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Rapid, accurate and convenient fluid dynamical modelling for real-world applications

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Abstract: Designing new or improved industrial processes and devices invariably requires (at least some amount of) theoretical or computer-based modelling. In the past this may have been through importation of a CAD model of the device into a suitable numerical solver which after some onerous refinement of the mesh to overcome non-continuous or non-smooth points may yield a solution which can be used to improve the process.

With the advent of Additive Manufacturing (AM) much more complex device geometries can be manufactured and with the input of Artificial Intelligence (AI) bespoke devices may be predicted from a plethora of possibilities. However, to complete the loop we need to assess each of the possibilities through a computer based numerical solver which will seamlessly interface with other components (AI and AM). Ideally this process should be automated with limited (or no) human intervention. This relies on developing an accurate, rapid, and convenient numerical solver which can easily assess the performance of devices for real-world applications.

A multitude of industrial processes involve fluids (liquids, gases, granular fluids) and can be modelled via a wide range of numerical techniques which require solving the Navier-Stokes equation, Newton’s equations or Boltzmann Transport equations. As stated above, an autonomous physics-based numerical solver is necessary and there exists a myriad of Computational Fluid Dynamical (CFD) methods which may be selected. However, we are aiming for a robust and stable methodology which is repeatable over multiple possibilities.

The Lattice Boltzmann (LB) method has been developed over the last 50 years or so, and we believe has several advantages over more traditional CFD methods such as Finite Element, Finite Volume, Smoothed Particles Hydrodynamics or Direct Numerical Simulations in the context of rapid, accurate, convenient solutions. LB works on a cartesian grid where each grid point represents a region (square in two-dimensions or cube in three-dimensions) which can be either solid or void (available for fluid flow). Vital for the LB method is a voxelised representation of the device but once that is obtained, through robust boundary conditions (such as bounce-back conditions for no-slip) one can model a wide range of fluid flow and heat transport scenarios.

We demonstrate the combined voxelisation and LB method for solving industrial problems involving fluid flow, fluid mixing, adsorption, and heat transfer. To begin with we have representation of the geometry surface, which comes as Stereo Lithographic (STL) format. This may consist of multiple intersecting solid objects, which is quite typical in our design method, as we aim to handle highly complex designs. We have developed a robust and fast voxel grid generator that takes this type of surface as input and produces a voxelised volume grid as output, which is a set of voxels that have been identified as either solid or fluid. The LB methodology is subsequently applied to this voxelised representation and has the advantages of being (i) easily coded, (ii) with robust boundary conditions and (iii) highly parallelizable.

The methodology is applied to microfluidic devices which are now being increasingly used for chemical, pharmaceutical and biological processing, and manufacture. Besides understanding the nature of how fluids flow and heat is transported in these devices, one also needs to determine a host of other, more specific characteristics such as fluid mixing, adsorption, shear, and residence times. We demonstrate how this combined methodology may be applied to these devices to extract both qualitative and quantitative data from these models.

Results are given for a series of well-known mixers such as the Staggered Herringbone Mixer, Kenics Mixer and SMX mixer as well as mixers that have been developed within CSIRO. From these results we can obtain performance measures for specific applications.

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