

Validation and Application of Lagrangian Stochastic Methods for Indoor Air Quality

Harriet Jones, Gregory Cartland-Glover and Stefano Rolfo

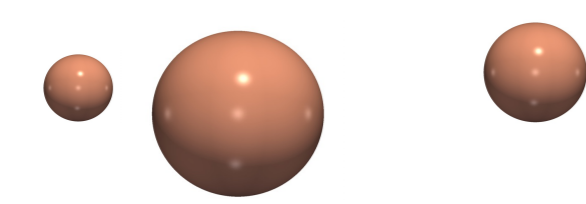
Computational Engineering Group, Scientific Computing Department, STFC Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK

The project



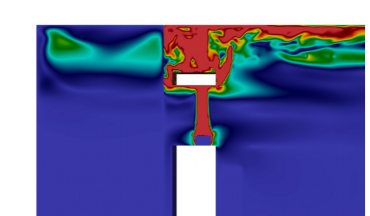
- Computational Fluid Dynamics (CFD) simulations are used to replicate fine particulate matter (PM_{2.5}) dispersion from a cooking pot in the DOMESTIC air quality test house. Various ventilation scenarios are tested. The validated CFD model will ultimately feed data back into the experimental work at DOMESTIC.

Tracking PM_{2.5} dispersion



2.5 µm or less in diameter

- It may be invisible to the naked eye, but PM_{2.5} is a serious health hazard. Regular exposure to concentrations of over 15 µg m⁻³ is correlated with an increased risk of chronic obstructive pulmonary disorder (COPD), coronary heart disease, stroke, and lung cancer [1]. But cooking activities can cause local PM_{2.5} concentrations of more than 350 µg m⁻³ [2].
- Lagrangian particle tracking is highly computationally intensive, but enables individual particle trajectories to be calculated. Hence it is very suitable for air quality studies.



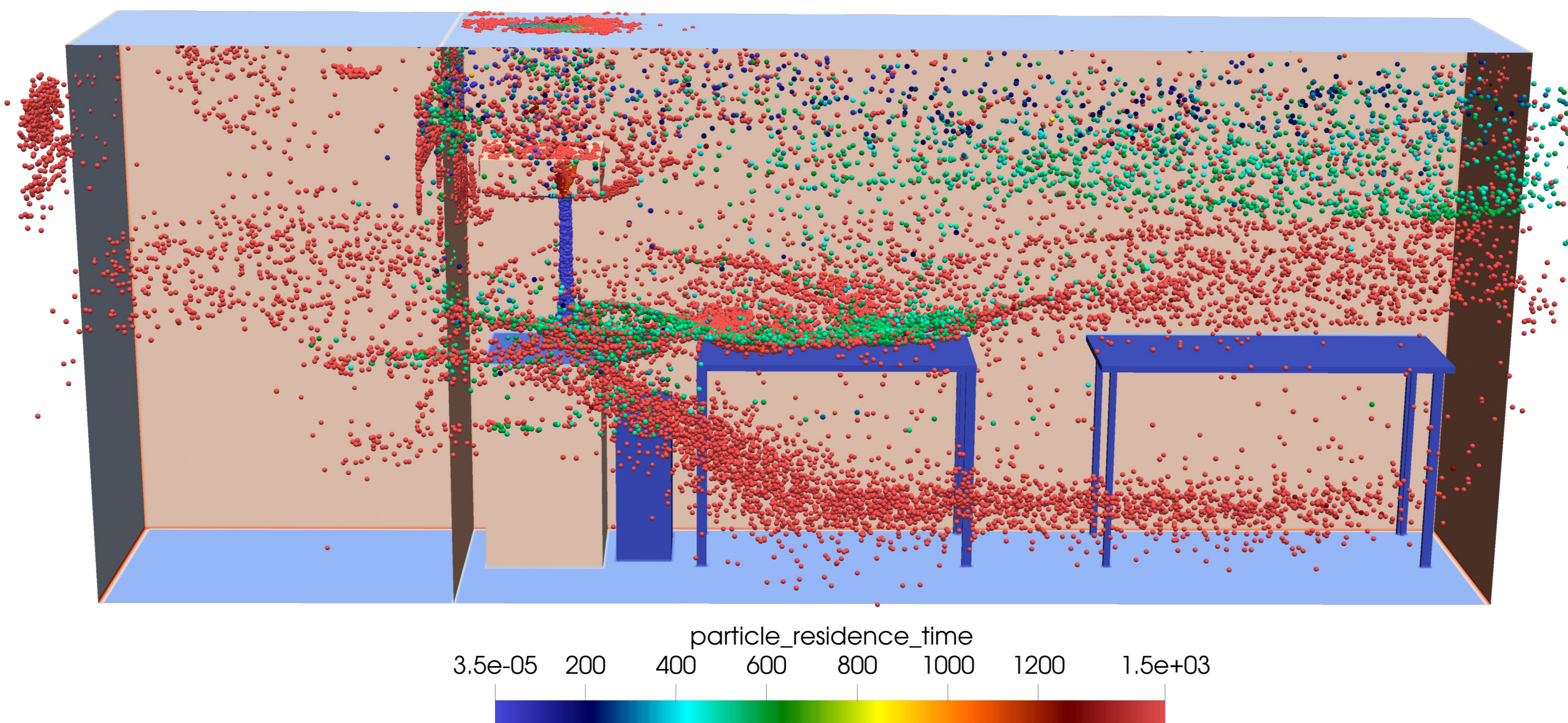
Code_Saturne



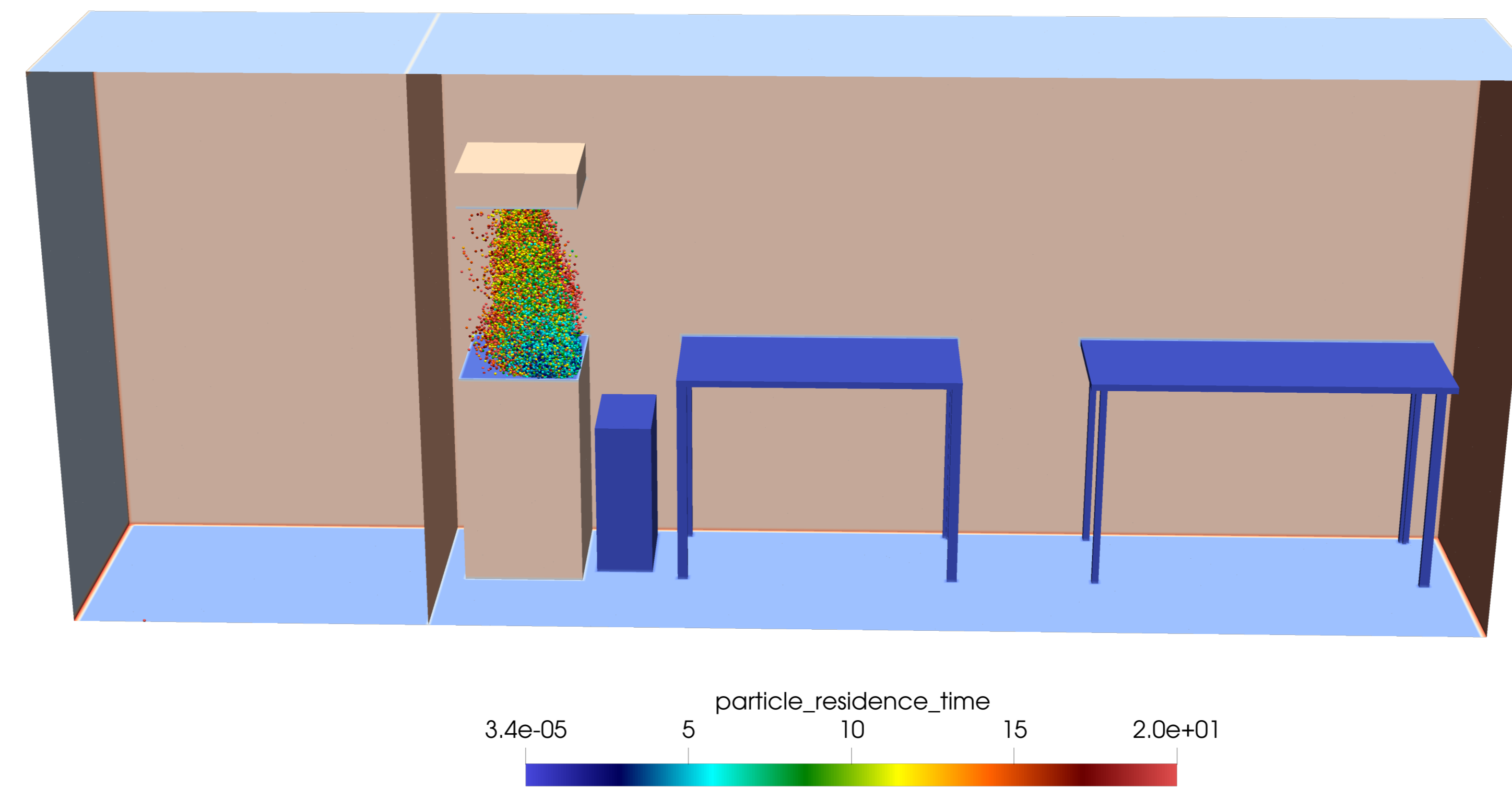
- Calculations have been performed using the open source CFD solver *Code_Saturne*, which is based on a finite volume discretisation. Second order central differencing is used for the convective terms, whereas an implicit Euler scheme is used for the time advance. The solver also includes a Lagrangian Particle Tracking (LPT) module [3].

Initial results – impact of ventilation on kitchen PM_{2.5} concentrations during cooking

No ventilation...

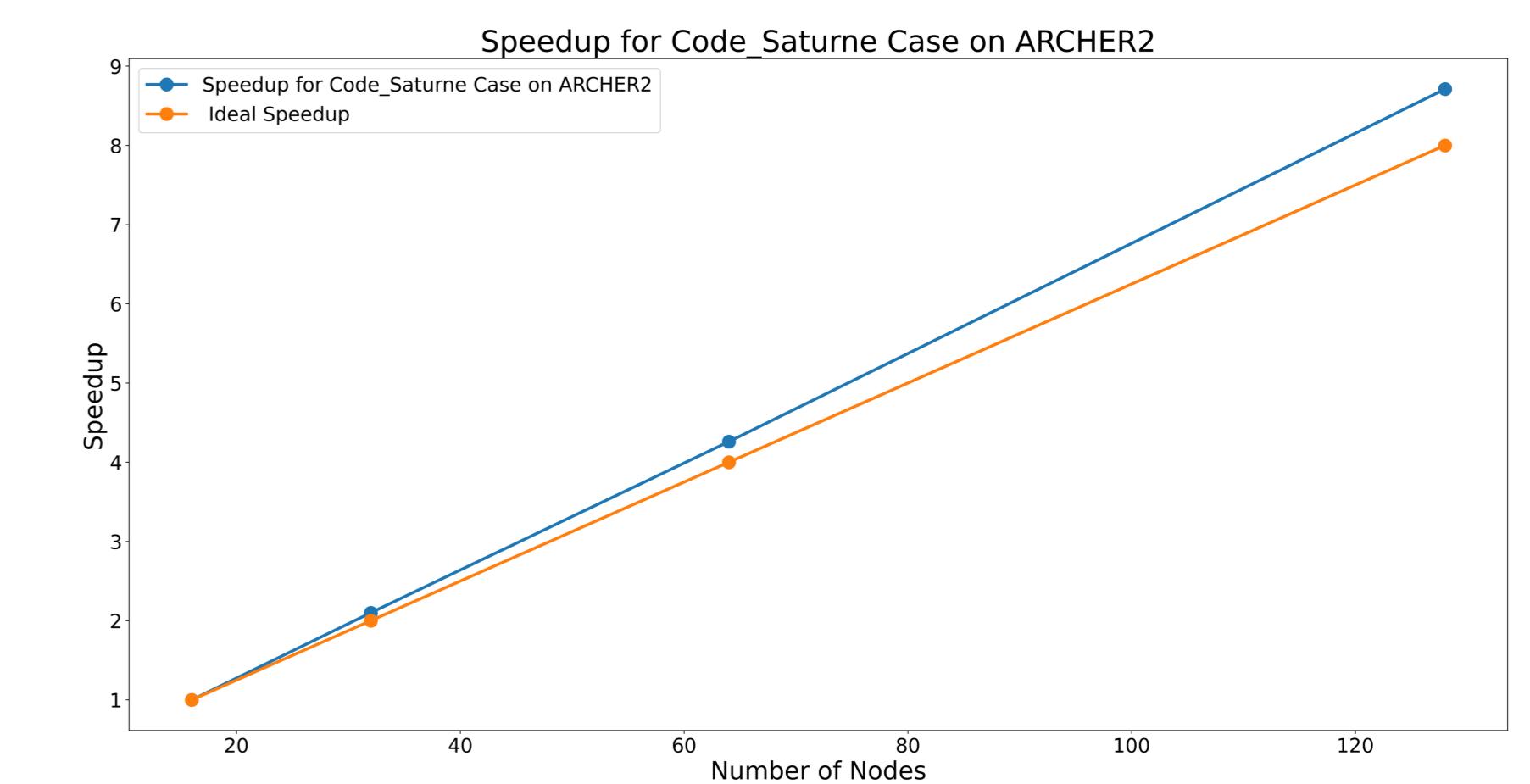


Versus hood extractor fan on (375 m³hr⁻¹)

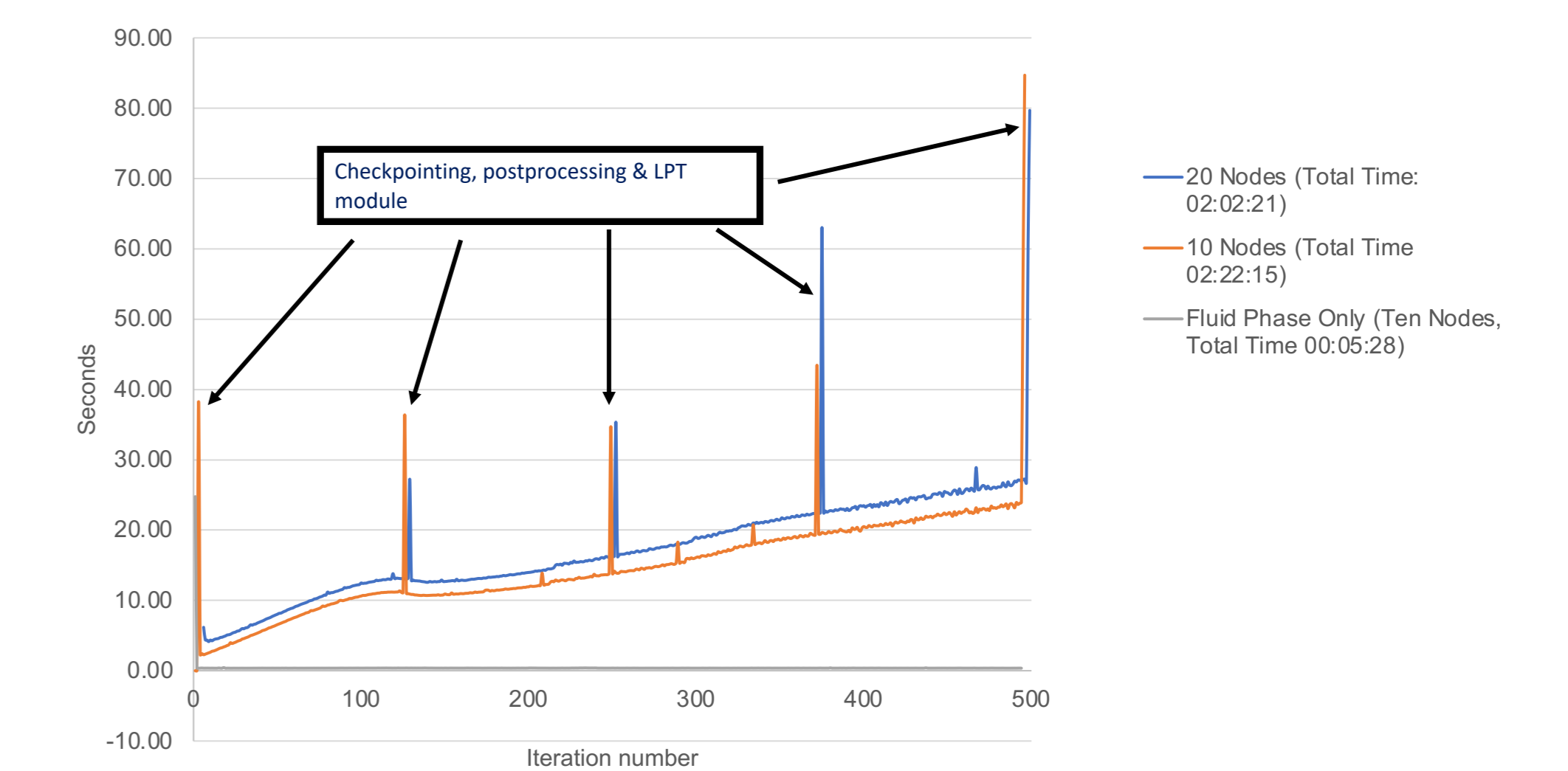


Cases use a ten million cell mesh, the EBRSM turbulence model and one-way fluid-particle coupling. 10,000 particles were injected per second, with a statistical weighting of 100. Simulations were run for 25 in-simulation minutes on twenty 32-core AMD nodes on STFC's Scientific Computing Application Resource for Facilities (SCARF) cluster.

Efficiency



- *Code_Saturne* scales excellently, with project cases showing a super-ideal speedup over a 16 -128 node range on ARCHER2. (Time step: 0.005 s, mesh size: 130 million cells)



- Efficient parallelization relies on the number of particles in the domain. Over the first 500 iterations of the case above, 20 nodes gave a 20-minute reduction in compute time, but the majority of iterations were slightly slower than for the 10-node case.
- It may be more energy efficient to initially run on fewer nodes, restarting on a higher number once the particle load is sufficiently high.

Acknowledgements

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References

[1] World Health Organisation, 2021, *WHO Air Quality Guidelines*. [2] Y. Omelekina et al., *Environmental Science: Processes & Impacts* 2020, 22, 1382-1396. [3] *Code_Saturne*, 2022, <https://www.code-saturne.org/cms/web/>