Optimisation of LESsCOAL for large-scale high-fidelity simulation of coal pyrolysis and combustion

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Outline

• Background information
• Motivation of the project
• Project targets
• The optimization strategies adopted
• Optimization of the pressure module
• Optimization of the radiation module
• Optimization of the particle module
• Parallel performance after optimization
• Conclusions
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Coal particles (75-90 micron) are fed into a premixed methane air flame at a rate of 100 g/m³. 

https://www.youtube.com/watch?v=dtIdyVsO26k
What is coal combustion?

- **Moisture:** Removed in the drying
- **Ash:** No reaction
- **Residual:** Combustible

Residual coal → **pyrolysis** → volatile fuel → Gas Fuel

Gas React. → Surface React. → Product: $\text{H}_2\text{O CO}_2$
Pyrolysis models

**SFOM model**

\[ \frac{dm_{vol}}{dt} = A_v \exp\left(-\frac{E_v}{RT_p}\right)(m_{vol}^* - m_{vol}), \quad m_v^* = Qm_v' \]

- Kinetic: \( A_v, E_v \) and \( Q \)
- Need to be calibrated

**Chemical Percolation Devolatilization model**

- Current **state-of-the-art** model
- **General** kinetic parameters
- **5** chemical **structural** parameters
  
  \( (MW_{cl}, MW_{\delta}, p_0, \sigma + 1, c_0) \)

- \( ^{13}\)C Nuclear Magnetic Resonance
- Nonlinear correlation of \( ^{13}\)C NMR
  
  - volatile matter content
  - ultimate analysis

http://www.et.byu.edu/~tom/devolatilization/CPD%20model.html
Simulation setup

• Primary Inlet \((D = 13 \text{ mm})\)
  - **Gas**: \(N_2, 10 \text{ m/s, } 300 \text{ K, Re } \approx 8200\)
  - **Coal**: \(5.1 \times 10^{-4} \text{ kg/s, } 300 \text{ K, } d_{\text{min}} = 10 \mu\text{m, } d_{\text{max}} = 100 \mu\text{m, } d_{\text{mean}} = 45 \mu\text{m, } \rho = 1400 \text{ kg/m}^3\)

• Co-flow
  - **Gas**: \(N_2, 0.2 \text{ m/s, } 2000 \text{ K}\)

• Outlet
  - Convective boundary condition

• CPD model

• SFOM model calibrated by CPD-LES

• Grid: \(~1.56\text{ million cells}\)
Pyrolysis case

• LES of pulverized-coal pyrolysis
  – Online CPD model => describe pyrolysis of coal particles

Pyrolysis Occurs
SFOM vs. CPD

The calibrated SFOM cannot fully represent the pyrolysis characteristics considered in CPD.

Combustion case

• LES of pulverized-coal combustion
  – Online CPD model => describe pyrolysis of coal particles
  – PaSR combustion model => volatile (gas phase) combustion
  – Kinetic/diffusion model => char (surface) reaction
Validation with exp.

Large difference in the instantaneous pyrolysis characteristics.

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Motivation

• Pulverized-coal combustion (PCC) is important
  – For UK, 25% of electricity power
  – For China, the figure is 70%

• Poor optical access in coal-fired furnaces
  – Difficult to apply advanced laser diagnostics

• High-fidelity simulation
  – Enabled by high-performance computing
  – Large-eddy simulation (LES) of PCC in industrial furnace
  – Computational study of advanced clean coal technologies
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LESsCOAL

• **Large-Eddy Simulations** of **COAL** combustion
  
  – Momentum module => Navier-Stokes equations
    (low Mach number form)
  
  – Scalar module => transport gas species and temperature
  
  – Particle module => trace coal particles
    (two-way coupling)
  
  – Radiation module => solve radiative heat transfer
  
  – Pressure module => solve Poisson equation
  
  – SGS module => calculate subgrid-scale model terms
Original scaling performance

- Good: scalar, momentum and SGS modules
- Poor: particle, radiation and pressure modules
- Overall: satisfactory scaling up to 200 cores
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Project targets & strategies

• Achieve 80% of the theoretical parallel efficiency when up to 3,000 computing cores are used on ARCHER
  – Develop and implement a new parallel particle-tracing algorithm to radically improve the load balance among processor cores.
  – Implement a three-dimensional domain decomposition approach. (more efficient information transfer)
  – Improve the pressure solver, considering both robustness and efficiency.
  – Improving the radiation module.
  – Implement new MPI and FORTRAN functionalities. (One-Sided Communications, non-blocking collectives, C-like pointers, etc)
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Pressure module

• The pressure equation is a Poisson’s equation:

\[ \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2} = S \]

• Solved by calling **HYPRE** – an open-source software package for solving large, sparse linear equations in parallel.

• **https://github.com/LLNL/hypre**
  – Written in C. (provides an interface for Fortran)
  – Require MPI library.
  – Multigrid and Krylov-based solvers: SMG, PFMG, PCG, GMRES, BICGSTAB, HYBRID.
  – Preconditioners: DIAGONAL, PFMG.
• 14 setups with different solvers and preconditioners.
• Least number of iterations: SMG-none.
• Least time consuming: GMRES-PFMG & PCG-PFMG.
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Radiation module

- Discrete ordinates method (DOM) with S4 scheme (24 directions):
  \[
  c_1 \frac{\partial I}{\partial x} + c_2 \frac{\partial I}{\partial y} + c_3 \frac{\partial I}{\partial z} + c_4 I = S
  \]

- The first-order upwind scheme is employed and the finite-difference form of the equations is
  \[
  b_1(I_{i,j,k} - I_{i-1,j,k}) + b_2(I_{i,j,k} - I_{i,j-1,k}) + b_3(I_{i,j,k} - I_{i,j,k-1}) + c_4 I_{i,j,k} = S
  \]
  \[
  (b_1 + b_2 + b_3 + c_4)I_{i,j,k} - b_1 I_{i-1,j,k} - b_2 I_{i,j-1,k} - b_3 I_{i,j,k-1} = S
  \]

- The method is inherently serial, each processor requires the data on its upwind boundaries becoming available before it can begin “meaningful” computations.

- Speedup is limited when large number of cores are used, as cores at the downwind side need to wait for the boundary data to be updated.
1. Priority queuing

- 24 rays.

- Different directions.

- *Priority optimized queuing.*

- Different cores compute different rays at the same time.

- Optimized transport efficiency of the radiation information:
  - Before: once per 24 ray calculations.
  - After: once per ray calculation.
2. Wavefront sweep algorithm

- Cells of the same color are independent and may be processed in parallel once preceding slices are complete.

- Boundary data can be sent to downwind neighbors before all the boundary updated.

**CON:**

- 2D domain decomposition.

- Inefficient memory access.
Diagonal slicing

- More frequent transport of radiation information
- \( N\)block value \( \Rightarrow \) Tuning parameter
  - The frequency of MPI communications between CPU cores.
Recent code optimization work

- Number of grid cells: 10 million
- Method 2: more suitable for modeling radiation in a long channel/tube.
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Particle module

- Lagrangian particle tracing

- Two parallel strategies:
  - Particle decomposition
    - Perfect load balance
    - Access to whole gas field for each core
  - Domain decomposition
    - Gas phase: perfect load balance and efficient
    - Particle phase: load imbalance issue
Load imbalance

• Significant load imbalance issue in the particle module.
  – *LES of gas-solid multiphase turbulent jet.*
  – *Two-way coupling between gas and particle phases.*

  – Distribute particles evenly to each core?
  – How to consider the two-way coupling?
• Particles will be sent from heavy-loaded cores to light-loaded cores.
  – Corresponding gas properties and source terms will also be transferred.
  – Transfer scheme determined by an open-source library: OhHelp.
One-sided communications

- Bookkeeping step in the particle transfer scheme.
- MPI collective communication function: MPI_Allgather
- MPI one-sided communication function: MPI_Put
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Optimized performance

- **Strong scaling test:** Good up to 1200 cores (> 82%).
- **Weak scaling test:** Achieved 80% of the theoretical parallel efficiency when using 3072 cores on ARCHER.
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• The parallel efficiency and optimization work of the LESsCOAL code for LES of pulverized-coal combustion has been presented and discussed.
• The original code has a satisfactory scaling up to 200 cores.
• Good scaling: scalar, momentum and SGS modules;
• Poor scaling: particle, radiation and pressure modules.
• 5 optimization strategies have been employed.
• Parallel efficiency of LESsCOAL has been significantly improved.
• Project target has been achieved: 80% of the theoretical parallel efficiency when using 3072 cores on ARCHER.
Acknowledgements

• The embedded CSE programme of ARCHER UK (0513)

• K.D.W. acknowledge the support from the Engineering and Physical Sciences Research Council (EPSRC) of the UK

• ARCHER UK National Supercomputing Service
  (http://www.archer.ac.uk)
THANK YOU.

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2017-3-22