TOWARDS EXASCALE ENGINE SIMULATIONS WITH NEK5000

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OUTLINE

• Internal Combustion Engine Research – Trends and Challenges
• Role of Simulations in Engine Research
• Do Engine Simulations Need Exascale Computing?
• Need for High-order Numerics
• Nek5000: High-order Scalable Spectral Element Code for Exascale Computing
• TCC Engine Simulations using Nek5000
• Future Work
• Summary
IC engines will continue to be an ubiquitous powertrain component for many decades due to:

- Competitive well-to-wheel energy efficiency
- Potential for near-zero harmful emissions
- Cost-effectiveness
- Highly developed fueling infrastructure

Over-arching objective:
- Speed the advancement of these positive attributes
- Provide powertrain solutions that maximize efficiency
- Minimize emissions at the lowest possible cost

Objective of this project: Develop the next generation engine simulation code that can scale well on the future exascale platforms
Engine power density has been increasing
Faster acceleration

Vehicle size and weight have increased, but fuel economy has improved

Total highway vehicle emissions have declined (from 2002 to 2015), even as the number of vehicles and VMT have increased.

NEW CARS CLEAN THE AIR!

Tailpipe Emissions are Lower than Ambient Levels on the LA Freeway

Measurement sample on Los Angeles Highway

Source: Gurpreet Singh, DOE Vehicle Technologies Office Annual Merit Review, 2018
REMAINING TECHNICAL CHALLENGES

- Improve understanding of, and ability to manipulate, combustion processes.
- Improve understanding of how fuel properties impact the efficiency of modern engines.
- Generate knowledge and insight necessary for industry to develop the next generation engines and fuels capable of improving the fuel economy of passenger and commercial vehicles.

Source: Gurpreet Singh, DOE Vehicle Technologies Office Annual Merit Review, 2018
Accurate, science-based, simulations using CFD can shed light on the complex phenomena within an ICE by improving the fundamental understanding that will help to establish and characterize the physical causes of stochastic events.

Predictive simulations were identified as an important tool in enabling increased engine efficiency [U.S. DOE – Office of Science]

Advanced simulation of processes such as the turbulent gas-exchange process, heat transfer, and fluid interactions with the cylinder walls are critical to realizing efficient engines with greater power density.
**Challenges:** Two-phase flows, all modes of heat-transfer, combustion chemistry for different fuels, turbulent - reacting flows, material issues (conjugate heat transfer) ...
Moving boundaries, grid convergence is challenging, ...
CO-DESIGN OF ENGINES AND FUELS: AN EXASCALE PROBLEM

According to John Deur, Director of Engine Research at Cummins Inc., the following levels of speedup are needed to significantly impact today’s engine development:

- [10x] 360 degree cylinder geometry
- [10x] multiple cycle variations
- [10x] more accurate turbulence model (LES)
- [10x] accurate spray dynamics
- [50x] detailed chemical kinetics for real transportation fuels

TOTAL Speedup needs are 500,000 times TODAY’S standard (today’s industry standard is 64 cores with 24 hour turnaround)

OUR PROBLEM IS EXASCALE => 30 million cores for 24 hour turnaround!

In general scalable codes are highly desirable since today’s cluster will be tomorrow’s laptop

* DOE Engine Simulation Roadmap Workshop - August 18, 2014
HIGH-FIDELITY MODELS ACROSS THE DESIGN SPACE
(Capability Computing)

High-order, scalable codes:
Nek5000

DNS

LES

206 CAD

HIGH THROUGHPUT SIMULATIONS TO EXPLORE THE FULL DESIGN SPACE
(Capacity Computing)

Low-order codes:
Converge, OpenFOAM, etc.
NEK5000
Where do High-Order and Low-Order methods part ways?

Large problem sizes enabled by peta- & exascale computers allow propagation of small features (size $\lambda$) over distances $L \gg \lambda$. If speed $\sim 1$, then $t_{\text{final}} \sim L / \lambda$.

- Dispersion errors accumulate linearly with time:
  $\sim |(\text{correct speed} - \text{numerical speed}) \times t|$ (for each wavenumber)
  $\Rightarrow \text{error}_{t,\text{final}} \sim (L / \lambda) \times |\text{numerical dispersion error}|$
- For fixed final error $\varepsilon_f$, require: numerical dispersion error $\sim (\lambda / L) \varepsilon_f \ll 1$.

High-order methods can efficiently deliver small dispersion errors.
(Kreiss & Oliger 72, Gottlieb et al. 2007)
SPECTRAL ELEMENT CONVERGENCE: EXPONENTIAL WITH $N$

- 4 orders-of-magnitude error reduction when doubling the resolution in each direction

- For a given error,
  - Reduced number of gridpoints
  - Reduced memory footprint.
  - Reduced data movement.

Exact Navier-Stokes Solution (Kovazsnay '48)

\[ \nu_x = 1 - e^{\lambda x} \cos 2\pi y \]
\[ \nu_y = \frac{\lambda}{2\pi} e^{\lambda x} \sin 2\pi y \]
\[ \lambda := \frac{Re}{2} - \sqrt{\frac{Re^2}{4} + 4\pi^2} \]
SPECTRAL ELEMENT METHOD

Costs

- Cost dominated by iterative solver costs, proportional to
  - iteration count
  - matrix-vector product + preconditioner cost

- Locally-structured tensor-product forms:
  - minimal indirect addressing
  - fast matrix-free operator evaluation
  - low-cost local operator inversion via fast diagonalization method \( (Lynch \textit{et al.} \ '64) \)
ADVANTAGE OF HIGH-ORDER CODES

OpenFOAM vs. Nek5000

➢ Problem Description: Incompressible viscous flow driven by a constant pressure gradient between two infinite parallel plates (Kim, Moin & Moser, JFM 1987, MKM 1999)

➢ Computational domain: \((L_x, L_y, L_z) = (4\pi\delta, 2\delta, 2\pi\delta)\)

➢ Reynolds number: \(Re = U_m \delta / \nu = 2800\)

➢ Performance and accuracy comparison of Nek5000 and OpenFOAM for turbulent channel flow at \(Re = 2800\) [Sprague et al. 2010 @ Nek5000 users meeting].

➢ For a given accuracy, turbulent channel flow simulations using SEM (Nek5000) requires half as many gridpoints in normal direction (1/8th as many for total domain)

➢ Nek5000 is more efficient, requiring 1/8th the computational resources for the simulation results.
NEK5000: HIGHLIGHTS

➢ Nek5000 is a spectral element code that has been under active development for 30+ years
➢ Applications span a wide range of fields, including fluid flow, thermal convection, combustion and magnetohydrodynamics
➢ User community includes over 400+ scientists and engineers in academia, laboratories and industry
  ➢ Annual user meetings and hackathons
➢ Currently part of codesign center funded by the exascale computing project – CEED (Center for Efficient Exascale Discretizations) and PSAAP-II Center for Multiphase Turbulence
  ➢ Part of the European ExaFLOW program for external aerodynamics simulations
➢ Heavily used by the nuclear energy community, and is part of the NEAMS (Nuclear Energy Advanced Modeling and Simulations Program) Center of Excellence
➢ Current version can handle low-Mach and incompressible flows; compressible version under validation at UIUC and UF
➢ Combustion model development at ETH-Zürich
NEK5000: NUMERICAL APPROACH

- **Spatial Discretization:** Spectral Element Method (SEM) (*Patera* 84, *Maday & Patera* 89)
  - Body-fitting capabilities for complex geometries
  - Solution is represented as $N$th-order tensor-product polynomials inside each element (typically $N \sim 4 – 15$)
  - Delivers minimal numerical dispersion (*Kreiss & Oliner* 72, *Gottlieb et al.* 2007)
    - **Exponential convergence** with $N$ for smooth solutions

- **Temporal Discretization**
  - Semi-Implicit & Characteristic-Based Schemes
    - 2nd or 3rd

- **ALE formulation for moving geometries**

- **Low-Mach number formulation**
  - Scale separation between fluid and acoustic wave propagation
  - Variable density (due to heat release) (*Rehm & Baum* 78)

- **High-order splitting scheme**
  - Continuity & momentum: semi-implicit
  - Species & energy: fully implicit (CVODE) (*Tomboulides et al.*, 97)
Mesh Generation

- **Genbox**: Simple box-type meshes
- **Prenek**: Dedicated Nek5000 meshing software for slightly more complex meshes
- **Mesh converters**: Nek5000 provides utilities to seamlessly convert meshes generated from several 3rd party mesh generators to Nek meshes
  - ICEM
  - CUBIT
  - HOPR
- High-order grid-to-grid interpolation utility to use several sequential SEM meshes for a transient moving geometry simulation

Post-Processing

- Nek5000 results can be visualized using ParaView or Visit
Cycle to cycle variation of incompressible flow in a piston-valve assembly experiment performed at Imperial College in London.

Good agreement in terms of flow structure as well as mean and rms velocities at different piston positions and measurement locations.
NEK5000: SCALABILITY

217 Pin Problem, N=9, E=3e6:

- 2 billion points

- BGQ – 524288 cores
  - 1 or 2 ranks per core

- A mixture of CG / multigrid

- 60% parallel efficiency at 1 million processes

- 2000 points/process
ICE SIMULATIONS USING NEK5000
Motored TCC-III Engine

Geometry and Valve Timings

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (L_b)</td>
<td>9.2 cm</td>
</tr>
<tr>
<td>Stroke</td>
<td>8.6 cm</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>23.1 cm</td>
</tr>
<tr>
<td>Geometric Compression Ratio</td>
<td>10:1</td>
</tr>
<tr>
<td>Clearance Height</td>
<td>0.95 cm</td>
</tr>
<tr>
<td>RPM</td>
<td>500</td>
</tr>
<tr>
<td>Max. Piston Velocity (U_p)</td>
<td>229.017 (cm/s)</td>
</tr>
<tr>
<td>Intake Valve Opening (IVO)</td>
<td>0 CAD</td>
</tr>
<tr>
<td>Intake Valve Closing (IVC)</td>
<td>180 CAD</td>
</tr>
<tr>
<td>Exhaust Valve Opening (EVO)</td>
<td>540 CAD</td>
</tr>
<tr>
<td>Exhaust Valve Closing (EVC)</td>
<td>720 CAD</td>
</tr>
</tbody>
</table>

- 21 cycles of motored operation
- Characteristic Time-Stepping for ALE (Patel et al. 2017)
  - CFL = 3.5

Boundary Conditions for Air

<table>
<thead>
<tr>
<th>Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake Pressure</td>
<td>101.325 kPa</td>
</tr>
<tr>
<td>Intake Temperature</td>
<td>400 K</td>
</tr>
<tr>
<td>Pipe Temperature</td>
<td>400 K</td>
</tr>
<tr>
<td>Cylinder Wall Temp</td>
<td>500 K</td>
</tr>
</tbody>
</table>

Presented at the VERIFI 2017 Workshop
# TCC-III: COMPUTATIONAL SET-UP

<table>
<thead>
<tr>
<th>Resolution Parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Polynomial Order (N)</td>
<td>5</td>
</tr>
<tr>
<td>Min # of Elements</td>
<td>68K @ TDC Intake</td>
</tr>
<tr>
<td>Max # of Elements</td>
<td>210K @ TDC Compression</td>
</tr>
<tr>
<td>Min # of Total Points</td>
<td>7.5 M @ TDC Intake</td>
</tr>
<tr>
<td>Max # of Total Points</td>
<td>23 M @ TDC Compression</td>
</tr>
<tr>
<td>Element Size (h)</td>
<td>0.75mm – 1.5mm</td>
</tr>
<tr>
<td>Effective Resolution</td>
<td>0.05 – 0.25mm @ TDC Intake</td>
</tr>
<tr>
<td></td>
<td>0.03 – 0.12mm @ TDC Compression</td>
</tr>
</tbody>
</table>

➢ 28 SEM grids constructed a priori in CUBIT
- High-Order g2gi
➢ Computational Cost:
- **54K CPUhr/Cycle** on Theta (KNL)
- **13 Hours/Cycle**, Using 4,096 processors
TCC-III
4-Stroke Cycle

➢ Intake Stroke: $\lambda_2$ vortex criterion (Jeong & Hussein '95) involves velocity gradients

$$\lambda_2(S^2 + \Omega^2) < 0$$

$$S := \frac{1}{2}[\nabla u + (\nabla u)^T]$$

$$\Omega := \frac{1}{2}[\nabla u - (\nabla u)^T]$$

➢ Comp/Exp Stroke:

▪ Heat Flux along the Boundary
▪ Temperature within the cylinder

➢ Exhaust Stroke:

▪ $\lambda_2$ vortices in the exhaust pipe
TCC-III

Cycle-to-Cycle Results – Velocity Magnitude, 25 CAD, y=0

➢ Intake Jet Variability
  ▪ Flapping motion
  ▪ Penetration and Orientation

Cycle 3 - 68.7 (m/s)
Cycle 4
Cycle 5
Smaller eddies develop during compression stroke

- $Re$ increases 5x due to decrease in kin. viscosity ($v = \mu(T)/\rho(P,T)$)
- Max Resolution at TDC

Results – Heat Flux on the Cylinder Head, $z=0$
SCALABILITY

Strong Scaling on Theta (ALCF)

This work: production runs at 18.8K pts/process (80% efficiency)
NEXT STEPS

- Code development
  - Compressibility formulation
  - Lagrangian phase – spray and ignition submodels
  - Combustion models – premixed, non-premixed, advanced chemistry solvers

- Validation
  - Real engine platforms
  - Spray flames

- Scalability
  - Demonstrate scalability on next-generation platforms
SUMMARY

• Trends and challenges in IC engine research was demonstrated
• Simulations will continue to play an important role in IC engine research
• Predictive and high-throughput engine simulations require exascale computing.
• There is a need for highly parallel, and highly accurate (higher order methods) code such as Nek5000 code for exascale computing.
• Lower order commercial codes can also utilize exascale computing in a “capacity fashion” wherein multiple jobs are bundled together and submitted.
• Nek5000 was used to perform multi-cycle LES for a motored engine. Strong scalability was demonstrated up to 32,768 cores.
• Future plans include incorporating advanced spray, combustion, and ignition models.
ACKNOWLEDGEMENTS

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Gurpreet Singh, Michael Weismiller

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G. Giannakopoulos (ETH Zurich), M. Min (Argonne)
THANK YOU

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SPECTRAL ELEMENT METHOD

Fast “Matrix-Free” Stiffness Matrix in 3D

- For a deformed spectral element, $\Omega^e$, never form local stiffness matrix.

$$A^e u^e = \begin{pmatrix} D_r \\ D_s \\ D_t \end{pmatrix}^T \begin{pmatrix} G_{rr} & G_{rs} & G_{rt} \\ G_{sr} & G_{ss} & G_{st} \\ G_{tr} & G_{ts} & G_{tt} \end{pmatrix} \begin{pmatrix} D_r \\ D_s \\ D_t \end{pmatrix} u^e$$

$$D_r = (I \otimes I \otimes \hat{D}) \quad G_{rs} = J \circ B \circ \left( \frac{\partial r}{\partial x} \frac{\partial s}{\partial x} + \frac{\partial r}{\partial y} \frac{\partial s}{\partial y} + \frac{\partial r}{\partial z} \frac{\partial s}{\partial z} \right)$$

Through use of chain rule + GLL quadrature:

- Matrix-free operator evaluation.
- Operation count is only $O(N^4)$ not $O(N^6)$ [Orszag '80, F'89, DFM02]
- Memory access is $7n$ ($G_{rr}, G_{rs},$ etc., are diagonal)
- Work is dominated by matrix-matrix products involving $D_r$, $D_s$, etc.
NEK5000

Flops Are Free Model

• $C = A \times B$:
  - Two $N \times N$ matrices,
  - $2N^2$ memory references
  - $2N^3$ ops

• $C = A + B$
  - Two $N \times N$ matrices,
  - $2N^2$ memory references
  - $N^2$ ops

**Times are the same, out to $N=14$.**
  - noncached data…
### EXASCALE APPLICATIONS ARE TARGETING NATIONAL PROBLEMS IN SIX KEY STRATEGIC PILLARS

<table>
<thead>
<tr>
<th>National security</th>
<th>Energy security</th>
<th>Economic security</th>
<th>Scientific discovery</th>
<th>Earth system</th>
<th>Health care</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stockpile stewardship</td>
<td>Turbine wind plant efficiency</td>
<td>Additive manufacturing of qualifiable metal parts</td>
<td>Cosmological probe of the standard model of particle physics</td>
<td>Accurate regional impact assessments in Earth system models</td>
<td>Accelerate and translate cancer research</td>
</tr>
<tr>
<td>Next-generation electromagnetics simulation of hostile environment and virtual flight testing for hypersonic re-entry vehicles</td>
<td>Design and commercialization of SMRs</td>
<td>Urban planning</td>
<td>Validate fundamental laws of nature</td>
<td>Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Nuclear fission and fusion reactor materials design</td>
<td>Reliable and efficient planning of the power grid</td>
<td>Plasma wakefield accelerator design</td>
<td>Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Subsurface use for carbon capture, petroleum extraction, waste disposal</td>
<td>Seismic hazard risk assessment</td>
<td>Light source-enabled analysis of protein and molecular structure and design</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>High-efficiency, low-emission combustion engine and gas turbine design</td>
<td></td>
<td>Find, predict, and control materials and properties</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Carbon capture and sequestration scaleup</td>
<td></td>
<td>Predict and control stable ITER operational performance</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Biofuel catalyst design</td>
<td></td>
<td>Demystify origin of chemical elements</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
TURBULENT ROUND JET SIMULATIONS
Computational Setup

- Objective: Utilize Nek5000 to simulate reacting fuel jets
- As a preliminary study, LES of turbulent non-reacting round jets were performed with Nek5000
- Prenek utility used for mesh generation
- Boundary layers accurately resolved using a stretched body-fitting mesh
Simulations show good agreement with experimental measurements
Performing convergence study with respect to grid size and polynomial order
This setup will be used as a starting point for the combustion model development
NEK5000 IS NO STRANGER TO COMBUSTION COMMUNITY

• Has been coupled with CHEMKIN-based libraries to compute reaction and diffusion rates
USING HIGH-ORDER CODES TO IMPROVE THE PERFORMANCE OF LOW-ORDER CODES

INTRODUCTION

- Most engine CFD codes employ low-order discretization schemes and implicit solvers to ensure numerical stability.
- These low-order schemes tend to add large numerical viscosity to the solution.
- This is ideal for RANS since the turbulent viscosity is much higher than numerical viscosity for high Re engine flows, but can be troublesome for LES.

![Diagram showing comparison between using a RANS code for LES and a good LES code.] 

Courtesy: T. Poinsot, LES4ICE 2016
# NUMERICS OF THE CODES

## Comparison of Low-order and high-order codes

<table>
<thead>
<tr>
<th></th>
<th>High-order code(^1)</th>
<th>Low-order code(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>Finite difference method</td>
<td>Finite volume method</td>
</tr>
<tr>
<td>Spatial discretization</td>
<td>6(^{th})-order Pade scheme</td>
<td>2(^{nd})-order central scheme and 1(^{st}) order upwind</td>
</tr>
<tr>
<td>Temporal discretization</td>
<td>4(^{th})-order Runge-Kutta scheme</td>
<td>1(^{st})-order</td>
</tr>
<tr>
<td>Inflow/outflow BC</td>
<td>Navier-Stokes Characteristic BC</td>
<td>Dirichlet / Neumann</td>
</tr>
<tr>
<td>Time-step</td>
<td>Acoustically-limited</td>
<td>Convection/Diffusion CFL</td>
</tr>
<tr>
<td>Language</td>
<td>Fortran 90</td>
<td>C</td>
</tr>
</tbody>
</table>


LES OF TURBULENT ROUND JET

Comparison of Codes

➢ The same grid setup was used for both the codes
➢ The high-order code shows excellent agreement with the experiments
➢ The low-order code shows earlier jet break-up and larger spreading rates

<table>
<thead>
<tr>
<th>Case</th>
<th>Potential Core Length ($d_j$) [6.2]</th>
<th>Spreading Rate (S) [0.094-0.102]</th>
</tr>
</thead>
<tbody>
<tr>
<td>High-order</td>
<td>5.5</td>
<td>0.104</td>
</tr>
<tr>
<td>Low-order</td>
<td>15.5</td>
<td>0.115</td>
</tr>
</tbody>
</table>
LES OF TURBULENT ROUND JET

Low-order code:
Baseline setup

Low-order code:
Improved setup

➢ High-order code simulations motivated improvements in the low-order code setup
➢ Low-order code provides similar jet structure as the high-order code by modifying the perturbation scheme and subgrid model