Redesigning Combustion Modeling Algorithms for GPU Computing and Application in Multi-dimensional HCCI engine Simulations with Very Detailed Reaction Mechanisms

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Research motivations

- Solving reaction mechanisms (chemical kinetics of fuels) in reacting flow simulations is expensive due to stiff ODEs (i.e. many reaction rates must be computed for many species, many times!)

\[
\begin{align*}
\frac{dy_1}{dt} &= f_1(T, P, y_1, \ldots, y_{N_s}) \\
& \vdots \\
\frac{dy_{N_s}}{dt} &= f_{N_s}(T, P, y_1, \ldots, y_{N_s}) \\
\frac{dT}{dt} &= f_{N_s+1}(T, P, y_1, \ldots, y_{N_s})
\end{align*}
\]

\[f_i = \sum_{j=1}^{N_s} \nu_{ij} \omega_j, f_{N_s+1} = \frac{1}{C_v} \sum_{i=1}^{N_s} u\dot{y}_i\]

\[
\omega_j = k_j^f \left( \prod_{i=1}^{N} c_i^{\nu_{ij}} - K_c^{-1} \prod_{i=1}^{N} c_i^{\nu_i} \right),
\]

\[
k_j^f = P_{cor,j} A_j T^{n_j} \exp\left( \frac{-E_j}{R_0 T} \right)
\]

- \[\text{IC8H18} + H = \text{C8H17} + H_2 \quad 4.38 \times 10^7 \quad 2.0 \quad 7760.0 \]

- \[\text{IC8H18} + O_2 = \text{C8H17} + HO_2 \quad 2.22 \times 10^{15} \quad 0.0 \quad 42904.0 \]

- \[\text{C8H17} + O_2 = \text{C8H17}O_2 \quad 1.05 \times 10^{11} \quad 0.0 \quad 0.0 \]

- \[\text{CH3} + HO_2 = \text{CH3O} + OH \quad 9.60 \times 10^{13} \quad 0.0 \quad 30950.0 \]

- \[\text{CO} + OH = \text{CO}_2 + H \quad 1.26 \times 10^7 \quad 1.3 \quad -758.0 \]

...
Research motivations

- In reacting flow simulations, over 95% simulation time is spent on solving the stiff ODEs (operator splitting scheme).
- In practice, it is affordable (but still expensive) to solve reaction mechanisms with only a few tens species and hundreds reactions using implicit stiff ODE solvers.

- Poor scaling of implicit ODE solvers (super-quadratically with species number).

Detailed reaction mechanisms of hydrocarbon fuels contain thousands species and reactions e.g., C16H34 (hexadecane)
- 2115 species and 8157 reactions

C11H22O2 (methyl decanoate)
- 2877 species and 8555 reactions
Research motivations

- There is an urgent need to improve the computational efficiency of stiff ODE solvers to incorporate large detailed reaction mechanisms in reacting flow CFD simulations.

Take advantage of many-core structure of GPU and parallel computing.
GPU-accelerated chemical kinetics ODE solver (Identify parallelism)

- Solving chemical kinetics problem is essentially to solve stiff ODEs subject to initial conditions

\[
y' = \frac{dy}{dt} = f_1(T, y), \quad y(0) = C_1 \\
T' = \frac{dT}{dt} = f_2(T, y), \quad T(0) = C_2
\]

- Implicit backward Euler method for solving stiff ODEs is popular in the community, the existing solvers include DASSL (DASAC in Senkin), DVODE, and etc.

\[
\frac{dy}{dt} = \frac{y_n - y_{n-1}}{h} = f_1(T_n, y_n) \\
y_n - y_{n-1} - h \times f_1(T_n, y_n) = 0
\]
Newton iteration

\[ y_{n+1} = y_n - (I - h \frac{\partial f}{\partial y})^{-1} (y_n - y_{n-1} - h \times f(T_n, y_n)) \]

Linear system

\[ -(I - h \frac{\partial f}{\partial y})^{-1} (y_n - y_{n-1} - h \times f(T_n, y_n)) = \delta \]

\[ (I - h \frac{\partial f}{\partial y}) \delta = -(y_n - y_{n-1} - h \times f(T_n, y_n)) \]

\[ y_{n+1} = y_n + \delta \]

Function evaluation involves species rate calculation essentially, reaction rates calculation

Reactions are independent

Solving the linear equation system

Heavily rely on LU decomposition on LHS

Matrix elements are independent

These two parts take over 97% time when solving large mechanisms
GPU-accelerated chemical kinetics ODE solver

- Reaction rate evaluations
  C kernel function to evaluate reaction rates in parallel (with Fortran wrapper)
- Accelerated linear algebra
  CULA library is employed to supersede LAPACK LU factorization subroutine which is originally used in most implicit ODE solvers, such as DASAC and DVODE tested in the present study
- Apply GPU-accelerated DASAC and DVODE solvers to Senkin code (Chemical kinetics simulation code in Fortran)

Redesigning Combustion Modeling Algorithms for the Graphics Processing Unit (GPU): Chemical Kinetic Rate Evaluation and Ordinary Differential Equation Integration, Combustion and Flame, 2011 (Accepted)
Comparison study

- Constant-volume ignition simulations with CPU, CPU+GTX260, CPU+Tesla C2050

  - Test conditions: stoichiometric fuel/air mixtures under 1200 K and 20 bar for 0.003 second simulation time
  - Hardware: Intel I7-930 (only use single-core)
    GTX 260 (Capacity 1.3)
    Tesla C2050 (Capacity 2.0, ECC off (5% performance boost))
  - Compiler: Intel Fortran + GCC (NVCC) + O3 optimization, on Ubuntu 64bit system
## Comparison study

- **Tested reaction mechanisms**

<table>
<thead>
<tr>
<th>Reaction mechanism</th>
<th>Species number</th>
<th>Reaction number</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRI-mech 3.0</td>
<td>53</td>
<td>325</td>
</tr>
<tr>
<td>n-butane</td>
<td>155</td>
<td>689</td>
</tr>
<tr>
<td>n-pentane</td>
<td>385</td>
<td>1896</td>
</tr>
<tr>
<td>n-heptane</td>
<td>561</td>
<td>2539</td>
</tr>
<tr>
<td>Iso-octane</td>
<td>857</td>
<td>3606</td>
</tr>
<tr>
<td>n-hexadecane</td>
<td>2115</td>
<td>8157</td>
</tr>
<tr>
<td>methyl decanoate</td>
<td>2877</td>
<td>8555</td>
</tr>
</tbody>
</table>
Comparison study (CPU VS GTX 260)

Simulation time (left Y axis) and Speed-up factor (right Y axis)

DASAC solver with Senkin

DVODE solver with Senkin
Comparison study (CPU VS Tesla C2050)

Simulation time (left Y axis) and Speed-up factor (right Y axis)

DASAC solver with Senkin

DVODE solver with Senkin

Tesla C2050 simulation only ~ 1.5 to 1.8 times faster than GTX 260?!
Comparison study (CPU VS Tesla C2050)

Computational time scaling with the species number

DASAC solver with Senkin

DVODE solver with Senkin
Application in HCCI engine simulations

- Homogeneous Charge Compression Ignition Engine

Combustion performance and emissions are mainly characterized by the chemical kinetic behavior of fuels in HCCI engines.
On-the-fly mechanism reduction method + GPU-assisted chemistry solver

- Apply graph theory based model reduction method to reduce the number of species and reactions on-the-fly in engine combustion simulations
  - At each simulation time step, species and reaction number vary from thousands to tens.
  - GPU-assisted ODE solver is called to solve large dynamically-formed mechanisms
  - CPU-only ODE solver is called to solve small mechanisms
  - Threshold: 300 species and 1000 reactions
### Engine specifications and test conditions

<table>
<thead>
<tr>
<th>Specifications</th>
<th>Value 1</th>
<th>Value 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (cm) x Stroke (cm)</td>
<td>13.716 x 16.51</td>
<td></td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>16.1</td>
<td></td>
</tr>
<tr>
<td>IVC</td>
<td>143 BTDC</td>
<td></td>
</tr>
<tr>
<td>EVO</td>
<td>130 ATDC</td>
<td></td>
</tr>
<tr>
<td>Speed (rev/min)</td>
<td>821</td>
<td>1737</td>
</tr>
<tr>
<td>Intake temperature (K)</td>
<td>350</td>
<td>350</td>
</tr>
<tr>
<td>Intake pressure (bar)</td>
<td>1.9</td>
<td>1.4</td>
</tr>
<tr>
<td>Equivalence ratio</td>
<td>0.2</td>
<td>0.6</td>
</tr>
<tr>
<td>Load (bar)</td>
<td>5</td>
<td>11</td>
</tr>
<tr>
<td>EGR (%)</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Caterpillar 3400E
Single-zone simulations

Solve ODEs with varied volume

Detailed methyl decanoate (biodiesel) mechanism with 2877 species and 8555 reactions

<table>
<thead>
<tr>
<th>Methods</th>
<th>Slow speed (in minutes)</th>
<th>High speed (in minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full Chemistry (CPU)</td>
<td>784.85</td>
<td>827.21</td>
</tr>
<tr>
<td>Full Chemistry (GPU)</td>
<td>41.23</td>
<td>43.41</td>
</tr>
<tr>
<td>On-the-fly reduction (GPU/CPU)</td>
<td>3.47</td>
<td>2.72</td>
</tr>
</tbody>
</table>
Single-zone simulations (species number)

Number of species and reactions

8555 reactions for full chemistry

- species
- reactions

2877 species for full chemistry

Crank Angle (degree)

Low speed case

High speed case

GPU-assisted chemistry solver
Single-zone simulations (pressure trace)

Low speed case

High speed case
Multi-dimensional simulations

650 cells using KIVA-Chemkin code with GPU-assisted DVODE solver

Detailed methyl decanoate (biodiesel) mechanism with 2877 species and 8555 reactions
Adaptive multi-grid chemistry model

Mapping cells to a group (2-D illustration)

Center cell
Thermodynamically similar cells (cells with similar temperature and equivalence ratio $\phi$)

$\phi = \frac{2C_{\text{CO}_2}^\# + H_{\text{H}_2O}^\#/2 - z'C_{\text{CO}_2}^\#}{O_{\text{CO}_2-H_2O}^\# - z'C_{\text{CO}_2}^\#}$

Computational domain
mass conservation and species gradient preservation

Chemkin Solver
(Using on-the-fly reduction and GPU-assisted ODE solver)

Remapping back to individual cells
Multi-zone simulations
(AMC model + on-the-fly reduction + GPU)

Stratified charge

<table>
<thead>
<tr>
<th>Methods</th>
<th>Slow speed case (in hours)</th>
<th>High speed case (in hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>W/O AMC model (GPU/CPU)</td>
<td>166.04</td>
<td>56.64</td>
</tr>
<tr>
<td>AMC model (GPU/CPU)</td>
<td>14.73</td>
<td>10.75</td>
</tr>
</tbody>
</table>
Multi-dimensional simulations (zone number)

Low speed case

High speed case

Solve much less grids
Multi-dimensional simulations (pressure trace)

Low speed case

High speed case

Pressure (MPa)

Crank Angle (degree)
Conclusions

- Significant simulation acceleration are obtained by exploiting GPUs in combustion simulations.

- The computational time is seen to scale less than quadratically with the number of chemical species in the kinetic mechanism when using the GPU, as compared to the super-quadratic scaling normally seen with CPU-only chemical kinetics computations.
Conclusions (Cont.)

- The combination of the on-the-fly model reduction scheme with the GPU/CPU hybrid ODE solver accelerated the single-zone HCCI engine simulations with the detailed methyl decanoate mechanism by up to 300-fold!

- By using the AMC model together with the model reduction method and the GPU/CPU ODE solver, we completed 2-D HCCI engine simulations within only 15 hours on a PC with a Tesla C2050 GPU card.
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