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CFD Multiphysics Tool

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Introduction

The recent bold initiatives to expand the human presence in space require innovative approaches to the design of propulsion systems whose underlying *technology* is not yet mature. The space propulsion community has identified a number of candidate concepts. A short list includes solar sails, high-energy-density chemical propellants, electric and electromagnetic accelerators, solar-thermal and nuclear-thermal expanders. For each of these, the underlying *physics* are relatively well understood. One could easily cite authoritative texts, addressing both the governing equations, and practical solution methods for, e.g. electromagnetic fields, heat transfer, radiation, thermophysics, structural dynamics, particulate kinematics, nuclear energy, power conversion, and fluid dynamics. One could also easily cite scholarly works in which “complete” equation sets for any *one* of these physical processes have been accurately solved relative to complex engineered systems.

The Advanced Concepts and Analysis Office (ACAO), Space Transportation Directorate, NASA Marshall Space Flight Center, has recently released the first alpha version of a set of computer utilities for performing the applicable physical analyses relative to candidate deep-space propulsion systems such as those listed above. PARSEC, Preliminary Analysis of Revolutionary in-Space Engineering Concepts, enables rapid iterative calculations using several physics tools developed in-house. A complete cycle of the entire tool set takes about twenty minutes.

PARSEC is a level-zero/level-one design tool. For PARSEC’s proof-of-concept, and preliminary design decision-making, assumptions that significantly simplify the governing equation sets are necessary. To proceed to level-two, one wishes to retain modeling of the underlying physics as close as practical to known *applicable* first principles. This report describes results of collaboration between ACAO, and Embry-Riddle Aeronautical University (ERAU), to begin building a set of level-two design tools for PARSEC. The “CFD Multiphysics Tool” will be the propulsive element of the tool set. The name acknowledges that space propulsion performance assessment is primarily a fluid mechanics problem. At the core of the CFD Multiphysics Tool is an open-source CFD code, HYP, under development at ERAU.

ERAU is renowned for its undergraduate degree program in Aerospace Engineering – the largest in the nation. The strength of the program is its applications-oriented curriculum, which culminates in one of three two-course Engineering Design sequences: Aerospace Propulsion, Spacecraft, or Aircraft. This same philosophy applies to the HYP Project, albeit with fluid physics modeling commensurate with graduate research. HYP’s purpose, like the Multiphysics Tool’s, is to enable calculations of real (three-dimensional; geometrically complex; intended for hardware development) applications of high speed and propulsive fluid flows.

Grid Generation

Resident grid generation capability is a goal of the CFD Multiphysics Tool Project. A number of rudimentary code fragments previously written by the author were assembled into a baseline grid generator. The tool is described in some detail, and a tutorial is presented, in reference [1]. A brief summary is given here.

The user specifies, through namelist input: the overall dimensions in each coordinate direction; the coordinates of the eight corner points of a structured hexahedral blocking topology; the types of segments defining the edges of the block. Currently these types are limited to line segments and circular arcs, each with options for equal grid spacing, or clustering via geometric progressions, for resolution of boundary, free shear, or mixing layers, for example.

The tool employs linear trans-finite interpolation for the surface mesh fill-in on each of the six block sides. There is also an elliptical smoothing option. Similarly, the volume mesh is initially filled with 3-D linear TFI, and a 3-D elliptic smoothing option exists.

A present limitation is that the surface mesh utilities do not have the ability to constrain the mesh to a general geometry. That is, whereas surfaces are *topologically* two-dimensional, they are *geometrically* three-dimensional in general. At present, contoured surfaces cannot be reliably captured without hardwiring the code to do so. For example, in one trial, the outer surface mesh for a converging/diverging rocket combustor and nozzle configuration was generated by hardwiring the code to rotate the block edge contour about the centerline - this in lieu of the usual TFI procedure.

General Description of the CFD Code

More detailed descriptions of the governing equations solved by the code are given in references [3] and [4]. HYP solves the conservation law equations in general coordinates, for a set of conserved variables specified by the user. The fundamental governing equation is

$$\frac{\partial \bar{Q}}{\partial t} + \frac{\partial \bar{E}'}{\partial \xi} + \frac{\partial \bar{F}'}{\partial \eta} + \frac{\partial \bar{G}'}{\partial \zeta} = \bar{W} \quad (1)$$

where \bar{Q} denotes the vector of conserved variables, $\bar{E}', \bar{F}', \bar{G}'$ denote the fluxes of conserved variables in the coordinate directions ξ, η, ζ respectively, and \bar{W} is the vector of source terms. In a relatively simple calculation, the conserved variables might be a number of chemical species mass densities, three momentum components, and total energy.

$$\bar{Q} = [\rho_1 \quad \dots \quad \rho_{ns} \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T \quad (2)$$

$$E_T = \sum_{s=1}^{ns} \rho_s \left(h_s(T) + h_{s_0}^f - \frac{R_u}{M_s} T \right) + \rho \frac{u^2 + v^2 + w^2}{2} \quad (3)$$

The code uses a finite volume formulation. Mathematically, this means that the spatial derivatives are evaluated according to the divergence theorem. Physically, this approach can be thought of as simple accounting for the conserved variables comprising the \bar{Q} vector: mass, momentum, and energy. The flow field is divided into a computational mesh, with a number of small hexahedral “cells.” The rate of change of the \bar{Q} variables within each cell (the leading term in equation (1)) is equal to the rates at which quantities flow in, minus the rate at which they flow out. This difference is the divergence of the fluxes. The source vector \bar{W} contains terms for the rate of production of the conserved variables within the cell.

Electromagnetic Field Modeling

This involves addition of the magnetic induction equation to the set of conservation equations. The magnetic induction equation is derived from Maxwell's electromagnetic field equations. It adds the three components of a "magnetic flux" to the conserved variables. The wave speeds of the equation set thus extended now include the convective velocity as before, plus two Alfvén waves, four magneto-acoustic waves, and one magnetic flux wave [5]. Deriving these wave speeds and the associated flux magnitudes was a primary task of this research. Progress to date is reported in reference[2].

Internal Energy Modeling

The default method of treating the molecular internal energies is according to the equilibrium assumption. That is, one temperature characterizes all of the internal energy states – vibrational, rotational, and electrical. In this case, the internal energy is given by the summation in equation (3).

The specific enthalpies $h_s(T)$ are calculated as cubic splines, fit to the values in the JANAF Thermochemical Tables in increments of 100 K.

For calculations of high speed flows, HYP has an option to treat molecular vibrational energy independently of the molecular translational energy. We say that the gas is in "vibrational non-equilibrium," meaning that the gas translational and vibrational energies are characterized by two different temperatures. The vibrational energy is

$$E_{vib} = R_u \sum_{s=1}^{ns} \frac{\rho_s}{M_s} \sum_{m=1}^{nm} \frac{g_{sm} \theta_{vsm}}{\exp\left(\frac{\theta_{vsm}}{T_{vib}}\right) - 1} \quad (4)$$

Under construction are options for rotational and electron/electronic non-equilibrium. These energies are

$$E_{rot} = R_u T_{rot} \sum_{s=1}^{ns} \frac{\rho_s}{M_s} \frac{r m_s}{2} \quad (5)$$

$$E_{elec} = R_u \sum_{s=1}^{ns} \frac{\rho_s}{M_s} \theta_{elec,s} \frac{\frac{g_{1,s} \exp\left(\frac{-\theta_{elec,s}}{T_{elec}}\right)}{g_{0,s}}}{1 + \frac{g_{1,s} \exp\left(\frac{-\theta_{elec,s}}{T_{elec}}\right)}{g_{0,s}}} + \frac{3}{2} \rho_e \frac{R_u}{M_e} T_{elec} + \rho_e e_k \quad (6)$$

The summation term in equation (7) is the energy of the electron cloud – the ground and first excited states only - surrounding the molecular nuclei. The last two terms are the free electron translational, and kinetic energies, respectively. Considering Hatfield's findings [1], we adopt the

practice of holding the free and bound electrons in equilibrium (at the same temperature), rather than conserving their energies independently.

Conclusions

A CFD code for aerospace propulsion applications under development at Embry-Riddle Aeronautical University, is being adapted for use by the Advanced Concepts and Analysis Office, as the core of the CFD Multiphysics Tool, the propulsive element of a level-two iterative design software package intended for analyzing deep space propulsion concepts. The entire level-two tool set will be incorporated into PARSEC, the recently operational package of level-zero and level-one tools.

Future Work

The continuation of this project during summer 2005 is anticipated. Much of the basic code modification for an MPD Thruster application is being pursued as a Master's thesis project under the author's supervision. A completion date in December 2004 is expected. Discussions are ongoing about possible funding of additional Master's thesis projects, and Graduate Student Research Program (GSRP) topics, related to the Multiphysics Tool. A proposal for advanced MPD computational work and experimental benchmarking in collaboration with UAH and ACAO is in preparation, in response to the recent Human and Robotic Technology Broad Agency Announcement.

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