PhD outline

Development of modular and scalable hybrid numerical algorithms for flow simulation, combining continuum approaches with particle methods.

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This PhD project aims to develop modular and scalable hybrid numerical algorithms for flow simulation by combining continuum approaches (such as finite-volume) with particle methods (such as lattice Boltzmann, Monte Carlo, vortex method).

Computational fluid dynamics (CFD) methods are predominantly based on the continuum formulation of the Navier-Stokes equations. Standard methods include finite-volume and finite-element discretizations in addition to several approaches for turbulence modelling.

However, CFD methods need to be both faster and more accurate if more simulation and less physical testing are to be used in the design process. Being a mature discipline, CFD will need fundamental changes to deliver such an increase in simulation capability.

This PhD project is aimed at investigating one such fundamental change, which is to incorporate non-continuum representations of the fluid quantities with the standard continuum approach. The non-continuum, or particle simulation, approach has in the main been developed separately from traditional CFD, apart from some exceptions - we reference some examples below. Several special features of these alternatives seem very attractive as possible means for increasing the simulation capability of CFD. In particular, reduced numerical diffusion often means that high-accuracy can be obtained with a smaller computational footprint compared to traditional methods as the latter may require extremely fine meshes for the resolution of flow features such as large flow gradients.

Hybrid methods are an area of research where there is an expectation that an increase in simulation capacity is achievable. For example, there have been attempts to combine Navier-Stokes solvers with direct simulation Monte-Carlo for hypersonic flows [3], looking to produce a physically accurate and numerically efficient tool in this domain. This application domain is very special, however, because the rarified gas gives a straightforward criterion for choosing between continuum and particle representations. A similar situation arises in micro-scale gas flows, where hybrid approaches have also been investigated recently [2]. In the application domains of CFD where there is no physical continuum breakdown, there has been little effort yet for development of continuum-particle hybrid methods.

In fact, the bulk of available literature on hybrid methods applies domain coupling, in which the particle representation is used either where the continuum hypothesis breaks down, or where the scales are too small, and the continuum method is used in the "far field". For example, molecular dynamics description near a carbon nanotube, and finite volume Navier-Stokes at the larger scales [4]. An exception, unique as far as we know, is the use of particle-grid domain decomposition with overlapping in [1], which applies finite differences near a bluff solid object, and vortex particle method in the wake of the body.

The other major objective of this work is to explore possible increases in simulation capability by employing advanced algorithm concepts and designs aimed at high-performance computing implementation —not by designing software to fit a particular hardware architecture but rather by writing software within a framework that can incorporate the properties and capabilities of general novel architectures such as multi-core processors and heterogeneous computing:

Multi-core processors Tightly-coupled multiprocessor systems; performance gain is obtained through the integration of multiple processors on the same chip.

Heterogeneous Computing Achieve high performance through the use of diverse computing resources such as Graphical Processor Units (GPU), ClearSpeed coprocessor technology, IBM Cell architecture.

We aim to design codes in a manner that will enable the exploitation of novel hardware architectures and that will use component interfaces to gain abstraction from any software libraries or hardware specific implementations that perform computationally intensive processes.

The approach for the research will be an integrated consideration of all aspects of flow simulation software; i.e. the mathematical models, the numerical algorithms and also computer architecture and software engineering. Algorithmic scalability will be ensured by aiming for operation count complexities that grow linearly with respect to the discrete problem size. It has been recognized that only hierarchical algorithms, such as multigrid, multipole, and FFT, are algorithmically scalable. Therefore, the component-based integration of these types of algorithms will be explored. Furthermore, the implementation will seek to integrate high-level parallel libraries, and will employ modern software engineering approaches such as version control.

References

[1] M. L. Ould-Salihi, G.-H. Cottet, and M. El Hamraoui. Blending finite-difference and vortex methods for incompressible flow computations. *SIAM J. Sci. Comput.*, 22(5):1655–1674, 2000.

[2] Q. Sun, I. D. Boyd, and G. V. Candler. A hybrid continuum/particle approach for micro-scale gas flows. In *Proceedings of the* 23^{rd} *International Symposium on Rarefied Gas Dynamics*, Whistler, Canada, July 2002.

[3] W.-L. Wang, Q. Sun, and I. D. Boyd. Towards development of a hybrid DSMC-CFD method for simulating hypersonic interacting flows. AIAA paper #2002-3099, 8^{th} AIAA/ASME Joint Thermophysics and Heat Transfer Conference, St. Louis, MO, June 2002.

[4] T. Werder, J. H. Walther, and P. Koumoutsakos. Hybrid atomistic-continuum method for the simulation of dense fluid flows. *J. Comput. Phys.*, 205:373–390, 2005.

The Candidate

Felipe Cruz holds a Bachelor and an Engineering degree in Informatics (Computer Science) from Univerisdad Técnica Federico Santa María, Chile. This is one of the most prestigious technical universities of Chile and Latin America, whose graduates are very sought after in the region. Founded in 1932, it was the first university in Latin America to confer the degree of Doctor in Engineering in 1963.

Felipe has an outstanding academic record –a very good First Class degree, and has continued to do a Master's degree with full merit-based scholarship. He is currently in Bristol thanks to a mobility grant awarded by the European project of the ALFA Programme "Scientific Computing Advanced Training, SCAT". He is in the process of completing a MSc thesis based on his research project during his mobility grant.

The professional engineering degree completed by Felipe consists of a twelve semester programme of courses including, among others:

- Foundations of informatics: logic, formal languages, automata theory, multiple programming languages.
- Scientific computing: numerical linear algebra, numerical methods for ordinary and partial differential equations, nonlinear optimisation.
- Wavelet theory, filter banks.
- Estimation, tracking, data fusion.
- Artificial inteligence, quantitative methods, operation research.

Moreover, Felipe already has considerable research experience for a PhD candidate. He has worked as a research assistant in a project involving the modelling of the public transportation system of the city of Santiago. The models were implemented in clusters of computers using C++/MPI, at the Centre for Mathematical Modelling, University of Chile. See: `http://www.cmm.uchile.cl/`
Another research project in which Felipe worked as collaborator involved a Data Fusion problem related to a large number of tracking radars. This project carried out at Univerisdad Técnica Federico Santa María funded by a Chilean company specializing in defense systems.