

LES/FDF/ISAT computations of turbulent flames

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The *in situ* adaptive tabulation (ISAT) algorithm is incorporated in the Stanford structured large eddy simulation (LES) code for the large eddy simulation of turbulent combustion. The subgrid scale (SGS) closure implemented by Raman is based on the scalar filtered mass density function (FDF) methodology. The FDF represents the joint probability density function of the subgrid-scale scalar quantities and is obtained by solution of its modelled transport equation. In this equation, the effect of chemical reactions appears in closed form and the chemistry mechanism is implemented via ISAT; the influences of SGS mixing and convection are modelled. The modelled FDF transport equation is solved by the Lagrangian Monte Carlo scheme which solves the statistically equivalent stochastic differential equations (SDEs). The numerical simulation of a spatially developing mixing layer with a 9-species detailed hydrogen mechanism is performed to examine computational issues arising in the LES/FDF/ISAT methodology. It is shown that the filtered mixture fraction field obtained via the FDF agrees well with that obtained by the ‘conventional’ LES in which the finite difference solution of the transport equation of the filtered mixture fraction is obtained. The performance and load balancing of both the serial and parallel ISAT strategies are investigated. For the simulation in which cheap retrievals are dominant, a speed-up factor of about 300 is obtained for the combustion chemistry compared to using direct integration. And compared to the LES (without FDF), the relative cost of LES/FDF (without reaction) is about 2.8, and the relative cost of LES/FDF/ISAT is about 4.3. For the simulation in which there is a significant fraction of direct integrations, the halving of the time in combustion chemistry is achieved by using the parallel ISAT strategy compared to serial ISAT.

1. Introduction

For the modeling of turbulent combustion, large eddy simulation (LES) has the advantage of accounting for the large scale unsteady motions, which account for the bulk of the spatial transport. Within the past decade, large eddy simulation of turbulent reacting flows has been the subject of widespread investigation. And there are significant recent developments of subgrid scale (SGS) modelling for the large eddy simulation of turbulent reacting flows. One such closure is based on the “filtered density function” (FDF) method, first introduced by Pope (Pope 1990). This method is analogous to the probability density function (PDF) modeling (Pope 1985) which has proved very effective in Reynolds averaged simulations. The composition FDF is considered by many investigators and it provides a complete description of the subfilter-scale composition fluctuations (Gao & O’Brien 1993; Colucci *et al.* 1998; Jaber *et al.* 1999; Zhou & Pereira 2000; James & Jaber 2000; Cha & Trouillet 2003; Givi 2003; Raman *et al.* 2003a). Due to this property, the effect of chemical reactions appears in closed form and the FDF offers the ability to treat finite-rate chemistry and the turbulence-chemistry interactions. This combined methodology LES/FDF (with very simple chemistry) has been applied to

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the Sandia D flame by Sheikhi *et al.* (Sheikhi *et al.* 2004), and to the Sydney bluff-body by Raman *et al.* (Raman *et al.* 2004a; Raman *et al.* 2004b).

While desirable, the computational cost of directly using realistic combustion chemistry in the LES/FDF simulation of turbulent combustion is expensive and usually prohibitive due to strong non-linearities of the reaction source term and the wide range of time scales in the chemical kinetics. The *in situ* adaptive tabulation (ISAT) algorithm (Pope 1997) greatly facilitates the incorporation of realistic combustion chemistry (e.g., of order 10 and 20 species for hydrogen and methane, respectively) and reduces the CPU time dramatically, which makes the LES/FDF simulation of turbulent combustion with realistic chemistry feasible.

In this work, the LES/FDF/ISAT capability for the numerical simulations of turbulent reactive flows with realistic combustion chemistry is developed by incorporating ISAT into the Stanford structured LES code with a Lagrangian Monte Carlo implementation of the composition FDF method. The numerical simulation of a simple spatially developing mixing layer is performed to verify this capability. A detailed hydrogen mechanism, the Li mechanism (Li *et al.* 2003), which has 9 species and 21 reactions, is incorporated via ISAT. In the next sections, the three important ingredients of the LES/FDF/ISAT capability (the LES solver, the FDF formulation and the ISAT algorithm) are briefly reviewed. Then, the results from the mixing layer are discussed, and the ISAT performance and load balancing are investigated.

2. The LES solver

The Stanford parallel structured finite volume code (Pierce 2001; Pierce & Moin 2004), developed specifically for LES of variable density low Mach-number flows, is used in this work. The second order LES scheme uses an energy conserving formulation for the momentum equation. The eddy viscosity and diffusivity are computed using the dynamic Smagorinsky model (Moin *et al.* 1991). The LES scheme also solves the scalar transport equation of filtered mixture fraction $\langle \xi \rangle_L$ using a semi-implicit scheme. The numerical implementation uses an upwind based QUICK scheme that is designed to reduced numerical oscillations but also leads to some amount of numerical dissipation.

3. The filtered density function (FDF) and its Monte Carlo solution

Let ϕ denotes the composition, which consists of species mass fractions and enthalpy in the simulation. The filtered density function (FDF), which describes the sub-filter joint composition density function, is defined as (Pope 1990; Gao & O'Brien 1993)

$$F_L(\psi; \mathbf{x}, t) = \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) \delta[\psi - \phi(\mathbf{x}', t)] G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}', \quad (3.1)$$

where F_L denotes the filtered mass density function, δ denotes the Dirac delta function, ψ is the sample-space variable corresponding to ϕ and $G(\mathbf{x}' - \mathbf{x})$ is the filter. This definition implies that the FDF is the mass-weighted spatially filtered value of the fine-grained density and the integral properties of the FDF is such that

$$\int_{-\infty}^{+\infty} F_L(\psi; \mathbf{x}, t) d\psi = \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}' = \bar{\rho}, \quad (3.2)$$

where $\bar{\rho}$ is the filtered density. Using the above definitions, the transport equation for F_L can be derived (Colucci *et al.* 1998; Jaber *et al.* 1999). In the transport equation

for F_L , if the effects of SGS convection are modelled by a gradient diffusion model and and the SGS mixing is closed via the interaction by exchange with the mean (IEM or LMSE) (Villermaux & Devillon 1972; Dopazo & O'Brien 1974) model, the final modelled FDF transport equation is

$$\frac{\partial F_L}{\partial t} + \frac{\partial[\langle u_i \rangle_L F_L]}{\partial x_i} = \frac{\partial}{\partial x_i} \left[(\gamma + \gamma_t) \frac{\partial(F_L/\bar{\rho})}{\partial x_i} \right] + \frac{\partial}{\partial \psi_\alpha} [\Omega_m (\psi_\alpha - \langle \phi_\alpha \rangle_L) F_L] - \frac{\partial[S_\alpha F_L]}{\partial \psi_\alpha}, \quad (3.3)$$

where $\langle u_i \rangle_L$ is the Favre filtered velocity component, $\langle \phi \rangle_L$ is the Favre filtered composition and \mathbf{S} is the rate of change of composition given by the detailed chemical mechanism. The molecular and turbulent diffusivities are denoted by γ and γ_t respectively. The term Ω_m is the SGS mixing frequency (as required in IEM) and is modelled by $\Omega_m = C_\Omega (\gamma + \gamma_t) / (\bar{\rho} \Delta_G^2)$, where C_Ω is a model parameter and Δ_G is the filter width.

The Lagrangian Monte Carlo procedure (Pope 1985) using an ensemble of notional particles is employed for the solution of the high-dimensional equation Eq. 3.3. In this procedure, each of the particles obeys the evolution equations which is obtained from Eq. 3.1 by using techniques similar to the RANS based method. These particles undergo motion in physical space by convection due to the filtered flow velocity and diffusion due to molecular and subgrid diffusivities. The particles move in physical space according to

$$d\mathbf{x}^* = \left(\langle \mathbf{u} \rangle_L + \frac{1}{\bar{\rho}} \nabla (\gamma + \gamma_t) \right) dt + \sqrt{2 \frac{(\gamma + \gamma_t)}{\bar{\rho}}} d\mathbf{W}, \quad (3.4)$$

where \mathbf{x}^* is the instantaneous particle position, $\bar{\rho}$ is the filtered density and \mathbf{W} represents the Wiener process. The particle composition is changed due to mixing and reaction.

$$d\phi^* = [\Omega_m (\langle \phi \rangle_L - \phi^*) + \mathbf{S}(\phi)] dt, \quad (3.5)$$

where ϕ^* is the composition of the particle with the position \mathbf{x}^* . A splitting operation is employed in which the transport in physical and composition space are treated separately (Raman *et al.* 2003b). The transfer of information from the fixed finite difference grid points to the locations of the Monte Carlo particles is conducted via interpolation. Whereas the Favre-filtered statistics such as the filtered species mass fractions on the fixed grid points are obtained via ensemble averaging all the particles in the grid cells.

4. In situ adaptive tabulation (ISAT)

In LES/FDF simulations of turbulent combustion, if a splitting scheme is used to separate the combustion chemistry from other processes such as convective and diffusive species transport as depicted in Fig. 1, the reaction fractional step corresponds to a homogeneous, adiabatic, isobaric system consisting of n_s chemical species. At time t , the full composition is represented by the $n_\phi = n_s + 1$ variables $\phi(t) \equiv \{\phi_1, \phi_2, \dots, \phi_{n_\phi}\}$, which can be taken to be the species mass fractions and enthalpy. Modeling reaction kinetics in this system leads to a set of stiff ordinary differential equations (ODEs)

$$\frac{d\phi(t)}{dt} = \mathbf{S}(\phi(t)), \quad (4.1)$$

where \mathbf{S} is the rate of change of composition given by the detailed chemical mechanism. The task in the reaction fractional step is to determine the solution to Eq. 4.1, the composition $\phi(t + \Delta t)$ after reaction has occurred for the time-step interval Δt starting from the initial composition $\phi(t)$ at time t . Due to strong non-linearities of the reaction

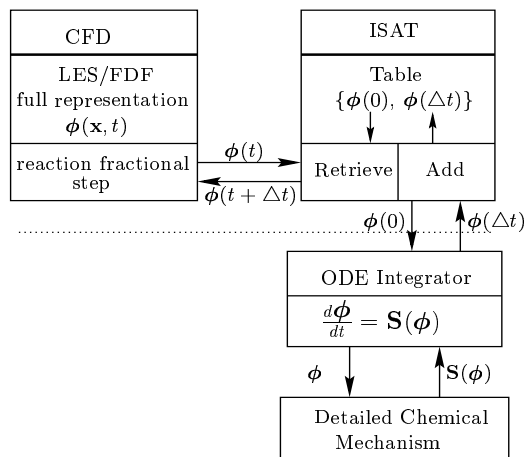


FIGURE 1. Schematic of *in situ* adaptive tabulation used in the reaction fractional step of a CFD computation using LES/FDF approach.

source term and the wide range of time scales in the chemical kinetics, direct integration (DI) of Eq. 4.1 using an ODE integrator is computationally expensive. Further, when the reaction fractional step is performed a huge number of times with many different initial compositions, significant computational resources are required.

An alternative to DI for computing the solution $\phi(t + \Delta t)$ is ISAT, which is a storage-retrieval methodology (with error control) introduced by Pope (1997). As depicted in Fig. 1, an ISAT table stores pairs of values of ϕ before and after reaction $\{\phi(0), \phi(\Delta t)\}$, so that given $\phi(t)$ the corresponding value $\phi(t + \Delta t)$ can be retrieved from the table. (Since the governing ordinary differential equations (ODEs) are autonomous, the value of t is immaterial, and without loss of generality we can set $t = 0$.) As needed, pairs of values $\{\phi(0), \phi(\Delta t)\}$ are added to the table by integrating the governing ODEs with the detailed chemistry. In a large-scale numerical simulation, the reaction fractional step is predominantly treated by retrieving from the ISAT table, which is many orders of magnitude less expensive than performing an ODE integration. As a result, ISAT makes the use of realistic combustion chemistry in the LES/FDF simulation of turbulent combustion feasible.

Both the serial and parallel ISAT strategies have been developed. In a parallel LES/FDF simulation of a combustion problem, each processor has its own ISAT table. For the serial ISAT strategy, in the reaction fractional step, particle compositions on one processor are locally processed by using the local ISAT table and there is no message passing. Whereas for the parallel ISAT, the particle composition $\phi(t)$ on one processor may be passed to another processor (using MPI), processed there using the local ISAT table, and then $\phi(t + \Delta t)$ is passed back to the original processor. Two different parallel ISAT strategies are used in this study. One is the uniform random distribution (URAN) method in which all the particle compositions in the simulation are randomly distributed uniformly among the processors to be processed during the reaction fractional step. The other strategy is the local level distribution (LOCLEV) method in which message passing is minimized by passing particle compositions to nearby processors so that all processors have close to the same number of particle compositions to be processed during the reaction fractional step.

5. Flow configuration and numerical specification

The LES/FDF simulation of a two-dimensional, spatially developing, reacting, plane mixing layer is considered. In the simulation, the effect of heat release is neglected and the density is taken to be constant: therefore there is no feedback from the FDF to the LES computation. The primary objective of the simulation is to test the computational performance of the new LES/FDF/ISAT approach and to investigate the ISAT performance for serial and parallel ISAT strategies. No attempt is made to study the numerical accuracy, investigate the effect of models and model parameters, or make comparison with the experimental data.

The flow configuration is set to mimic the Cabra flame which is a turbulent lifted flame of H_2/N_2 issuing into a vitiated co-flow (Cabra *et al.* 2002). In the simulations, a reacting planar mixing layer composed of cold diluted hydrogen in one stream (fuel stream) and hot lean combustion product in the other stream (oxidant stream) is considered. The composition for the fuel stream is taken to be (in volume percentage) N_2 (75%) and H_2 (25%); the temperature is 305K. The composition for the oxidant stream is taken to be (in volume percentage) N_2 (75%), O_2 (15%) and H_2O (10%); the temperature is 1045K.

In the simulation, the flow variables are normalized with respect to selected reference quantities, denoted by the subscript r . The reference velocity U_r is chosen to be the fuel stream velocity 66 m/s, the reference length L_r is taken to be 3.3mm. And the non-dimensional time is given by $t^+ = U_r t / L_r$. The kinematic viscosity ν_r in the simulation is taken to be a constant throughout, which is based on the fuel stream properties. The Reynold number $Re = U_r L_r / \nu_r$ is 15200. The two-dimensional computational domain in non-dimensional units in the simulation is the rectangular region: x^+ from -10 to 50 and y^+ from 0 to 15, where the splitter plate lies in the region: x^+ from -10 to 0 and y^+ from 7.2 to 7.8. The present two-dimensional calculations are performed on a nonuniform mesh with 128 grids nodes in the streamwise direction (x^+) and 64 grid nodes in the tranverse direction (y^+). The mesh in the small region near the splitter plate is refined. The simulation uses parallel computation with 8 processors, and the computational domain is decomposed into 8 blocks in the x^+ direction with each block having the same number of grid cells.

In the simulation, the inlet velocity profiles at $x^+ = -10$ are taken to be laminar plug profiles and turbulence develops in the downstream layer due to the instability of the shear layer. The ratio of oxidant and fuel stream velocities is fixed at 0.4, with the non-dimensional fuel stream velocity being unity, and oxidant stream velocity being 0.4. These values of the free stream velocities are selected so that the flame exists throughout most of the flow, as shown in Fig. 3. The wall boundary conditions at the splitter plate are Neumann conditions for all scalars and pressure, and no-slip Dirichlet conditions for velocity. All the open and outflow boundaries use the convective boundary condition.

In FDF, the Monte Carlo particles are distributed at $t=0$ throughout the calculation domain. The nominal particle number density of 30 particles per cell is use in the simulation. Particle cloning and clustering are utilized to minimize the fluctuation in the number density. New particles are introduced at the inlet at a rate proportional to the local mass flow rate, and the composition of incoming particles is set according to the composition of the fluid at the point of entry. To save computational time, the LES simulation without FDF/ISAT is carried out until the flow field reaches statistical stationarity. Then the LES/FDF simulation without reaction fractional steps is carried out for 1000 time steps. Finally the full LES/FDF/ISAT simulation is performed.

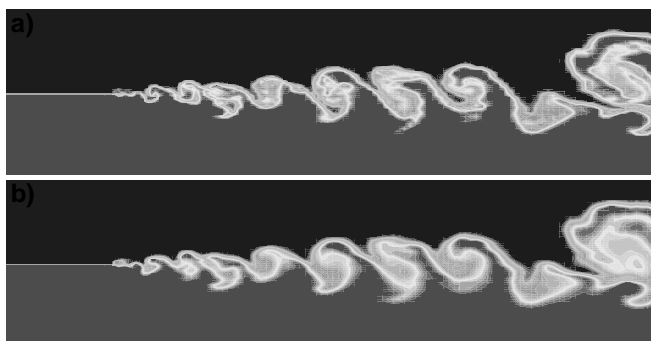


FIGURE 2. Contours of the instantaneous filtered mixture fraction field as predicted by the LES/FDF/ISAT approach via (a) FDF, (b) the LES solver using a standard finite difference scheme.

6. Assessment of the LES/FDF/ISAT approach

To demonstrate the consistency of the FDF formulation, the mixture fraction results obtained via FDF and via the LES solver using the standard finite difference scheme are compared to each other. For the mixing layer studied, any deviations between the results from the FDF and the LES solvers are attributed to the differences in the numerical procedures. Since the accuracy of the finite difference scheme is well established, this comparative analysis provided a means of assessing the performance of the Monte Carlo solution of the FDF. In the FDF for this two-stream problem, the filtered mixture fraction is constructed based on the filtered N_2 mass fraction, $\langle \xi \rangle_L = \frac{\langle Y_{N_2} \rangle_L - Y_{N_2}^o}{Y_{N_2}^f - Y_{N_2}^o}$, where $Y_{N_2}^o$ and $Y_{N_2}^f$ are the N_2 mass fractions of the fuel and oxidant streams respectively. In Fig. 2, the instantaneous contour plots of the mixture fraction are shown as determined by the FDF and LES solvers. This figure provides a simple visual demonstration of consistency of the FDF formulation as the results via the particle method are in agreement with those obtained by the finite difference scheme. In fact, results from the LES solver are somewhat more smeared partially due to the numerical diffusion. Further work should include a quantitative comparison between the filtered mixture fraction fields obtained via FDF and LES as a function of the numerical parameters (e.g., grid size and particle number density).

The LES/FDF/ISAT approach is able to predict the compositional structure of the flame once realistic combustion chemistry is employed. In the simulation, the OH mass fraction, Y_{OH} , is used as a marker of the flame (Cabra *et al.* 2002). Figure 3, which shows one instantaneous filtered OH contour from the particle method, provides a simple visual demonstration of the flame structure. The cold fuel and hot vitiated products mix together with the development of mixing layer and the flame occurs some distance downstream. The reactants must be mixed at the molecular level for reactions to occur. Free-stream fluid that has been entrained into the mixing layer, but remains unmixed, will not undergo reaction as shown in the figure.

7. ISAT performance

One full LES/FDF/ISAT simulation (denoted as CASE1) with constant non-dimensional time step $dt^+ = 0.06$ is performed for 6000 time steps (about two flow-through times). In this simulation, the nominal particle number density of 30 particles per cell is used.

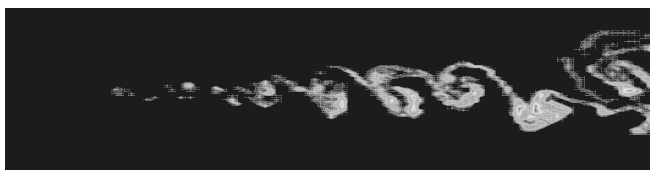


FIGURE 3. The instantaneous filtered OH contour as predicted by the LES/FDF/ISAT approach via FDF.

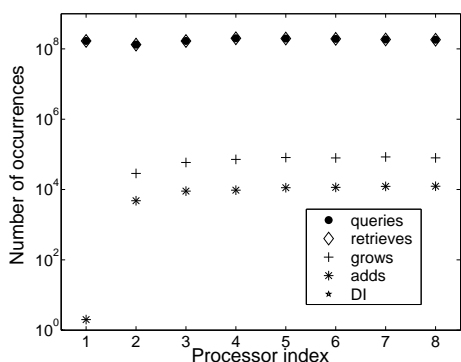


FIGURE 4. Number of occurrences of different events in ISAT (serial) for each processor of CASE1.

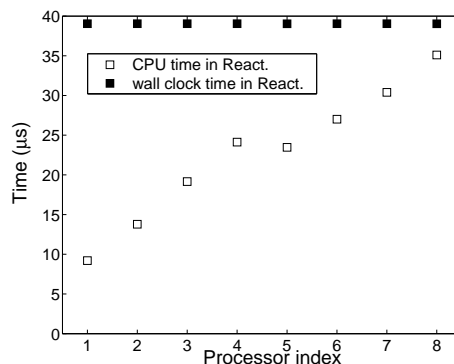


FIGURE 5. The CPU time and wall clock time in reaction fractional step (in microseconds per particle step) for each processor of CASE1.

Each processor has one ISAT table with the maximum assigned storage 300 Mbytes and the ISAT error tolerance used is $\epsilon_{tol} = 1 \times 10^{-5}$.

Figure 4 shows the number of occurrences for different events in ISAT (serial) for each processor. As may be seen from this figure, the number of reaction fractional steps (number of queries) performed is about 2×10^8 for each processor; the cheap retrieves are dominant and there are no direct integrations in the simulation (because the tables are not full).

In the parallel simulations of turbulent combustion, one computational difficulty is how to ensure good load balancing, especially for combustion chemistry. Figure 5 shows the CPU time and wall clock time (per particle step) in the reaction fractional steps for each processor. As may be seen from this figure, even for this simple geometry and chemistry case, the load balancing is not good. The CPU time spent by processor 7 is almost 4 times the CPU time spent by processor 1. And processor 1 has a significant amount of idle time. This is due to the following fact: in the active flame region there are strong chemical reactions and so the reaction fractional step is usually computationally expensive; in the computational domain of processor 1 (adjacent to the inlet), there is no flame at all; whereas for processor 7 (adjacent to the outlet), there is significant flame activity (see Fig. 3).

The load balancing issue for combustion chemistry motivates the development of parallel ISAT strategies. The objective of parallel ISAT strategies is to minimize the wall clock time by trying to achieve good load balancing for the combustion chemistry (i.e., for the reaction fractional step). However, the optimal strategy, which minimizes the wall clock time for the combustion chemistry, may not give the best load balancing. For the two parallel ISAT strategies studied, the uniform random distribution (URAN) method

guarantees good load balancing but requires a large amount of message passing, whereas the local level distribution (LOCLEV) method tries to minimize message passing. A further strategy which can be used in combination with both URAN and LOCLEV is called “Quick Try”. This is done by looping over all the particle compositions on each processor and trying to retrieve by using the local ISAT table before performing the parallel ISAT strategies. Then the parallel ISAT strategies are applied only to those particle compositions whose queries cannot be resolved by retrieves from the local ISAT table. In this study, Quick Try is combined with the parallel ISAT strategies yielding five different modes of ISAT: serial, URAN, URAN-Quick, LOCLEV and LOCLEV-Quick. These parallel strategies are implemented using the *x2f_mpi* software developed by Pope & Lantz (Pope & Lantz 2004).

The success of the parallel ISAT strategies depends on three key time parameters: the average CPU time per retrieve (t_{ret}); the average message passing time per particle composition (t_{MPI}); and the average CPU time per direct integration (t_{DI}). The time t_{ret} increases with n_ϕ^2 ; t_{MPI} increases linearly with n_ϕ ; and t_{DI} increases at least with n_ϕ^3 . Generally, t_{ret} is much smaller than t_{DI} ; and for a combustion process with large n_ϕ , t_{MPI} is smaller than both t_{ret} and t_{DI} . For a particular simulation, if t_{MPI} is greater than both t_{ret} and t_{DI} , then parallel ISAT strategies have no advantages over serial ISAT. (Even though parallel ISAT strategies may achieve better load balancing, the wall clock time for combustion chemistry is larger compared with serial ISAT. As far as wall clock time is concerned, for this case serial ISAT is optimal.) If t_{MPI} is greater than t_{ret} but smaller than t_{DI} , parallel ISAT strategies have no advantages over serial ISAT if the cheap retrieves are dominant and there are no direct integrations in the simulation; however the performance (both for load balancing and wall clock time) of parallel ISAT strategies is better than serial ISAT if there is a significant fraction of direct integrations in the simulation.

For the simulation of the mixing layer with H_2 detailed mechanism, these three key time parameters are listed in the Table 1. As may be seen from the table, the message passing time per particle step is of the same order as the retrieve time (a little more expensive) and both the retrieve time and message passing time are two order of magnitude smaller than the direct integration time. Under these circumstances, for the above simulation (CASE1) where the cheap retrieve is dominant and there are no direct integrations, we observed that serial ISAT is optimal even though the load balancing is not good. For this simulation with simple H_2 chemistry, by using serial ISAT, a speed-up factor of about 300 is obtained for the combustion chemistry compared to using direct integration for the reaction fractional step. The performance of URAN-Quick and LOCLEV-Quick modes is similar to serial ISAT because about 99.5% of particle compositions can be retrieved by Quick Try. Even though the URAN mode achieves the best load balancing, the wall clock time for the combustion chemistry using the URAN mode is about twice the wall clock time using serial ISAT.

In order to study and compare the different ISAT strategies when there is a significant fraction of direct integrations, another simulation (denoted as CASE2) is carried out. In this simulation, all the settings are the same as CASE1 except that the assigned ISAT table storage is 20 Mbytes, the ISAT error tolerance is $\epsilon = 5 \times 10^{-6}$ and the simulation is performed for 4000 time steps. As may be seen from Fig. 6 a, there is a significant number of direct integrations (about 1% for some processors) in the simulation. Figure 6 b-f show the CPU time and wall clock time in combustion chemistry, and the CPU time in Quick Try for each processor for different ISAT strategies. As may be seen from the figure, all

Direct integration (t_{DI})	retrieve (t_{ret})	message passing (t_{MPI})
$\sim 6000\mu s$	$\sim 15\mu s$	$\sim 20\mu s$

TABLE 1. Time (in microseconds per particle step) for DI, retrieve and message passing.

the parallel ISAT strategies have advantages over serial ISAT both for load balancing and wall clock time. For this particular case, the URAN-Quick is best (in that it gives the smallest wall clock time) whereas URAN gives the best load balancing. For the URAN-Quick and LOCLEV-Quick modes, even though about 98% percents of particle compositions are retrieved using Quick Try, the CPU time of Quick Try accounts for only about 30% of the total CPU time in the reaction fractional step. The effect of quick try depends on the different parallel ISAT strategy. For the case simulated, URAN-Quick gives smaller wall clock time than URAN whereas LOCLEV-Quick gives larger wall clock time than LOCLEV.

8. LES/FDF performance

Besides studying the different ISAT strategies for the combustion chemistry, the computational performance of the LES/FDF methodology in the mixing layer simulation is also analyzed. Figure 7 shows the CPU time and wall clock time in the LES part, in the particle part excluding reaction part and in the reaction fractional part for the simulation CASE1. As may be seen from the figure, the LES solver accounts for less than 25% of the wall clock time, and most time is spent in the particle part. Besides the load balancing issue for the combustion chemistry part, the load balancing of the particle part excluding reaction is also not good, and the fist processor takes much more CPU time than other processors. This clearly is a topic for further investigation. Also observe that the LES wall clock time is several times the LES CPU time. The particle wall time excluding the reaction is greater than the wall time in the reaction fractional steps. Compared to the LES (without FDF), the relative cost of LES/FDF (without reaction) is about 2.8, and the relative cost of LES/FDF/ISAT is about 4.3.

9. Conclusion

The LES/FDF/ISAT capability for the numerical simulations of turbulent combustion with realistic chemistry is developed by incorporating ISAT into the Stanford structured LES code with a Lagrangian Monte Carlo implementation of the composition FDF method. The numerical simulation of a two-dimensional spatially-developing mixing layer with a 9-species detailed hydrogen mechanism is performed to examine computational issues arising in the LES/FDF/ISAT methodology. It is shown that there is good consistency between the filtered mixture fractions obtained both from the FDF and LES solvers.

Both the serial ISAT and two different parallel ISAT strategies are studied and compared. For the mixing layer with the simple H_2 chemistry, when the cheap retrieves are dominant and there are no direct integrations in the simulation (such as CASE1), se-

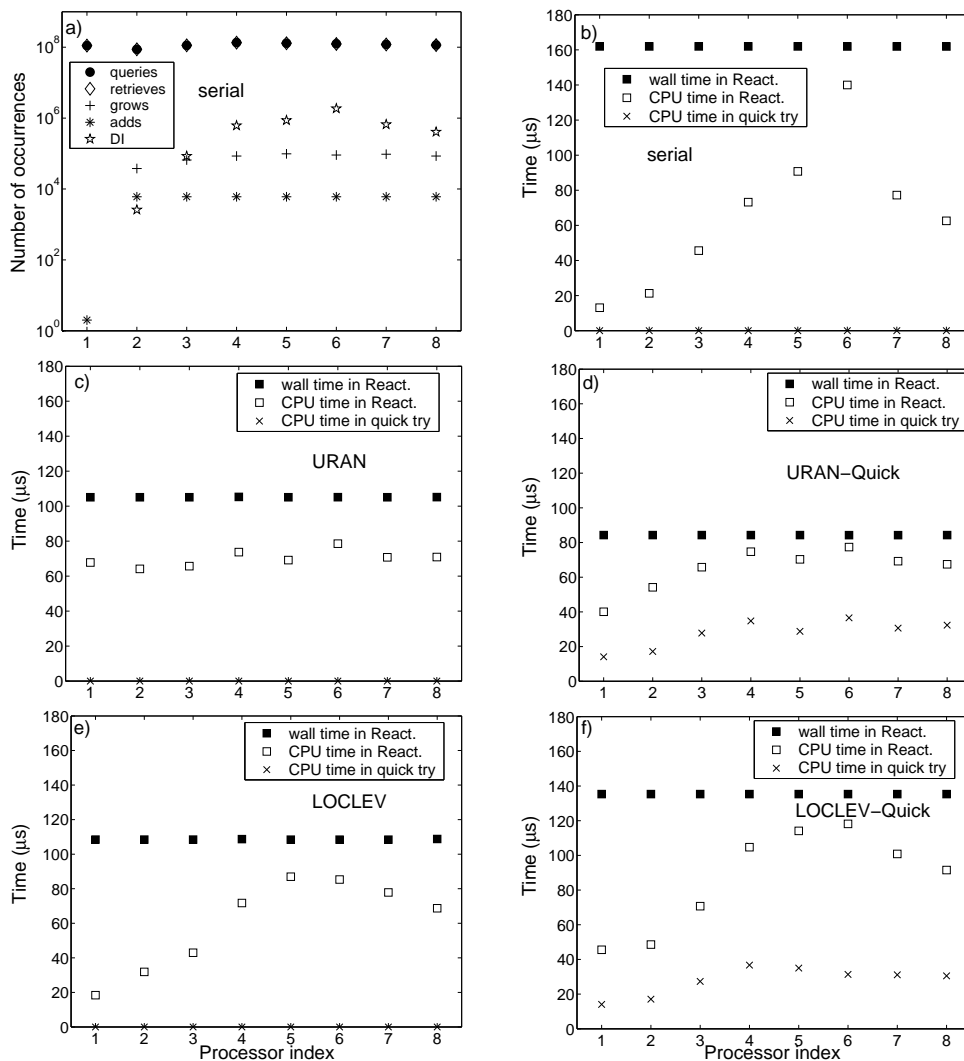


FIGURE 6. (a) Number of occurrences for different events in ISAT (serial) for each processor. (b)-(f) The CPU time and wall clock time in reaction fractional step, and the CPU time in the quick try (in microseconds per particle step) for each processor of CASE2.

rial ISAT gives a smallest wall clock time for the combustion chemistry and therefore is optimal, even though the parallel ISAT strategies may achieve better load balancing. For the simulation CASE1 with serial ISAT, a speed-up factor of about 300 is obtained for the combustion chemistry compared to using direct integration for the reaction fractional step. When there is a significant fraction of direct integrations in the simulation (such as CASE2), all the parallel ISAT strategies have advantages over serial ISAT both for load balancing and in terms of wall clock time. The effect of quick try depends on the different parallel ISAT strategy. For the simulation CASE2, URAN-Quick gives a smaller wall clock time than URAN whereas LOCLEV-Quick gives a larger wall clock time than LOCLEV. For the simulation CASE2, the URAN-Quick is optimal (in that it

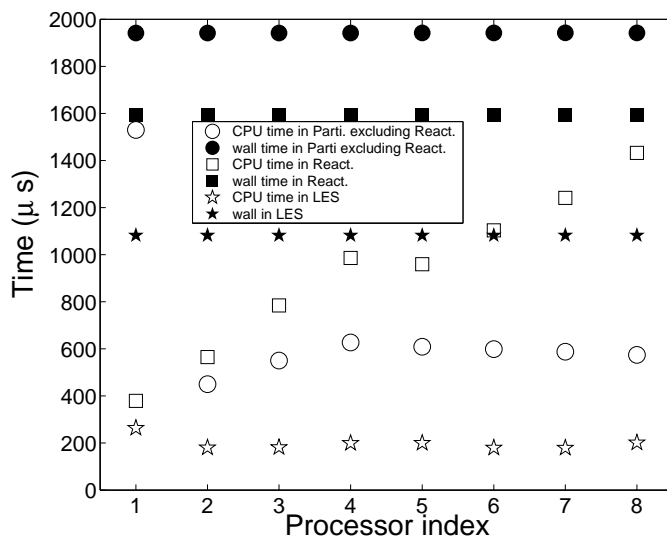


FIGURE 7. The CPU time and wall clock time in the LES solver, in the Monte Carlo particle part (excluding the reaction fractional step) and in the reaction fractional step (in microseconds per cell per time step) of CASE1.

gives the smallest wall clock time) whereas URAN gives the best load balancing. For the simulation CASE1, compared to the LES (without FDF), the relative cost of LES/FDF (without reaction) is about 2.8, and the relative cost of LES/FDF/ISAT is about 4.3.

In the future work, for the LES/FDF, the coupling (such as density) between the LES and FDF should be implemented and more quantitative testing of accuracy and efficiency would be performed. For the ISAT, the quantitative study of the performance of different strategies for different chemical mechanism and in different circumstance would be performed.

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REFERENCES

- CABRA, R., MYRVOLD, T., CHEN, J. Y., DIBBLE, R. W., KARPETIS, A. N. & BARLOW, R. S. 2002 Simultaneous laser Raman-Rayleigh-Lif measurements and numerical modeling results of a lifted turbulent H-2/N-2 jet flame in a vitiated coflow. *Proc. Combust. Inst.* **29**, 1881-1888
- CHA, C. M. & TROUILLET, P. 2003 A subgrid-scale mixing model for large-eddy simulations of turbulent reacting flows using the filtered density function. *Phys. Fluids* **15**, 1496-1504.
- COLUCCI, P. J., JABERI, F. A., GIVI, P. & POPE, S. B. 1998 Filtered density function for large eddy simulation of turbulent reacting flows. *Phys. Fluids* **10**, 499-515.

- DOPAZO, C. & O'BRIEN, E. E. 1974 Approach to autoignition of a turbulent mixture. *Acta Astronaut.* **1**, 1239-1266.
- GAO, F. & O'BRIEN, E. E. 1993 A large-eddy simulation scheme for turbulent reacting flows. *Phys. Fluids A* **5**, 1282-1284.
- GIVI, P. 2003 Subgrid scale modeling in turbulent combustion: A review. *AIAA Paper*, 2003-5081.
- JABERI, F. A., COLUCCI, P.J., JAMES, S., GIVI, P. & POPE, S. B. 1999 Filtered mass density function for large eddy simulation of turbulent reacting flows. *J. Fluid Mech.* **401**, 85-121.
- JAMES, S. & JABERI, F. A. 2000 Large scale simulations of two-dimensional nonpremixed methane jet flames. *Combust. Flame* **123**, 465-487.
- LI, J., ZHAO, Z., KAZAKOV, A. & DRYER, F. L. 2003 An updated comprehensive kinetic model for H_2 combustion. *Fall Technical Meeting of the Eastern States Section of the Combustion Institute, Penn State University, University Park, PA, October 26-29, 2003*.
- MOIN, P., SQUIRES, K., CABOT, W. & LEE, S. 1991 A dynamic subgrid-scale model for compressible turbulence and scalar transport. *Physics of Fluids A* **3**, 2746-2757.
- PIERCE, C. D. 2001 Progress-variable approach for large-eddy simulation of turbulent combustion. PhD thesis, Stanford University.
- PIERCE, C. D. & MOIN, P. 2004 Progress-variable approach for large-eddy simulation of non-premixed turbulent combustion. *J. Fluid Mech.* **504**, 73-97.
- POPE, S. B. 1985 PDF methods for turbulent reactive flows. *Prog. Energy Combust. Sci.* **11**, 119-192.
- POPE, S. B. 1990 Computations of turbulent combustion: Progress and challenges. *Proc. Combust. Inst.* **23**, 591-612.
- POPE, S. B. 1997 Computationally efficient implementation of combustion chemistry using *in situ* adaptive tabulation. *Combust. Theo. Modelling* **1**, 41-63.
- POPE, S. B. & LANTZ, S. R. 2004 *x2f-mpi* Software for the efficient load distribution of function evaluations in a multi-processor MPI environment. (in preparation)
- RAMAN, V., PITSCH, H. & FOX, R. O. 2003a Quadrature moments method for the simulation of turbulent reactive flows. in: *CTR Annual Research Briefs, Center For Turbulence Research*, 261-275.
- RAMAN, V., FOX, R. O., HARVEY, A. D. & WEST, D. H. 2003b Effect of feed-stream configuration on gas-phase chlorination reactor performance. *Industrial and Engineering Chemistry Research*, **42**, 2544-2557.
- RAMAN, V., PITSCH, H. & FOX, R. O. 2004a LES-transported FDF simulations of a bluff-body stabilized flame. *TNF7 Workshop Proceedings*, 56-57.
- RAMAN, V., PITSCH, H. & FOX, R. O. 2004b Hybrid large-eddy simulation/lagrangian filtered density function approach for simulating turbulent combustion. (submitted)
- SHEIKHI, M. R. H., DROZDA, T. G., GIVI, P., JABERI, F.A. & POPE, S. B. 2004 Large eddy simulation of a turbulent nonpremixed piloted methane jet flame (Sandia flame D). *Proc. Combust. Inst.* **30**, in press.
- VILLERMAUX, J. & DEVILLON, J. C. 1972 in: *Proc. 2nd Int. Symp. on Chemical Reaction Engineering*. Elsevier, New York.
- ZHOU, X. Y. & PEREIRA, J. C. F. 2000 Large eddy simulation (2D) of a reacting plane mixing layer using filtered density function. *Flow, Turbulence and Combustion* **64**, 279-300.