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IMPROVEMENTS AND NEW FEATURES IN THE PDF MODULE

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Overview

- Modeling: What models are used in this package and what are their advantages and disadvantages.

- Numerics: Describe how the PDF model is implemented and what are the features of the program.

- Future Developments: What can be expected in the future from the NASA Lewis PDF code.

PDF Modeled Equations.

- Exact scalar PDF transport equation is:

$$\begin{aligned}\frac{\partial}{\partial t}(\bar{\rho}P) \; + \; & \frac{\partial}{\partial x_i}(\bar{\rho}\bar{U}_i P) + \frac{\partial}{\partial \phi_\alpha}(\bar{\rho}S_\alpha(\underline{\hat{\psi}}, p, \eta)P) \\ = \; & \frac{\partial}{\partial x_i}(\langle \bar{\rho}\tilde{u}_i | \underline{\psi}, \eta \rangle P) + \frac{\partial}{\partial \phi_\alpha}(\langle \frac{\partial J_i^\alpha}{\partial x_i} | \underline{\psi}, \eta \rangle P) \\ + \; & \frac{\partial}{\partial \eta}(\langle \frac{\partial q_i^\alpha}{\partial x_i} | \underline{\psi}, \eta \rangle P) + \frac{\partial}{\partial \eta}(\langle \frac{Dp}{Dt} | \underline{\psi}, \eta \rangle P)\end{aligned} \tag{1}$$

- Terms on the LHS exact - need to model the four terms on RHS, corresponding to turbulent convection, molecular mixing and the pressure term.

Turbulent Convection

- This term is modeled as a simple gradient diffusion process.

$$\langle \bar{\rho}\tilde{u}_i | \underline{\psi}, \eta \rangle P \approx D_t \frac{\partial P}{\partial \psi_\alpha} \tag{2}$$

- D_t is the turbulent diffusion coefficient, equal to the eddy viscosity. (Assume unity Schmidt)

- Disadvantage: Counter-gradient diffusion known to occur in some pre-mixed flames.

Molecular Mixing.

• Molecular mixing can be viewed as process which changes the shape of the scalar PDF without affecting the mean.

• Molecular mixing is modeled by two models: A coalescence/ dispersion model (Hsu and Chen) and a relax-to-mean model (Dopazo).

• Advantages of both models is that they are simple and readily adaptable to any number of scalars.

• Disadvantages are the relative lack of physics in the models.

Pressure Term.

• Pressure term model is based on second order closure models for compressible flows (eg. Sarkar).

$$\langle \frac{Dp}{Dt} | \underline{\psi}, \eta \rangle \approx \frac{\partial \langle p \rangle}{\partial t} + \langle U_i \rangle \frac{\partial p}{\partial x_i} + 0.8\rho\langle k \rangle \frac{\partial \langle U_i \rangle}{\partial x_i} + 0.15\rho P_r M_t - 0.2\rho\epsilon M_t^2 \qquad (3)$$

• Advantages are that model is tried and tested in finite volume codes. Disadvantage is that only the mean pressure can be used for model. Idealy we would like a stochastic process for two state variables.

Numerics

- Solution of scalar PDF transport equation achieved by a particle based Monte Carlo scheme.

- PDF represented by an ensemble of particles, each with a composition and enthalpy.

- PDF evolves by the motion of these particles in physical, scalar and enthalpy space, by exact and modeled processes. eg. Convection, reaction, mixing.

- Statistics (eg. means) obtained by averaging over ensemble of particles.

Numerical Details - Monte Carlo Scheme

- Module based on cell-centered quantities.

- PDF method is a nodal one. ie. All particles reside at the center of the cell, and can move only to neighboring cells.

- Number of particles at each node is the same and the number remains fixed.

- Statistics obtained by averaging over particles at each node, and also by time-averaging.

Numerics - Convection

• Upwind scheme used for mean convection, and central difference for turbulent convection.

• Evolution achieved by moving particles in from adjacent nodes. Particles are selected at random.

• Fractions of particles are treated by random convection.

$$\text{if 6.3 particles then} \begin{cases} 6.0 & 70\% \text{ of the time} \\ 7.0 & 30\% \text{ of the time} \end{cases} \qquad (4)$$

Numerics - Reaction

• Although reaction source term treated exactly, several different numerical schemes are needed. Timing figures are for % of time spent in the PDF part of the code on SPARC II workstation.

• No reaction: For scalar mixing calculations.
(Timing: 17.2 %)

• Equilibrium reaction: Assume reaction proceeds at infinite speed. Table of equilibrium composition as a function of mixture fraction obtained from seperate CHEMKIN routine.
(Timing: 24.4 %)

Numerics - Reaction Cont.

• One-step global reaction schemes. Westbrook and Dryer global reactions integrated for each time-step.
(Timing: 51.1 %)

• Tabulated reaction incriments. Users create their own table of composition incriments as a function of scalars using the adaptive tabulation scheme provided, plus the users favourite reduced mechanism.
(Timing: 58.9 %)

• Chemkin full mechanism integration. Very slow and not recomended except for parallel applications.
(Timing: 97.8 %)

Numerics - Averaging

• To reduce statistical error in the evaluation of the mean scalar quantities (without increasing the number of particles per node), time averaging is employed.

• A weighted time average is used to give more weight to recient values and less to those in the far past.

$$\langle\langle\phi\rangle\rangle_t = \frac{1}{w_t + 1}(\langle\phi\rangle_t + w_t\langle\langle\phi\rangle\rangle_{n-1}) \tag{5}$$

$$w_t = c_t(w_{t-1} + 1) \tag{6}$$

Numerics: Misc.

- A portable random number generator is now included in the module, set up for 32 bit machines.

- A time step check is now performed to ensure boundedness of the PDF solution. ie. no negative numbers of particles.

- Rplus/PDF release ported to workstation enviroment. K-epsilon now standard turbulence model.

Future Work.

- Release of 3D version with new improvements.

- Implimentation of parallel processing for distributed cluster environment. (PVM based)

- Include model for another state variable to close PDF modeling.

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