

Large-Scale Parallel Simulations of Turbulent Combustion using Combined Dimension Reduction and Tabulation of Chemistry

Varun Hiremath^{a,*}, Steven R. Lantz^b, Haifeng Wang^a, Stephen B. Pope^a

^a*Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY 14853, USA*

^b*Center for Advanced Computing, Cornell University, Ithaca, NY 14853, USA*

Abstract

Simulations of turbulent reacting flows with chemistry represented using detailed kinetic model involving a large number of species and reactions are computationally expensive. Here we present a combined dimension reduction and tabulation strategy for implementing chemistry in large scale parallel *Large-Eddy Simulation* (LES)/*Probability Density Function* (PDF) computations of turbulent reacting flows. In this approach, the dimension reduction is performed using the *Rate Controlled Constrained-Equilibrium* (RCCE) method, and tabulation of the reduced space is performed using the *In Situ Adaptive Tabulation* (ISAT) algorithm. In addition, we use *x2f-mpi* – a Fortran library for parallel vector-valued function evaluation (used with ISAT in this context) – to efficiently redistribute the chemistry workload among the participating cores in parallel LES/PDF computations to reduce the overall wall clock time of the simulation. We test three parallel strategies for redistributing the chemistry workload, namely (a) PLP, purely local processing; (b) URAN, the uniform random distribution of chemistry computations among all cores following an early stage of PLP; and (c) P-URAN, a Partitioned URAN strategy that redistributes the workload within partitions or subsets of the cores. To demonstrate the efficiency of this combined approach, we perform parallel LES/PDF computations (on 1,024 cores) of the Sandia Flame D with chemistry represented using a 38-species C_1 - C_4

*Corresponding author

Email address: `vh63@cornell.edu` (Varun Hiremath)

Report Documentation Page		Form Approved OMB No. 0704-0188
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1. REPORT DATE 22 MAY 2012	2. REPORT TYPE	3. DATES COVERED 00-00-2012 to 00-00-2012
4. TITLE AND SUBTITLE Large-Scale Parallel Simulations of Turbulent Combustion using Combined Dimension Reduction and Tabulation of Chemistry		5a. CONTRACT NUMBER
		5b. GRANT NUMBER
		5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER	
	5e. TASK NUMBER	
	5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Cornell University, Sibley School of Mechanical and Aerospace Engineering, Ithaca, NY, 14853		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited		
13. SUPPLEMENTARY NOTES		
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15. SUBJECT TERMS		

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Same as Report (SAR)	18. NUMBER OF PAGES 22	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

skeletal mechanism. We show that relative to using ISAT alone with the 38-species full representation, the combined ISAT/RCCE approach with 10 represented species (i) predicts time-averaged mean and standard deviation statistics with a normalized root-mean-square difference of less than 3% (30 K) in temperature, less than 2% (0.02 kg/m³) in density, less than 2.5% in mass fraction of major species, and less than 8% in mass fraction of minor species of interest; and (ii) reduces the simulation wall clock time by over 40% with the P-URAN strategy.

Keywords: Large-eddy simulation, Probability density function method, In situ adaptive tabulation, Rate controlled constrained-equilibrium, Parallel function evaluation

Manuscript Word Count

Item	Method	Words
Main text	(440 lines) $\times$ (10 words/line)	4400
References	(41 refs) $\times$ (1.5 lines/ref) $\times$ (8 words/line)	492
Captions	(20 lines) $\times$ (10 words/line)	200
Tables	(14 lines) $\times$ (5 words/line)	70
Figures*	(2 large) $\times$ (400 words) + (1 small) $\times$ (200 words)	1000
Total		6162

* smaller figures will be provided if there is space restriction.

1. Introduction

Detailed chemical mechanisms of hydrocarbon fuels may involve hundreds or thousands of species and thousands of reactions [1, 2]. Incorporating directly such detailed chemistry in the combustion flow calculations is computationally prohibitive, even using distributed parallel computing. The current efforts aimed at reducing the computational cost of representing chemistry can be placed under three main categories: (1) *mechanism reduction*, the generation of reaction mechanisms involving fewer species and reactions [3, 4, 5]; (2) *dimension reduction*, the representation of chemistry using a reduced number of variables [6, 7, 8, 9]; and (3) *tabulation*, the use of storage-retrieval methods to reduce significantly the cost of expensive evaluations of the reaction mappings involving ODE integrations [10, 11, 12, 13].

13 Combined methodologies have also been developed to use reduced reaction
14 mechanisms or dimension reduction methods in conjunction with tabulation
15 [14, 15, 16, 17].

16 Since most of the modern day reactive flow simulations are performed
17 in parallel on multiple cores using distributed computing, in addition to the
18 aforementioned techniques, strategies are needed to efficiently distribute the
19 chemistry workload among the participating cores to reduce the overall wall
20 clock time of the simulation [18, 19, 20, 21]. We recently demonstrated
21 scalable parallel strategies implemented using *x2f-mpi* for the efficient redis-
22 tribution of chemistry workload in large scale parallel Large-Eddy Simulation
23 (LES)/Probability Density Function (PDF) computations [22].

24 In this paper we further extend our LES/PDF solver with the capa-
25 bility of representing chemistry using our combined dimension reduction
26 and tabulation approach [15]. In this approach, the dimension reduction
27 is performed using the Rate Controlled Constrained-Equilibrium (RCCE)
28 [6, 23, 24] method followed by tabulation using the *In Situ* Adaptive Tab-
29 ulation (ISAT) [10, 11] algorithm. In [15], we tested our combined dimen-
30 sion reduction and tabulation approach using the partially-stirred reactor for
31 methane and ethylene chemistry, and the main conclusions drawn from this
32 work are that the ISAT/RCCE approach

- 33 • yields the same level of accuracy as other reduced (based on the Quasi-
34 Steady State Assumption, QSSA) or skeletal mechanisms with rela-
35 tively fewer represented species;
- 36 • yields significant speedup relative to using ISAT alone with the detailed
37 mechanism.

38 Here, for the first time, the ISAT/RCCE approach is being demonstrated
39 in the context of full-scale LES/PDF simulations of turbulent reacting flows
40 using realistic chemistry. In this study, the accuracy and efficiency of this
41 combined approach is demonstrated by performing full-scale LES/PDF sim-
42 ulation of the Sandia Flame D [25].

43 The outline of the remainder of the paper is as follows: in Section 2 we
44 describe our combined LES/PDF solver; in Section 3 we describe the com-
45 bined dimension reduction and tabulation strategy; in Section 4 we briefly
46 describe the parallel strategies implemented using *x2f-mpi* for redistributing
47 the chemistry workload in large scale LES/PDF computations; in Section
48 5 we present computational details for simulating the Sandia Flame D; in

49 Section 6 we present simulation results; and finally in Section 7 we state our
50 conclusions.

51 2. Combined LES/PDF Solver

52 In this study we use a combined LES/PDF solver developed at Cornell
53 as described in more detail in [22, 26]. Below we mention some of the key
54 aspects of this solver.

55 2.1. LES Solver

56 The LES solver is based on the Stanford LES code [27, 28]. The solver
57 uses structured non-uniform grids; supports cylindrical coordinate system; is
58 second-order accurate in space and time; and is parallelized (using MPI) by
59 domain decomposition in two dimensions.

60 2.2. PDF Solver

61 The PDF solver, *HPDF* [26], has second-order accuracy in space and
62 time; supports Cartesian and cylindrical coordinate systems; is parallelized
63 (using MPI) by domain decomposition in two dimensions; and has a general
64 interface to facilitate coupling with existing LES (or RANS) solvers.

65 In the PDF approach, the thermochemical composition of the fluid within
66 the solution domain is represented by a large number of particles. The HPDF
67 solver has three main components

- 68 1. *transport*: to account for the change in *position* of a particle due to
69 advection in the physical space (including a random-walk component to
70 represent the effects of subgrid-scale turbulent advection and molecular
71 diffusion);
- 72 2. *mixing*: to account for change in the *composition* of a particle due to
73 mixing with neighboring particles (which models the effects of molecu-
74 lar mixing); and
- 75 3. *reaction*: to account for change in the *composition* of a particle due to
76 chemical reaction.

77 These components are implemented in *fractional steps* using splitting schemes
78 [29]. In this study, to simulate the Sandia Flame D, we use the first-order
79 TMR splitting scheme (which is found to perform as well as the second-order
80 splitting scheme for jet flames [26]). The TMR splitting scheme denotes tak-
81 ing fractional steps of *transport*, $\mathbb{T}$; *mixing*, $\mathbb{M}$; and *reaction*, $\mathbb{R}$ in this order

on each time-step. The Kloeden and Platen (KP) [30] stochastic differential equation (SDE) scheme is used to integrate the *transport* equations; and the *mixing* is represented using the modified Curl [31] mixing model. The *reaction* fractional step is implemented using the combined dimension reduction and tabulation approach which we will discuss in more detail in the later sections.

2.3. Domain Decomposition

The LES computations are performed on a structured non-uniform grid in the cylindrical coordinate system. We denote the grid used for LES computations by $N_x \times N_r \times N_\theta$ (in the axial, radial and azimuthal directions). In performing parallel LES/PDF computations (using the combined LES/HPDF solver) on N_c cores, the computational domain is decomposed into N_c sub-domains and each core performs the computations of one sub-domain. The domain decomposition is done in the first two principal directions x and r , and is denoted by $D_x \times D_r$, where $D_x D_r = N_c$. For instance, in this study we perform LES/PDF simulations of the Sandia Flame D using a non-uniform LES grid of size $N_x = 192$, $N_r = 192$, $N_\theta = 96$ on $N_c = 1,024$ cores using a domain decomposition with $D_x = 64$ and $D_r = 16$.

3. Combined Dimension Reduction and Tabulation

In this section we briefly describe the combined dimension reduction and tabulation approach used for representing chemistry using ISAT/RCCE. More detailed description can be found in [15].

3.1. Particle Representation

We consider a reacting gas-phase mixture consisting of n_s chemical species, composed of n_e elements. We consider an isobaric system with a fixed specified pressure p , and so the thermochemical state of the mixture (at a given position and time) is completely characterized by the mixture enthalpy h , and the n_s -vector $\mathbf{z}$ of specific moles of the species.

In the *reaction fractional step*, a particle's chemical composition $\mathbf{z}$ evolves (at constant enthalpy h) in time according to the following set of n_s coupled ordinary differential equations (ODEs)

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{S}(\mathbf{z}(t)), \quad (1)$$

113 where $\mathbf{S}$ is the n_s -vector of chemical production rates determined by the
 114 chemical mechanism used to represent the chemistry.

115 Given a reaction fractional time step Δt , the *reaction mapping*, $\mathbf{z}(\Delta t)$, is
 116 defined to be the solution to Eqn.1 after time Δt starting from the initial
 117 composition $\mathbf{z}(0)$. The reaction mapping obtained by directly integrating the
 118 set of ODEs given by Eqn.1 is referred to as a *direct evaluation* (DE). We
 119 use DDASAC [32] for performing ODE integration.

120 Owing to the large cost of direct evaluation of reaction mappings involv-
 121 ing large numbers of species, we use a combined dimension reduction (us-
 122 ing RCCE) and tabulation (using ISAT) strategy for representing chemistry.
 123 This combined methodology can be applied to chemical systems involving a
 124 large number of species (100 to 1000) by first applying the dimension reduc-
 125 tion to reduce the dimensionality of the system to say around 20 (depending
 126 on the level of accuracy needed) and then using ISAT to tabulate the reaction
 127 mappings in the reduced dimension.

128 3.2. Dimension Reduction

129 In this section we briefly describe the procedure followed for dimension
 130 reduction in our implementation of the RCCE method; a more detailed de-
 131 scription can be found in [14, 15].

132 In our implementation of RCCE, to perform the dimension reduction we
 133 specify a set of n_{rs} *represented* (constrained) species selected from the full set
 134 of n_s species. Consequently, we have $n_{us} = n_s - n_{rs}$ *unrepresented* species.

135 The selection of good represented species is crucial for the accuracy of
 136 the RCCE dimension reduction method. We have devised an automated
 137 Greedy Algorithm with Local Improvement (GALI) [14, 15] to select good
 138 represented species based on a specified measure of dimension reduction error.
 139 The greedy algorithm selects represented species in stages one-by-one which
 140 minimizes the specified measure of dimension reduction error [14].

141 The *reduced representation* of the species composition is denoted by $\mathbf{r} \equiv$
 142 $\{\mathbf{z}^r, \mathbf{z}^{u,e}\}$, where $\mathbf{z}^r$ is an n_{rs} -vector of specific moles of the represented species;
 143 and $\mathbf{z}^{u,e}$ is an n_e -vector of specific moles of the elements in the unrepresented
 144 species (for atom conservation). Thus, $\mathbf{r}$ is a vector of length $n_r = n_{rs} + n_e$,
 145 and the dimension of the system is reduced from n_s to n_r . At any time t ,
 146 the *reduced representation*, $\mathbf{r}(t)$, is related to the *full representation*, $\mathbf{z}(t)$, by

$$\mathbf{r}(t) = \mathbf{B}^T \mathbf{z}(t), \quad (2)$$

147 where $\mathbf{B}$ is a constant $n_s \times n_r$ matrix which can be determined for a specified
 148 set of represented species. (In general, the reduced representation in RCCE
 149 can be a linear or non-linear function of the full representation [33].)

150 In the HPDF solver, with dimension reduction, the particles carry only
 151 the reduced representation $\{\mathbf{r}, h\}$. Given the reduced representation $\mathbf{r}$, the
 152 temperature T and density ρ are approximated using the method described
 153 in the Appendix of [15]. Later in the Results (Section 6.1) we show that this
 154 approximation method yields values of temperature and density that match
 155 closely with those obtained with the full representation $\mathbf{z}$.

156 Given the reduced representation at the beginning of the reaction frac-
 157 tional step $\mathbf{r}(0)$, and the reaction fractional time step Δt , the *reduced reaction*
 158 *mapping* $\mathbf{r}(\Delta t)$ (at constant enthalpy) is computed using the following steps:

- 159 1. *species reconstruction*: given $\mathbf{r}(0)$, we compute the constrained-equilibrium
 160 composition at constant enthalpy, $\mathbf{z}^{CE}(\mathbf{r}(0))$, using CEQ [34];
- 161 2. *reaction mapping*: starting from $\mathbf{z}^{CE}(\mathbf{r}(0))$, we solve the full system of
 162 n_s ODEs Eqn.1 to obtain the reaction mapping, $\mathbf{z}(\Delta t)$;
- 163 3. *reduction*: we obtain the *reduced reaction mapping* as, $\mathbf{r}(\Delta t) = \mathbf{B}^T \mathbf{z}(\Delta t)$.

164 The above steps of course make the computation of the reaction mapping
 165 even more expensive than directly solving the full set of ODEs Eqn.1, due
 166 to the additional species reconstruction and reduction steps. However, when
 167 ISAT is used in conjunction with dimension reduction, the computational
 168 cost is reduced significantly as explained in the next section.

169 A more efficient way of obtaining the reduced reaction mapping, $\mathbf{r}(\Delta t)$,
 170 is to directly solve a reduced system of n_r ODEs for the constraints, $\mathbf{r}$, or for
 171 the constraint-potentials (as is done in the classical RCCE approach [35, 36]).
 172 We are currently working on implementing this method which should give
 173 a further improvement in performance. Nevertheless, even with our current
 174 implementation of RCCE, we achieve significant reduction in computational
 175 cost relative to the detailed chemistry calculation as shown in this work.

176 3.3. Tabulation

177 We use *in situ* adaptive tabulation (ISAT) [10] for tabulating the reac-
 178 tion mappings. The ISAT algorithm has been successfully applied in many
 179 combustion chemistry calculations involving up to $n_s \leq 50$ species [11, 15].
 180 However, with chemistry involving more than 50 species, the direct use of
 181 ISAT may not be very efficient, due to the large table size and search times
 182 [15].

Hence, for chemistry involving more than say $n_s \geq 30$ species, we use the RCCE dimension reduction method to represent the chemistry using a reduced representation involving fewer n_r variables. Note, for very large mechanisms involving thousands of species, the direct use of RCCE/GALI may still result in $n_r \gg 30$ to achieve an acceptable level of accuracy. In such cases it will be more efficient to use ISAT/RCCE with a skeletal mechanism (based on the detailed mechanism) involving hundreds of species.

We use ISAT to tabulate the *reduced reaction mapping* in the reduced dimension n_r , which reduces significantly the overall computational cost because

1. the exact reduced reaction mapping is computed (using the steps listed in the previous section) only for a small fraction of particles (typically less than 1%); and for the majority of the particles a linear approximation to the reduced reaction mapping is obtained using the tabulated data;
2. since the tabulation is performed in a reduced dimension, n_r , the ISAT table size is reduced, which in turn reduces the table search and retrieve times; and
3. since the particle compositions are also stored in a reduced dimension, fetching particles from the memory is faster.

Consequently, the combined dimension reduction and tabulation approach using ISAT/RCCE is found to give an additional speedup by a factor of $\mathcal{O}(10)$ relative to using ISAT alone with the full representation for tests performed using the 111-species C_1 - C_4 USC Mech II detailed mechanism [15]. A more detailed description of our combined dimension reduction and tabulation approach is provided in [15].

4. Parallel Strategies for Implementing Chemistry

In performing parallel LES/PDF computations on multiple cores using our LES/HPDF solver with chemistry represented using the combined dimension reduction and tabulation approach, each core has its own ISAT table for tabulating the chemistry. On the reaction fractional step, the reaction mappings for all the particles in the computational domain need to be evaluated. However, the chemical reactivity is in general not uniform across the entire domain. For example, in simulation of jet flames, the sub-domains in the flame front are chemically more reactive than sub-domains in the outer

218 coflow/air. Thus, a direct call to ISAT on each core at the reaction fractional
 219 step can create *load imbalance* among the cores, leading to increase in the
 220 overall simulation wall clock time. Hence, at the reaction fractional step, we
 221 use parallel strategies implemented using *x2f_mpi* to redistribute the parti-
 222 cles among the participating cores for reaction mapping evaluation, thereby
 223 achieving a better load balance and reducing the overall simulation wall clock
 224 time.

225 In [22], we presented three parallel strategies, denoted by PLP, URAN
 226 and P-URAN, for redistributing the chemistry workload. We give a brief
 227 description of these strategies below.

228 1. Purely Local Processing (PLP):

229 In this strategy, the reaction mapping of all the particles on a core
 230 is evaluated using the local ISAT table without any message passing or
 231 load redistribution. This in some sense is the same as invoking ISAT
 232 directly from HPDF on each core without using the *x2f_mpi* interface.
 233 This strategy thus leads to significant load imbalance.

234 2. Uniform Random (URAN):

235 This strategy is the extreme opposite of the PLP strategy and aims
 236 at achieving statistically ideal load balancing by evenly distributing
 237 the chemistry workload among all the participating cores. The strategy
 238 involves one initial step of PLP to initialize the local ISAT tables. In the
 239 subsequent steps, on each core, first an attempt is made to retrieve the
 240 reaction mapping of particles from the local ISAT table (also referred to
 241 as a “quick try”). Following this, there is a uniform random distribution
 242 of all the unresolved particles (for which “quick try” failed) to all the
 243 cores. This strategy thus ensures that the workload is evenly balanced
 244 over all the cores, however, it also results in a large amount of all-to-all
 245 message passing.

246 3. Partitioned Uniform Random (P-URAN):

247 This strategy aims at achieving a balance between communication
 248 cost and load imbalance by using the PLP and URAN strategies over
 249 smaller partitions of cores. The P-URAN strategy works in two stages:
 250 in stage 1, for a specified duration of time τ (hours) the PLP strategy is
 251 used to resolve particles; then in stage 2, for the remainder of the time,
 252 the participating cores are partitioned into smaller groups of κ cores,
 253 and within each partition the URAN strategy is used to uniformly
 254 distribute the chemistry workload among the cores in that partition.
 255 We use the notation P-URAN[τ, κ] to describe the P-URAN strategy.

256 In [22], based on LES/PDF simulations of Sandia Flame D using ISAT
 257 alone we showed that among the aforementioned three strategies, the P-
 258 URAN strategy yields the lowest wall clock time. We also showed that the
 259 P-URAN strategy shows good scaling up to 9,000 cores. In this work we
 260 use these strategies in conjunction with combined dimension reduction and
 261 tabulation to compare their relative performance. Here we focus more on
 262 the gains achieved using the combined dimension reduction and tabulation
 263 approach and show that the simulation wall clock time can be further reduced
 264 using our combined ISAT/RCCE approach without losing too much accuracy.

265 5. LES/PDF Simulation of Sandia Flame D

266 To test the chemistry implementation we perform LES/PDF simulations
 267 of the Sandia Flame D.

268 5.1. Sandia Flame D

269 The Sandia Flame D is a piloted CH_4 /Air jet flame operating at a jet
 270 Reynolds number, $Re = 22,400$. All the details about this flame and the
 271 burner geometry can be found at [25]. Here we mention only some of the
 272 important aspects of this flame.

273 The jet fluid consists of 25% CH_4 and 75% air by volume. The jet flows
 274 in at 49.6 m/s velocity at 294 K temperature and 0.993 atm pressure. The
 275 jet diameter, $D = 7.2$ mm. The pilot is a lean (equivalence ratio, $\Phi = 0.77$)
 276 mixture of C_2H_2 , H_2 , air, CO_2 , and N_2 with the same nominal enthalpy and
 277 equilibrium composition as that of CH_4 /Air at this equivalence ratio. The
 278 pilot velocity is 11.4 m/s. The coflow is air flowing in at 0.9 m/s at 291 K
 279 and 0.993 atm.

280 5.2. Computational Details

281 We perform LES/PDF simulation of the Sandia Flame D using the cou-
 282 pled LES/HPDF solver. The simulation is performed in a cylindrical co-
 283 ordinate system. A computational domain of $80D \times 30D \times 2\pi$ is used in the
 284 axial, radial and azimuthal directions, respectively. A non-uniform struc-
 285 tured grid of size $192 \times 192 \times 96$ (in the axial, radial and azimuthal directions,
 286 respectively) is used for the LES solver. In the HPDF solver, the number of
 287 particles per LES cell (N_{pc}) used is $N_{pc} = 40$. With a total of $192 \times 192 \times 96$
 288 $\approx 3.5 \times 10^6$ LES cells, an overall 140×10^6 particles are used in the computa-
 289 tional domain. The simulations are performed on 1,024 cores using a domain

decomposition of 64×16 in the axial and radial directions, respectively. All the simulations are performed on the Texas Advanced Computing Center (TACC) Ranger cluster.

The chemistry is represented using the combined dimension reduction (using RCCE) and tabulation (using ISAT) approach with a C_1 - C_4 skeletal mechanism [37] involving $n_s = 38$ species composed of $n_e = 5$ elements. This mechanism is developed especially for ethylene combustion, but is also applicable to methane flames. In the future, we want to apply the methodology developed here to study ethylene combustion.

The RCCE dimension reduction is performed by specifying $n_{rs} = 10$ represented species (which is found to be a good number of represented species to achieve less than 2% dimension reduction error based on our previous tests with chemical mechanisms involving around 30 species [14, 15, 16, 17]), and so the reduced representation has a dimension $n_r = n_{rs} + n_e = 15$. This dimension reduction from $n_s = 38$ to $n_r = 15$ results in a 60% reduction in the storage needed for particle composition and an 84% reduction in the storage per ISAT table entry. In this preliminary study, we specify the represented species manually (to include the major species of interest for which statistics had already been collected in some of our previous LES/PDF simulations and for which experimental data is available). However, in future studies with bigger mechanisms we will use GALI [15] to select the represented species. In this work, we use the following 10 species as the represented species: CH_4 , O_2 , CO_2 , H_2O , CO , H_2 , OH , H , O and HO_2 .

A fixed ISAT error tolerance, $\epsilon_{tol} = 10^{-4}$, is used in this study. At this error tolerance, the ISAT *tabulation error* relative to direct evaluation (as defined in [15]) is found to be less than 3%. In addition, we specify a maximum ISAT table size of 1000 MB per core. In simulations with the 38-species full representation, some ISAT tables become completely filled. However in simulations with the combined ISAT/RCCE approach with 10 represented species, none of the ISAT tables have a size of more than 200 MB.

6. Results

In this section we compare the computational time and statistics of thermochemical quantities obtained using the combined dimension reduction and tabulation approach with 10 represented species relative to using tabulation alone with the 38-species C_1 - C_4 skeletal mechanism.

326 In order to make the comparisons, we perform separate LES/PDF sim-
 327 ulations of the Sandia Flame D on 1,024 cores with chemistry represented
 328 using the following two methods

- 329 1. ISAT: tabulation alone (no dimension reduction) with the 38-species
 330 full representation; and
- 331 2. ISAT/RCCE: combined dimension reduction and tabulation with a re-
 332 duced representation involving 10 represented species (specified in the
 333 previous section) and 5 elements.

334 In each case, we perform LES/PDF simulation to reach a statistically sta-
 335 tionary state. We then collect statistics for thermochemical quantities like
 336 temperature, density, and species mass fractions time-averaged over 10,000
 337 time steps. In addition, in each case we perform simulations for 2,000 time
 338 steps using the three parallel strategies PLP, URAN and P-URAN to com-
 339 pare their relative performance. These simulations start from the statistically
 340 stationary state with empty ISAT tables.

341 6.1. Comparison of Statistics

342 In this section we compare the radial profiles of mean and standard devi-
 343 ation statistics of thermochemical quantities obtained from the PDF particle
 344 data from the LES/PDF simulation using ISAT alone and using the combined
 345 ISAT/RCCE approach.

346 The radial statistics are azimuthally-averaged at each time step, and are
 347 also time-averaged over 10,000 time steps after reaching the statistically
 348 stationary state. For a quantity ξ , we denote the density-weighted mean
 349 statistics by $\langle \xi \rangle$, and the standard deviation by $\langle \xi'' \rangle$ which is defined as
 350 $\langle \xi'' \rangle \equiv \sqrt{\langle \xi^2 \rangle - \langle \xi \rangle^2}$.

351 In Fig.1 and Fig.2, we show respectively the radial profiles of mean and
 352 standard deviation of temperature T , density ρ , and mass fraction of species
 353 CH_4 , O_2 , CO_2 , H_2O , CO , H_2 , OH at axial locations $x/D = 15, 30, 45, 60$
 354 obtained from (i) an LES/PDF simulation using ISAT alone with the 38-
 355 species full representation; (ii) an LES/PDF simulation using ISAT/RCCE
 356 with 10 represented species; and (iii) experimentally measured statistics [25]
 357 (for reference).

358 We notice that the statistics obtained with ISAT/RCCE using 10 rep-
 359 resented species match very closely with the statistics obtained using ISAT
 360 alone with the 38-species full representation. To quantify the difference be-
 361 tween the statistics obtained using ISAT/RCCE and ISAT alone, for each

362 quantity ξ (mean or standard deviation), we compute the normalized root-
 363 mean-square difference (RMSD) denoted by $\epsilon(\xi)$ as follows

$$\epsilon(\xi) = \frac{[\xi^r - \xi^f]_{rms}}{\xi_{ref}}, \quad (3)$$

364 where ξ^r and ξ^f denote respectively the quantities obtained using the re-
 365 duced representation with ISAT/RCCE and the full representation with
 366 ISAT alone; and the operator $[\]_{rms}$ denotes the RMSD computed over all the
 367 radial locations at all the considered axial locations $x/D = 15, 30, 45, 60$.
 368 Here ξ_{ref} is a reference value used for normalization, which is taken to be
 369 1000 K for temperature and 1 kg/m³ for density. For the species mass frac-
 370 tions, we take ξ_{ref} to be the maximum value of the mean statistics obtained
 371 for that species, $\max(\langle \xi \rangle^f)$.

372 The reference value and the normalized RMSD computed using the above
 373 expression Eqn.3 for all the quantities of interest is summarized in Table 1.
 374 We notice that the normalized RMSD in the mean and standard deviation
 375 statistics is less than 3% (i.e. 30 K) for temperature; less than 2% (i.e. 0.02
 376 kg/m³) for density; less than 2.5% for species mass fractions of major species
 377 CH_4 , O_2 , CO_2 , H_2O ; and less than 8% for species mass fractions of minor
 378 species CO , H_2 , OH . In summary, these results show that the combined
 379 ISAT/RCCE approach shows good error control and the predicted statistics
 380 are well within acceptable level of accuracy (relative to using ISAT alone with
 381 the full representation) for most engineering applications. These results also
 382 show that the density and temperature approximation method used with the
 383 reduced representation in ISAT/RCCE [15] yields values that match closely
 384 with those obtained with the full representation. A more careful selection of
 385 represented species using GALI [15] should help further reduce the differences
 386 between the reduced and full descriptions.

387 The experimentally measured statistics are qualitatively well captured
 388 by the LES/PDF simulation, yet quantitatively we notice that some of the
 389 statistics differ by around 20%. The discrepancies between the LES/PDF
 390 simulation statistics and experimentally measured statistics can be attributed
 391 to (i) numerical and statistical errors in the simulation; (ii) experimental
 392 measurement errors; and (iii) errors in the chemical kinetic models. However,
 393 study of these errors is not the primary focus of this work. Similar level of
 394 agreement between the simulated and experimentally measured statistics is
 395 found in some of the previous studies of Sandia Flame D [38, 39, 40, 41].

6.2. Computational Performance

In this section we compare the wall clock time required to perform LES/PDF simulation of Sandia Flame D for 2,000 time steps using the combined ISAT/RCCE approach relative to using ISAT alone. In addition we compare the relative performance of the PLP, URAN and P-URAN parallel strategies. In each case, the LES/PDF simulation is started from a fixed statistically stationary state with empty ISAT tables. We measure a moderate ISAT *build time* (see [15]) of about 1 hour in these simulations, i.e., after 1 hour of simulation, most of the particles are resolved by ISAT retrieves.

In Fig.3, the bottom three bars show the wall clock time taken to perform 2,000 simulation time steps using the combined ISAT/RCCE approach with 10 represented species with the PLP, URAN and P-URAN[0.2h,32] parallel strategies. In each case, we also show the breakdown of time spent in LES, HPDF (outside reaction), Reaction (including *x2f_mpi* communication), and Waiting (average idle time) as defined in [22]. We see that the P-URAN strategy yields the lowest wall clock time among the three strategies. The Waiting time (average idle time), which is indicative of the *load imbalance* is maximum for PLP, minimum for URAN and moderate for P-URAN (as also seen in our previous studies [22]).

The LES/PDF simulation of Sandia Flame D using ISAT alone with the 38-species full representation is performed using the PLP, URAN and P-URAN strategies [22]. Among these the P-URAN strategy again yields the lowest wall clock time. In Fig.3, for comparison, the top bar shows the wall clock time for 2,000 time steps using the 38-species full representation with the P-URAN[0.2h,32] strategy.

We notice that relative to the simulation using ISAT alone with the 38-species full representation, the combined ISAT/RCCE approach with 10 represented species using the P-URAN strategy

1. yields more than 40% reduction in HPDF time (outside Reaction). This is because with dimension reduction, the particles in PDF simulation carry only the reduced representation (in this case involving 15 variables). As a result, a) particles require 60% less storage, which in turn reduces the particle communication cost; and b) less time is required for collecting species (LES cell mean) statistics.
2. reduces the Reaction time by over 40% due to smaller ISAT table sizes and faster retrieve times (statistics given in Table 2 and explained below); and

433 3. consequently, reduces the overall wall clock time of the simulation by
434 more than 40%.

435 In Table 2, we list the ISAT statistics collected from the simulations
436 with the P-URAN strategy using a) ISAT alone with the 38-species full
437 representation; and b) ISAT/RCCE with 10 represented species. We see that
438 in both the cases, over 99.9% of the queries result in retrieves which shows
439 the high efficiency of ISAT tabulation. Compared to ISAT/RCCE with 10
440 represented species, the simulation with 38-species full-representation results
441 in almost twice the number of adds, and also results in some direct evaluations
442 because some of the tables get completely filled. The average retrieve time
443 with ISAT/RCCE is only 3 μ s compared to 8 μ s with ISAT alone.

444 7. Conclusions

445 We have successfully extended our LES/PDF solver with the capability
446 of performing turbulent combustion calculations with realistic combustion
447 chemistry, wherein the chemistry in the PDF solver is represented using the
448 combined dimension reduction (using RCCE) and tabulation (using ISAT)
449 approach. The chemistry workload is efficiently redistributed using the P-
450 URAN strategy implemented using the *x2f_mpi* library. We have shown that
451 for performing LES/PDF simulation of Sandia Flame D, relative to using
452 ISAT alone with the 38-species full representation, the ISAT/RCCE approach
453 with 10 represented species (i) yields acceptable level of accuracy in mean
454 and standard deviation statistics of major thermochemical quantities of in-
455 terest like temperature, density and species mass fractions; and (ii) reduces
456 the overall simulation wall clock time by more than 40% with the P-URAN
457 strategy.

458 8. Acknowledgments

459 V.H.’s work on dimension reduction methodologies is supported by Office
460 of Energy Research, Office of Basic Energy Sciences, Chemical Sciences, Geo-
461 sciences and Biosciences Division of the US Department of Energy (DOE)
462 under Grant No. DE-FG02-90ER. The work of V.H. and S.R.L. on the ethy-
463 lene mechanism is supported by Grant No. FA9550-09-1-0611 funded by the
464 National Center for Hypersonic Combined Cycle Propulsion, sponsored by
465 the AFOSR and NASA ARMD. S.R.L.’s initial work on this project was

466 supported by NASA Grant No. NNX08AB36A. This research was also sup-
467 ported in part by the National Science Foundation through TeraGrid re-
468 sources provided by the Texas Advanced Computing Center under Grant
469 No. TG-CTS090020. S.B.P. has a financial interest in Ithaca Combustion
470 Enterprise, LLC., which has licensed the software ISAT-CK and CEQ used
471 in this work.

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Table 1: Normalized root-mean-square difference (RMSD) (see Eqn.3) in mean and standard deviation statistics obtained using the reduced representation with ISAT/RCCE relative to full representation with ISAT alone. The quantities listed are temperature T , density ρ , and mass fraction of species CH_4 , O_2 , CO_2 , H_2O , CO , H_2 , OH .

Quantity ξ	Reference Value ξ_{ref}	RMSD in $\langle \xi \rangle$ $\epsilon(\langle \xi \rangle)$, percent	RMSD in $\langle \xi'' \rangle$ $\epsilon(\langle \xi'' \rangle)$, percent
T (K)	1000.0	2.92	1.95
ρ (kg/m ³)	1.0	1.72	1.07
Y_{CH_4}	1.5×10^{-1}	1.47	1.17
Y_{O_2}	2.4×10^{-1}	2.10	0.93
Y_{CO_2}	1.2×10^{-1}	1.50	0.81
Y_{H_2O}	1.3×10^{-1}	2.24	0.92
Y_{CO}	5.7×10^{-2}	6.36	4.10
Y_{H_2}	3.7×10^{-3}	7.87	5.29
Y_{OH}	2.7×10^{-3}	2.18	1.92

Table 2: Cumulative ISAT statistics for the LES/PDF simulation of Sandia Flame D using (i) ISAT alone and (ii) ISAT/RCCE with the P-URAN parallel strategy.

method	variables	queries	retrieves (percent)	adds (percent)	direct evals ^(*) (percent)	retrieve time (μs)
ISAT	38	3×10^{11}	99.974	5.572×10^{-3}	1.665×10^{-3}	8
ISAT/RCCE	15	3×10^{11}	99.984	2.742×10^{-3}	0.0	3

(*) performed only if the ISAT table is completely filled.

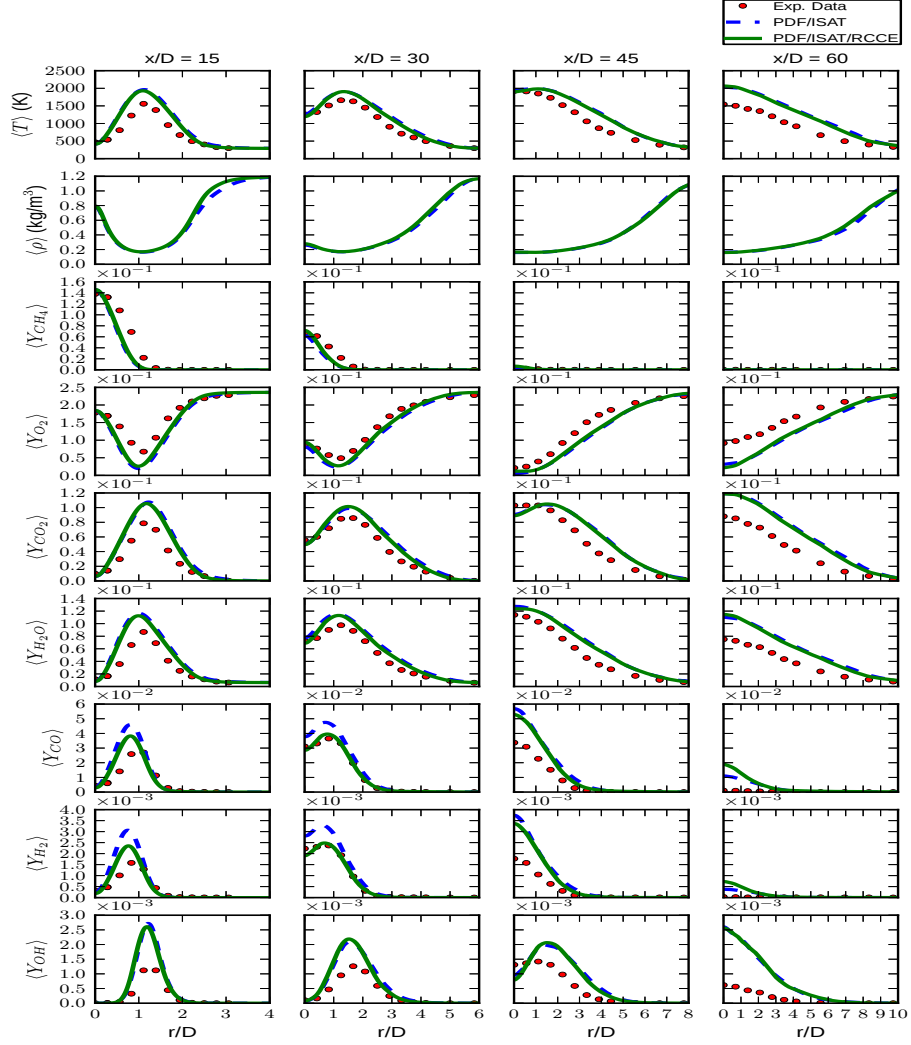


Figure 1: Radial profiles of time-averaged mean temperature T , density ρ , and mass fraction of species CH_4 , O_2 , CO_2 , H_2O , CO , H_2 , OH at axial locations $x/D = 15, 30, 45$ and 60 obtained from (i) experimental data; (ii) an LES/PDF simulation using ISAT alone with the 38-species full representation; and (iii) an LES/PDF simulation using ISAT/RCCE with 10 represented species.

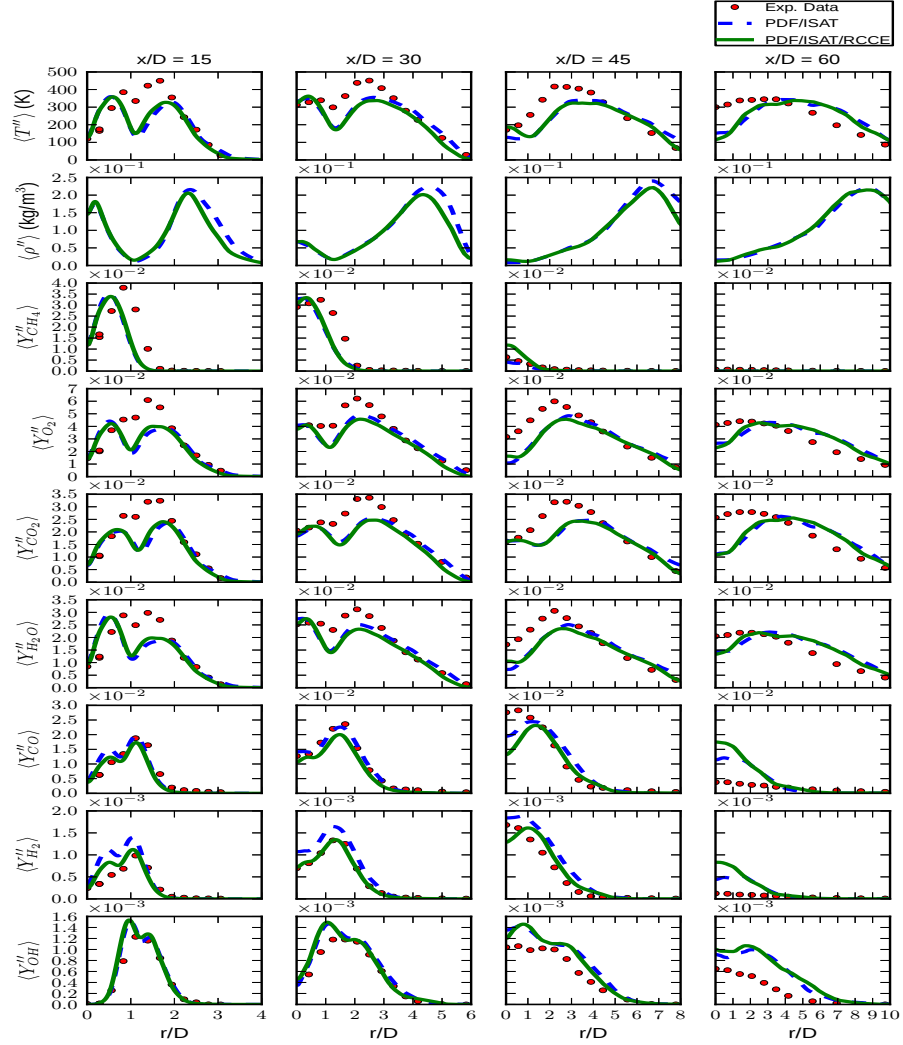


Figure 2: Radial profiles of time-averaged standard deviation of temperature T , density ρ , and mass fraction of species CH_4 , O_2 , CO_2 , H_2O , CO , H_2 , OH at axial locations $x/D = 15, 30, 45$ and 60 obtained from (i) experimental data; (ii) an LES/PDF simulation using ISAT alone with the 38-species full representation; and (iii) an LES/PDF simulation using ISAT/RCCE with 10 represented species.

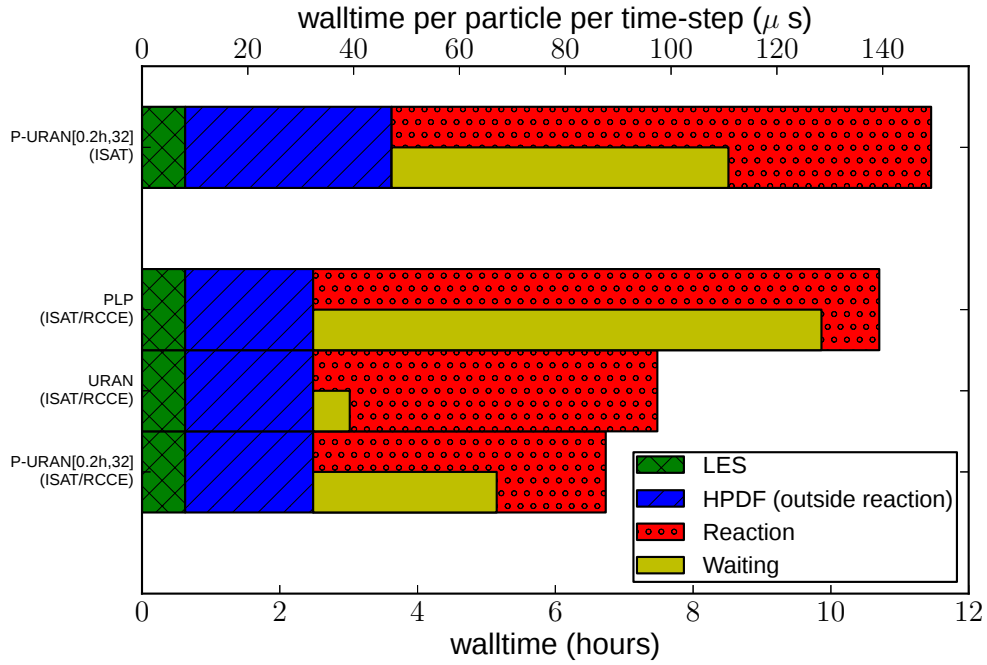


Figure 3: For LES/PDF simulation of Sandia Flame D, wall clock time for 2,000 time steps along with breakdown of time spent in LES, HPDF (outside reaction), Reaction (including *x2f_mpi* communication) and Waiting (average idle time) using different parallel strategies. Top: using ISAT alone with the 38-species full representation with the P-URAN[0.2h, 32] parallel strategy. Bottom three: using combined ISAT/RCCE with 10 represented species using (i) PLP; (ii) URAN; and (iii) P-URAN[0.2h, 32] parallel strategies.