Adaptive parameterization of combustion chemistry with lower order polynomials

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1 Summary

We present a new method to approximate the solution to the initial value ordinary differential equation system that represents chemical kinetics. In this method, the approximation is performed with zero order, first order and second order algebraic polynomial expressions. The method is adaptive polynomial tabulation (APT). The polynomials are created on the fly from a look-up table. To achieve fast and efficient searching, the chemical composition space is partitioned online into local regions. The sizes of the local regions are calculated from the mapping gradients. In this approach, stored data points are used to construct polynomials. Each stored data point is encircled by two concentric ellipsoids namely, IDENTICAL and ISAT ellipsoids with radii $\delta\phi^0$ and $\delta\phi^1$ respectively. Another local region, the PRISM ellipsoid with radius $\delta\phi^2$ is also considered. There could be several ISAT ellipsoids within each PRISM ellipsoid. The chemical ODE solver receives as input a mixture point, at a time t, and evolves it after a time interval Δt, given a new mixture point, the ODE solution using the time demanding numerical integration. Meanwhile, APT provides a computationally cheaper alternative by approximating the ODE solution with local polynomials. APT uses binary search tree functions to identify local regions. During computation mixture points enter these regions. When a mixture point enters the IDENTICAL ellipsoid of a stored data point, the ODE solution at the mixture point is approximated by zero order polynomials. Similarly, when a mixture point enters the ISAT ellipsoid of a stored data point, its ODE solution is approximated by first order polynomials. Mixture points will be accumulatated in the PRISM ellipsoid, if they fall outside the IDENTICAL and ISAT ellipsoids of other stored points. The accumulated data points are later used to construct second order polynomials for the PRISM ellipsoid. In this case, the ODE solutions at other mixture points which encounter this PRISM ellipsoid are approximated by the second order polynomials. The memory for the point-slope data of the PRISM ellipsoid is freed when the second order polynomials are constructed. APT can be adapted to use a reduced number of variables to access local regions and construct polynomials. In the test calculations, APT replaced the chemical ordinary equation (ODE) solver in a two zone model for spark ignition engine. In this model each zone is treated as a stochastic reactor, flame propagation is calculated from a Wiebe function. The engine is fueled with hydrogen. For this problem, a speed up factor of 3-5 is reported. The chemical species, temperature and pressure profiles are in very good agreement with those of the model calculations that used the chemical ODE solver

2 Introduction

Solving for the initial value chemical ordinary differential equation system using detailed chemistry is computationally demanding. This is because most chemical mechanisms are large in size, and the associated rate equations are stiff and non-linear. There is a growing need for the coupling detailed chemistry into multi-dimensional CFD codes for different engineering applications. For example, in the prediction of auto-ignition, pollutant formation and emissions in realistic models for Diesel and HCCI engines, engine knock in realistic models for spark-igniton engines. This type of calculations may require several millions of ODE solver calls, and may take several months of CPU time, which is deemed prohibitive. To overcome these difficulties, some scientists have proposed surrogate models, which mimic the ODE solutions with computationally inexpensive

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polynomial expressions valid for local regions. The tools PRISM and ISAT fall under this category. In PRISM, the ODE solutions at mixture points are approximated locally by second order polynomial expressions. The second order polynomial coefficients have limited region of validity, which is a hypercube in the chemical composition space. The polynomial coefficients are created on the fly from carefully selected points with the hypercube and their ODE solutions. The points are selected using central composite design [3]. In [4] computational gain of 15 is reported using PRISM. However, the memory burden in this approach is also a concern, the coefficients are stored in a direct access disk file and in memory. In ISAT, the ODE solutions at mixture points are approximated locally by first order polynomial expressions. The polynomials are also created on the fly from a look-up table. The size of the region of validity of the local polynomials depends on the mapping gradients and a specified error tolerance, This region is known as the ellipsoid of accuracy, EOA. If the mixture points falls within the EOA, its ODE solution is approximated by first order polynomial. If the mixture point is outside the EOA, the EOA is either grown or a new record is added to the table. Searching the record in the table is not a primary concern since binary search tree is used, because it does only $\log_2 N$ searches, where N is the number of records. The memory increases quadratically with the number of variables.
In the present work, we combine ISAT and PRISM into a computer code called adaptive polynomial tabulation. Herein, ISAT is called with PRISM, and PRISM is reformulated to use stored data points to construct second order polynomials instead of points selected by central composite design. In this case, no extra ODE solver calls are required. The local region of validity of second order polynomial coefficients, that is the PRISM hypercube fully covered by PRISM ellipsoid is calculated online from the mapping gradient. Furthermore, regions of validity of zero order polynomials are introduced. These are called IDENTICAL ellipsoids, their sizes are also calculated from the mapping gradients. The magnitude of the initial memory burden is significantly reduced because point-slope data for each PRISM hypercube is deleted after its second order polynomials are constructed. In the next section APT is described. This is followed by a brief description of the stochastic reactor – spark ignition engine model in section 4. The description of the test case, results and discussions are given in section 5 and conclusion is given in section 6.

3 Adaptive Polynomial Tabulation (APT)

In this work, PRISM and ISAT are combined into one computer code called adaptive polynomial tabulation. It provides lower order polynomial approximations to the solution to the chemical kinetic ordinary differential equation system. The polynomials for each local region are constructed on the fly from the library of stored data. The chemical composition space is partitioned online into local regions. The local regions are of three different types, which include IDENTICAL, ISAT and PRISM ellipsoids. The PRISM ellipsoids contain may the stored points, the chemical ODE solutions at the stored points, the sensitivities with respect to the initial conditions at the stored points, the mean of the stored points and their standard deviation.

Suppose $\phi_q = (Y_1^t, \ldots Y_{n_s}^t, H^t, p^t)$ is a query mixture point whose time evolution $R(\phi_q)$ is required from APT. Where Y_i^t are chemical specie mass fractions, H^t is the enthalpy, p^t is the pressure and n_s is the number of chemical species. The algorithm proceeds as follows, a multidimensional binary tree search function is employed to determine the index of the PRISM ellipsoid that contains ϕ_q. It is should be noted that the PRISM ellipsoids are replaced by PRISM hypercube, which are fully covered by the PRISM ellipsoids. If the polynomial coefficients for this hypercube has been calculated, then the polynomials are retrieved from memory and evaluated at ϕ_q using equation (1)

$$Y_i^{t+\Delta t} = a_{i,0} + \sum_j^d a_{i,j} \tilde{Y}_i^t + \sum_j^d \sum_{k \le j}^d a_{i,jk} \tilde{Y}_j^t \tilde{Y}_k^t \qquad (1)$$

Where ϕ_q has been transformed to $\phi_q^{'} = (\tilde{Y}_1^t, \tilde{Y}_2^t \ldots, \tilde{Y}_d^t)$ and Δt is the time step.

On the other hand if the second degree polynomials have not been constructed, the list of stored points for the PRISM hypercube is scanned until a stored point is found, such that, the query point ϕ_q lies inside its IDENTICAL or ISAT ellipsoid. If ϕ_q is within the ISAT ellipsoid (with radius $\delta\phi_s^1$) of a stored point ϕ_s. The ODE solution at ϕ_q is approximated by using equation (2), but if ϕ_q lies within the IDENTICAL ellipsoid (with radius $\delta\phi_s^0$), the ODE solution at the stored point is taken as the ODE solution at ϕ_q

$$Y_i^{t+\Delta t} = Y_{s^1,i} + \sum_{j=1}^{n_s} A_{ij}(\phi_s)(Y_i^t - Y_{s^0,i}) \tag{2}$$

Here $Y_{s^1,i}$ and $Y_{s^0,i}$ are the elements of ϕ_s and $R(\phi_s)$ respectively. Where $R(\phi_s)$ is the ODE solution at ϕ_s. The matrix $A(\phi_s)$ is the mapping gradient at ϕ_s. However, if the query point, ϕ_q is not within the ISAT ellipsoid of any of the stored points, and the number of stored points is less than $\tilde{N}$ (the number of stored points required to construct second degree polynomials). The chemical ODE solver is called to compute the ODE solution $R(\phi_q)$ and mapping gradient $A(\phi_q)$ at ϕ_q, followed by the computation of the ISAT radius $\delta\phi_q^1$ for this point. The ISAT radius $\delta\phi_q^1$ is obtained by solving equation 3 by using Lower Upper (LU) decomposition and back substitution (see Pope 1997).

$$A(\phi_q)\delta\phi_q^1 = \varepsilon_{tol} R(\phi_q) \tag{3}$$

Here ε_{tol} is the ISAT error tolerance. Before the point-slope data is stored, it is tested if the radius of the PRISM ellipsoid that contains ϕ_q is small enough in each dimension to allow second degree polynomials to be accurate within the PRISM ellipsoid. For this, we calculate the radius of the new PRISM ellipsoid ($\delta\phi_q^2$) using $\delta\phi_q^2 = \eta\delta\phi_q^1$, where η is in the range $100 \le \eta \le 1000$. Finally point-slope data is stored.

In reduced APT or RAPT, a reduced set of variables are used to access local regions and construct polynomials. In this case, a smaller system of equations is obtained, therefore a gain in computational efficiency.

4 Stochastic-reactor-spark ignition (SRM-SI) engine model

The stochastic-reactor-spark-ignition engine model is rigorously explained in [3] and the references there in. The stochastic-reactor-spark ignition engine model is a zero dimensional model. The mixture in the cylinder is partitioned into two zones, burned and unburned gas zones, each zone is modeled as a stochastic reactor. In this model the scalars such as chemical species mass fractions and temperature are treated as random variables, and a PDF transport equation for these scalars is derived using the assumption of statistical homogeneity. Meanwhile, quantities such as mass, mean density, volume and pressure are considered as global variables. In variable density flows, stochastic reactors are usually represented in terms of the mass density function $F_\phi(\varphi;t)$ where the local quantities are given by $\phi(t) = (\phi_1, \phi_2, ..., \phi_{n_s}, \phi_{n_s+1}; t)$.

The transport equation of the mass density function is given by

$$\frac{\partial F_\phi(\varphi;t)}{\partial t}+\frac{\partial}{\partial \varphi_i}\left(Q(\varphi)F_\phi(\varphi;t)\right)=\frac{\partial}{\partial \varphi_i}\left(\frac{1}{2}\frac{C_\phi}{\tau}\left(\varphi-\langle\phi_i\rangle\right)F_\phi(\varphi;t)\right)$$
$$F_\phi(\varphi;0)=F_\phi^0(\varphi) \qquad (4)$$

Here the right hand side of the first part of equation (4) represents transport of mass density due to micro-molecular mixing. The term Q_i denotes the transport of the mass density function (MDF) due to chemical reactions, heat losses and volume work. An equi-weighted Monte Carlo particle method is used to solve equation (4) numerically. In this method, the initial mass density function is approximated by a stochastic particle ensemble, and the particles are moved according to the time evolution of the density function. The evolution of the cylinder gas is divided in a number of time steps by the operator splitting algorithm [5]. With time marching, turbulent mixing, convective heat loss, flame propagation and chemical reactions events are performed on the particle ensemble for each global time step (from inlet valve closing to exhaust valve opening).

5 Test cases, calculations and results

The purpose of these tests is to verify the fidelity of the end gas auto-ignition predictions of the APT (and RAPT) compared to the chemical ODE solver and further to quantify associated computational speed up. The engine used in the simulations is a port injected **FORD ZETEC 2.0 L** engine [5]. The engine settings and the stochastic reactor parameters are the same as those in Table 1of [5]. A hydrogen mechanism of 9 chemical species and 38 elementary reactions is used as in [5]. In the RAPT, the progress variables are H_2, H_2O, O_2. In each case enthalpy and pressure serve as parameters.

In using the tools APT and RAPT within two zone spark-ignition engine model, end gas auto-ignition is reported as with the model calculations with the chemical ODE solver. This temperature and pressure profiles are shown in Fig. 1a and 1b. In the figures, the agreement between APT (RAPT) and ODE solver is very good. In the problem considered a speed up factor in the range of 3-5 is reported, a speed up factor in the chemistry subroutines in the range of 6-9 is also reported. This is shown in Table 1 for different values of $\tilde{N}$ (the number of stored points required to construct second order polynomials). As compared to APT, RAPT demonstrates better time savings, because it uses a reduced set of variables to identify local regions and evaluate polynomials.

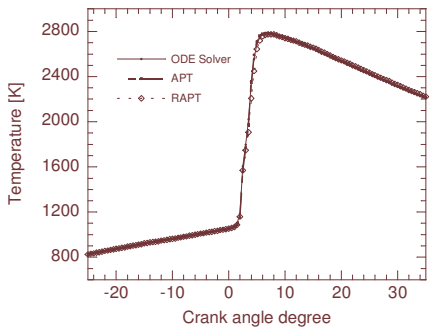

Fig. 1a

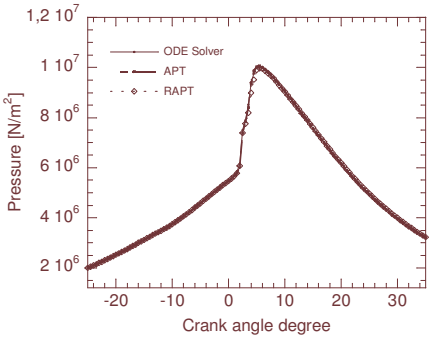

Fig. 1b

Fig. 1a (1b) : Temperature (Pressure) history for spark ignition calulations using APT, RAPT and the ODE solver.

Table 1. The speed up factors for the chemistry and the two zone spark-ignition engine

Ñ	APT speed-up factor	SRM-SI/APT speed-up factor	RAPT speed-up factor	SRM-SI/RAPT speed-up factor
281	6.46	3.94	8.13	4.67
306	7.32	4.35	8.25	4.71
459	6.30	3.98	7.88	4.60
562	6.25	4.03	8.04	4.33

Conclusions

A new method to approximate the solution of the initial value ordinary equation system that represents chemical kinetics, adaptive polynomial tabulation has been presented and described. It has demonstrated robustness and adaptability, with the capability of reducing the computational cost without sacrificing chemical fidelity. It can use a reduced number of variables to access local regions and construct polynomials. APT constructs polynomials only as needed and the sizes of local regions are calculated dynamically from the mapping gradients. The method demonstrates better memory economy than PRISM and ISAT.

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