Towards a Comprehensive Modelling and Simulation Approach for Turbulent Nonequilibrium Plasma Flows

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Abstract: Variational Multiscale Large Eddy Simulation (VMS-LES) is investigated as a comprehensive methodology for the simulation of turbulent nonequilibrium plasma flows. The method circumvents the assumptions in traditional LES by using a variational decomposition of scales and a residual-based approximation of the sub-grid scales. The initial evaluation of a parallel Finite Element implementation in C++ is presented.

Keywords: Plasma turbulence, sub-grid scale modelling, thermodynamic non-equilibrium.

1. Introduction

Plasmas at atmospheric or higher pressures, typically denoted as thermal plasmas, are partially ionized gases in which the high collision frequency among its constituents (molecules, atoms, ions, and electrons) causes them to be in a state of Local Thermodynamic Equilibrium (LTE) [1]. Thermal plasma flows, often generated by electric arcs, are at the core of diverse technologies, such as plasma cutting, spraying, circuit breakers, lighting, fuel reforming, and gasification. The interaction of the plasma with the process environment causes deviations from the LTE state, and therefore prompts the plasma to be in a state of kinetic nonequilibrium. Non-LTE (NLTE) plasmas present significant differences in the temperature of the electrons compared to that for the heavy-species (molecules, atoms, ions). Plasma flows are inherently multiscale, i.e., various physical phenomena are associated with characteristic temporal and spatial extents (e.g., from charge dynamics and molecular diffusion at microscopic scales, to advective transport within the spatial domain size), and are often unstable and turbulent, particularly at industrially relevant conditions. These characteristics make the computational simulation of turbulent NLTE plasma flows exceedingly challenging.

One of the most common plasma sources is the plasma torch, a device that generates a directed flow of plasma from a stream of working fluid. These torches are used in diverse applications such as plasma spraying and particle and chemical synthesis. Figure 1 schematically depicts a direct-current (DC) non-transferred arc plasma torch and the associated plasma flow with some of its features.

![Fig. 1. Schematic representation of the flow from a non-transferred arc plasma torch.](image)

Kolmogorov presented a theory for turbulent fluid motion that describes how energy is transferred from the larger to the smaller eddies and how much energy is contained and dissipated by eddies of a given size [2]. Methods for the numerical modelling and simulation of turbulent flows can be divided among Direct Numerical Simulation (DNS), which resolves all the scales of the flow (i.e. all eddy sizes), and is therefore the most accurate method; Large-Eddy Simulation (LES), which resolves the large scales and models only the small scales; and Reynolds-Averaged Navier-Stokes (RANS), which models all scales and is therefore the least computationally expensive technique, yet of limited accuracy and generality. Fig. 2 shows the distribution of energy associated to a given eddy as function of its rotational frequency $k$ (the smaller the eddy, the larger its rotational frequency), as well as the difference between the range of resolved scales for DNS and LES. The intractable computational demands of DNS have led LES, which is typically orders of magnitude less computationally expensive than DNS, as the de facto standard for the exploration of most turbulent flows. Nevertheless, the vast majority of LES techniques rely on assumptions that are not valid for plasma flows, such as isotropy and constancy of material properties, and therefore cannot provide adequate descriptions of them.

![Fig. 2. Turbulent energy cascade: energy associated to a given eddy as function of its size, and the extents of resolution aimed by Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES).](image)
This article presents preliminary work in the development of a comprehensive (i.e., consistent and complete) methodology for the coarse-grained simulation of NLTE turbulent plasma flows. The approach is based on the Variational Multi-Scale Large Eddy Simulation (VMS-LES) framework, the state-of-the-art method for the modelling and simulation of turbulent non-plasma flows. The proposed VMS-LES method circumvents the assumptions in traditional LES by using a variational decomposition of scales, and a residual-based approximation of small scales without the need for empirical parameters, which makes it promising for the modelling of multiphysics turbulent flows, particularly nonequilibrium plasma flows.

2. Nonequilibrium Plasma Flow Model

The nonequilibrium plasma flow model in the present study is given by the set of conservation equations for conservation of total mass, mass-averaged momentum, internal energy of heavy-species, and internal energy of electrons (i.e., two-temperature plasma model); together with the equation of conservation of total charge and the magnetic induction equation (both expressed in terms of electromagnetic potentials). The complete set of coupled fluid – electromagnetic equations describing the NLTE plasma flow is listed in Table 1.

Table 1. Set of equations of the nonequilibrium plasma flow model, for each equation:

<table>
<thead>
<tr>
<th>Equation</th>
<th>Transient</th>
<th>Adective</th>
<th>Diffusive</th>
<th>Reactive</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conservation total mass</td>
<td>$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>Conservation momentum</td>
<td>$\rho \frac{\partial \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V} \mathbf{V}) = \frac{\partial p}{\partial t} + \nabla \cdot (\mathbf{F} - \mathbf{V} \mu \nabla \phi) + \mathbf{J} \times \mathbf{B}$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>Energy heavy-species</td>
<td>$\rho \frac{\partial e}{\partial t} + \nabla \cdot (\rho u e) = \frac{\partial e}{\partial t} + \nabla \cdot (\frac{\partial e}{\partial t} u) + \nabla \cdot (\mathbf{F}_e - \mathbf{V}_e \mu \nabla \phi) + \mathbf{J}_e \times \mathbf{B}$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>Energy electrons</td>
<td>$\rho_e \frac{\partial e_e}{\partial t} + \nabla \cdot (\rho_e u_e e_e) = \frac{\partial e_e}{\partial t} + \nabla \cdot (\frac{\partial e_e}{\partial t} u_e) + \nabla \cdot (\mathbf{F}<em>{e_e} - \mathbf{V}</em>{e_e} \mu \nabla \phi) + \mathbf{J}_{e_e} \times \mathbf{B}$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>Conservation charge</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>Magnetic induction</td>
<td>$\mu_0 \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mu_0 \mathbf{B} \times \mathbf{H}) = \mathbf{J}$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
</tbody>
</table>

The nomenclature and details of the mathematical model are presented in [3]. The equations in Table 1 represent transport equations composed of transient, advective, diffusive, and reactive (TADR) terms. These equations can be expressed in compact form as a coupled system for the vector of unknowns $\mathbf{Y}$, as indicated in Eq. [1]. The set of variables to be used is the set of primitive variables given by Eq. [2]; where $A_b$, $A_v$, $K_b$, $S_1$ are coefficient matrices used to describe each transport process and are presented in [3, 4].

3. Variational Multiscale (VMS) Formulation

The strong form of the plasma flow model for the array of unknowns $\mathbf{Y}$ is given by Eq. [3], where $\mathcal{L}$ represents the TADR transport operator. Using the variational form of $\mathcal{L}(\mathbf{Y})$, decomposing the solution field $\mathbf{Y}$ into a large (coarse, grid-scale) component $\overline{\mathbf{Y}}$ and a small (fine, sub-grid) scale component $\mathbf{Y}'$ (i.e., $\mathbf{Y} = \overline{\mathbf{Y}} + \mathbf{Y}'$), and applying the same decomposition to the basis function (characteristic of the weak form of the problem), two equations, one for the large scales and one for the unresolved scales, are obtained. The solution for the small scales problem is given by Eq. [4]. With this approximation, the Variational Multiscale formulation of Eq. [1] for $\mathbf{Y}$ leads to a problem in terms of the large scales only. In particular, the algebraic VMS formulation relies on approximating $\mathcal{L}^{-1}$ with an algebraic operator $\tau$. The intrinsic time scales operator $\tau$ is the main modelling component of the VMS formulation. The role of this operator is to approximate the inverse of the TADR operator $\mathcal{L}$. There are numerous approaches to obtain an expression for $\tau$; most of them require certain amount of empiricism for multi-dimensional coupled problems. The formulation for $\tau$ used in the present work borrows ideas from the work of Hughes and collaborators [5] and is presented in [3].

4. Variational Multiscale Large Eddy Simulation (VMS-LES)

It has been recognized that the VMS framework offered a natural foundation for the development of comprehensive coarse-grained turbulence models [6]. The major challenge is due to the dominant and highly nonlinear role of the small scales. The VMS-LES formulation has to address $ab initio$ the nonlinear nature of the transport operator $\mathcal{L}$, i.e., $\mathcal{L}(\mathbf{Y}) = \mathcal{L}(\overline{\mathbf{Y}} + \mathbf{Y}')$; and therefore, the set of procedures followed in the classical VMS formulation are no longer valid. However, when the nonlinearities are properly addressed, a VMS formulation still provides a comprehensive coarse-grained model of turbulent flows. The nonlinearities in the NLTE plasma flow model (Table 1) make it necessary to use a frontal approach for the handling of the nonlinearity of $\mathcal{L}$. To address the nonlinearity of $\mathcal{L}$, a fixed-point procedure for the modelling of the small scales is being investigated. This procedure represents an extension of the classical VMS formulation and is depicted in Fig. 3.

Fig. 3. VMS-LES formulation as a generalization of the original VMS formulation.

The iterative loop in Fig. 3 implies attaining progressively more accurate approximations of the small scales within some given tolerance $\varepsilon$. It can be noticed
5. Computational Implementation

The algebraic VMS formulation has been implemented in TPORT (TransPORT solver), an in-house developed C++ code for the solution of general systems of TADR equations based on a Finite Element Method (FEM) discretization. TPORT allows sequential as well as parallel processing in both, shared-memory architectures, using OpenMP, and in distributed-memory architectures, using PETSc, the Portable, Extensible Toolkit for Scientific Computation [7]. PETSc is a freely available software package that provides a robust and flexible suite of data structures and routines for the large-scale massively-parallel solution of scientific applications modelled by Partial Differential Equations (PDEs), as required in turbulent flow simulations. As part of the present research, the implementation of PETSc linear solvers in TPORT has been accomplished.

6. Preliminary Results

Before proceeding to the implementation of the VMS-LES formulation as an extension of the classical VMS approach, the VMS implementation in TPORT has been verified and validated. The algebraic VMS method has been verified with the simulation of the compression ramp flow problem, a standard benchmark for compressible flows. Fig. 4 presents the problem set-up, boundary conditions, computational discretization and solution fields for the reference solution, using the commercial software Fluent® [8], and the solution obtained using the VMS formulation. The problem was solved using air as the working fluid. The results show that despite the use of an advective formulation, which arguably does not produce the correct shock location (angle), as so-called conservative formulations do, the VMS simulation produces the correct shock angle.

The VMS implementation has also been verified with the simulation of the magnetohydrodynamic (MHD) benchmark problem known as the Hartmann flow. Fig. 5 presents the problem set-up and the TPORT simulation results together with the corresponding analytical solutions for different values of the Hartmann number. The velocity profiles in this figure are plotted as function of the average velocity. According to Fig. 5, it can be concluded that there is a good agreement between the analytical and numerical solutions.

Fig. 6 presents simulation results of the flow from a non-transferred arc plasma torch impinging on a flat surface. The distribution of the nonequilibrium parameter \( \theta = T_e/T_h \) (i.e. the ratio of electron to heavy-species temperatures) indicates that thermodynamic nonequilibrium is very significant along the plasma – cold flow interface. No explicit turbulence model or forcing of inflow conditions has been included in the simulations. Nevertheless, the images in Fig. 6 show significant resemblance with experimental observations of the dynamics of plasma jets [9, 10].
The results in Fig. 4, Fig. 5, and Fig. 6 indicate that the VMS method provides a reasonable coarse-grained representation of the flow, and therefore is a suitable platform for the development of more comprehensive turbulent plasma flow models, particularly of the proposed VMS-LES formulation.

Ongoing work includes the implementation and optimization of the procedure in Fig. 3 for the modelling of the small scales, and the validation of overall VMS-LES approach with DNS of isotropic plasma turbulence and with experimental data from collaborators of the flow form a non-transferred arc plasma torch [9, 10].

7. Summary

Nonequilibrium plasma flows are inherently multiscale and are often turbulent, particularly at industrially relevant conditions. The computational exploration of turbulent plasma flows with Direct Numerical Simulation (DNS) will remain unfeasible with current and foreseeable computational resources. In contrast, Large Eddy simulation (LES) is considered as the sensible alternative to DNS. Nevertheless, the vast majority of LES techniques rely on assumptions that are not valid for plasma flows, and therefore classical LES cannot provide adequate descriptions of them. This paper presents preliminary work on the use of Variational Multiscale Large Eddy Simulation (VMS-LES) as a modelling and simulation methodology for the comprehensive and computationally feasible description of turbulent nonequilibrium plasma flows. The plasma is modelled as a compressible, electromagnetic, reactive fluid in chemical equilibrium and thermodynamic nonequilibrium. The equations describing the flow are treated in a monolithic approach as a transient–advective–diffusive–reactive (TADR) transport system. The VMS-LES formulation is being implemented in the TPORT code, which is capable of solving general systems of TADR equations using the Finite Element Method. In order to allow massively-parallel computation, the PETSc numerical library has been incorporated in TPORT. The overall VMS-LES approach will be validated with DNS of isotropic plasma turbulence and with experimental data for the flow form a non-transferred arc plasma torch.

8. Equations

\[ \mathcal{R}(\mathbf{Y}) = \mathbf{A}_t \partial_t \mathbf{Y} + (\mathbf{A}_a)\mathbf{Y} \]

\[ -\partial_j (\mathbf{K}_{ij} \partial_j \mathbf{Y}) - (\mathbf{S}_Y - \mathbf{S}_b) = 0 \]

where \( \mathbf{Y} = [ p \ u^T \ T_h \ T_e \ \phi_p \ \mathbf{A}^T ]^T \).

9. Acknowledgements

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10. References

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