Model Development and Analysis of Clean & Efficient Engine Combustion

2016 DOE Hydrogen and Fuel Cells Program and Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting

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Lawrence Livermore National Laboratory

Overview

Timeline

- Ongoing project with yearly direction from DOE

Barriers

- Inadequate understanding of the fundamentals of HECC
- Inadequate understanding of the fundamentals of mixed mode operation
- Computational expense of HECC simulations

Budget

- FY15 funding: $508K
- FY16 funding: $508K

Partners

- AEC Working Group:
  - Sandia NL, GM, Oak Ridge NL
- Industrial:
  - Convergent Science Inc.
  - Nvidia

Relevance – Enhanced understanding of HECC requires expensive models that fully couple detailed kinetics with CFD

Objective

Reduce time to solution for advanced engine combustion simulations.

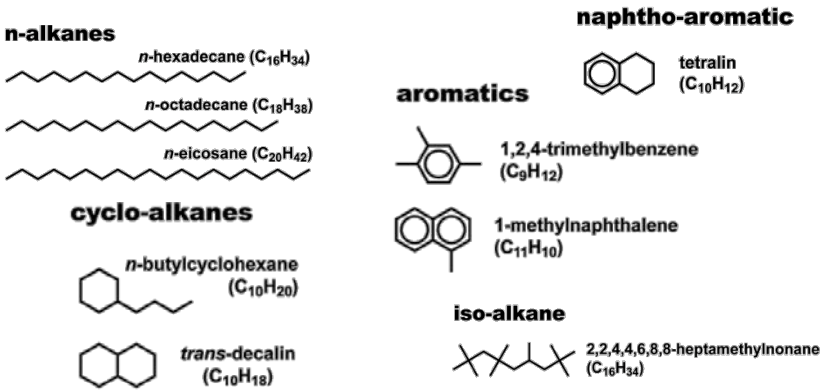
- Accelerates R&D on three major challenges identified in the VT multi-year program plan:

  A. *Lack of fundamental knowledge of advanced engine combustion regimes*

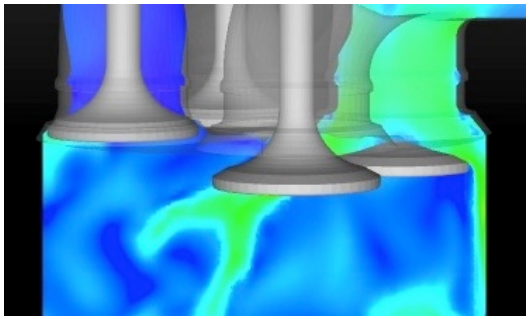
  C. *Lack of modeling capability for combustion and emission control*

  D. *Lack of effective engine controls*

We want to use detailed chemistry



in highly resolved engine simulations



Accurate simulations yield improved engine designs.

Milestones

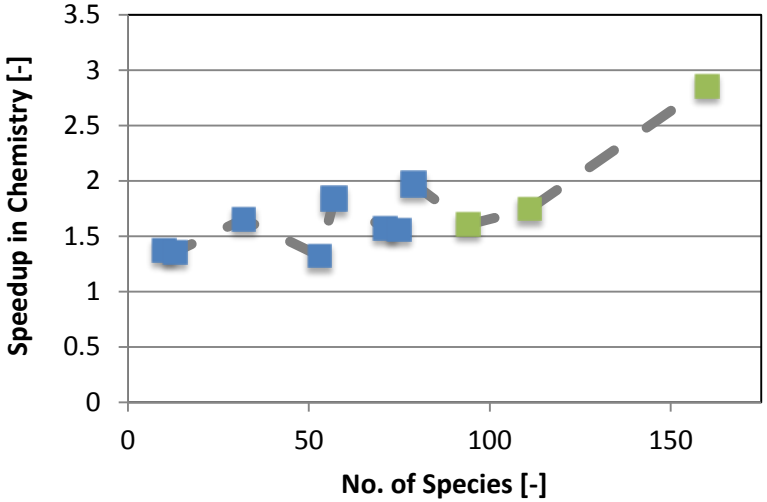
Milestone Name/Description	End Date	Type	Project	Status
Improved mechanism for iso-cetane	12/31/2015	Quarterly	ACE013	✓
Create a technical report on mechanism repair and user guide for the LLNL inspection and repair utility	6/30/2016	Quarterly	ACE076	on schedule
Evaluate different load-balancing schemes for chemical kinetics in parallel CFD simulations and implement most promising technique.	9/30/2016	Quarterly	ACE012	on schedule
Evaluate research progress and impact	3/31/2016	Annual	ACE012, ACE013, ACE076	✓

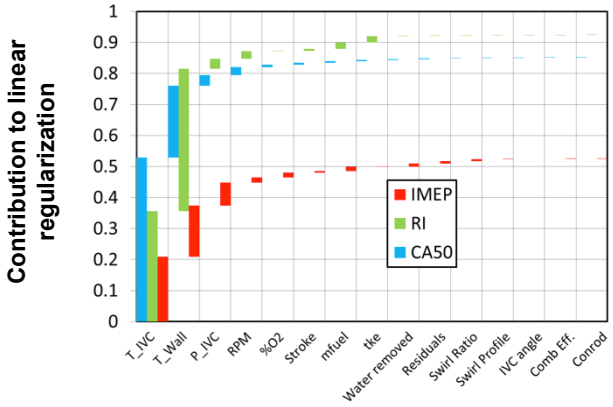
Approach: Develop analysis tools leading to clean, efficient engines in collaboration with industry, academia and national labs.

- Gain fundamental and practical insight into HECC regimes through numerical simulations and experiments
- Develop and apply numerical tools to simulate HECC by combining multidimensional fluid mechanics with chemical kinetics
- Reduce computational expense for HECC simulations
- Make accurate and efficient models accessible to industry
- Democratize simulation: bring chemical kinetics-fluid mechanics computational tools to the desktop PC

Accomplishments presented at 2015 AMR

- Fast chemistry in CFD
  - 1.5-2x speedup for "engineering" size mechanisms (10-100 species) on CPU
  - Additional speedup using GPU accelerator
- Uncertainty Quantification in HCCI engine simulation
  - Fast chemistry enabled large sampling of HCCI engine sensitivity
  - Results indicate that large uncertainty in temperature leads to high variability in key engine performance metrics (IMEP, RI, CA50)

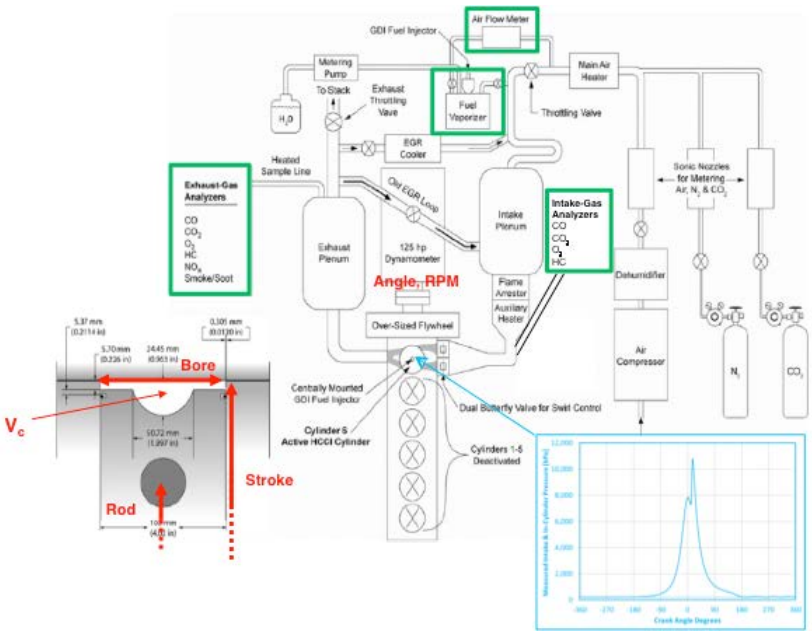




Technical Accomplishments

Uncertainty analysis of HCCI experiments at SNL

- Need to understand uncertainty in model inputs
- Need basis for comparing model outputs to experimental outputs



Measured Quantities

Crank angle
Engine speed
Geometry (Bore, stroke, rod, V_c)
Intake air and fuel flow
X_i (dry), i=CO,CO_2,O_2, Nox, HC
Intake pressure
In-cylinder pressure

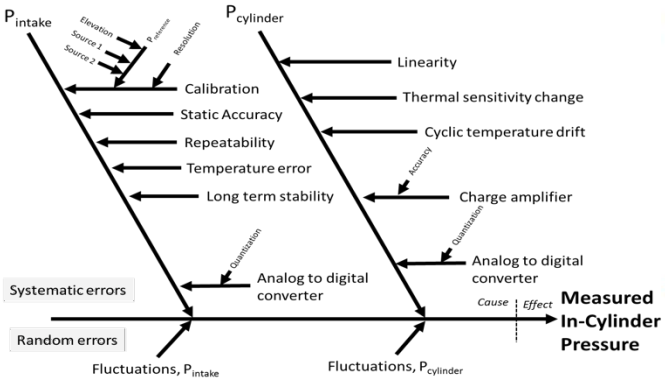
Derived Quantities

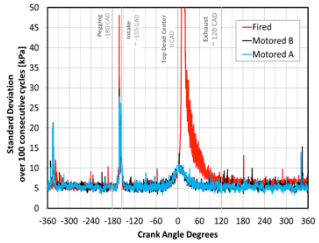
Compression Ratio
Air/fuel mixture (phi)
T_{IVC}, T_{EVO}, $T_{exhaust}$, $T_{residuals}$, T_{BDC}
X_i (actual)
%residual, %EGR
%water removal in EGR loop
%water removal upstream gas analyzers
IMEP, heat release, Ringing Intensity

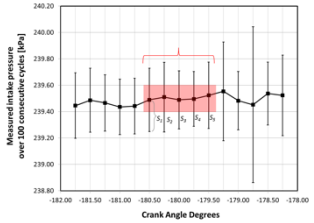
Technical Accomplishments

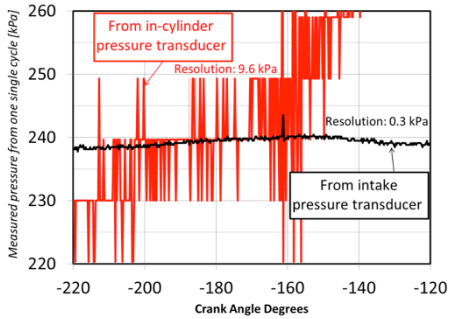
Uncertainty analysis of HCCI experiments at SNL

- First: "bottom up" analysis of measurement uncertainty
- Shown here, in-cylinder pressure measurement
- Many sources of uncertainty must be identified and quantified
- Combined uncertainties provide confidence interval for P_{cyl}









Technical Accomplishments

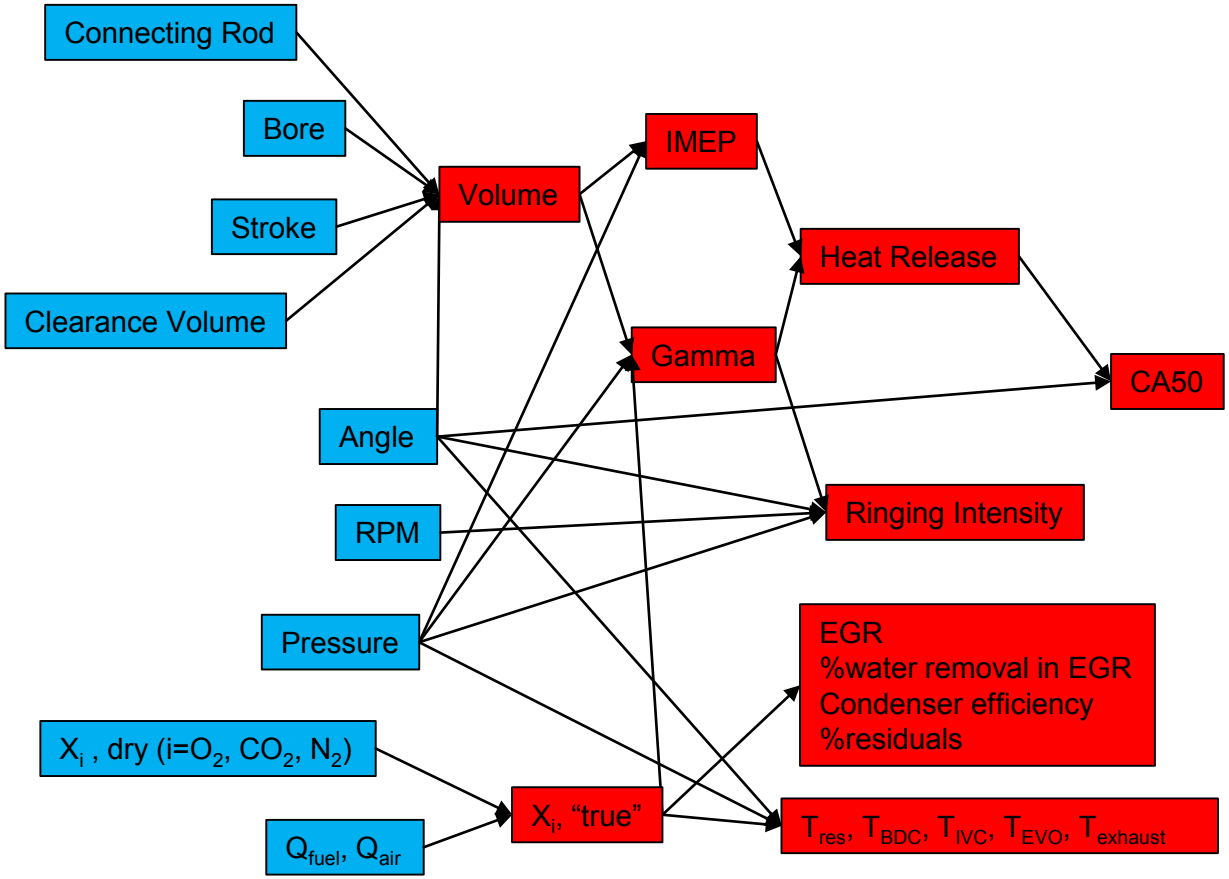
Uncertainty analysis of HCCI experiments at SNL

- Same "bottom-up" approach must be used for each measured quantity, reported here
- Each measurement presents its own challenges
- Assumptions necessary in some cases (e.g. machining tolerances)

	Experimentally measured quantity	Typical Mean Value	Experimental error	Assumed Distribution	Standard uncertainty
Geometry	Bore	0.10223 m	±3e-6 m	Uniform	1.7e-6 m
	Stroke	0.12 m	±2.5e-5 m	Uniform	1.4e-5 m
	Connecting rod	0.192 m	±2.5e-5 m	Uniform	1.4e-5 m
	Clearance volume	75.77 mL	±0.25 mL	Uniform	0.14 mL
	Crank angle	0 to 360 CAD	±0.05 CAD	Uniform	0.03 CAD
	Engine speed	1200 RPM	±24 RPM	Normal (95%)	12.2 RPM
Pressure	BDC Pressure	240 kPa	±6.62 kPa	Normal (95%)	3.31 kPa
	In-cylinder Pressure	240 to 10,900 kPa	±60 to 320 kPa	Normal (95%)	31 to 162 kPa
Composition	Air flow intake	10.98 g/s	±0.02 g/s	Normal (95%)	0.01 g/s
	Fuel flow intake	0.59 g/s	±2% (relative)	Normal (95%)	6 mg/s
	CO_2 intake	5.59%	±0.075 % (absolute)	Normal (95%)	0.04%
	O_2 intake	12.5%	±0.22 % (absolute)	Normal (95%)	0.11%
	CO_2 exhaust	11.4%	±0.16 % (absolute)	Normal (95%)	0.08%
	O_2 exhaust	5.01%	±0.22 % (absolute)	Normal (95%)	0.11%
	Combustion efficiency	98.42 %	1 % (absolute)	Triangular	0.4%

Uncertainty analysis of HCCI experiments at SNL

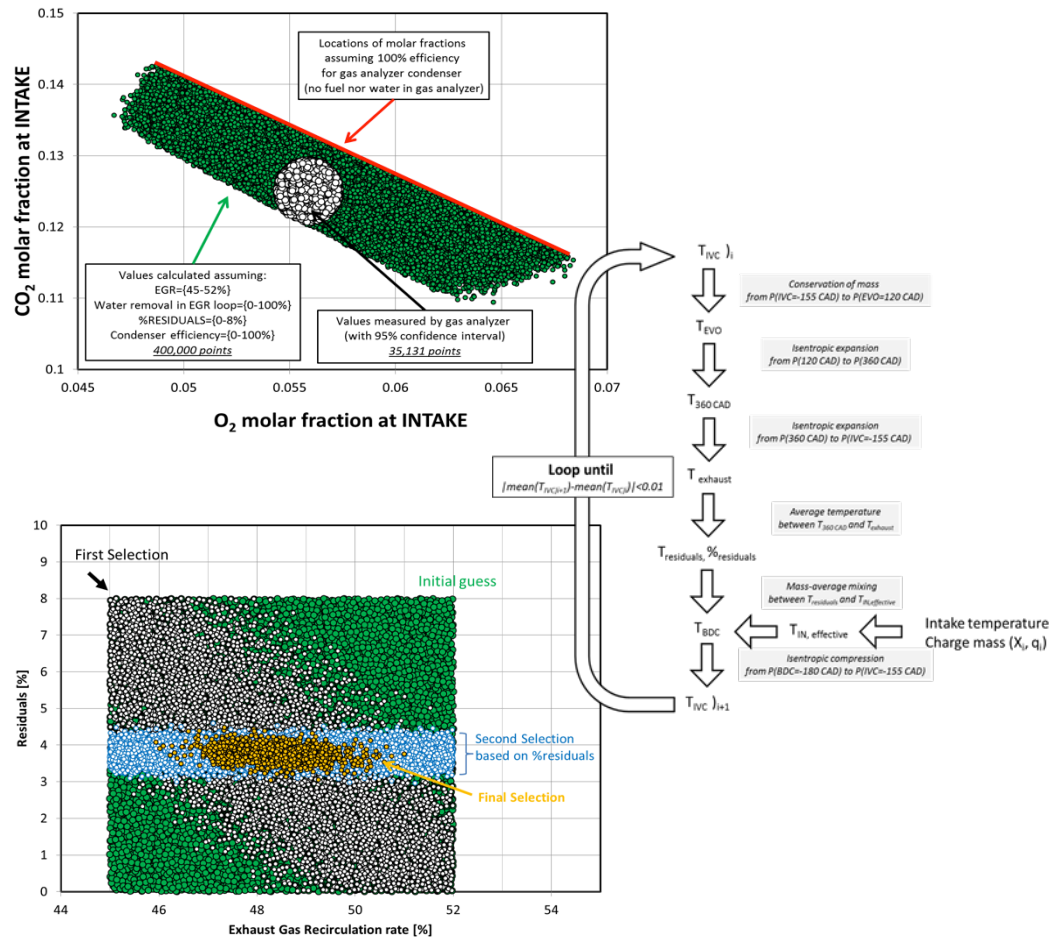
- Measured uncertainty propagated to determine uncertainty in derived quantities
  - Linear method
  - Monte Carlo method
  - Bayesian inference



Technical Accomplishments

Uncertainty analysis of HCCI experiments at SNL

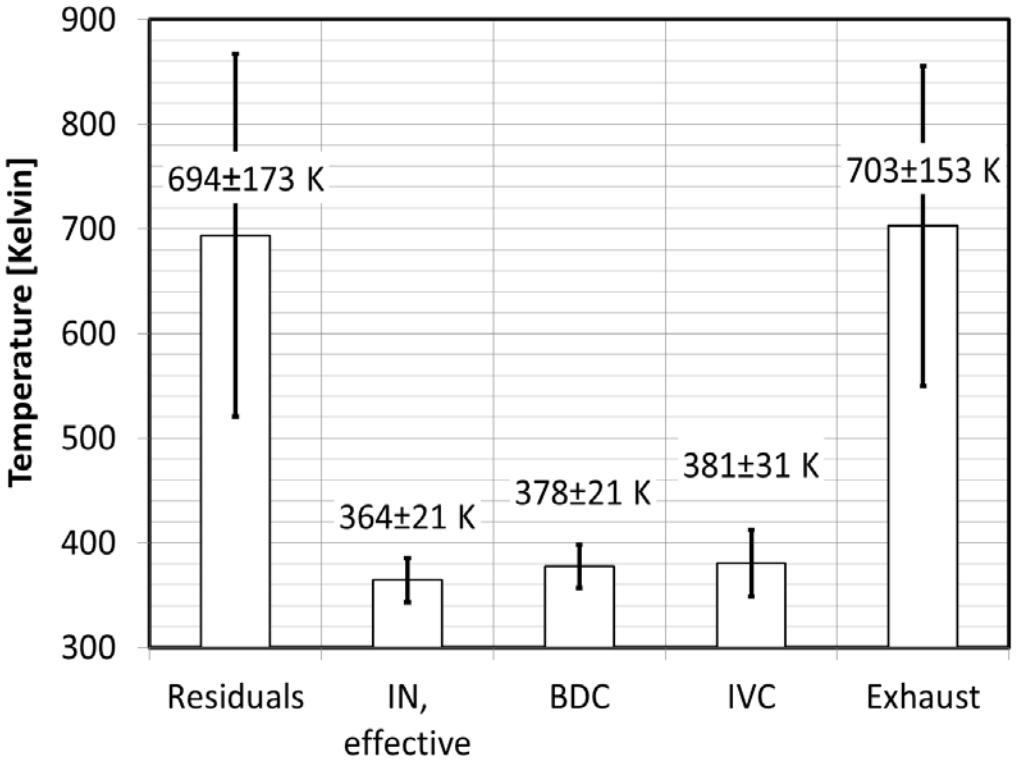
- Uncertainty in EGR loop (EGR rate and condensation) increases complexity of analysis
- Bayesian inference and Monte Carlo sampling used to constrain resulting uncertainty in mixing model



Technical Accomplishments

Uncertainty analysis of HCCI experiments at SNL

- Analysis leads to strongly supported estimates of temperature including confidence intervals
- First full accounting of uncertainties in quantities vital to advanced engine combustion models
- Promises to enhance our ability to understand and predict combustion phenomena in difficult regimes.

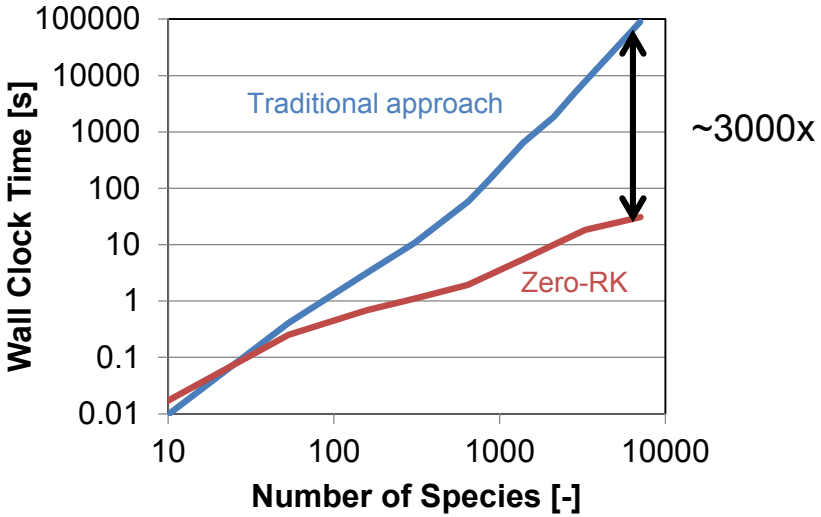


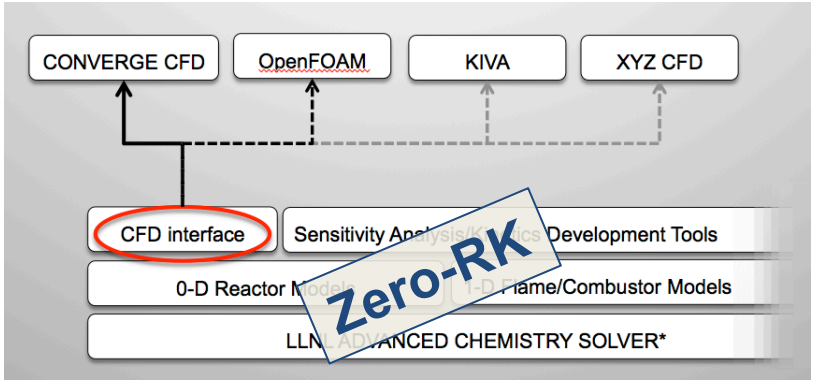
error bars indicate 95% confidence interval

Technical Accomplishments

LLNL fast-solver (Zero-RK) wins R&D 100

- Joint development between this project and ACE076 (McNenly)
- This project focuses on interface to CFD and GPU acceleration
- ACE076 focused on numerics, canonical reactors, and mechanism tools

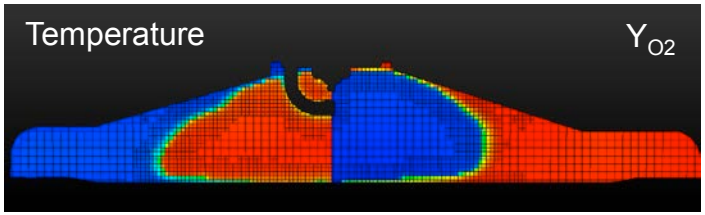


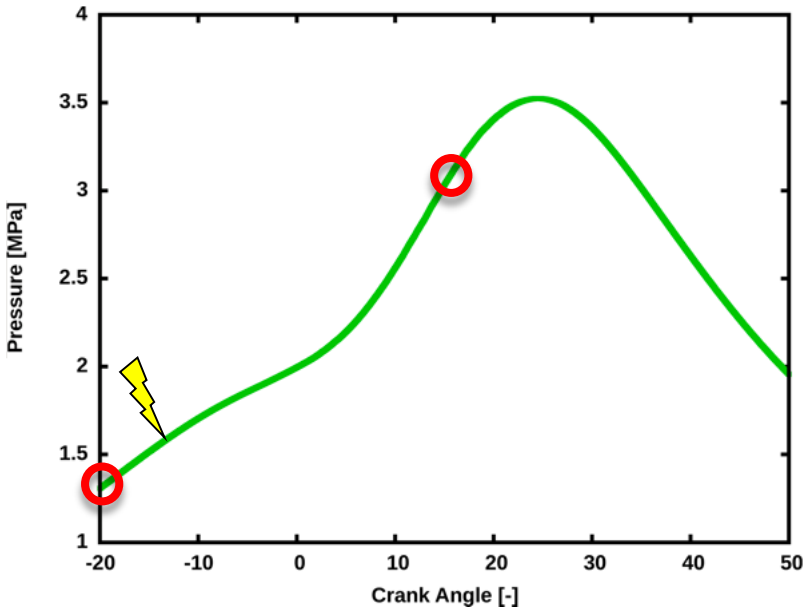


Technical Accomplishments

Development of GPU accelerated chemistry for engine simulation

- Building on accomplishment from FY15, first engine simulation using all CPU and GPUs on compute cluster node
- 16 CPU cores solved in 21.2 hours
- 16 CPU cores + 2 GPU solved in 17.6 hours
- Speedup = 21.2/17.6 = 1.20
- Not as good as hoped/expected
- Why? Explanation follows…





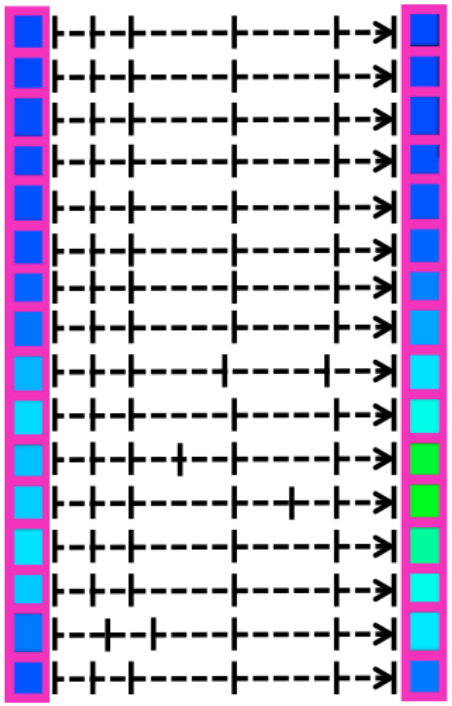
start/end of simulation time in test case spark timing

Technical Accomplishments

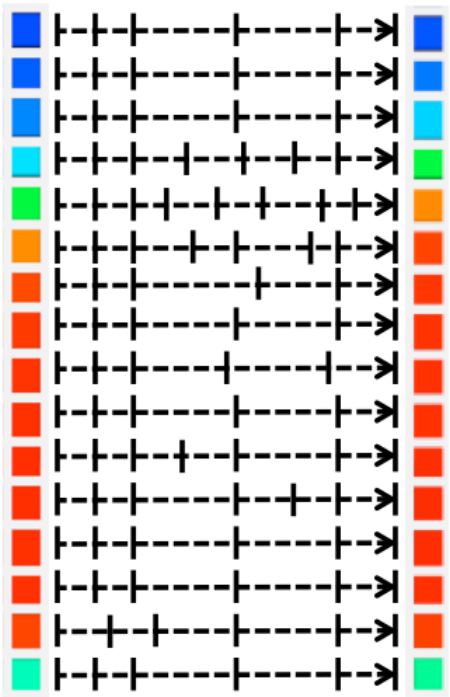
Development of GPU accelerated chemistry for engine simulation

Background/Example

- Calculating chemical source terms for single CFD time step
- Each vertical line represents sub-step in chemistry solver
- On CPU, all reactors treated independently and take their own steps



reactor set 1

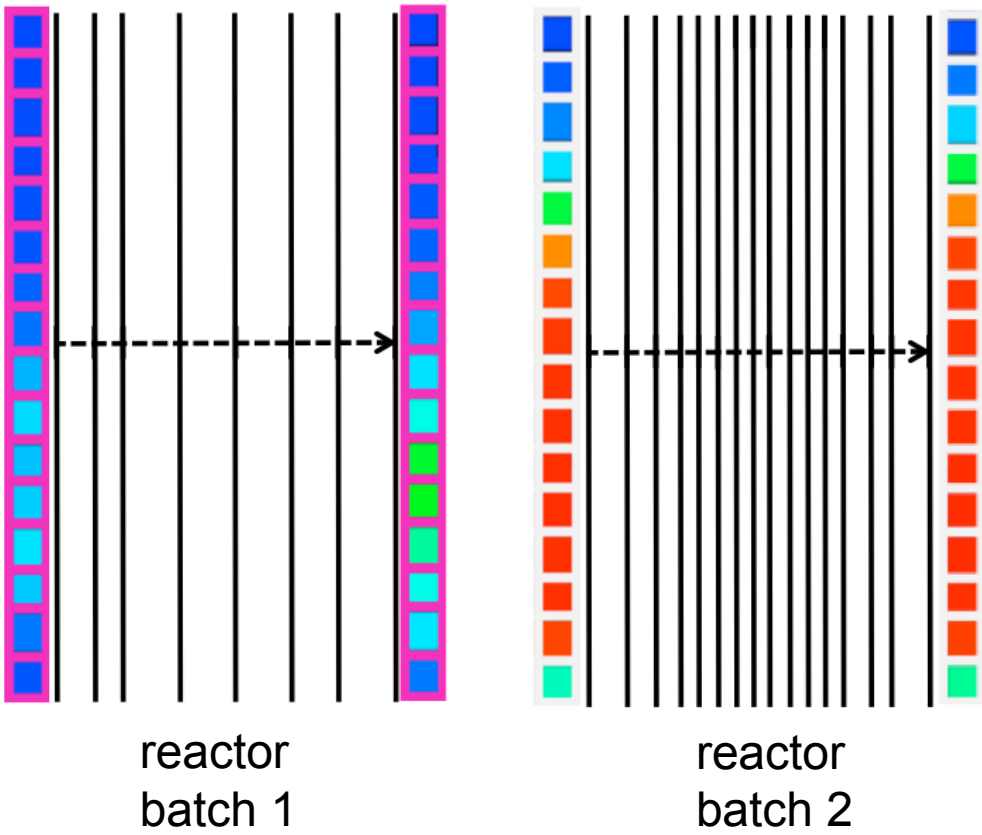


reactor set 2

Development of GPU accelerated chemistry for engine simulation

Background/Example

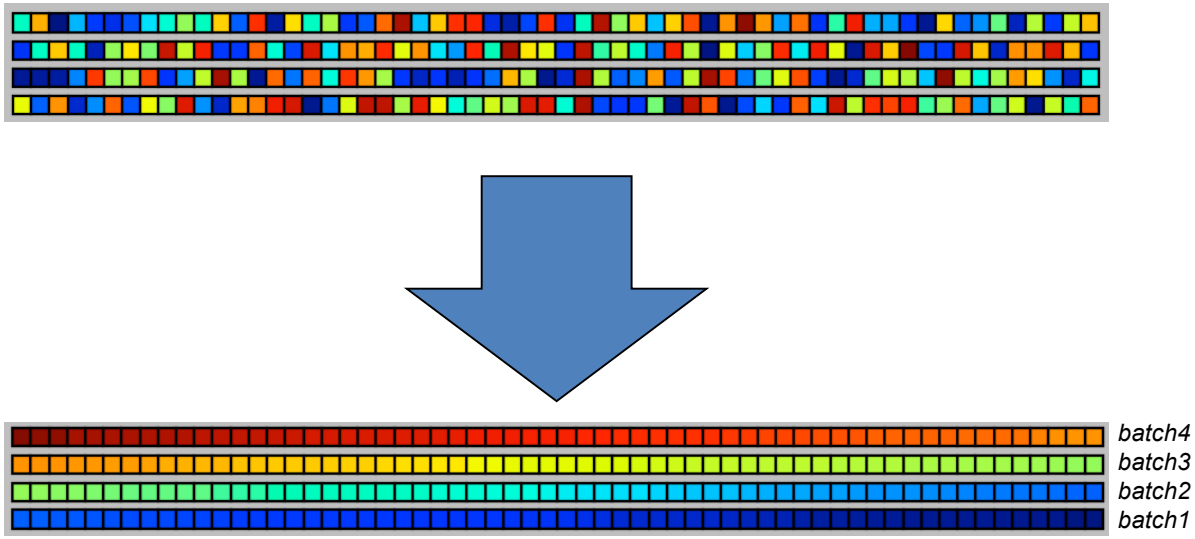
- On GPU, reactors are batched together, forcing them to take the same sub-steps
- Some batches may take excessive extra sub-steps as a result
- Extra steps cut into acceleration offered by GPU
- This is the reason why our test case was slower than expected

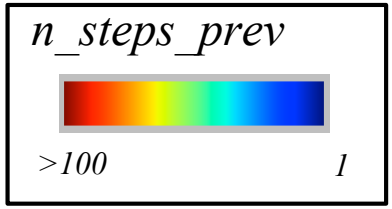


Development of GPU accelerated chemistry for engine simulation

Smart batching

- Sort reactors/cells by number of sub-steps taken on previous time step
- Sub-steps on previous cycle found to be good predictor of sub-steps required on current cycle

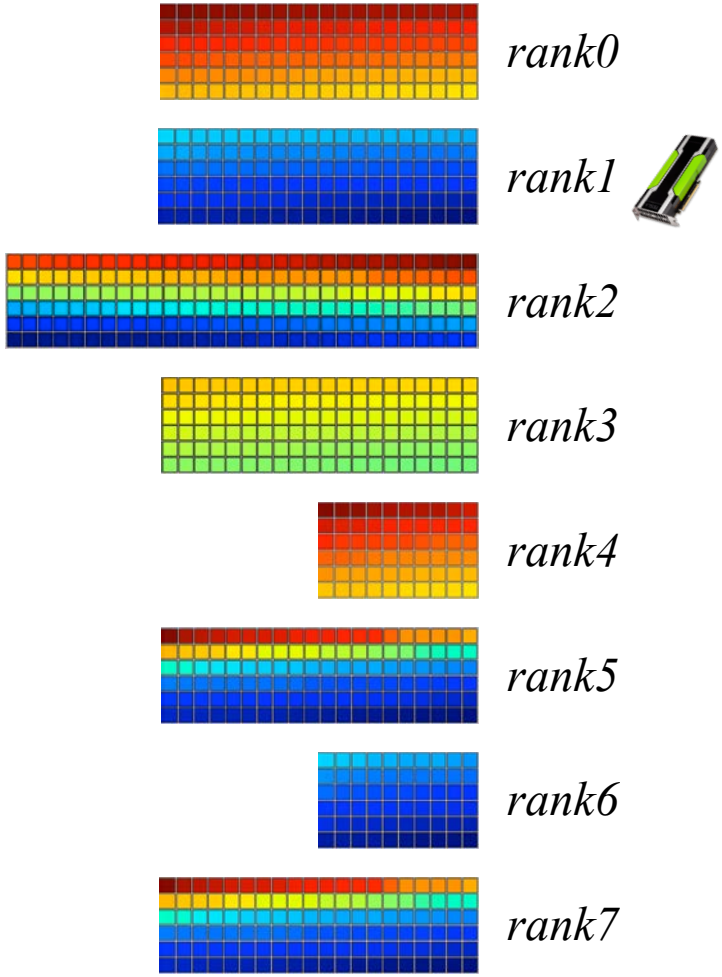




Development of GPU accelerated chemistry for engine simulation

Smart batching in practice

- Modern CFD works on distributed memory architectures
- Adding GPU's results in "heterogeneous" compute environment
- Chemistry starts unevenly balanced because not all cells have active chemistry, and not all chemistry equal cost

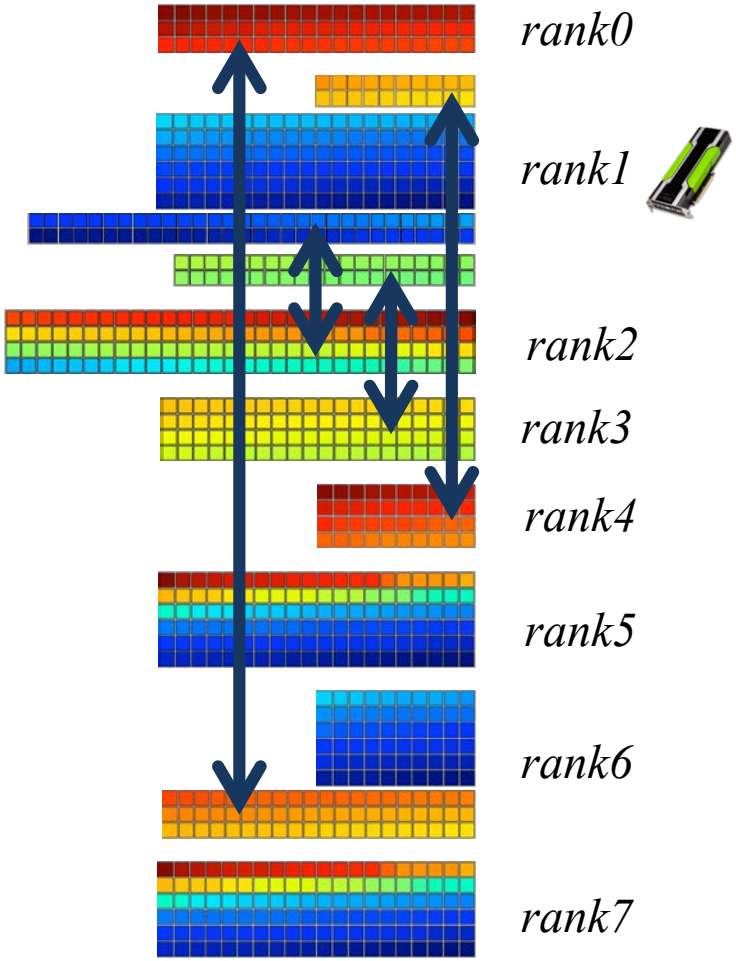


Technical Accomplishments

Development of GPU accelerated chemistry for engine simulation

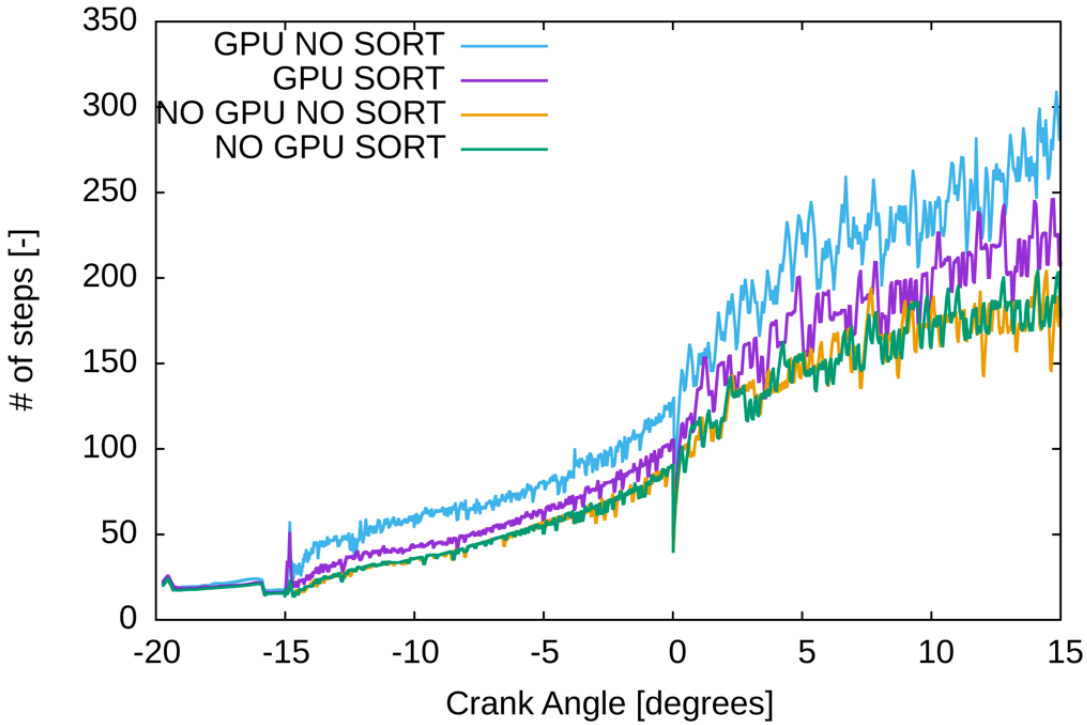
Smart batching in practice

- Use Message Passing Interface (MPI) to balance chemistry load across all “ranks”
- Balancing takes account for expected cost of cells based on previous sub-step counts
- GPU gets more work because it can process faster
- Batches on GPU are sorted to achieve best speed up



Development of GPU accelerated chemistry for engine simulation

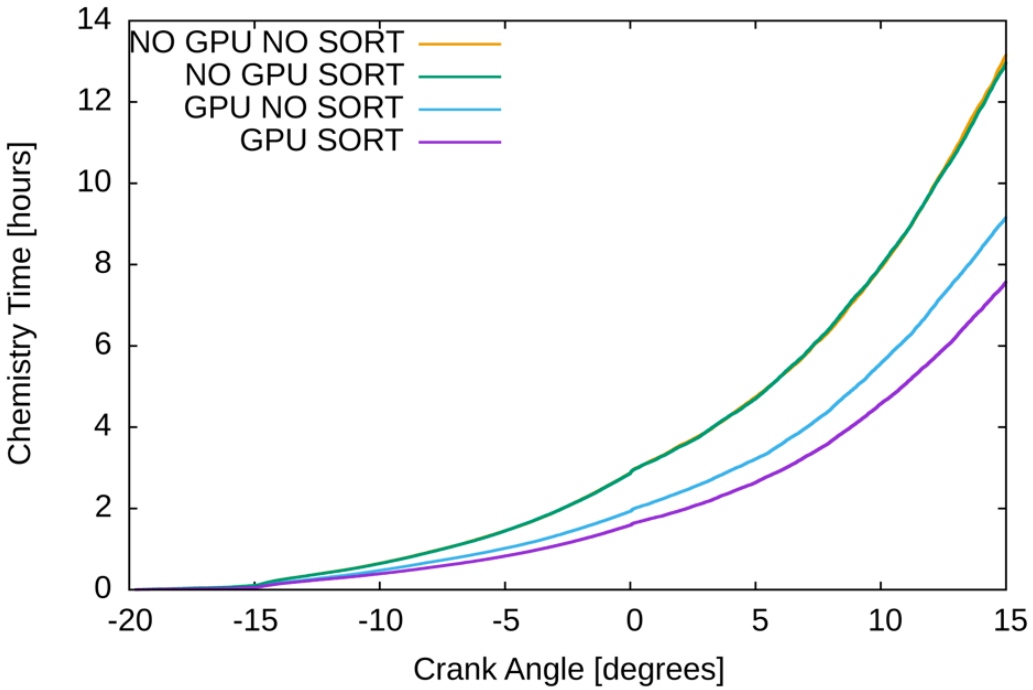
- Sorting doesn't change results if only using CPU
- Unsorted batches on GPU take 2-4x more steps than un-batched on CPU.
- Smart batches on GPU brings step counts back down; only 1.25-1.5x CPU.



Technical Accomplishments

Development of GPU accelerated chemistry for engine simulation

- New work-sharing scheme brings CPU time down from 21.2 hours to 13.1 hours
- GPU with sorted batches now < 8 hours speeding up total solution time by 1.7x
- Slope of chemistry time shows that for longer run even more reduction in time comparing CPU to GPU
- 16 CPU's + 2 GPUs (workstation class hardware)

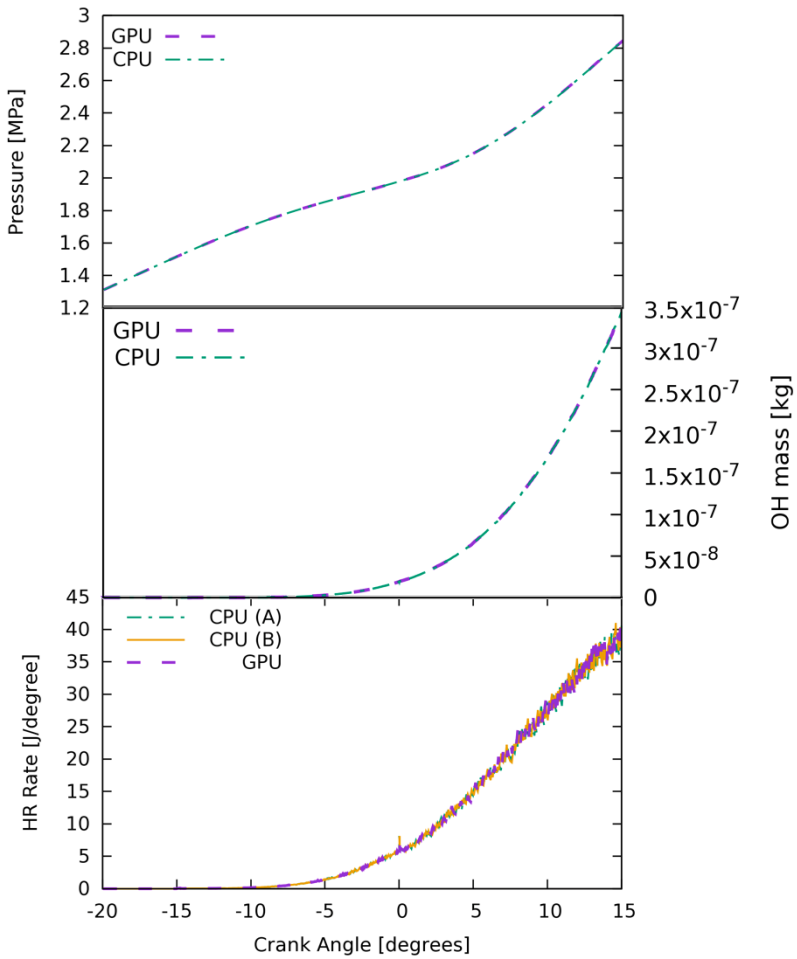


Technical Accomplishments

Development of GPU accelerated chemistry for engine simulation

Verification

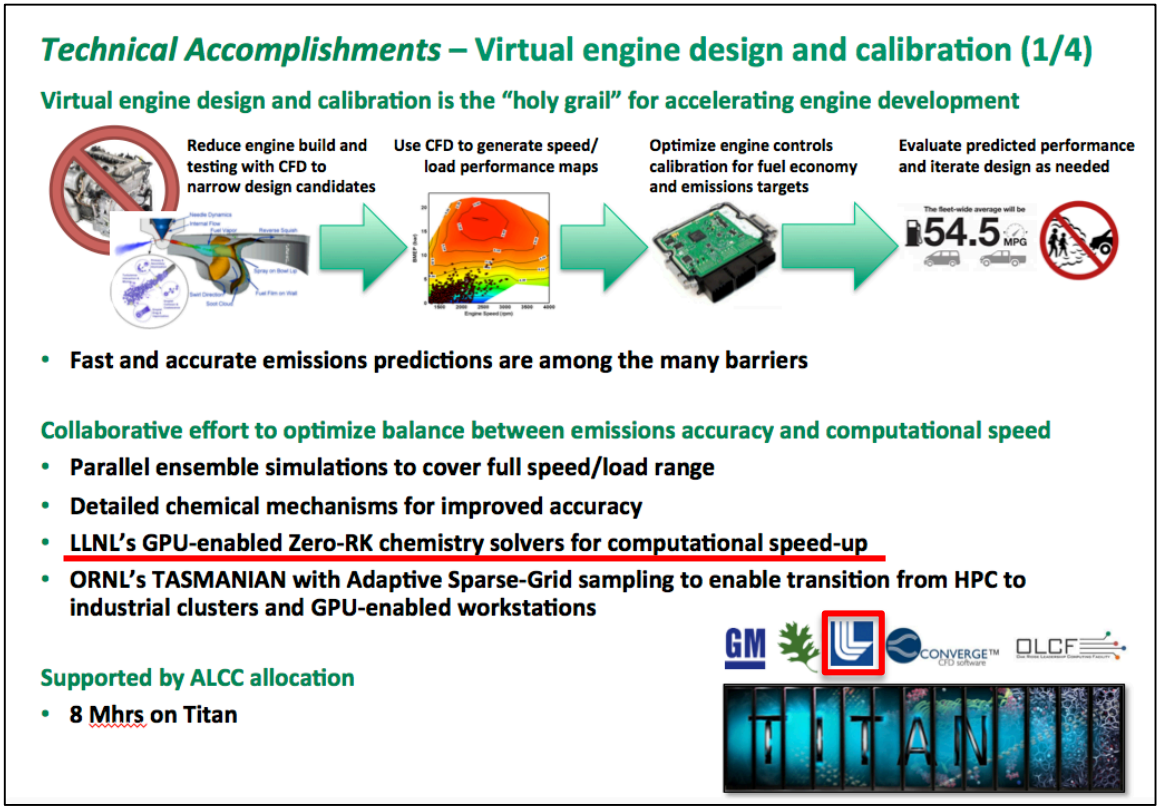
- GPU produces same result as CPU
- GPU solves same problem as CPU, just in less time
- Outputs for all quantities of interest overlap
- Heat release (HR) rate is noisy based on CFD time step selection, so match is not exact but also true in comparing two CPU runs.



Technical Accomplishments

Development of GPU accelerated chemistry for engine simulation

- Hundreds of simulations running on fastest US supercomputer
- GPU acceleration reduces time per simulation, increasing number of sims run in allocation
- Collaboration of laboratories and industry to tackle big engine combustion problems



courtesy K. Dean Edwards ACE017

FY2015 Reviewer's comments and our response

- This reviewer pointed out that the uncertainty analysis is interesting, but just running it does not teach much. There needs to be significant work to interpret the results and to show why such a wide range of results could be obtained for a relatively small space of inputs for each variable. It was mentioned depending on the outcome of such an analysis; this could open up a new area of work that could be valuable.
  - We agree that the uncertainty analysis needs to be extended to gain further insight. We have continued our application of these tools to engine experiments this year and hope to continue in future years.

- The reviewer questioned if there is a way to incorporate soot emissions in the predictions.
  - It is already possible to include phenomenological soot models with our fast solver tools. This year ACE076 (McNenly) added several capabilities to Zero-RK to handle large, detailed soot mechanisms efficiently to accelerate model development. We are also in discussions with Converge CFD to make their detailed soot models compatible with the solver and new soot models are being developed as part of ACE012 (Pitz) that will be compatible with our solver.

- The reviewer stated that the emphasis seems to be on smaller mechanisms as it is apparently not cost effective for large mechanisms which are a reasonable perspective. That said, there are other groups which seem to be incorporating large reaction mechanisms in their simulations. For example in project ace007 RAPTOR simulations of ignition delay time were reported using almost 3,000 reactions for dodecane. It was suggested it would help to place the performance of the chemistry solver in RAPTOR or other codes in the context of the chemistry solver being developed here.
  - The focus of last years work was on smaller mechanisms as many industrial users do fast turn-around simulations with 30-100 species. However, as discussed in previous AMR presentations and ACE076, the solver is very efficient for large mechanisms. The recent work shown in ACE007 on chemistry in RAPTOR is an extremely *reduced* chemical scheme starting from a large dodecane mechanism. This reduction is necessary as even normally cheap chemistry leads to unmanageable runtimes for the highly resolved LES simulations RAPTOR is used for. The reduction comes at the expense of predictive capability, especially in terms of emissions (e.g. NOx and soot).

- The reviewer suggested that some discussion of the possible overlap or distinction with the future work of ace076 should be provided.
  - The two projects benefit from each other but are distinct. ACE076 is focused on numerics, canonical reactors, and mechanism tools. This project applies the work produced in ACE076 to engine simulations, with extension to GPU and provides feedback on performance.

- The reviewer suggested that there also should be some interaction with the end-user industry. Part of the work DOE can be doing is to speed up simulations for what is currently done in industry, but part can also be making the tools faster and better for higher fidelity simulations. Without that interaction, there is little opportunity for impact.

  The reviewer reported that the collaboration with code vendors has already been noted, but should be expanded to include more. This reviewer also suggested that while some industrial partners are engaged, more need to be solicited to increase the scale of testing against real engine problems to continue validation and performance testing.
  - We are always open to more collaboration. On the industry side we have had valuable interaction with GM in the current fiscal year. On the code vendor side we are in process with LLNL IP office to make the fast solver (Zero-RK) available for wide distribution to software vendors.

Mostly positive comments and above average scores.

Collaboration – Ongoing interactions with industry, national laboratories, and universities

- Advanced Engine Combustion (AEC) working group (Industry, National labs, Univ. of Wisc., Univ of Mich., MIT, UC Berkeley) – semiannual meetings and informal collaboration
- Sandia National Laboratory – J. Dec HCCI UQ information exchange
- General Motors/Oak Ridge National Lab – Ron Grover/K. Dean Edwards "Virtual Engine Design and Calibration"; Testing CPU solver package for ConvergeCFD engine simulations with large mechanisms (>1000 species)
- Convergent Science Inc. (CSI) – Multi-zone model development, thermo-chemical functions, coupling detailed soot to Zero-RK in ConvergeCFD
- NVIDIA – Hardware, software and technical support for GPU chemistry development

Remaining Challenges and Barriers

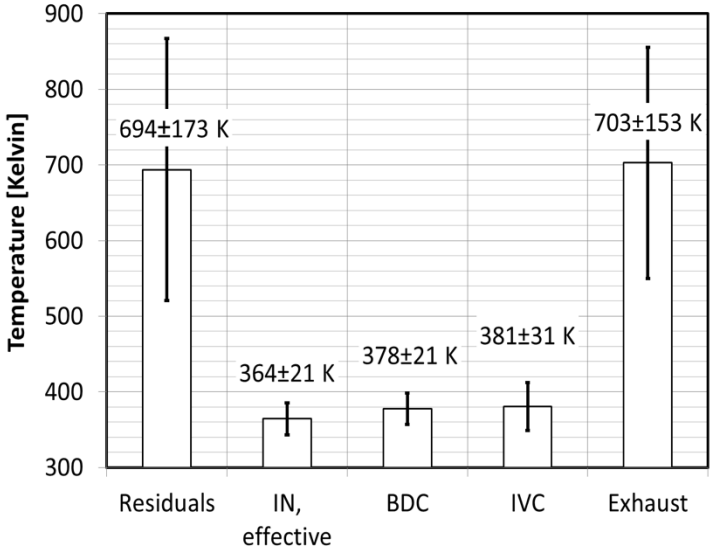
- Chemistry still not fast enough
  - In current test case chemistry still >80% of total time
  - Want to add more chemistry (100-1000's of species)
  - Want to include detailed soot
- Uncertainties analysis incomplete
  - Link uncertainty in models with uncertainty in experiments
  - Currently limited to single set of HCCI engine experiments

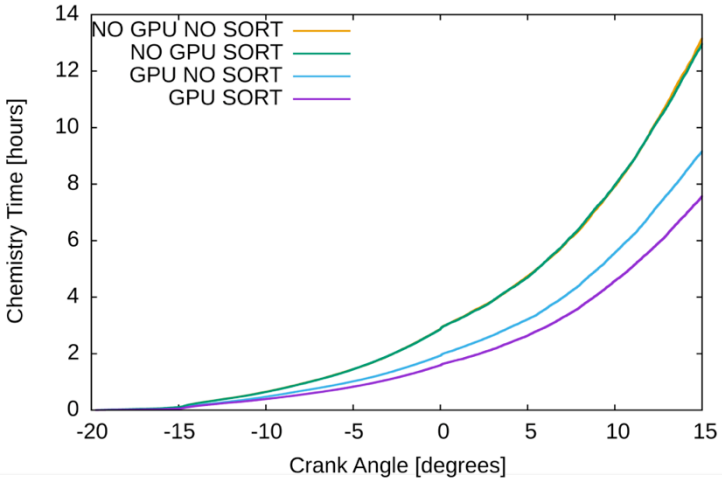
Future Work

- Continue to reduce time to solution for combustion chemistry
  - Alternate time integration schemes (CPU+GPU)
  - Continue to tune GPU for better acceleration
  - More collaboration with industry and labs
- More UQ work to inform both experiments and simulations
  - Close the uncertainty loop: experiments ⟷ models
  - Expand analysis to other engine configurations
  - Help make UQ analysis in engine research "standard" practice

Summary: Our work continues to improve state of the art in advanced engine combustion modeling

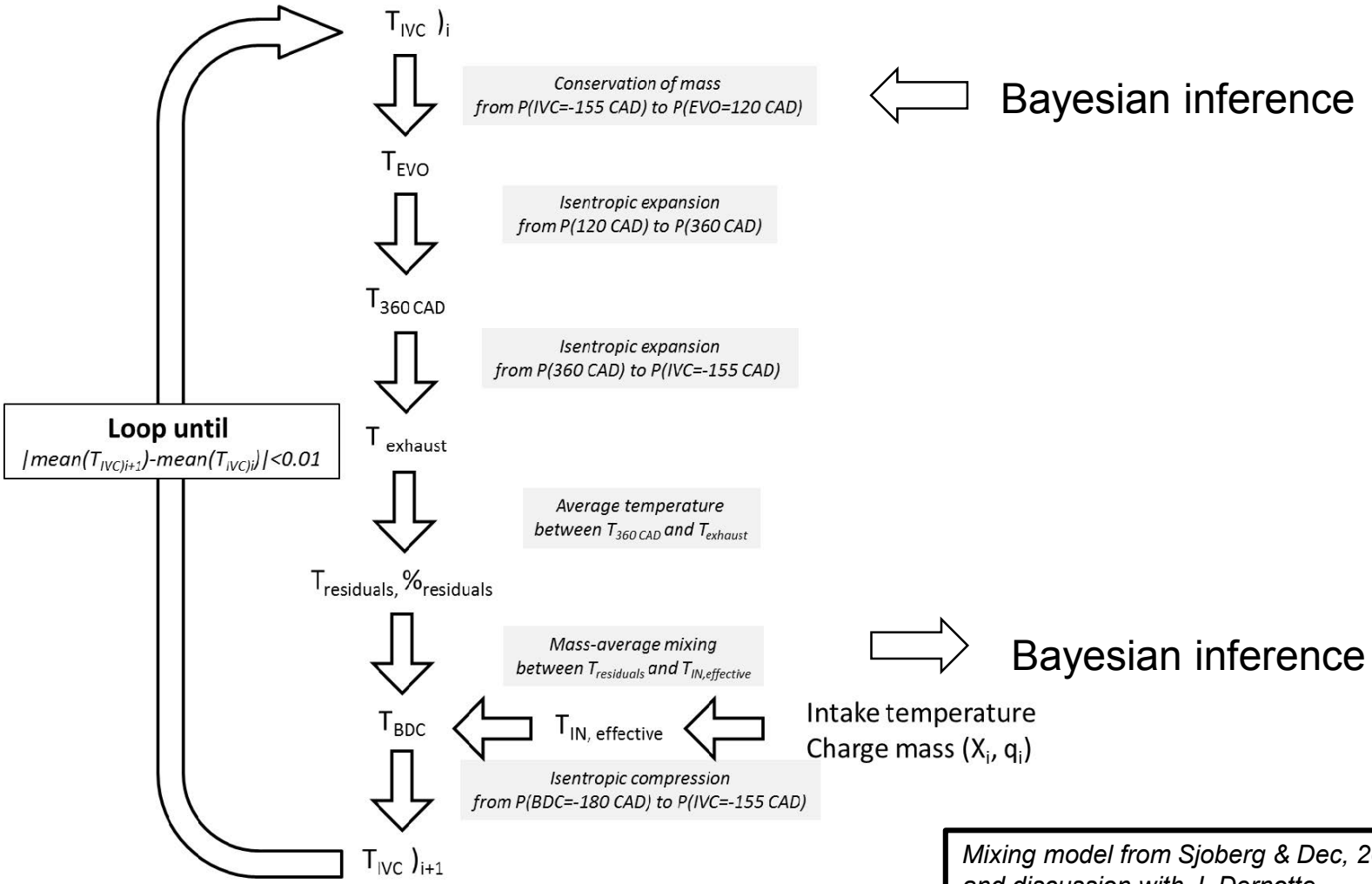
- Uncertainty analysis:
  - First full accounting of uncertainties in quantities vital to advanced engine combustion models
  - Promises to enhance our ability to understand and predict combustion phenomena in difficult regimes.
- GPU fast chemistry solution:
  - Continued reduction in time to solution
    - More fidelity in the same time
    - Faster turn-around for designers
  - Partnering with industry and other labs to prove applicability in range of engine configurations





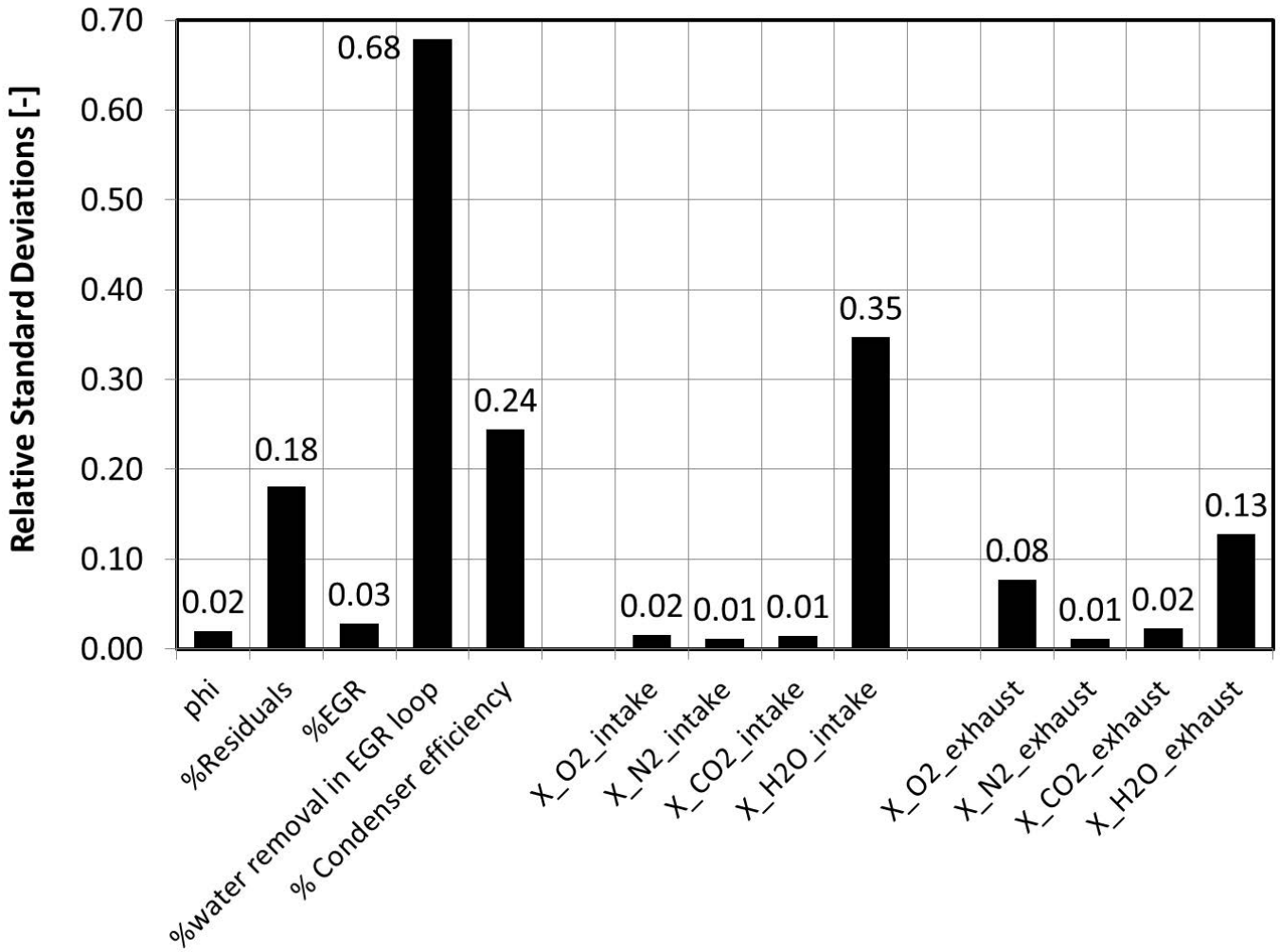
Technical Backup Slides

An iterative method, coupled with Monte Carlo methods, is used to estimate temperatures

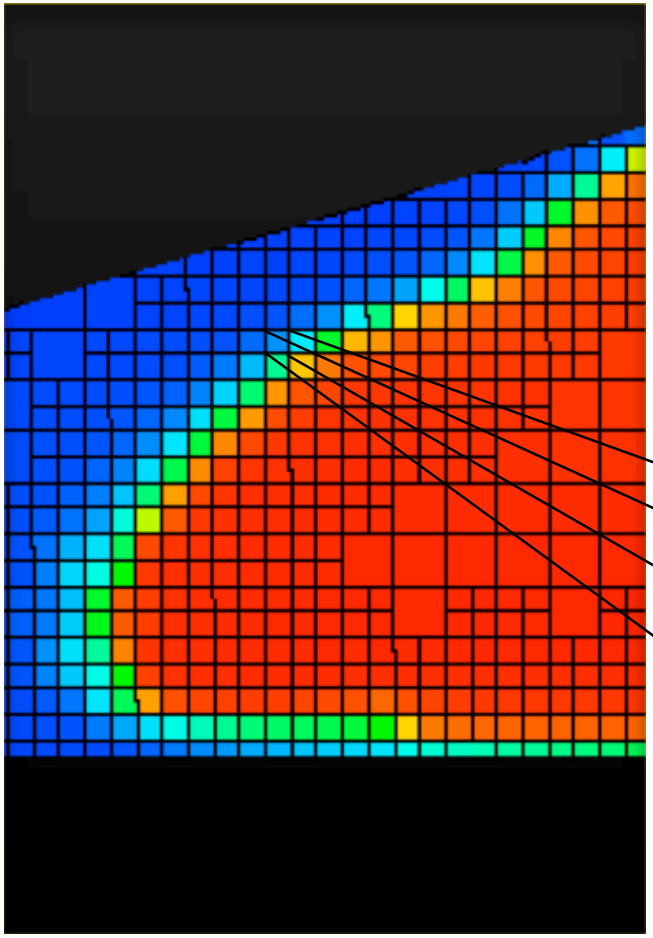


Mixing model from Sjoberg & Dec, 2004-01-1900 and discussion with J. Dernotte

Bayesian inference, coupled with Monte Carlo methods, enables to characterize true composition

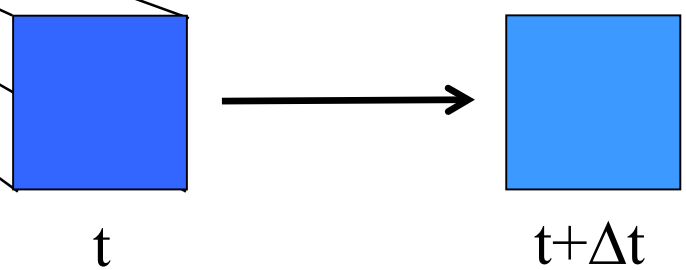


Detailed Chemistry in Reacting Flow CFD:



Operator Splitting Technique:

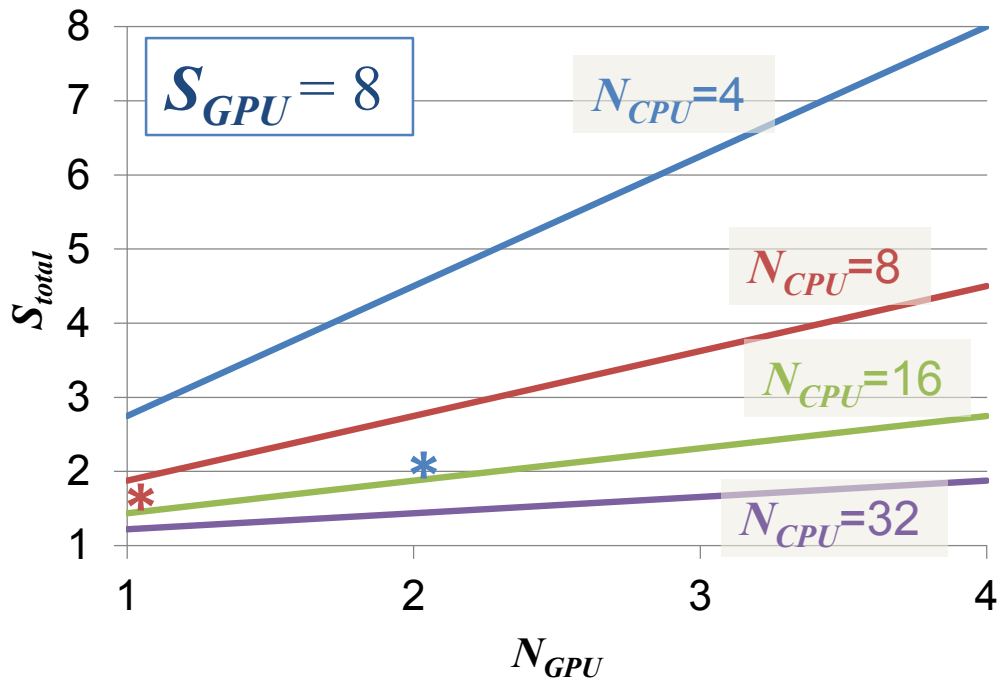
Solve independent set of ordinary differential equations (ODEs) in each cell to calculate chemical source terms for species and energy advection/diffusion equations.



Ideal CPU-GPU Work-sharing

$$S_{GPU} = \frac{walltime(CPU)}{walltime(GPU)}$$

$$S_{total} = \frac{\left(N_{CPU} + N_{GPU}\left(S_{GPU} - 1\right)\right)}{N_{CPU}}$$



- # CPU <u>cores</u> = N_{CPU}
- # GPU <u>devices</u> = N_{GPU}

```
* TITAN   (1.4375)
* surface (1.8750)
```