Simulating Multi-Component Systems to Study Turbulence

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In the inaugural editorial of this journal, it was suggested that non-elastic collisions of molecules may modify the traditional continuum model of a turbulent fluid. Non-elastic collisions of molecules violate the historic assumption that molecular properties do not matter for as long as viscosity and density are used as macroscopic parameters, contributing to the dimensionless Reynolds number. In fact, inelastic collisions presume the existence of quantum states of molecules. An energetic gas consists of molecules in various quantum states. The gas is therefore composed of different components, each component belongs to an excited state, and the gas may be considered multi-component. An accurate physical description will consist of different species of what used to be considered a single specie of unexcited molecules, as in the Navier-Stokes equation. Note that traditional numerical simulations only assume a single specie. The purpose of this guest editorial is to suggest that if computational fluid dynamics admits the existence of several interacting species, very rich results, including turbulence, will be found.

We illustrate this suggested new approach with a simple example. Let there be a gas consisting of two species: ground state molecules, and excited state molecules. The velocity of ground state molecules is v_1, while the velocity of excited state molecules is v_2. Transport equations describing the time evolution of the two velocities may be modeled by the following equations in one dimension:

$$\frac{\partial v_1}{\partial t} + \frac{1}{2}\frac{\partial \left(v_1^2\right)}{\partial x} = (A + \rho B)v_2 - \rho B v_1 \tag{1}$$

$$\frac{\partial v_2}{\partial t} + \frac{1}{2}\frac{\partial \left(v_2^2\right)}{\partial x} = (A + \rho B)v_1 - \rho B v_2 \tag{2}$$

A and B are analogues of the Einstein A and B coefficients used in laser physics, ρ is a radiation density that couples the two states. If *A* and *B* are zero – *no quantum mechanics (!)* – the model equations reduce to the

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classical uncoupled Burgers equations [1], a simplification of the Navier-Stokes equation by making the pressure term a constant. The steady states are exactly solvable, resulting in multivalued velocity fields. The steady state solutions are Lambert functions indexed by a branch number [2,3].

There are no known solutions for the fully time-dependent case, but simulation experiments may be done to yield some interesting behavior. One such result is the velocity at a specific position, showing the time evolution of the velocity at that position. We show one such computation – *simpler than any CFD study* – for the velocities v_1 and v_2. With initial data using a simple gradient of velocities as a function of position, and an imposed periodic boundary condition, the result is surprising. A turbulent region is sandwiched between steady states, caricaturing the occurrence of "plugs" in pipe flow [4].

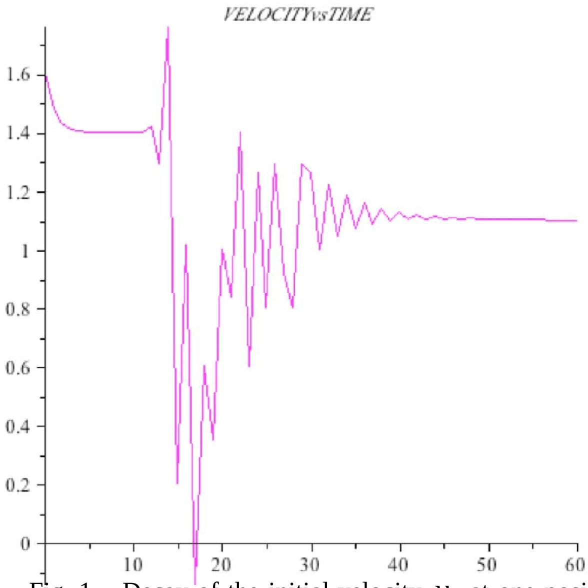

Fig. 1 – Decay of the initial velocity v_1 at one position to a quasi-steady state and subsequent turbulent period, followed by decay to another quasi-steady state.

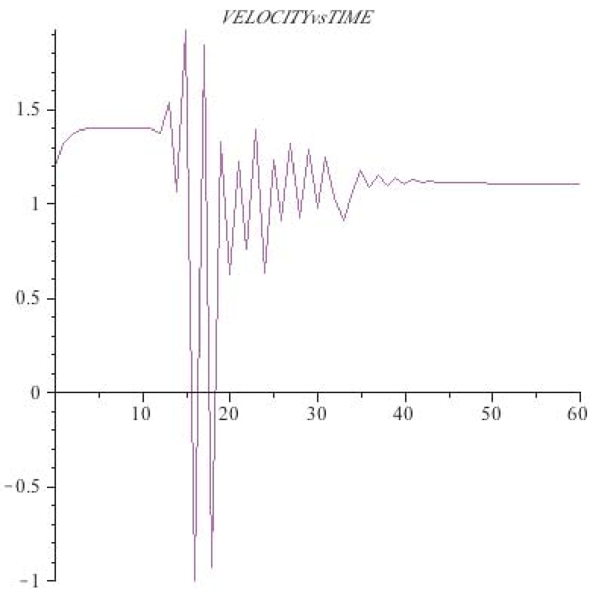

Fig. 2 – Growth of the initial velocity v_2 of the excited state atom at the same position to a quasi-steady state and subsequent turbulent period, followed by a decay to another quasi-steady state.

How do we know that the solutions of the equations are turbulent? By inspection, just like the entire history of turbulence! But in fact the solution satisfies a new precise, unique definition of turbulence [2,3]: (I) when the steady-state solution of a transport equation is multivalued, the system described is turbulent. Furthermore, (II) the system consists of ground state and excited state molecules, which is yet another physical condition for turbulence. Both (I) and (II) are manifestations of the quantum mechanical description of matter.

If nothing else, the lives of CFD specialists will become more challenging and interesting if CFD addresses interacting multicomponent systems, as our simple example illustrates.

Finally, on a related matter, it is curious that the Clay Institute challenge to find solutions of the Navier-Stokes equation -- presumably to explain turbulence -- does not define turbulence. Perhaps we might make a somewhat self-serving proposal [5] that turbulence be defined by (I) and (II) above, filling the absence of a rigorous definition. With this definition, we may be able to answer the philosophical question: how does one solve a problem that has not been precisely defined mathematically? Perhaps our field of research could advance if we start with a precise definition of turbulence.

References

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