

Accelerating reactive-flow simulations using vectorized chemistry integration

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Abstract

The high cost of chemistry integration is a significant computational bottleneck for realistic reactive-flow simulations using operator splitting. Here we present a methodology to accelerate the solution of the chemical kinetic ordinary differential equations using single-instruction, multiple-data vector processing on CPUs using the OpenCL framework. First, we compared several vectorized integration algorithms using chemical kinetic source terms and analytical Jacobians from the `pyJac` software against a widely used integration code, `CVODEs`. Next, we extended the `OpenFOAM` computational fluid dynamics library to incorporate the vectorized solvers, and we compared the accuracy of a fourth-order linearly implicit integrator—both in vectorized form and a corresponding method native to `OpenFOAM`—with the community standard chemical kinetics library `Cantera`. We then applied our methodology to a variety of chemical kinetic models, turbulent intensities, and simulation scales to examine a range of engineering and scientific scale problems, including (pseudo) steady-state as well as time-dependent Reynolds-averaged Navier–Stokes simulations of the Sandia flame D and the Volvo Flygmotor bluff-body stabilized, premixed flame. Subsequently, we compared the performance of the vectorized and native `OpenFOAM` integrators over the studied models and simulations and found that our vectorized approach performs up to 33–35 $\times$ faster than the native `OpenFOAM` solver with high accuracy.

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1. Introduction

Developers of next-generation combustion devices have increasingly turned to new operating regimes—e.g., low-temperature combustion [1]—to achieve higher efficiencies and reduced emissions. Computational reactive-flow modeling has been used to rapidly develop these new combustion concepts into functional prototypes [2], but accurately predicting combustion processes at these regimes depends on realistic chemical kinetics models. This places a large computational burden on reactive-flow modeling, since solving the ordinary differential equations (ODEs) governing chemical kinetics can dominate the overall cost of simulations. For example, in a study of *n*-dodecane spray injection, a high-resolution large-eddy simulation (LES) using a 54-species skeletal model and up to 22 million cells took around 48,000 CPU hours (or about 20 days of wall-clock time) to complete a single realization of just 2 ms after start of injection [3]. Large model size and high numerical stiffness further increase computational cost, and unfortunately chemical kinetic models relevant to transportation or power-generation applications exhibit these characteristics [4].

Many strategies have been developed to reduce the cost of using realistic, detailed chemical kinetic models in reactive-flow simulations [4, 5]. Skeletal reduction methods aim to remove unimportant species and reactions from a chemical kinetic model while maintaining fidelity to the base detailed model [6–9]. In addition, species with similar thermochemical properties may also be lumped together [10–12], time-scale methods can be used to reduce numerical stiffness [13–16], and tabulation/interpolation methods reuse previously computed results to accelerate simulations [17–19]. Often, several of these techniques are combined to achieve better performance [20–22], or are even applied dynamically throughout a simulation to achieve greater local computational savings [23–25].

In addition to methods that reduce or approximate the base chemical kinetic model, performance can be increased by improving the ODE integration algorithms used to solve the chemical-kinetic equations. Some researchers have developed new integration algorithms specifically for efficiently solving chemical kinetics [16, 26, 27], while others have examined the performance of existing algorithms for use in reactive-flow simulations [28–33]. Further,

several codes have recently been developed for analytically evaluating the chemical-kinetic Jacobian matrix [34–36], which may be used to improve the performance of implicit ODE integration schemes [4].

In recent years, high-performance computing hardware has been evolving from a homogeneous, CPU-based paradigm to one dominated by heterogeneous processing architectures. In particular, single-instruction multiple-thread (SIMT) processors have become widely available, such as graphics processing units (GPUs), and many studies have leveraged their high floating-operation throughput to accelerate chemical-kinetics integration. Early work used GPUs to evaluate chemical-kinetic source terms or factorize the Jacobian matrix, but found significant speedups only for large chemical kinetic models [37, 38]. Later, several studies implemented GPU-based explicit integration techniques to achieve order-of-magnitude or more speedups when integrating non-stiff or moderately-stiff chemical kinetics [28, 30, 39]. Further work followed that developed GPU-based implicit integration schemes, but these exhibited decreased performance with increasing numerical stiffness due to thread divergence [40–42].

In contrast, vectorization based on the single-instruction multiple-data (SIMD) paradigm, like that found on modern CPUs, has not been as extensively investigated for use in chemical-kinetic integration, though SIMD vectorization has been used for ODE integration in related contexts [43–45]. Che et al. [46] used loop-unrolling/rearrangement, aligned arrays, and OpenMP [47] compilation directives (i.e., `#pragmas`) to achieve SIMD vectorization for accelerating an LES solver on the Intel Xeon Phi Many Integrated Core (MIC) co-processor. Stone et al. [33] used the OpenCL [48] framework to vectorize a linearly implicit Rosenbrock integration method [49] on the CPU, GPU, and MIC architectures. In addition, we developed the open-source platform `pyJac` that can generate vectorized, OpenCL-based chemical kinetic source term and Jacobian evaluation codes [35].

In this work, we describe a method to implement SIMD-based vectorized ODE integration methods—coupled with vectorized, analytical chemical kinetic Jacobian and source-term evaluations—for use in realistic reactive-flow simulations. Our primary focus is finding the acceleration and performance scaling achievable by the vectorized methods, so we examine these in applications with different turbulent and chemical time scales, mesh resolutions, and chemical-kinetic model sizes to assess their performance in a variety of engineering and scientific contexts. To do so, we extended the open-source computational fluid dynamics (CFD) code `OpenFOAM` [50] to use the vector-

ized methods.

Our goal here is to demonstrate the significant reduction in computational cost achievable by fully vectorized chemical-kinetic integration on CPUs without compromising accuracy, rather than to perform high-fidelity studies with the aim of investigating the combustion physics involved. Although the open-source nature of **OpenFOAM** is advantageous for these purposes—allowing modification to enable the vectorized ODE integration methods—it lacks some commonly used models (e.g., multi-component and mixture-averaged species transport [51]) and boundary conditions (e.g., Navier–Stokes Characteristic Boundary Conditions [52, 53]). It has to be pointed out that the impact of the interaction of errors from computational grid size, subgrid models, numerical schemes, and chemical kinetic model selection on the accuracy of reactive-flow simulations is not well understood. For instance, Cocks et al. [54] demonstrated that four different numerical schemes (as provided by industry, research, and open-source CFD codes) are unable to produce consistent reactive-flow LES solutions for the commonly used Volvo bluff-body stabilized flame [55–57], even when using the same computational grid, subgrid, and chemistry models. Similarly, Rochette et al. [58] found that the numerical scheme and chemical kinetic model have a large effect on the agreement of the solution with experimental data used in a reactive-flow LES solution of the Volvo bluff-body stabilized flame problem. The focus of this work is not model validation, so we will use only built-in **OpenFOAM** numerical schemes, subgrid models, and boundary conditions—substituting in our vectorized ODE solver—to simulate selected reactive-flow problems, demonstrating that the techniques developed here can further aid the development of standard models in **OpenFOAM**.

The rest of this article is organized as follows. Section 2 describes the numerical methods and software used in this study. Subsequently, Section 3 first verifies the vectorized solvers against a typical implicit integration algorithm, then confirms their coupling to the CFD code **OpenFOAM** [50]. Then, Section 4 presents two case studies that compare the performance of the vectorized solvers with those built into **OpenFOAM**: Sandia flame D [59–61] in Section 4.1 and the Volvo Flygmotor bluff-body flame [55–57] in Section 4.2. Finally, in Section 6 we identify and discuss directions for future efforts.

2. Numerical methods and software

2.1. *pyJac* code-generation platform

pyJac [35] is an open-source software package that generates code for evaluating the chemical-kinetic source terms and analytical Jacobian matrix for a variety of execution, data-ordering, and matrix-format patterns. For full details, we direct readers to our prior work focusing on *pyJac* [34, 35]; however, here we highlight key points relevant to this work. When using the constant-pressure assumption¹, the resulting thermochemical state vector in *pyJac* is

$$\Phi = \{T, V, n_1, n_2, \dots, n_{N_{\text{sp}}-1}\} , \quad (1)$$

where T is the temperature of the gas mixture, V is the volume, n_i is the moles of species i , and N_{sp} is the number of species in the model. The last species in the model is typically the bath gas— N_2 in this study—and omitted from the state vector, as it is calculated implicitly via the ideal gas equation of state:

$$n = \frac{PV}{\mathcal{R}T} = \sum_{i=1}^{N_{\text{sp}}} n_i , \quad (2)$$

where n is the total number of moles of the gas mixture and $\mathcal{R}$ is the universal gas constant. The moles of the last species in the model $n_{N_{\text{sp}}}$ is then calculated as

$$n_{N_{\text{sp}}} = \frac{PV}{\mathcal{R}T} - \sum_{i=1}^{N_{\text{sp}}-1} n_i . \quad (3)$$

This formulation explicitly conserves mass in *pyJac*, and also ensures that the system of equations is not overconstrained [36].

Given a thermochemical state vector, *pyJac* can evaluate the chemical kinetic source rates

$$\frac{d\Phi}{dt} = f(\Phi) = \left\{ \frac{dT}{dt}, \frac{dV}{dt}, \frac{dn_1}{dt}, \frac{dn_2}{dt}, \dots, \frac{dn_{N_{\text{sp}}-1}}{dt} \right\} , \quad (4)$$

which form the autonomous chemical kinetic ODEs. In addition, *pyJac* can

¹In this context, “constant pressure” refers to the solution of chemical kinetics within a reaction sub-step of an operator-splitting scheme, rather than a general constant-pressure reactive-flow simulation.

calculate the analytical chemical kinetic Jacobian

$$\mathcal{J}_{i,j} = \frac{\partial f_i}{\partial \Phi_j}, \quad i, j = 1, \dots, N_{\text{sp}} + 1. \quad (5)$$

Although `pyJac` can evaluate the Jacobian in a sparse-matrix format (e.g., compressed row storage), we used a dense-matrix format to simplify implementing linear-algebra operations; extending this effort to use a sparse matrix is a goal for future studies. We used `pyJac` to generate an explicit “shallow”-vectorization, as described in Section 2.2, using a vector width of eight double-precision floating-point operations¹, and “C” (or row-major) data ordering.

2.2. OpenCL and vectorization

The parallel programming standard OpenCL [48] provides a common interface to execute vectorized code on a variety of different platforms (e.g., CPU, GPU, MIC). For a detailed overview of different vectorization patterns and their applications to different hardware platforms for integrating chemical kinetic ODEs, we refer the reader to past works [35, 40, 42, 62]. Here we will discuss only the so-called “shallow”-vectorization pattern for SIMD processors (e.g., CPUs) using OpenCL.

This method groups together the thermochemical state vectors of several chemical kinetic ODE systems:

$$\Phi_{\text{vec}} = \left\{ \begin{aligned} &\{\Phi_{1,1}, \Phi_{2,1}, \dots, \Phi_{N_v,1}\}, \\ &\{\Phi_{1,2}, \Phi_{2,2}, \dots, \Phi_{N_v,2}\}, \dots, \\ &\{\Phi_{1,N_{\text{sp}}+1}, \Phi_{2,N_{\text{sp}}+1}, \dots, \Phi_{N_v,N_{\text{sp}}+1}\} \end{aligned} \right\}, \quad (6)$$

where N_v is the number of elements in the vector, also known as the vector width, and $\Phi_{j,i}$ is the i th component of the thermochemical state vector (Eq. (1)) for the j th state.

These modified state vectors can be loaded into OpenCL vector data types, e.g., `double8`, allowing floating-point math operations to be performed

¹If the OpenCL vector width is longer than that implemented on the underlying hardware, the vector operation is implicitly converted to multiple smaller vector operations, similar to loop-unrolling optimizations.

concurrently over the vector (by specialized vector processors present on all modern CPUs), thus accelerating computations. The OpenCL runtime (e.g., as supplied by Intel [63]) then transforms the OpenCL code into vectorized operations using the vector-instruction set present on the device.

2.3. *accelerInt* ODE integration library

Efficiently and accurately integrating the autonomous chemical kinetic ODEs is critical to simulating reactive flows. Integration advances the source rates—described in Section 2.1—from an initial time t_i to a final time t_f :

$$\frac{d\Phi}{dt} = f(\Phi), \quad t_i \leq t \leq t_f. \quad (7)$$

We have implemented several previously developed vectorized OpenCL-based ODE integration methods [33] in the *accelerInt* software library [42]: a fourth-order explicit Runge–Kutta method and several third- and fourth-order linearly implicit Rosenbrock methods [49, 64, 65]. Table 1 lists the OpenCL-based solvers available in *accelerInt*, as well as their orders, solver types, and references.

Solver name	Order	Solver type	Reference(s)	Short name
Rosenbrock	3	Linearly implicit	[64, 65]	ROS3
Rosenbrock	4	Linearly implicit	[49]	ROS4
RODAS	3	Linearly implicit	[64, 65]	RODAS3
RODAS	4	Linearly implicit	[49]	RODAS4
RKF45	4	Explicit	[66]	RKF45

Table 1: List of vectorized OpenCL integration methods incorporated into *accelerInt*.

Runge–Kutta methods include both implicit and explicit solvers, and are widely used to solve systems of stiff and non-stiff ODEs. A Runge–Kutta method with s stages may be written as

$$\Phi(t_{n+1}) = \Phi(t_n) + \sum_{i=1}^s b_i \mathbf{k}_i, \quad (8)$$

where each stage is computed as

$$\mathbf{k}_i = h f \left(\Phi(t_n) + \sum_{j=1}^s a_{ij} \mathbf{k}_j \right), \quad (9)$$

where h is the time-step size, and a_{ij} and b_i are method coefficients that define the algorithm.

The explicit solver included in `accelerInt` is a five-stage, fourth-order-accurate embedded Runge–Kutta–Fehlberg method (RKF45) [66]. Explicit Runge–Kutta methods are obtained when the coefficient matrix a_{ij} in Eq. (9) is strictly lower triangular (i.e., $a_{ii} = 0$). While explicit integration methods are efficient for non-stiff problems, they are only conditionally stable and perform poorly for stiff problems where the step size h is limited by stability concerns rather than the desired accuracy.

Implicit Runge–Kutta methods result from a fully populated coefficient matrix a_{ij} , resulting in a system of non-linear equations that are typically solved via Newton–Raphson iteration. This technique requires the repeated evaluation and factorization of the chemical-kinetic Jacobian matrix $\mathcal{J}$ (see Eq. (5)). As such, implicit methods cost more per integration step, but their improved stability typically makes them more efficient for solving stiff ODEs. Implicit methods commonly reuse the Jacobian matrix (and its factorization) for multiple time steps to reduce the computational overhead.

Rosenbrock (ROS and RODAS)¹ methods are more similar in structure to Runge–Kutta methods than to fully implicit techniques. They solve a linearized form of Eq. (8) and are therefore known as “linearly implicit” techniques. An s -stage Rosenbrock method is formulated as

$$\mathbf{k}_i = h f \left(\Phi(t_n) + \sum_{j=1}^{i-1} \alpha_{ij} \mathbf{k}_j \right) + h \mathcal{J} \sum_{j=1}^i \gamma_{ij} \mathbf{k}_j, \quad i = 1, \dots, s \quad (10)$$

$$\Phi(t_{n+1}) = \Phi(t_n) + \sum_{i=1}^s b_i \mathbf{k}_i, \quad (11)$$

where α_{ij} , γ_{ij} , and b_i are the method parameters. Typically Rosenbrock methods are constructed with $\gamma_{11} = \dots = \gamma_{ss} = \gamma$, a constant parameter,

¹Here we adopt the naming convention of Hairer and Wanner [49].

such that only one LU decomposition must be performed per time step [49].

To avoid solving a linear system and performing matrix-vector multiplication at each stage of the method [49, 67], Eq. (10) may be transformed:

$$\left(\frac{1}{h\gamma_{ii}}\mathbf{I} - \mathcal{J}\right)\mathbf{u}_i = f\left(\Phi(t_n) + \sum_{j=1}^{i-1} a_{ij}\mathbf{u}_j\right) + \sum_{j=1}^i \frac{c_{ij}}{h}\mathbf{u}_j, \quad i = 1, \dots, s \quad (12)$$

$$\Phi(t_{n+1}) = \Phi(t_n) + \sum_{j=1}^s m_j \mathbf{u}_j, \quad (13)$$

where $\mathbf{\Gamma} = (\gamma_{ij})$ is an intermediate matrix constructed from the γ_{ij} values,

$$\mathbf{u}_i = \sum_{j=1}^i \gamma_{ij} \mathbf{k}_j, \quad (14)$$

$$a_{ij} = \alpha_{ij} \mathbf{\Gamma}^{-1}, \quad (15)$$

$$c_{ij} = \gamma \mathbf{I} - \mathbf{\Gamma}^{-1}, \text{ and} \quad (16)$$

$$m_j = b_j \mathbf{\Gamma}^{-1}. \quad (17)$$

Directly using the Jacobian matrix in Rosenbrock solvers avoids the need for Newton iteration, making these methods particularly well-suited for SIMD and SIMT vectorization due to the low levels of divergence between vector lanes/threads [29]. However, ROS solvers are formulated around using an exact (analytical) Jacobian, since a finite-difference Jacobian may impact the solver's order and convergence [49, 68]. Further, the Jacobian must now be evaluated/factorized at each step, adding to the cost per time step. W-methods may be a suitable technique to avoid these costs, since they are formulated around using an inexact Jacobian [49]; these should be investigated for vectorized ODE integration in the future.

These Runge–Kutta and Rosenbrock solvers, coupled with OpenCL source-code/Jacobian evaluation code generated by the latest version of pyJac [35], form the basis of the accelerated ODE integration techniques used here.

2.4. *OpenFOAM*

OpenFOAM [50] is an open-source C++ library capable of solving a variety of continuum mechanics problems, and is designed to allow straightforward extension and implementation of custom solvers. In this work, we extend the

`OpenFOAM` applications for solving reactive-flow CFD problems to incorporate the vectorized ODE integration techniques outlined in Section 2.3. The reactive-flow solver `reactingFoam` supports using a variety of boundary conditions, models, solution techniques, and turbulence descriptions, including Reynolds-averaged Navier–Stokes (RANS) and LES simulations. For comprehensive details on these models and their implementation in `OpenFOAM` we refer readers to dedicated articles on these topics [50, 69–71]. Here we focus on the models relevant to incorporating `accelerInt` into `OpenFOAM` for solving chemical kinetic ODEs.

2.4.1. Chemistry solvers

`OpenFOAM` has a number of built-in solvers for integrating the chemical kinetic ODEs, including C++ implementations of the third- and fourth-order linearly implicit Rosenbrock solvers in `accelerInt`. However, the implementations differ in a number of key aspects. First, and most obviously, the difference in programming languages results in different execution patterns: serial evaluation in `OpenFOAM` vs. vectorized/batched integration in `accelerInt`. Second, the `ROS4` solver in `OpenFOAM` uses a different set of method coefficients [68] than those used in `accelerInt` [49]. Third, `OpenFOAM v6.x` includes an analytical Jacobian evaluation code¹, but it uses a different state vector composed of the species concentrations, temperature, and pressure (which is assumed constant, as in `pyJac`). Finally, `OpenFOAM` does not employ the explicit mass-conservation formulation employed by `pyJac`, i.e., the concentration of the last species in the model is solved for directly in `OpenFOAM`.

We created a new chemistry model for `OpenFOAM` by extending the base class `BasicChemistryModel`: `BatchedChemistryModel`. This new model performs the chemical-kinetic integration of the thermochemical state vectors for the domain (or sub-domain, in the case of runs parallelized with the message passing interface, MPI [72]) in a single batched call to the `accelerInt` library, instead of evaluating them sequentially as in the base `OpenFOAM` code. The `accelerInt` library returns the updated thermochemical state vectors for the domain, as well as the final internal integration time step taken for

¹Previous versions of `OpenFOAM` used a semi-analytical approach, where most Jacobian values were computed analytically but the temperature derivatives were evaluated using finite differences. The fully analytical Jacobian was introduced on the `OpenFOAM-Dev` channel in June 2018, and is built into `OpenFOAM v6.x`.

each cell in the domain. The time-step values are used as an initial time step for the next ODE integration of this cell (as in the `BasicChemistryModel`¹ used in the `OpenFOAM` code), as well as to adaptively limit the overall CFD time-step size for certain `OpenFOAM` solvers (e.g., `chemFoam`).

2.4.2. Turbulent combustion model

`OpenFOAM` implements multiple turbulent combustion models for simulating turbulence-chemistry interactions in reactive-flow simulations, ranging from a simple infinitely fast chemistry model to the more-complex flame surface density formulation [73]. We selected the eddy-dissipation concept (EDC) [74] as a robust and relatively computationally expensive combustion model to demonstrate the performance of the vectorized ODE solvers. EDC is a commonly used technique for modeling turbulence-chemistry interaction, and has been applied to a large variety of combustion problems [75–77]. Conceptually, EDC is based upon the idea of the turbulent energy cascade [74] and involves both a fine-scale reactor and its non-reacting surroundings [75]. EDC models molecular mixing between the fine scales and their surroundings by mass transfer between the two. When using a detailed chemical kinetic model, the fine-scale reactor is typically treated as a perfectly stirred reactor and solved to equilibrium, imposing significant computational overhead [78].

The mean reaction rate for species i in the EDC model [74, 75], $\bar{R}_i$, is given by²

$$\bar{R}_i = \frac{\bar{\rho}}{\tau^*} \frac{\gamma_L^2 \chi}{1 - \gamma_L^2 \chi} (\bar{Y}_i - Y_i^*) , \quad (18)$$

where $\bar{\rho}$ is the mean fluid density; $\bar{Y}_i$ and Y_i^* are the fluid mean and fine-structure mass fractions of species i , respectively; τ^* and γ_L are the fine-structure residence time and dimensionless length fraction, respectively; and χ is the fraction of fine-structure regions that interact with the rest of the fluid, typically assumed to be unity [75].

¹Technically, this re-use takes place in the `StandardChemistryModel` in `OpenFOAM`, which is the sub-class of the `BasicChemistryModel` corresponding to our own `BatchedChemistryModel` implementation.

²Here we only consider Magnussen’s 2005 EDC model [74]. `OpenFOAM` implements other versions of the EDC model (Bösenhofer et al. [75] provided a good overview of the available versions), but the version selected does not affect the derivation of $\bar{R}_i$, as the chemical kinetic model is only responsible for evaluating the thermodynamic components of Eq. (20).

By definition, for the concentration of species i we have

$$[C_i] = \rho \frac{Y_i}{W_i} = \frac{n_i}{V} ,$$

and

$$\rho Y_i = W_i \frac{n_i}{V} , \quad (19)$$

where W_i is the molecular weight of species i and the volume V is that of the corresponding CFD cell. Combining Eq. (19) with Eq. (18) gives the mean reaction rate in terms of species moles (the species state variable used in `pyJac`):

$$\overline{R}_i = \frac{1}{\tau^*} \frac{\gamma_L^2 \chi}{1 - \gamma_L^2 \chi} \frac{W_i}{\overline{V}} (\overline{n}_i - n_i^*) . \quad (20)$$

where $\overline{n}_i$ and n_i^* are the mean and fine-structure moles of species i , respectively. Both $\overline{n}_{N_{\text{sp}}}$ and $n_{N_{\text{sp}}}^*$, the numbers of moles of the last species in the model in the mean and fine structures, respectively, are calculated using Eq. (3) to be consistent with `pyJac`.

3. Verification

In this section, we will verify the accuracy of the vectorized ODE solvers in two contexts. First, we will directly compare the vectorized solvers implemented in `accelerInt` against the commonly used high-order implicit solver `CVODEs` [79–81], to verify their accuracy and examine their relative performance. Then, we will compare the accuracy of the vectorized `ROS4` solver coupled to `OpenFOAM` (using the methods described in Section 2.4) and the same `ROS4` solver natively implemented in `OpenFOAM` to a reference chemical kinetics code `Cantera` [82] for constant-pressure homogeneous ignition problems.

3.1. *accelerInt* verification

To verify the new solvers, we sampled 100,000 thermochemical conditions from a previously generated database [83], created using constant-pressure partially stirred reactor simulations [34] with the GRI-Mech 3.0 [84] chemical kinetic model, which consists of 53 species and 325 reactions. The database covers a pressure range of 1–25 atm and a range of temperatures and compositions from a cold unburned CH_4/air mixture to states of ignition and

equilibrium. These conditions were integrated using **CVODEs** [79–81] with tight integration tolerances (absolute tolerance of 10^{-20} , relative tolerance of 10^{-15}) for a single global time step of 10^{-6} sec to form a reference solution.

We then used the OpenCL solvers to integrate the same initial values to the same end time, varying the tolerances given to the adaptive time-stepping algorithm over 10^{-4} , 10^{-5} , $\dots$, 10^{-15} . We set both the relative and absolute tolerances for the OpenCL solvers to this tolerance value for the verification effort; in general these can be (and often are) different, e.g., as in the computation of the reference **CVODEs** solution.

The error of each initial value problem (IVP) was then measured as

$$\|E_j\| = \left\| \frac{|y_{i,j}^\circ(t) - y_{i,j}(t)|}{10^{-10} + 10^{-6} \times |y_{i,j}^\circ(t)|} \right\|_2, \quad (21)$$

where $y_{i,j}^\circ(t)$ is the i th component of the solution computed by **CVODEs** for the j th IVP and $y_{i,j}(t)$ is the solution computed by the solver being tested. The “tolerances” used for calculating the weighted reference solution components in Eq. (21) are for normalization purposes only, and are selected solely because they are the tolerances that will be used for the reactive-flow test-case (Section 4.2.2). The error over all IVPs was then calculated using the infinity norm

$$\|E\| = \|E_j\|_\infty = \max_j |E_j|. \quad (22)$$

The tested solvers used the same vectorization settings described in Section 2.1. Figure 1 shows the work-precision diagram for the **accelerInt** solvers: the vertical axis shows the error (as measured by Eqs. (21) and (22)) for the solvers over the various tolerances tested, while the horizontal axis shows the mean CPU runtime (averaged over five individual runs) on a single core of an Intel[®] Xeon[®] X5650 CPU (with SSE4.2 vector instructions), using **v16.1.1** of the Intel OpenCL runtime [63]. We omitted **RKF45** from this test, as the stiffness of the chemical kinetic ODEs caused prohibitive computational costs; this solver will be examined in future work for less-stiff problems.

For loose tolerances (10^{-4} – 10^{-6}), the tested solvers all exhibit similar performance and error. However, for intermediate tolerances (10^{-7} – 10^{-11} , marked in grey on Fig. 1) the **ROS3** solver consistently has the lowest error compared with the reference solution; the fourth-order solvers (**ROS4**, **RODAS4**) tend to be slightly faster for a minor increase in error in this region. The

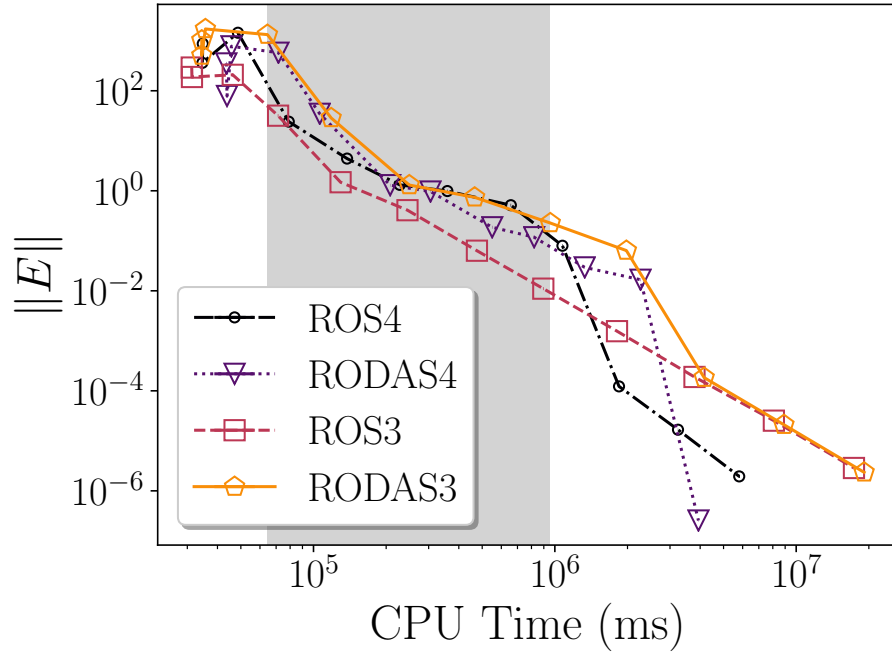


Figure 1: Work-precision diagram for the implicit OpenCL solvers in **accelerInt**. The vertical axis shows the error norm computed by Eqs. (21) and (22), while the horizontal axis shows the mean runtime of the solver, measured in ms. The region marked in grey corresponds to “intermediate” tolerances, ranging from 10^{-7} – 10^{-11} (with equal absolute and relative tolerances in the adaptive time-stepping algorithm).

higher accuracy of the ROS3 solver in this region is likely due to using a different set of method coefficients (see Table 1). At strict tolerances, i.e., less than 10^{-11} , the ROS4 solver is both faster and more accurate than the third-order methods, while the RODAS4 solver is the most accurate for the strictest tolerance of 10^{-15} .

3.2. Constant-pressure ignition in *OpenFOAM*

To verify the coupling of the `accelerInt` solvers to the `OpenFOAM` chemistry model (see Section 2.4), we ran a series of constant-pressure homogeneous ignition problems over initial temperatures of $T_0 = 850, 1100$, and 1500 K, initial pressures of $P_0 = 1, 10$, and 25 atm, and equivalence ratios of $\phi = 0.5, 1.0$, and 1.5 in air, using the GRI-Mech 3.0 chemical kinetic model [84] and CH_4 as the fuel. These conditions cover low-, intermediate-, and high-temperature ignition, as well as lean, stoichiometric, and rich fuel-air mixtures to test the accuracy of the solvers over different chemical kinetic regimes. To test the relative accuracy of the various solvers, the ignition problems were simulated to near chemical equilibrium (post-ignition) with both `accelerInt` and the built-in `OpenFOAM` integrators. The values of the thermochemical-state vectors for each solver were sampled 10 times, equally distributed over the entire simulated time span (excluding the initial state); Fig. 2a shows an example of the time sampling. We compared the sampled values of both approaches with a reference solution computed using the open-source, community chemical kinetics code `Cantera`¹ [82]. In this example we used the fourth-order linearly implicit Rosenbrock solver (ROS4) in both `OpenFOAM` and `accelerInt`, and set the absolute and relative integration tolerances to 10^{-10} and 10^{-6} , respectively, for the `OpenFOAM` and `accelerInt` solvers, and to 10^{-20} and 10^{-15} for `Cantera`.

Figure 2 compares the values of the temperature and species mass fractions of CH_4 , OH , and NO for several initial conditions, showing that all three solvers agree qualitatively. To quantify this comparison, the supremum and mean L^2 norms of the (filtered) relative error between the tested solvers and

¹`Cantera` internally uses `CVODEs` for ODE integration.

Cantera were calculated respectively as

$$\|E\|_{\infty} = \left\| \frac{|\Phi_i^{\circ}(t_j) - \Phi_i(t_j)|}{|1 \times 10^{-10} + \Phi_i^{\circ}(t_j)|} \right\|_{\infty} \quad (23)$$

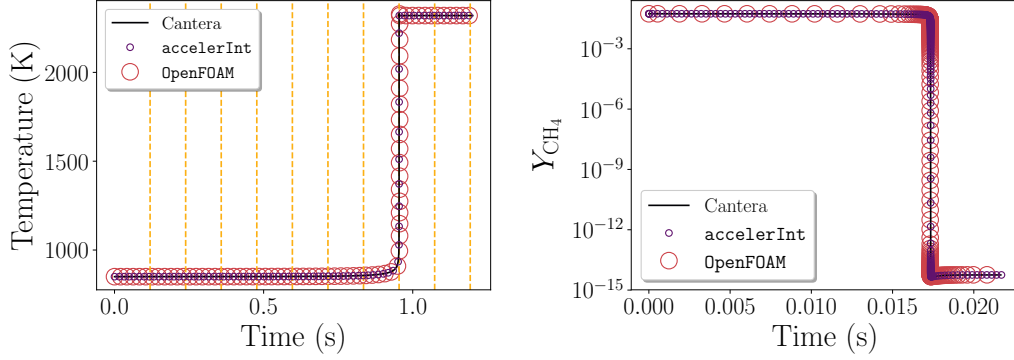
$$\|E\|_{\text{mean}} = \frac{1}{N_s(N_{\text{sp}} + 1)} \left\| \frac{|\Phi_i^{\circ}(t_j) - \Phi_i(t_j)|}{|1 \times 10^{-10} + \Phi_i^{\circ}(t_j)|} \right\|_2, \quad (24)$$

where N_s is the total number of sampled points, $N_{\text{sp}} + 1$ is the size of the thermochemical state vector used in **OpenFOAM** (i.e., the temperature and all species concentrations), $\Phi_i(t_j)$ is the i th entry of the state vector calculated by either the built-in **OpenFOAM** or coupled **accelerInt ROS4** solver at the j th sampled point, and $\Phi_i^{\circ}(t_j)$ the reference value calculated by **Cantera**.

Table 2 shows the values of these norms for both solvers; the coupled **accelerInt** solver agrees much better with the reference solution computed by **Cantera** than the built-in **OpenFOAM** solver. Although the computed error norms for **OpenFOAM** are several orders of magnitudes larger (i.e., $\mathcal{O}(10^5)$ – $\mathcal{O}(10^6)$ versus $\mathcal{O}(10^{-1})$ – $\mathcal{O}(1)$ for **accelerInt**), this does not imply that the built-in **OpenFOAM ROS4** solver is grossly inaccurate; indeed, a visual comparison of the solutions over the entire simulation (Figs. 2a to 2c) show no easily discernible discrepancies. Instead, this difference largely results from more-accurate predictions of ignition delay time on the part of **accelerInt**. For instance, Fig. 2d shows the predicted mass fraction of NO during ignition for the stoichiometric case with an initial pressure of 25 atm and temperature of 850 K. The **OpenFOAM** solver predicts ignition about 1.8 ms later than either **accelerInt** or **Cantera**, a mere 0.21 % difference. Nonetheless, we conclude that the coupled **accelerInt ROS4** solver is more accurate than the corresponding built-in **OpenFOAM** implementation.

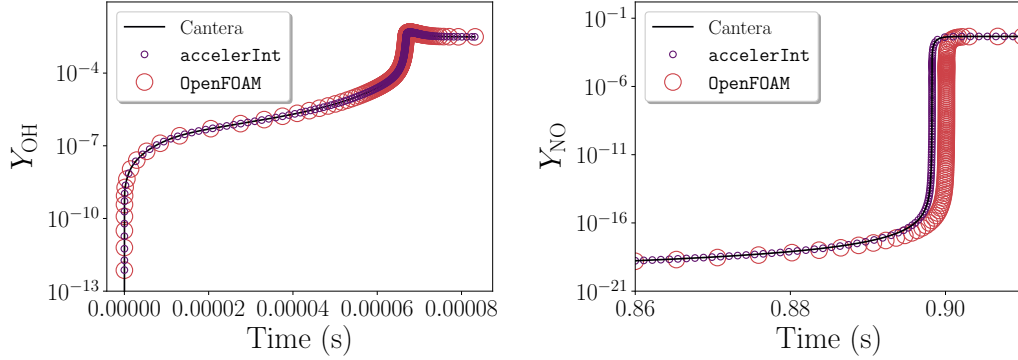
Solver	$\ E\ _{\text{mean}}$	$\ E\ _{\infty}$
OpenFOAM	4.68×10^5	9.49×10^6
accelerInt	3.39×10^{-1}	8.12×10^0

Table 2: The filtered mean and supremum relative error norms comparing the computed solutions of the built-in **OpenFOAM** and coupled **accelerInt ROS4** solvers to those of **Cantera** for the homogeneous constant-pressure ignition problems.



(a) The predicted temperature traces at $P_0 = 25$ atm, $T_0 = 850$ K, and CH₄/air of $\phi = 1.5$. The vertical dashed lines show the points at which the solution was sampled for error evaluation.

(b) The CH₄ mass-fraction profiles predicted by the various solvers at $P_0 = 10$ atm, $T_0 = 1100$ K, and CH₄/air of $\phi = 1.0$



(c) The OH mass-fraction profiles predicted by the various solvers at $P_0 = 25$ atm, $T_0 = 1500$ K, and CH₄/air of $\phi = 0.5$

(d) A zoomed-in look at the NO mass-fraction profiles predicted by the various solvers during the ignition event, for $P_0 = 25$ atm, $T_0 = 850$ K, and CH₄/air of $\phi = 1.0$.

Figure 2: Comparison of constant-pressure homogeneous ignition problem with various solvers using GRI-Mech 3.0. The plotted points for the built-in OpenFOAM and coupled accelerInt ROS4 solvers were thinned somewhat for visibility.

4. Case studies

After verifying the accuracy of the `accelerInt` solvers, we next compare the performance of the built-in `OpenFOAM` and `accelerInt ROS4` solvers on realistic reactive-flow simulations: the Sandia flame D and the Volvo Flygmotor bluff-body stabilized flame. Our objective in both cases is to determine the potential speedup offered by the vectorized solver.

4.1. Sandia flame D

The Sandia Flame D [59–61] is a well-characterized piloted CH_4/air jet flame with a turbulent Reynolds number of $\text{Re}_t = 22000$. `OpenFOAM v5.x` (the 2017 release from the OpenFOAM foundation [85]) and later include a case modeling this flame as a tutorial, providing a relatively inexpensive but more-realistic proving ground for the coupled `accelerInt` solvers. Table 3 and Table 4 list the operating conditions and key dimensions of the case, and Fig. 3c shows a schematic of the configuration superimposed over the simulation mesh.

	Source		
	Jet	Coflow	Pilot
Composition	CH_4/Air : 25/75 % [†]	Dry air	Equil. [‡]
Velocity	49.6 m/s	0.9 m/s	11.4 m/s
Temperature	294 K	291 K	1880 K
Pressure	0.993 atm	0.993 atm	0.993 atm

Table 3: Operating conditions for the Sandia Flame D case.

[†] The jet composition is measured by percent volume.

[‡] Equilibrium state of CH_4/air at $\phi = 0.7$.

The mesh for this case, pictured in Fig. 3a, is fully orthogonal with 5170 cells, ranging in size from roughly 5 mm on a side to 0.72 mm tall near the wall. The solution domain is a thin three-dimensional wedge, with axi-symmetric boundary conditions on the front and back faces, and zero-gradient/total-pressure boundary conditions on the outlet. The case, as packaged with `OpenFOAM`, uses second-order interpolation and gradient schemes for all variables, but a strongly limited scheme (tending towards first-order) for divergence calculations. In addition, the simulation uses a standard $k-\varepsilon$

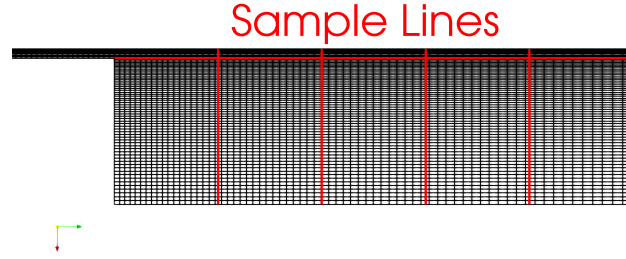
Dimension	Value
$D_{\text{jet, inner}}$	7.2 mm
$D_{\text{pilot, inner}}$	7.7 mm
$D_{\text{pilot, outer}}$	18.2 mm
$D_{\text{wall, outer}}$	18.9 mm
Exit	30 mm $\times$ 30 mm

Table 4: Diameter of the jet, pilot, and wall, and exit-plane dimensions for the Sandia Flame D case.

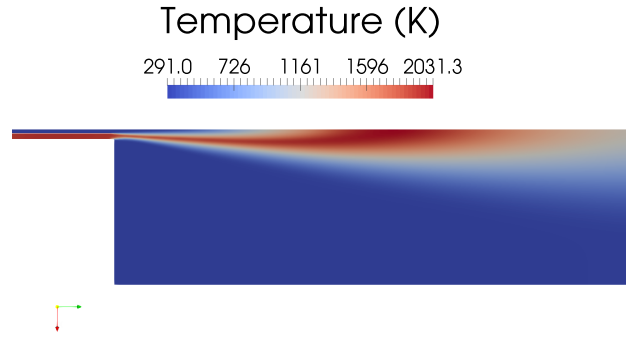
RANS model to model turbulence and a pseudo-transient, first-order time-stepping scheme to initially advance to a steady-state solution.

We modified the baseline case slightly to better suit the purposes of this study. First, we substituted the full GRI-Mech 3.0 chemical kinetic model [84] for the 36-species skeletal methane model originally used in **OpenFOAM**. Second, the base **OpenFOAM** case uses a tabulated dynamic adaptive chemistry scheme [18, 19] to accelerate the solution process; we disabled this to directly compare the performance and accuracy of the ODE solvers. Finally, after reaching steady state, we switched the time-stepping scheme to the second-order implicit method, set the minimum reacting temperature to 500 K, and ran the case for an additional 10 ms of simulated time using a CFD time step of $\Delta t = 10^{-6}$ sec.

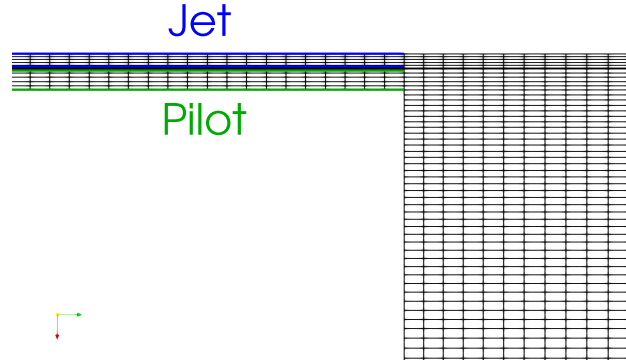
Using this case, we tested the performance of the various **OpenFOAM** and **accelerInt** solvers. Our goal here is to demonstrate the performance enhancement achievable through vectorized chemical kinetic integration, using available Intel CPUs; though dated, the **AVX2** instruction set remains broadly relevant for CPUs that do not support the newer **AVX-512** set. We ran the performance studies on 10 cores of an Intel E5-2690 V3 CPU, with **AVX2** vector instructions, 128 Gbit of RAM, and **v16.1.1** of the Intel OpenCL runtime. We used **OpenFOAM** version **6.x** with **v2.1.0** of the OpenMPI library [86], compiled with **gcc v5.4.0** [87]. We instrumented the **reactingFoam** solver with the MPI profiling library **IPM v2.0.6** [88] by placing profiling sections (via **MPI_PControl**) around the calls to the turbulent combustion model, ODE integration, and other key parts of the CFD time step (e.g., convection evaluation). Section S1 of the Supplemental Material compares in detail the predicted results for the different solvers; here, we focus on the computational cost/performance.



(a) The mesh for the Sandia Flame D case. The red line denotes where we sampled the solution for validation.



(b) The steady-state temperature profile in K, as solved by the base `OpenFOAM` fourth-order Rosenbrock ODE integrator.



(c) A close-up view of the inlet to the domain. The jet and pilot flames are marked in blue and green, respectively. The sample lines are marked in red, as in Fig. 3a

Figure 3: The mesh and steady-state temperature profile of the Sandia Flame D case.

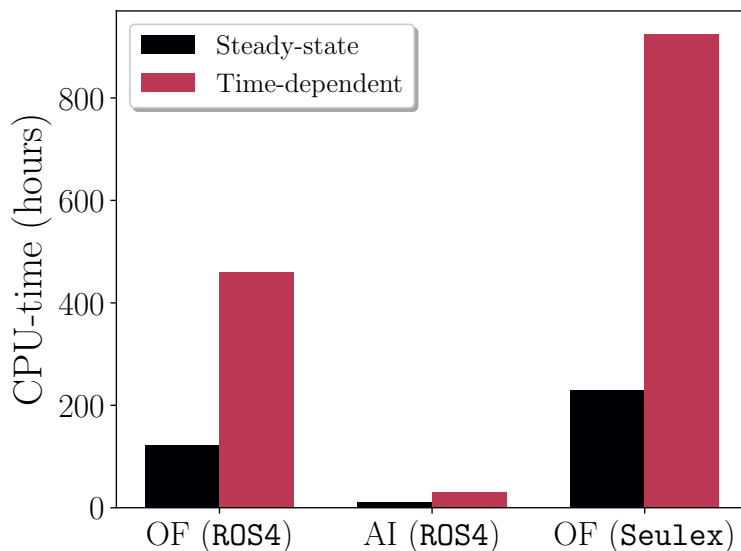


Figure 4: Total CPU hours spent evaluating chemistry in the Sandia Flame D case. AI is `accelerInt` and OF is `OpenFOAM`.

Figure 4 shows the total wall-clock execution time (over all 10 processors) spent by each solver integrating the chemical kinetic ODEs. The `accelerInt` solver spends just 10.2 and 31.1 h solving chemistry for the steady-state and time-dependent cases, respectively, while both the `OpenFOAM` solvers take over 100 h in all cases. The slowest integration method is the `OpenFOAM Seulex` solver, which takes over 923 h to complete the time-dependent solution. The chemistry evaluation time includes time spent idle due to the poor load balancing of chemistry present in most `OpenFOAM` simulations¹.

Table 5 compares the speedups of the solvers, reported against the `OpenFOAM ROS4` solver as the baseline. The `accelerInt ROS4` solver performs 12.0–14.8 $\times$ faster than the `OpenFOAM` equivalent. In addition, the `OpenFOAM Seulex` solver runs roughly 2 $\times$ slower than the `OpenFOAM ROS4` solver in both cases. Finally, the `accelerInt` solver spends 94–96 % in chemistry integration, while both `OpenFOAM` methods use over 99 % of the runtime solving chemistry.

¹`OpenFOAM` uses a simple static decomposition of the domain, which is to say there is no chemistry load-balancing occurring.

	Solver		
	AI (ROS4)	OF (ROS4)	OF (Seulex)
Steady-state	$12.0 \times$	–	$0.53 \times$
Time-dependent	$14.8 \times$	–	$0.50 \times$
Chemistry time	93.9–95.8 %	99.3–99.6 %	99.7–99.9 %

Table 5: Speedups of the chemistry solvers (AI is `accelerInt` and OF is `OpenFOAM`), normalized by the `OpenFOAM ROS4` solver and the percent of total execution time spent integrating the chemical-kinetic ODEs.

4.2. Volvo bluff-body stabilized flame

Next, we will use the Volvo Flymotor bluff-body stabilized premixed flame experiment [55–57] as a second test case. We simulated a reacting case, and used this to study the speedup of the coupled `accelerInt` solver compared to the built-in `OpenFOAM` method.

4.2.1. Case description

The Volvo Flymotor bluff-body stabilized premixed flame experiments include many phenomena found in practical combustors, such as anchored flames, recirculation regions, and shear layers [55–57]. The computational domain is relatively simple and inexpensive to simulate, though, and it is a well-studied test case for non-swirling turbulent flames [54, 58, 89–92]. Furthermore, experimental velocity, turbulence statistics, and temperature measurements are available for two inlet velocities and temperatures for validation purposes [55–57]. Section S2 of the Supplemental Material contains a validation of our setup using the non-reacting simulated velocity and turbulence statistics, compared with available experimental data; we did not include this in the main text, since our main focus is computational performance of the reacting solver.

Figure 5a shows the computational domain we used here, which omits the fuel injection, seeding, and flow-straightener parts upstream of the bluff body. Instead, we set steady inflow boundary conditions at $5D$ —where $D = 40$ mm is the bluff-body height—upstream of the trailing edge of the bluff body, as used in previous studies [54, 90, 93]. The domain extends 0.662 m downstream of the trailing edge of the bluff body, where we used wave-transmissive outflow conditions as suggested in previous work [90, 92, 93]. The domain is

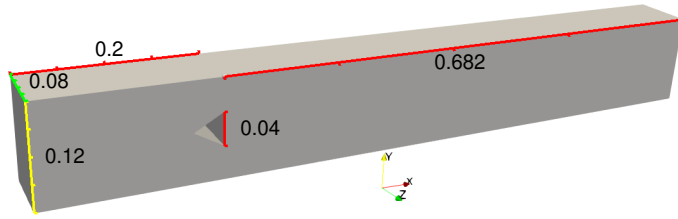
2D wide in the span-wise direction; the front and back faces of the domain use periodic boundary conditions to reduce computational effort [54, 93]. The walls of the domain use adiabatic and no-slip boundary conditions. Table 6 lists the inlet conditions, based on the available experimental conditions [94].

We developed the computational mesh (shown in Fig. 5b) based on recommendations from previous studies [54, 93]; it uses hexagonal cells nominally 2 mm large and a maximum wall-normal distance of 0.3 mm. Grading clusters the cells near the walls and bluff-body edges, as well as the shear layers downstream of the bluff body; the domain is as isotropic as possible elsewhere, resulting in a total of 2,365,000 mesh cells.

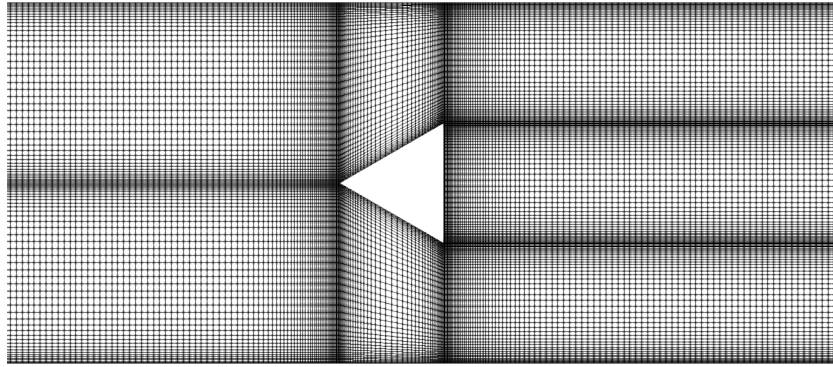
Parameter	Non-reactive	Reactive
Pressure	1 bar	1 bar
Temperature	288 K	288 K
U_{bulk}	16.6 m/s	17.3 m/s

Table 6: Inlet conditions for non-reactive and reactive cases [93], selected to match the available archived experiment data [94]. U_{bulk} is the bulk inlet velocity.

To simulate this case we used the `OpenFOAM` solver `reactingFoam` with the LES turbulence model, along with a Smagorinsky subgrid scale model [95]. A second-order accurate central-differencing scheme discretized the Laplacian terms, while the solver used a second-order bounded cell-based Green-gauss method for gradient calculations. We used a second-order weakly-limited central scheme to calculate the velocity advection divergence and strong limiting for turbulent kinetic energy, species, and energy scalars. The solver advanced in time with a blended first- and second-order Crank–Nicolson scheme, and we handled pressure-velocity coupling with the PISO (pressure-implicit with split operator) algorithm [96]. Using a fully implicit second-order time-stepping method (along with an unlimited velocity advection scheme) was possible with multiple outer corrector steps—i.e., the PIMPLE algorithm in place of PISO—to avoid breakup of the flow due to pressure-velocity decoupling. However, this would require multiple solutions of the chemical kinetic ODEs at each step of the simulation, and consequentially make completing a single time step using the `OpenFOAM` ODE solvers take longer than the largest available time reservation on the computing cluster we used here. Hence, we used the blended time stepping and weakly limited velocity advection schemes instead.



(a) Schematic of the computational domain for the Volvo bluff-body stabilized flame case. All distances are in meters.



(b) A close up of the computational mesh near the bluff body. The cells are gradually stretched from a maximum wall-normal distance of 0.3 mm near the walls and bluff body to a nominal mesh size of 2 mm.

Figure 5: The computational (a) domain and (b) mesh for the Volvo bluff-body stabilized flame case.

4.2.2. Results

We ran the performance studies on 96 cores (i.e., four nodes with 2×12 cores on each) of an Intel E5-2690 V3 CPU, with AVX2 vector instructions, 128 GB of RAM, and using the Intel OpenCL runtime v16.1.1. We used `OpenFOAM` version 6.x [97] with v2.1.0 of the OpenMPI library [86], compiled with `gcc` v5.4.0 [87]. We instrumented the `reactingFoam` solver with the MPI-profiling library `IPM` v2.0.6 [88] by placing profiling sections (via `MPI_PControl` calls) around the calls to the turbulent combustion model, ODE integration, and other key parts of the CFD time step (e.g., convection evaluation). The absolute and relative tolerances of the `OpenFOAM` and `accelerInt` `ROS4` solvers were 10^{-10} and 10^{-6} , respectively.

Although the Volvo bluff-body reactive flame experiments used a lean propane-air mixture (overall global equivalence ratio of $\phi = 0.6$), here we chose a stoichiometric CH_4 /air combustion case for this study. Previous studies have shown mixed agreement between simulated and experimental results using `OpenFOAM` on this configuration [54, 92]. Considering the many potential sources of error in a reactive-flow simulation [58]—e.g., the quality of chemical kinetic model, the turbulence-chemistry interaction model, and the numerical solver itself [54]—we opted to focus on the performance of the ODE integration algorithms instead of a detailed comparison of the reactive-flow case to the experimental data (as done for the non-reactive case as shown in the Supplemental Material). While we expect that these results could be reproduced for, e.g., the UCSD propane model [98] with 57 species and 268 reactions, we prefer to simply use the comparably sized GRI-Mech 3.0 [84] for our demonstration.

We initialized the reactive-flow case using a RANS simulation with the coarse (4 mm nominal cell size) mesh and the base `OpenFOAM` `ROS4` integrator. A two-step methane model [99] ignited the flame via a spherical high-temperature kernel placed behind the bluff body. After the flame stabilized and attached to the bluff body, we ran the RANS simulation using the two-step methane model for a single flow-through time to develop the temperature field. Next, we mapped the RANS solution onto the same coarse mesh using the full GRI-Mech 3.0 model with the numerical schemes and LES setup described above; we reduced the CFD time-step size to 3×10^{-7} s such that the maximum Courant number remained under 0.05, and set a minimum reacting temperature threshold of 550 K. As species transport is more relevant in the reactive case, we used the Sutherland transport model in `OpenFOAM`, and de-

terminated species coefficients by a non-linear least squares fit [100, 101] to the species viscosities versus temperature relation obtained from **Cantera** [82].

For the reactive case, the **OpenFOAM** ROS4 solver proved too slow to advance the solution in a reasonable time frame, so the **accelerInt** solver was used instead to run the coarse LES mesh for a full flow-through time to develop the solution. Next, the coarse solution was mapped onto the finer grid described in Section 4.2.1 and run for 3 ms of simulated time using the **accelerInt** ROS4 solver to obtain baseline timing and solution data. Figure 6 shows an instantaneous snapshot of the temperature field on the finer LES grid. For the fine mesh however, the **OpenFOAM** ROS4 solver was incapable of finishing more than a single CFD time step in the maximum allotted time reservation (6 h) on the computing cluster used here, with each step taking on average, 3.02–3.80 h of wall-clock time¹; in contrast, we note that a single time step using the **accelerInt** solver took only an average of 6.5 min of wall-clock time. Thus, simulating the entire 3 ms duration with the **OpenFOAM** solver would have required the completion of over 10,000 individual job submissions. To get around this issue, 150 evenly spaced solution points were selected throughout the 3 ms duration, from each of which the solution was computed for a single CFD time step using the **OpenFOAM** ROS4 solver for comparison with **accelerInt**.

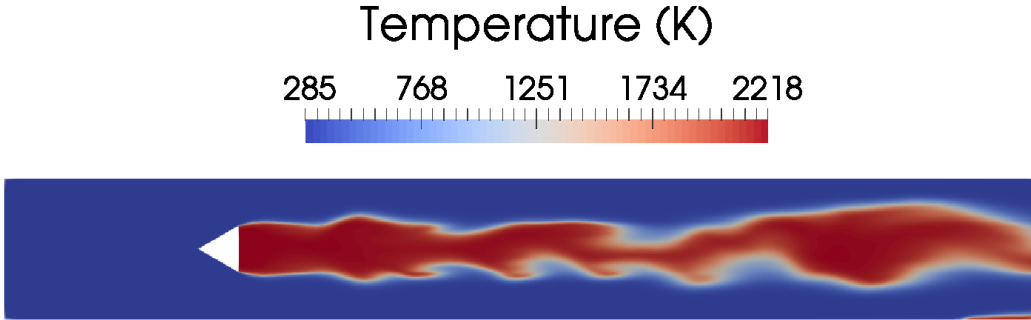


Figure 6: Instantaneous temperature contour of the reactive case on the finer LES grid.

The IPM library provides the total wall-clock execution time spent in

¹Here, the mean wall-clock time per CFD step is normalized by the total number of MPI ranks in the simulation such that it can be directly compared to the maximum time-reservation on the cluster. The mean wall-clock times per CFD step later reported in Table 7 do not have this normalization applied.

user-designated MPI profiling sections for each MPI rank in the simulation over a single job run. Therefore, the computational time spent in, e.g., solving the chemical kinetic ODEs for each individual CFD time step cannot be obtained directly. Instead, we normalized the total wall-clock execution time by the number of CFD time steps completed in a run, and averaged the normalized wall-clock time per CFD time step over the total number of runs (150 for the `OpenFOAM` solver, and 175 for `accelerInt`).

Region	Quantity	<code>accelerInt</code>	<code>OpenFOAM</code>
ODE solution	Time	1.900 ± 0.192 h	58.95 ± 8.05 h
	Speedup	$31.06 \pm 5.27 \times$	–
	% of total	18.79 ± 3.32 %	20.86 ± 2.93 %
Load balancing	Time	7.11 ± 0.77 h	254.34 ± 28.60 h
	Speedup	$35.82 \pm 5.59 \times$	–
	% of total	81.06 ± 12.89 %	78.06 ± 11.64 %
Total	Time	9.10 ± 0.94 h	313.76 ± 35.28 h
	Speedup	$34.48 \pm 5.25 \times$	–
	% of total	100 %	100 %

Table 7: The mean wall-clock execution time per CFD time step, speedup, and percent of total runtime spent in ODE integration and load balancing for both the `accelerInt` and `OpenFOAM ROS4` ODE integration solvers averaged over ten runs. The times are reported in CPU hours per step, and were run on 96 Intel E5-2690 V3 CPU cores with `AVX2` vector instructions.

Table 7 presents the average wall-clock execution time per CFD time step for the `accelerInt` and `OpenFOAM` solvers. The `accelerInt ROS4` solver performs, on average, $32.65\times$ faster (with a variation of $\pm 1.87\times$ depending on the run) in solving the chemical kinetic ODEs than the corresponding `OpenFOAM` approach. In addition, `OpenFOAM` poorly balances the load of the chemistry integration, with both the `accelerInt` and `OpenFOAM` chemistry solvers spending upwards of 75 % of the total computational time waiting on the solution of the chemical kinetic ODEs from other MPI ranks. `OpenFOAM` uses a simple static decomposition of the domain to distribute the computational cells to the various MPI ranks; hence, if a majority of the cells on an MPI rank are considered “non-reactive” (i.e., the temperature of the cell is less than the 550 K threshold) the CPU core will sit idle during chem-

istry integration. A stiffness-based chemical kinetic load balancing scheme (e.g., as implemented by Kodavasal et al. [102]) could further improve the computational efficiency of reactive-flow simulations in `OpenFOAM`, and merits future investigation. Finally, Table 7 shows that the bluff-body simulation in `OpenFOAM` using the `accelerInt` solver spends $35.82 \pm 5.59\times$ less time waiting due to poor chemical kinetic load balancing, while the overall simulation is $34.48 \pm 5.25\times$ faster.

5. Lessons learned

Our strategy for vectorizing chemistry integration focused on building a solver based on extended versions of existing models in `OpenFOAM`. This consisted of

- existing turbulence-combustion interaction models (e.g., EDC, partially stirred reactor [PaSR]) to enable profiling via IPM [88];
- a batched chemistry model, based on the `StandardChemistryModel` class in `OpenFOAM` that additionally enables optional IPM profiling, that (1) scans the list of cells to determine the list of interacting cells based on the temperature cut-off, (2) converts the state variables to the form expected by `pyJac`, (3) passes the complete list of reacting cells to the `accelerInt` solver(s), and (4) finally converts state variables for the integration back to the native `OpenFOAM` format and stores them in the appropriate buffers;
- three solvers (each with optional IPM profiling):
 - `testODE`, used to verify the accuracy of the `accelerInt` solvers when converting to and from the `OpenFOAM` state variables (as compared to Cantera),
 - `chemFoam`, used to verify the `accelerInt` solver(s) coupling to `OpenFOAM` (i.e., integrating the system of equations), and
 - `reactingFoam`, used to enforce the explicit mass conservation in `pyJac`’s state variables, and enable the coupling to `accelerInt` for production simulations.

This strategy allowed us to vectorize chemistry integration while modifying little of `OpenFOAM` itself. Instead, almost all the logic for enabling alternate

models and solvers was contained in the `reactingFoamIPM` module. Simultaneously, because we built the `reactingFoamIPM` module against existing `OpenFOAM` classes, we had to implement few new features there, instead using calls to the parent class wherever possible. For example, a call to the IPM-profiling-enabled PaSR class’s correction method just required placing `MPI_Pcontrol` calls around a call to the base PaSR class’s correction method. Thus, we did not need to vectorize `OpenFOAM` itself—the OpenCL code was entirely contained within the `accelerInt` and `pyJac` libraries.

We pursued an OpenCL-based strategy here to vectorize code, with the intent of supporting portability to different platforms. However, in practice, we found that this led to frequent problems involving segmentation faults during compiling, program crashes, incorrect compiled code, and more, in addition to the associated increase in complexity of the source code. Ultimately, this limited the utility of our approach. Moving forward, we recommend examining a pure OpenMP-based implementation to enable broad adoption; OpenMP version 5.0 [47, 103] might also support offloading calculations to GPUs.

6. Conclusions

This work adapted several previously developed linearly implicit and explicit OpenCL-vectorized ODE integration methods [33] into the `accelerInt` library [104]. We verified the accuracy of these solvers for the solution of the chemical kinetic ODEs (using source-rate and analytical Jacobian evaluation codes from the `pyJac` code-generation platform [35]) for a variety of cases in this effort. We developed `OpenFOAM`-based models of the Sandia Flame D [59–61] stabilized jet flame and Volvo bluff-body stabilized premixed flame [105]. Furthermore, we used a vectorized solver to accelerate chemical-kinetic integration of these reactive simulations, resulting in large performance improvements.

The major contributions of this work are

- Incorporating vectorized chemical kinetic ODE integration methods (provided by the `accelerInt` and `pyJac` libraries) into a publicly available `OpenFOAM` solver [106];
- Achieving significant speedups (33–35 $\times$) via the vectorized solvers over built-in `OpenFOAM` integration methods on the same hardware (an Intel Xeon CPU with AVX2 vector instructions); and

- Profiling the solution of realistic reactive-flow simulations in `OpenFOAM`, demonstrating the need for chemical kinetic load-balancing.

Future extensions to this work should focus on a few key aspects. First, this study has demonstrated that one of the largest bottlenecks of realistic reactive-flow simulations in `OpenFOAM` is the poor chemical kinetic load balancing based on static decomposition. Over 75 % of the overall computational time is wasted using either the `accelerInt` or native `OpenFOAM` solvers due to this issue. A number of chemical kinetic load balancing algorithms exist [107, 108], but the stiffness-based load-balancing technique of Kodavasal et al. [102] seems particularly promising.

More generally, this work has shown that vectorized, linearly implicit ODE integration (paired with analytical Jacobian evaluation) can greatly accelerate reactive-flow simulations. Developing vectorized sparse linear algebra/matrix factorization codes would be an excellent—while challenging—extension of this work, further speeding up the integration of larger detailed chemical models. More advanced integration algorithms should also be investigated; W-methods [49] are particularly promising for their ability to re-use previously evaluated Jacobians and LU-factorizations without needing Newton iteration.

We also found challenges in the OpenCL-based programming approach, which we originally pursued for portability. Moving forward, we recommend using pure OpenMP for vectorization, which should avoid substantially increasing source complexity and also may enable offloading of calculations to GPUs.

Acknowledgments

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Appendix: Availability of material

The vectorized ODE integration methods used in this work are available in version 2.0-beta of the `accelerInt` library [104], while `pyJac-v2.0` [109]

provides the chemical kinetic source terms and Jacobian evaluation. The `OpenFOAM` case modeling the Volvo bluff-body flame is available for download via GitHub [105], and the coupled `OpenFOAM/accelerInt` solver (with IPM-based profiling) is also made available for public use [106]. Finally, the data, figures, and plotting scripts used to generate this paper are similarly available for public use [110].

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