Accelerating the Computation of Detailed Chemical Reaction Kinetics for Simulating Combustion of Complex Fuels

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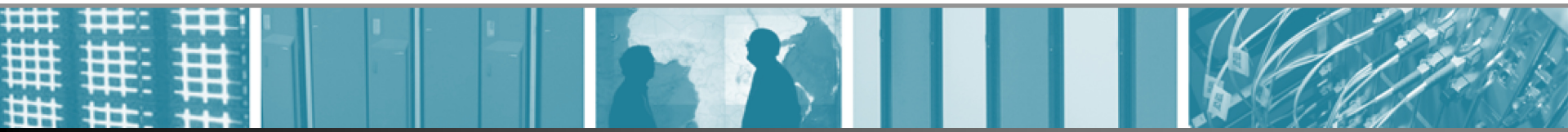
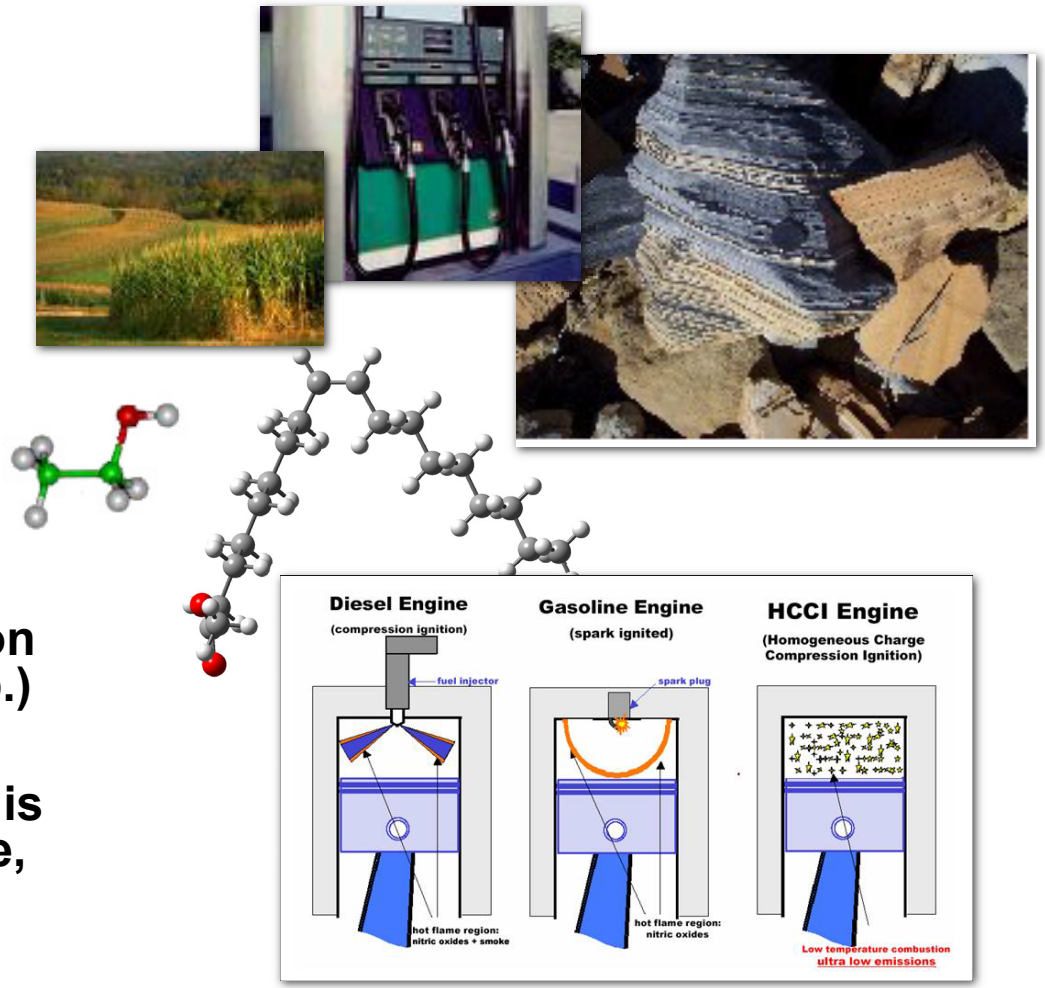


Motivation: Changing World of Fuels and Engines

- Fuel streams are rapidly evolving
  - Heavy hydrocarbons
    - ✓ Oil sands
    - ✓ Oil shale
    - ✓ Coal
  - New renewable fuel sources
    - ✓ Ethanol
    - ✓ Biodiesel
- New engine technologies
  - Direct Injection (DI
  - Homogeneous Charge Compression Ignition (HCCI)
  - Low-temperature combustion
- New mixed modes of combustion (dilute, high-pressure, low-temp.)
- Sound scientific understanding is necessary to develop predictive, validated multi-scale models!



Combustion chemistry

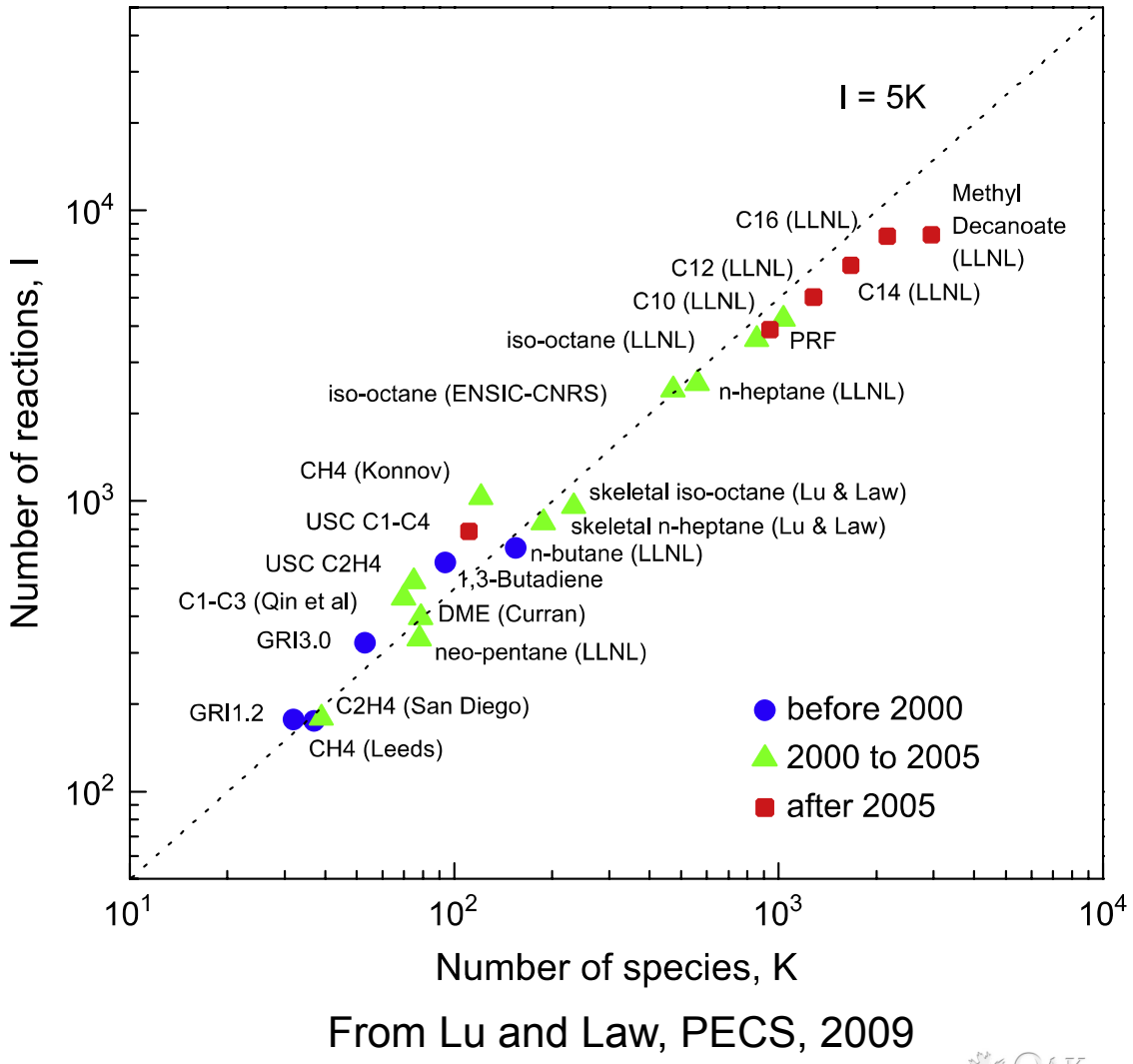
- Example, natural gas combustion

$$CH_4 + 2O_2 \Rightarrow CO_2 + H_2O$$

- Occurs through a reaction network producing and consuming intermediate species
  - CO, OH, H_2O_2, HO_2, CH_3, …
- Detailed chemical mechanisms are needed to compute
  - Flame structure and stability
  - Emissions
  - Validate reduced reaction mechanisms

Detailed chemical kinetics are expensive

- Chemical source term evaluation is computationally intensive
- Thousands of elementary reaction steps accumulated to global species reaction rates
- Often the target for model reductions or algorithmic improvements
- How fast can we compute detailed chemical kinetics on accelerators?



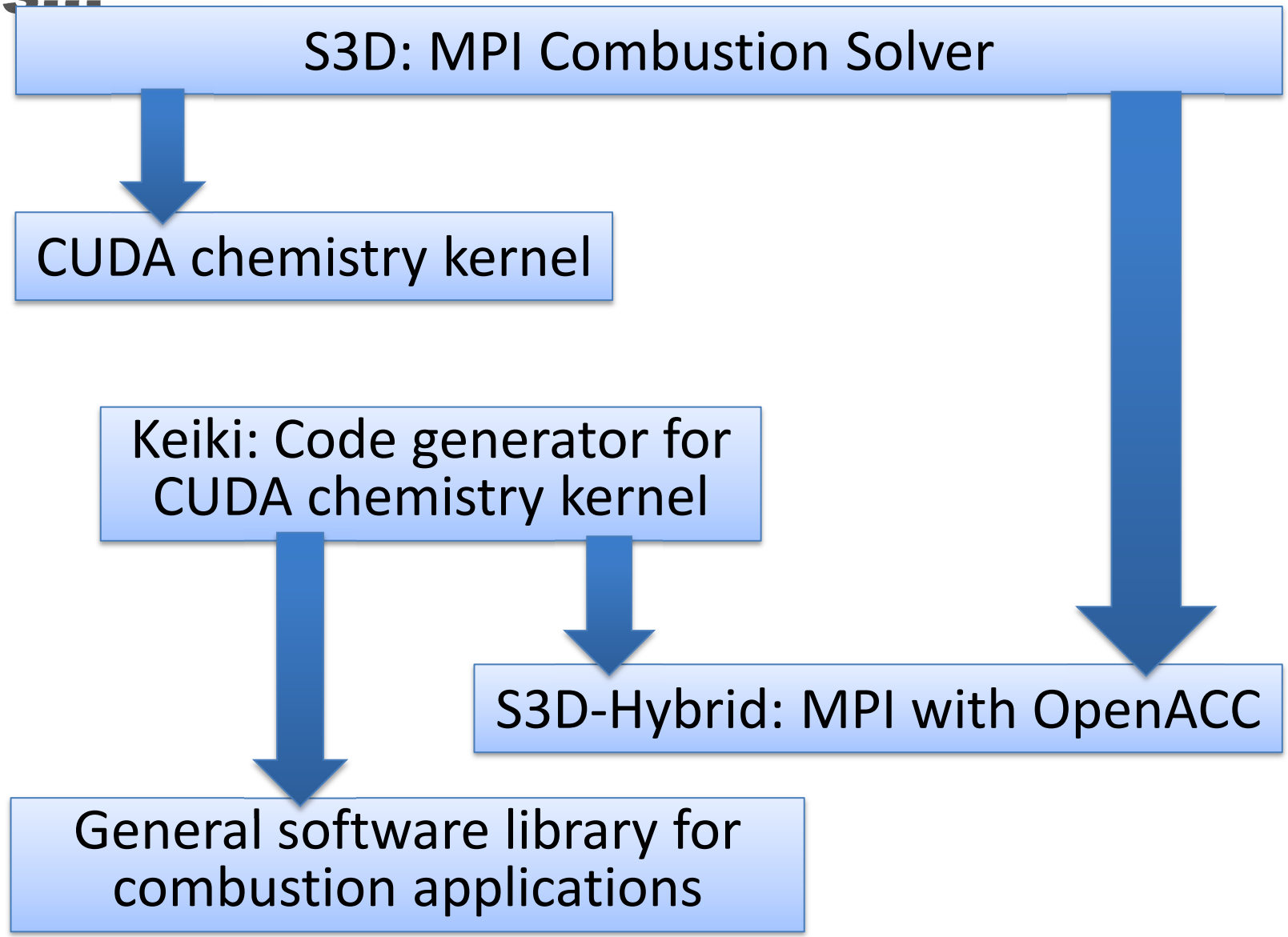
From Lu and Law, PECS, 2009

Chemistry Kernels

- Reaction rates, thermodynamic properties and transport coefficients account for 55% of time.
  - Complex chemical kinetic models needed to address multi-stage ignition and flame dynamics
- Point-wise functions that are independent of DNS software's mesh data structure and MPI-layer
  - Uses Chemkin API
- Used across other combustion codes in the community.
  - Impacts other HPC and workstation-scale combustion applications.
- Accelerator library targets the DNS chemistry needs and beyond

Kyle Spafford (ORNL) et al., "Accelerating S3D: A GPGPU Case Study," in Seventh International Workshop on Algorithms, Models, and Tools for Parallel Computing on Heterogeneous Platforms (HeteroPar 2009). Delft, The Netherlands, 2009

Background: In the beginning there was…



Accelerator library for combustion kinetics

- Conservation equation in a typical combustion application

$$\frac{\partial Q}{\partial t} + u\frac{\partial Q}{\partial x} + \cdots = \dot{\omega}_Q$$

$$\dot{\omega}_Q = f\left(\dot{\omega}_C\right)$$

where $\dot{\omega}_C$ is the rate of chemical kinetics

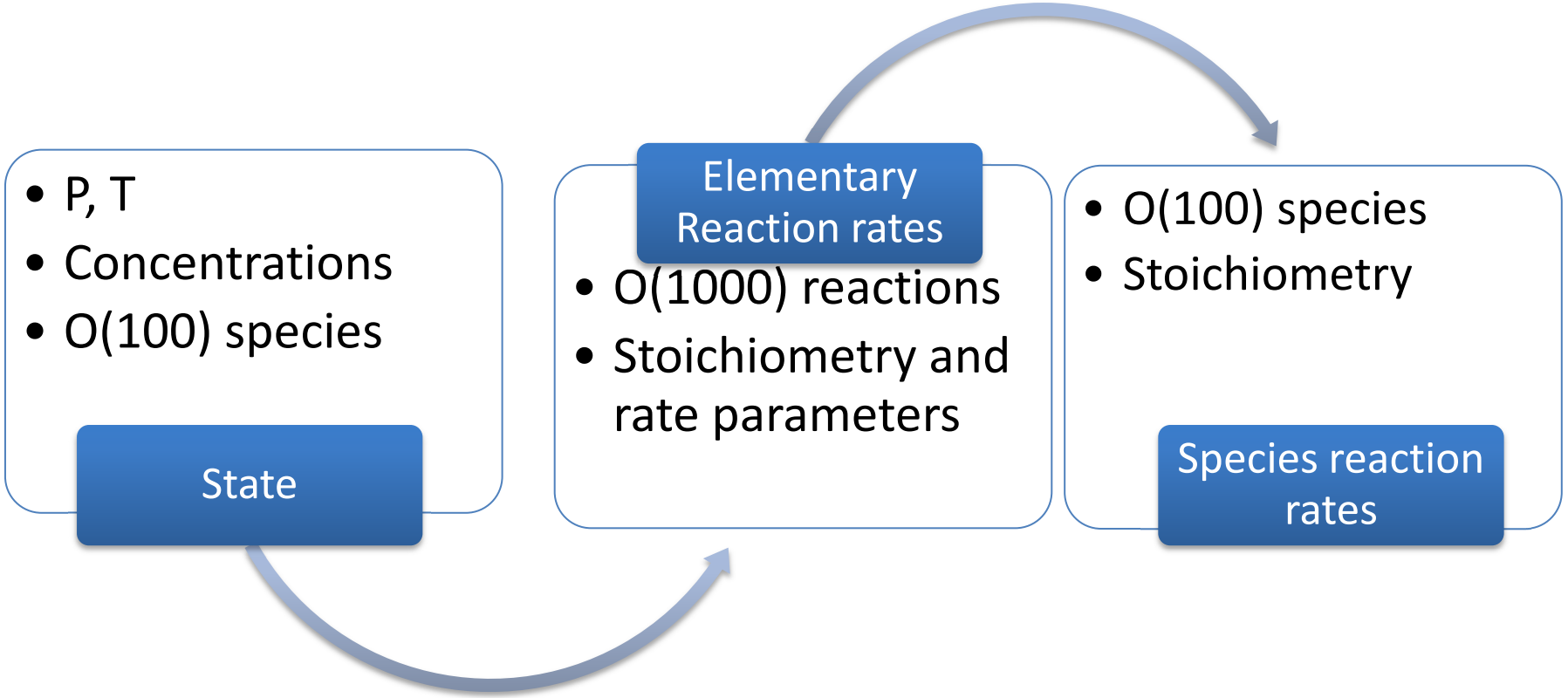
- Chemistry kernel evaluates the chemical kinetics for large mechanisms.
- Well optimized on CPUs and achieves more than 20% of peak on AMD opterons
- Porting to GPU and larger chemistry requires higher levels of parallelism

Parallelizing reaction kinetics (CKWYP)

$$\dot{\omega}_M = \sum_N \Omega(P, T, Y_M)$$

- Grid-level parallelism (several independent states)
  - Will provide MPI parallelism
  - In some cases, also SMP-like parallelism
- Grid-level vectorization does not provide sufficient performance
  - 32(states) * 4000 variables * 8bytes = 1000 kB
- Current capacity in shared memory/L1 cache = 64kB
- Need to go deeper for vector parallelism
  - Equation level parallelism

Data flow in the rates kernel



- Data movement should be minimized while also vectorizing
- Expose concurrency (independent blocks) within the reaction network
- Redundant computation to achieve parallelism

Partitioning at species/reaction level

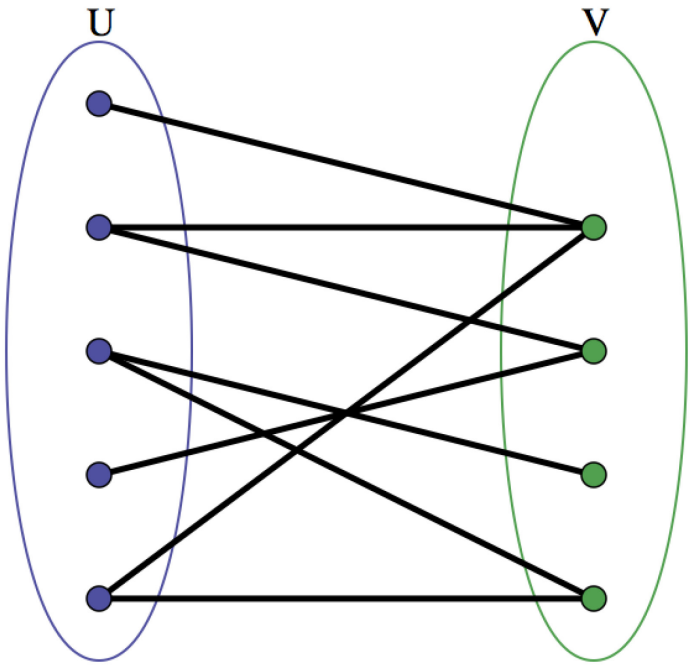
- Similar to partitioning the grid for distributed memory parallelism (MPI)
- Why partition the computation at species/reaction level?
  - Asynchronous execution to hide latencies and data transfers (memcpy across PCI)
  - Distribute work to multiple accelerators assigned to a single host
  - Allow finer grained parallelism at the chemistry level to multiply the scalability of the flow solver
- **Keiki** treats the chemical kinetics as a graph and partitions it to minimize edgecut and maximize parallel performance

Reaction network as a graph

- Chemical reaction network is a bi-partite graph between two sets of vertices
  - The species form one set
  - The reactions form the second set
  - Stoichiometry of the reaction network defines the graph
- The adjacency matrix of the graph is

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

- Where B is the M x N stoichiometry matrix

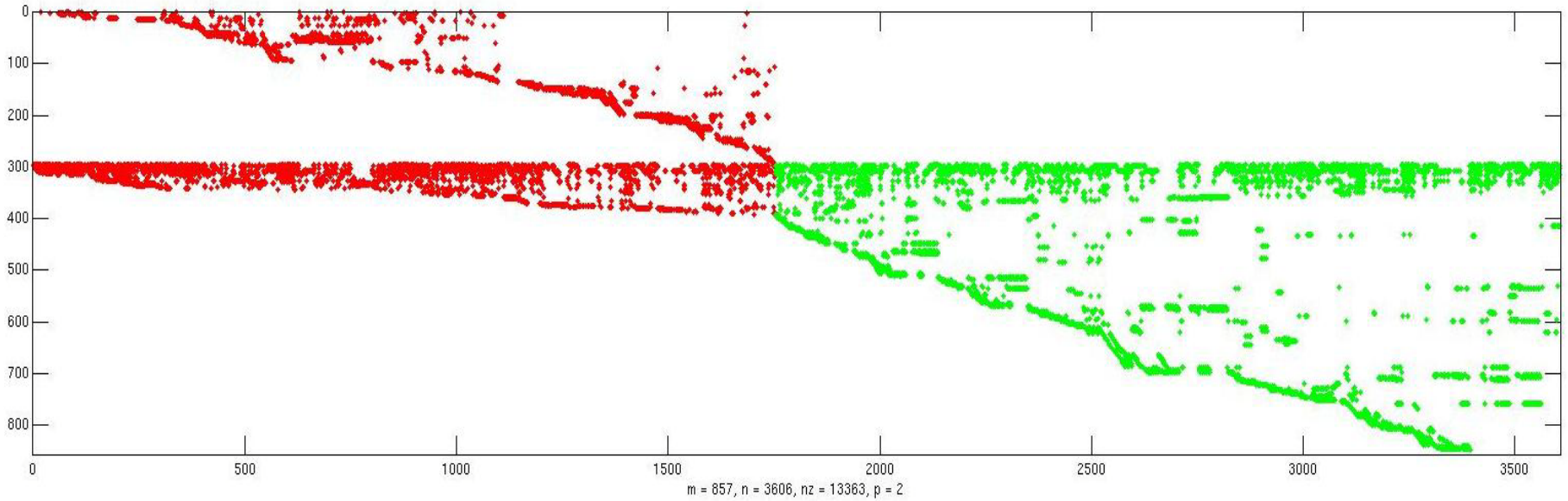


Partitioning the graph

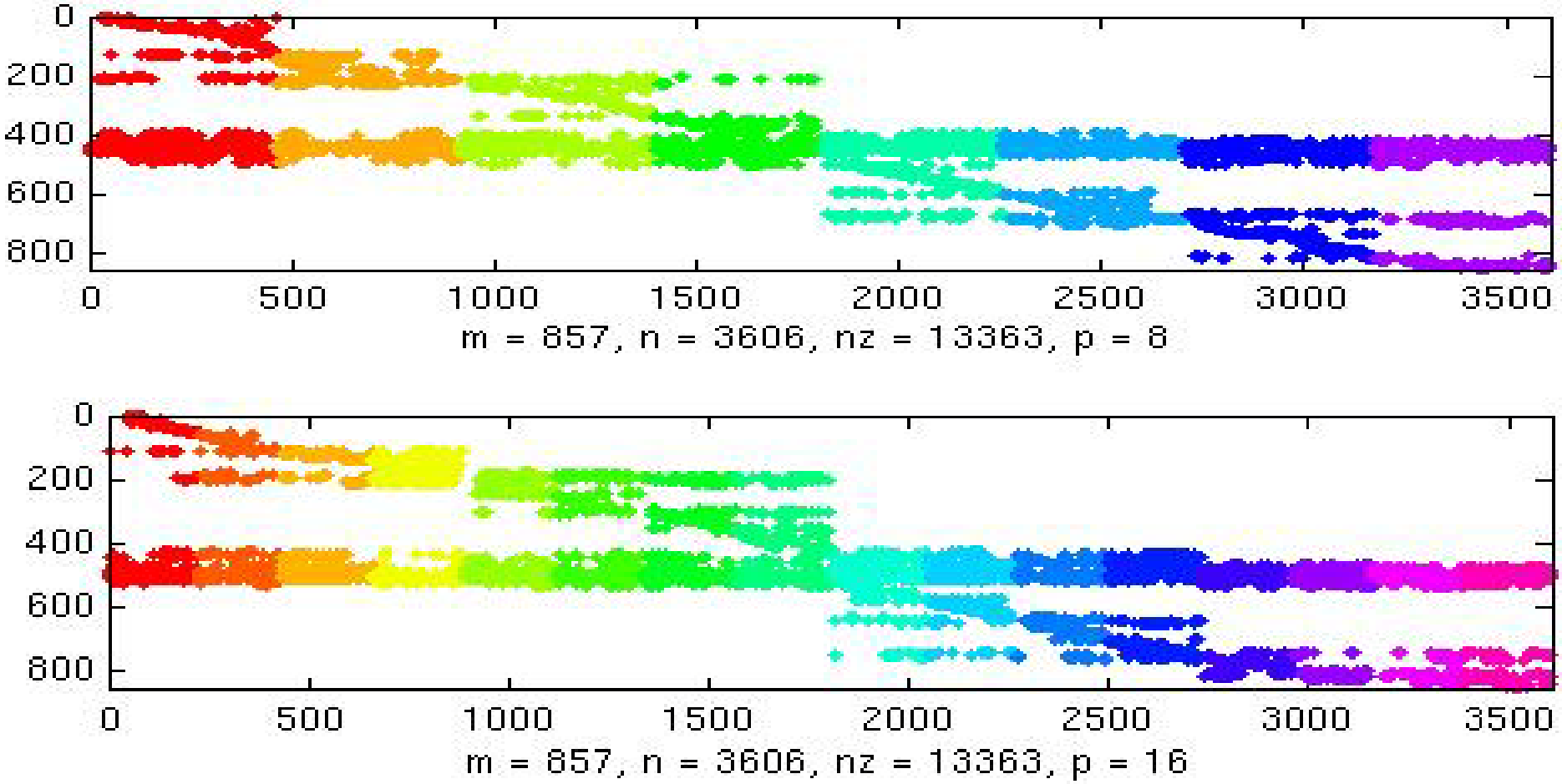
- Graph partitioning software Metis and PaToH were used to partition the bi-partite graph
  - A good quality partition minimizes edge-cut with maximum load balance
  - Reorders the network, without changing the answers
- Edge-cut induces redundant computation or synchronization points
- Partitions should be sized to meet the vector length and memory requirement
  - Large enough to have enough number of threads per thread block
  - Control shared memory requirement to obtain high occupancy
- Need a sufficient number of partitions that can execute concurrently

Partitioning iso-octane chemistry

- LLNL's detailed mechanism for gasoline surrogate composed of 858 species and 3606 reactions

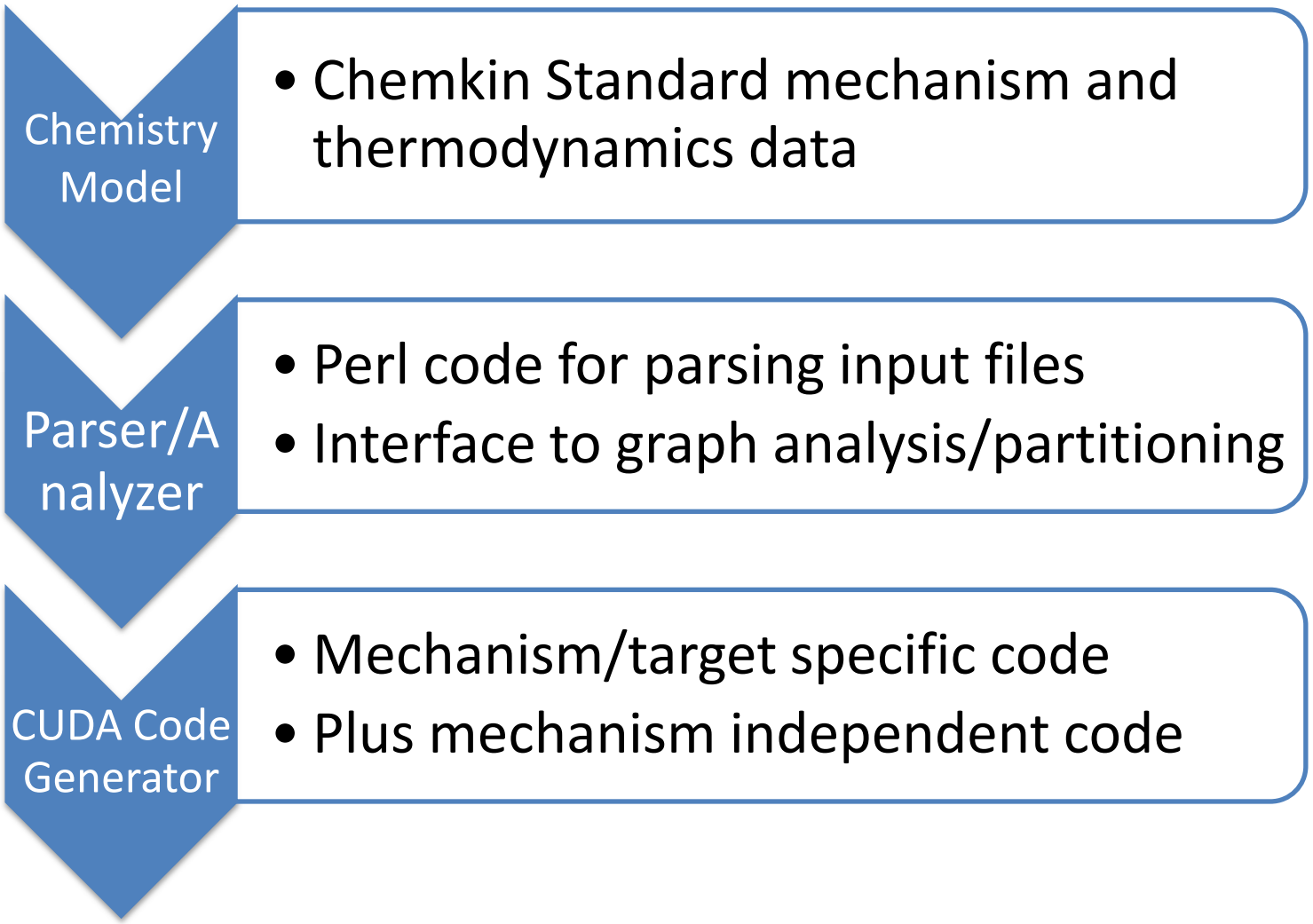


Partitioning iso-octane chemistry (contd)



- The quality of partitioning gets better as the chemistry model gets bigger

Keiki – Code Generator

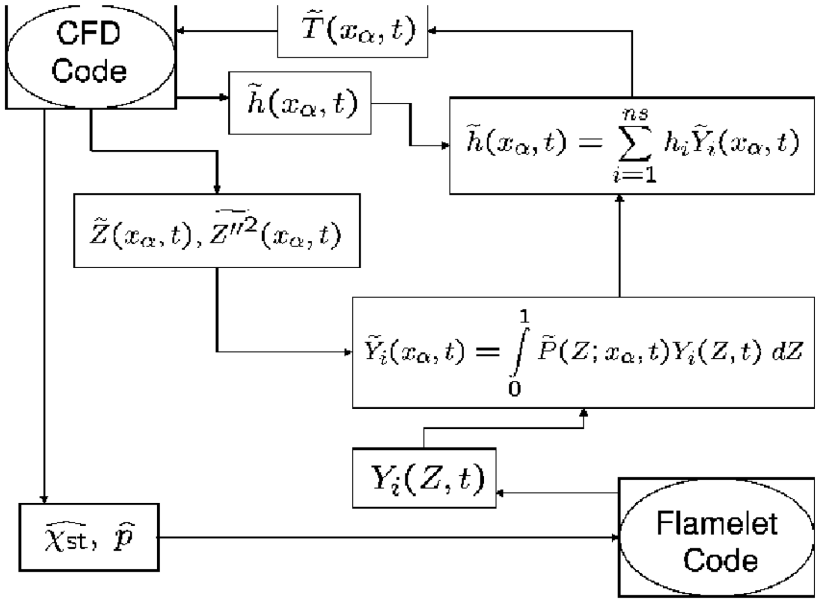


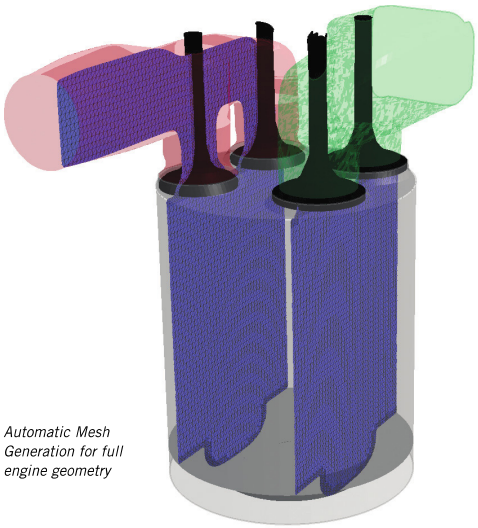
Performance results

- Performance on dual 6-core Opteron CPU and Fermi GPU were compared for 52-species n-heptane and 858 species iso-octane chemistry
  - CPU peak = 2*62.4 = 125 GF
  - GPU peak = 515 GF
- The CPU code was well optimized and tuned for performance
- The execution times on GPU were 3X faster than the CPU
- Work in progress to measure and tune performance on Kepler

GPU library coupled to combustion CFD

- Work in progress:
- A flamelet equation solver is being developed around the CUDA library
- CUDA library for chemical kinetics is being coupled to Forte in partnership with Reaction Design
  - Forte ported to Jaguar (Cray XK6)
  - Software linking and API are being explored





Automatic Mesh Generation for full engine geometry

Summary

- New software and techniques were developed to enable the computation of combustion chemistry on GPU accelerators using the CUDA programming model
- Significant potential to accelerate the computation of very large detailed mechanisms
- What started out as an effort to accelerate S3D has been extended to much larger chemical mechanisms.