SpeedCHEM
A Sparse Analytical Jacobian Chemistry code for Engine Simulations with Detailed Chemistry

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Outline

- Motivation and challenges

- The Sparse Analytical Jacobian approach
  - Chemical Kinetics for Internal Combustion Engine simulations
  - Sparsity and structure of the problem’s Jacobian matrix
  - Effect of reaction mechanism size on sparsity

- A code for the solution of chemical kinetics using SAJ
  - Validation at adiabatic constant-volume reactors
  - ODE solver choice, accuracy and problems

- Modelling of a Heavy-Duty Diesel Engine
  - CFD simulation methodology and grid characteristics
  - Impact of grid resolution, and mechanism dimensions

- Conclusions
Motivation and challenges

- New combustion concepts (HCCI/PCCI, RCCI) show impressive improvements in conversion efficiency
  - ICE indicated efficiency >50%
  - strong dependency on fuel chemistry and local mixture reactivity

- Simple/phenomenological combustion models lack of resolution in modelling:
  - the whole range of operating conditions of practical systems
  - presence of exhaust gases in the mixture
  - simultaneous operation with multiple fuels

- Practical reaction mechanisms for Internal Combustion Engine simulations range from ~30 to ~200 species
  - Total CPU times typically unviable for practical engineering design (cases should run overnight)

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Sizes of biofuels mechanisms
(from Perini, Ph.D. Thesis, 2011)

\[
\text{n_s} = 30 \div 200
\]
Chemical Kinetics in ICE CFD

\[ \frac{\partial Y_i}{\partial t} = - \nabla \cdot (Y_i \mathbf{v}) - \nabla \cdot Y_i \mathbf{v}_{d,i} + \frac{1}{\rho} \omega_i \mathbf{W}_i \]

\[ \frac{\partial E}{\partial t} = - \nabla \cdot (E \mathbf{v}) - \nabla \cdot (\mathbf{v} \cdot \mathbf{T}) - \nabla \cdot (\dot{\mathbf{Q}} + \dot{\mathbf{Q}}_r) + \mathbf{v} \cdot \sum_j m_j a_j + \sum_j \mathbf{v}_{d,i} \cdot m_j a_j \]

- Usually part of an operator-splitting scheme
- Each cell is treated as an adiabatic well-stirred reactor
  - embarassingly parallel problem
  - very stiff IVP
  - only overall changes in species mass fractions and internal energy are passed to the flow solver
- Approach to the solution should be tailored to the problem
Sparse Analytical Jacobian approach

- Chemical Kinetics is a **sparse** problem => **Jacobian** matrix

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>(n_s)</th>
<th>(n_r)</th>
<th>non-zero</th>
<th>sparsity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. ERC n-heptane</td>
<td>29</td>
<td>52</td>
<td>412</td>
<td>54.2%</td>
</tr>
<tr>
<td>2. LLNL n-heptane</td>
<td>160</td>
<td>1540</td>
<td>3570</td>
<td>86.2%</td>
</tr>
<tr>
<td>3. LLNL PRF</td>
<td>1034</td>
<td>4236</td>
<td>22551</td>
<td>97.9%</td>
</tr>
<tr>
<td>4. LLNL MD</td>
<td>2878</td>
<td>8555</td>
<td>166703</td>
<td>99.4%</td>
</tr>
</tbody>
</table>

- Usually, not more than 3-4 species per reaction
- Significant even at small mechanisms
Jacobian matrix sparsity effects

- Reduce scaling of the computational demand for evaluating the Jacobian matrix: \( n_s^2 \Rightarrow n_s \)
- Reduce matrix storage requirements: \( n_s^2 \Rightarrow n_s \)
- Scaling of the costs for matrix factorization: \( n_s^3 \Rightarrow n_s \)
- Improve (quadratic) convergence of Newton’s iterative method
Tabulation of temperature-dependent quantities

- Interpolation errors can be very low e.g. at degree-4 interpolation
- Fixed temperature steps make storage simpler, data contiguous, and interpolating polynomial coefficients simple to compute
- CPU time reduction of more than 1 order of magnitude
Tabulation of temperature-dependent quantities II – effect on total CPU time

- The relative importance of tabulation decreases at increasing mechanism dimensions
- Anyway, it accounts for about 50% CPU time in comparison with the non-tabulated case
- At large reaction mechanisms, the solution of the linear system accounts for almost 50% time
Results: constant-volume reactors

- 18 ignition cases for each mechanism
- \( P_0 = 2.0, 20.0 \) bar
- \( T_0 = 750, 1000, 1500 \) K
- \( \phi_0 = 0.5, 1.0, 2.0 \)

<table>
<thead>
<tr>
<th>Program</th>
<th>CHEMKIN-II</th>
<th>present code</th>
</tr>
</thead>
<tbody>
<tr>
<td>ODE solver</td>
<td>VODE</td>
<td>LSODES</td>
</tr>
<tr>
<td>relative tolerance</td>
<td>( 10^{-4} )</td>
<td>( 10^{-4} )</td>
</tr>
<tr>
<td>absolute tolerance</td>
<td>( 10^{-13} )</td>
<td>( 10^{-13} )</td>
</tr>
</tbody>
</table>
Results: constant-volume reactors II

- Almost linear speedup in comparison with a reference code that uses FD

- At typical mechanism dimension, the speedup is of almost one order of magnitude

- Nota Bene: two different solvers were used!
Results: constant-volume reactors III

![Graph showing CPU time vs. n_s for different programs]

<table>
<thead>
<tr>
<th>Program</th>
<th>Cantera</th>
<th>Chemkin-PRO</th>
<th>CHEMKIN-II</th>
<th>SpeedCHEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>ODE solver</td>
<td>CVODE</td>
<td>Internal (DASPK?)</td>
<td>VODE</td>
<td>LSODES</td>
</tr>
<tr>
<td>relative tolerance</td>
<td>10^{-4}</td>
<td>10^{-4}</td>
<td>10^{-4}</td>
<td>10^{-4}</td>
</tr>
<tr>
<td>absolute tolerance</td>
<td>10^{-13}</td>
<td>10^{-13}</td>
<td>10^{-13}</td>
<td>10^{-13}</td>
</tr>
</tbody>
</table>

*All cases run on a 32-bit 3.0GHz Pentium IV machine with 1GB RAM*
Different solvers do have different performance…

- All of the solvers have been implemented sparse solution of linear systems (Yale sparse matrix package, 1983)
- The same truncation error handling has different meanings

\[ |y(t_n) - \hat{y}(t_n)| \leq RTOL \cdot |y(t_n)| + ATOL \]
... and stricter tolerances do not always mean better results

LLNL n-heptane mech
SpeedCHEM + LSODES solver
Reference solution has RTOL = 1d-15
Modelling of a Heavy-Duty Diesel Engine

Caterpillar SCOTE 3401 Engine details

<table>
<thead>
<tr>
<th>Details</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine type</td>
<td>direct-injection diesel</td>
</tr>
<tr>
<td>Number of cylinders</td>
<td>1</td>
</tr>
<tr>
<td>Valves per cylinder</td>
<td>4</td>
</tr>
<tr>
<td>Bore x Stroke [mm]</td>
<td>137.2 x 165.1</td>
</tr>
<tr>
<td>Conrod length [mm]</td>
<td>261.6</td>
</tr>
<tr>
<td>Compression ratio [-]</td>
<td>16:1</td>
</tr>
<tr>
<td>Unit displacement [L]</td>
<td>2.44</td>
</tr>
<tr>
<td>Chamber Turbulence</td>
<td>Quiescent</td>
</tr>
<tr>
<td>Piston bowl geometry</td>
<td>Mexican hat</td>
</tr>
</tbody>
</table>

- Extensive experimental measurements by Hardy, UW-ERC (SAE 2006-01-0026)

<table>
<thead>
<tr>
<th>Engine operating conditions</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotating speed [rev/min]</td>
<td>1737</td>
</tr>
<tr>
<td>Engine load [-]</td>
<td>57%</td>
</tr>
<tr>
<td>Intake temperature [K]</td>
<td>305.15</td>
</tr>
<tr>
<td>Injection rate [g/s]</td>
<td>1.94</td>
</tr>
<tr>
<td>Pilot injection start [°atdc]</td>
<td>-65 ± -50</td>
</tr>
<tr>
<td>Pilot injection length [μs]</td>
<td>1000 ± 1450</td>
</tr>
<tr>
<td>Main injection start [°atdc]</td>
<td>-5 ± 20</td>
</tr>
<tr>
<td>Main injection length [μs]</td>
<td>1950</td>
</tr>
<tr>
<td>EGR fraction</td>
<td>0 %</td>
</tr>
<tr>
<td>Boost pressure [kPa]</td>
<td>186.2 ± 220.6</td>
</tr>
</tbody>
</table>

- Two-stage combustion
  - High sensitivity to emissions
  - No interaction between spray jets

- Pilot SOI, main SOI, boost pressure sweeps
CFD simulation setup

- **KIVA-4 code developed at LANL** *(Torres & Trujillo, JCP 2006)*

- **Model improvements**
  - Detailed chemistry capability using CHEMKIN-II (CONV) or present code
  - Dynamic injection spray angle computation *(Reitz and Bracco, SAE790494)*
  - Smooth grid snapping algorithm

- **Diesel fuel modelling**
  - tetradecane *(C14H30)* liquid spray properties
  - n-heptane *(nC7H16)* ignition chemistry

- **NO\textsubscript{x} formation mechanism from GRI-mech**
  - 5 additional species, 12 reactions

<table>
<thead>
<tr>
<th>Grid</th>
<th>Coarse</th>
<th>Refined</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cells at BDC</td>
<td>16950</td>
<td>42480</td>
</tr>
<tr>
<td>Average resolution</td>
<td>2.2 mm</td>
<td>1.1 mm</td>
</tr>
<tr>
<td>Azimuth resolution</td>
<td>4.0 deg</td>
<td>~ 3.3 deg</td>
</tr>
</tbody>
</table>
Results: Caterpillar SCOTE 3401

- Excellent agreement of the new solver coupling vs. Chemkin-II
- Average CPU time reduction (included flow-field part):
  - 75.4% (LLNL) 48.8% (ERC)
Caterpillar SCOTE 3401: coarse vs. refined

- Refined grid's peak in AHRR due to ignition of almost-quiescent mixture in the squish region
- Volume averaging and reduced spray penetration in the coarse grid reduces the AHRR peak and delays ignition

![Injection axis cutplane, -16° ATDC]

**LLNL n-heptane mech., present code**

<table>
<thead>
<tr>
<th>CA degrees ATDC</th>
<th>In-cylinder pressure (bar)</th>
<th>Rate of Heat Release (J/CA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-80</td>
<td>0</td>
<td>-60</td>
</tr>
<tr>
<td>-60</td>
<td>20</td>
<td>-20</td>
</tr>
<tr>
<td>-40</td>
<td>40</td>
<td>-60</td>
</tr>
<tr>
<td>-20</td>
<td>60</td>
<td>-20</td>
</tr>
<tr>
<td>0</td>
<td>80</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>100</td>
<td>20</td>
</tr>
<tr>
<td>40</td>
<td>120</td>
<td>40</td>
</tr>
<tr>
<td>60</td>
<td>140</td>
<td>60</td>
</tr>
<tr>
<td>80</td>
<td>160</td>
<td>80</td>
</tr>
</tbody>
</table>

- In both grids the fuel vapor jet is deviated to the cylinder head
Caterpillar SCOTE 3401: NO\textsubscript{x} emissions

- Parameter sweeps
  - pilot pulse SOI
  - main pulse SOI
  - boost pressure

- ERC mechanism
  - refined grid case
    - peak in AHRR after pilot injection leads to mismatched NO\textsubscript{x} trend

- Coarse grid has greater temperature distribution mixing
  - NO\textsubscript{x} are underestimated

Very good agreement between chemistry solvers
Conclusions

- A new code for the integration of **sparse** reaction kinetics of gaseous mixtures has been developed.
- The code has been coupled with KIVA-4, to model a heavy-duty Diesel engine operated in a two-stage combustion mode.

- Comparison with a reference academic chemistry code showed excellent agreement.
- Speedups of the order of **2 times** => **30+ times** were achieved at a range of mechanism dimensions vs. FD code.
- CPU times for refined grid + detailed mech. were < **25h on 4CPU**

*The solver is suitable to incorporate semi-detailed reaction mechanisms in practical engine simulations.*
There’s plenty of room at the bottom

- Find out optimal ODE integration method at different reactivity (and stiffness) conditions
- Investigate the accuracy of sparse semi-implicit integrators
- Find suitable Jacobian preconditioners
- Explore ODE solvers accuracy using quadruple-precision arithmetics
- Investigate the role of transport in ICE simulations with detailed chemistry integration
Thanks for your attention! Questions?

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Backup
Jacobian matrix sparsity assumption

- Three-body and more complex pressure-dependent reactions involve the whole mixture concentration

\[ C_{tot} = \sum_{i=1}^{n_s} \frac{\rho Y_i}{W_i} \]

- In constant-pressure environments, \( C_{tot} \) is constant
- In constant-volume environments, \( C_{tot} \) has non-negative derivative with each species

\[ \frac{\partial C_{tot}}{\partial Y_j} = \frac{\partial}{\partial Y_j} \left( \sum_{i=1}^{n_s} \frac{\rho Y_i}{W_i} \right) = \frac{\rho}{W_j} \quad \forall \ j = 1, \ldots, n_s \]

- Dense lines in the Jacobian matrix
Jacobian matrix sparsity assumption

- Simplifying assumption: \[
\frac{\partial C_{tot}}{\partial Y_j} \approx 0
\]

- Affected is the Jacobian only, not the problem formulation
Jacobian matrix sparsity assumption

- Comparison between complete and sparser formulation
Chemical Kinetics IVPs

Chemical kinetics IVPs in adiabatic environments

- For an arbitrary reaction mechanism,
  \[ \sum_{i=1}^{n_s} v'_{k,i} M_i \Rightarrow \sum_{i=1}^{n_s} v''_{k,i} M_i, \quad k = 1, \ldots, n_r \]

- Mass conservation:
  \[ \frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} \left( v''_{k,i} - v'_{k,i} \right) q_k(Y, T), \quad i = 1, \ldots, n_s \]

- Energy conservation:
  \[ \frac{dT}{dt} (Y, T) = -\frac{1}{\bar{c}_v(Y, T)} \sum_{i=1}^{n_s} \left( \frac{U_i(T)}{W_i} \frac{dY_i}{dt} (Y, T) \right) \]

- Integrated with stiff ODE solvers (VODE, LSODE, RADAU5...)

- Only species and internal energy sources are linked to the CFD solver
Interpolation of temperature-dependent quantities

- Species thermodynamic potentials are polynomial functions of temperature
  in JANAF format, e.g.
  \[ U_i = R_{mol} \left[ (a_i - 1) T + \frac{b_i}{2} T^2 + \frac{c_i}{3} T^3 + \frac{d_i}{4} T^4 + \frac{e_i}{5} T^5 + f_i \right] ; \]

- Equilibrium constant is an exponential function of the reaction’s free energy delta:
  \[ K_{c_{eq}, k} (T) = \exp \left( -\Delta g_k^0 \right) \left( \frac{p_{atm}}{RT} \right) \sum_{i=1}^{n_s} (v''_{k,i} - v'_{k,i}) ; \]

- Reaction rates are exponentials too:
  \[ \kappa_{f, k} (T) = A_k T^{b_k} \exp \left( -\frac{E_k}{RT} \right) . \]
Interpolation of temperature-dependent quantities

- Then, the interpolation errors can be very low e.g. at degree-4 interpolation
- Fixed temperature steps make storage simpler and data contiguous
- CPU time reduction of more than 1 order of magnitude with -O3
Interpolation of temperature-dependent quantities

\[ p_n(x) = \sum_{i=0}^{n} a_i x^i = a_0 + a_1 x + a_2 x^2 \ldots + a_n x^n \]
Species thermodynamic properties databases
Effect of RTOL and ATOL on local error constraint

\[ |y(t_n) - \hat{y}(t_n)| \leq RTOL \cdot |y(t_n)| + ATOL \]