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

Kaidi Wan[1], Jun Xia[2], Neelofer Banglawala[3], Zhihua Wang[1], Kefa Cen[1]

1. Zhejiang University, Hangzhou, China
2. Brunel University London, Uxbridge, UK
3. Edinburgh Parallel Computing Centre (EPCC), Edinburgh, UK

Jun.Xia@brunel.ac.uk

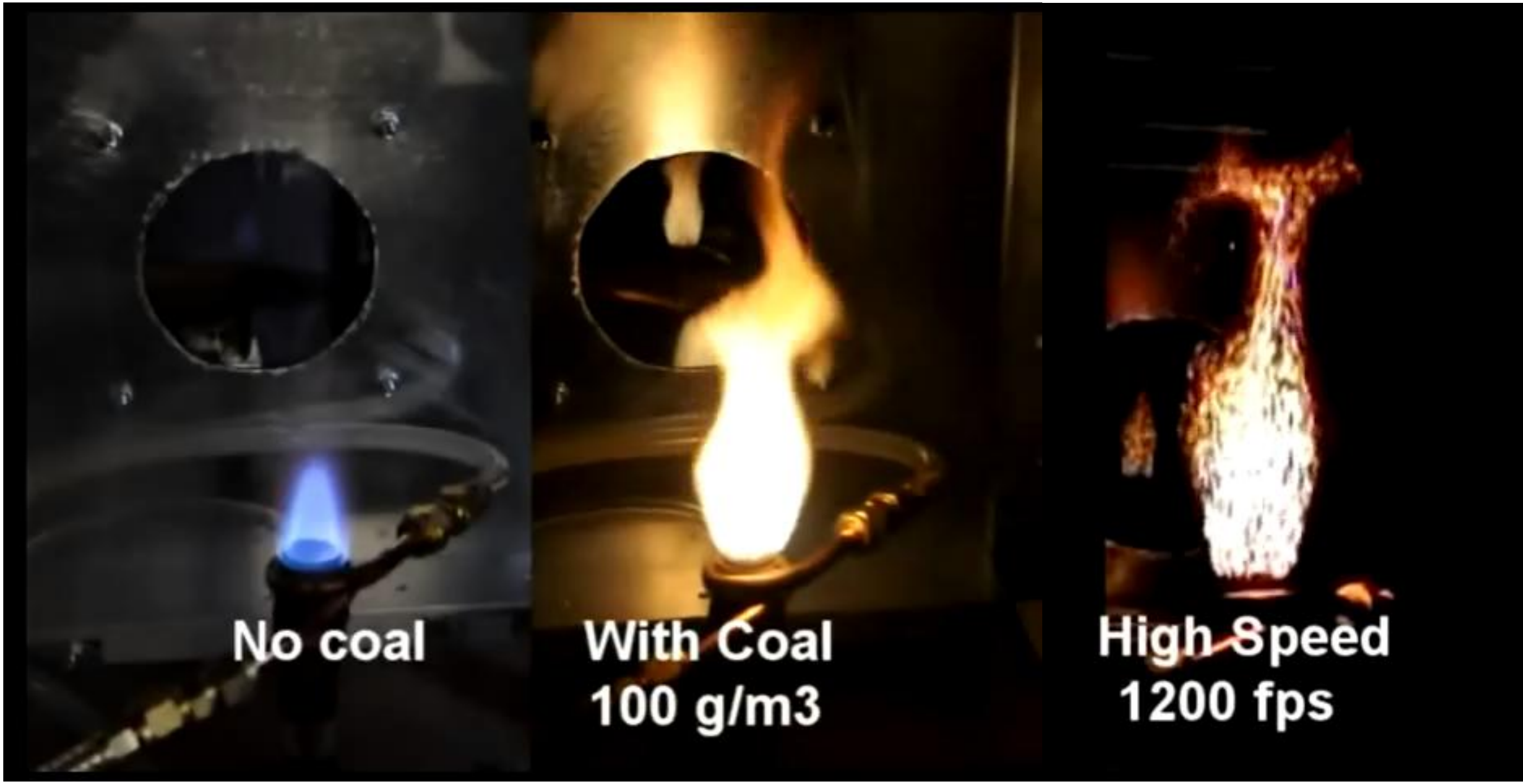
Outline

- 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

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

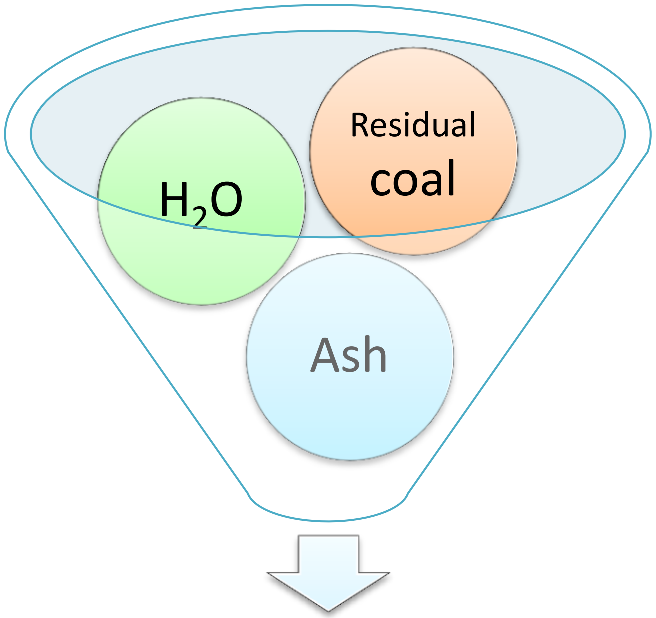
Pulverized-coal combustion



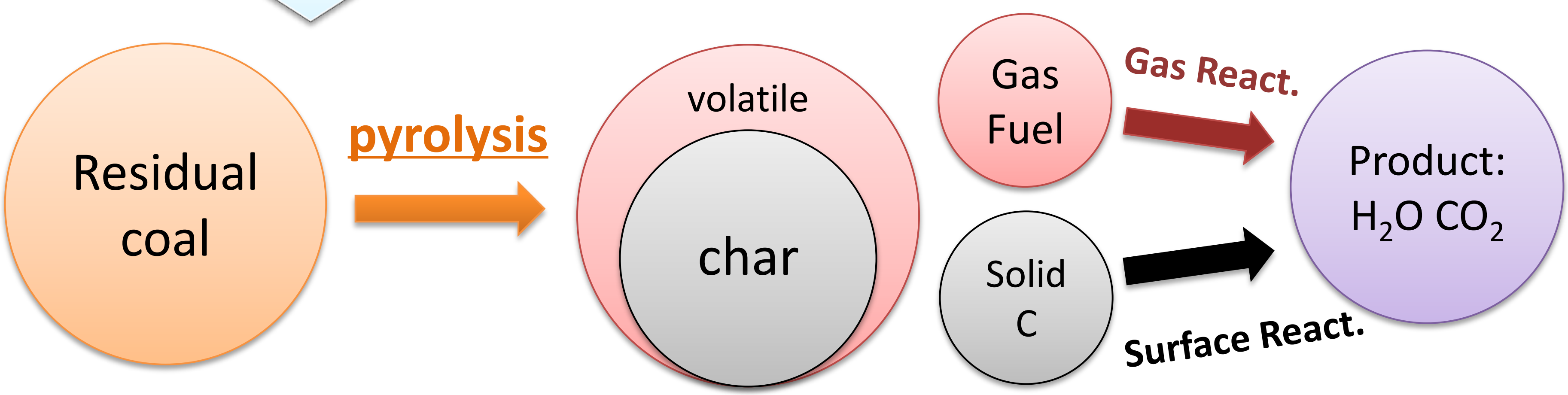
Coal particles (75-90 micron) are fed into a premixed methane air flame at a rate of 100 g/m^3.

https://www.youtube.com/watch?v=dtIdyVk026k

What is coal combustion?



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

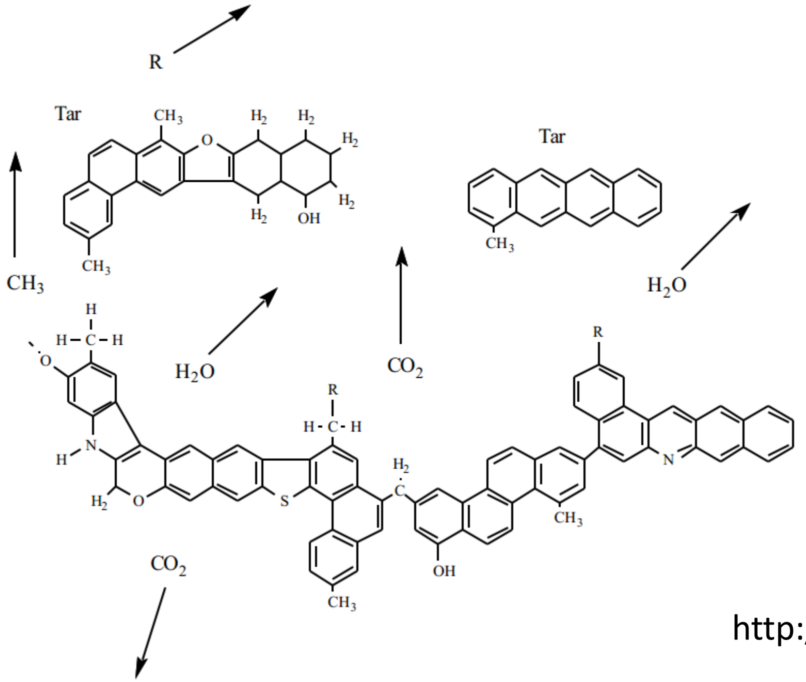


Pyrolysis models

SFOM model

$$\frac{dm_{vol}}{dt} = A_v \exp(-\frac{E_v}{RT_p})(m_{vol}^* - m_{vol}) \ , \ m_v^* = Qm_v^{*\prime}$$

- 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
- <u>Nonlinear correlation of ^{13}C NMR</u>
  - volatile matter content
  - ultimate analysis

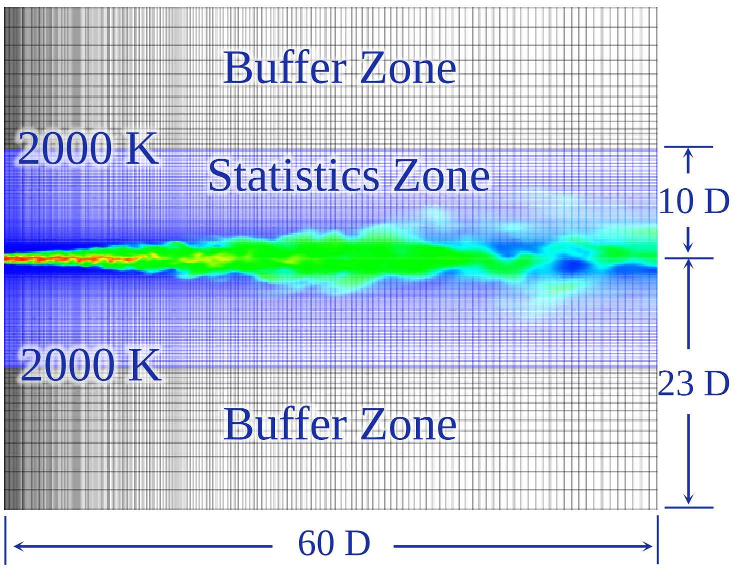
http://www.et.byu.edu/~tom/devolatilization/CPD%20model.html

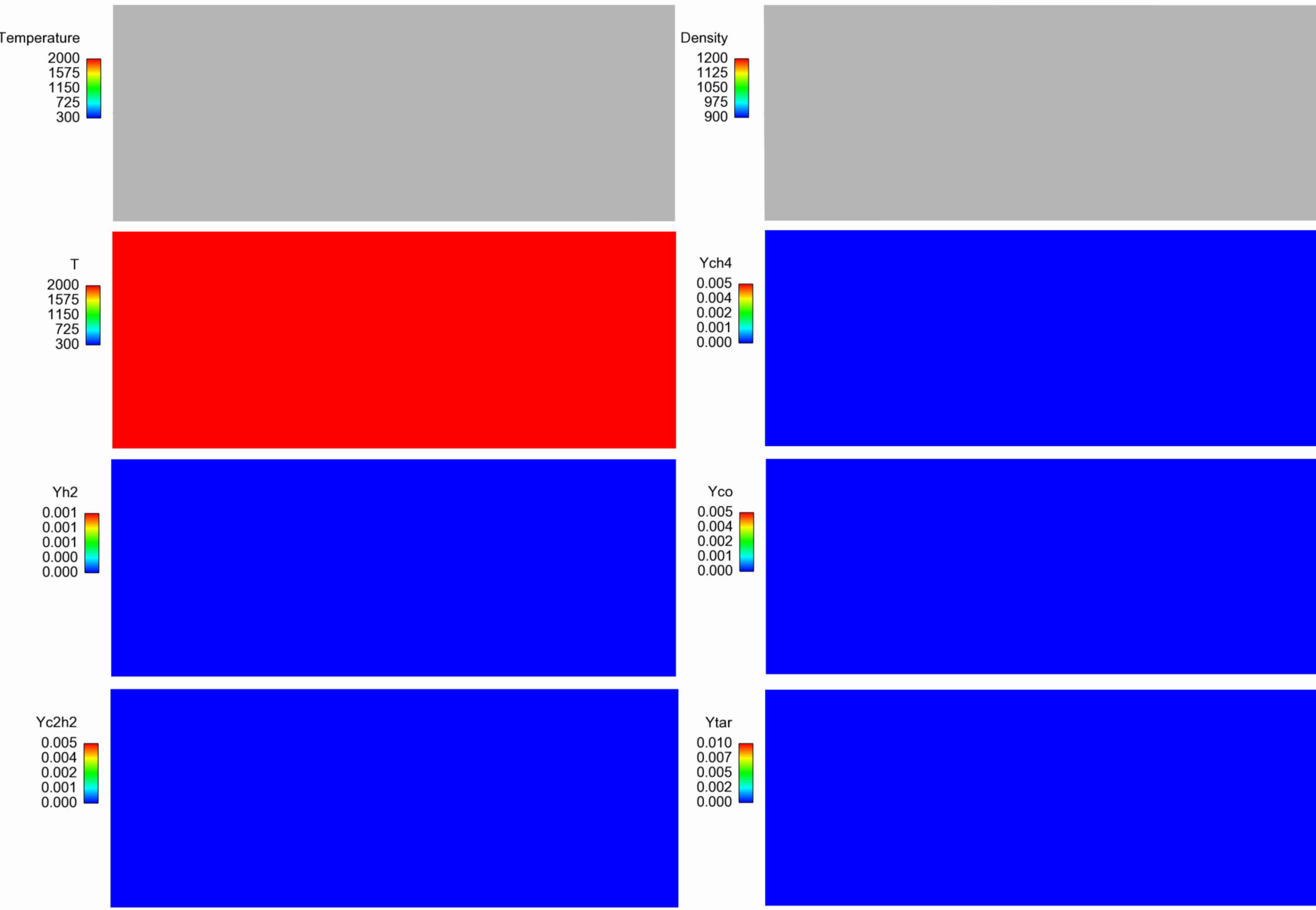
Simulation setup

- Primary Inlet (*D* = **13** mm)
  - **Gas:** N_2, 10 m/s, 300 K, **Re ≈ 8200**
  - **Coal:** 5.1×10^{-4} kg/s, 300 K, d_{min} = 10 μm, d_{max} = 100 μm, d_{mean} = 45 μm, ρ = 1400 kg/m^3
- Co-flow
  - Gas: N_2, 0.2 m/s, **2000 K**
- Outlet
  - Convective boundary condition
- CPD model
- SFOM model calibrated by CPD-LES

- Grid: ~**1.56** million cells

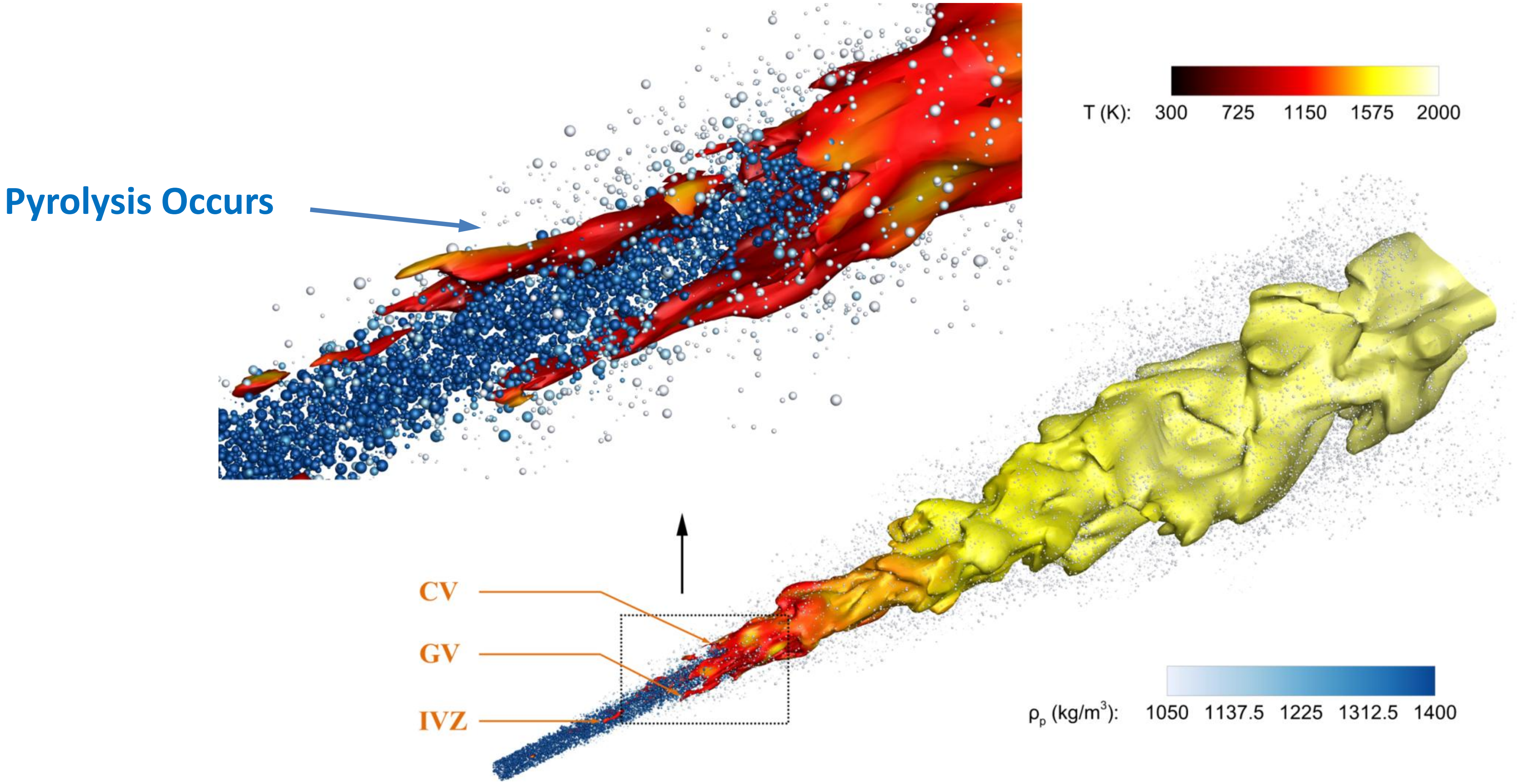
Computational Domain




Temperature
2000
1575
1150
725
300
Density
1200
1125
1050
975
900
T
2000
1575
1150
725
300
Ych4
0.005
0.004
0.002
0.001
0.000
Yh2
0.001
0.001
0.001
0.000
0.000
Yco
0.005
0.004
0.002
0.001
0.000
Yc2h2
0.005
0.004
0.002
0.001
0.000
Ytar
0.010
0.007
0.005
0.002
0.000

Pyrolysis case

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

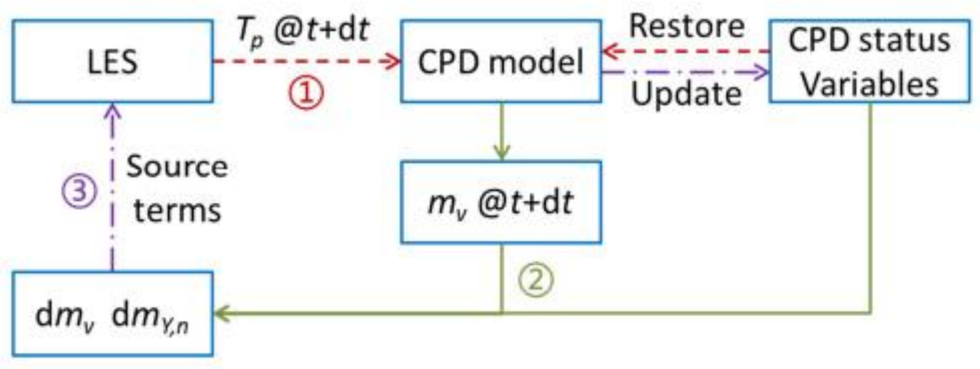


K.D. Wan et al. ***Combust. Sci. Technol.*** *2017.*

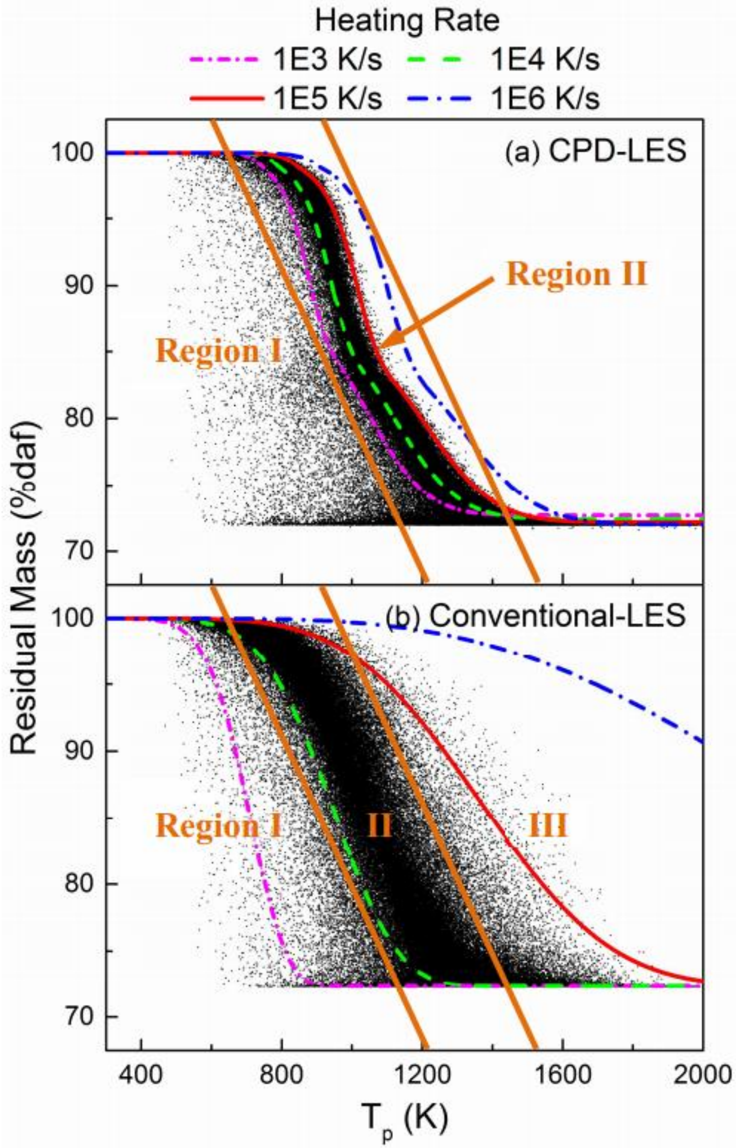
SFOM vs. CPD

The coupling between CPD and LES.

⇓



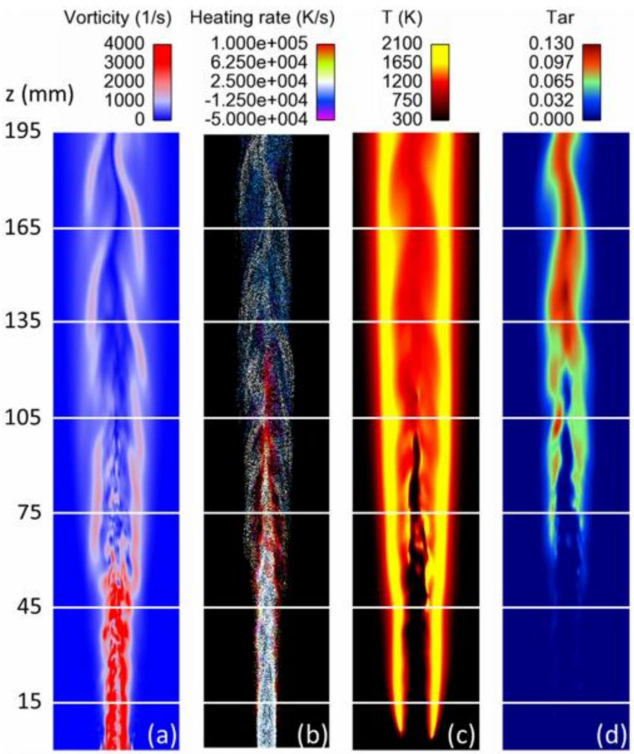
The calibrated SFOM cannot fully represent the pyrolysis characteristics considered in CPD. =>

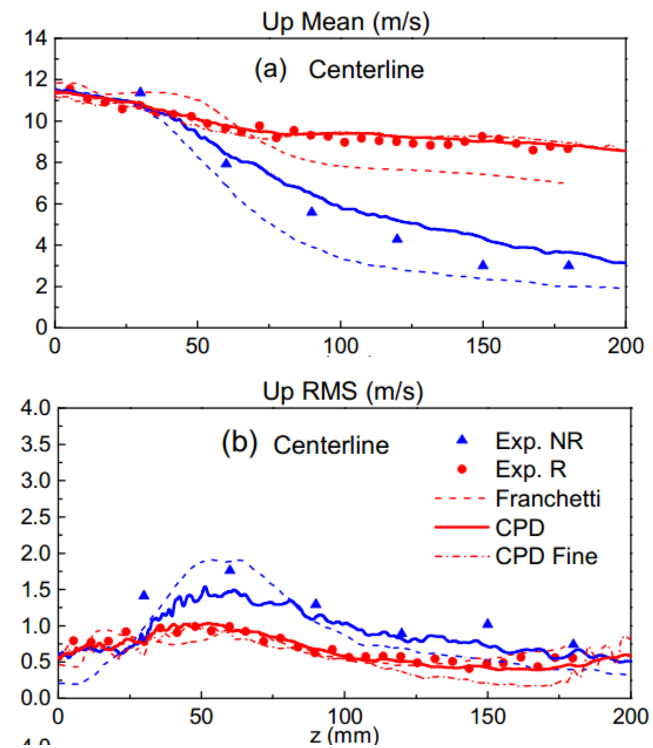


K.D. Wan et al. ***Combust. Sci. Technol.*** *2017.*

Combustion case

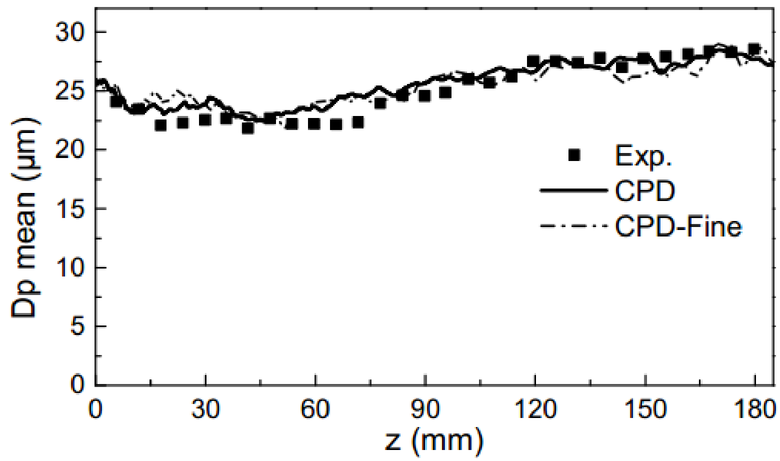
- LES of pulverized-coal combustion
  - Online CPD model => describe pyrolysis of coal particles
  - PaSR combustion model => volatile (gas phase) combustion
  - Kinetic/diffusion model => char (surface) reaction

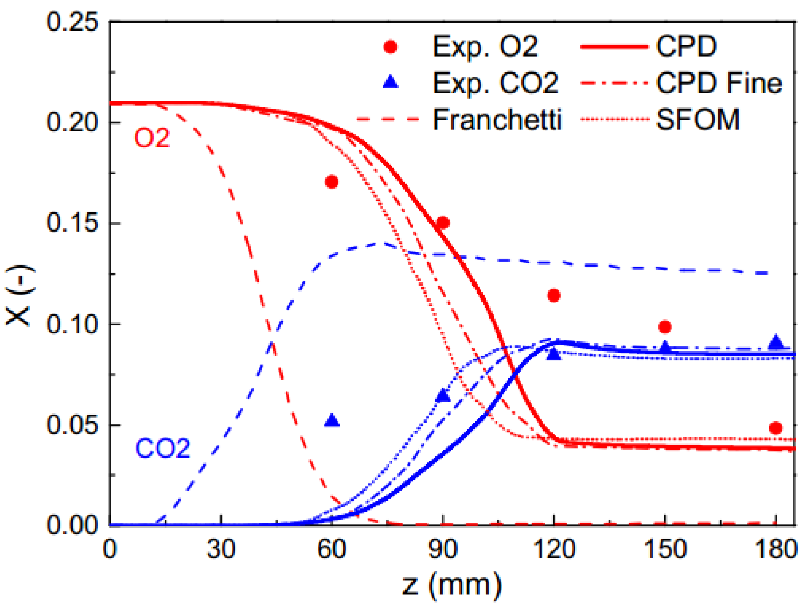


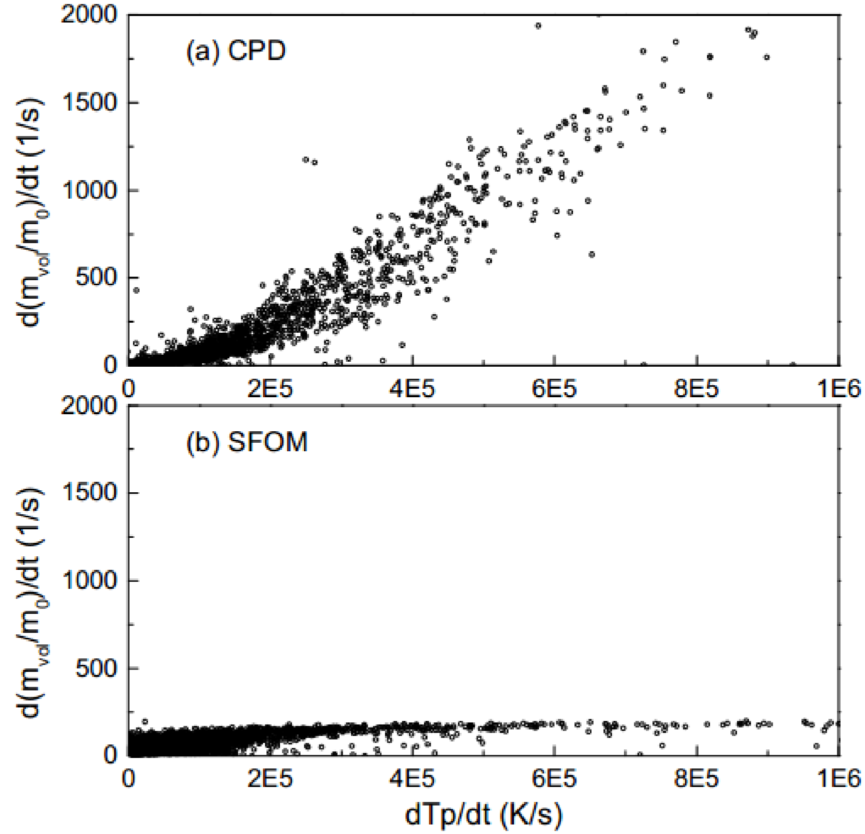


K.D. Wan et al. ***Flow Turbul. Combust.*** *(revision submitted)*

Validation with exp.







Large difference in the instantaneous pyrolysis characteristics.

K.D. Wan et al. ***Flow Turbul. Combust.*** *(revision submitted)*

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

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

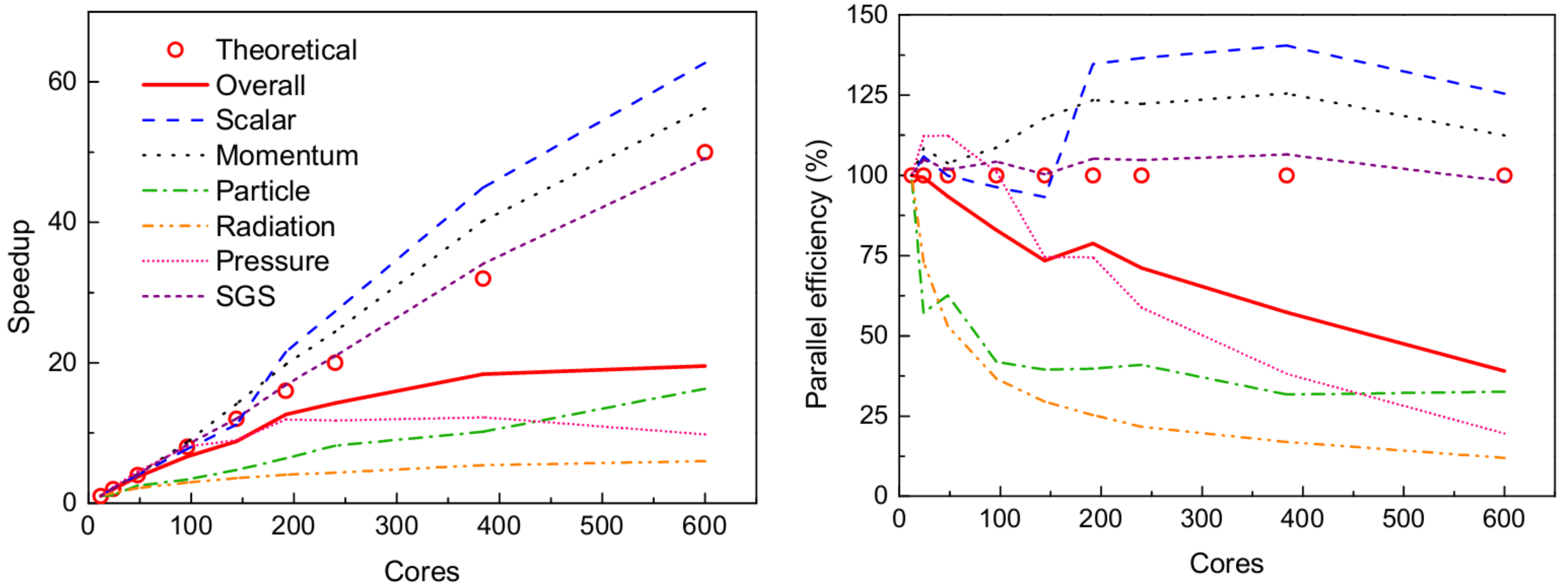
Outline

- Background information
- Motivation of the project
- The LESsCOAL code
- Project targets & optimization strategies
- Optimization of the pressure module
- Optimization of the radiation module
- Optimization of the particle module
- Parallel performance after optimization
- Conclusions

LESsCOAL

- **L**arge-**E**ddy **S**imulation**s** 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

Outline

- Background information
- Motivation of the project
- The LESsCOAL code
- Project targets & optimization strategies
- Optimization of the pressure module
- Optimization of the radiation module
- Optimization of the particle module
- Parallel performance after optimization
- Conclusions

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)

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

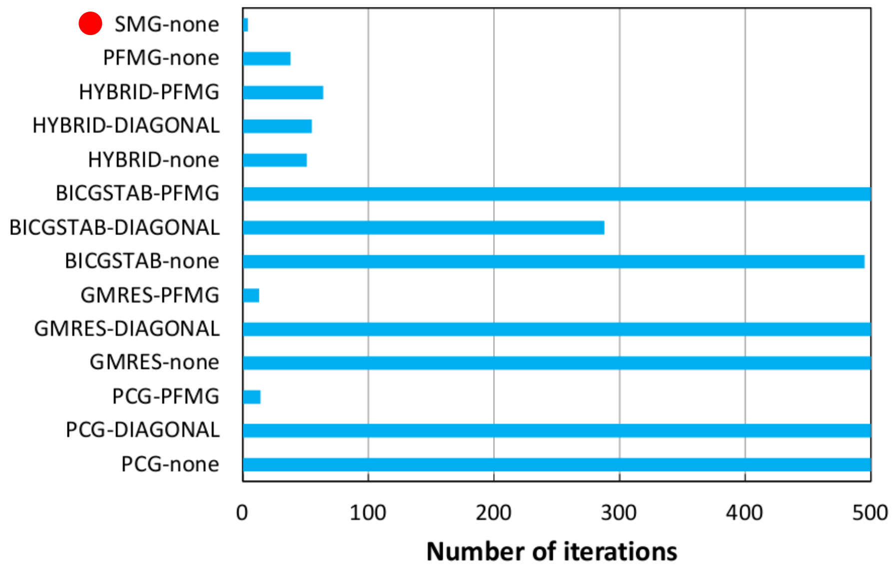
Pressure module

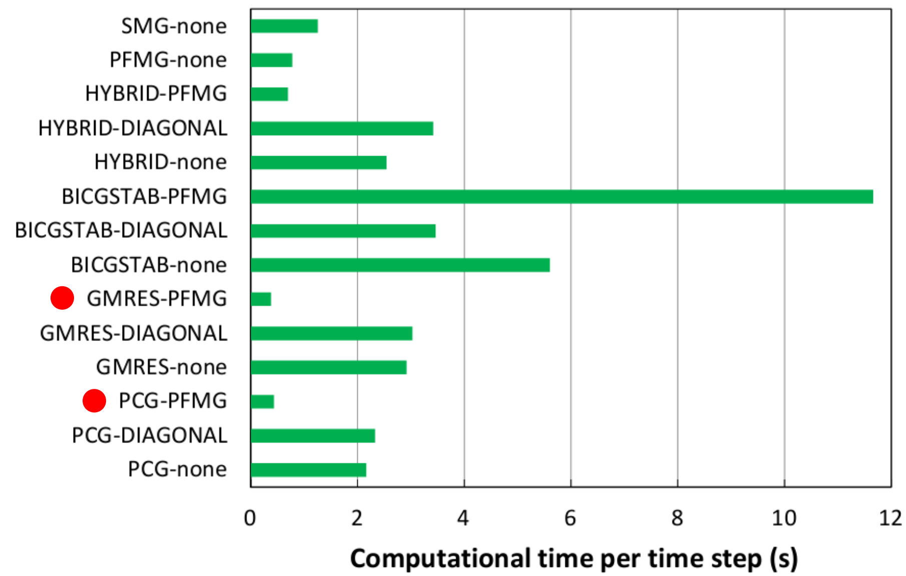
- The pressure equation is a Poisson's equation:

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

- 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.

HYPRE





- 14 setups with different solvers and preconditioners.
- Least number of iterations: SMG-none.
- Least time consuming: GMRES-PFMG & PCG-PFMG.

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

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

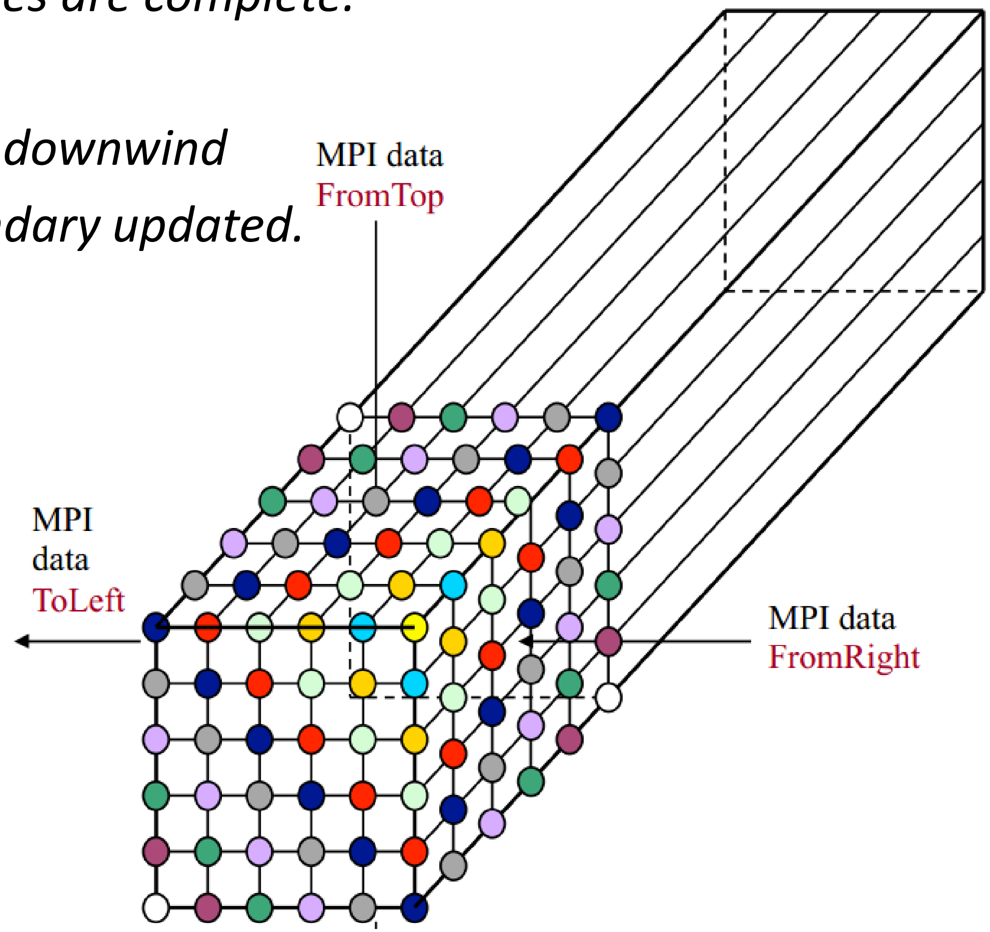
- 24 rays.
- Different directions.
- *Priority optimized queuing.*

4	5	6	7	8	9
3	4	5	6	7	8
2	3	4	5	6	7
1	2	3	4	5	6

- 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.*

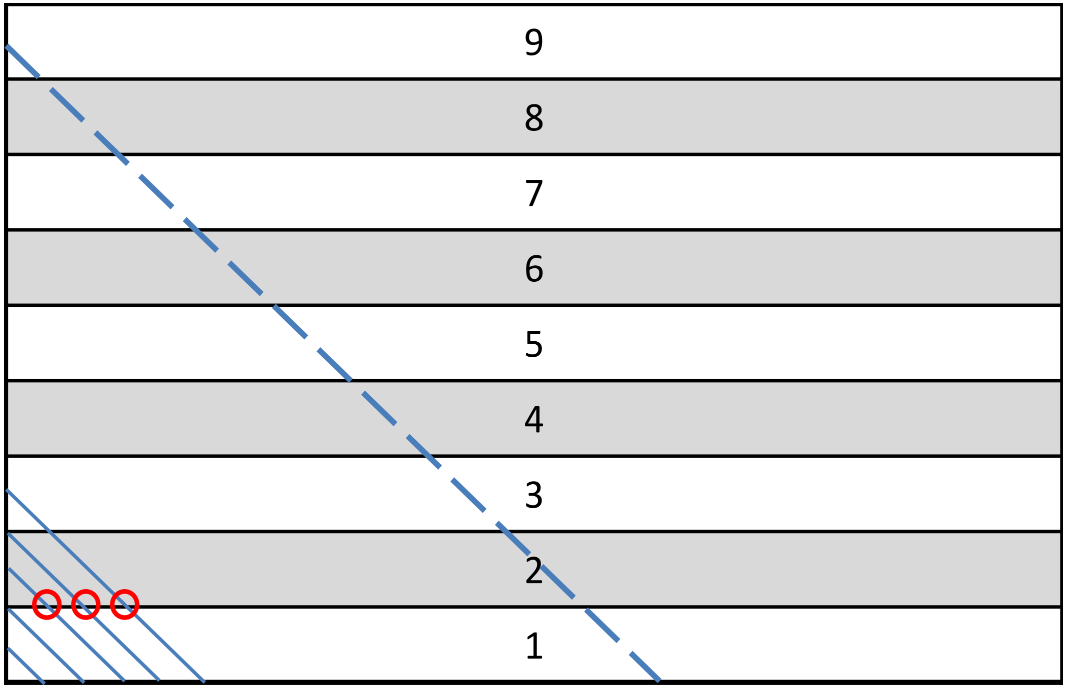


CON:

- *2D domain decomposition.*
- *Inefficient memory access.*

G. Pringle. ***PPAR Lunchtime Seminar Series, EPCC***

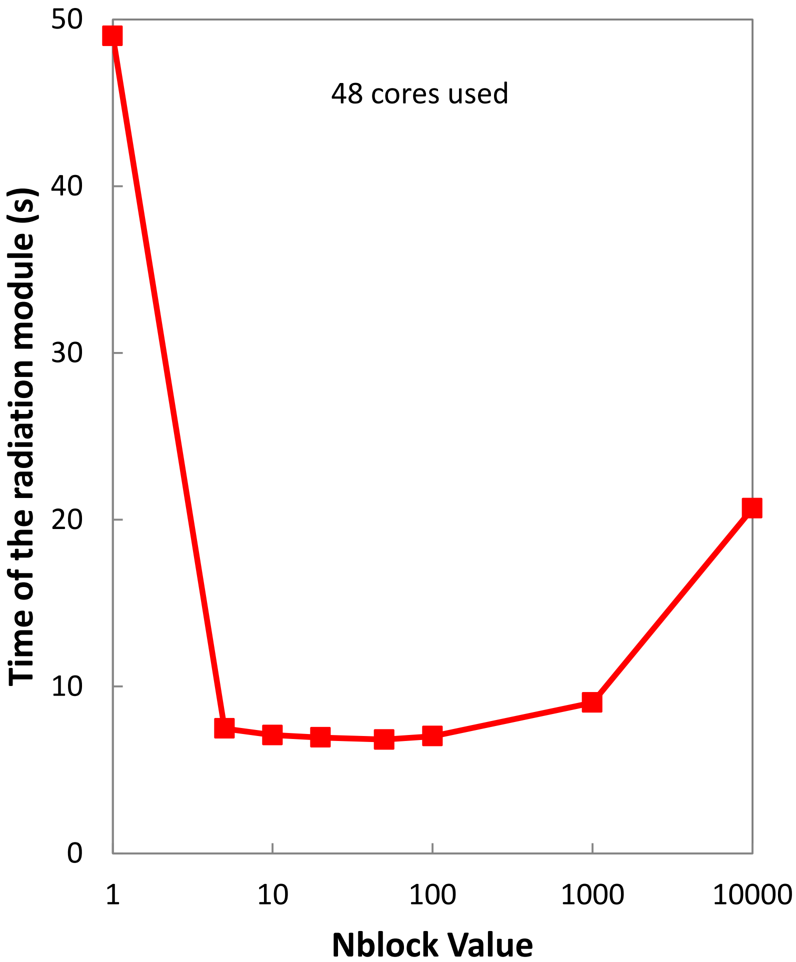
Diagonal slicing

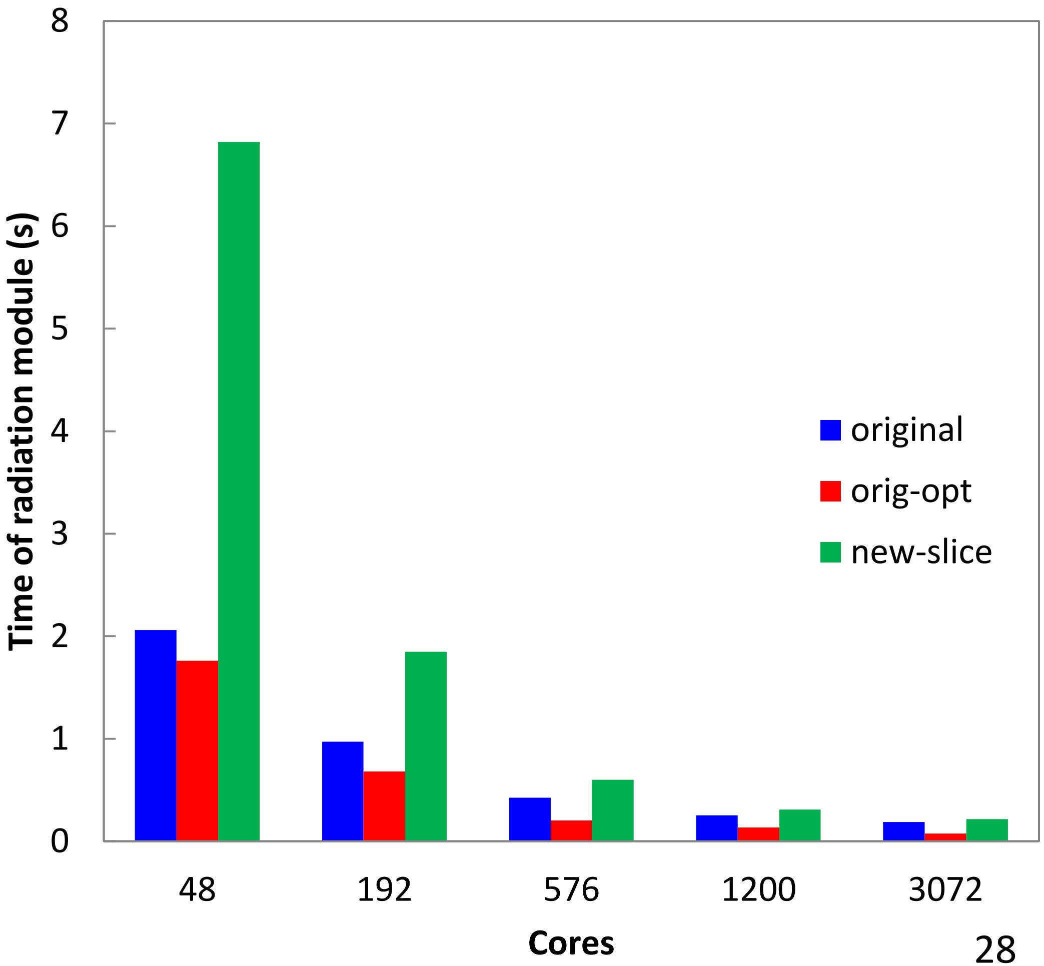


- *More frequent transport of radiation information*
- *Nblock value => Tuning parameter*
  - *The frequency of MPI communications between CPU cores.*

Recent code optimization work

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



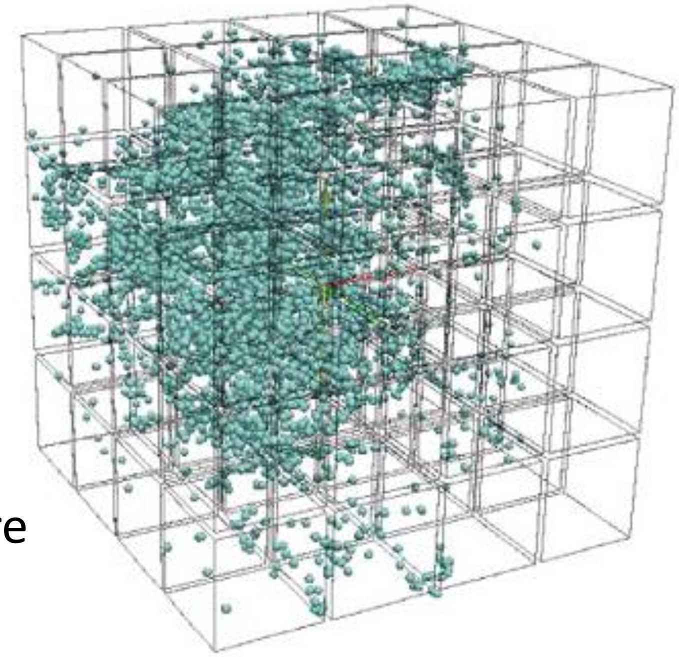


Outline

- 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

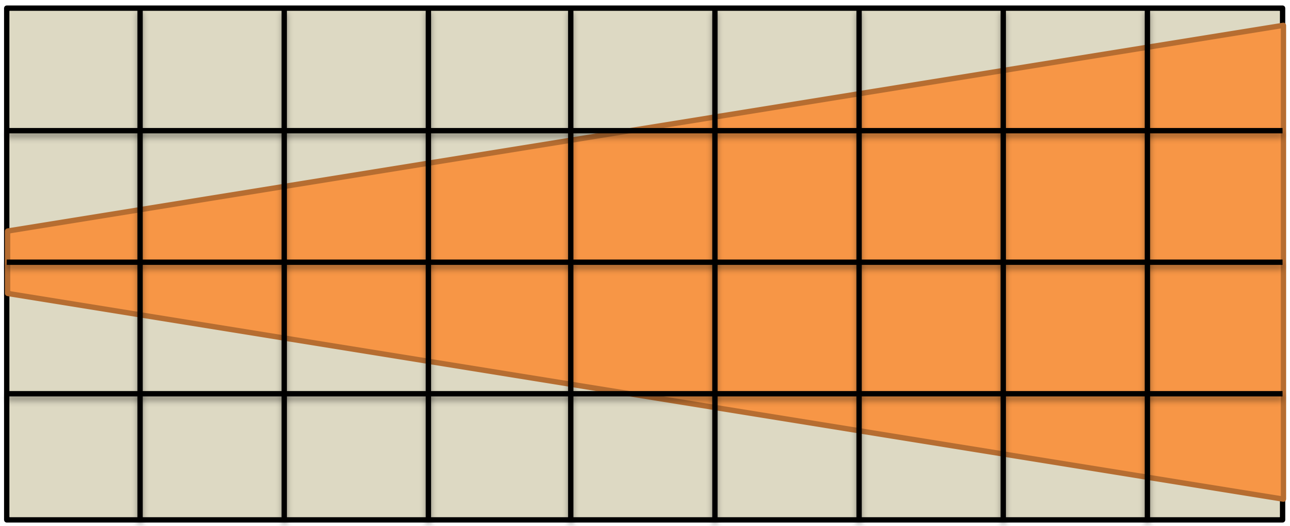
Particle module

- 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

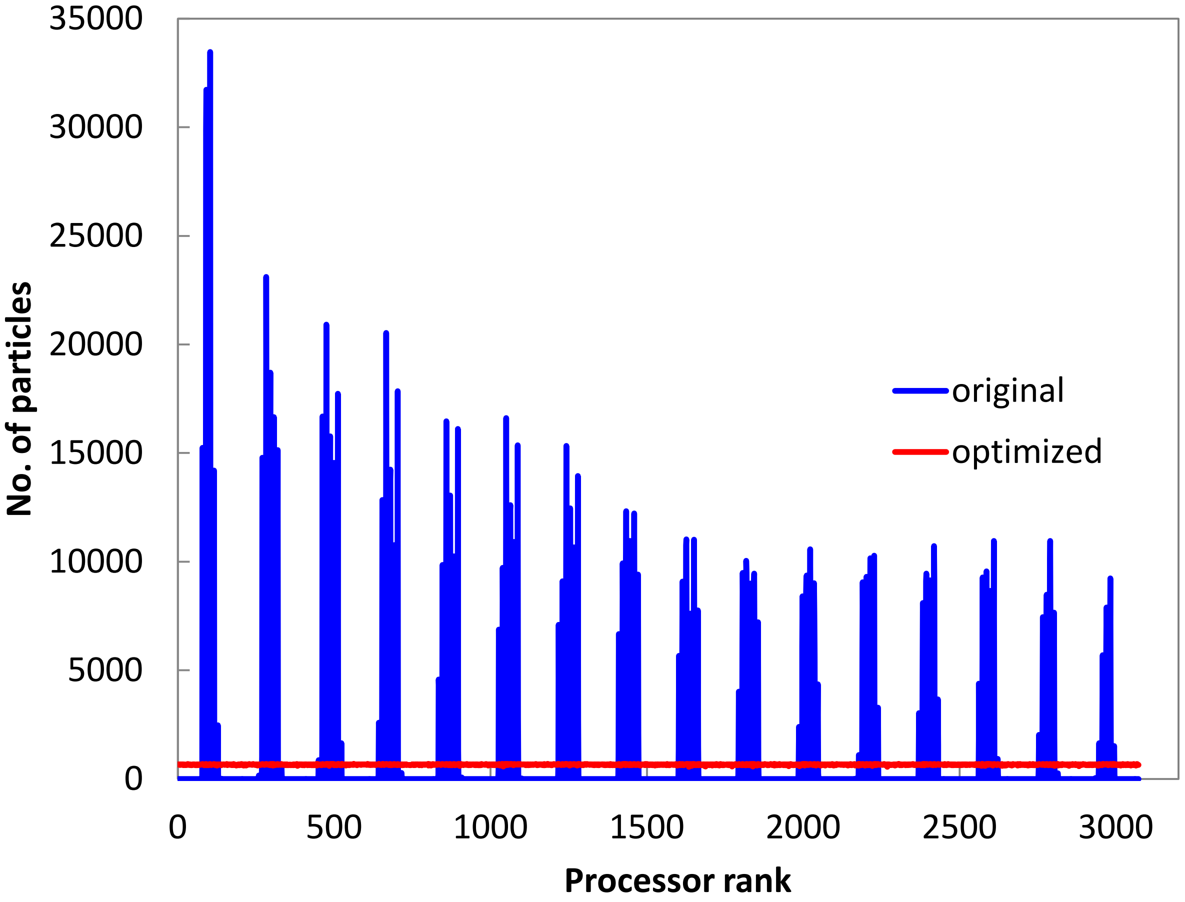
- Significant load imbalance issue in the particle module.
  - *LES of gas-solid multiphase turbulent jet.*
  - *Two-way coupling between gas and particle phases.*

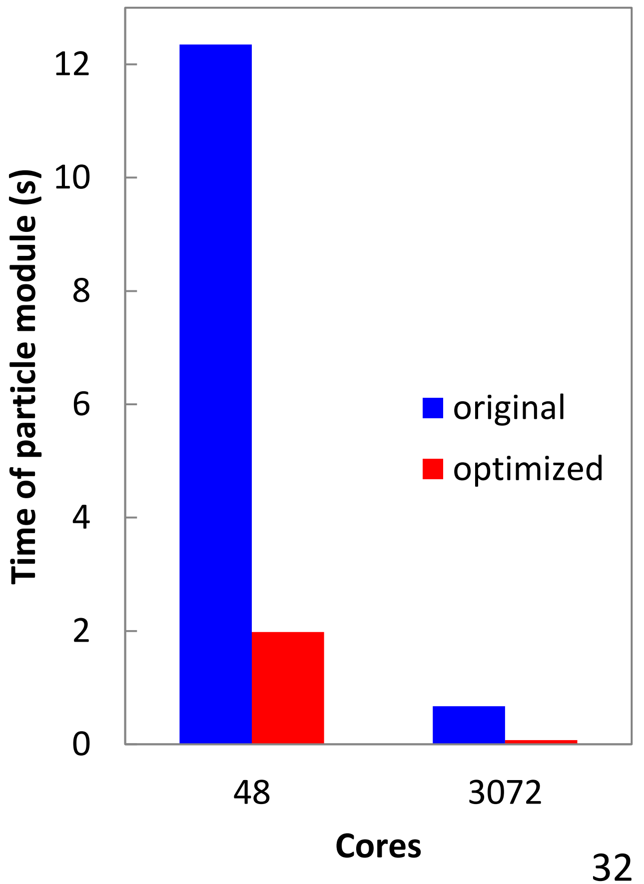


  - *Distribute particles evenly to each core?*
  - *How to consider the two-way coupling?*

OhHelp

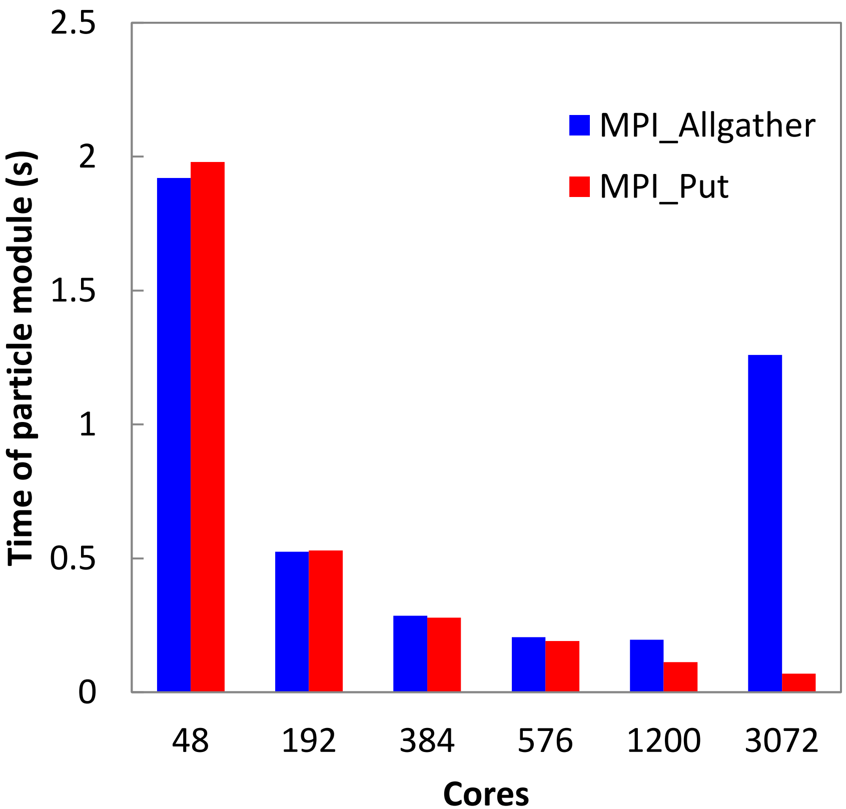
- Particles will be sent from heavy-loaded cores to light-loaded cores.
  - *Corresponding gas properties and source terms will also be transferred.*
  - *Transfer scheme determined by an open-source library: OhHelp.*

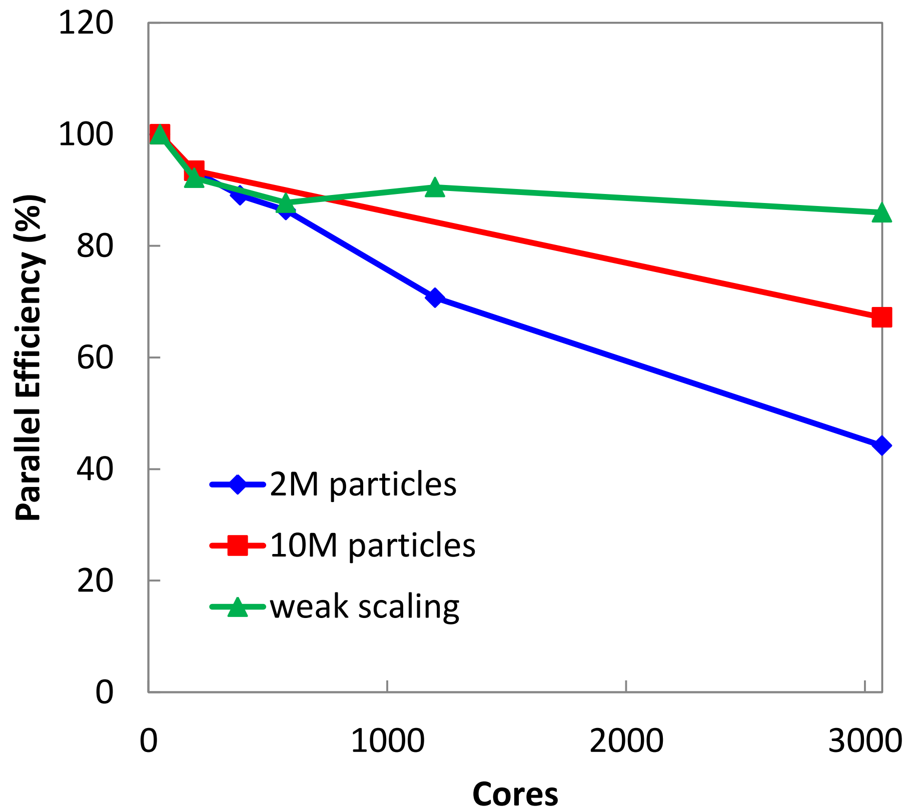




One-sided communications

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

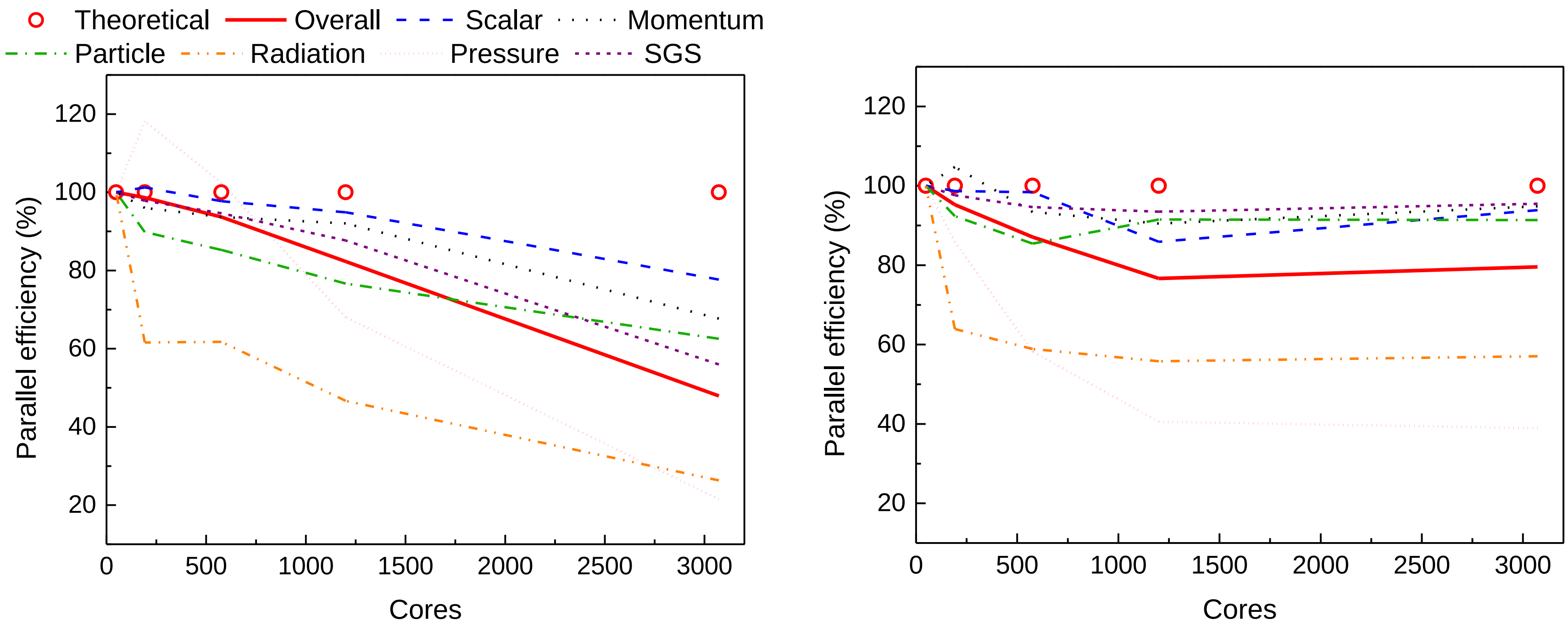




Outline

- 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

Optimized performance



- Strong scaling test: Good up to 1200 cores (> 82%).
- Weak scaling test: Achieved 80% of the theoretical paralle efficiency when using 3072 cores on ARCHER.

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

Conclusions

- 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)

谢 THANK YOU.

@K.D. Wan
2017-3-22