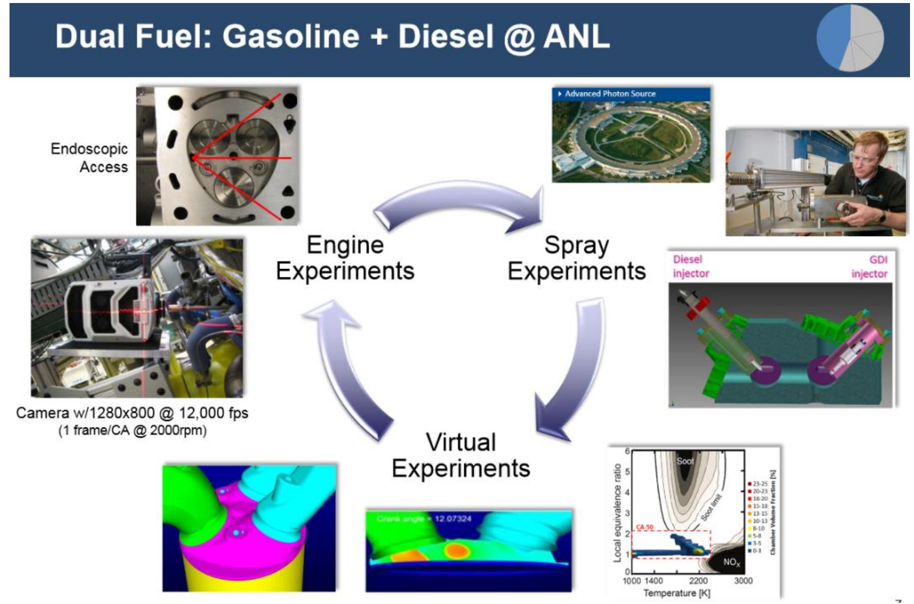
Use CONGO and let your cluster find the optimum design

CONGO Genetic Algorithm

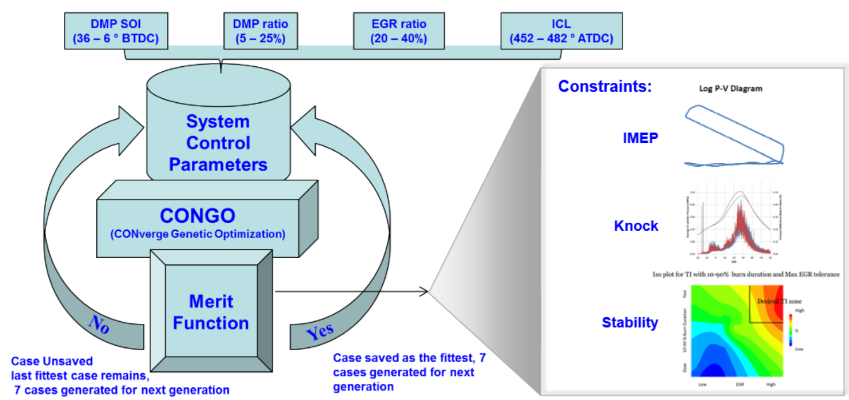
CHRYSLER

A MultiAir / MultiFuel Approach to Enhancing Engine System Efficiency

Chrysler (PI): Ronald A. Reese, II
DOE Technology Development Manager: Ken Howden
DOE NETL Project Officer: Ralph Nine



- Objective is to improve engine efficiency AND improve control robustness
- Includes both the DASI transition mode and the DMP mode
- Approach outlined below is underway, and will be verified *via* engine test



11

Use CONGO and let your cluster find the optimum design

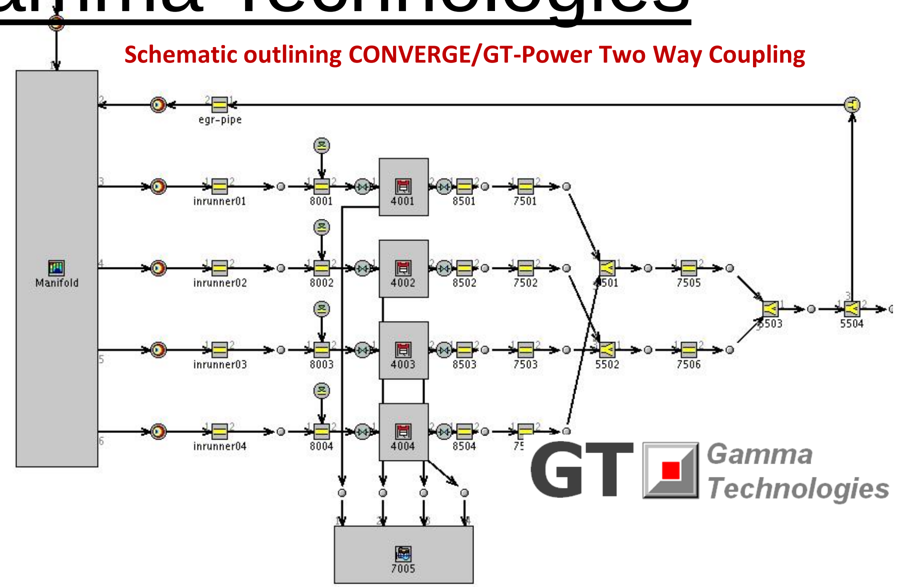
CONVERGENT SCIENCE

http://www4.eere.energy.gov/vehiclesandfuels/resources/merit-review/sites/default/files/ace062_reese_2013_o.pdf

Collaboration with Gamma Technologies

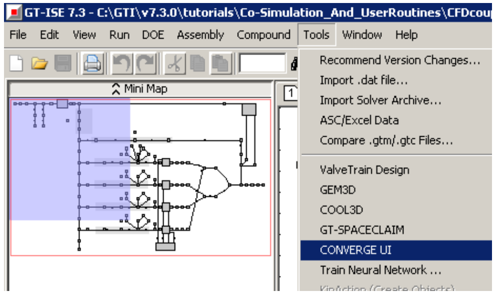
- GT-Power is commonly used to generate boundary conditions for CONVERGE simulations
- Historically, the coupling with GT-Power was done in a “one way” fashion (CONVERGE influenced by GT-Power only)
- Through a recent collaboration with Gamma Technologies, two way interactive coupling with GT-POWER is now possible.
- Running GT-Power with CONVERGE can be used to more accurately simulate multiple cycles and multiple cylinders
- A limited version of CONVERGE called CONVERGE-Lite is embedded into GT-SUITE

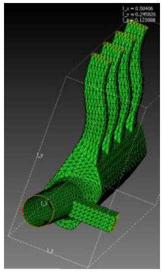
Schematic outlining CONVERGE/GT-Power Two Way Coupling



GTLINK
- Full GT-SUITE model, with in-cylinder CFD performed with CONVERGE
- With all CONVERGE features and models
- Good for in-cylinder 3D simulations

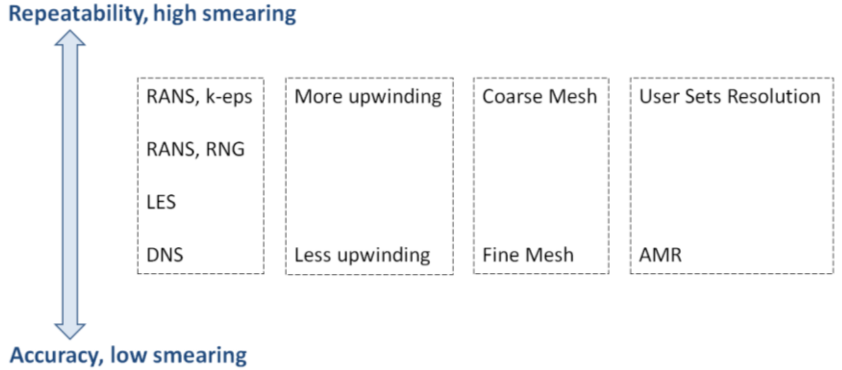
CONVERGE-Lite
- Simplified version of CONVERGE embedded within GT-SUITE
- Limited CONVERGE features and models
- Good for intake/exhaust manifold 3D simulations



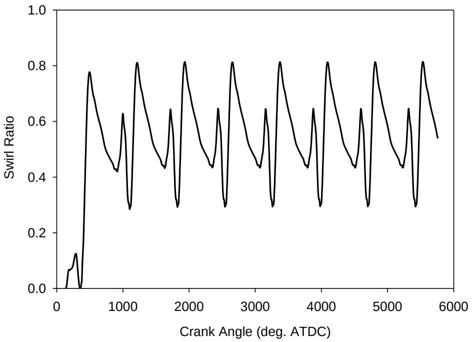


Accuracy vs Repeatability

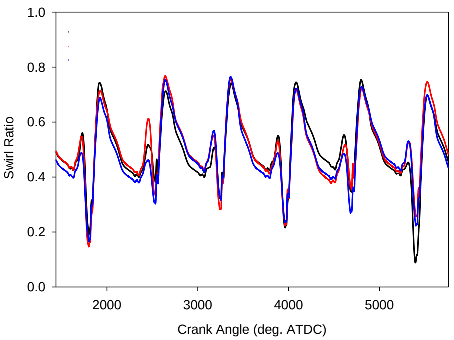
- Running multiple cylinders and multiple cycles to study cycle to cycle variations is becoming very common with CONVERGE
  - Very important for GDI engines
  - Auto-ignition studies
- This brings up an important tradeoff between repeatability and accuracy
  - Repeatable results require fewer cycles, yet missed important phenomena
  - Accurate results require more cycles to be run
- For repeatable results, smearing is desirable which is promoted by: course mesh, upwinding, large timesteps
- Accurate results can be promoted by using smaller cells, smaller timesteps and central differencing.
- CONVERGE can be run in either mode: highly accurate (recommended) or repeatable
  - For repeatable results, disable AMR, use a course mesh, upwinding and constant dt
  - For accurate results, enable AMR, variable dt and central differencing



All combinations of the above can be run in CONVERGE, depending on the user's desire for more repeatability or more accuracy

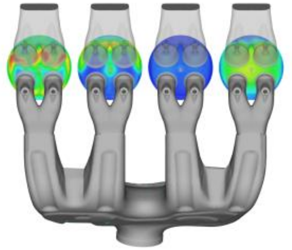


Repeatable solution (no cycle to cycle variations)



Accurate solution showing cycle variations

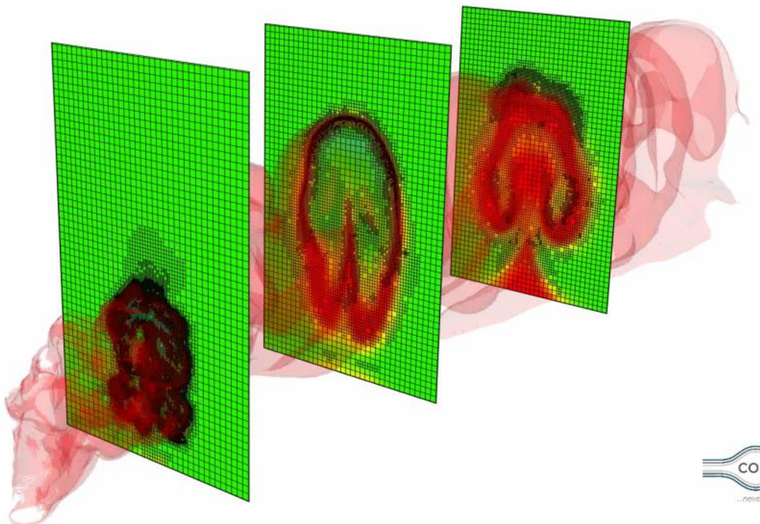
CONVERGENT SCIENCE

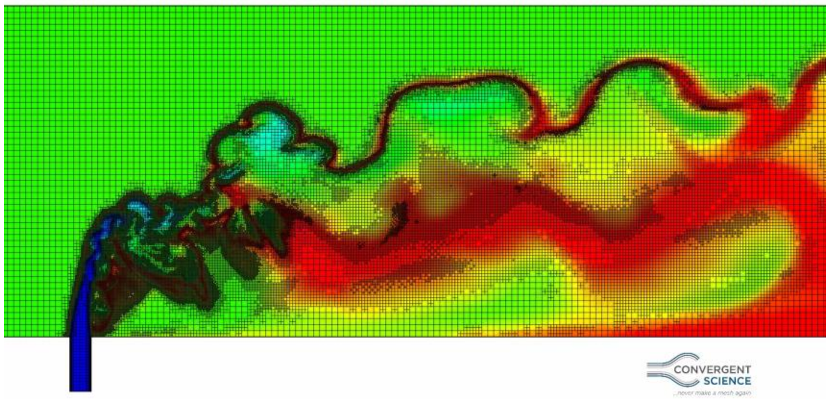


Multiple cylinder simulation: Courtesy Chrysler

Overview of Presentation

- Company Overview
- Technology Overview
- Combustion Modeling
- Spray modeling
- Optimization



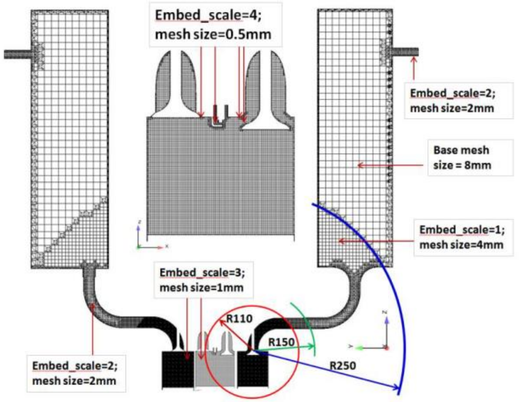


Jet in crossflow detailed chemistry simulation

CONVERGE Combustion Modeling Overview

- CONVERGE has extensive modeling capabilities for the combustion phenomena:
    - Ignition modeling
    - Knock modeling
    - Mixing-controlled combustion
    - Flame propagation
    - Emissions formation

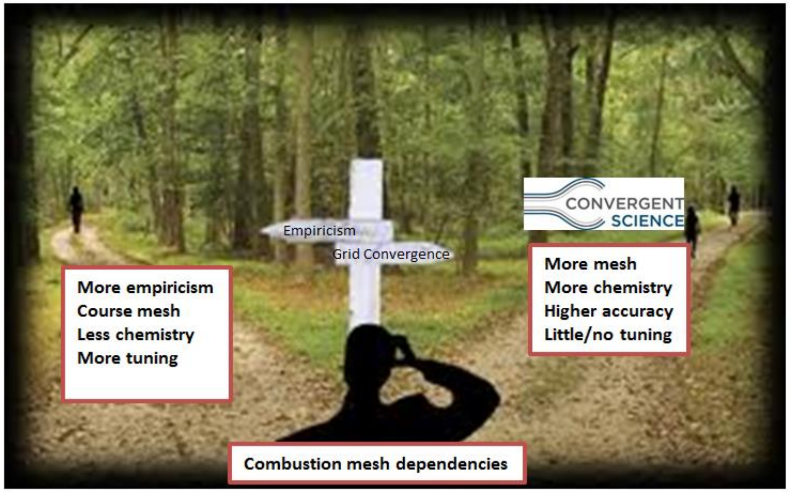
- CONVERGE combustion models allow the user to choose the compromise of accuracy and speed:
    - SAGE detailed chemistry solver – generally applicable/highly accurate
    - Shell ignition model (Diesel Autoignition)
    - Characteristic Time Model (Diesel combustion)
    - G-Equation model (Premixed combustion)
    - RIF Model (Diesel combustion)
    - ECFM-3Z -under development – General combustion

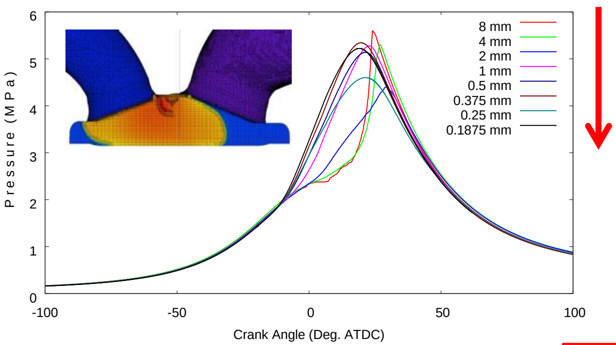


LES test case from ICEF2013-19043
Courtesy General Motors

Grid Convergent Combustion Modeling

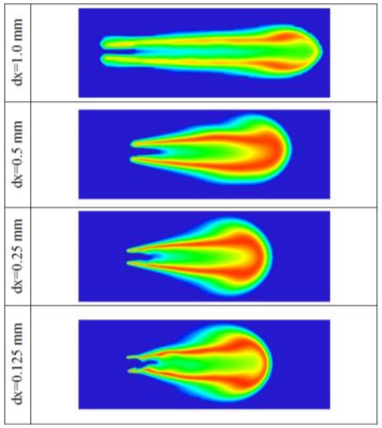
- Combustion models are often sensitive to the mesh
  - This often leads to model tuning and more empiricism
- The recommended approach with CONVERGE is to use:
  - More chemistry
  - Sufficient mesh to resolve flame
  - Less empiricism

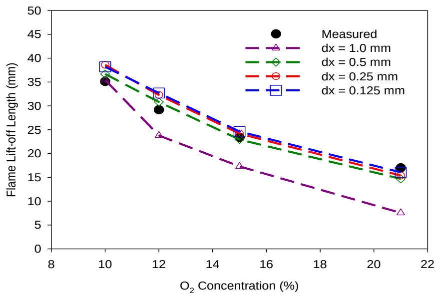




Premixed gasoline engine grid convergence study

For both premixed and diffusion flames, as mesh is refined, grid convergent behavior is approached





Diffusion flame grid convergence study

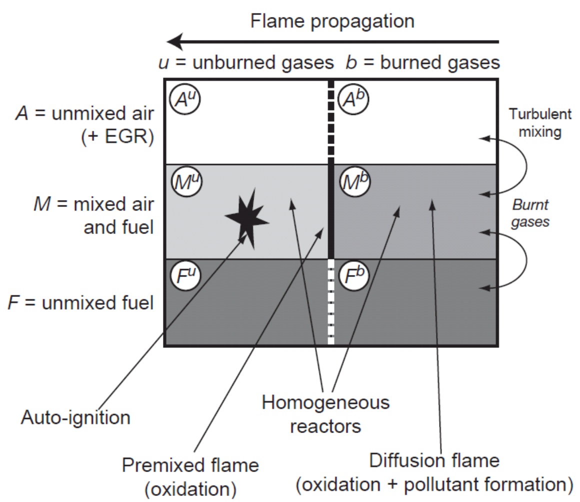
CONVERGENT SCIENCE

14PFL-0442
Modeling Turbulent Combustion Using a RANS Model, Detailed Chemistry, and Adaptive Mesh Refinement

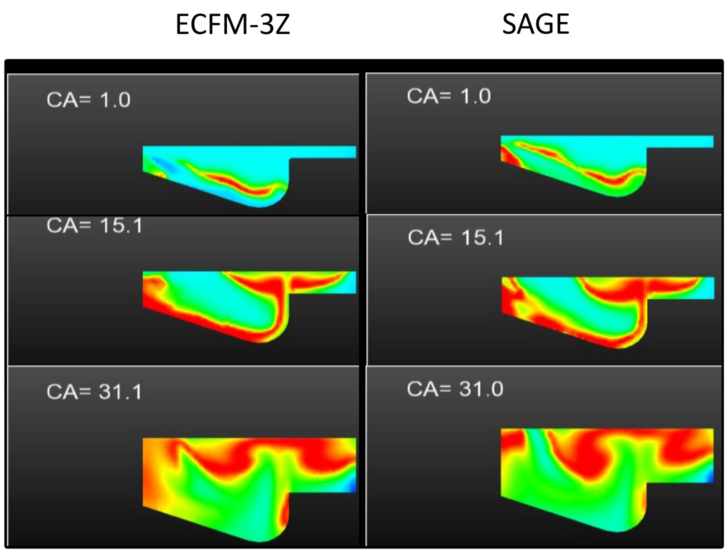
ECFM-3Z Model Overview

- Premixed combustion - Extended Coherent Flamelet Model (ECFM) [1]
- Partially Premixed combustion
- Non Premixed combustion

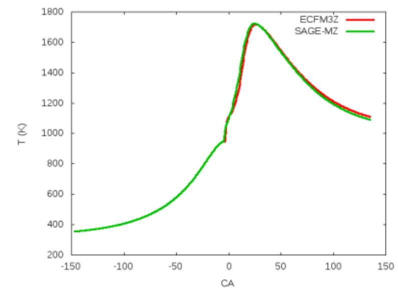
(Partially Premixed and Non Premixed combustion:) Mixing Model + Flamelet Model (ECFM-3Z) [2]

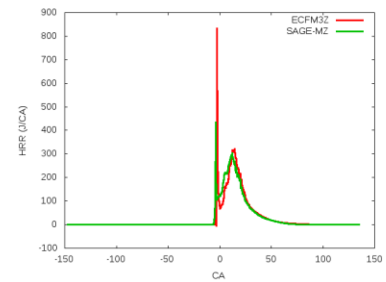


Schematic of ECFM3Z model computational cell (from [2]).



Diesel sector test cases using ECFM-3Z model

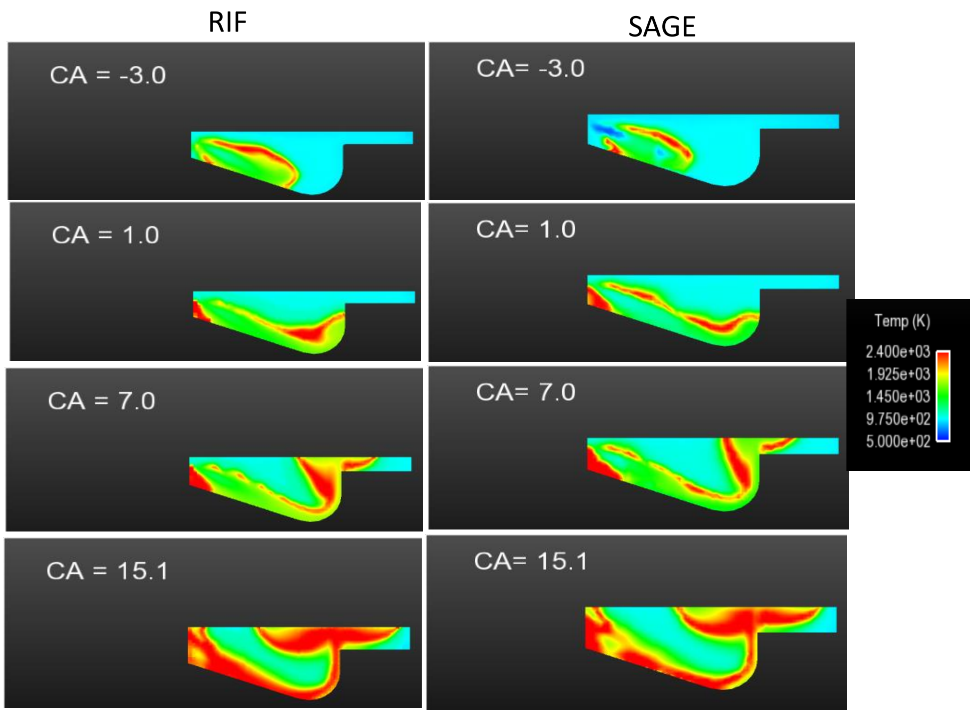




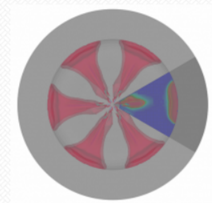
[1] O. Colin, A. Benkenida and C. Angelberger, "A 3D Modeling of Mixing, Ignition and Combustion Phenomena in Highly Stratified Gasoline Engines," *Oil & Gas Science and Technology, Rev. IFP*, Vol. 58, No. 1, pp. 47-62, 2003.
[2] O. Colin and A. Benkenida, "The 3-Zones Extended Coherent Flame Model (Ecfm3z) for Computing Premixed/Diffusion Combustion," *Oil & Gas Science and Technology - Rev. IFP*, Vol. 59, No. 6, pp. 593-609, 2004.

Representative Interactive Flamelet (RIF) Model

- Non-Premixed Combustion model including single and multiple flamelets
- CONVERGE 2.1 includes the FORTRAN-based RIF model from Norbert Peters (RWTH Aachen)
- Re-implementing a C version of RIF and parallelizing it to gain advantage over multiple processors
  - The 1d flamelet chemistry is parallelized in the new version
  - Makes use of analytical evaluation of Jacobian matrix



Convergent Science integrates the Representative Interactive Flamelet combustion model of Advanced Combustion GmbH into CONVERGE™



Convergent Science Inc. has announced that it has integrated the Representative Interactive Flamelet (RIF v4.0) model of Advanced Combustion GmbH into the CONVERGE™ CFD software. RIF can be used to model the ignition, combustion and emissions within a diffusion flame, such as those found within a Diesel engine. RIF maps the multidimensional flame front to one dimensional flamelet equations based upon mixture fraction. This decoupling of chemical and turbulent time scales greatly reduces the computational expense associated with combustion modeling. RIF 4.0 allows for multiple flamelets and multiple spray injections. RIF 4.0 also has been optimized to run more efficiently in parallel and now makes use of the analytical evaluation of the Jacobian matrix.

Dr. Daniel Lee, Vice President at Convergent Science stated “We are very pleased to integrate RIF 4.0 into CONVERGE. This will offer our users more options for modeling combustion from which they can choose the desired tradeoff of accuracy and speed. Advanced Combustion GmbH has a proven track record of producing cutting edge combustion models and we are excited to offer this technology to our users.”

Dr. Norbert Peters, CEO of Advanced Combustion commented “The collaboration with the people from Convergent Science in implementing RIF v4.0 into the Converge code was what we had expected from them: professional and efficient. It has been a pleasure to work with them.”

CONVERGE™ is an innovative CFD software that automates the meshing at runtime with a perfectly orthogonal Cartesian mesh, eliminating the need for a user defined mesh. This combined with its Adaptive Mesh Refinement technology allows for easy analysis of complex geometries and moving boundaries. CONVERGE™ is also equipped with extremely fast and efficient detailed chemistry, an extensive set of physical sub-models, a genetic algorithm optimization module, and fully automated parallelization.

Flamelet Equations

$$\rho \frac{\partial Y_i}{\partial t} = \underbrace{\rho \frac{\chi}{2L\hat{e}} \frac{\partial^2 Y_i}{\partial z^2}}_{transport} + \underbrace{\dot{\omega}_i}_{chemical}$$

$$\rho \frac{\partial T}{\partial t} = \underbrace{\rho \frac{\chi}{2} \frac{\partial^2 T}{\partial z^2} + \rho \frac{\chi}{2c_p} \frac{\partial T}{\partial z} \frac{\partial c_p}{\partial z} + \sum_{i=1}^{N} \rho \frac{\chi}{2L\hat{e}} \frac{c_{p_i}}{c_p} \frac{\partial Y_i}{\partial z} \frac{\partial T}{\partial z} + \frac{1}{c_p} \frac{\partial p}{\partial t}}_{transport} - \underbrace{\frac{1}{c_p} \sum_{i=1}^{N} \dot{\omega}_i h_i}_{chemical}$$

CONVERGENT SCIENCE

G-Equation Combustion Model

• The G-Equation combustion model of Peters has been implemented as an alternative to SAGE detailed chemistry for faster runtimes through coarser meshes

• The turbulent flame front can be tracked by solving for the non-reacting scalar, G (i.e., the distance to the flame):

$$\frac{\partial \rho \tilde{G}}{\partial t} + \frac{\partial \rho \widetilde{u_i} \tilde{G}}{\partial x_i} = -D_t^{'} \kappa \left|\frac{\partial \tilde{G}}{\partial x_i}\right| + \rho_u s_t \left|\frac{\partial \tilde{G}}{\partial x_i}\right|$$

Influence of curvature on the flame front

averaged turbulent mass burn rate

$$\kappa = \frac{\partial}{\partial x_i}\left(\frac{\partial \tilde{G}}{\partial x_i} \Big/ \left|\frac{\partial \tilde{G}}{\partial x_i}\right| \right)$$

Mean flame front curvature

$$D_t^{'} = \frac{c_\mu}{Sc}\frac{k^2}{\varepsilon}$$

• The level set method is used to solve the G-equation in order to track and maintain a sharp interface (i.e., the flame front where G=0). The interface divides the flow field into two regions: an unburned region (G<0) and a burned region (G>0)

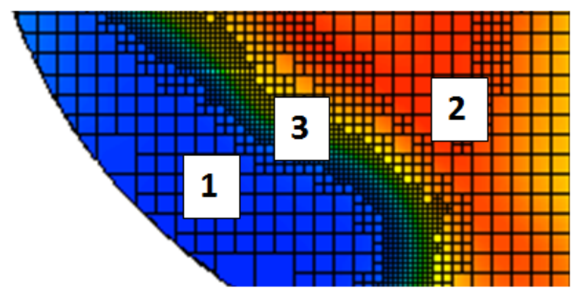
• The turbulent flame speed is calculated with the expression (Peters):

$$s_t = s_l + u^{'}\left\{ -\frac{a_4 b_3^2}{2b_1} Da + \left[\left(\frac{a_4 b_3^2}{2b_1} Da \right)^2 + a_4 b_3^2 Da \right]^{1/2} \right\}$$

•There are three options for species conversion:

- If only flame propagation (i.e., heat release) is of interest: equilibrium is solved in region 2 (CEQ solver)

- If emissions are of interest: detailed chemistry is solved in region 2 (SAGE solver)



- If auto-ignition (knock) is of interest: detailed chemistry is solved in both regions 1 and 2 (SAGE solver)

SAGE Detailed Chemistry

• For combustion modeling, the SAGE detailed chemistry solver is available as a standard feature:

- Imports mechanism in CHEMKIN format
- Parallelized independently from the flow for maximum efficiency
- Does not require empirical modeling for different combustion regimes
- For reasonable mechanisms and sufficient mesh resolution, no model tuning is required

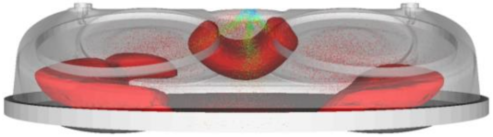
• Convergent Science recommends that SAGE is used for all engine types (assuming the additional runtime can be afforded and a valid chemical mechanism is available)

• SAGE is commonly used to model all combustion regimes (Diesel, natural gas, dual fuel, gasoline, auto-ignition etc)

• Significant resources are devoted to making the SAGE chemistry solver as fast as possible without compromising accuracy (SAGE run times are approaching those of empirically based models)

- Multi-zone solver
- Iterative solver
- Dynamic mechanism reduction (v2.2)

• The goal is to use bigger mechanisms, more cycles, more cylinders



Auto-ignition locations (red) and liquid spray droplets for dual fuel (Iso-octane+Diesel) test case. Courtesy Chrysler Group LLC.

CONVERGENT SCIENCE

Mechanism Reduction

• When using the SAGE detailed chemistry solver with CONVERGE, the user must supply a reaction mechanism

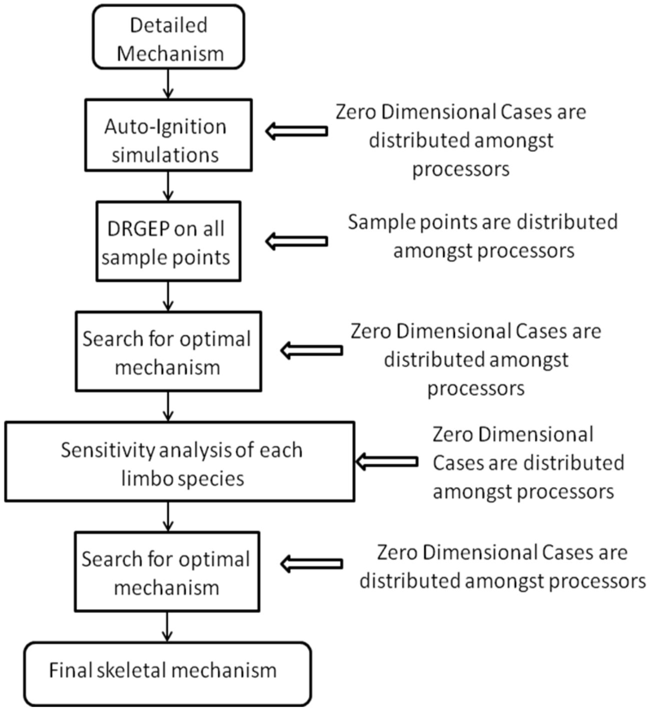
• There is no theoretical limit to the number of species and reactions used in CONVERGE

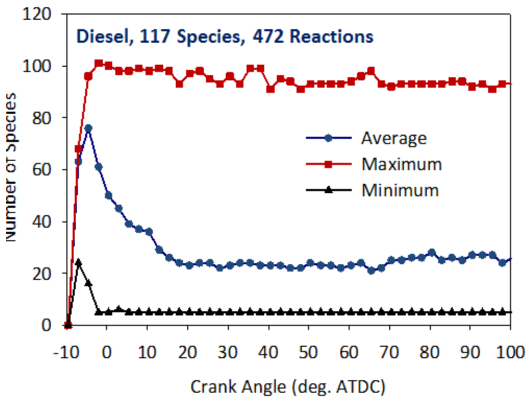
• CSI has developed a mechanism reduction toolkit with the goal of minimizing the mechanism size while maximizing the accuracy

• This toolkit is called Parallel Directed Relation Graph with Error Propagation and Sensitivity Analysis (PDRGEPSA)

• Unimportant species and reactions are removed to generate a skeleton mechanism

• In v2.2, dynamic mechanism reduction is available



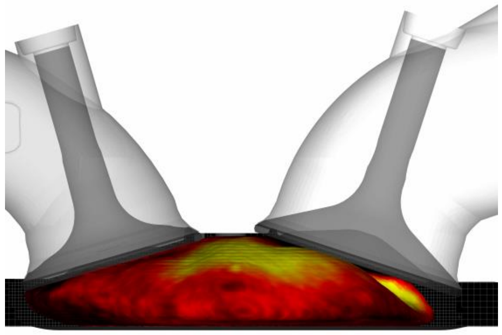


Number of species vs crank angle showing the computational speed provided by dynamic mechanism reduction

CONVERGENT SCIENCE

SAGE – Speed Improvements

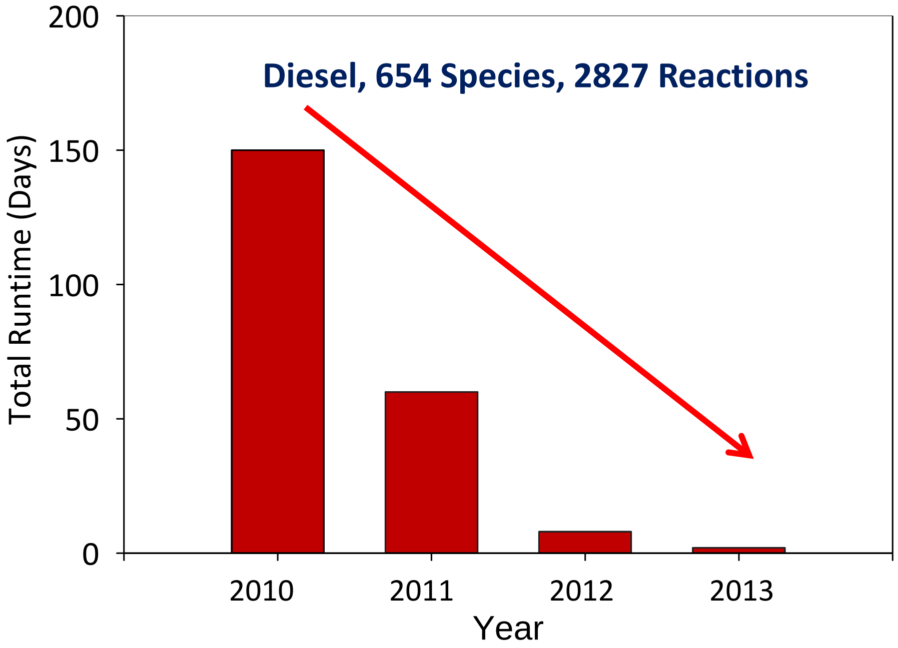
654 Species, 2827 Reactions	Total Time (days)
SAGE detailed chemistry solver	150
SAGE-Multizone, Direct solver	60
SAGE-Multizone, Iterative solver	8
SAGE-MZ-Dynamic mechanism reduction, Iterative	2 (v2.2)
SAGE-Multizone running on GPU	?? (results soon)



- Mechanisms with up to 1,000 species can now be simulated

Detailed chemistry in CONVERGE is getting faster and faster

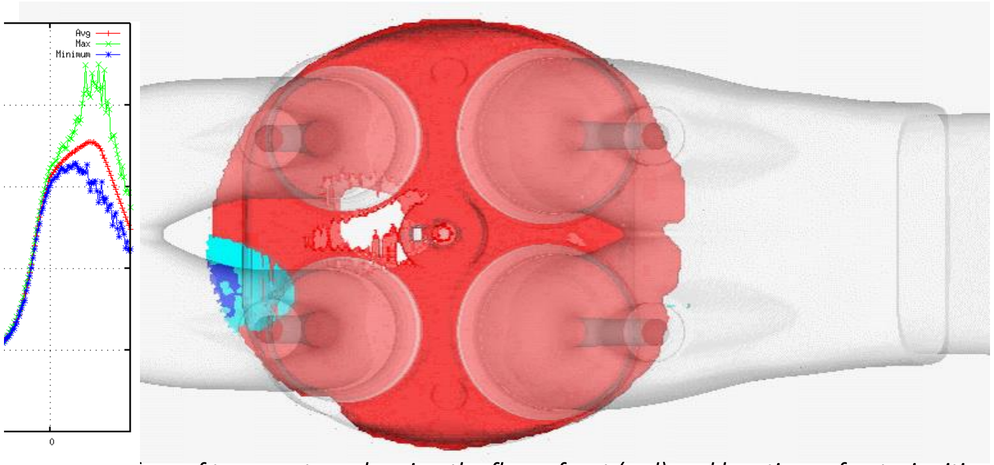
The goal is for detailed chemistry to be as fast (or faster) than empirically based models



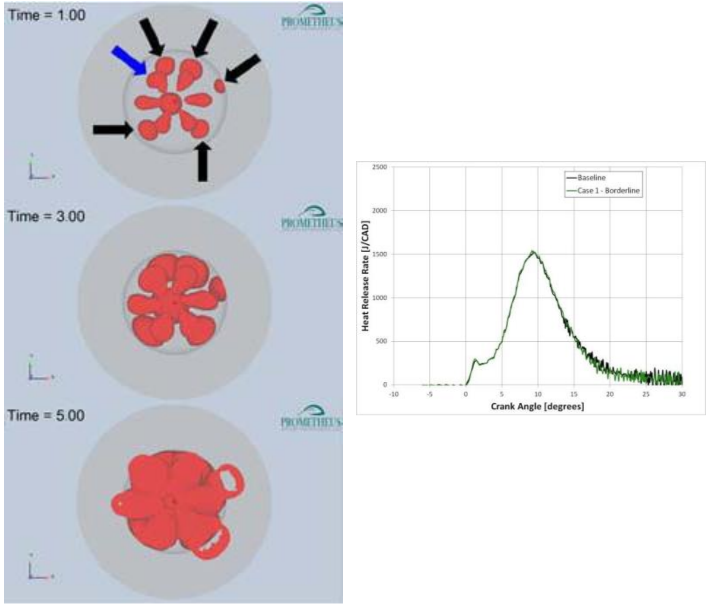
CONVERGENT SCIENCE

Auto-Ignition Modeling in CONVERGE

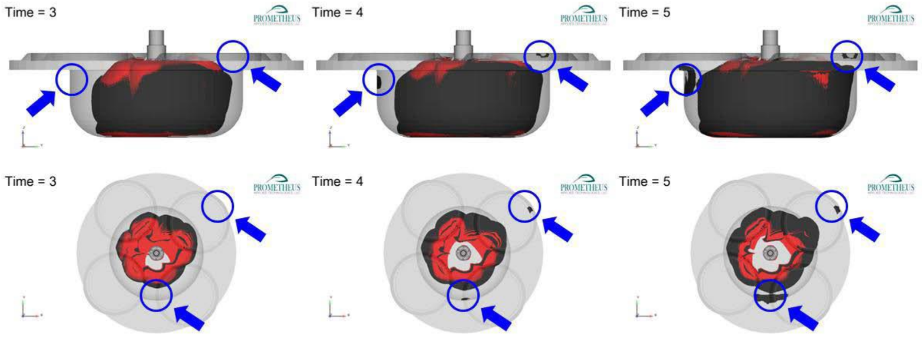
- If SAGE is used, auto-ignition is predicted directly without any other submodels required



Iso-surface of temperature showing the flame front (red) and locations of auto-ignition (blue) for spark ignited engine. Courtesy Chrysler Group LLC.



Lube oil autoignition locations and heat release rate
Courtesy Prometheus Applied Technologies

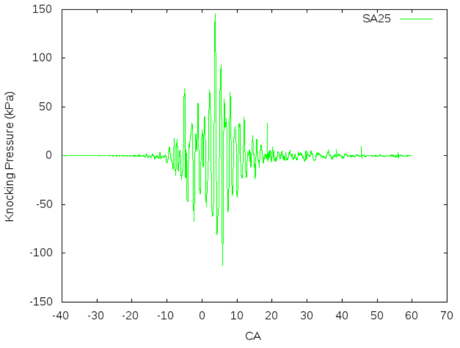


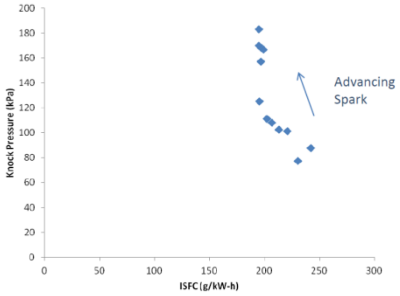
Flame propagation with multiple autoignition events (flame is a red isosurface, H2O2 is a black isosurface) . Courtesy Prometheus Applied Technologies

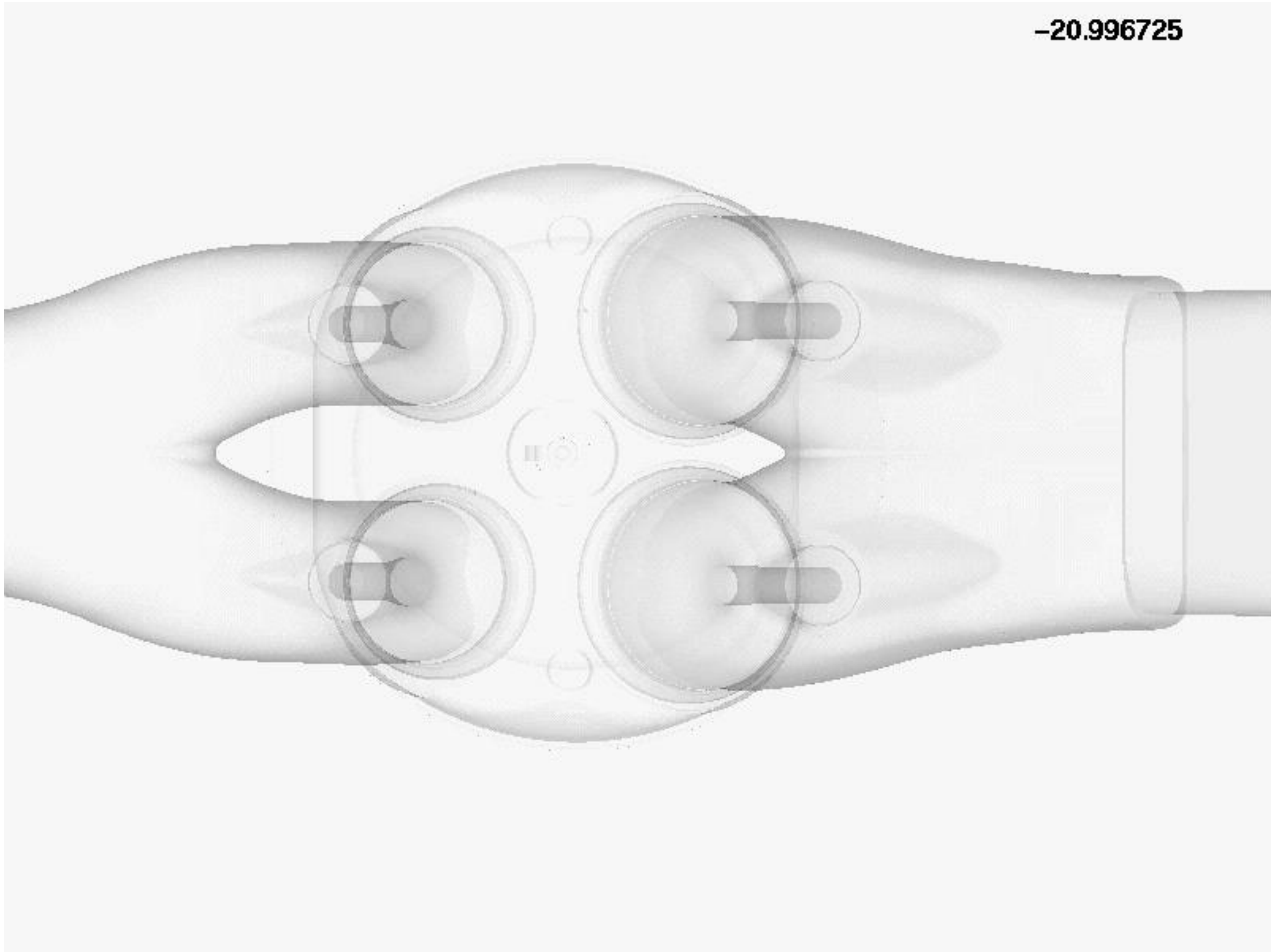
CONVERGENT SCIENCE

Auto-Ignition Modeling in CONVERGE

SAGE and Adaptive Mesh Refinement for Flame Propagation Simulation







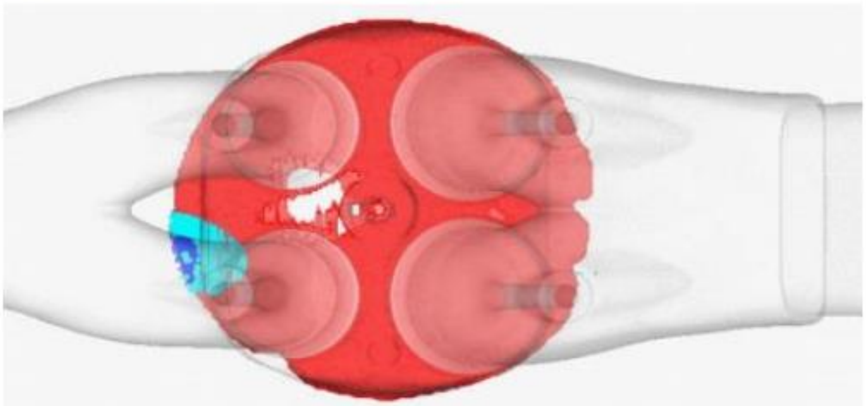
CONVERGENT SCIENCE

Iso-surface of temperature showing the flame front (red) and locations of auto-ignition (blue) for spark ignited engine. Courtesy Chrysler Group LLC.

Convergent Science in the News

Finding the virtual knock-limit

04-Sep-2013 16:21 GMT



Iso-surface of temperature showing the flame front (red) and locations of auto-ignition (blue) for spark ignited engine. (Chrysler Group LLC)

Pushed by a competitive need for better fuel economy coupled with emissions regulations, engine developers are taking conventional internal-combustion engine (ICE) technologies to the limit. This means a greater risk of knock—that rattling, tinny sound of an engine in distress. What causes it? Uncontrolled ignition during combustion. Instead of a smooth flame front moving through the combustion chamber, hot spots will auto-ignite unpredictably in the remaining air-fuel mixture ahead of the flame front. Excessive temperature and pressures in localized spots result. Besides annoying drivers, excessive knock can wear engines faster and even catastrophically damage pistons and cylinders.

Boosting, higher compression ratios, geometry of the piston, injection strategies, spark timing, and octane levels of fuels are just some of the design factors that affect knocking. "All efficient engines have knock, it is a

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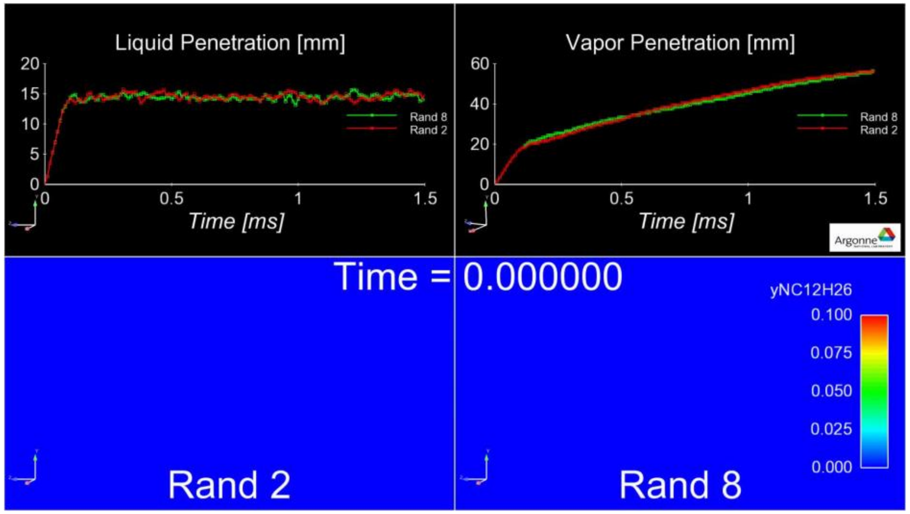
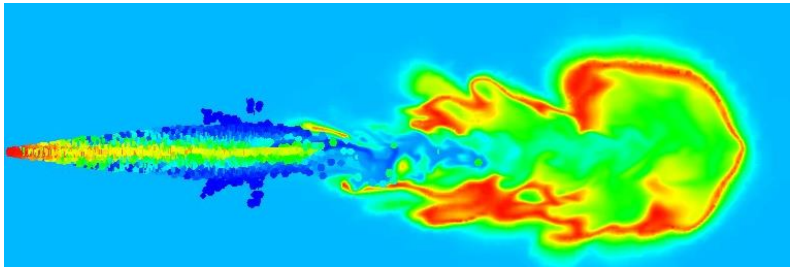
CONVERGE with SAGE detailed chemistry solver used for auto-ignition prediction

CONVERGENT SCIENCE

Overview of Presentation

- Company Overview
- Technology Overview
- Combustion Modeling
- Spray modeling
- Optimization



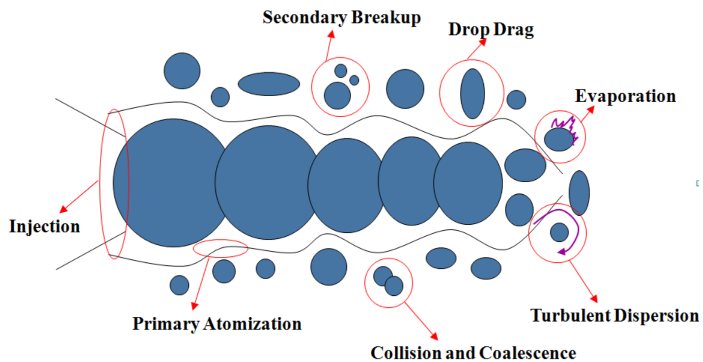


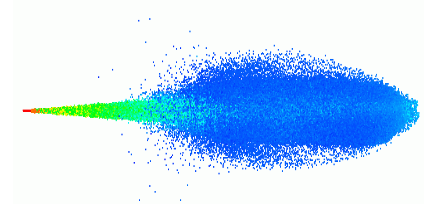
Spray combustor simulated with LES and detailed chemistry

CONVERGENT SCIENCE

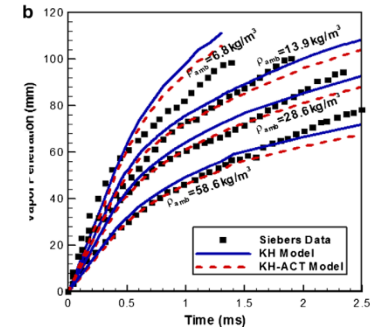
Spray Modeling Overview

- CONVERGE has a rich set of models to simulation spray injection and atomization
- Breakup
  - Kelvin-Helmholtz breakup
  - Rayleigh-Taylor breakup
  - LISA sheet breakup
  - TAB breakup
- Drop collision and coalescence
  - O'Rourke numerical algorithm
  - Collision mesh option
- Wall Film model
  - A particle-based wall film model is available in CONVERGE
  - Film splashing, separation and evaporation is included
- Nozzle flows
  - Cavitation modeling
  - Moving nozzles readily handled
- Great care is taken to assure spray models are grid convergent

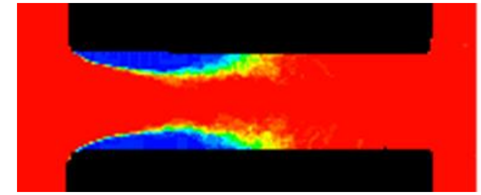




Diesel spray simulation

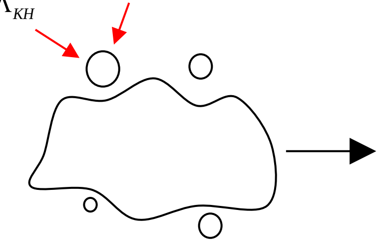


Som et al., Combustion and Flame 157 (2010) 1179–1193



Cavitating nozzle simulation Zhao et al. ASME 2013

$$r = B_0 \Lambda_{KH} \qquad v_n = C_1 \Lambda_{KH} \Omega_{KH}$$



LARGE EDDY SIMULATION OF VAPORIZING SPRAYS CONSIDERING MULTI-INJECTION AVERAGING AND GRID-CONVERGENT MESH RESOLUTION

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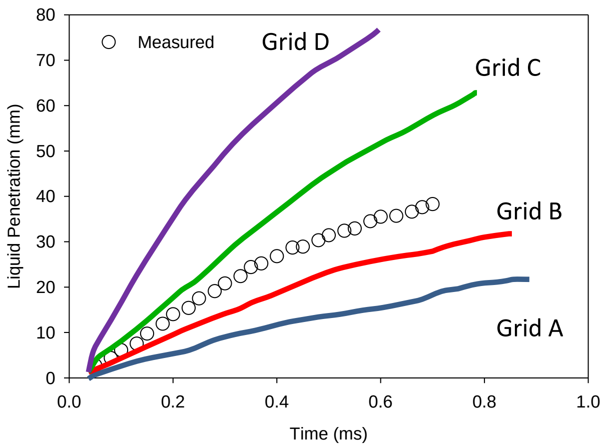
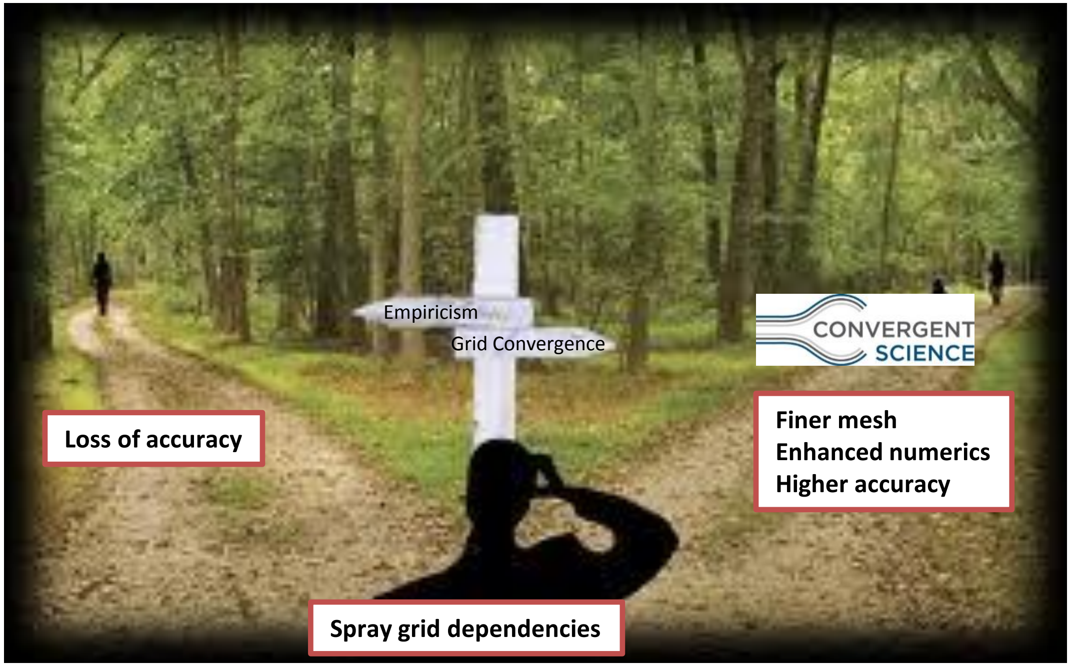
CONVERGENT SCIENCE

Spray Modeling

- Lagrangian spray models are known to be extremely grid sensitive
- One option is to introduce more empiricism in the spray models => this is against the CONVERGE modeling philosophy
- The CONVERGE approach is to utilize meshing tools, numerics and physical models to create a grid-convergent approach
- Run simpler test cases (both RANS and LES) such as spray bombs to understand the mesh requirements for grid convergent answers and the tradeoff in run times
- Use knowledge about run time vs accuracy learned from the simpler cases to full engine analysis (run with confidence)



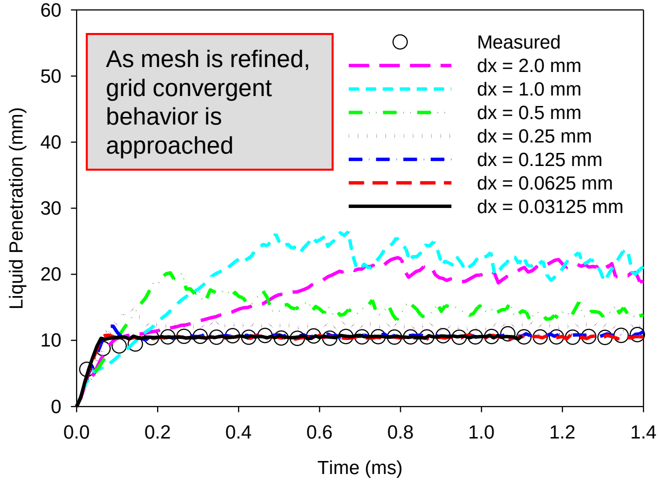
Other CFD codes show large grid dependencies for spray simulations



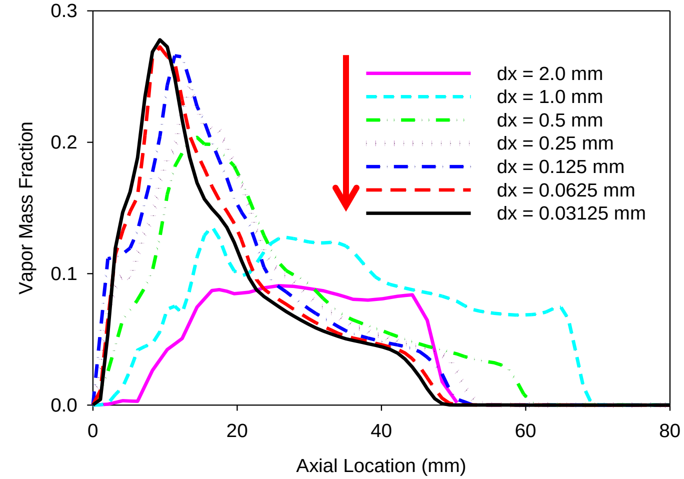
CONVERGENT SCIENCE

Grid Convergent Spray Modeling

- Adaptive Mesh Refinement (AMR)
  - Must be able to run cell sizes below the point of convergence
  - Allows the use of very fine grids near the spray while keeping the overall cell count low
- Fully Implicit Momentum Coupling
- Improved Liquid-Gas Coupling
  - Taylor series expansion to calculate the gas-phase velocity
- Temporal Liquid Mass Distribution
  - A common error is to keep the number of injected parcels the same as the mesh is refined
  - Current approach significantly increases the injected number of parcels as the embed scale is increased
- Spatial Liquid Mass Distribution



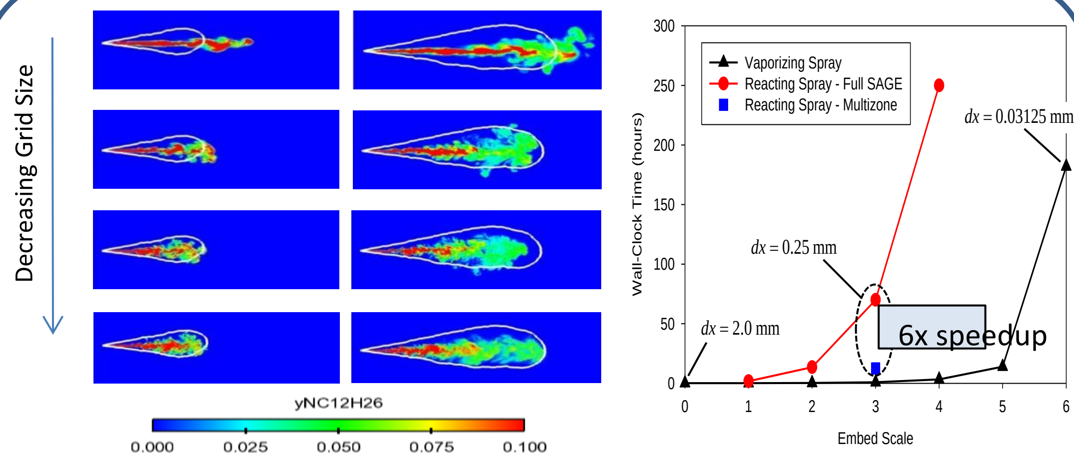
Comparison of measured and predicted liquid penetration for evaporating spray case



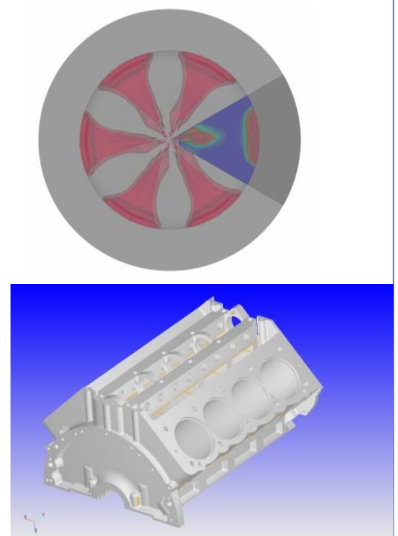
Comparison of spray centerline vapor mass fraction for a range of mesh resolutions.

CONVERGENT SCIENCE

Spray Modeling



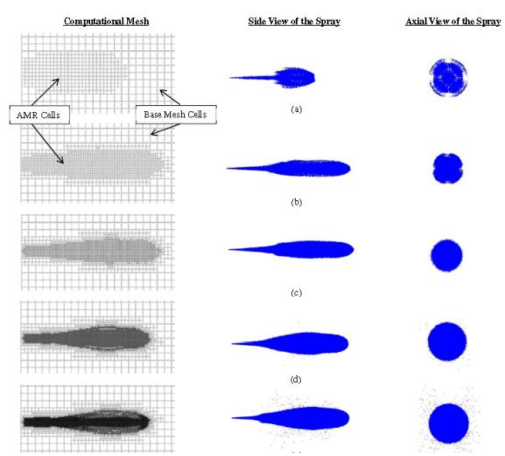
Knowledge of run time & accuracy tradeoff for spray modeling grid effects



Mesh size influence on run time and accuracy for simpler test case

Full engine simulations done with confidence

CONVERGE offers meshing tools other codes don't have, allowing for mesh elements to be added when and where they are needed to minimize grid dependencies.



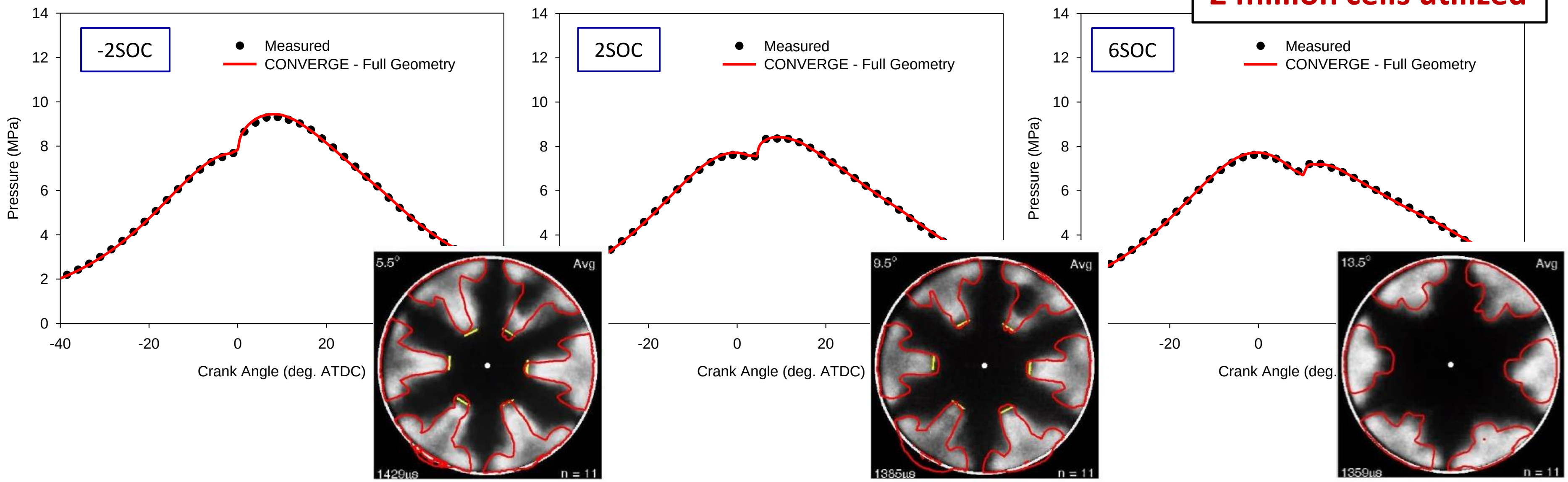
As mesh is refined, grid convergent behavior is approached

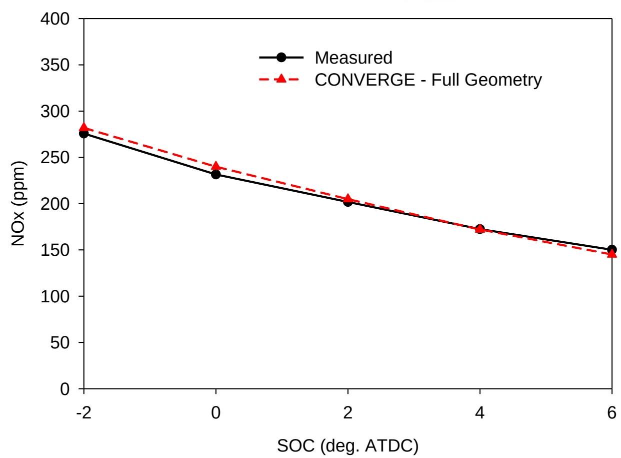
CONVERGENT SCIENCE

Grid Convergent Engine Modeling

- **Grid-Convergent Engine Simulations**

2 million cells utilized





OH* Chemiluminescence vs. OH iso-surface, 7.5 degrees after SOC

The grid-convergent methodology results in excellent agreement with global combustion behavior as well as flame lift-off length and flame location with no model tuning

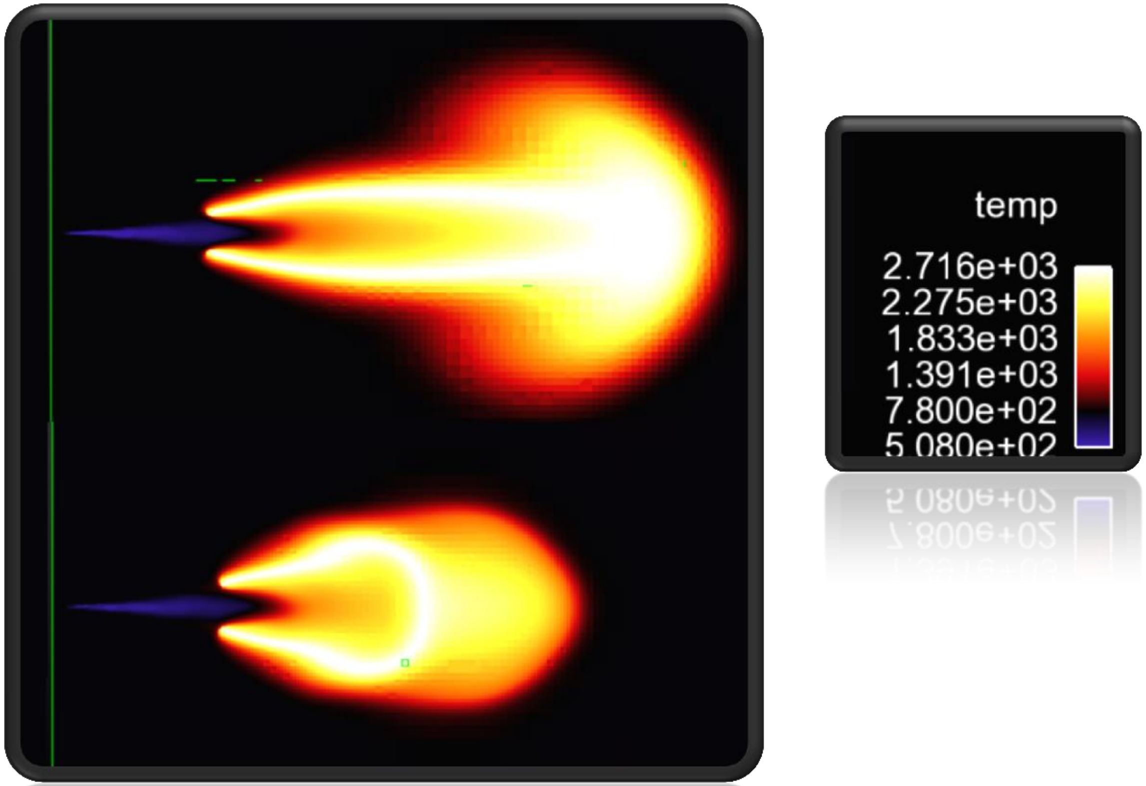
CONVERGENT SCIENCE

Collaboration with Caterpillar Inc. and Sandia National Laboratories

*Senecal et al. ASME 2013

1-D Spherical Droplet Heating

- Current method is 0-D, assuming uniform temperature.
- New method is 1-D, assuming spherical symmetry for more realistic heating and evaporation.
- User can choose number of cells for FV heat equation solver and threshold below which model switches back to 0-D.
- Effects of droplet recirculation can be simulated via effective thermal conductivity model.

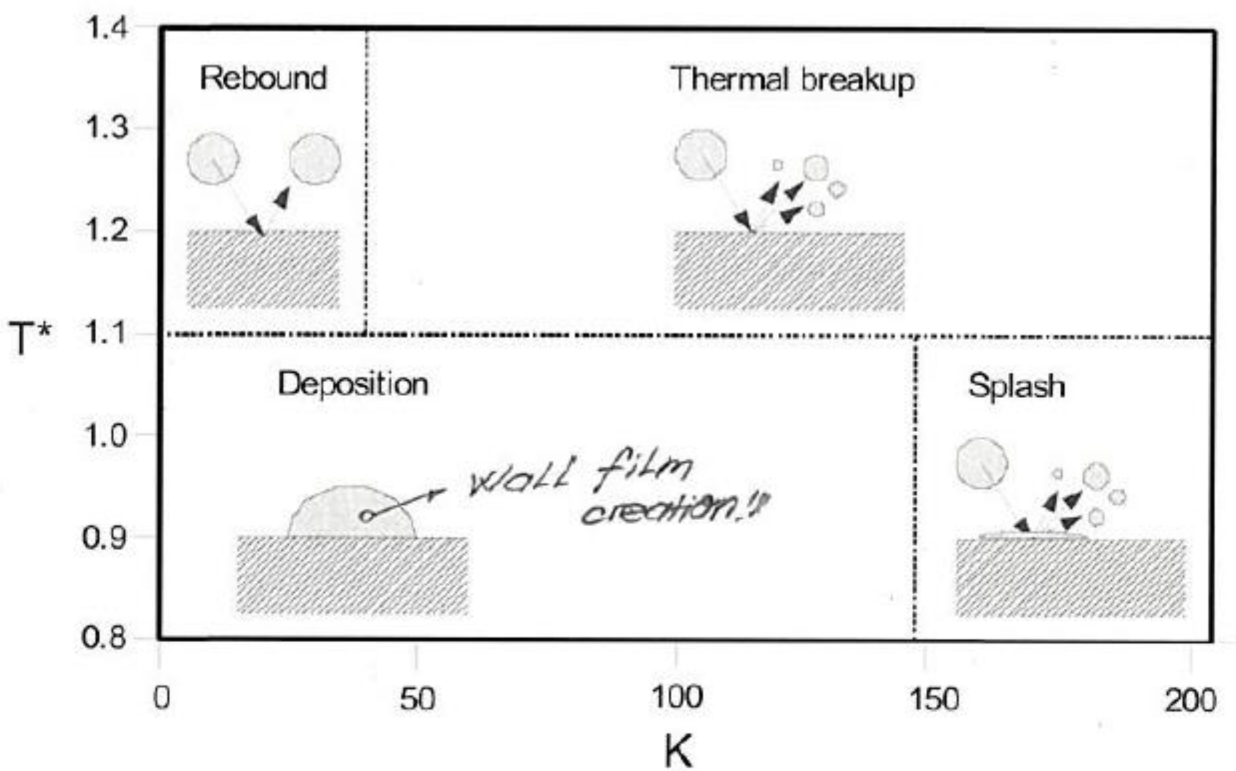


1D model (bottom) results in more rapid surface heating, which speeds up evaporation, enhancing the cooling the gas, resulting in a delayed flame as compared to the 0D model (top).

CONVERGENT SCIENCE

New Spray/Wall Interaction Model

Dominik Kuhnke, *Spray/Wall-interaction Modeling by Dimensionless Data Analysis*, Shaker, Aachen, 2004 [Ph.D.Thesis]



Regime Map for Spray/Wall Interaction According to Kuhnke

- K number :

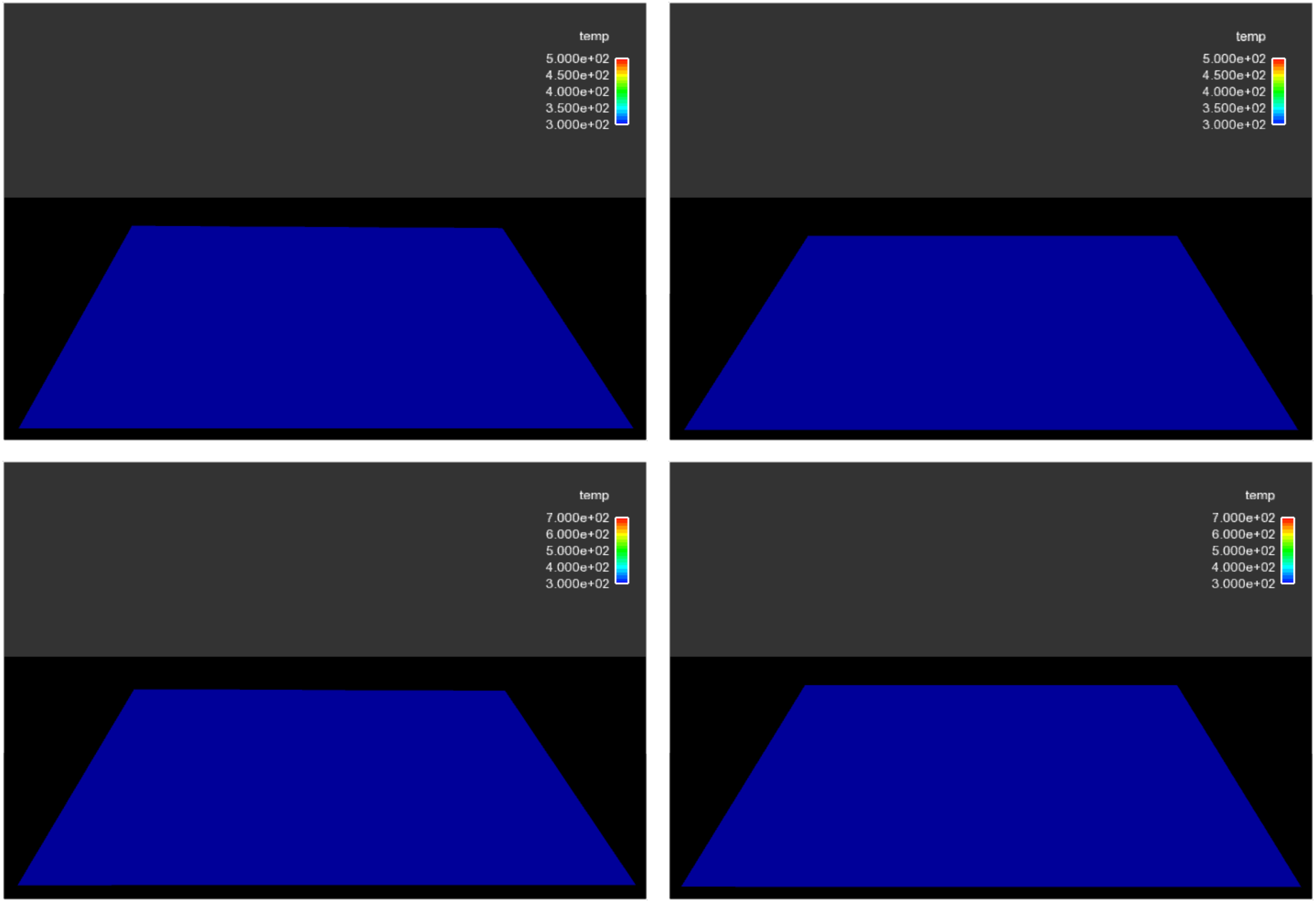
$$K = \frac{(\rho d)^{3/4} U^{5/4}}{\sigma^{1/2} \mu^{1/4}}$$

- combination of Weber number and Laplace number:

$$K = We^{5/8} La^{1/8}$$

- accounts for the effects of both kinematic condition and size of the spray droplets.

New Spray/Wall Interaction Model



$$\frac{T_w}{T_{boil}} = 0.9$$

$$\frac{T_w}{T_{boil}} = 1.25$$

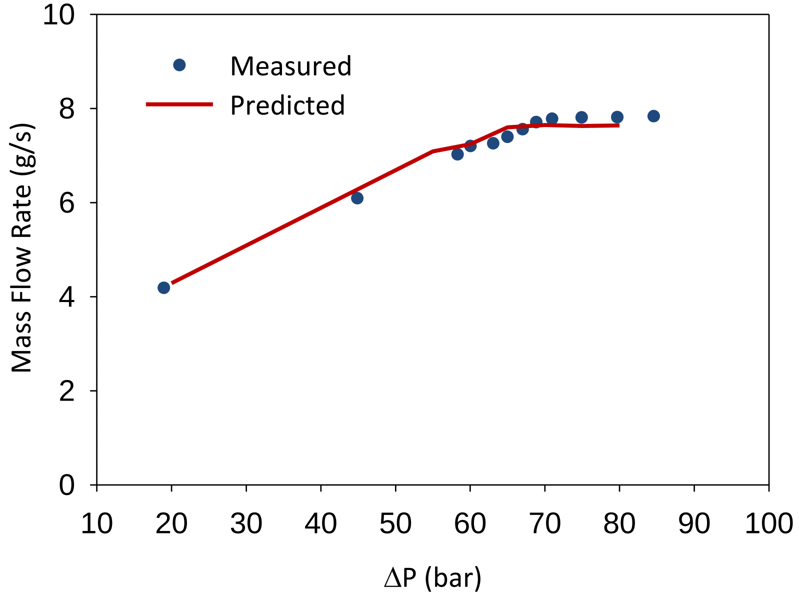
Old model

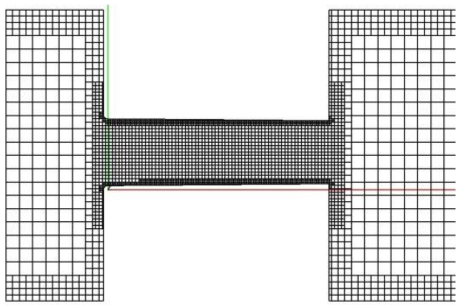
New model

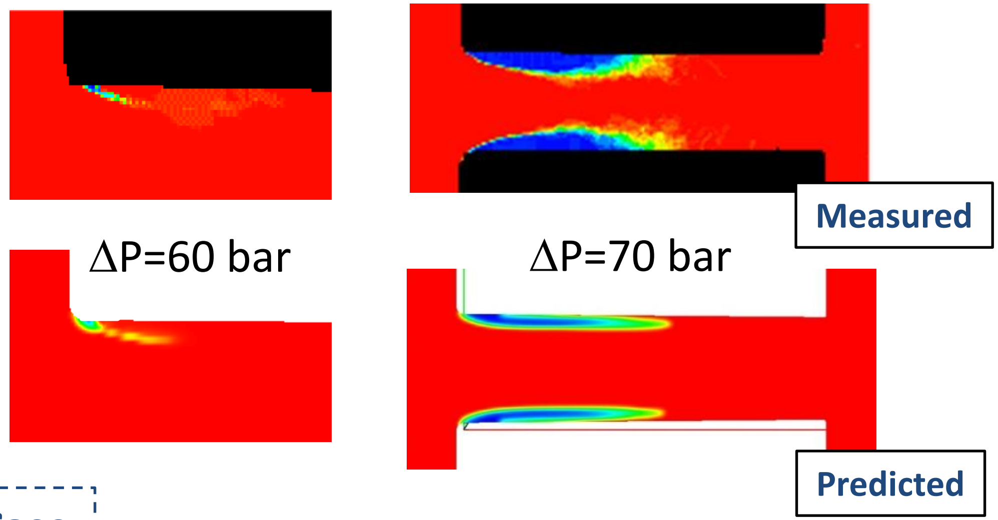
CONVERGENT SCIENCE

Fuel Injection Modeling

- **Internal Nozzle Flow Simulations**
  - Volume of Fluid (VOF) method to model two-phase flow
  - Cavitation is modeled with the Homogeneous Relaxation Model (HRM) of Schmidt
  - High Resolution Interface Capturing (HRIC) is used to sharpen the gas-liquid interface
  - Void fraction AMR is used to sharpen the gas-liquid interface







Winklhofer Nozzle Test Case

*Zhao et al. ASME 2013

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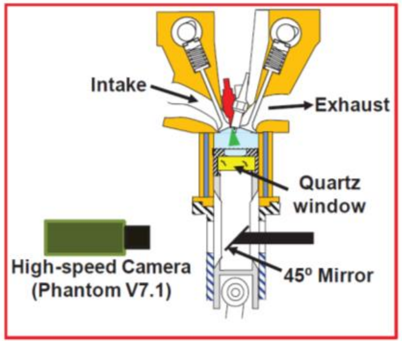
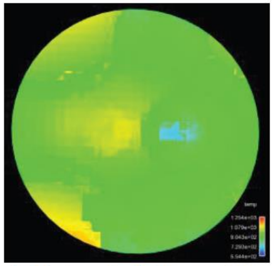
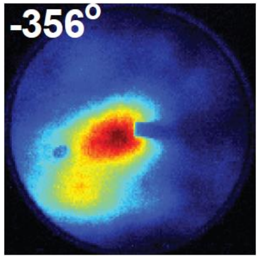
- Emissions modeling
- Conjugate heat transfer





(a) Integrated temperature at -356 CA aTDC



(b) Optical Image at -356 CA aTDC

Comparison of CFD temperature and optical image for HCCI engine (from ICEF2013-19216)
Courtesy General Motors

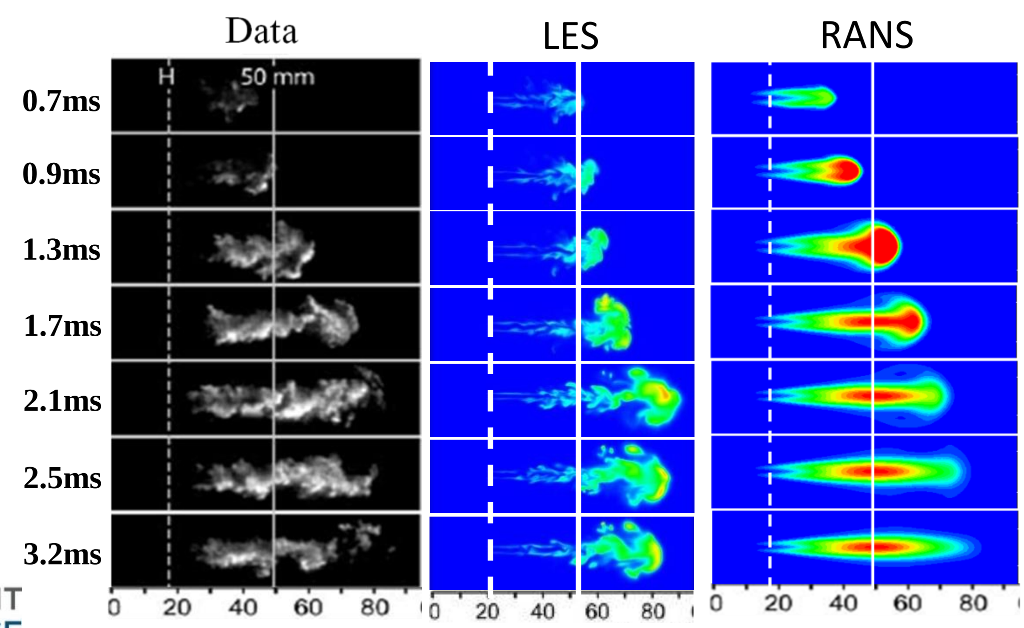
Emissions Modeling – Current Approach

- **NO_x Calculations**
  - Extended Zel'dovich reactions
  - More complicated NO_x chemistry (e.g., including NO_2) can be included through the chemical mechanism
- **Soot Calculations**
  - Two step model using fuel or C_2H_2 as the formation species and the NSC model for oxidation

$$\frac{dM_s}{dt} = \dot{M}_{sf} - \dot{M}_{so}$$

$$\dot{M}_{sf} = A_{sf} P^{0.5} \exp\left(-E_{sf}/R_u T\right) M_{form}$$

$$\dot{M}_{so} = A_{so} \frac{6M_s}{\rho_s D_s} R_{total} MW_c$$



Soot Data from LM Pickett & DE Siebers, Combustion and Flame 2004

Collaboration with Argonne National Lab

CONVERGENT SCIENCE

Partnership with Prof. Mauss

Convergent Science integrates advanced soot modeling capability into CONVERGE™

Convergent Science Inc. has announced that it is collaborating with Professor Fabian Mauss of Brandenburg Technical University in Cottbus, Germany (BTU-Cottbus) to integrate advanced soot models into the CONVERGE™ CFD software. The advanced models will improve the accuracy of emissions predictions by incorporating detailed descriptions of the soot formation processes. For example, soot inception is modeled through the prediction of Polycyclic Aromatic Hydrocarbons (PAHs) formed from a complex set of chemical reactions.

Historically, obtaining accurate predictions of soot has been one of the most challenging aspects of internal combustion engine modeling. Emissions mandates are becoming exceedingly stringent, pushing soot levels lower and increasing the level of accuracy needed in predictions. As a result, simplified two-step soot models, while still providing trends for traditional engine designs, often break down when advanced combustion strategies are employed.

Dr. P. Kelly Senecal, Vice President at Convergent Science stated "*We are very pleased to integrate Professor Mauss' advanced soot models into CONVERGE™. The models are a natural extension of our SAGE detailed chemistry solver which efficiently calculates large sets of chemical reactions. Our goal is to provide our users with the most predictive combustion and emissions models available. We believe that the combination of CONVERGE™'s industry-leading CFD technology and Professor Mauss' cutting edge models will deliver this level of accuracy.*"

Dr. Fabian Mauss, Professor at BTU-Cottbus commented "*I am glad to see the results of our research integrated in CONVERGE™. I am excited that the model integration will support engineers to meet their emission targets in the future.*"

CONVERGE™ is innovative CFD software that automates the meshing at runtime with a perfectly orthogonal Cartesian mesh, eliminating the need for a user defined mesh. This combined with its Adaptive Mesh Refinement technology allows for easy analysis of complex geometries and moving boundaries. CONVERGE™ is also equipped with extremely fast and efficient detailed chemistry, an extensive set of physical sub-models, a genetic algorithm optimization module, and fully automated parallelization.

Convergent Science is working closely with Prof. Fabian Mauss of BTU-Cottbus on soot modeling

CONVERGENT SCIENCE

Emissions Modeling – Roadmap

Empirical model (Hiroyasu Soot model)	Semi-empirical/semi-detailed model(Phenomenological models)	Detailed model (Mauss soot model/Section rate model)
Single rate expression; no sub-processes information	Single rate expression for different sub-processes	Detailed mathematical methods for different sub-processes
Based on empirical correlation	Only good for certain applications	Can be applied for various applications
Fast and simple	Moderate high computation cost	High computational cost
Available in CONVERGE 2.1 and previous version	Will be available for CONVERGE 2.2	

CONVERGENT SCIENCE

Mauss Soot Model (1)

- Method of Moments is used in Mauss soot model.
  - Method of Moments solves global quantities for large population of soot.

- Define *r*-th moment as:

i: particle size class
N: number density of soot particles

$$M_r = \sum_{i=1}^{\infty} i^r N_i$$

M_0 is related to mean number density of soot;
M_1 is related to mean mass/volume of soot;
…

In most practical applications, the properties of interest are fully determined by just the first few moments.

↓

Only need to solve a small number of equations for the lowest-order moments.

CONVERGENT SCIENCE

Mauss Soot Model (2)

- For different moments:

$$\frac{dM_r}{dt} = \frac{dM_{r,pi}}{dt} + \frac{dM_{r,con}}{dt} + \frac{dM_{r,coag}}{dt} + \frac{dM_{r,sg}}{dt}$$

- Summary of moment rate expression:

$M_{r,pi}$: soot inception	$M_{r,pi} = \frac{1}{2}\alpha C(2\langle i\rangle)^r \langle i\rangle^{1/6} M_0^2$
$M_{r,\,con}$: soot condensation	$M_{r,con} = C_{lib}\sum_{k=0}^{r-1}\langle j\rangle^{r-k-1/2} M_{k+2/3}$
$M_{r,\,coag}$: soot coagulation	$M_{r,coag} = M_{r,coag}^{fm} M_{r,coag}^{c} \Big/ (M_{r,coag}^{fm} + M_{r,coag}^{c})$
$M_{r,\,sg}$: soot surface growth	$M_{r,sg} = \alpha k[C2H2] f_{3a} A \sum_{k=0}^{r-1}\binom{r}{k} M_{k+2/3}\Delta m^{r-k}$

Detailed derivations can be found in :

Mauss F., *Entwicklung eines kinetischen Modells der Russbildung mit schneller Polymerisation*, PhD thesis, RWTH Aachen, Department of Mechanical Engineering, 1998.

CONVERGENT SCIENCE

Mauss Soot Model (3)

- The transport equations for moments will also be solved:

$$\frac{\partial M_r}{\partial t} + \nabla \cdot (M_r \cdot v) = \nabla \cdot \left(\frac{\mu}{SC} \nabla \left(\frac{M_r}{\rho} \right) \right) + \dot{s}_M$$

μ: cell viscosity;
SC: Schmidt number;

- Important soot parameters obtained by Mauss model:

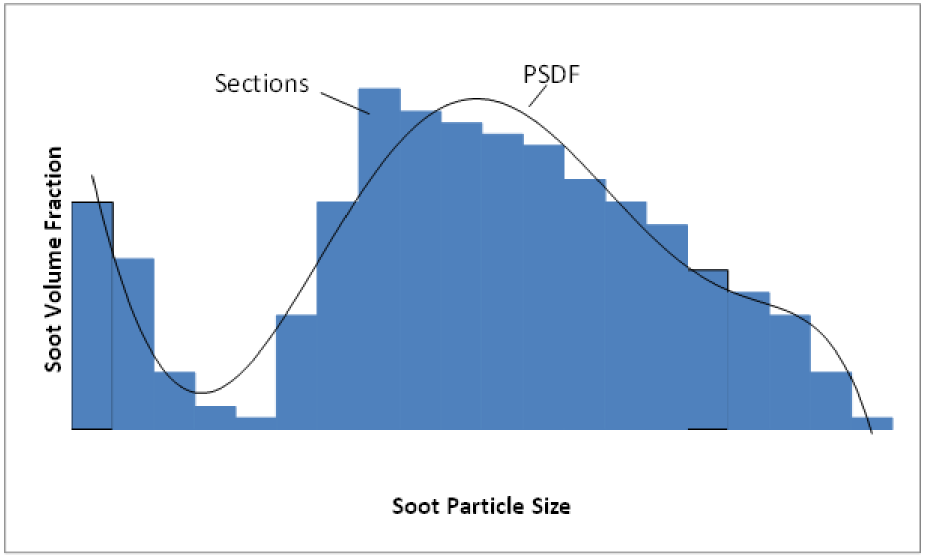
Parameters	Related moment
Soot number density	M0
Soot volume fraction	M1
Total soot mass	M1
Total soot surface	M0, M1, M2, M3
Mean diameter d	M0, M1, M2, M3
Dispersion	M0, M1, M2, M3

CONVERGENT SCIENCE

Section Rate Soot Model

- Divided the soot particle distribution function(PSDF) into different sections.
  - Section: soot particles with similar size, solved as volume fractions of soot

- Sections will be solved as additional transport passives.



Detailed derivations can be found in :
Caroline M., *MODELISATION DE LA FORMATION ET DE L'OXYDATION DES SUIES DANS UN MOTEUR AUTOMOBILE,* PhD thesis, UNIVERSITE D'ORLEANS, ENERGETIQUE, 2008.

CONVERGENT SCIENCE

Mauss Model vs. Section Rate Model

	Mauss Soot Model(PM)	Section Rate Model(PSM)
Number of variables to be solved	Moments (2-4)	Sections (more than 20)
Global parameters obtained	Soot mass, number density, volume fraction, total surface area, etc.	Soot mass, number density, volume fraction, total surface area, etc.
Particle size distribution function in each computational cell	Assumed as log-normal distribution.	Obtained based sections solution.
Computation time	Expensive compared to Hiroyasu and other Phenomenological models	More expensive compared to Mauss mdoel.

CONVERGENT SCIENCE

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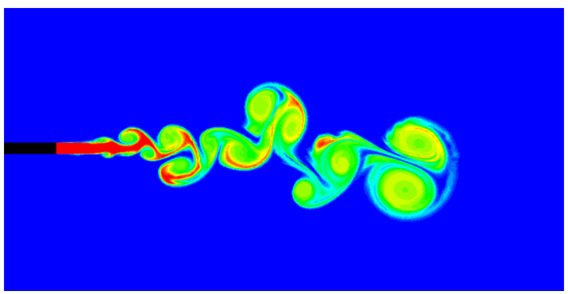
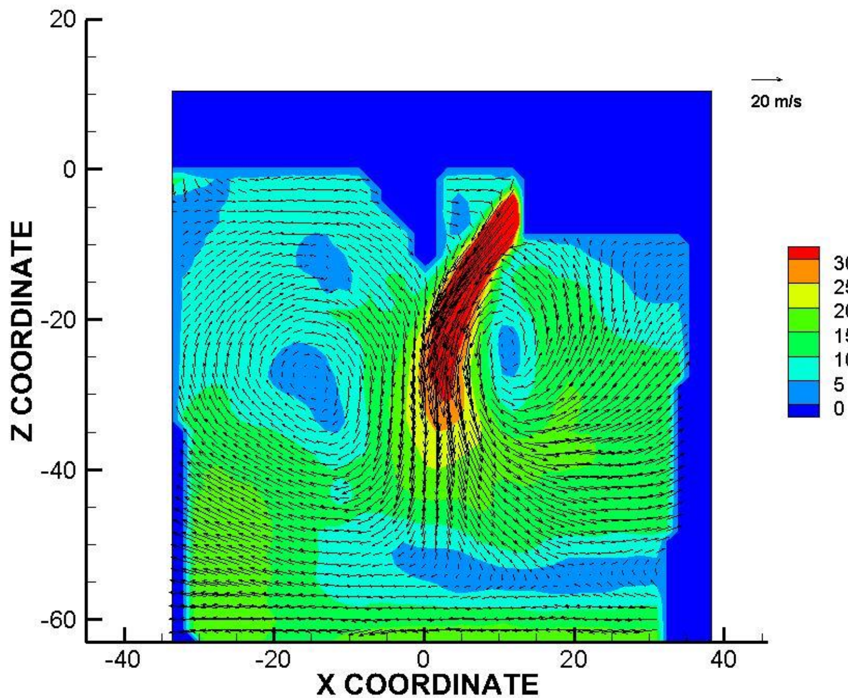
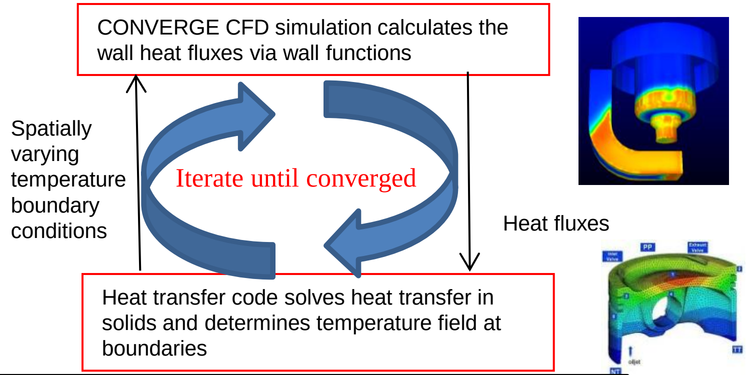




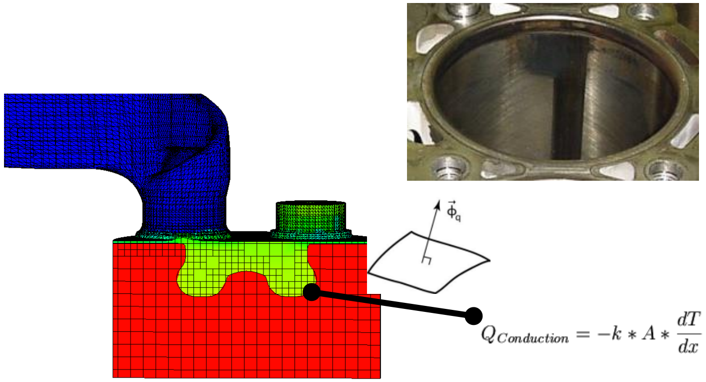
CONVERGENT SCIENCE

Conjugate Heat Transfer (CHT)

- Older versions of CONVERGE could only simulate the fluid flow (no solids)
- Appropriate wall thermal conditions must be specified
- Many clients currently couple CONVERGE with a separate heat transfer code (such as NASTRAN) to determine the solid metal temperature
- The coupling process is as follows:
    - CONVERGE is run (fluid only) using assumed wall thermal boundary conditions
    - CONVERGE exports the wall heat fluxes to the separate heat transfer tool
    - The metal temperature is calculated using (outside of CONVERGE) and new thermal boundary conditions are passed to CONVERGE
    - The process it repeated until the metal temperature is converged
- This process works, but is less than ideal
    - Interpolations must be done at the solid/fluid interface
    - Code coupling required
    - Run times can be long as many iterations are required
- A significantly better approach is available in CONVERGE 2.1, making the above coupling obsolete
- Let's first provide an overview of the challenges associated with CHT



Conjugate heat transfer coupling CONVERGE (fluid portion) with other simulation tools (solid portion)



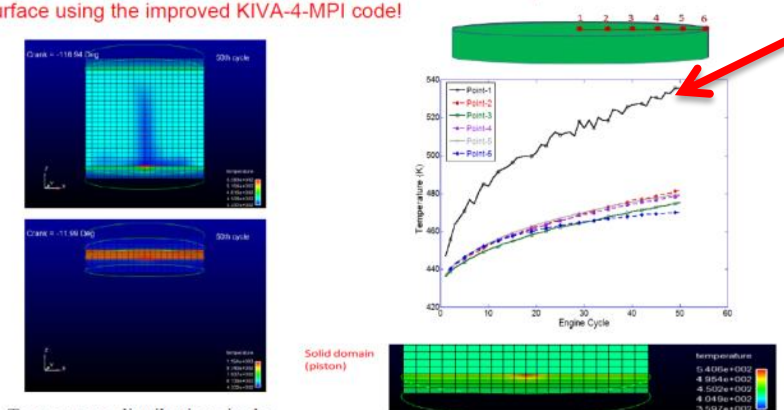
Conjugate heat transfer (both fluid and solid) simulated in CONVERGE without any coupling with other tools

CONVERGENT SCIENCE

Conjugate Heat Transfer (CHT)

- It is well known that fluid flow and heat transfer are associated with drastically disparate timescales (fluid flow is fast, heat transfer is slow)
- As an example, when a car starts in the winter, the combustion happens immediately yet many seconds (and piston revolutions) go by until the engine block temperature reaches steady state
- One option for modeling this CHT process is to couple the heat flux every boundary cell every timestep
- However, this approach will produce excessive run times as many thousands of piston revolutions much be modeled
- Another approach is to time average the heat fluxes and couple every piston iteration but this is less than ideal

- Model predicts thermal gradients from heat transfer between in-cylinder gas and solids.
- Highest T occurs where at piston surface where spray combustion takes place most vigorously.
- Model predicts in-cylinder spray combustion and determines Temperature distribution on the solid surface using the improved KIVA-4-MPI code!



Temperature distributions in the gas and solid phases for selected timings at the 50th simulation cycle

Temperature distributions on the piston surface after 50 simulation cycles

10

50 engine cycles are run and steady CHT results are still not reached

http://www1.eere.energy.gov/vehiclesandfuels/pdfs/merit_review_2012/adv_combustion/ace014_carrington_2012_o.pdf

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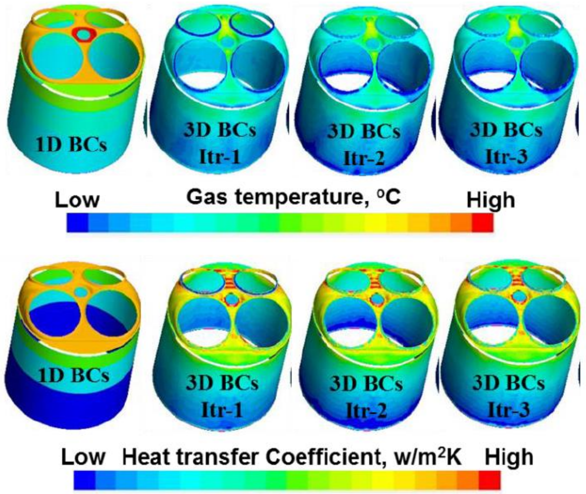
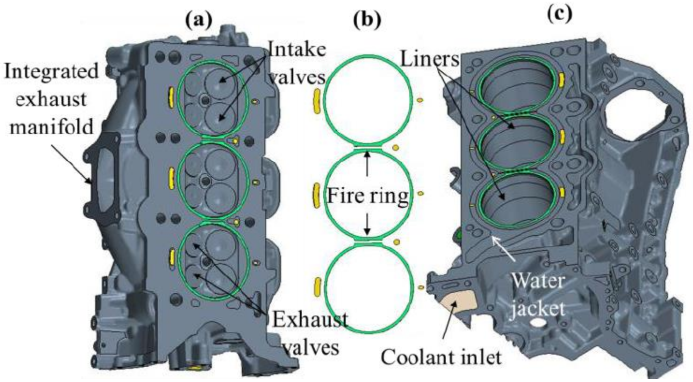
Conjugate Heat Transfer

- In v2.1 CONVERGE can perform conjugate heat transfer (fluid and solid portions) all is one simulation
- Therefore, coupling with other heat transfer tools will no longer be necessary to determine the metal/fluid temperatures
- Like the fluid flow, all meshing for conjugate heat transfer will be fully automated and done by CONVERGE at runtime
- Appropriate super-cycling techniques for handling the disparate time-scales of heat transfer and fluid flow will be available to minimize run times
    - The super-cycling averages heat fluxes and periodically freezes the fluid flow and solves the energy equation steady state
    - Then fluid and solid regions are solved together to adjust to the new solid temperature field, and prepare for the next super-cycle stage
    - The user controls the averaging periods and coupling frequency
    - Testing has shown that steady metal temperature can be achieved in approximately three piston revolutions
- Current testing is done on simulating the combustion and heat transfer to the block and coolant flows (results coming soon)

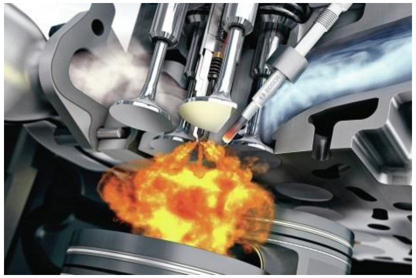




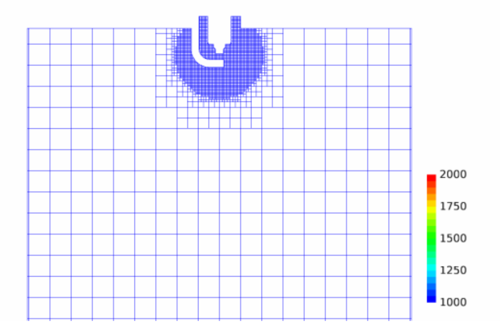
ICEF2013-19227

Conclusion

- CONVERGE is a powerful tool for rapidly and accurately simulating ICengine flow, spray and combustion
  - CONVERGE users can perform engine analysis cheaper, faster and better than with competitors' products
  - Leverage economies of scale by using one common CFD tool for all engine types
  - With geometry/meshing issues largely removed, clients are free to perform simulations which push the technical envelope (knocking, multi-cylinder, detailed chemistry etc)
  - By using CONVERGE, engine manufacturers can design engines instead of making meshes



- There are many exciting new developments with CONVERGE:
  - CONVERGE Studio for setup
  - Gamma Technologies collaboration (CONVERGE-Lite & Two way coupling)
  - CONGO for genetic algorithm optimization
  - SAGE continues to get much faster
  - Injector modeling with cavitation
  - Grid convergent spray modeling
  - Conjugate heat transfer
  - Eulerian spray modeling
  - HPC performance improvements (METIS etc)
  - Advanced emissions modeling



- CONVERGE will continue to push the technical envelope with goal of helping our clients' in their never ending quest to provide cleaner and more fuel efficient engines to the global marketplace

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Use CONVERGE CFD and never make a mesh again