Model Development and Analysis of Clean & Efficient Engine Combustion

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Project ID # ACE012

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

- FY13 funding: $740K
- FY14 funding: $475K

Partners

- AEC Working Group:
  - Sandia NL, Cummins
- Universities:
  - UC Berkeley, Univ. of Wisconsin, Clemson Univ., SFSU

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

Objective

Create faster and more accurate combustion solvers.

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

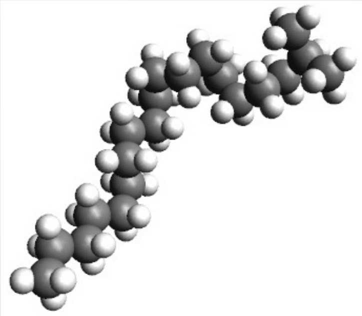
  A. Lack of fundamental knowledge of advanced engine combustion regimes

  C. Lack of modeling capability for combustion and emission control

  D. Lack of effective engine controls

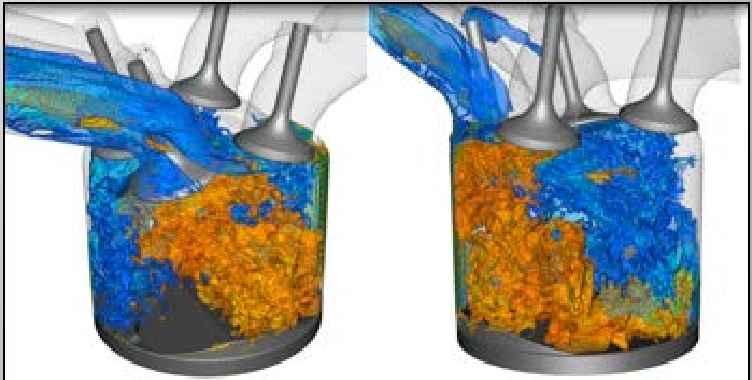
We want to use…

Detailed chemistry



Ex. Biodiesel component $C_{20}H_{42}$ (LLNL)
7.2K species
53K reaction steps

in highly resolved 3D simulations



Ex. SI/HCCI transition ~10M cells for Bosch in LLNL's hpc4energy incubator

Accurate simulations yield improved engine designs

Objective: Enhance understanding of clean and efficient engine operation through detailed numerical modeling

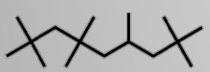
n-alkanes

n-hexadecane ($C_{16}H_{34}$)

n-octadecane ($C_{18}H_{38}$)

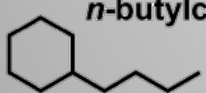
n-eicosane ($C_{20}H_{42}$)

iso-alkane

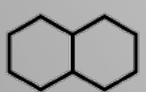


2,2,4,4,6,8,8-heptamethylnonane ($C_{16}H_{34}$)

cyclo-alkanes

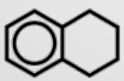


n-butylcyclohexane ($C_{10}H_{20}$)



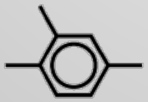
trans-decalin ($C_{10}H_{18}$)

naphtho-aromatic

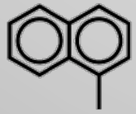


tetralin ($C_{10}H_{12}$)

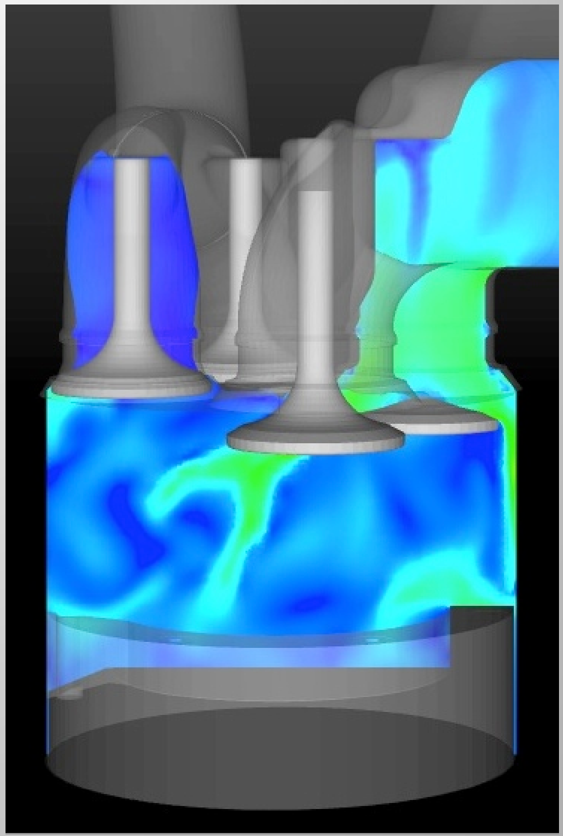
aromatics



1,2,4-trimethylbenzene (C_9H_{12})



1-methylnaphthalene ($C_{11}H_{10}$)



Representative Detailed Chemical Kinetics

High-Fidelity Fluid Mechanics

Accurate simulations yield improved engine designs

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

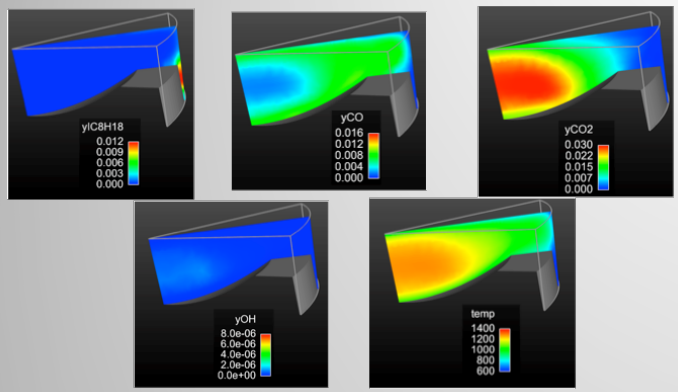
Enable more accurate simulations via more detailed physical representation

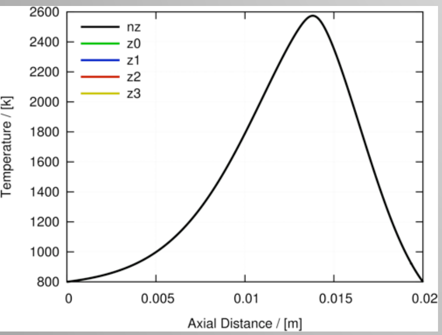
Milestones: We are developing and validating detailed engine and combustion modeling tools

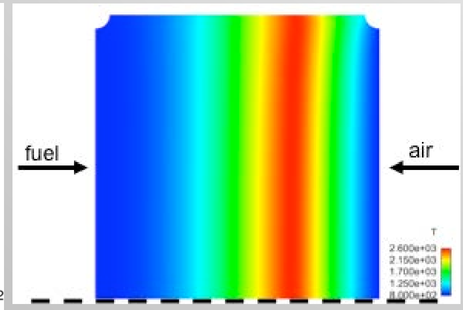
- ✓ GPU chemistry solver development
- ✓ CFD-model interface improvements
- Simulations of fuel effects in PCCI experiments
- Simulations of surrogate diesel engine experiments

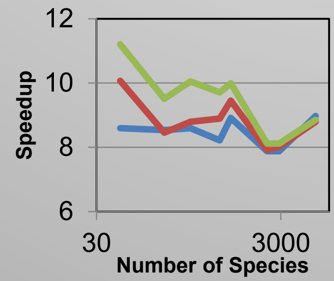
We are on track.

FY2013 Accomplishments





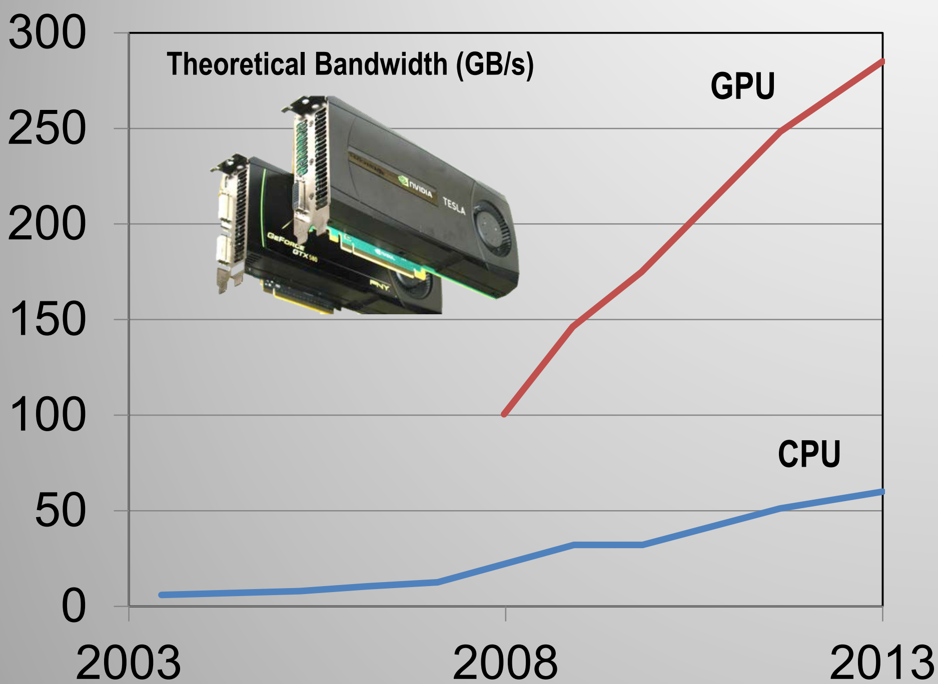




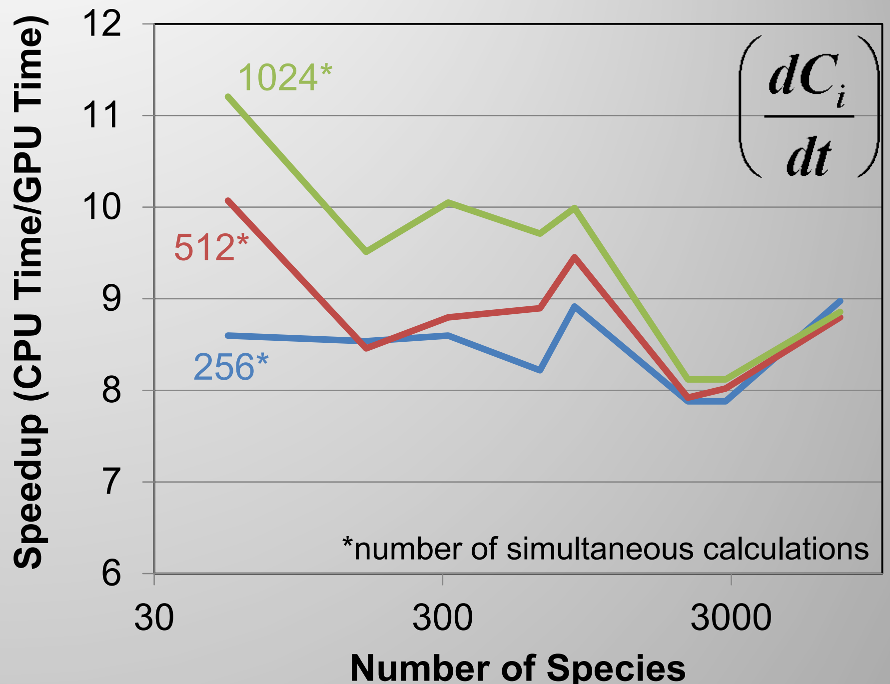
- Implemented advanced solvers with Converge multi-zone, ***orders of magnitude reduction in simulation time***
- Partnered with Cummins/Converge to integrate GPU-based solver into multidimensional CFD, **developed and tested GPU combustion chemistry with *potential 10x speedup***
- ***New license agreement*** for advanced CPU/GPU solvers **with Convergent Science Inc.**
- Validated Multi-dimensional simulations of iso-octane PCCI using Converge multi-zone with detailed chemistry
- Demonstrated CFD/multi-zone applied to GDI SI and PCCI operation
- Validated new multi-zone scheme, quantified accuracy and fidelity for zone strategies

Significant achievements in simulation performance and efficiency.

Technical Accomplishment: We are advancing our work using GPU accelerators to bring more capability to the engine designer



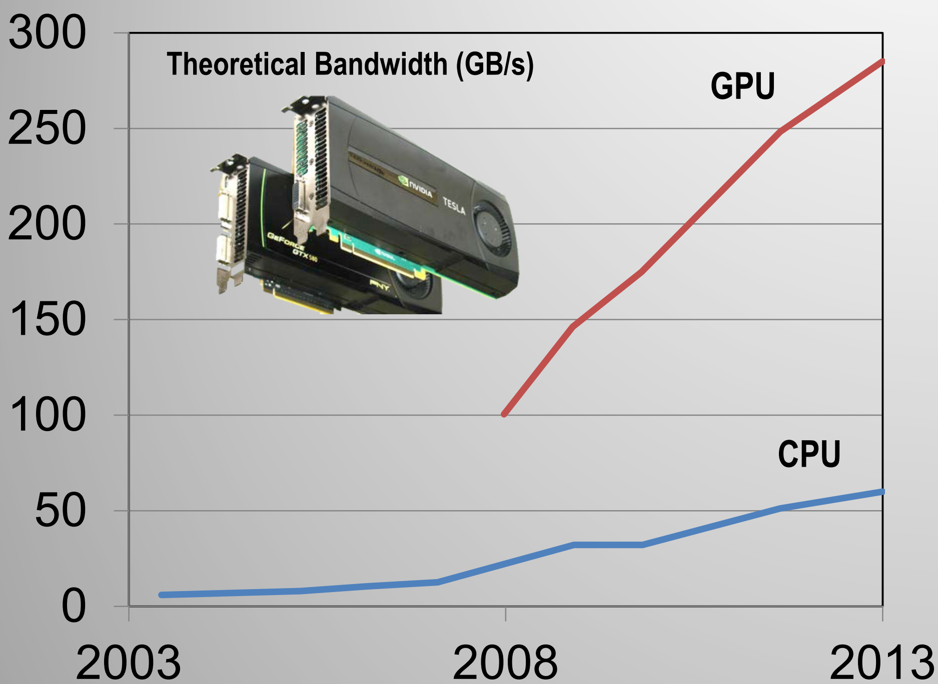
The high performance computing hardware landscape is changing.

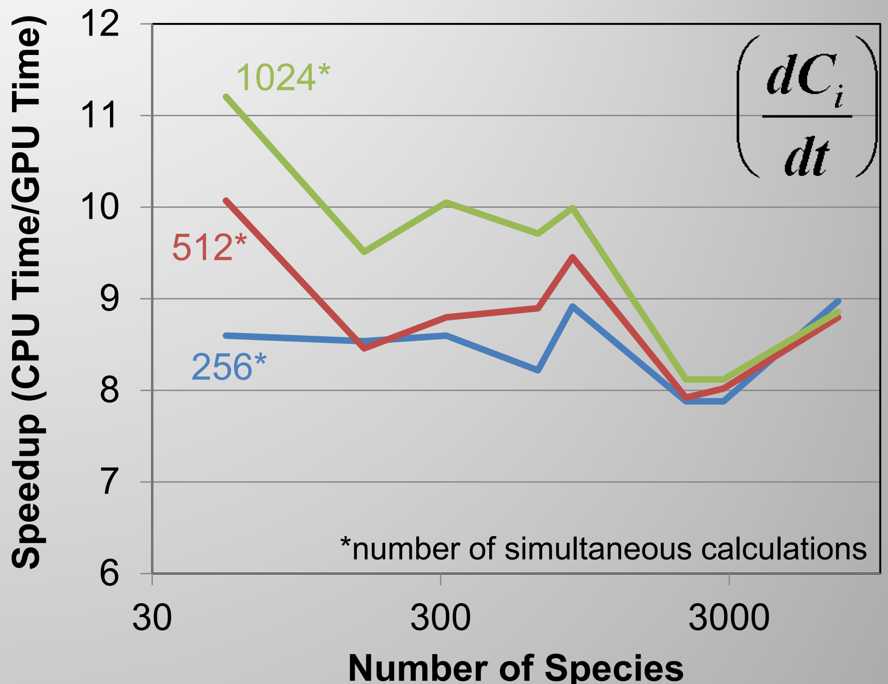


In FY13: We showed potential of GPU for combustion chemistry with ~10x speedup of chemical derivative calculation.

Towards Next Generation Computing Architectures

Technical Accomplishment: We are advancing our work using GPU accelerators to bring more capability to the engine designer





In order to take advantage of GPU capabilities we have to solve many chemical integration problems simultaneously. This lends itself directly to application in CFD where chemistry is solved on a per cell or per zone basis.

Towards Next Generation Computing Architectures

Technical Accomplishment: All significant chemistry integration calculations have been ported to GPU

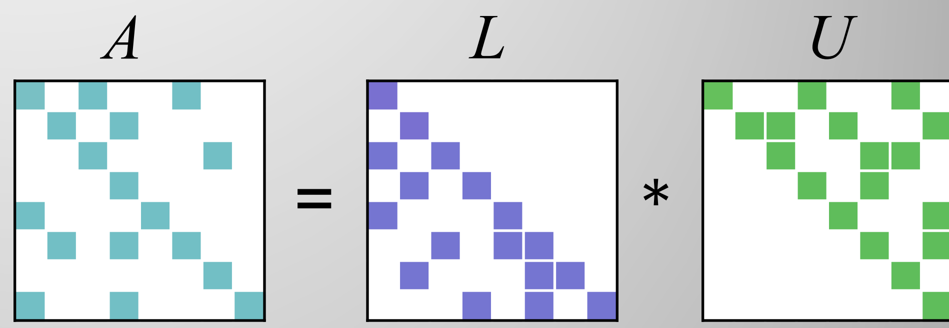
Derivative Calculation (vector equations)

$$\frac{dy_i}{dt} = \frac{w_i}{\rho}\frac{dC_i}{dt}$$

$$\frac{dT}{dt} = -\frac{RT}{\rho c_v}\sum_{i}^{species} u_i \frac{dC_i}{dt}$$

Derivative represents system of equations to be solved.

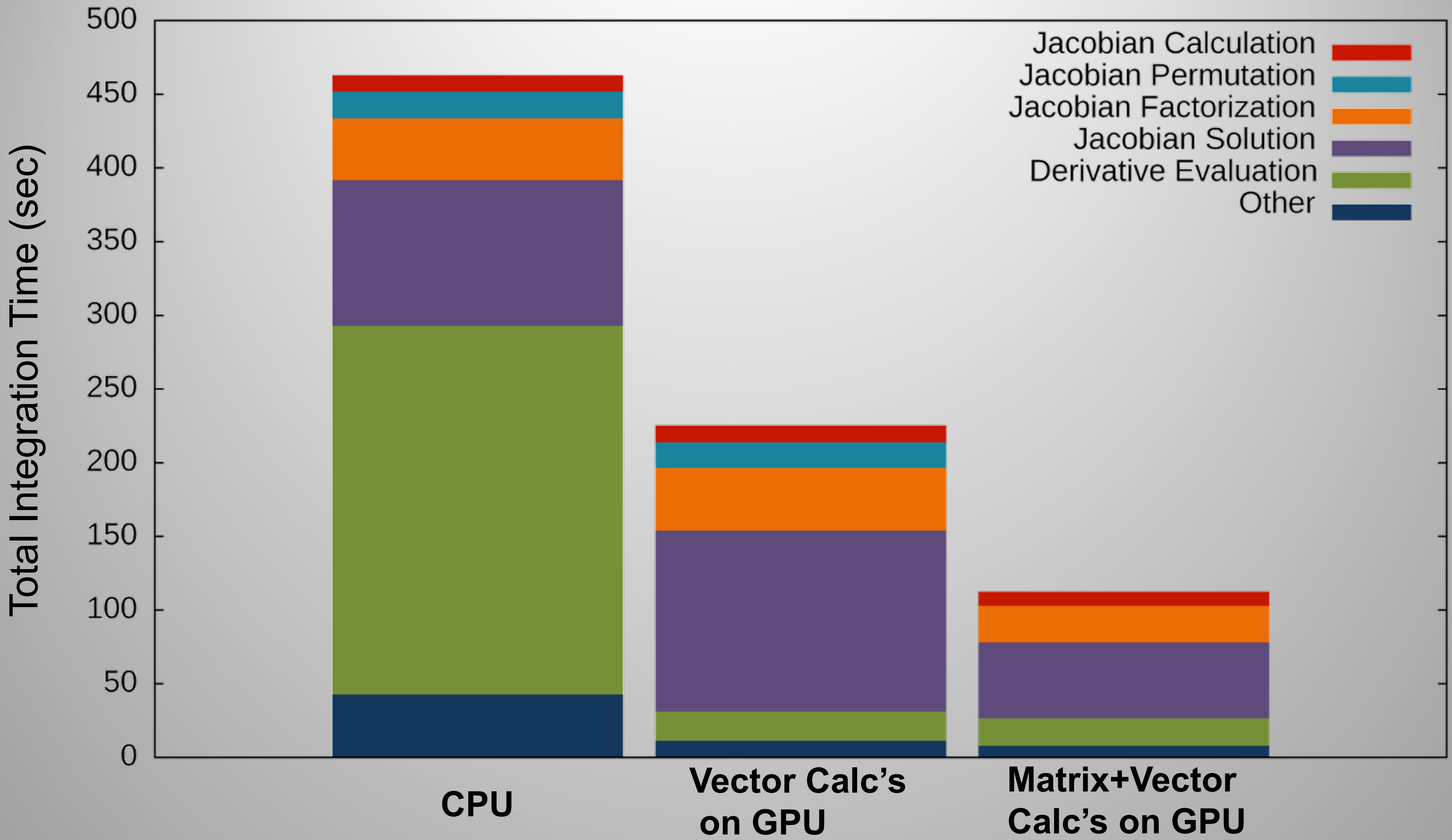
Jacobian Sparse Matrix Solution



- Matrix solution required for efficient time-stepping (variable-order implicit method)
- We exploit sparsity of matrices to reduce number of calculations and memory required
- GPU sparse matrix package developed by NVIDIA and provided to LLNL as beta testers

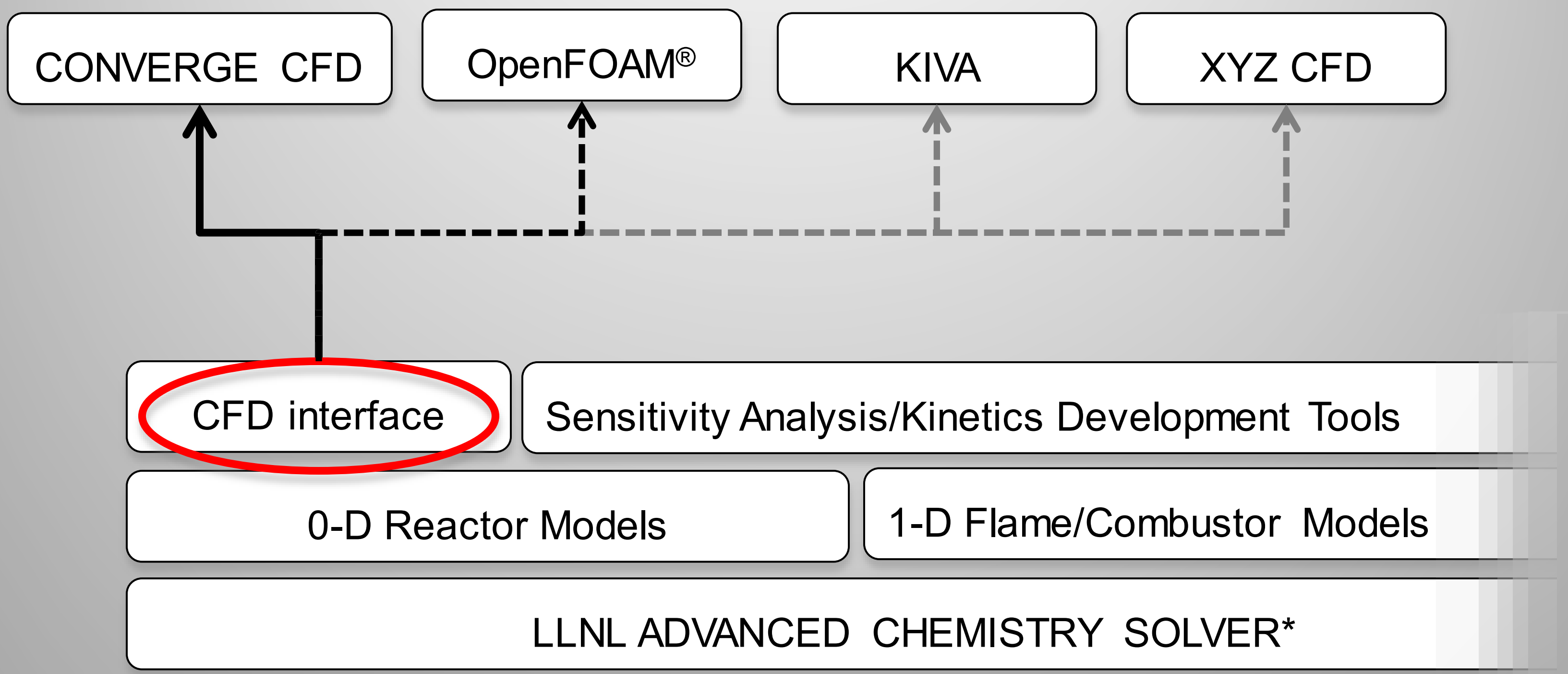
Significant effort to transform fastest CPU algorithms to GPU appropriate versions.

Technical Accomplishment: ~5x decrease in simulation time for parallel chemical integration



~10x improvement for vectors; 2-3x for sparse matrices

Technical Accomplishment: Improved interface has been created to more easily couple the advanced solvers to engine relevant CFD software

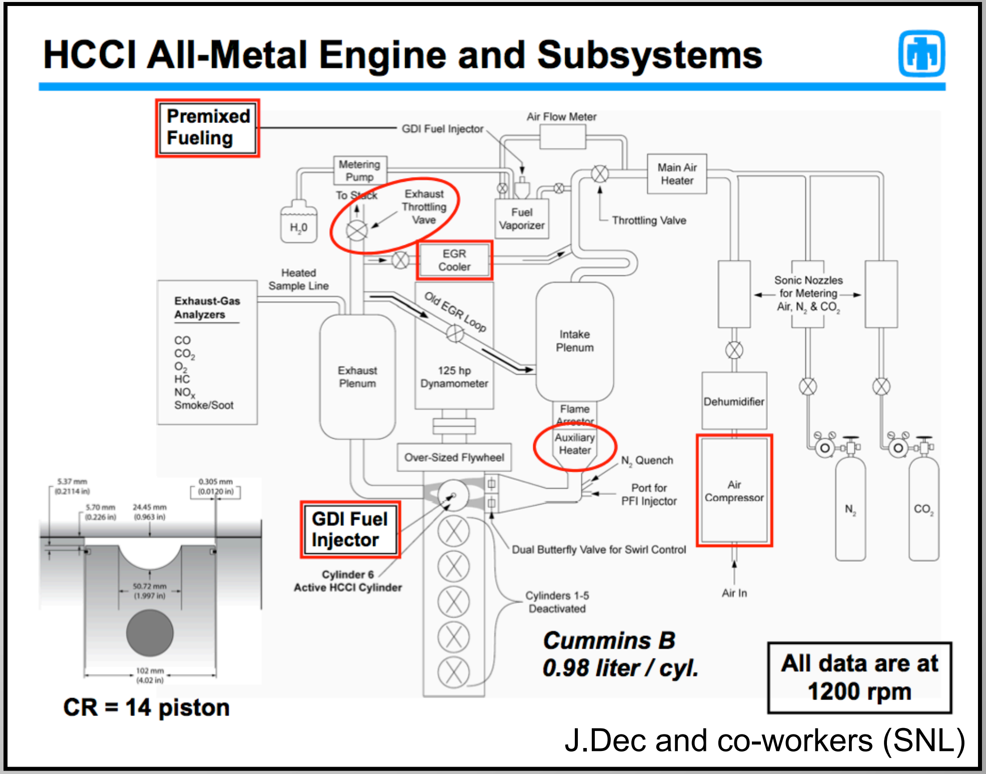


*ACE076: McNenly (PI)

Making advanced solver work more accessible to more people

Technical Accomplishments/Progress: Detailed modeling of HCCI/PCCI Experiments performed by Dec at Sandia NL

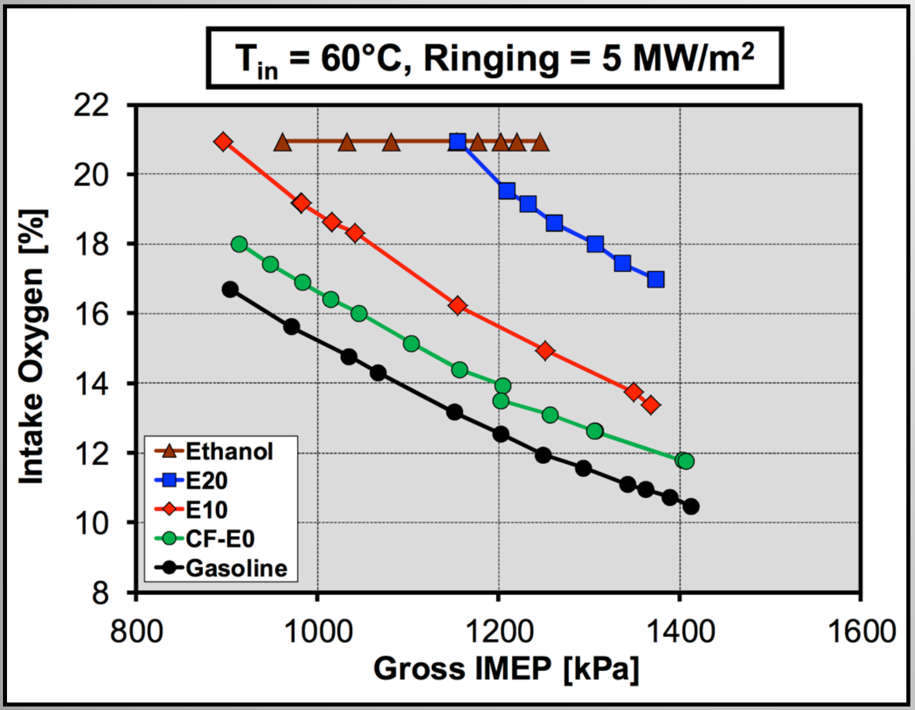
- Experiments explore fuel/mixing effects on combustion timing, stability and heat release rate
- Simulations focused on quantitative agreement of combustion timing, heat release rate, and thermal efficiency.
- HCCI/PCCI configuration allows examination of much of the parameter space with detailed chemistry (1400 species LLNL mech.)



Applying modeling tools to recent advanced engine experiments.

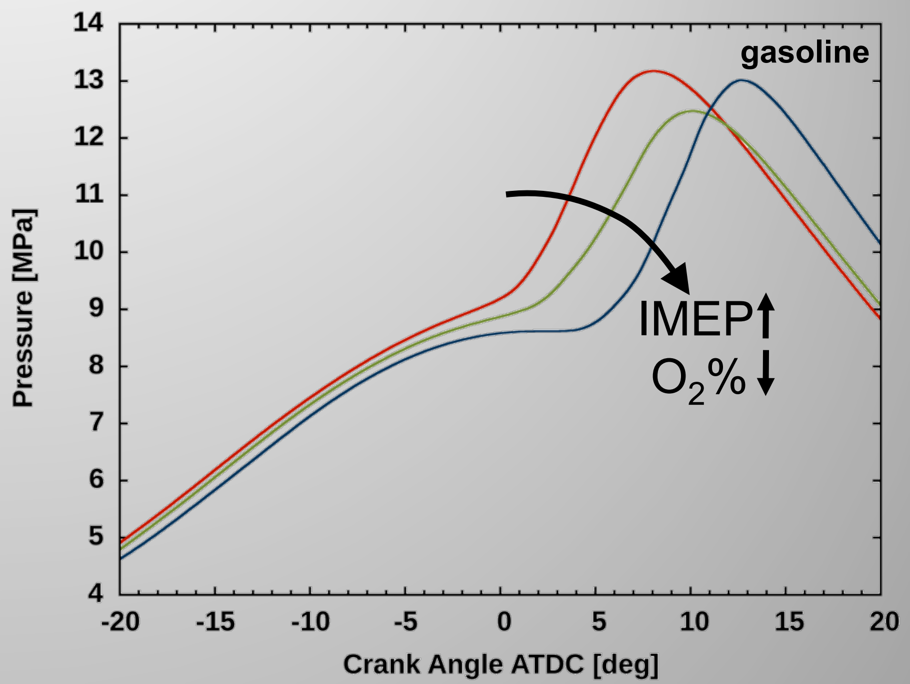
Technical Accomplishments/Progress: Initial model results show qualitative agreement for fuel/oxygen ratio, load and timing data

Range of experimental conditions



J.Dec and co-workers (SNL)

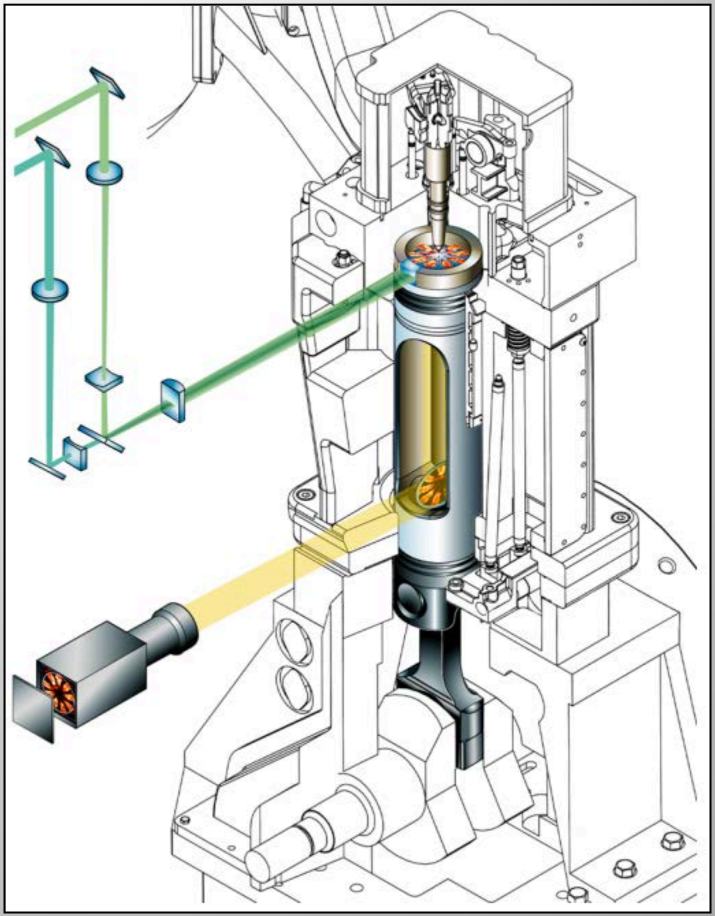
Preliminary LLNL Model Results



Targeting quantitative agreement for range of fuels and operating conditions

Technical Accomplishments/Progress: Developing a detailed model of recent experiments in the Sandia light duty optical diesel engine

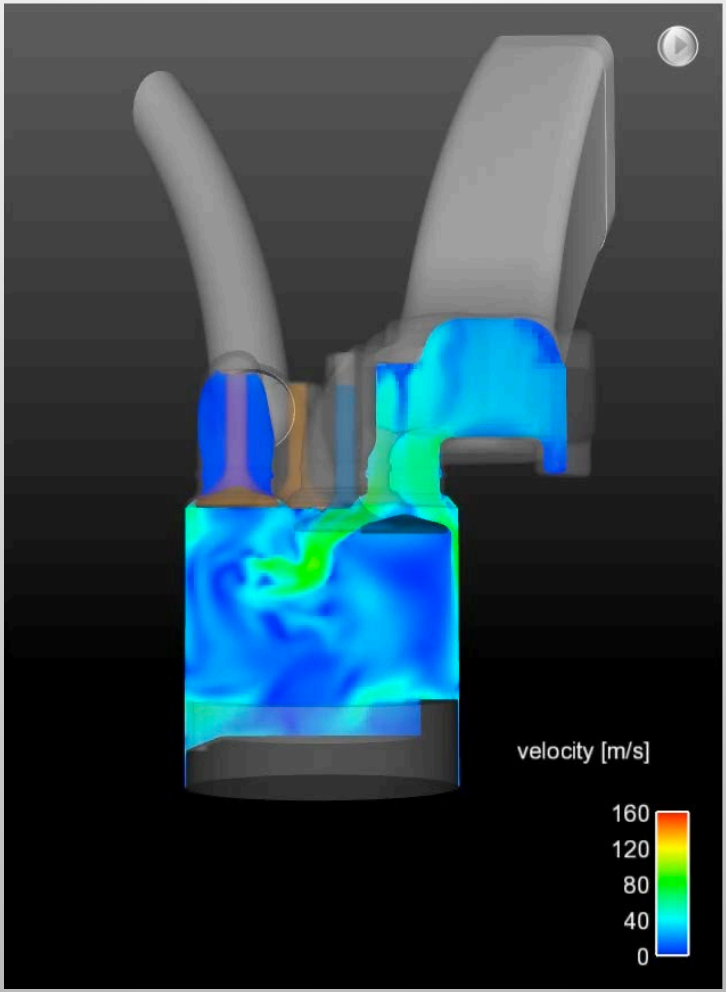
- Experiments employ pure component and well defined surrogates to study diesel combustion phenomena
- Simulations focused on affects of fuel chemistry with detailed mechanisms.
- Allows us to examine impact of detailed chemistry in mixing controlled engine configuration.



C.Mueller and co-workers (SNL)

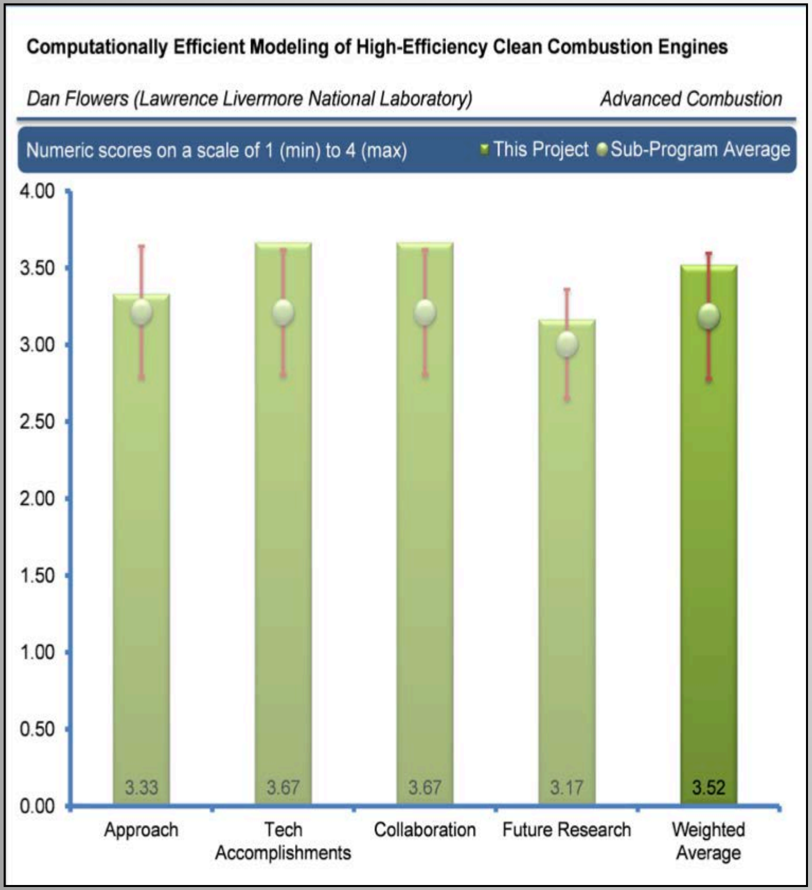
Extending the applicability limits of fast solvers and multi-zone.

Technical Accomplishments/Progress: Full breathing simulation with accurate engine geometry



Resolving intake process critical to subsequent simulation.

FY2013 Reviewer's comments and our response



- Mostly positive comments in all categories.
- The reviewer voiced: "that this ongoing project had demonstrated good progress in improving computational efficiency. … The missing ingredient [is a] lack of validation for engine operating conditions."
- The reviewer observed: "that the multi-zone scheme was working well and that orders-of-magnitude reductions in simulation runtime had been achieved with the advanced GPU-solvers. … This reviewer added that it seemed like progress on applying the models to real-world problems and the evaluation of models could be faster."
- Response: While our recent focus has been on model tool development and on making these tools available to other researchers, we continually evaluate the performance of the tools. In addition, we are currently applying these tools to a variety of conditions from recent experiments that highlight fundamental aspects of engine simulation and design.

We appreciate the reviewer's guidance and are striving to meet their requests.

Collaboration – We have 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 presentations
- **Cummins**; supporting proposal to DOE VTP wide-area call. CPU/GPU solvers for Converge CFD on Indiana Univ. GPU supercomputer.
- **Convergent Science Inc. (CSI)**; Multi-zone model development, thermo-chemical functions (CPU/GPU), adaptive preconditioners (CPU/GPU).
- **NVIDIA:** Hardware, software and technical support for GPU chemistry development
- **EFRC Proposal:** Fundamental Chemical Kinetic Mechanisms of Next Generation Fuels (4 national labs, 3 universities)
- **Universities**: UC Berkeley, Univ. Wisconsin, Clemson Univ., SFSU
- **Sandia National Laboratory**: engine experiments
- **Fuels for Advanced Combustion Engines (FACE)** working group

We collaborate broadly and are eager for interaction with interested groups.

Remaining Challenges and Barriers

- ***In engine simulations with large mechanisms that employ multi-zone and advanced solvers: species advection/diffusion can be as expensive as chemistry.***
- ***GPU effectiveness depends on coupling together integration of many CFD cells and on hybrid GPU/CPU algorithms to determine optimal coupling/workload balance.***
- ***Need for systematic reconciliation of uncertainties in experimental and modeling parameters and results.***
- ***Non-chemistry sub-models lack general predictive capability (e.g. fuel sprays and soot models).***

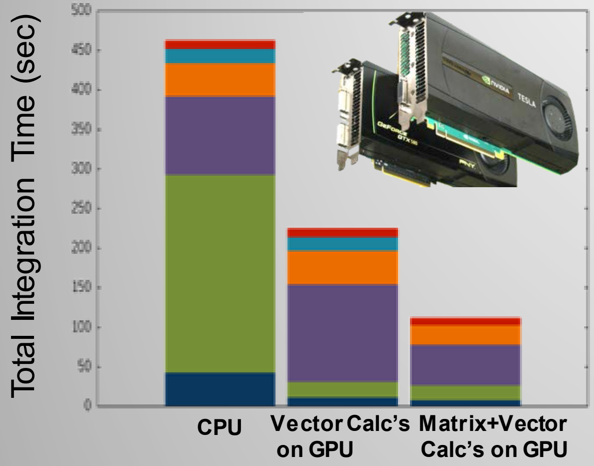
We will address these issues in our future work.

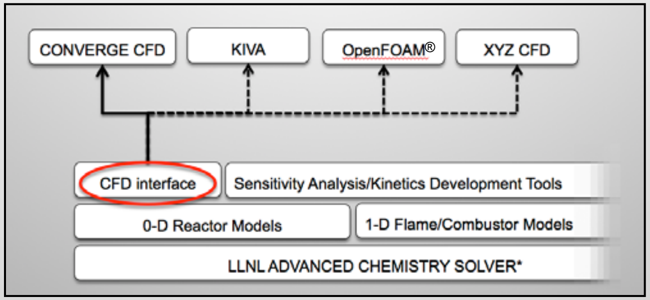
Future work: Improve physical accuracy and computational efficiency of engine combustion modeling tools

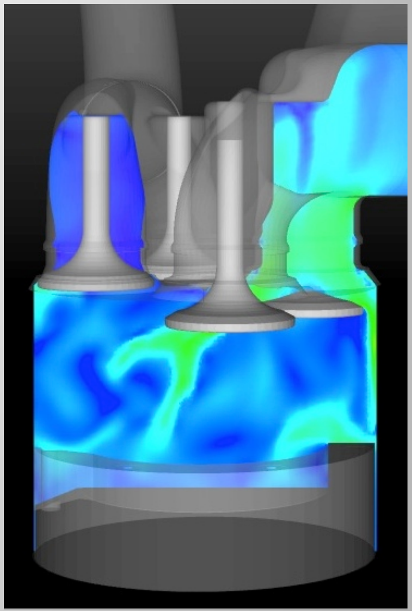
- ***Improved parallel CFD with chemistry***
  - Continue implementation plan for GPU chemistry solver in engine CFD
    - — Reactor/cell grouping algorithms
    - — CPU/GPU work sharing optimization
  - Improve computational performance for species advection/diffusion calculations.
- ***Engine simulation with LLNL parallel CFD with chemistry***
  - Continue engine modeling efforts (HCCI/PCCI and diesel) and publish findings
  - Develop framework for identifying and reconciling experimental and model parameter uncertainties and sensitivities.
- ***Continue technology transfer and licensing activities***

We continue improving model efficiency and accuracy.

Summary: We are providing industry and researchers with accurate and efficient engine combustion modeling tools







- Proven ~5x speed-up for GPU accelerated chemical integration
- Developed general interface for incorporation of advanced chemistry into CFD
- On schedule for targeted simulations of advanced engine experiments utilizing advanced modeling tools

Thank You.

Technical Back-Up Slides

Problem: Can't directly port CPU chemistry algorithms to GPU

- CPU algorithms take advantage of sparsity.
- GPUs need dense data access for speed.
- How can we maintain low number of operations while improving data access pattern?

Solution: Re-frame series of sparse reactor calculations into system of coupled reactors.

Technical Approach: GPU chemistry solution – simultaneous solution of multiple reactors

Matrix Algebra : CPU *vs.* GPU

$$Ax = b$$

Want to solve for x.
(A is a matrix;
x and b are vectors)

$$A \Rightarrow LU$$

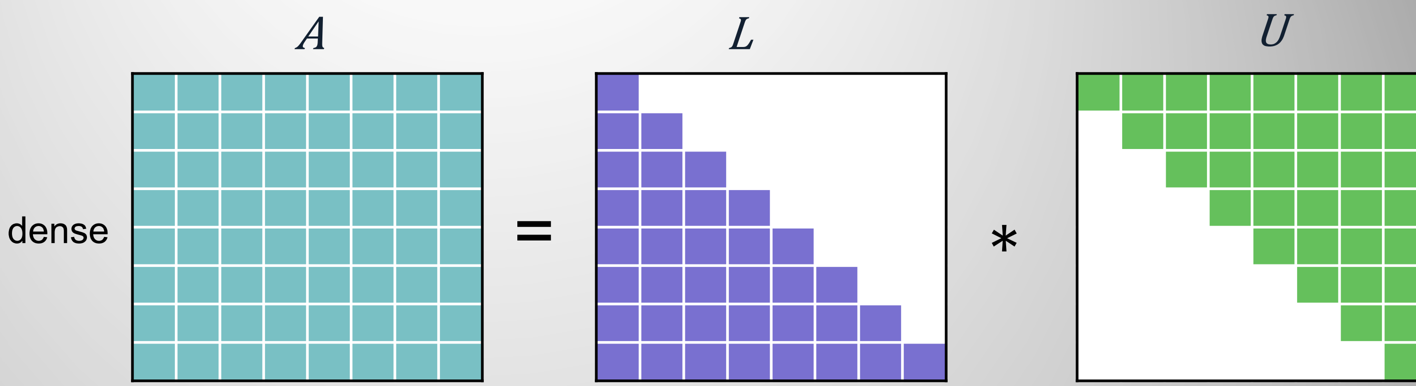
factorization

Separate A into lower (L) and upper (U) triangular matrices.

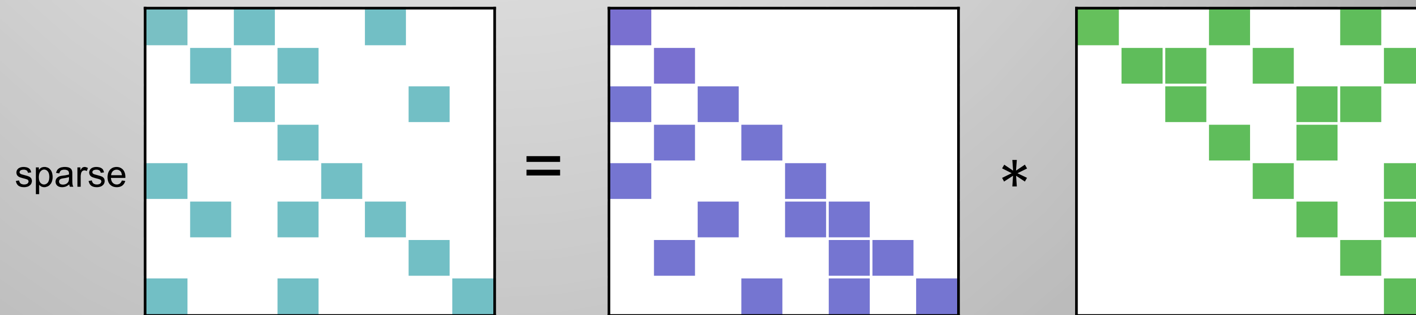
$$x = f(L, U, b)$$

solution

x can be determined efficiently via algebraic manipulation of L, U and b.



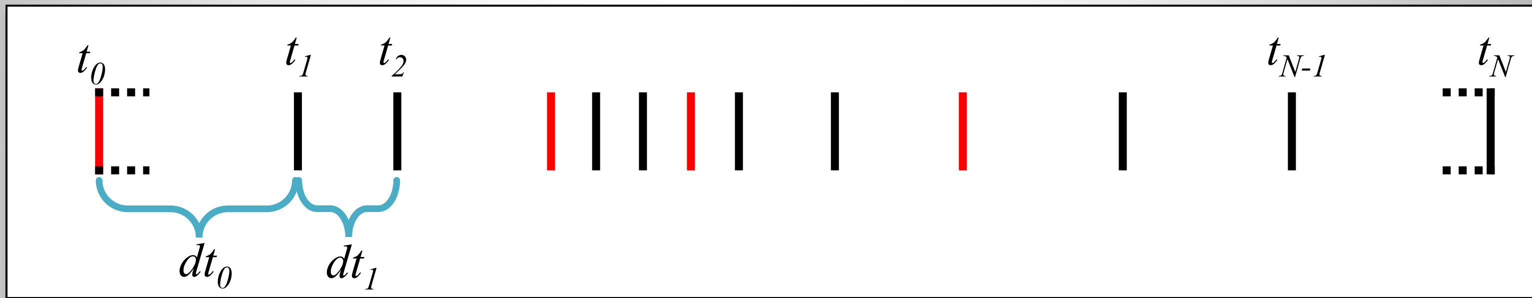
CPU Packages: LAPACK (serial) ScaLAPACK (parallel)
Highly tuned for architecture, easily ported to GPU



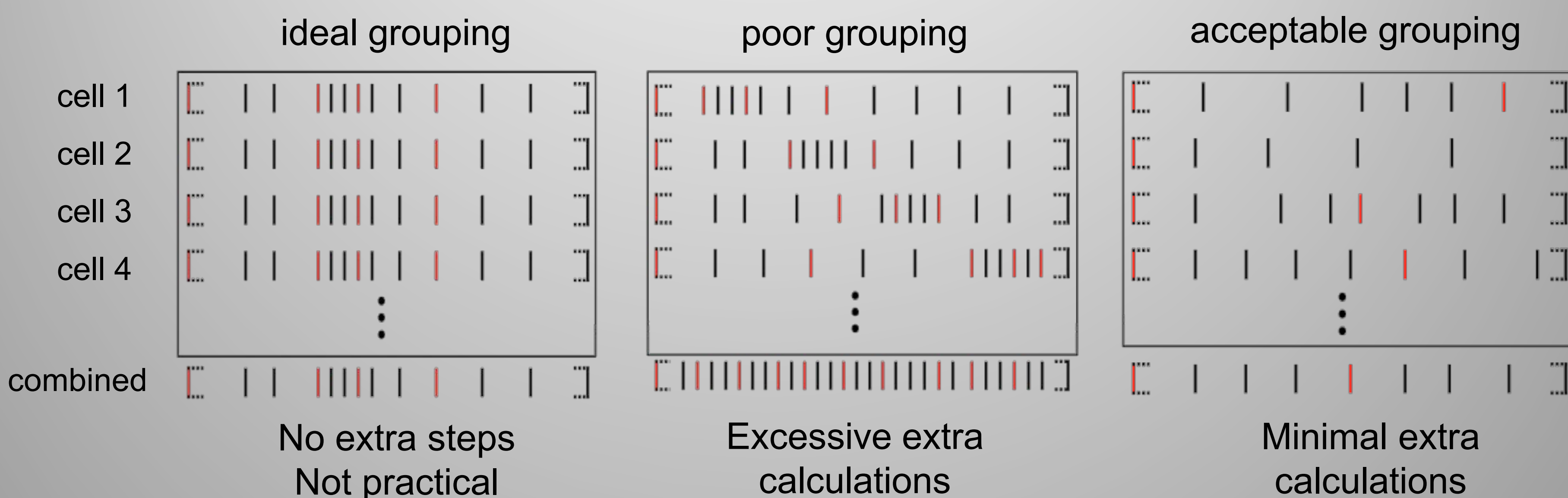
CPU Packages: PARDISO, Watson, SuperLU, KLU, …
Problem specific performance, more challenging for GPU
(due to irregular data access patterns)

What works on CPU doesn't necessarily work on GPU.

Single chemical reactor

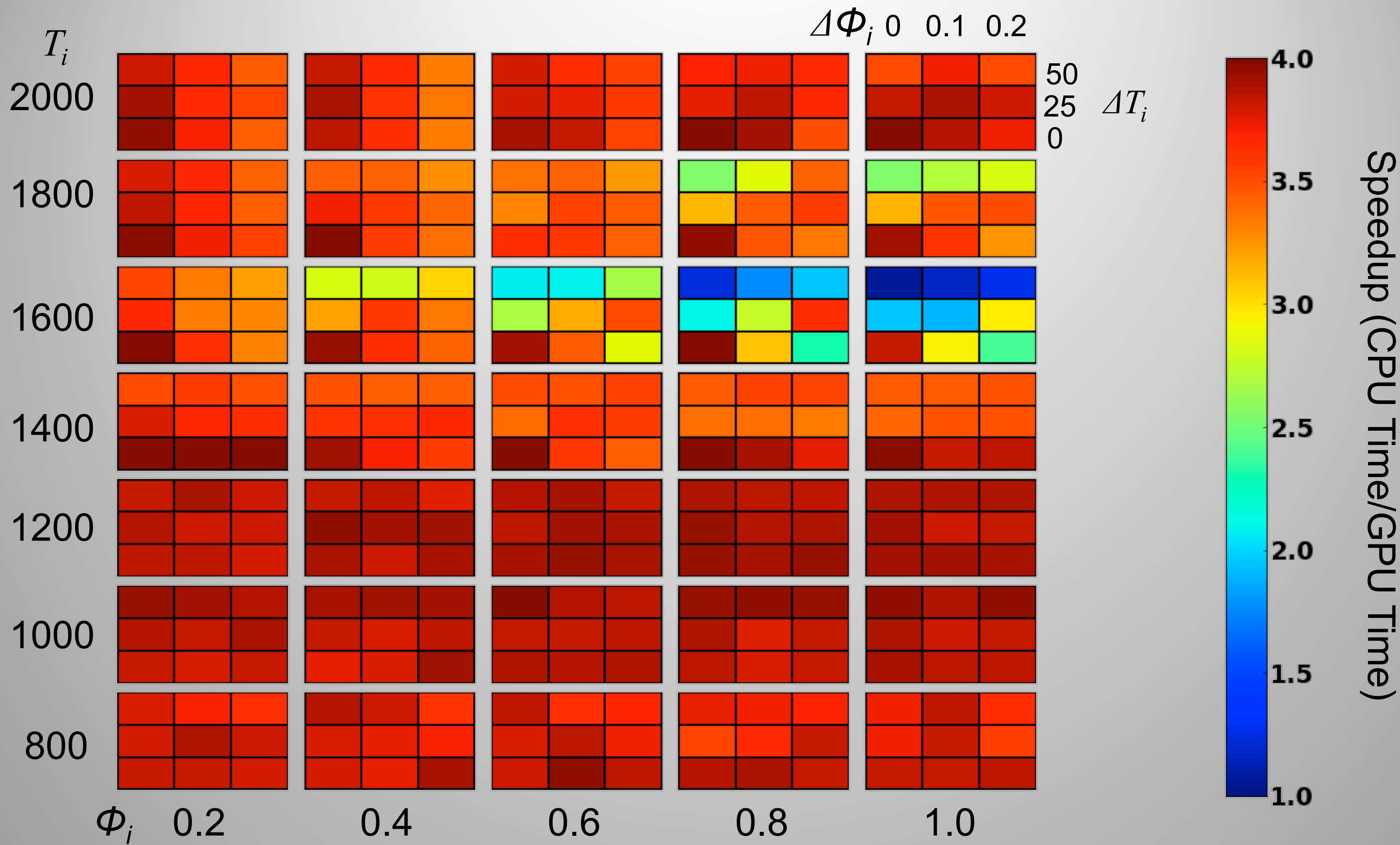


- Red lines indicate matrix factorization (expensive).
- Integrator decides:
  - how long a step to take
  - when to perform new factorization



Caveat: Simultaneous solution may incur time-stepping or "coupling" penalty

Cell coupling penalty: Test Case



Testing spread in initial conditions relevant to engine CFD for simultaneous solution